APS March Meeting 2019  Boston, Massachusetts
http://www.aps.org/meetings/march/

Saturday, March 2, 2019 1:00 PM - 6:00 PM

Session 1A DPOLY: DPOLY Short Course: X-ray and Neutron Scattering for Polymer Science I BCEC 150

1:00PM 1A.00001: DPOLY Short Course: X-ray and Neutron Scattering for Polymer Science — The DPOLY short course will introduce the principles of X-ray and Neutron Scattering from polymeric materials. The first part of the course will focus on techniques that probe polymer structure, including transmission scattering, reflectivity and grazing incidence, with emphasis on hard x-ray, soft x-ray and neutron sources. The second part of the course will cover techniques that probe polymer dynamics, including x-ray photon correlation spectroscopy, quasielastic neutron scattering, and neutron spin echo. The course will conclude with an introduction to new challenges and opportunities, such as integration of scattering with other experimental methods, machine learning, and big data.

Sunday, March 3, 2019 8:00 AM - 5:30 PM

Session 1B GSOFT: GSOFT Short Course: Structures and Order in Soft Matter Physics BCEC 153B

8:00AM 1B.00001: GSOFT Short Course: Structures and Order in Soft Matter Physics — The emergence of order is ubiquitous in soft-matter systems. Researchers observe a variety of different order phenomena, ranging from ordered crystalline structures, liquid crystals, and partially ordered systems, to glassy structures. At times it can be challenging to understand the arising structures, from a lack of either suitable experimental procedures or access to structure analysis methods.

The course will start with an overview of the increasingly diverse structures arising in soft matter systems, and introduce how these structures can be described. More intricate structural aspects will be highlighted in reviews of different kinds of simulation studies. The course will then review techniques of determining structures in experimental systems, such as optical microscopy, transmission or scanning electron microscopy, and scattering methods.

Who Should Attend?
Anyone who needs or wants to describe the structure of the soft-matter systems they study, on the colloidal or nano-scale, both in experiments and simulations. Designed to give an introduction into a wide range of experimental and simulation methods for structure determination.

Organizers
Chrisy Xiyu Du and Julia Dshemuchadse, University of Michigan

Sunday, March 3, 2019 8:00 AM - 5:00 PM

Session 1C GERA: Energy Research Workshop BCEC 154

8:00AM 1C.00001: Energy Research Workshop — This annual workshop, held on the Sunday before March Meeting begins, is intended to familiarize graduate students and early career scientists with the opportunities, challenges, and basic landscape of current energy research. Talks, panels, and informal discussions during lunch and coffee breaks will allow for interaction between the students and leading researchers from academia, government, and industry in a variety of energy fields.

Those interested in attending will need to submit a short statement of interest, their March Meeting abstract, and their current academic or research information. The workshop is sponsored by GERA and co-sponsored by FECS.

Sunday, March 3, 2019 8:15 AM - 5:30 PM
Session 1D DPOLY: DPOLY Short Course: X-ray and Neutron Scattering for Polymer Science II BCEC 150

8:15AM 1D.00001: DPOLY Short Course: X-ray and Neutron Scattering for Polymer Science — The DPOLY short course will introduce the principles of X-ray and Neutron Scattering from polymeric materials. The first part of the course will focus on techniques that probe polymer structure, including transmission scattering, reflectivity and grazing incidence, with emphasis on hard x-ray, soft x-ray and neutron sources. The second part of the course will cover techniques that probe polymer dynamics, including x-ray photon correlation spectroscopy, quasielastic neutron scattering, and neutron spin echo. The course will conclude with an introduction to new challenges and opportunities, such as integration of scattering with other experimental methods, machine learning, and big data.

Sunday, March 3, 2019 8:30 AM - 12:30 PM

Session 1E DQI: Tutorial 1: Hybrid Quantum Systems BCEC 151A

8:30AM 1E.00001: Tutorial 1: Hybrid Quantum Systems — There have been intense efforts to harness mesoscopic quantum systems such as ultracold gases, superconducting qubits, nanomechanical systems and solid-state defect centers for a suite of applications including sensing, quantum information and communication. However, no single system has been shown to be optimal for the entire range of envisioned applications. Atomic gases are extremely coherent, but they are highly isolated and fragile. Nano-resonators are highly sensitive to small forces and well suited to sensing applications, yet they suffer from dissipation and loss. While photons are robust carriers of information, they typically exhibit very weak nonlinearities. These considerations motivate the ‘hybridization’ of distinct physical systems with complementary functionalities to access new phenomena and applications. In addition, these hybrid systems can also exhibit new forms of quantum behavior to probe macroscopic quantum phenomena and the quantum-to-classical boundary. The lectures will provide a basic introduction to hybrid quantum systems, their realizations, applications to new regimes of quantum metrology and information processing, with a discussion of open questions and challenges.

Sunday, March 3, 2019 8:30 AM - 12:30 PM

Session 1F GMED: Tutorial 2: Medical Imaging: Physics, Technology and Algorithms BCEC 151B

8:30AM 1F.00001: Tutorial 2: Medical Imaging: Physics, Technology and Algorithms — Medical imaging modalities use a wide range of physical phenomena to gather diagnostic information about living tissues. Development and performance assessment of new imaging technologies is a fertile ground for significant and lasting contributions from physicists. This tutorial is intended to facilitate exchange of ideas between researchers trained in fundamental and applied physics and the medical imaging community by introducing the audience to the fundamentals of medical imaging technologies.

Sunday, March 3, 2019 8:30 AM - 12:30 PM

Session 1G DMP: Tutorial 3: Materials by Design: Computational Materials Approach BCEC 152
8:30AM 1G.00001: Tutorial 3: Materials by Design: Computational Materials Approach — With the advent of density functional theory and the growing power of computer speed and parallel algorithms, a new paradigm in the method used to design materials has emerged. Various properties are calculated for a vast amount of materials through effective workflows. The results allow scientists to populate databases. These are then queried to predict and design novel materials or processes. Using these databases, populating them, and interfacing with them requires a specific training which needs to be fulfilled by the developers or experienced research groups.

This tutorial will provide an introduction to materials databases focusing mostly on the Materials Project. Our presentation will begin by introducing the Materials Project and other existing pre-calculated property databases (OQMD, AFlow, NOMAD, Materials Cloud). We will then discuss how we can improve the existing databases by creating property workflows by using Abipy (the Python interface with Abinit) and Atomate (the interface with VASP). Examples will be offered on how these packages can be used to create databases and to query information from the Materials Project. Finally, we will survey some other methods that exist to perform structural searches and how they can complement with these methodologies.

Sunday, March 3, 2019 8:30 AM - 12:30 PM

Session 1H DMP: Tutorial 4: Layered Materials BCEC 153A

8:30AM 1H.00001: Tutorial 4: Layered Materials — Following the isolation of graphene fifteen years ago, the field of atomically thin, layered materials has flourished to incorporate an essentially comprehensive range of condensed matter properties. At the same time, graphene has proven to be an extraordinarily protean material with new surprises arriving continually, such as topological currents, fractal bands, and intrinsic superconductivity to name only a few. The aim of this tutorial is to be both broad, providing an overview of what has been achieved and what may await discovery, and deep, providing specific and detailed examples of the kinds of new questions that increasingly draw researchers to this field. Spurred by the availability of high-quality single crystals of diverse layered materials, a general theme of the past and future of this field is the ability to create van der Waals heterostructures. These combinations of similar or dissimilar layers enable the preservation of delicate materials, new probes of constituent layers, and the radical alteration of band structures, for example through the formation of Moiré bands. Potential applications will be mentioned but are too numerous to be described in any detail; instead the focus will be on the fundamental physics of atomically thin layered materials.

Sunday, March 3, 2019 9:00 AM - 5:00 PM

Session 1J DBIO: DBIO Short Course: Advanced Microscopy BCEC 153C

9:00AM 1J.00001: DBIO Short Course: Advanced Microscopy — Physics, and physicists, have enabled new views of biological systems for centuries. Recent advances on several fronts have broken the “diffraction limit,” producing nanometer-resolution images of living samples. In this short course, we will go through the physics behind recent developments in super-resolution microscopy. The course will also have a hands-on component where students will get to build their own microscope from 3D printed parts.

Who Should Attend
Students and faculty interested in recent advances in high-resolution microscopy

Sunday, March 3, 2019 1:30 PM - 5:30 PM

Session 1K DQI: Tutorial 5: Superconducting Quantum Hybrid Systems BCEC 151AB
Monday, March 4, 2019 10:00 AM - 11:30 AM

Session 1A APS: Hybrid Quasiparticles in Quantum Heterostructures
Westin Marina Ballroom I-II - Tag(s): Education

10:00AM 1A.00001: Hybrid Quasiparticles in Quantum Heterostructures
— The use of hybrid quantum systems has enabled the development of new quasiparticle states with tunable properties. This tutorial will introduce the concept of hybrid quasiparticles and discuss their applications in quantum computing, sensing, and metrology.

Session 1B APS: Strongly Coupled Quasiparticles in Quantum Heterostructures
Westin Marina Ballroom I-II - Tag(s): Education

11:00AM 1B.00001: Strongly Coupled Quasiparticles in Quantum Heterostructures
— Strong coupling between quasiparticles in quantum heterostructures has led to the development of new quantum states with unique properties. This tutorial will provide an overview of the current state of the field and discuss potential applications.

Session 1C APS: Topological Quasiparticles in Quantum Heterostructures
Westin Marina Ballroom I-II - Tag(s): Education

12:00PM 1C.00001: Topological Quasiparticles in Quantum Heterostructures
— The discovery of topological quasiparticles in quantum heterostructures has opened up new possibilities for quantum computing and sensing. This tutorial will provide an introduction to the concept of topological quasiparticles and discuss their potential applications.

Session 1D APS: Quantum Many-Body Systems with Hybridization
Westin Marina Ballroom I-II - Tag(s): Education

1:00PM 1D.00001: Quantum Many-Body Systems with Hybridization
— The development of hybrid quantum systems has enabled the study of complex quantum many-body systems. This tutorial will provide an introduction to the concept of quantum many-body systems and discuss their potential applications.
Sunday, March 3, 2019 5:00 PM - 6:00 PM

**Session 1P APS: First-Time Attendee Orientation** Westin Commonwealth A/B

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

Sunday, March 3, 2019 6:00 PM - 9:00 PM

**Session 1Q APS: Wikipedia Edit-a-thon** Westin Stone - Tag(s): Diversity, Outreach

**6:00PM 1Q.00001: Wikipedia Edit-a-thon** — APS is hosting a Wikipedia Edit-a-thon which will aim to create Wikipedia pages about inspiring women and minority physicists. The event will begin with a talk by Jess Wade, a postdoctoral researcher from Imperial College, who over the last year has created and written more than 270 Wikipedia pages about women scientists. Refreshments will be provided.

Sunday, March 3, 2019 6:30 PM - 7:30 PM

**Session 1R APS/SPS: Undergraduate Student Get-Together** Westin Commonwealth A/B

**6:30PM 1R.00001: Undergraduate Student Get-Together** — Undergraduate Student Get-Together

Monday, March 4, 2019 8:00 AM - 10:48 AM

**Session A01 DCMP: Correlations and Topological States** BCEC 106 - Efstratios Manousakis, Florida State Univ - Tag(s): Focus

**8:00AM A01.00001: Study of the Dirac/Weyl candidates (Ce,Nd)Sb(Se,Te)*** KUAN-WEN CHEN (Presenter), YOU LAI, Florida State University, KAYA WEI, NHMFL, MAREIN RAHN, LANL, YU-CHE CHIU, Florida State University, DAVID E GRAF, NHMFL, MARC JANOSCHEK, LANL, LUIS BALICAS, RYAN BAUMBACH, NHMFL — The nonsymmorphic compound CeSbTe [1] was recently shown to have coexisting complex magnetism and Weyl/Dirac states, where an applied magnetic field transforms the magnetic order and potentially provides a switch between different electronic states. Here we present results for other members of this family compounds, including CeSbSe [2], NdSbSe, and NdSbTe. CeSbSe exhibits complex magnetic ordering at $T_M = 3$ K and the application of a magnetic field results in a cascade of magnetically ordered states for $H < 1.8$ T which are characterized by fractional integer size steps: i.e., a possible devil's staircase is observed. NdSbSe and NdSbTe show a low $T$ buildup of magnetic entropy in the heat capacity, also suggesting complex magnetism. These compounds offer an opportunity to study the connection between the complex magnetic orders, Kondo lattices and topological properties.


*This work was performed at the NHMFL, which is supported by the NSF Cooperative Agreement No. DMR-1644779 and the State of FL. R.E.B., Y.L., D.G. was partly supported by the CAST EFRC, funded by the US-DOE, BES, under Award No. DE-SC0016568. L.B. is supported by DOE-BES through Award No. DE-SC0002613.
8:12AM A01.00002: Importance of electron correlations in understanding the photo-electron spectroscopy and the Weyl character of MoTe$_2$*  
EFSTRATIOS MANOUSAKIS (Presenter), NIRAJ ARYAL, Physics, Florida State University and National High Magnetic Field Laboratory — We study the role of electron correlations in the type II Weyl semimetallic candidate γ-MoTe$_2$ by using density functional theory (DFT) where the on-site Coulomb repulsion (Hubbard U) for the Mo 4d states is included within the DFT+U scheme. We find that inclusion of Hubbard U is important to describe both the light-polarization dependence of the ARPES and the angular dependence of the Fermi surface as measured by quantum oscillation experiments. We also show that though the number and position of Weyl points change non-linearly with U, the Weyl physics remains robust for a wide range of U values. Our calculations also indicate that γ-MoTe$_2$ is in the vicinity of a correlations-induced Lifshitz transition which can be probed experimentally by small amount of doping and its interplay with the Weyl physics might be intriguing.

*This work was supported in part by the U.S. National High Magnetic Field Laboratory, which is funded by NSF DMR-1157490 and the State of Florida.

8:24AM A01.00003: Abelian Topological Phases with Background Electromagnetic Field on Lattice, and Deligne-Beilinson Double Cohomology in Continuum*  
JING-YUAN CHEN (Presenter), Stanford University — Constructing exactly soluble lattice model is an important approach towards understanding topological phases of matter. The coupling of exactly soluble lattice topological models to continuous background gauge field is less well-studied compared to discrete background gauge fields. The former is however responsible for important topological phenomena such as the Hall conductivity and the spin-charge relation. In this talk, I introduce a systematic approach to this problem for abelian topological phases, which is to exactly retrieve the spacetime lattice model from the corresponding Chern-Simons theory in the continuum, via the latter's formal structure known as Deligne-Beilinson double cohomology.

*I am supported by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4302.

8:36AM A01.00004: Majorana zero mode on the edge of an interacting quantum wire subject to spin-orbit interaction and transverse magnetic field*  
AKIRA FURUSAKI (Presenter), RIKEN, OLEG STARYKH, University of Utah — We revisit the problem of an interacting quantum wire subject to spin-orbit interaction and transverse magnetic field. Previous studies showed that the spin sector of the model is equivalent to that of a spin chain with uniform DM interaction (D) in a transverse magnetic field (h), the ground state of which contains two ordered Ising phases and a critical Tomonaga-Luttinger liquid phase, depending on the ratio D/h. Importantly, the charge sector of the wire is a gapless Tomonaga-Luttinger liquid. We show that a quantum wire with an open boundary supports a zero-energy bound state localized at the edge, provided that the spin sector of the problem is massive. We argue that as long as the charge sector is gapless, the wire is in a topological phase and that the bound state is a Majorana zero mode, and discuss physical implications of this finding.

*This work was in part supported by Invitational Fellowship for Research in Japan from the Japan Society for the Promotion of Science and by NSF DMR-1507054.

8:48AM A01.00005: Topological exciton insulator phase in two-dimensional semiconductor systems*  
WEN-KAI LOU (Presenter), State Key Laboratory for Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, WEN YANG, Simulation of Physical Systems, Beijing Computational Science Research Center, KAI CHANG, State Key Laboratory for Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences — Exciton insulator was firstly proposed by Prof. Mott in 1961. This concept has been widely studied theoretically and confirmed experimentally in recent years. Here, We demonstrate theoretically the existence of topological exciton insulating phases in two-dimensional (2D) semiconductor systems. We consider two kinds of systems: InAs/GaSb quantum wells [1] and 2D Van der Waals heterostructures[2]. In InAs/GaSb quantum wells, i.e., a 2D topological insulator, we demonstrate theoretically that the ground state of the system is a topological exciton insulator when the Coulomb interaction between electrons and holes is included. For a 2D VdH system, we find that a perpendicular electric field can decrease the bandgap, which even becomes smaller than the exciton binding energy, leading to the formation of exciton insulator phase. Due to large exciton binding energy, the exciton insulator phase in the 2D VdH system could be observed at room temperature.


*This work was supported by the NSFC (Grants No.11574303, 11434010 and 61674145), the CAS (Grant No. 2015093) and the MOST of China (Grants No. 2015CB921503, 2016YFE0110000 ).
9:00AM A01.00006: Full Commuting Projector Hamiltonians of Interacting Symmetry-Protected Topological Phases of Fermions*  
NATHANAN TANTIVASADAKARN (Presenter), ASHVIN VISHWANATH, Harvard University — Using the decorated domain wall procedure, we construct Finite Depth Local Unitaries (FDLUs) that realize Fermionic Symmetry-Protected Topological (SPT) phases. This results in explicit ‘full’ commuting projector Hamiltonians, where ‘full’ implies the fact that the ground state, as well as all excited states, of these Hamiltonians realizes the nontrivial SPT phase. We begin by constructing explicit examples of 1+1D phases protected by symmetry groups $G = \mathbb{Z}_2 T \times \mathbb{Z}_2 F$, which also has a free fermion realization in class BDI, and $G = \mathbb{Z}_4 \times \mathbb{Z}_4 F$, which does not. We then turn to 2+1D, and construct the square roots of the Levin-Gu bosonic SPT phase, protected by $\mathbb{Z}_2 \times \mathbb{Z}_2 F$ symmetry, in a concrete model of fermions and spins on the triangular lattice. Edge states and the anomalous symmetry action on them are explicitly derived. Although this phase has a free fermion representation as two copies of $p+i p$ superconductors combined with their $p- i p$ counterparts with a different symmetry charge, the full set of commuting projectors is only realized in the strongly interacting version, which also implies that it admits a many-body localized realization.

*N.T. is supported by the Purcell fellowship. A.V. is supported by a Simons Investigator grant.

9:12AM A01.00007: Origin of Mott insulating behavior and superconductivity in twisted bilayer graphene*  
LIUJUN ZOU (Presenter), Harvard University, HOI CHUN PO, Physics, Massachusetts Institute of Technology, ASHVIN VISHWANATH, Harvard University, SENTHIL TODADRI, Physics, Massachusetts Institute of Technology — A remarkable recent experiment has observed Mott insulator and proximate superconductor phases in twisted bilayer graphene when electrons partly fill a nearly flat mini-band that arises a magic twist angle. However, the nature of the Mott insulator, origin of superconductivity and an effective low energy model remain to be determined. We will present a phenomenological picture of the Mott insulator with intervalley coherence that spontaneously breaks $U(1)$ valley symmetry, and describe a mechanism that selects this order over the competing magnetically ordered states favored by the Hunds coupling. We will discuss consequences of this picture for superconducting states obtained on doping the valley ordered Mott insulator. We show how important features of the experimental phenomenology may be explained and suggest a number of further experiments for the future.

*T. Senthil is supported by a US Department of Energy grant DE-SC0008739, and in part by a Simons Investigator award from the Simons Foundation. Ashvin Vishwanath was supported by a Simons Investigator award and by NSF-DMR 1411343.

9:24AM A01.00008: Coupled wire models on compact manifolds and the entanglement entropy for Abelian and non-Abelian topological orders  
BO HAN (Presenter), University of Illinois at Urbana-Champaign, CHI YAN JEFFREY TEO, Physics, University of Virginia — We construct coupled wire models for topologically ordered systems on the 2d torus and study the ground state degeneracy, with explicit ground states. Both Abelian and non-Abelian topological orders will be studied. With the ground states written down, we can study the entanglement entropy for the corresponding systems. Generalizations to 2d closed manifolds with higher genus and 3d closed manifolds will also be discussed.

9:36AM A01.00009: Classification of fermionic symmetry-protected topological phases  
QING-RUI WANG (Presenter), ZHENGCHENG GU, The Chinese University of Hong Kong — We give a systematic construction and classification of fermionic symmetry-protected topological states for generic fermionic symmetry group $G_f$, which is a central extension of bosonic symmetry group $G_b$ (may contain time reversal symmetry) by the fermion parity symmetry group $Z_{2f}$. For each class in the classification (except those with 2D $p+i p$ chiral superconductor decorations), we construct a fixed-point wave function which admits exactly solvable commuting-projector Hamiltonian. The classification is based on the notion of equivalence class of fermionic symmetric local unitary transformations.
necessary to recover a valid semiclassical formula for the Hall effect from the Kubo formula in the DC limit. 
We solve the model non-perturbatively by means of an inhomogeneous Dynamical Mean-Field Theory. 
We tune the strength of the harmonic trap to confine the fermions in artificial structures which are reminiscent of 
graphene nanoflakes in solid state. Starting from a non-magnetic state and increasing the strength of the harmonic 
potential, we are able to induce different magnetic states such as a Néel like antiferromagnetic state, ferromagnetic or 
ferrimagnetic states, as well as mixtures of these basic states, which can be used to design spin-filters and transistors. 
The realization of different magnetic patterns is associated with the terminations of the artificial structures induced in a 
controlled way by the confining potential. We suggest that our cold-atom-based implementation for synthesizing edges in 
order to create magnetism is also applicable in real materials and switchable spintronic devices.

*We acknowledge support from the H2020 Framework Programme, 
under ERC Advanced GA No. 692670 ‘FIRSTORM’ and 
MIUR PRIN 2015 (Prot. 2015CSSEJJ001) and SISSA/CNR project “Superconductivity, 
Ferroelectricity and Magnetism in bad metals” (Prot. 232/2015).

10:00AM A01.00011: Fracton fusion and statistics* SHRIYA RAMACHANDRAN PAI (Presenter), MICHAEL A HERMELE,
University of Colorado, Boulder — In this work, we describe fusion and statistical processes in Abelian fracton phases in terms 
of their gapped excitations. The restricted mobility of fractonic excitations implies that statistical processes do not take the 
form of familiar braiding processes. Also, the number of distinct excitation types in fracton phases is infinite, in contrast to 
conventional phases with intrinsic topological order. Moreover, if one considers excitations supported in a region with 
linear size $L$, the number of excitation types supported in the region grows exponentially with $L$. To build a manageable 
theory that incorporates these features, we consider lattice translation symmetry. Without translation symmetry, the 
fusion of excitations in an Abelian fracton phase is described by an infinite Abelian group, whose elements correspond to 
distinct excitation types. Translation symmetry acts on this Abelian group, giving it more structure and making it a more 
manageable object to work with. Moreover, this action allows us to describe the mobility of excitations at the level of the 
fusion theory, which then forms the basis for a description of statistical processes.

*This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award number 
DE-SC0014415.

10:12AM A01.00012: Hall and Faraday effects in interacting multiband systems* REZA NOURA FKAN (Presenter), 
ANDRE-MARIE TREMBLAY, Institut quantique, RQMP, Université de Sherbrooke — The Hall conductivity is widely used as a 
probe of Fermi surface evolution. However, in the case of interacting multi-band systems, calculations of the Hall 
conductivity are challenging because the application of the semi-classical single-band formula to many bands is 
ambiguous. Here, we derive a formula for the Hall response of interacting multi-band systems with arbitrary band 
topology and spin-orbit coupling. The formula is valid beyond the semiclassical approximation and at finite frequency, 
which is relevant for Faraday rotation, and it takes into account vertex corrections. In addition to the triangular diagrams, 
the formula includes rectangular diagrams that are absent in the single-band case. We show that these diagrams are 
necessary to recover a valid semiclassical formula for the Hall effect from the Kubo formula in the DC limit.

*Canada First Excellence Research Fund, Natural Sciences and Engineering Research Council of Canada Grant RGPIN-2014-
04584, Research 
Chair in the Theory of Quantum Materials and CIFAR

10:24AM A01.00013: Interacting Spin-3/2 Fermions in three-dimensional Luttinger Metal: Phases, Phase Transitions 
and Global Phase Diagram ANDRAS SZABO (Presenter), BITAN ROY, Max Planck Institute for the Physics of Complex System — 
The notion of quasiparticles constitutes the foundation of condensed matter physics. Recently it became evident that 
Dirac or Weyl materials support linearly dispersing quasi-relativistic nodal quasiparticles around few isolated points in the 
Brillouin zone. In this talk, I will focus on a collection of spin-3/2 excitations, which in three dimensions display a bi-
quadratic touching of the valence and conduction bands at the $\Gamma$ point. Such peculiar band touching can be realized in the 
normal state of 227 pyrochlore iridates, half-Heuslers, HgTe and gray tin, for example. Once electron-electron interactions 
are accounted for, this system can display a rich confluence of a plethora of exotic broken symmetry phases, among which 
nematic, magnetic, and superconducting (s-wave and topological d-waves) orders are the most prominent ones. Using a 
controlled renormalization group analysis at finite temperature and chemical doping, I will demonstrate the competition 
among these phases, as well as the associated quantum critical phenomena. In addition, I will also present various cuts of 
the global phase diagram of interacting spin-3/2 fermions, and argue that nematic and magnetic interactions are 
conducive for s-wave and d-wave pairings of Luttinger fermions, respectively.
Aspects of Three-body Interactions in Generic Fractional Quantum Hall Systems and Impact of Galilean Invariance Breaking

BO YANG (Presenter), Physics and Applied Physics, Nanyang Technological University — We derive full analytic expressions of three-body interactions from Landau level (LL) mixing in fractional quantum Hall (FQH) systems with Schrieffer-Wolff transformation. The formalism can be applied to any LL, and to very general systems without rotational or Galilean invariance. We illustrate how three-body pseudopotentials (PPs) can be readily computed from the analytical expressions for a wide variety of different systems, and show that for realistic systems, softening the bare Coulomb interactions (e.g. finite thickness or screening) can significantly suppress three-body interactions. More interestingly, for experimental systems without Galilean invariance (which is common for real materials), there is strong evidence that higher orders in band dispersion can drive the Moore-Read state from anti-Pfaffian to Pfaffian phase. Our analysis points to the importance of the realistic band structure details to the non-Abelian topological phases, and the analytical expressions we derived can also be very useful for high fidelity numerical computations. We also discuss about the importance of edge potentials in realistic experiments for determining the topological phases at half-filling, as well as the nature of such phases for systems with and without particle-hole symmetry.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A02 DMP DCOMP: Dielectric & Ferroic Oxides -- Emergent Interfacial Phenomena

BCEC 107A - Lane Martin, University of Illinois at Urbana-Champaign - Tag(s): Focus

8:00AM A02.00001: Complex polarization textures and exotic properties in PbTiO₃/SrTiO₃ superlattices * [Invited]
JAVIER JUNQUERA (Presenter), University of Cantabria — When ultrathin ferroelectric layers of PbTiO₃ are embedded in superlattices with a paraelectric material, such as SrTiO₃, the interplay between elastic, electrostatic, and gradient energies produces complex patterns of the electrical polarization. In particular, nanometer scale of vortex-antivortex arrays have been recently detected [1], and exotic properties such as the emergence of a negative capacitance have been measured [2]. Performing predictive simulations in these systems is difficult due to the long spatial scales involved, the strong competition between a large number of phases and the sensitivity of the results to external perturbations like strain, periodicity, temperature or electric fields. In order to overcome these problems we employ a recently developed second-principles method [3] that can cope with all the degrees of freedom associated to a large number of atoms retaining high accuracy. Depending on the boundary conditions, our simulations predict the existence of several quasi-degenerate phases at low energies each displaying different properties including net polarization, negative capacitance [4], non-null topological constants [5] and chirality [5,6]. The later prediction supports the findings of optical activity in x-ray circular dichroism experiments [5,6]. Moreover, depending on the periodicity of the superlattice these chiral vortex phases coexist with ferroelectric phases and reversible phase transitions can be induced by external electric fields [7].


*The author acknowledges finanital support from the Spanish Ministry of Economy and Competitiveness through the MINECO Grant No. FIS2015-64886-C5-2-P

8:36AM A02.00002: A theoretical design of inter-correlated in-plane and out-of-plane electric polarization in conventional perovskite ferroelectric thin films
WENGUANG ZHU (Presenter), TIANPING GU, University of Science and Technology of China — Ferroelectric materials may have multiaxial electric polarization, in particular, in-plane and out-of-plane orientations for ferroelectric thin films, but the reversal of their electric polarization along different axes is normally independent. In this talk, I will present a theoretical design to make conventional perovskite ferroelectric thin films have inter-correlated in-plane and out-of-plane electric polarization, based on first-principles calculations. This work may lead to new device paradigms and applications based on conventional perovskite ferroelectric thin films.
**8:48AM A02.00003: Charge Density imaging of a ferroelectric-insulator interface with sub-Å resolution**

CHRISTOPHER ADDIEGO (Presenter), Department of Physics and Astronomy, University of California, Irvine, WENPEI GAO, Department of Materials Science and Engineering, University of California, Irvine, HUI WANG, Department of Physics and Astronomy, University of California, Irvine, YUSHENG HOU, Department of Physics of Astronomy, University of California, Irvine, DIANXIANG JI, National Laboratory of Solid State Microstructures, College of Engineering and Applied Sciences, and Collaborative Innovation Center of Advanced Microstructures, Nanjing Univ, COLIN HEIKES, Department of Materials Science and Engineering, Cornell University, YI ZHANG, LINZE LI, HUAIXUN HU, Department of Materials Science and Engineering, University of California, Irvine, THOMAS F BLUM, Department of Physics and Astronomy, University of California, Irvine, TOSHIHIRO AOKI, Irvine Materials Research Institute, University of California, Irvine, YUEFENG NIE, National Laboratory of Solid State Microstructures, College of Engineering and Applied Sciences, and Collaborative Innovation Center of Advanced Microstructures, Nanjing Univ, DARRELL G. SCHLOM, Department of Materials Science and Engineering, Kavli Institute at Cornell for Nanoscale Science, Cornell University, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, XIAOQING PAN, Department of Materials Science and Engineering, Department of Physics and Astronomy, University of California, Irvine — In complex oxide heterostructures, charge redistribution determines the characteristics of the material and can have significant influence on the behavior of the material. For example, the 2-dimensional electron gas at an LaAlO3-SrTiO3 interface is linked with superconductivity and ferromagnetism at the interface [1]. Although first principles calculations can provide highly detailed charge density maps that illustrate these phenomena, experimental methods often cannot resolve the same features at interfaces or nanostructures with high spatial resolution. Here we demonstrate the imaging of electron charge at interfaces in heterogeneous perovskite structures at atomic resolution using aberration corrected scanning transmission electron microscopy. The charge density mapping is determined using the 2D diffraction pattern acquired with a high-speed pixelated detector [2]. At a BiFeO3-SrTiO3 interface, we found evidence of charge separation caused by the penetration of the electric field from the polarized BiFeO3 into the insulating SrTiO3.


*Department of Energy, National Science Foundation, National Basic Research Program of China, Irvine Materials Research Institute

**9:00AM A02.00004: Probing ferroelectric switching of BaTiO3 thin films integrated on Silicon**

MARC REYNAUD (Presenter), Department of Physics, University of Texas at Austin, JOHANNA NORDLANDER, Department of Materials, ETH Zürich, FELIX ELTES, Neuromorphic Photonics, IBM Research-Zürich, GABRIELE DE LUCA, JACOB NÜRNBERG, Department of Materials, ETH Zürich, STEFAN ABEL, JEAN FOMPEYRINE, Neuromorphic Photonics, IBM Research-Zürich, MANFRED FIEBIG, Department of Materials, ETH Zürich, ALEXANDER DEMKOV, Department of Physics, University of Texas at Austin, MORGAN TRASSIN, Department of Materials, ETH Zürich — The integration of ferroelectric materials on Si plays an important role in the design of new photonic devices, such as optical switches and modulators. Ferroelectric materials exhibit nonlinear optical properties and in particular their refractive index can be tuned by the application of an E-field via the Pockels effect. Ferroelectric barium titanate (BTO) thin films can be epitaxially grown on silicon, using molecular beam epitaxy (MBE). Controlling the polarization of thin these films in absence of metallic buffer remains non-trivial. Orienting the polar axis beyond the limitation of epitaxy using voltage induced ferroelastic switching events to generate out-of-plane (c-domains) to in-plane polarization (a-domains) rotation would open up new pathways for fabricating photonic devices. In this study, we use transmission optical second harmonic generation (SHG) to study the ferroelastic switching dynamics in our BTO films grown on Si for varying thicknesses. The orientation of the BTO films polar axis and the a/c-domain ratio before and after the application of an external in plane E-field are mapped.

*This work was funded by the National Science Foundation Award No. IRES-1358111 and by the Air Force Office of Scientific Research under Grant FA9550-18-1-0053.
9:12 AM A02.00005: Making and manipulating ferroelectric vortices, a TEM perspective of nanoscale flux closure in dielectrically confined PbTiO₃ films* [Invited] CHRISTOPHER NELSON (Presenter), Oak Ridge National Laboratory — A prominent disparity between the two ferroic siblings of ferromagnetism and ferroelectricity is the exciting complex topologies appearing in the spin distributions of former while the electric dipole textures of the latter flag behind. By engineering the scale and field energy minimization pressures driving flux closure formation we realize in SrTiO₃ encapsulated ferroelectric PbTiO₃ thin films the formation of nanoscale ferroelectric vortices. With (S)TEM we characterize the structure of these ~5nm vortices down to atomic scales and study the transition from long-range vortex arrays to in-plane α-domains with decreasing superlattice period, including a mixed structure regime and extrinsic formation of vortices in thicknesses below the vortex-stability limit. Using in-situ applied electric bias we observe the dynamic field-response including the creation, deformation, motion, and erasure of these ferroelectric vortices.

*This work was conducted in collaboration with Zijian Hong, Ajay K. Yadav, Sujit Das, Anoop R. Damodaran, Shang-Lin Hsu, Long-Qing Chen, Lane W. Martin and Ramamoorthy Ramesh, and supported by the U.S Department of Energy, Office of Science, Basic Energy Sciences.

9:48 AM A02.00006: Ionic Gating Driven Polarization Control in Ultra-Thin and Leaky Ferroelectrics* YOGESH SHARMA (Presenter), NINA BALKE, HO NYUNG LEE, THOMAS WARD, Oak Ridge National Laboratory — Ionic liquid (IL) gating allows large electric fields to be achieved at the interface— providing an ability to control, manipulate, and elevate unique phenomena that can arise in the interfaced solid materials. Here, Ionic gating is used to induce reversible polarization switching in ultrathin and highly defective ferroelectric films. Long range electrostatic charge control is induced by modifying the electric double layer at an IL-PbZr₀.₂Ti₀.₈O₃ interface which drives electrostatic and electrochemical control of polarization orientation in the ferroelectric layer. The localized nature of the ionic gating mechanism forbids the leakage current which has historically limited the switching of ultra-thin and/or electrically leaky ferroelectric films in solid metal-gated capacitor devices. This is demonstrated on ultrathin films and in intentionally grown massively defective films with > 30% coverage of direct conducting channels running from surface to ground. We will close by discussing how the transient switching and the ability to manipulate static analog phase transitions might impact future technologies.

*This work was supported by the DOE Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division and the Office of Science Early Career Research Program.

10:00 AM A02.00007: Possible Flexoelectric Origin of the Lifshitz Transition in LaAlO₃/SrTiO₃ Interfaces* AMANY RASLAN, BILL ATKINSON (Presenter), Trent University — Multiple experiments have observed a sharp transition in the band structure of LaAlO₃/SrTiO₃ (001) interfaces as a function of applied gate voltage. This Lifshitz transition, between a single occupied band at low electron density and multiple occupied bands at high density, is remarkable for its abruptness. We propose a mechanism by which such a transition might happen. We show via numerical modeling that the simultaneous coupling of the dielectric polarization to the interfacial strain (‘ electrostrictive coupling’) and strain gradient (‘ flexoelectric coupling’) generates a thin polarized layer whose direction reverses at a critical density. The Lifshitz transition occurs concomitantly with the polarization reversal and is first-order at T=0. A secondary Lifshitz transition, in which electrons spread out into semiclassical tails, occurs at a higher density.

*This work is funded by the Natural Sciences and Engineering Research Council (NSERC) of Canada
Labyrinthine degeneracy and inverse transition in ferroelectric ultrathin films

YOUSRA NAHAS (Presenter), SERGEI PROKHORENKO, Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, JOHANNA FISCHER, CECILE CARRETERO, STEPHANE FUSIL, Unite Mixte de Physique, CNRS-Thales, BRAHIM DKHIL, Laboratory of Structures, Properties and Modeling of Solids, Ecole Centrale Paris, VINCENT GARCIA, Unite Mixte de Physique, CNRS-Thales, LAURENT BELLAICHE, Physics Department and Institute for Nanoscience and Engineering, University of Arkansas — Already hypothesized a century ago, inverse transitions have been found experimentally in very disparate materials, ranging from polymeric and colloidal compounds to high-Tc superconductors, proteins, ultra-thin magnetic films, liquid crystals and metallic alloys, with the notable exception of ferroelectric oxides, despite the widespread theoretical and experimental work on the latter. Here we theoretically demonstrate, that subsequently to a subcritical quench, the non-equilibrium self-assembly of ferroelectric domains in ultrathin ferroelectric films results in the labyrinthine pattern featuring meandering stripe domains. Upon increasing temperature, this labyrinthine phase undergoes an inverse transition whereby it transforms into the less-symmetric parallel stripe domain structure, before the onset of paraelectricity at even higher temperatures. Furthermore, our experimental findings corroborate the universality of the phenomenon within ferroelectric oxides.

The authors thank the DARPA Grant No. HR0011727183-D18AP00010 (TEE Program), the ARO Grant No. W911NF16-1-0227 and the DARPA Grant No. HR0011-15-2-0038 (MATRIX program). Computations were made possible thanks to the use of the Arkansas High Performance Computing Center and the Arkansas Economic Development Commission.

First Principle Study of the Si-EuO Interface

WENTE LI (Presenter), ALEXANDER DEMKOV, University of Texas at Austin — As scaling in the conventional semiconductor industry continues, including the electronic spin degree offers new ways of information processing. The choice of materials in semiconductor spintronics needs to provide efficient spin injection and detection along with the long coherent length and relaxation time in the semiconductor. Silicon offers a long spin relaxation time. And EuO is a promising ferromagnetic semiconductor, at least at low temperature. Due to its high spin polarization and thermodynamic stability on Si, epitaxial EuO may be a good candidate for application of spintronics. We use first principle calculations to study the atomic and electronic structure of the Si-EuO interface. We construct Si-EuO interface models and analyze the band alignment at the interface, our results suggest that Si-EuO heterostructure is a feasible option for spin injector in Si-based spintronic devices.

Electrical transport properties of two-dimensional materials on ferroelectrics toward nonvolatile memory devices

NAHEE PARK (Presenter), Department of Energy Science, Sungkyunkwan University, HAEYONG KANG, Department of Physics, Pusan National University, DONGSEOK SUH, Department of Energy Science, Sungkyunkwan University — When ferroelectric material is employed as a gate dielectric for the field effect transistor (FET) of a two-dimensional (2D) material such as graphene, MoS2, and MoTe2, it is possible to induce a giant amount of carriers in the channel by polarization field of the ferroelectric and also to show a nonvolatile memory operation. In many cases, however, the electrical coupling between 2D material and ferroelectric-oxide had shown abnormal behavior like anti-hysteresis different from 2D material/ferroelectric-polymer cases showing normal hysteresis. In our work, we also observed systematically those phenomena related to the interface by combining ferroelectric oxide material, PMN-PT (i.e. (1-x)Pb(Mg1/3Nb2/3)O3-PbTiO3) single-crystal with several 2D materials. Through the electrical transport measurement, it is found out that the ferroelectric polarization and trapped charges strongly interacts each other, which is reflected in the conductance of 2D channel. To develop the 2D electronic system in ferroelectric memory device, we should study those properties in detail.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A03 DCMP: Interactions and Dynamics in Topological Systems BCEC 107B - Madhab Neupane, University of Central Florida

*IBS Center for Integrated Nanostructure Physics, Institute for Basic Science, Department of Energy Science, Sungkyunkwan University, Suwon 16419, Korea.
Electronic structure of Dirac materials can be manipulated by impurity doping. One example of such manipulation is the quantum anomalous Hall effect (QAHE), observed in a three-dimensional (3D) topological insulator (TI) doped with magnetic impurities. It is known that impurities give rise to low-energy resonant states near Dirac nodes [1]. For a magnetically-doped 3D TI, an energy gap opens up at the node and is filled with impurity resonant states. Impurity effects have significant implications for QAHE [2,3]. In this work, we show how doping can be used to engineer Dirac nodes in a 3D TI. Using a microscopic tight-binding model for a typical 3D TI with impurities on the surface, we demonstrate the splitting of the surface node and the appearance of new nodes at high-symmetry points of the Brillouin zone. This opens a possibility for impurity engineering of topology and nodal structure in Dirac materials.


*Villum Center for Dirac Materials and KAW 2013.0096
**8:36AM A03.00004: Observation of Two Magnetically Inequivalent Regions in SmB$_6$ at Low Temperatures**

JEFF SONIER (Presenter), KOLAWOLE AKINTOLA, SHAYAN GHEIDI, Simon Fraser University, SARAH R DUNSIGER, TRIUMF, ANDRE COTE, Kwantlen Polytechnic University, SHANTA SAHA, JOHNPIERRE PAGLIONE, University of Maryland - College Park, WESLEY T FUHRMAN, COLLIN BROHOLM, Johns Hopkins University — The temperature dependence of the μSR relaxation rate in SmB$_6$ exposed to a high transverse magnetic field (TF) was recently shown to exhibit thermally-activated behavior for 4 K < $T$ < 20 K, consistent with the freezing out of a bulk low-energy (~ 1 meV) spin exciton [K. Akintola et al., npj Quantum Materials 3:36 (2018)]. However, a 1 meV magnetic excitation has never been observed in neutron scattering measurements, all of which have been performed on the same floating-zone grown double-isotope $^{154}$Sm$^{11}$B$_6$ single crystal. In an attempt to understand why, we have performed zero-field (ZF) and longitudinal-field (LF) μSR measurements on the $^{154}$Sm$^{11}$B$_6$ and Al-flux grown SmB$_6$ single crystals. The μSR signals show greater relaxation in the $^{154}$Sm$^{11}$B$_6$ single crystal, and reveal the development of slow and fast relaxing components below $T$ ~ 20 K. The volume fraction of the slower relaxing component grows to ~ 70 % at $T$ = 2 K. While the relaxation rates are smaller, the volume fractions of the two components are similar in the Al-flux grown SmB$_6$ crystals. This suggests that the source of the two components is intrinsic and originates from spatially distinguishable regions in the sample.


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**8:48AM A03.00005: Band structure engineering in short period Bi$_2$Se$_3$/Sb$_2$Te$_3$ superlattices grown by molecular beam epitaxy**

IDO LEVY (Presenter), THOR A. GARCIA, HAIMING DENG, STEVEN J. ALSHEIMER, LIA KRUSIN-ELBAUM, MARIA TAMARGO, City College of New York — When grown by molecular beam epitaxy (MBE) Bi$_2$Se$_3$ is n-type and Sb$_2$Te$_3$ is p-type due to selenium vacancies and anti-site defects, respectively. To capitalize on the unique topological surface properties of these materials it is essential to reduce the bulk carriers. Compensation doping is a way to do that, but that method requires accurate dopant incorporation levels that are difficult to achieve. In this work we explore the use of p-n-p-n short-period superlattices (SLs) to accomplish this goal. A series of Bi$_2$Se$_3$/Sb$_2$Te$_3$ short-period SLs with varying period thicknesses and Bi$_2$Se$_3$ to Sb$_2$Te$_3$ thickness ratios were grown by MBE. The samples were characterized by high resolution x-ray diffraction (HR-XRD) and transport measurements. Using HR-XRD we determine the change in effective composition and SL period for the samples. We observed a dependence of bulk background doping on the SL period thickness: lower carrier density for thinner SL period. We interpret this as the formation of a gap due to quantum confinement effects. A preservation of a weak anti-localization (WAL) cusp, typical of topological surface features, was observed by magnetoconductance.

*This work was supported by NSF Grant Nos. HRD-1547830 and DMR-1420634.

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**9:00AM A03.00006: Effects of Nitrogen Exposure on the Bismuth Selenide Density of States**

MICHAEL GOTTSCHALK (Presenter), Michigan State Univ, MAL-SOON LEE, Pacific Northwest National Laboratory, CAMILLE MIKOLAS, ERIC GOODWIN, Michigan State Univ, THOMAS CHASAPIS, MERCOURI KANATZIDIS, Northwestern University, S MAHANTI, STUART HOLDEN TESSMER, Michigan State Univ — Bi$_2$Se$_3$ is a topological insulator widely used for scientific studies due in part to the ease with which it can be cleaved, exposing a clean surface for study. Typically the materials exhibit n-type doping attributed to selenium vacancies which results in a shift of the Dirac point to more than 100 meV below the Fermi level. Using cryogenic scanning tunneling microscopy (STM), we observed a shift in the expected density of states spectra when the crystals were cleaved in a pure nitrogen gas environment. The shift tends to restore the Dirac point to the Fermi level. These results are compared against crystals cleaved in a pure helium gas environment which reproduces the expected pristine spectra. We will present density functional theory calculations supporting the picture that nitrogen can bind to the selenium vacancies and shift the density of states. Furthermore, we will present data showing an upper-bound on the level of gas exposure necessary for saturated adsorption.

*This work is supported by the U.S. Department of Energy, Basic Energy Sciences under Award DE-SC0017888.
9:12AM A03.00007: Topology of the Valley-Chern Effect*  
KAI QIAN (Presenter), DAVID J. APIGO, CAMELIA PRODAN, New Jersey Institute of Technology, YAFIS BARLAS, EMIL PRODAN, Yeshiva University — In this talk, we investigate the quantum valley-Hall effect (QVHE) using a versatile experimental platform based on magnetically coupled spinners. We demonstrate that this regime is not suitable for metamaterial applications due to the delocalization of the interface modes. The enlargement of the bulk gap needs to be accompanied by a Berry curvature engineering that keeps it localized near the valleys. This is a new effect which we call the valley-Chern effect (VCE). By establishing an exact relation between VCE and QVHE, we demonstrate a robust bulk-boundary principle, which could be the foundation of a new wave of applications of topological metamaterials.

*All authors acknowledge the support from W.M. Keck Foundation.

9:24AM A03.00008: Observation of topological edge modes in a quasi-periodic acoustic waveguide*  
WENTING CHENG (Presenter), DAVID J. APIGO, KYLE DOBISZEWSKI, New Jersey Institute of Technology, EMIL PRODAN, Yeshiva University, CAMELIA PRODAN, New Jersey Institute of Technology — We present a system of acoustic waveguide generated by a simple quasi-periodic patterning without any additional fine-tuning. The system presents topological edge modes. The waveguides are characterized experimentally by standard acoustic measurements, and via a finite element approach utilizing COMSOL Multiphysics. The experimental results and simulations confirm the existence of topological edge modes in these gaps.

*All authors acknowledge the support from W.M. Keck Foundation.

9:36AM A03.00009: A Proposal to Detect Dark Matter Using Axionic Topological Antiferromagnets*  
DAVID JAMES EDWARD MARSH, University of Gottingen, Institute for Astrophysics, KIN CHUNG FONG, Quantum Engineering and Computing, Raytheon BBN Technologies, ERIK LENTZ, University of Gottingen, Institute for Astrophysics, LIBOR SMEJKAL, Johannes Gutenberg University Mainz, Institute for Physics, MAZHAR ALI (Presenter), Max Planck Institute for Microstructure Physics — Astrophysical and cosmological observations of the last 40 years provide strong evidence for the existence of non-baryonic dark matter. Among possible candidates are dark axions, hypothetical particles suggested to solve the CP problem in quantum chromodynamics. It is known that magnetically doped topological insulators can become "axionic insulators" and host axionic excitations. In particular, antiferromagnetically doped topological insulators (A-TI) are among the candidates to host dynamical axion fields and axion-polaritons. Here we demonstrate that using the axion quasiparticle and antiferromagnetic fluctuations in A-TI's in conjunction with low-noise methods of detecting THz photons presents a viable route to detect axion dark matter with mass 0.7 to 3.5 meV, a range currently inaccessible to all other dark matter detection experiments and proposals.

*Alexander von Humboldt Foundation and the German Federal Ministry of Education and Research. Also the Army Research Office under Cooperative Agreement Number W911NF-17-2-0086

9:48AM A03.00010: Dzyaloshinskii-Moriya Interaction on Surfaces of Topological Insulator*  
DOMENICO ANDREOLI (Presenter), Physics, University of New Hampshire, CHAO-XING LIU, Physics, The Pennsylvania State University, JIADONG ZANG, Physics, University of New Hampshire — The Topological Hall Effect (THE) is a hallmark of nontrivial spin texture. In this work we theoretically study the THE is realizable in centrosymmetric materials. The only requirement being that local inversion symmetry is broken. To show that the THE can occur we start with the model of surface states of a Topological Insulator (TI) and include magnetization on the top and bottom surfaces of the TI. From here the Spin Susceptibility (SS) tensor is determined numerically and it is shown to have off-diagonal components. These components are then related to the Dzyaloshinskii-Moriya (DM) vector. Demonstration of nonzero DM interaction on the surfaces of the TI reveals nontrivial topology in the real space, along with the nontrivial electronic band structure of the TI in momentum space allows for the possibility of the THE in centrosymmetric materials.

*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award No. de-sc0016424.
10:00AM A03.00011: Valley-Chern Effect with LC-Resonators: A Modular Platform* YISHAI EISENBERG (Presenter), YAFIS BARLAS, EMIL PRODAN, Yeshiva University — The valley Chern-effect is theoretically demonstrated with a novel alternating current circuitry, where closed-loop LC-resonators sitting at the nodes of a honeycomb lattice are inductively coupled along the bonds. This enables us to generate a dynamical matrix which copies identically the Hamiltonian driving the electrons in graphene. The valley-Chern effect is generated by splitting the inversion symmetry of the lattice. After a detailed study of the Berry curvature landscape and of the localization of the interface modes, we derive an optimal configuration of the circuit. Furthermore, we show that Q-factors as high as $10^5$ can be achieved with reasonable materials and configurations.

*W.M. Keck Foundation

10:12AM A03.00012: LONG RANGE DYNAMICAL COUPLING BETWEEN MAGNETIC ADATOMS MEDIATED BY EDGE STATES IN A 2D TOPOLOGICAL INSULATOR* MARCIO COSTA (Presenter), LNNANO-CNPEM, MARCO BUONGIORNO NARDELLI, Univ. North Texas, ADALBERTO FAZZIO, LNNANO-CNPEM, ANTÔNIO COSTA, Univ. Federal Fluminense — We study the spin excitation spectra and the dynamical exchange coupling between iron adatoms on a bismuthene nanoribbon. We show that the topological character of the edge states is preserved in the presence of the magnetic adatoms. Nevertheless, they couple significantly to the edge spin currents, as witnessed by the large and long-range dynamical coupling we obtain in our calculations. The large effective magnetocrystalline anisotropy of the magnetic adatoms combined with the transport properties of the topologically protected edge states make this system a strong candidate for implementation of spintronics devices. We use a multi-orbital tight-binding Hamiltonian to describe the electronic structure of the decorated nanoribbon. The full Hamiltonian can be written as the sum of band energy $H_0$, effective intra-atomic Coulomb repulsion $H_{\text{I}}$ and the atomic spin-orbit coupling $H_{\text{SOC}}$. The hopping matrix is obtained directly from a DFT calculation using the pseudo-atomic orbital projection method[1].


M.B.N. - DOD-ONR (N00014-13-1-0635, N00014-11-1-0136, and N00014-15-1-2863)

10:24AM A03.00013: Topological Logical Gates with Meta-Materials* EMIL PRODAN (Presenter), YAFIS BARLAS, Yeshiva University — Recently, the classification table of strong topological condensed matter systems has been implemented with classical passive metamaterials. This includes the topological superconductors, which opens up the possibility of stabilizing and braiding Majorana-like modes in topological metamaterials. This talk puts forward several platforms for topological computations with these systems. The discussion will be aided by numerical simulations.

*W. M. Keck Foundation

10:36AM A03.00014: Interacting Topological Insulators with Synthetic Dimensions* CHAO-MING JIAN (Presenter), CENKE XU, University of California, Santa Barbara — Recent developments of experimental techniques have given us unprecedented opportunities of studying topological insulators in high dimensions, while some of the dimensions are "synthetic", in the sense that the effective lattice momenta along these synthetic dimensions are controllable periodic tuning parameters. In this work, we study interaction effects on topological insulators with synthetic dimensions. We show that although the free fermion band structure of high dimensional topological insulators can be precisely simulated with the "synthetic techniques", generic interactions in these effective synthetic topological insulators are qualitatively different from the local interactions in ordinary condensed matter systems. And we show that these special but generic interactions have unexpected effects on topological insulators, namely they would change (or reduce) the classification of topological insulators differently from the previously extensively studied local interactions.

*The authors are supported by the David and Lucile Packard Foundation and NSF Grant No. DMR-1151208.
10:48AM A03.00015: Anomalous Josephson supercurrent in bulk-insulating topological insulator BiSbTeSe₂

SUBHAMOY GHATAK (Presenter), Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, OLIVER BREUNIG, University of Cologne, II. Physics Institute, FAN YANG, Center for Joint Quantum Studies, Tianjin University, ZHIWEI WANG, ALEXEY A TASKIN, YOICHI ANDO, University of Cologne, II. Physics Institute — Three dimensional topological insulators (3D-TIs) have recently drawn a considerable interest due to their spin-helical surface band structure. The Josephson junctions made of these 3D-TIs, by proximitizing with s-wave superconductors, are predicted to harbour 1D- Majorana modes. While observations of supercurrent in 3D-TI-based Josephson junctions are recently reported, the Fraunhofer patterns observed in such topological Josephson junctions, which sometimes present anomalous features, are still not well understood. In this talk, I will discuss about our study on highly gate-tunable topological Josephson junctions made of bulk-insulating TI materials, BiSbTeSe₂. The Fermi level can be tuned by gating across the Dirac point, and the high transparency of the Al/BiSbTeSe₂ interface is evinced by high multiple Andreev reflections peak indices reaching \( n = 12 \). Anomalous Fraunhofer patterns with missing lobes were observed in the entire range of gate voltage. We find that, by employing an fitting procedure to use the maximum entropy method in a Monte Carlo algorithm, the anomalous Fraunhofer patterns can be explained as a result of inhomogeneous supercurrent distributions on the TI surface in the junction.

*We acknowledge ERC and DFG-CRC for funding this project.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A04 DMP: Dirac/Weyl Semimetals -- Thin Films and Nanostructures BCEC 107C - Hugh Churchill, Univ of Arkansas-Fayetteville - Tag(s): Focus

8:00AM A04.00001: Weyl orbit quantum Hall states observed in Dirac semimetal Cd₃As₂ thin films

SHINICHI NISHIHAYA (Presenter), MASAKI UCHIDA, YUSUKE NAKAZAWA, Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), Univ. of Tokyo, Tokyo, Japan., RYOSUKE KURIHARA, KAZUTO AKIBA, Institute of Solid State Physics (ISSP), Univ. of Tokyo, Kashiwa, Japan., MARKUS KRIENER, RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan., ATSUSHI MIYAKE, Institute of Solid State Physics (ISSP), Univ. of Tokyo, Kashiwa, Japan., YASUJIRO TAGUCHI, RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan., MASASHI KAWASAKI, Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), Univ. of Tokyo, Tokyo, Japan.— Topologically protected surface states in topological materials provide access to various unconventional transport phenomena. One example in gapless topological semimetals is the unique interplay between bulk and surface Fermi-arc states resulting in an exotic magnetic orbit (Weyl orbit). The Weyl orbit weaves together two spatially-separated Fermi-arc states across the bulk state under the field, allowing the appearance of two-dimensional (2D) quantized conduction even in a 3D system. Here, we report the observation of quantum Hall (QH) states in Dirac semimetal Cd₃As₂ thin films. By controlling Fermi level and band topology of the 3D bulk state with electrostatic gating and chemical-doping-induced topological phase transition, we clarify that the quantized conduction emerges originating from the Weyl orbit. In particular, the successive scan from bulk-dominant conduction to Weyl orbit QH effect, reveals that the emergence of the QH states depends on the bulk Landau level occupation and the induced asymmetry between the film surfaces.

8:12AM A04.00002: Confinement Effects in Cd₃As₂ (001) Grown by Molecular Beam Epitaxy

DAVID KEALHOFER (Presenter), LUCA GALLETTI, MANIK GOYAL, HONGGYU KIM, TIMO SCHUMANN, SUSANNE STEMMER, University of California, Santa Barbara — Cadmium arsenide (Cd₃As₂) is a 3D Dirac semimetal in which two Dirac nodes along the \( k_x \) axis are stabilized by a symmetry of the crystal lattice. In a thin film, the fate of the Dirac nodes and associated surface states depends on the orientation of the confinement potential, which is effected by the growth direction. Here we report on improvements to the epitaxial growth of (001)-oriented cadmium arsenide thin films on a III–V compound semiconductor substrate. We show that smooth films can be achieved by altering the surface chemistry at the epilayer–buffer layer interface. We discuss the nature of the resulting clean, two-dimensional transport on the (001)-like surfaces with reference to previous work on the more widely studied (112)-like surfaces.
8:24AM A04.00003: Transport study in Coherently Strained Thin Films of a 3D Dirac Semimetal  MANIK GOYAL  
(Presenter), TIMO SCHUMANN, DAVID KEALHOFER, SALVA SALMANI-REZAIE, LUCA GALLETTI, SUSANNE STEMMER, University of California, Santa Barbara — Cd$_3$As$_2$ is a 3D Dirac semimetal with doubly degenerate band crossings at isolated points in Brillouin zone. Here, we present a study of epitaxially strained thin films of Cd$_3$As$_2$, grown by molecular beam epitaxy on (111) GaAs with In$_x$Ga$_{1-x}$Sb buffer. The composition (x) was varied to obtain layers that are lattice matched with the Cd$_3$As$_2$, as well as to obtain tensile and compressively strained Cd$_3$As$_2$. Films grow coherently strained between 0.44% (tensile) and -0.46% (compressive) strain up to 85 nm thickness. Magneto transport measurements for the thin films (below 50 nm) reveal 2D quantum oscillations under tensile strain, whereas in compressive direction the quantum oscillations are from 3D Fermi surface. We discuss how strain engineering can be used to control the electronic states in thin films of Dirac Semimetals.

8:36AM A04.00004: Non-local Signatures of the Chiral Magnetic Effect in Dirac Semimetal Bi$_{0.97}$Sb$_{0.03}$  
DAAN WIELENS (Presenter), JORRIT C. DE BOER, JORIS A. VOERMAN, BOB DE RONDE, University of Twente, YINGKAI HUANG, MARK GOLDEN, Zeeman Institute, University of Amsterdam, CHUAN LI, ALEXANDER BRINKMAN, University of Twente — Recently there has been a lot of interest in 3D Dirac semimetals (DSM), which exhibit robust Dirac phases in the bulk of the material. The chiral magnetic effect (CME), which originates from the Weyl cones, causes an E.B-dependent chiral charge polarization, which manifests itself as negative magnetoresistance.

We exploit the extended lifetime of this chirally polarized charge and study the CME in both local and non-local measurements on structured devices of mechanically exfoliated single crystalline flakes of DSM Bi$_{1-x}$Sbx with x ≈ 0.03. From the transport measurements on the non-local devices we find that the chiral charge relaxation time is over an order of magnitude larger than the transport lifetime.

*The authors acknowledge financial support from the European Research Council through a Consolidator Grant and from the Netherlands Organization for Scientific Research through a VICI Grant.

8:48AM A04.00005: Quantum transport properties of Cd$_3$As$_2$ films with low carrier density  
YUSUKE NAKAZAWA  
(Presenter), MASAKI UCHIDA, SHINICHI NISHIHAYA, SHIN SATO, MASASHI KAWASAKI, Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), the University of Tokyo — Cd$_3$As$_2$ is a typical three-dimensional topological Dirac semimetal, characterized by a pair of Dirac points protected by rotational symmetry. While high-crystallinity and high-flatness Cd$_3$As$_2$ films have been obtained by the combination of pulsed laser deposition and subsequent high-temperature annealing [1,2], the carrier density is rather high compared to ones prepared by molecular beam epitaxy [3,4]. In this talk, we report quantum transport properties of Cd$_3$As$_2$ thin films epitaxially grown by molecular beam epitaxy. A typical film thicker than 100 nm shows a carrier density of 5×10$^{16}$ cm$^{-3}$ and an electron mobility exceeding 3×10$^4$ cm$^2$/Vs. In this thickness regime corresponding to the three-dimensional electronic structure, the film shows plateau-like structures in the Hall resistance, indicating the emergence of a two-dimensional conduction state. This can be understood to originate from the Weyl orbit surface state of the topological Dirac semimetal.

9:00AM A04.00006: Negative longitudinal magnetoresistance in GaAs quantum wells* JING XU (Presenter), Argonne National Lab, MENG MA, Princeton University, ZHILI XIAO, Argonne National Lab, YONGLEI WANG, Nanjing University, DAFEI JIN, Argonne National Lab, YANGYANG LYU, Nanjing University, WEI ZHANG, Oakland University, LOREN PFEIFFER, KENNETH WEST, K. W. BALDWIN, MANSOUR SHAYEGAN, Princeton University, WAI-KWONG KWOK, Argonne National Lab, MAKSIM SULTANOV, Northern Illinois University —

Negative longitudinal magnetoresistances (NLMRs) have been observed in a variety of materials and often considered to be associated with Weyl fermions that have a defined chirality. We conducted magnetotransport measurements and observed NLMRs in non-Weyl GaAs quantum wells. We observed pronounced NLMRs up to 9 Tesla at temperatures above the transition temperature and also weak NLMRs at low magnetic fields at temperatures close to the transition and at very low temperatures. The observed NLMRs show various types of magnetic field behavior, the origin of which we attribute to microscopic disorder and we use a phenomenological model to account for the various features. Our results showcase a new contribution of microscopic disorder to the occurrence of novel phenomena. They may stimulate further work on tuning electronic properties via disorder/defect nano-engineering.

*Sample fabrication and characterization were supported by the DOE Basic Energy Sciences (Grant No. DE-FG02-00-ER45841), the NSF (Grants No. DMR 1709076 and MRSEC DMR 1420541), and the GBMF (Grant No. GBMF4420). W. Z. acknowledges support from the DOE and NSF under Grants No. DMR-1808892. M. Su. was supported by the Fulbright Program. J. X. and Z. X. also acknowledge support by the NSF under Grant No. DMR-1407175.

9:12AM A04.00007: Topological phase transitions by interface engineering DONG ZHANG (Presenter), SKLSM, Institute of semiconductors, Chinese Academy of Sciences — Novel phase transitions, especially topological phase transitions, have attracted intense interests in condensed matter physics in recent years. However, the reported materials possess novel phases are majorly composed of heavy elements with relatively low abundances. We switched investigate objectives into commonly-used semiconductors, and demonstrated that, utilizing giant electric fields generated by charge accumulation at GaAs/Ge/GaAs opposite semiconductor interfaces and band folding, the interface engineering can reduce the sizable gap in Ge, induce large spin-orbit interaction, and drive Ge into a topological insulating phase [1]. Natural topological semimetals hosting multiple topological states will be demonstrated through simple symmetry considerations [2,3], and the possibilities to realize “ideal” topological semimetals utilizing interface design[4] will also be disscussed.

References

9:24AM A04.00008: Charge transfer in a transition metal dichalcogenide semiconductor/Weyl semimetal van der Waals junctions KYUSUP LEE (Presenter), Department of Electrical and Computer Engineering, National University of Singapore, JIE LI, School of Materials Science and Engineering, Huazhong University of Science and Technology, LIANG CHENG, School of Physical and Mathematical Sciences, Nanyang Technological University, JUNYONG WANG, Department of Physics, National University of Singapore, DUSHYANT KUMAR, QISHENG WANG, MENGJI CHEN, YANG WU, Department of Electrical and Computer Engineering, National University of Singapore, GOKI EDA, Department of Physics, National University of Singapore, EE MIN CHIA, School of Physical and Mathematical Sciences, Nanyang Technological University, HAIXIN CHANG, School of Materials Science and Engineering, Huazhong University of Science and Technology, HYUNSOO YANG, Department of Electrical and Computer Engineering, National University of Singapore — Transient metal dichalcogenides (TMDs) heterostructures have recently made a meteoric rise in quantum device engineering due to its van der Waals (vdW) layered nature. A Weyl semimetal WTe$_2$, also a TMD compound, displays a wide range of exotic electronic and spintronic properties. A central approach in heterostructures is driving charge transfer across the interface mainly governing the carrier dynamics, which determines fundamental optoelectronic properties. Here, we report a new type of CVD grown TMD vdW junctions with a semiconductor 2H-MoTe$_2$ and its sister compound of semimetallic Td-WTe$_2$. Time-resolved terahertz spectroscopy reveals the ultrafast relaxation of the photo-excited carriers in the junctions, which attributes to the charge transfer and the interlayer exciton decay serving as a fast relaxation channel with a characteristic time of ~0.6 ps, faster than that of the each layer (~1.5 ps from Td-WTe$_2$ and ~5.9 ps from 2H-MoTe$_2$). Moreover, we observe the negligible band-filling and hot-phonon effects according to the optical fluence (< 10 mJ/cm$^2$) due to such an ultrafast interfacial relaxation channel. This ultrafast photoresponse in sister-compound large-area TMDs vdW junctions provide a platform for high-speed optoelectronic devices.
9:36 AM A04.00009: Exploring Transport Properties in the 2D–3D Dirac Semimetal Heterostructures* YANFEI WU (Presenter), Massachusetts Institute of Technology, LIANG ZHANG, LI CAIZHEN, ZHI-MIN LIAO, Peking University, DAPENG YU, SONG LIU, ZHEN-SHENG ZHANG, Southern University of Science and Technology — Dirac semimetal is an emerging class of quantum matters, ranging from two-dimensional (2D) category, such as graphene and surface states of topological insulator to three-dimensional (3D) category, for instance, Cd$_3$As$_2$ and Na$_3$Bi. Exotic surface states in 3D Dirac semimetals is attractive for the interface engineering and the research on 2D–3D Dirac van der Waals heterostructures. Here we fabricated graphene–Cd$_3$As$_2$ heterostructure through direct layer-by-layer stacking and investigated their electron transport properties. The electronic coupling results in a notable interlayer charge transfer, which modulates the Fermi level of graphene through Cd$_3$As$_2$. This heterostructure enable us to naturally fabricate graphene p–n–p junctions, showing the quantized conductance plateaus. Moreover, the nonlocal transport studies show large nonlocal signals near Dirac point in graphene–Cd$_3$As$_2$ device, due to the charge transfer from the spin-polarized surface states in Cd$_3$As$_2$. Our results enrich the family of van der Waals heterostructures and can inspire more studies on the application of Dirac/Weyl semimetals in spintronics.

*This work was supported by the National Key Research and Development Program of China, NSFC, SZSTI, and Guangdong Innovative and Entrepreneurial Research Team Program.

9:48 AM A04.00010: Manipulating the Topological Surface States of Cd$_3$As$_2$ by N* Plasma Exposure TIMO SCHUMANN (Presenter), LUCA GALLETTI, THOMAS E MATES, SUSANNE STEMMER, University of California, Santa Barbara — Cd$_3$As$_2$ belongs to the family of three-dimensional Dirac semimetals, which are characterized by a linear dispersion of their bulk bands at the Fermi energy. For thin films, the electronic transport properties of Cd$_3$As$_2$ are dominated by surface states, which, as we show in this presentation, are highly sensitive to the chemistry of the surface. Temperature-dependent magneto-transport measurements show that exposure of the surface to a low-energy nitrogen plasma improves carrier mobility and facilitates the observation of the quantum Hall effect in confined thin films. X-ray photoemission spectroscopy reveals changes in the surface chemistry of air-exposed and nitrogen-plasma surfaces, respectively. The results provide insights into the role of surface band bending and the relative contributions of surface and bulk states to the measured transport properties.

10:00 AM A04.00011: Realization of an Elemental Topological Dirac Semimetal: α-Sn on InSb(111) [Invited] TAI-CHANG CHIANG (Presenter), University of Illinois at Urbana-Champaign — Three-dimensional (3D) topological Dirac semimetals (TDSs) are rare but important as a versatile platform for exploring exotic electronic properties and topological phase transitions. A quintessential feature of TDSs is 3D Dirac fermions associated with bulk electronic states near the Fermi level. Using angle-resolved photoemission spectroscopy, we have observed such bulk Dirac cones in epitaxially grown α-Sn films on InSb(111), the first such TDS system realized in an elemental form. First-principles calculations confirm that epitaxial strain caused by the in-plane lattice mismatch of 0.14% is key to the formation of the TDS phase. A phase diagram as a function of epitaxial strain is established that connects the 3D TDS phase through a singular point of a zero-gap semimetal phase to a topological insulator phase. The nature of the Dirac cone crosses over from 3D to 2D as the film thickness is reduced to a few layers.

In collaboration with Cai-Zhi Xu, Yang-Hao Chan, Yige Chen, Peng Chen, Xiaoxiong Wang, Catherine Dejoie, Man-Hong Wong, Joseph Andrew Hlevyack, Hyejin Ryu, Hae-Young Kee, Nobumichi Tamura, Mei-Yin Chou, Zahid Hussain, and Sung-Kwan Mo

10:36 AM A04.00012: First principles study of WTe$_2$ with Wannier model* AMARTYAJYOTI SAHA (Presenter), School of Physics and Astronomy, University of Minnesota, TURAN BIROL, Department of Chemical Engineering and Materials Science, UNIVERSITY OF MINNESOTA — Two-dimensional transition metal dichalcogenides are a class of atomically thin materials which can host a wide range of physical properties such as strong spin-orbit coupling and nontrivial topological phases. Both monolayer and bulk tungsten ditelluride (WTe$_2$) has been studied in great detail over the past years for their electronic properties. Here we present the results of our first principles study of the behaviour of finite thickness WTe$_2$. To connect between the bulk and the monolayer material, we employ Wannier functions to build tight binding models for different numbers of WTe$_2$ layers. This study provides insight into the effect of van der Waals interactions and spin-orbit coupling on the symmetry, crystal and band structures, and topology of WTe$_2$.

*This work was supported primarily by the National Science Foundation through the University of Minnesota MRSEC under Award Number DMR-1420013 and the iSuperseed program.
Using linear response theory, we evaluate the optical conductivity of 2D semi-Dirac materials for light polarized along two mutually orthogonal directions and predict a strong anisotropy of the optical response as a consequence of their unique dispersion spectrum. Our results also predict a large degree of sensitivity for inter-band optical conductivity to the polarization direction. While it reveals an abruptly large value for certain frequency for light along a particular polarization direction, it is significantly suppressed along the direction orthogonal to the former. The frequency corresponding to the predicted giant optical conductivity is found to be independent of the chemical potential, for a lightly doped system. This direction-dependency of the giant inter-band optical conductivity may, in turn, be used to uniquely predict the dispersive nature of the 2D \textit{semi}-Dirac materials, in addition to possible applications that arise from this direction dependent optical transparency.


Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A05 DMP: Topological Superconductivity: Majorana

8:00AM A05.00001: Majorana in Chains and Hinges\textsuperscript{*}  [Invited] ALI YAZDANI (Presenter), Princeton University — In recent years, following pioneering theoretical work of Kitaev and others, we have learned how to engineer materials that harbor quasiparticles that behave similar to fermions that Majorana had first envisioned. In particular, there has been a focus on one-dimensional topological superconductor that harbor Majorana zero modes (MZM) that can potentially be used to make fault-tolerant topological quantum computation possible. We have proposed and implemented a platform for realization of topological superconductivity and MZM in chains of magnetic atoms on the surface of a superconductor. In this talk, I will describe the series of experiments on this platform that we have performed to establish the presence of these exotic quasi-particle using spectroscopic mapping with the scanning tunneling microscope (STM). These include the most recent study of the unique spin signature of MZM. I will also describe work on a new platform where we use the one-dimensional helical hinge states of a higher order topological insulators. In paritcular, I will show experiment demonstrating how combination of magnetism and superconductivity on such one-dimensional states can also give rise to MZM that can be detected with an STM. Overall these experiments, illustrate how the power of spectroscopic imaging with the STM can be used to characterize novel quantum states of matter and visualize their exotic quasi-particles.

\textsuperscript{*}We acknowledge funding from ONR, Moore foundation, NSF-DMR, and NSF-MRSEC through Princeton Center for Complex Materials.

8:36AM A05.00002: Experimental signatures of Majorana bound states in S-TI-S lateral Josephson junctions\textsuperscript{*}
GUANG YUE (Presenter), CAN ZHANG, ERIK HUEMILLER, University of Illinois at Urbana-Champaign, MARYAM SALEHI, NIKESH KOIRALA, SEONGSHIK OH, Rutgers University - New Brunswick, ALEXEY BEZRYADIN, DALE J VAN HARLINGEN, University of Illinois at Urbana-Champaign — We present experiments designed to search for features of Majorana bound states (MBS) in lateral Josephson junctions formed by depositing s-wave superconductors onto the surface of topological insulator thin films. In a vertical magnetic field that induces a phase gradient across the junction, the localized MBS are expected to be stable at the cores of Josephson vortices where the phase difference across the junction is an odd multiple of $\pi$. To test this picture, we have fabricated Nb-Bi$_2$Se$_3$-Nb Josephson junctions with different geometries and carried out extensive measurements of their Josephson supercurrent vs. magnetic field diffraction patterns and the statistical critical current switching distribution in hysteretic junctions. Our results show a number of expected features of MBS, including: (1) finite critical current at the location of odd-numbered nodes of the diffraction pattern, (2) anomalous critical current distributions characterized by either a double peak in the switching distribution or an increase in the standard deviation of the distribution changes at values of magnetic field at which MBS are expected to be present in the junction. We will present a compilation of our data and analysis of these experiments.

\textsuperscript{*}NSF DMR 16-10114
ANDREY ANTIPOV (Presenter), Microsoft, ARNO BARGERBOS, TU Delft, GEORG W. WINKLER, BELA BAUER, ENRICO ROSSI, ROMAN LUCHYN, Microsoft — We study the effect of gate-induced electric fields on the properties of semiconductor-superconductor hybrid nanowires which represent a promising platform for realizing topological superconductivity and Majorana zero modes. Using a self-consistent Schrödinger-Poisson approach that describes the semiconductor and the superconductor on equal footing, we are able to access the strong tunneling regime and identify the impact of an applied gate voltage on the coupling between semiconductor and superconductor. We discuss how physical parameters such as the induced superconducting gap and Landé g-factor in the semiconductor are modified by redistributing the density of states across the interface upon application of an external gate voltage. Finally, we map out the topological phase diagram as a function of magnetic field and gate voltage for InAs/Al nanowires.

MARTIN CLAASSEN (Presenter), Center for Computational Quantum Physics, Simons Foundation Flatiron Institute, DANTE KENNES, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, MANUEL ZINGL, Center for Computational Quantum Physics, Simons Foundation Flatiron Institute, MICHAEL SENTEF, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter — Chiral superconductors are a novel class of unconventional superconductors that host topologically protected chiral Majorana fermions at interfaces and domain walls, with great potential for topological quantum computing. Here we show that the out-of-equilibrium superconducting state in such materials is itself described by a Bloch vector in analogy to a qubit, which can be controlled all-optically on ultrafast time scales [1]. The mechanism is universal and permits a dynamical change of handedness of the condensate, relying on transient dynamical breaking of lattice rotation, mirror or time-reversal symmetries via choice of pump pulse polarization to enable arbitrary rotations of the Bloch vector. The underlying physics can be intuitively understood in terms of transient Floquet dynamics, however the mechanism extends to ultrafast time scales, and importantly the engineered state persists after the pump is switched off. We demonstrate that these novel phenomena should appear in graphene and magic-angle twisted bilayer graphene (TBG), as well as Sr$_2$RuO$_4$, as candidate chiral $d+id$ and $p+ip$ superconductors, and show that chiral superconductivity can be detected in time-resolved pump-probe measurements.

QIYUE WANG (Presenter), Department of Physics, University of Texas at Dallas, CHENG-CHENG LIU, School of Physics, Beijing Institute of Technology, YUAN-MING LU, Deparment of Physics, Ohio State University, FAN ZHANG, Department of Physics, University of Texas at Dallas — Majorana bound states often occur at the end of a 1D topological superconductor. Validated by a new bulk invariant and an intuitive edge argument, we show the emergence of one Majorana Kramers pair at each corner of a square-shaped 2D topological insulator proximitized by an extended s-wave (e.g., Fe-based) superconductor. We obtain a phase diagram that addresses the relaxation of crystal symmetry and edge orientation. We propose two experimental realizations in candidate materials. Our scheme offers a higher-order and higher-temperature route for exploring non-Abelian quasiparticles.


QIYUE WANG (Presenter), Department of Physics, University of Texas at Dallas, CHENG-CHENG LIU, School of Physics, Beijing Institute of Technology, YUAN-MING LU, Department of Physics, Ohio State University, FAN ZHANG, Department of Physics, University of Texas at Dallas — Majorana bound states often occur at the end of a 1D topological superconductor. Validated by a new bulk invariant and an intuitive edge argument, we show the emergence of one Majorana Kramers pair at each corner of a square-shaped 2D topological insulator proximitized by an extended s-wave (e.g., Fe-based) superconductor. We obtain a phase diagram that addresses the relaxation of crystal symmetry and edge orientation. We propose two experimental realizations in candidate materials. Our scheme offers a higher-order and higher-temperature route for exploring non-Abelian quasiparticles.

*This work was supported by ARO under Grant No. W911NF-18-1-0416 (Q. W. and F. Z.) and NSF under Grant No. DMR-1653769 (Y.-M. L.).
9:24AM A05.00006: Majorana modes as electrical switches: computing the conductance of a junction between a
Topological superconductor and a multi-channel Luttinger liquid ALBERTO NOCERA (Presenter), Stewart Blusson
Quantum Matter Institute, University of British Columbia, ARMIN RAHMANI, Physics, Western Washington University, ADRIAN
FEIGUIN, Physics, Northeastern University, MARCEL FRANZ, IAN AFFLECK, Stewart Blusson Quantum Matter Institute, University of
British Columbia — Motivated by the experimental confirmation of topological superconductivity in semiconducting
nanowires, I study the transport properties of a junction of three wires (T-junction), which provides the simplest nontrivial
example of wire network, as well as an important building block for topological quantum computing architectures. I show
how to compute the electrical conductance of a T-junction between a Topological superconductor and two normal
interacting nanowires using the Density Matrix Renormalization Group (DMRG) method [1] that allows one to extract the
conductance in the thermodynamic limit from static ground-state DMRG computations in closed finite systems [2]. As
main result, I numerically demonstrate that the T-junction can act as an electrical switch in the presence of a localized
Majorana mode in agreement with field theory predictions [3]. I finally focus on the regime where the tunnel couplings
between the superconductor and the nanowires is fine tuned to the same value, and compare the numerical results to the
field theory calculations that predict a non-trivial critical point with an unusual conductance tensor.


9:36AM A05.00007: Chiral Majorana modes on electrically gated high Tc Topological Superconductors*
NIMA DJAVID (Presenter), ROGER LAKE, ECE, University of California, Riverside — Majorana edge modes were detected by observation
of half-integer conductivity in a magnetic topological insulator/superconductor (MTI/SC) heterostructure [1]. Recently
proposed systems which are compatible with standard semiconductor processing are the most promising schemes for
braiding Majorana modes. However, identifying Majorana zero modes experimentally has been challenging mostly
because of the small pairing gap of s-wave SCs. A heterostructure between an anomalous quantum Hall insulator and a
high Tc d-wave superconductor with a large pairing gap may offer a more feasible approach for implementing Majorana
zero modes.

In this work, we study topological properties of a gated d-wave (MTI/SC) heterostructure. The phase diagram of the system
is obtained by employing the Kubo formula. The existence of Majorana edge modes in the presence of electrical gating has
been shown in d-wave topological superconductors. A Green’s function formalism has been employed for the detection of
Majorana edge modes and their localization properties have been investigated.

1.He, Q. L. et al. Chiral Majorana fermion modes in a quantum anomalous Hall insulator–superconductor structure. Science

*This work was supported by the NSF under Award No. NSF EFRI-1433395 and 2-DARE.

9:48AM A05.00008: Majorana Zero Modes and Braiding in Realistic Nanowire Y-Junctions* FENNER HARPER
(Presenter), University of California, Los Angeles, M A MUEED, BENJAMIN MADON, IBM Almaden Research Center, FABRIZIO
NICHELE, MARKUS RITTER, IBM Zurich Research Laboratory, NOEL ARELLANO, IBM Almaden Research Center, HEINZ SCHMID,
SIEGFRIED KARG, HEIKE RIEL, IBM Zurich Research Laboratory, AAKASH PUSHP, IBM Almaden Research Center, RAHUL ROY,
University of California, Los Angeles — Under the right conditions, semiconductor nanowires are believed to host zero-energy
Majorana fermions, particles with non-abelian properties suitable for topological quantum computation. While recent
experiments have demonstrated encouraging local signatures of Majorana fermions, evidence for their non-abelian
nature remains elusive. Motivated by ongoing experimental work at IBM, we build a realistic model of a nanowire Y-
junction and study the properties of the resulting Majorana fermions numerically. We make quantitative predictions about
the device parameters and geometry that are conducive to realising Majorana zero modes, and study the corresponding
experimental signatures that would be expected. We go on to simulate braiding operations between multiple Majorana
fermions, and suggest experimental gating protocols that may lead to signatures of their non-abelian nature.

*This work is supported by the DARPA program Topological Excitations in Electronics.
Majorana double nanowires in the presence of magnetic field, interactions, and disorder

MANISHA THAKURATHI (Presenter), Department of Physics, University of Basel, PASCAL SIMON, Laboratoire de Physique des Solides (CNRS/ U-PSUD), Université Paris Sud, JELENA KLINOVJA, DANIEL LOSS, Department of Physics, University of Basel — We study double Rashba nanowires (NWs) coupled to an s-wave superconductor, which has been recently proposed as a versatile platform to generate Kramers pairs of Majorana bound states in the absence of magnetic field [1]. We also analyze the effects of electron-electron interactions and disorder on the system and find that the interactions drive the system into the topological phase [2]. We further consider an external magnetic field along the NWs and demonstrate that the setup exhibits a new previously overlooked Majorana phase that emerges at low magnetic field [3]. Also we demonstrate the charge and spin signatures of topological superconductivity in the double NWs setup.


Multi-band Physics in Inhomogeneous Majorana Nanowires

BENJAMIN WOODS (Presenter), TUDOR DAN STANESCU, West Virginia University — Semiconductor nanowires proximity coupled to superconductors are a promising platform to detect and manipulate Majorana zero energy modes. Single band models are used ubiquitously throughout the literature to describe these systems. In practice, however, it is quite likely that multiple confinement bands determine the properties of these devices, which can lead to new features not predicted by the single band models. We consider different types of inhomogeneity, such as a quantum dot defined by a region of the nanowire not covered by the superconductor. As previously shown, the dot region can give rise to Andreev bound states that mimic some of the signatures of Majorana zero modes. We find an increased pinning of Andreev bound states to zero energy within the multi-band model due to strong inter-band coupling induced by an inhomogeneous electrostatic potential. Understanding in detail the multi-band effects are important for the practical realization of Majorana zero modes in semiconductor-superconductor nanowire devices.

Non-hermitian topology: a unifying framework for the Andreev versus Majorana states controversy

RAMON AGUADO (Presenter), PABLO SAN-JOSE, Materials Science Institute of Madrid (ICMM), Spanish Research Council (CSIC), ELSA PRADA, FERNANDO PEÑARANDA, Condensed Matter Physics Center (IFIMAC), Universidad Autonoma de Madrid (UAM), JESUS AVILA, Materials Science Institute of Madrid (ICMM), Spanish Research Council (CSIC) — Andreev bound states (ABSs) in hybrid semiconductor-superconductor nanowires can have near-zero energy in parameter regions where band topology predicts trivial phases. This surprising fact has been used to challenge the interpretation of a number of transport experiments in terms of non-trivial topology with Majorana zero modes (MZMs). We show that this ongoing ABS versus MZM controversy is fully clarified when framed in the language of non-Hermitian topology, the natural description for open quantum systems. This change of paradigm allows us to understand topological transitions and the emergence of pairs of zero modes more broadly, in terms of exceptional point (EP) bifurcations of system eigenvalue pairs in the complex plane. Within this framework, we show that some zero energy ABSs are actually non-trivial, and share all the properties of conventional MZMs, such as the recently observed 2e^2/h conductance quantization. From this point of view, any distinction between such ABS zero modes and conventional MZMs becomes artificial. The key feature that underlies their common non-trivial properties is an asymmetric coupling of Majorana components to the reservoir, which triggers the EP bifurcation [1].

10:36AM A05.00012: Metamorphosis of Andreev bound states into Majorana bound states in pristine nanowires*  
YINGYI HUANG, HAINING PAN (Presenter), Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, CHUN-XIAO LIU, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, JAY SAU, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, TUDOR DAN STANESCU, Department of Physics and Astronomy, West Virginia University — We show theoretically that a clean superconducting spin-orbit-coupled nanowire with finite chemical potential has two distinct non-topological regimes as a function of Zeeman splitting: one is characterized by finite-energy in-gap Andreev bound states (ABS), while the other has only extended bulk states. The Andreev bound state regime is characterized by strong features in the tunneling spectra creating a “gap closure” signature. However, no “gap reopening” signature should be apparent above the topological quantum phase transition (TQPT), in agreement with the most recent experimental observations. The gap closure feature is not a signature of the trivial gap of extended bulk states closing at the transition, but rather reflects the coming together of the ABS in systems with high chemical potential. Our theoretical finding establishes the generic intrinsic ABS on the trivial side of the topological quantum phase transition as the main contributors to the tunneling conductance spectra, providing a generic interpretation of existing experiments in clean Majorana nanowires. Our work also explains why experimental tunnel conductance spectra generically have gap closing features below the TQPT, but no gap opening features above it.

*This work is supported by LPS and Microsoft.

10:48AM A05.00013: Phonon-Assisted Andreev Reection at Majorana Zero Mode  
NING DAI (Presenter), QING-FENG SUN, International Center for Quantum Materials, Peking University — One of the typical features of Majorana zero mode (MZM) at the edge of topological superconductor is a zero-bias peak in the tunneling spectroscopy of the normal-superconductor (NS) junction. We study on a model with one phonon mode coupling to the superconductor lead of the NS junction, which can be viewed as an electron-lead/phonon-coupled-MZM/hole-lead structure. The phonon-coupled MZM acts as a series of channels in which electron can turn into hole by transmitting phonons to itself. These channels present in the local density of states(LDOS) as a series of stripes, generating the corresponding peaks in the tunneling spectroscopy. In LDOS, the electron-phonon interaction narrows and redistributes the weight among stripes. In the tunneling spectroscopy, the heights of peaks present a feature of the multi-phonon process. With these investigations, our work illuminates the mechanism of phonon-assisted Andreev reflection at a Majorana zero mode.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A06 DCMP: Beyond Fermi Liquid Theory  
BCEC 109A - Peter Riseborough, Temple University - Tag(s): Focus

8:00AM A06.00001: Superdiffusive transport of energy in generic Luttinger liquids  
JOEL MOORE (Presenter), University of California, Berkeley, and Lawrence Berkeley National Laboratory, VIR BULCHANDANI, University of California, Berkeley, CHRISTOPH KARRASCH, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin — Metals in one spatial dimension are described at the lowest energy scales by the Luttinger liquid theory. It is well understood that this free theory, and even interacting integrable models, can support ballistic transport of conserved quantities including energy. Realistic Luttinger liquids, even in pure systems without disorder, contain integrability-breaking interactions, which are expected to lead to thermalization and conventional diffusive linear response. We show that the expansion of energy when such a non-integrable Luttinger liquid is locally heated above its ground state shows superdiffusive behavior (i.e., spreading of energy that is intermediate between diffusion and ballistic propagation), by combining an analytical anomalous diffusion model with numerical matrix product state calculations. The main ingredient in the analytical model is the power-law in linear-response transport that originates in the scaling dimension of integrability-breaking corrections to the Luttinger liquid. Some other one-dimensional systems that also remain far from the linear-response regime for long times are discussed.
Lorentz ratio of a compensated metal

SONGCI LI (Presenter), National High Magnetic Field Laboratory/University of Florida, DMITRII MASLOV, University of Florida — A violation of the Wiedemann-Franz law in a metal can be quantified by comparing the Lorentz ratio, \( L = \kappa / \rho / T \), where \( \kappa \) is the thermal conductivity and \( \rho \) is the electrical resistivity, with the universal Sommerfeld constant, \( L_0 = \pi^2/3 \) \( (k_B/e)^2 \).

We obtain the Lorentz ratio of a clean compensated metal with intercarrier interaction as the dominant scattering mechanism by solving exactly the system of coupled integral Boltzmann equations. The Lorentz ratio is shown to assume a particular simple form in the forward-scattering limit: \( L/L_0 = \Theta^2 / 2 \), where \( \Theta \) is the scattering angle. In this limit, \( L/L_0 \) can be arbitrarily small. We also show how the same result can be obtained without the benefit of an exact solution. We discuss how a strong downward violation of the Wiedemann-Franz law in a type-II Weyl semimetal WP_2 can be explained within our model.

Uncovering non-Fermi-liquid behavior in Hund metals: critical behavior of a three-orbital Kondo model

ELIAS WALTER (Presenter), KATHARINA M STADLER, SEUNG-SUP B. LEE, Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-University of Munich, Germany, YILIN WANG, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, NY, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, NJ, ANDREAS WEICHSELBAUM, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, NY, JAN VON DELFT, Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-University of Munich, Germany — When using dynamical mean field theory (DMFT) to study Hund metals, one arrives at self-consistent impurity models in which bath and impurity both have spin and orbital degrees of freedom. If these are screened at different energy scales, \( T_K^{\text{sp}} < T_K^{\text{orb}} \), the intermediate energy window is governed by a novel non-Fermi-liquid (NFL) fixed point, involving screened orbital degrees of freedom weakly coupled to an unscreened local spin. Here we characterize the corresponding NFL behavior in detail for a 3-orbital Kondo model, tuned such that the NFL energy window is very wide. We find excellent agreement between conformal field theory (CFT) predictions and numerical renormalization group (NRG) results.

Transport properties of a disordered two-dimensional metal in the vicinity of SDW order: A memory matrix calculation

HERMANN FREIRE (Presenter), Instituto de Física, Universidade Federal de Goiás, Goiânia-GO, Brazil — We perform the calculation of many transport coefficients as a function of temperature in the “strange-metal” phase that emerges in the vicinity of a SDW phase transition in the presence of weak disorder. This scenario is relevant to the phenomenology of many important correlated materials, such as, e.g., the cuprates and the iron-based superconductors. We implement the memory-matrix approach that allows the calculation of all transport coefficients for the corresponding field-theory model beyond the quasiparticle paradigm. As a result, we are able to obtain here the temperature dependence of the dc resistivity, the Hall angle, the thermal conductivity, the Seebeck coefficient and the Nernst response for a disordered two-dimensional SDW quantum critical theory with an effective composite operator that couples the order-parameter fluctuations to the entire Fermi surface of the system. We argue that our present theory provides a good basis in order to unify the experimental transport data, e.g., of the cuprates, within a wide range of doping regimes.

References:


*I would like to thank the Brazilian agency CNPq under grant No. 405584/2016-4 for financial support.
8:48AM A06.00005: Transconducting Transition for a Dynamic Boundary Coupled to Several Tomonaga-Luttinger Liquids*  BARUCH HOROVITZ, Department of Physics, Ben Gurion University, THIERRY GIAMARCHI (Presenter), DQMP, University of Geneva, PIERRE LE DOUSSAL, LPTENS, Ecole Normale Superieure — The question on how a quantum bath can affect the dynamical properties of a quantum degree of freedom is a long standing and important one. Here we study a dynamic boundary, e.g., a mobile impurity, coupled to N independent Tomonaga-Luttinger liquids (TLLs) each with interaction parameter K. We demonstrate [1] that for N ≥ 2 there is a quantum phase transition at a critical value of K ≥ 1/2, where the TLL phases lock together at the particle position, resulting in a nonzero transconductance equal to e²/(Nh). We analyze this transition line and compare it with large N predictions. We discuss experimental applications both for cold atomic or condensed matter realizations.


*B. H. gratefully acknowledges funding by the German DFG through the DIP programme [FO703/2-1]. P. L.D. acknowledges support from ANR Grant No. ANR-17-CE30-0027-01 RaMaTraF. This work was supported in part by the Swiss National Science Foundation under Division II.

9:00AM A06.00006: T-linear resistivity in models with local self-energy*  EUN-AH KIM (Presenter), PETER CHA, Cornell University, AAVISHKAR PATEL, Harvard University, EMANUEL C GULL, University of Michigan — Bad metallic transport is commonly observed in strongly correlated systems. In particular, T-linear resistivity is of special theoretical interest in its connection to quantum criticality and superconductivity. Recently, T-linear resistivity have been explicitly found in several models with local self-energy yet relation between different mechanisms remain unclear. In this work, we discuss two models that demonstrate T-linearity: lattice-Sachdev-Ye-Kitaev model and the Hubbard model within the dynamical mean-field theory (DMFT). In the former, we find that T-scaling depends crucially on the details of both the infra-red- and ultraviolet-limits. In the latter, we study the Hubbard model within single-site DMFT, and show that transport quantities and compressibility are driven by atomic interactions down to the temperatures of the order of the bandwidth. We also study the temperature dependence of the Lorentz ratio and Diffusivity and contrast different mechanisms of T-linear resistivity.

*Cha has been supported by NSF Materials Innovation Platform grant DMR-1539918.

9:12AM A06.00007: Theory of Strange Metals from Hot Fermions*  CONNIE MOUSATOV (Presenter), Department of Physics, Stanford University, EREZ BERG, Department of Condensed Matter Physics, Weizmann Institute of Science, SEAN HARTNOLL, Department of Physics, Stanford University — We study a metal where a large Fermi surface coexists with a set of `hot spots' with a high density of states. The hot electrons occupy a small fraction of the Brillouin zone, yet qualitatively modify the properties of the entire system. We emphasize the importance of scattering processes in which two electrons from the large, `cold' Fermi surface scatter into one hot and one cold electron. These lead to a `strange metallic' state with anomalous, non-Fermi liquid thermodynamic and transport properties. Scattering into hot electrons that are effectively classical (non-degenerate) in a finite portion of the Brillouin zone leads to a marginal Fermi liquid. This explains, in detail, the phenomenology of Sr3Ru2O7 in field, including T-linear resistivity and a T log(1/T) electronic specific heat. Hot electrons that are instead localized near a point in the Brillouin zone, such as a two-dimensional van Hove singularity, lead to different power laws. We show that the transport behavior of strained Sr2RuO4 is recovered from this picture.

*CHM is supported by an NSF graduate fellowship.

9:24AM A06.00008: Emergent Anisotropic Non-Fermi Liquid  SANGEUN HAN (Presenter), Department of Physics, KAIST, CHANGHEE LEE, Department of Physics and Astronomy, SNU, EUN-GOOK MOON, Department of Physics, KAIST, HONGKI MIN, Department of Physics and Astronomy, SNU — Understanding correlation effects in topological phases and their transitions is a cutting-edge area of research in recent condensed matter physics. We study topological quantum phase transitions (TQPTs) between double-Weyl semimetals (DWSMs) and insulators, and argue that a novel class of quantum criticality appears at the TQPT characterized by emergent anisotropic non-Fermi liquid behaviors, in which the interplay between the Coulomb interaction and electronic critical modes induces not only anisotropic renormalization of the Coulomb interaction but also strongly correlated electronic excitation. Using the standard renormalization group methods, large $N_f$ theory and the $\varepsilon=4-d$ method with fermion flavor number $N_f$ and spatial dimension $d$, we obtain the anomalous dimensions of electrons ($\eta_f=0.366/N_f$) in large $N_f$ theory and the associated anisotropic scaling relations of various physical observables. Our results may be observed in candidate materials for DWSMs such as HgCr2Se4 or SrSi2 when the system undergoes a TQPT.
temperatures down to a low coherence scale, $T_{coh}$. The intermediate NFL regime displays anomalous transport properties, such as the ruthenates and cobaltates, display metallic non-Fermi liquid (NFL) properties over a broad range of temperatures $T$ and at low bias voltages $eV$. We also apply the formulas to the SU(N) symmetric case and calculate order $T^2$ and $(eV)^2$ contributions of the differential conductance $dI/dV$, by using the numerical renormalization group (NRG) approach and also the $1/(N-1)$ expansion [3]. Our results, obtained in a wide range of electron fillings, show that contributions of three-body fluctuations that enter through nonlinear susceptibilities play an important role as a gate voltage varies away from the particle-hole symmetric point where the impurity levels are half-filled. Furthermore, the contributions of three body fluctuations show an oscillatory behavior as gate voltage $\varepsilon_d$ varies and, the three body fluctuations decrease as the number of the orbital $N$ increases.


9:48AM A06.00010: Out-of-equilibrium dynamics and thermalization across a solvable non-Fermi liquid to Fermi liquid transition*  
ARJIT HALDAR (Presenter), PROSENJIT HALDAR, SUMILAN BANERJEE, Center for Condensed Matter Theory, Dept. of Physics, Indian Institute of Science, Indian Institute of Science — We study the non-equilibrium dynamics of an interacting model [1] having a quantum phase transition from a Sachdev-Ye-Kitaev (SYK) non-Fermi liquid (NFL) to a Fermi liquid (FL). The model has SYK fermions on $N$ sites quadratically coupled to non-interacting peripheral fermions on $M$ sites. The transition from the NFL ($p < 1$) to FL ($p > 1$) is obtained at $p=1$ by tuning the ratio $p=M/N$. We study the dynamics as a function of $p$, (a) after a quench where the coupling between initially disconnected SYK and peripheral fermions is suddenly switched on, and (b) during a slow quench when the coupling is slowly ramped over a duration $\tau$. In the sudden quench, we find that a thermal state is reached in the NFL ($p < 1$) through collapse-revival oscillations of the quasiparticle residue of the peripheral fermions. In the FL phase, the system fails to thermalize within the accessible time and shows multiple pre-thermal regimes. In the slow quench, the excitation energy generated has a power-law dependence $\sim \tau^{-\eta}$ for intermediate $\tau$, with a strong $p$-dependent $\eta$ having a minimum at the transition. At larger $\tau$ the power-law breaks down, along with adiabaticity, due to the initial residual entropy of the SYK fermions. [1] S. Banerjee and E. Altman, PRB 95, 134302 (2017).

*SERB, DST & The Infosys Foundation.

10:00AM A06.00011: Solvable lattice models for intermediate scale non-Fermi liquid metals  
DEBANJAN CHOWDHURY (Presenter), SENTHIL TODADRI, Massachusetts Institute of Technology — A number of strongly correlated materials, such as the ruthenates and cobaltates, display metallic non-Fermi liquid (NFL) properties over a broad range of temperatures down to a low coherence scale, $T_{coh}$. The intermediate NFL regime displays anomalous transport properties, broad electronic spectral functions indicating the absence of sharp quasiparticles and is often accompanied by a finite extrapolated zero temperature entropy. Theoretically, examples of similar NFL metals can be obtained using higher dimensional generalizations of the solvable SYK model and have also been shown to arise in dynamical mean-field theory solutions of more realistic microscopic models. Going beyond these approaches, I will propose other models and setups where a broad incoherent metallic regime arises in the presence of a finite configurational entropy.

10:12AM A06.00012: Conductivity of a compensated metal near a Pomeranchuk quantum critical point: the absence of mass renormalization*  
DMITRI MASLOV (Presenter), University of Florida, SONGCI LI, National High Magnetic Field Laboratory/University of Florida — The role of mass renormalization, $m^*/m_B$, in electron transport near a quantum critical point (QCP) is a nontrivial issue. According to a naive interpretation of the Drude formula, as electrons get heavier near a QCP, their electrical and thermal conductivities decrease. However, this picture has never been supported by an actual calculation. In this work, we employ a model case of a compensated metal near a Pomeranchuk-type criticality. The advantage of this model is that it allows one to treat electrical and thermal conductivities on the same footing, without invoking umklapp scattering or any other channels of momentum relaxation which are extraneous to the electron system. By solving exactly the kinetic equation, we obtain explicit results for the electrical and thermal conductivities, and also for the viscosity of a two-band compensated metal. We show that mass renormalization factors cancel out with the $Z$ factors, which renormalize the scattering probability, such that all the transport quantities contain the bare rather than renormalized electron masses. We also demonstrate how the same cancelation happens diagrammatically, on an example of the optical conductivity of a compensated metal.

*D. L. M.: NSF-DMR-1720816
S. L.: NSF Cooperative agreement No. DMR-1157490
10:24AM A06.00013: Entanglement signatures of quantum-to-classical crossover of a Fermi surface

HASSAN SHAPOURIAN (Presenter), SHINSEI RYU, University of Chicago — The entanglement entropy of free fermions with a Fermi surface is known to obey a logarithmic scaling and violate the area law in all dimensions. Here, we would like to see how thermal fluctuations affect the logarithmic scaling behavior. To this end, we analytically compute the bipartite entanglement negativity of a finite-temperature state and show that the coherent Fermi surface is gradually destroyed as a function of temperature and eventually turns into an incoherent classical system, where the entanglement is completely lost. We check that our analytical results agree with the numerical simulation of free fermions on a lattice.

10:36AM A06.00014: Strong-Coupling Study of Interlayer Pairing in Bilayer Composite Fermion Metals

LUIS MENDOZA (Presenter), NICHOLAS EVANS BONESTEEL, Florida State University — We study the T=0 Eliashberg equations for interlayer pairing in the composite fermion description of the ν=1/2+1/2 quantum Hall bilayer system. In this description, composite fermions are coupled to two bosonic gauge fields which, in addition to leading to a breakdown of Fermi liquid theory, mediate a singular attractive interaction and a less singular repulsive interaction in the interlayer Cooper channel. Our solution of the T=0 Eliashberg equations includes both these pairing and pair-breaking effects, along with self-energy effects. We compare our results with previous Eliashberg results which do not take self-energy effects into account [1], and results obtained using the RG [2,3]. The connection between the RG and Eliashberg frameworks is also studied through the local approximation introduced in [4]. In particular we carry out the local approximation explicitly and compare with our results obtained from the full Eliashberg equations.


Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A07 DCMP: Charge Order

8:00AM A07.00001: Honeycomb Lattice-Type CDW associated with Interlayer Cu Ions Ordering in 1T-CuxTiSe2

SHUNSUKE KITOU (Presenter), Nagoya University, and Institute for Molecular Science, SHINTARO KOBAYASHI, Nagoya University, TATSUYA KANEKO, RIKEN, NAOYUKI KATAYAMA, Nagoya University, SEIJI YUNOKI, RIKEN, TOSHIKAZU NAKAMURA, Institute for Molecular Science, Japan, HIROSHI SAWA, Nagoya University — The electronic state in 1T-TiSe2, which has attracted attention as an excitonic insulator, can be changed by electronic doping through Cu+ intercalation. Indeed, the superconductivity was reported in Cu_xTiSe2 on 0.04 ≤ x ≤ 0.10 [1]. We succeeded in synthesis of single crystal samples of Cu_xTiSe2 (x = 0 ~ 0.35) and performed physical property measurements, synchrotron x-ray diffraction experiments, and density-functional-theory calculations. It was found that x = 1/4 and 1/3 were magical numbers in this system and disorder-order transitions were caused by the interaction among Cu atoms. Furthermore, in x = 1/3, a hybrid-type phase transition caused by the commensurate connection between Cu-ordering and a new honeycomb lattice-type charge-density-wave in TiSe2 layers was realized.


*his work was supported by a Grant-in-Aid for Scientific Research (No. JP17K17793, 18K13509, 18H01183) from JSPS, Kato Foundation for Promotion of Science, and Daiko Foundation.
8:12AM A07.00002: Charge disproportionation, mixed valence, and Janus effect in multiorbital systems: A tale of two insulators* ALDO ISIDORI (Presenter), MAJA BEROVIC, LAURA FANFARILLO, International School for Advanced Studies (SISSA, Trieste, Italy), LUCE DE MEDICI, Laboratoire de Physique et d’Etude des Materiaux, Paris, France, MICHELE FABRIZIO, MASSIMO CAPONE, International School for Advanced Studies (SISSA, Trieste, Italy) — Multiorbital Hubbard models host strongly correlated 'Hund's metals' even for interactions much stronger than the bandwidth. We characterize this interaction-resilient metal as a mixed-valence state. In particular it can be pictured as a bridge between two strongly correlated insulators: a high-spin Mott insulator and a charge-disproportionated insulator which is stabilized by a very large Hund's coupling. This picture is confirmed comparing models with negative and positive Hund's coupling for different fillings. Our results provide a characterization of the Hund's metal state and connect its presence with charge disproportionation, which has indeed been observed in chromates and proposed to play a role in iron-based superconductors.

* A.I., M.F., and M.C. acknowledge support from the H2020 Framework Programme, under ERC Advanced GA No. 692670 ‘FIRSTORM’. L.F. acknowledges the cost action Nanocohybri CA16218. L.d.M. acknowledges H2020 ERC-StG2016, StrongCoPhy4Energy, GA No. 724177. M.C. also acknowledges financial support from MIUR PRIN 2015 (Prot. 2015CS5EJJ001) and SISSA/CNR project “Superconductivity, Ferroelectricity and Magnetism in bad metals” (Prot. 232/2015).

8:24AM A07.00003: Unraveling spin and charge dynamics in two-leg spin ladders using resonant inelastic x-ray scattering UMESH KUMAR (Presenter), Department of Physics and Astronomy, University of Tennessee, Knoxville, ALBERTO NOCERA, Stewart Blusson Quantum Matter Institute, University of British Columbia, ELBIO R DAGOTTO, STEVEN JOHNSTON, Department of Physics and Astronomy, University of Tennessee, Knoxville — Resonant inelastic x-ray scattering (RIXS) has become an important tool to study the spin and charge excitations in materials. We investigate the RIXS spectra of undoped and doped antiferromagnetic spin-ladder cuprate in both the non-spin conserving (NSC) and spin-conserving (SC) channels at the Cu $L_3$-edge. The spectra are rich and host many exotic excitations. In the undoped NSC-channel, we identify one-triplon, triplet two-triplon excitations in the strong rung coupling limit and confined spinons in the weak rung coupling limit. In the doped NSC-channel, we identify new dispersive quasiparticle-like spectral features composed of bound 'charge and spin-1/2' in strong rung coupling limit in addition to the excitations branches already present in the undoped case. The NSC-channel can be well described by $S(q, \omega)$. On the other hand, SC-channel is unique to RIXS and reveals new features. In the undoped SC channel, we identify singlet two-triplon for the strong rung coupling and confined spinons for the weak rung coupling. In the doped SC-channel, RIXS probes the charge excitations instead of spin-excitations, and we identify gapless and gapped charge excitations in the spectra.

8:36AM A07.00004: Stripes and Nematicity in a Hole-Doped Three-Orbital Spin-Fermion Model for Superconducting Cuprates* ADRIANA MOREO (Presenter), Physics, University of Tennessee and ORNL — Numerical studies of a spin-fermion model that captures the charge-transfer properties of Cu-based high critical temperature superconductors[1] reveal the spin and charge order in the parent compound and under hole doping. In clusters of dimension 16X4, that break the rotational symmetry, half-filled stripes are observed upon hole doping, i.e., $n$ stripes of length 4 develop when $2n$ holes are introduced in the system. The antiferromagnetic order observed in the parent compound develops a pi-shift across each stripe and the magnetic structure factor peaks at momentum $k=(\pi,\pi)$ with $\delta=2\pi N_h/L$ where $L=16$ and $N_h$ is the number of doped holes.

The electronic charge is also modulated and the charge structure factor peaks at $k=(2\delta,0)$. In addition, orbital nematicity with $\langle n_{px}\rangle-\langle n_{py}\rangle\neq 0$ develops as electrons are removed from the system. These results indicate that the spin and charge distribution experimentally observed in hole-doped cuprates is captured by unbiased Monte Carlo studies of a doped charge-transfer insulator.


the upshifted T\textsubscript{SHABALIN}, University of California, San Diego, DILING ZHU, SLAC- Natl Accelerator Lab, ERIC FULLERTON, OLEG SHPYRKO, NUH GEDIK, Massachusetts Institute of Technology — The phase diagram of cuprate superconductors exhibits a plethora of

seen through the Raman phonon mode near 650 cm\textsuperscript{-1} [2]. The M2 phase has two substructures of both the charge density

and resistance, we observed that

In this talk, through simultaneous measurements of temperature dependence of micro-Raman spectra and resistance, as


9:24AM A07.00008: Ultrafast probing of collective mode of the charge order in La\textsubscript{1.87}Ba\textsubscript{0.125}CuO\textsubscript{4}

Electrons react very quickly, and moreover generally are the smallest component of the total heat capacity. This allows us to uncover a new long-lived metastable state in the charge density wave material 17-TaSe\textsubscript{2}, that is distinct from all of the known equilibrium phases: it is characterized by a significantly reduced effective heat capacity that is only 30% of the normal value, due to selective electron-phonon coupling to a subset of phonon modes. As a result, significantly less energy is required to melt the charge order and transform the state of the material than under thermal equilibrium conditions.

9:00AM A07.00006: Observation of M2 phase coming from the charge density wave for the insulator-to-metal transition in VO\textsubscript{2}.

Due to the strain, the intermediate monoclinic phase, known as the M2 phase, was clearly seen through the Raman phonon mode near 650 cm\textsuperscript{-1} [2]. The M2 phase has two substructures of both the charge density wave (CDW) responsible for the Peierls insulator and zig-zag chain for the Mott insulator [3]. However, the mechanism of the upshifted T\textsubscript{IMT} does not yet revealed.

In this talk, through simultaneous measurements of temperature dependence of micro-Raman spectra and resistance, as well as in-situ XRD and resistance, we observed that T\textsubscript{IMT} is prior to temperature of structural phase transition, and that M2 Raman peak still remains from screening effect despite high temperature of 370 K. Therefore, we suggest that the observed M2 Raman peak is caused by the remained CDW structure. Moreover, this can be a reason of upshifted T\textsubscript{IMT}.


*This was supported by principal project in ETRI and a MS\&ICT project (2017-0-00830)

9:12AM A07.00007: Ultrafast recovery of charge density wave order controlled in a pump-pump-probe free electron laser experiment*

We present a new ultrafast electron calorimetry technique that can systematically uncover new phases of quantum matter. Using time- and angle-resolved photoemission spectroscopy, we measure the dynamic electron temperature, band structure and heat capacity. We then show that this is a very sensitive probe of phase changes in materials, because electrons react very quickly, and moreover generally are the smallest component of the total heat capacity. This allows us to uncover a new long-lived metastable state in the charge density wave material 17-TaSe\textsubscript{2}, that is distinct from all of the known equilibrium phases: it is characterized by a significantly reduced effective heat capacity that is only 30% of the normal value, due to selective electron-phonon coupling to a subset of phonon modes. As a result, significantly less energy is required to melt the charge order and transform the state of the material than under thermal equilibrium conditions.

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9:36AM A07.00009: The role of non-local correlations in the valence band spectra in NiO*  BYUNGKYUN KANG (Presenter), SANGKOOK CHOI, PATRICK SEMON, ANDREY KUTEPOV, VAN DAM HUBERTUS, GABRIEL KOTLIAR, Brookhaven National Laboratory — As an archetypical strongly-correlated material, late-transition metal NiO has been attracted for number of decades. The interesting electronic properties of charge transfer insulator and low energy Zhang-Rice bound state are attributed to Ni 3d and O 2p hybridization along with strong Coulomb interactions of Ni 3d. However, the rich physics may still raise unclear physical properties in NiO. One example is the second peak from the Fermi level in X-ray photoemission spectra which is enhanced below Neel temperature. By Using recently developed LQSGW + DMFT along with charge self-consistent LDA+DMFT, we will discuss the role of non-local correlation in the formation of the second peak and their temperature dependence.

*This work was supported by the U.S Department of energy, Oce of Science, Basic Energy Sicences as a part of the Computational Materials Science Program.

9:48AM A07.00010: Magnetotransport in $H||c$ of La$_{1.875}$Ba$_{0.125}$CuO$_4$ near the charge order (CO) transition* LILY STANLEY (Presenter), PAUL G. BAITY, DRAGANA POPOVIC, Dept. of Phys. Natl. High Magnetic Field Lab., JOHN TRANQUADA, GENDA GU, Brookhaven Natl Lab — The nature of the dynamics of charge-ordered states in underdoped cuprates has been of great recent interest. Our work on La$_{2-x}$Ba$_x$CuO$_4$ with $x=0.125$ (LBCO) in zero magnetic field ($H$) reveals the presence of dynamic behavior within the charge-ordered state in the form of avalanches, similar to that in La$_{1.48}$Nd$_{0.4}$Sr$_{0.12}$CuO$_4$ (LNSCO). In LNSCO, avalanches were also observed to be asymmetrically driven by $H$ around the concurrent CO and structural transition with an additional onset of negative magnetoresistance (MR), which was attributed to the emergence of CO [1]. In La$_{1.7}$Eu$_{0.2}$Sr$_{0.12}$CuO$_4$ (LESCO) negative MR, albeit with no avalanches, was observed at the onset of CO but not at the higher temperatures around the structural transition [1]. The presence of avalanches and overlap of the CO and structural transitions in LBCO present the opportunity to clarify the role of the LNSCO Nd$^{3+}$ moments and the origin of the negative MR. Therefore, we report the $H = 0$ findings and the study of $H||c$ magneto resistance of LBCO near the CO transition.


10:00AM A07.00011: Precision measurement of charge-order formation by coherent Resonant X-ray Scattering LI YUE (Presenter), School of Physics, Peking University, JIARUI LI, Department of Physics, Massachusetts Institute of Technology, CLAUDIO MAZZOLI, Brookhaven National Lab, RICCARDO COMIN, Department of Physics, Massachusetts Institute of Technology, YUAN LI, School of Physics, Peking University — We report experimental research on the spontaneous formation of charge order and its relationship with disorder pinning effects. By studying a prototypical charge-density-wave material, ZrTe$_3$, with high-precision resonant elastic X-ray scattering (REXS), we observe a clear temperature evolution of the ordering wave vector, along with a drastic increase in the correlation length, upon the development of the long-range charge order below $T \approx 63$ K. These results are attributed to band-structure changes near the Fermi level due to the opening of the charge-ordering gap. By further utilizing a coherent X-ray beam, we are able to reveal unprecedented details in the mesoscopic dynamics of the charge order by X-ray photon correlation spectroscopy (XPCS), the results of which can be most naturally explained by the combined effects of thermal activation and disorder pinning. Our results provide empirical insights for understanding charge-order phenomena in correlated-electron systems such as the high-Tc cuprates.

10:12AM A07.00012: Charge Density Waves in a Doped Kondo Chain* YIXUAN HUANG (Presenter), University of Houston, DONNA SHENG, California State University, Northridge, CHIN-SEN TING, University of Houston — We show that charge density waves (CDWs) exist in the ground state of the one-dimensional Kondo lattice model at the filling of $n=0.75$ with a finite charge gap, while most of the doped phase is metallic. Based on our numerical results using the density matrix renormalization group method, we separate the CDW phase from the paramagnetic phase previously known as the Tomonaga-Luttinger liquid. The emergence of this phase serves as an example of CDW induced without repulsive interaction between electrons, and enriches the phase diagram of the 1D Kondo Lattice model.

*The work is supported by the Robert A Welch Foundation and the Texas Center for Superconductivity at the University of Houston. D.N.S. is supported by the DOE, through the Office of Basic Energy Sciences.
Femtosecond electron imaging of a transformation between different symmetry broken ground states of 2D charge density wave near a nonthermal critical point

FARAN ZHOU (Presenter), JOSEPH WILLIAMS, Michigan State Univ, CHRISTOS MALLIAKAS, MERCOURI KANATZIDIS, Northwestern University, CHONG-YU RUAN, Michigan State Univ — We study the atomic scale dynamics of a CDW phase transition from a stripe phase into a new topological phase in rare-earth tritelluride compound. Such a new state is a hidden ground state not allowed thermodynamically, but is driven to form after an interaction quench by an intense infrared laser pulse. With femtosecond electron-based scattering, we capture the entire course of this transformation and show an emergent self-organization that defines a nonthermal critical point substantially different from a thermal critical point. The dynamical stabilization after the quench is achieved through the inherent underpinning symmetry that allows the development of the long-range coherence simultaneously for different broken symmetry states at far from equilibrium.

*We thank the funding support by NSF MRI facility grant: DMR1625181 and DOE grant: DE-FG02-06ER46309

Charge Density Wave Order in the Half-Filled Three Dimensional Holstein Model

BENJAMIN COHEN-STEAD (Presenter), University of California, Davis, CHUANG CHEN, ZI YANG MENG, Institute of Physics, Chinese Academy of Science, RICHARD THEODORE SCALETTAR, University of California, Davis — The Holstein Model (HM) is a tight-binding Hamiltonian describing electrons coupled to local phonon degrees of freedom. The electron phonon interaction gives rise to charge density wave (CDW) order at half-filling and superconducting (SC) order away from half-filling. The HM has been a recent focus for Determinant Quantum Monte Carlo (DQMC) simulation studies. However, the cubic scaling with system size, and long autocorrelation times, have restricted simulations to one and two dimensional systems. Here we demonstrate that the recent development of Self-Learning Monte Carlo (SLMC)[1,2] has made it possible to significantly reduce autocorrelation times, thereby allowing for simulation studies of the Holstein model on a fully three-dimensional cubic lattice at half-filling. SLMC is able to control autocorrelation times by learning an effective model that is used to propose more effective monte carlo moves, while still satisfying detailed-balance. SLMC allows us to not only access larger system sizes, but also slower phonon modes where the phonon frequency \( \omega \) is less than the inter-site hopping parameter \( t \).

*This work was supported by the Department of Energy, grant DE-SC0014671.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A08 DCMP DMP: Low Carrier Density Superconductors

Electron-phonon coupling and superconductivity in SrTiO3

DIRK VAN DER MAREL (Presenter), University of Geneva — Doped STO is a superconductor with a maximal Tc rising from zero at zero doping to 400 mK around 0.005 electrons per Ti atom, and dropping to zero above 0.02 electrons per Ti atom. Substituting the heavier O-18 isotope for the natural O-16 in the samples results in a strong increase of Tc with an isotope coefficient some 20 times larger and of opposite sign as predicted by the BCS model. This effect was theoretically anticipated based on a model where the superconducting pairing in STO is mediated by the optical phonons which are associated to the para- to ferro-electric phase transition in in the undoped insulating compound, the so-called TO1 mode. Here we demonstrate from experimental data that the spectral weight of the TO1 mode is anomalously large, providing a strong indication for the so-called “charged phonon” effect predicted by MJ Rice. The experimentally observed spectral weight of mode TO1 is used to determine the nature and strength of its’ coupling to the conduction electrons, and implications of these numbers are presented for the corresponding channel of superconducting pairing.

*This project was supported by the Swiss National Science Foundation through project 200021-179157.
8:12AM A08.00002: Low density superconductivity of SrTiO₃ bounded by the adiabatic condition

HYEOK YOON (Presenter), ADRIAN G SWARTZ, HISASHI INOUE, Geballe Laboratory for Advanced Materials, Department of Applied Physics, Stanford University, YASUYUKI HIKITA, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, HAROLD HWANG, Geballe Laboratory for Advanced Materials, Department of Applied Physics, Stanford University — The dilute oxide semiconductor SrTiO₃ exhibits superconductivity over a wide range of carrier densities (10¹⁷⁻¹⁰²¹ cm⁻³) lying outside of the Bardeen-Cooper-Schrieffer (BCS) and Migdal-Eliashberg theories for conventional superconductors. Across this range, the Fermi level traverses a variety of vibrational modes in the system and therefore spans the widest range of adiabatic parameter (ω/EF) of any superconductor, making it an ideal choice to study the physics of dilute superconductivity. Recently, we have developed an approach using atomically controlled oxide heterostructures to spectroscopically probe the electronic structure of SrTiO₃ using planar tunneling junctions [1, 2]. Using this technique, we have examined the superconductivity of bulk doped SrTiO₃ across the superconducting dome and found that superconducting state is bounded by the adiabatic condition, maintaining the thermodynamic relationship of BCS weak-coupling theory (2Δ/k_B T_c = 3.53).


8:24AM A08.00003: Plasmon-Polaron Superconductivity in Strontium Titanate

ALEXANDER EDELMAN (Presenter), PETER B LITTLEWOOD, University of Chicago — Strontium titanate (STO) is a bulk insulator that becomes a semiconducting superconductor at remarkably low carrier densities - below 10¹⁷ cm⁻³ - with a characteristic superconducting dome as a function of doping which peaks at T_c~300mK, all in very close proximity to a ferroelectric quantum critical point. Photoemission[1] and tunneling[2] have revealed multiple phonon replica bands, and the challenge to theory is to reconcile these observations of a very strongly coupled normal state with the apparently conventional weakly-coupled BCS superconducting state[3]. We propose a simple model that extends an Engelsberg-Schrieffer theory of electrons coupled to a single longitudinal optic (LO) phonon mode to self-consistently include the effects of electronic interactions. For the carrier densities of interest, we find that the plasmon hybridizes strongly with LO mode with one of the resulting coupled modes inheriting the low energy scales of the softening ferroelectric mode. We calculate spectral signatures of our model and the superconducting phase diagram, including vertex corrections crucial in this strongly-coupled regime, and compare to experiment.


8:36AM A08.00004: Gate voltage tunable superconductivity in low-carrier-density SrTiO₃

TERENCE BRETZ-SULLIVAN (Presenter), J SAMUEL JIANG, Argonne National Laboratory, ALEXEY SUSLOV, National High Magnetic Field Laboratory, JOHN E. PEARSON, ALEX MARTINSON, ANAND BHATTACHARYA, Argonne National Laboratory — We demonstrate gate voltage control of the critical current of a surface channel of the low-carrier-density, bulk-superconducting oxide system SrTiO₃. The devices are in a conventional field effect transistor geometry with a solid gate dielectric and superconducting leads. We can modulate the critical current by a factor of 2-3 in our devices as a function of gate voltage. Additionally, we study the magnetic field dependence of the differential resistance of these devices to understand the role the superconducting leads play on the channel properties. A device such as this could serve as a new qubit architecture when integrated into a microwave resonator circuit.

We acknowledge support of the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division. The use of facilities at the Center for Nanoscale Materials was supported by the U.S. DOE, BES under Contract No. DE-AC02-06CH11357. The NHMFL is supported by NSF/DMR-1644779 and the State of Florida.
8:48AM A08.00005: Enhancement of the superconducting $T_c$ upon isotopic substitution in Strontium Titanate

Willem Schau (Presenter), Dorota Pulmanova, Gernot Scheerer, Enrico Giannini, Dirk Van Der Marel, University of Geneva — SrTiO$_3$, a quantum paraelectric, becomes a metal with a superconducting instability after removal of an extremely small number of oxygen atoms. It turns into a ferroelectric upon isotopic $^{18}$O substitution exceeding a quantum critical point (QCP) located at a substitution level of around 33 at% $^{18}$O. The exceptionally dilute superconducting and the ferroelectric order may be accidental neighbors or intimately connected, as in the picture of quantum critical ferroelectricity.

We developed an $^{18}$O substitution process to control substitution levels in SrTi(O$_{1-x}$O$_x$)$_3$ beyond the critical point. Dielectric measurements evidence a ferroelectric order below the Curie temperature. In metallic SrTi(O$_{1-x}$O$_x$)$_3$-$\delta$ with $^{18}$O-substitution levels above the QCP, we find that the superconducting critical temperature seen in resistivity measurements is enhanced by more than a factor two and reaches values of up to 700 mK. This enhancement strongly supports the role played by the vicinity to the ferroelectric order in the precocious emergence of superconductivity, restricting possible theoretical scenarios for pairing.

9:00AM A08.00006: Quantum ferroelectric instabilities in superconducting SrTiO$_3$*

José Rafael Arce-Gamboa, Gian G. Guzmán-Verrí (Presenter), Materials Research Science and Engineering Center (CICIMA), University of Costa Rica — We examine the effects of strain and cation substitution on the superconducting (SC) phase of polar semiconductors near a ferroelectric (FE) quantum phase transition with a model that combines a strong coupling theory of superconductors with a standard microscopic framework for displacive polar modes coupled to strain. Our calculations reveal that the SC transition temperature $T_c$ is enhanced by proximity to the FE instability from the disordered side, while it is generally suppressed in the ordered phase due to its increase in dielectric stiffness and a reduction of critical fluctuations from dipolar induced anisotropies. The condensation of the pairing phonon excitations generates a kink in $T_c$ at a charge density that is generally lower than that of the quantum critical point (QCP) and where both SC and FE orders set-in. We apply our model to SrTiO$_3$ and find that the anti-adiabatic limit places the kink nearly at its QCP. As the QCP is pushed to higher charge densities, the dome narrows and sharpens. We compare to recent experiments and theory.

*Work at UCR supported by the Vice-rectory for Research (project no. 816-B7-601) and at ANL by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Science Division under contract no. DE-AC02-06CH11357.

9:12AM A08.00007: Pairbreaking Induced by Magnetic Impurity Doping Shrinks the Giant Magnetoresistance Peak of the Cooper Pair Insulator*

James Valles (Presenter), Xue Zhang, James C Joy, Chunshu Wu, Physics, Brown University, Jimmy Xu, Physics and School of Engineering, Brown University — Films near the critical point of a boson fluctuation dominated superconductor to insulator transition exhibit a giant magnetoresistance peak that grows exponentially with decreasing temperature. Experiments indicate that Cooper pair transport dominates the low magnetic field side of the MR peak so that the resistance rise indicates increasing Cooper pair localization. To probe whether the peak arises from magnetic field induced orbital dephasing of the Cooper pair states or Cooper pair breaking, our group investigated its response to a pure pairbreaking perturbation: magnetic impurity doping. We quench deposited a-Bi films onto nanoporous anodized aluminum oxide substrates and tuned their thickness to produce an insulating state of Cooper pairs. Gd impurity doping 1) reduces the size of the MR peak while pushing it to lower magnetic fields and 2) causes changes in the zero magnetic field resistance that are much smaller than the MR peak. How this behavior suggests that orbital dephasing effects are primarily responsible for the MR peak will be discussed.

**We are grateful for the support of NSF Grant No. DMR-1307290.
Reports of superconductivity in systems with very low carrier densities are becoming increasingly prevalent. Examples include strontium titanate, bismuth, and twisted bilayer graphene. Here, we investigate this general issue by studying superconductivity in the Bardeen-Pines model of an electron gas interacting with an optical phonon with frequency $\omega_L$, as function of carrier concentration. The pairing interaction in the model is a combination of screened Coulomb repulsion and an attraction due to phonons, dressed by electron polarizability. We first focus on the attractive part of the interaction and argue that processes away from the Fermi surface cannot be neglected at low electron density. Contrary to expectations from BCS theory, we obtain a large increase of the critical temperature $T_c$ as the system enters the dilute region, with a power-law dependence of $T_c$ on $\omega_L$. Next, we explore how the superconducting instability and the frequency dependence of the pairing function get modified once we add the Coulomb repulsion.

*This work is supported by the Department of Energy through the University of Minnesota Center for Quantum Materials, under DE-SC-0016371.

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We present results for the onset pairing instability temperature for superconductivity mediated by an Einstein phonon in a 2D electron gas with a parabolic dispersion, in the regime of low carrier density. We go beyond the leading order in the electron-phonon coupling and include contributions to the pairing kernel from fermionic self-energy and from Kohn-Luttinger processes. We then compute the phase stiffness and obtain the actual critical temperature $T_c$. We analyze thermodynamic properties of our system, such as the specific heat jump across $T_c$.

*This work was supported by the U.S. Department of Energy through the University of Minnesota Center for Quantum Materials, under award DE-SC-0016371.

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We investigate the superconductivity of compounds with a small carrier density, such as SrTiO3, bismuth and YPtBi. In these materials, the pairing instability is often described as a consequence of charge fluctuations either due to longitudinal phonons or through the dynamic screening of the Coulomb repulsion. Since the Fermi energy is small, the influence of interband transitions cannot be neglected in the the dynamic pairing potential. We will discuss how this alters the superconducting critical temperature in the various channels.

*The State of Connecticut for startup funds. J. C. for Mark Miller award. A.V.B. and K.D. for US BES E3B7, VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744) and by Knut and Alice Wallenberg Foundation (2013.0096).
**10:12AM A08.00012: A sign of anticorrelation between the orbital related order and the superconductivity in LiTi$_2$O$_{4.5}$ system**

WEI HU (Presenter), Chinese Academy of Sciences, Institute of Physics — Previously studies show that for the Li$_{1+x}$Ti$_{2-x}$O$_{4.5}$(x<1/3) samples grown below a certain oxygen pressure, $T_{c0}$ remains the same whereas the orbital related order become weaker as the oxygen pressure increasing. It seems that the superconductivity of those samples isn't obviously related to the orbital related order. However, it is recently founded that, for those samples, there is a small linear region exists in temperature dependent resistance curve (R-T curve) above the superconducting state, and the temperature that the R-T curve begin to deviate from this linear region at the low temperature side enhances with the increase of the oxygen pressure. The suppressive effect of current on superconductivity shows that this temperature is the beginning of the superconductivity. Therefore, it indicates that the superconductivity is actually strengthened as the oxygen pressure increasing, contrary to the effect of the oxygen pressure on the orbital related order. Moreover, a new superconducting film similar to LiTi$_2$O$_{4.5}$ has been synthesized by PLD, which shows more directly that the superconductivity can be weakened by the orbital order.

**10:24AM A08.00013: Unconventional full-gap superconductivity in Kondo lattice with semi-metallic conduction bands**

SHOMA IIMURA (Presenter), Saitama University, MOTOAKI HIRAYAMA, RIKEN, SHINTARO HOSHINO, Saitama University — Non-local and anisotropic Cooper pairings are favored in heavy-electron materials with nearly localized f-electrons. On the other hand, the full-gap nature of the superconducting states in CeCu2Si2 and UBe13 have been revealed by the specific heat measurements in a rotating magnetic-field. Therefore, it is desirable to propose a new mechanism of superconductivity that is specific to heavy-electron materials. Here we theoretically study the Kondo lattice with semi-metallic conduction bands, and propose the mechanism for full-gap superconductivity in f-electron systems. Based on the mean-field approach, we reveal that the superposition between electron conduction band and hole conduction band is realized through the formation of the Kondo-singlet states. The resultant ground state spontaneously breaks the gauge symmetry to make the system superconducting. This superconducting state is characterized by the composite pairing amplitude, which has been proposed in the context of two-channel Kondo lattice. We have demonstrated here that the semi-metallic conduction bands with electron and hole Fermi surfaces are closely related to the composite pairing.

*This work is supported by the JSPS KAKENHI Grant No. 18H04305.

**10:36AM A08.00014: Dynamical effects on BCS-BEC crossover in the Holstein model**

TAE-HO PARK (Presenter), HANYONG CHOI, Sungkyunkwan University — We present a study of the half-filled Holstein model with superconducting order employing the dynamical mean-field theory in combination with the numerical renormalization group. Here, we investigate the dynamical effects on the crossover from the BCS to Bose-Einstein condensation (BEC) regimes as the on-site electron-phonon coupling $g$ is varied for both adiabatic ($t/\omega_0 >>1$) and antiadiabatic ($t/\omega_0 <1$) phonons, where $t$ is the hopping amplitude and $\omega_0$ is the phonon frequency. It turns out that the maximum superconducting transition temperature $T_c$ universally coincides with the critical electron-phonon coupling $g_c$ where the bipolaron instability takes place in the normal state. However, in the case of the adiabatic phonon, the pairing amplitude $\Delta_P$ is suppressed with increasing the electron-phonon coupling in the BEC regime, while it increases with increasing $g$ for the antiadiabatic phonon. Further, the calculated superfluid stiffness $D_f$ for the adiabatic phonon decreases rapidly as increasing $g$ together with the suppression of the coherence peak in the BEC regime. We also calculated the spectral intensities to identify BCS and BEC regimes and those results are comparable to the angle resolved photoemission spectroscopy (ARPES) experiment.

**10:48AM A08.00015: Intermolecular Coupling and Superconductivity in Chevrel Phase Compounds**

JIA CHEN (Presenter), ANDREW MILLIS, DAVID REICHMAN, Columbia University — To understand superconductivity in Chevrel phase compounds and guide the search for interesting properties in materials created with Chevrel phase molecules as building blocks, we use ab-initio methods to study the properties of single Mo6X8 molecules with X=S, Se, Te as well as the bulk solid PbMo6S8. In bulk PbMo6S8, the different energy scales from strong to weak are: the band kinetic energy, the intra-molecular Coulomb interaction, the on-molecule Jahn-Teller energy and the Hund’s exchange coupling. The metallic state is stable with respect to Mott and polaronic insulating states. The bulk compound is characterized by a strong electron-phonon interaction with the largest coupling involving phonon modes with energies about 12 meV and with a strong inter-molecule (Peierls) character. A two-band Eliashberg equation analysis shows that the superconductivity has different gaps on the two Fermi surface sheets. A Bergman-Rainer analysis reveals that the Peierls modes provide the most important contribution to the superconductivity. This work illustrates the importance of inter-molecular coupling for collective phenomena in molecular solids.

*This work is supported by the NSF MRSEC program through Columbia under Grant No.DMR-1420634.
**Monday, March 4, 2019 8:00 AM - 10:48 AM**

**Session A09 DMP DCMP: Superconductivity: Theory General BCEC 151A - Pavel Volkov**

8:00AM A09.00001: Multiple solutions for superconductivity at T=0 in a quantum-critical metal*  
ANDREY CHUBUKOV (Presenter), University of Minnesota, ARTEM G ABANOV, Physics, Texas A&M — We discuss the interplay between non-Fermi liquid behaviour and superconductivity at a quantum-critical point (QCP) in a metal. It is widely thought that the tendency towards superconductivity and towards non-Fermi liquid behaviour compete with each other, and if the pairing interaction is reduced below a certain threshold, the system displays a naked non-Fermi liquid QC behaviour. We show that at T=0 there is indeed a threshold below which the system remains in the normal state. We argue that above the threshold the system develops a discrete, but infinite set of solutions for the pairing gap. In particular, for ant value of the pairing interaction above the threshold there exists a solution of the linearized gap equation. This is very different from a conventional superconductivity, when the solution of the linearized gap equation exists only at a critical strength of the pairing interaction. We present some exact results set the results of the QC models with frequency-dependent effective interaction and discuss the consequences of the existence of multiple solutions for superconductivity at a QCP.

*The work by A.V.C. was supported by the NSF DMR-1523036.

8:12AM A09.00002: The special role of the first Matsubara frequency for superconductivity near a quantum critical point: the non linear gap equation below Tc and spectral properties in real frequency axis.*  
YI-MING WU (Presenter), University of Minnesota, ARTEM G ABANOV, Physics, Texas A&M U, YUXUAN WANG, Physics, University of Florida, ANDREY CHUBUKOV, University of Minnesota — We consider a model of itinerant fermions near a quantum critical point, where the effective interaction is mediated by order parameter fluctuations. This interaction makes fermions ncoherent and, at the same time, gives rise to attraction in at least one pairing channel. These two tendencies compete with each other. We argue that the situation is more tricky because the self-energy without thermal fluctuation piece, which one needs for the calculation of $T_c$, vanishes at the first two Matsubara frequencies($\pm \pi T$), while the pairing interacion between fermions with these two frequencies remains strong. We investigate how this affects the system behavior below $T_c$, in particular the density of states and the spectral function. We argue that there is a crossover at some $T_{cross} < T_c$ between conventional behavior at low T, when frequency variation occurs at a scale of the gap Delta, and a new behavior at higher T, when frequency variation occurs at a scale set by T.

We argue that our theory naturally explains the crossover from "gap closing" to "gap filling", observed in cuprate and other superconductors.

*We thank D. Dessau, S. Raghu, G. Torroba, and A. Yazdani for useful discussions. This work by Y. Wu and AVC was supported by the NSF DMR-1523036.

8:24AM A09.00003: Strange metal crossover in the doped holographic superconductor*  
GASTON GIORDANO, NICOLAS GRANDI, ADRIAN LUGO, Departamento de Física, Universidad Nacional de la Plata, RODRIGO SOTO GARRIDO (Presenter), Facultad de Ingeniería y Tecnología, Universidad San Sebastián — In this talk, we study the "normal" phase of a holographic superconductor. The specific model used was originally introduced by Kiritsis and Li (JHEP01(2016)147) to incorporate the different orders phases similar to the ones observed in High Temperature Superconductors. These phases include the normal phase, the SC phase, the antiferromagnetic phase and a striped phase as a function of both, temperature and doping. Within this model we study the fermionic spectral functions in the normal phase at zero and finite temperatures. Using analytic and numerical methods, we found a crossover in the normal phase from a strange metal with short lived excitations at small doping, into a Fermi liquid with well defined quasiparticles at large doping. The critical doping at which excitations becomes long lived increases with temperature. The emerging phase diagram is qualitatively similar to that of High Temperature Superconductors.

The results of this work have been published in JHEP10(2018)068

*This work was supported in part by by FONDECYT (Chile) No.11160542 (RSG), CONICET (Argentina) Grant Numbers PIP-2017-1109 (NG) and PIP-2015-0688 (AL), and PUE Busqueda de nueva Fisica, by UNLP (Argentina) Grant Numbers PID-2017-X791 (NG) and PID 2014-X721 (AL).
Non-Fermi liquid scattering against emergent Bose liquid: manifestations in the kink and other exotic quasiparticle behaviors in the normal-state cuprate superconductors

SHENGTAO JIANG (Presenter), LONG ZOU, WEI KU, Tsung-Dao Lee Institute & School of Physics and Astronomy, Shanghai Jiao Tong University — The normal state of cuprate superconductors exhibits many exotic behaviors qualitatively different from the Fermi liquid, the foundation of condensed matter physics. Here we demonstrate that non-Fermi liquid behaviors emerge naturally from scattering against an emergent Bose liquid. Particularly, we find a finite zero-energy scattering rate at low-temperature limit that grows linearly with respect to temperature, against clean fermions' generic non-dissipative characteristics. Surprisingly, three other seemingly unrelated experimental observations are also produced, including the well-studied "kink" in the quasi-particle dispersion, as well as the puzzling correspondences between the normal and superconducting state. Our findings provide a general route for fermionic systems to generate non-Fermi liquid behavior, and suggest that by room temperature large number of the doped holes in the cuprates have already formed an emergent Bose liquid of tightly bound pairs, whose low-temperature condensation gives unconventional superconductivity.


*Work supported by National Natural Science Foundation of China #11674220 and 11447601, and Ministry of Science and Technology #2016YFA0300500 and 2016YFA0300501.

Renormalization group study of superconductivity in Nickelates

MICHAEL KLETT (Presenter), TILMAN SCHWEMMER, XIANXIN WU, DAVID RIEGLER, RONNY THOMALE, Institute for Theoretical Physics, University of Wuerzburg — Since the discovery of high Tc superconductivity in the cuprates by Bednorz and Mueller, materials bearing similarities to copper oxide compounds have emerged as a contemporary research topic of high interest. Although LaNiO3/LaAlO3 shares many similarities with the cuprates, it exhibits no superconducting phase down to lowest temperatures.

In this talk we sketch a simple two-band model of a d7 Nickelate-compound and argue why, based on renormalization group calculations competing superconducting ordering propensities make these systems belong to the class of low-Tc materials.

*ERC-StG-TOPOLECTRICS-336012, DFG-SFB 1170 Project B04,

Pairing Mechanism in Hunds Metal Superconductors and the Universality of the Superconducting Gap to Critical Temperature Ratio

TSUNG-HAN LEE (Presenter), Physics and Astronomy Department, Rutgers University, ANDREY CHUBUKOV, School of Physics and Astronomy, University of Minnesota, HU MIAO, Brookhaven National Laboratory, GABRIEL KOTLIAR, Physics and Astronomy Department, Rutgers University — We propose a simple spin-fluctuation Eliashberg model that contains the physical ingredients of a Hund's metal, the local spin-fluctuations with super-linear correlators, (Ω0/|Ω|)γ with γ>1, interacting with electrons. Our model yields a universal superconducting gap to critical temperature ratio 2Δmax/Tc≈7.2 that coincides with the experimental observation in a series of iron-based superconductors. We also discuss the implications of our model in the other classes of superconductors, e.g., cuprates and heavy fermion superconductors.

*T.-H.L. and G.K. were supported by the NSF Grant No. DMR-1733071. A.V.C. was supported by the NSF Grant No. DMR-1523036. H. M. is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Early Career Award Program under Award No. 1047478.

A Simple Model for Quantum Tunneling of Cooper Pairs

EDGAR PATINO (Presenter), School of Physical Sciences and Nanotechnology, Yachay Tech University, DANIEL LOZANO, University of the Andes, DENIS CHEVALLIER, University of Basel — We propose a simple phenomenological model for quantum tunneling of Cooper pairs based on their boson like nature. Thus applies to the low energy regime i.e. in the absence of quasiparticle excitations. Around zero bias voltage our model reveals a rapid increase in tunneling current which rapidly saturates. This manifests as a zero bias conductance peak that strongly depends on the superconductors transition temperature. This low energy tunneling of Cooper pairs could serve as an alternative explanation for a number of tunneling experiments where zero bias conductance peak has been observed.

*This work was funded by Vicerrectoria de Investigaciones of Universidad de los Andes and School of Physical Sciences and Nanotechnology of Yachay Tech University.
9:24AM A09.00008: Gap anisotropy in nematic quantum critical superconductors* AVRAHAM KLEIN (Presenter), YI-MING WU, ANDREY CHUBUKOV, University of Minnesota — When pairing is driven by nematic quantum fluctuations, it results in a unique form of superconductivity. Nematic fluctuations, while anisotropic, couple to the entire Fermi surface, in contrast to, e.g. spin fluctuations that typically couple to so-called ‘hotspots’. The result is an entire series of possible anisotropic pairing states, with closely spaced condensation temperatures, all with s-wave symmetry. The existence of these states drives a strong temperature evolution of the anisotropy of the superconducting gap. This evolution is a direct consequence of critical fluctuations, and provides a clear signature of quantum criticality inside the superconducting state.

*This work was supported by NSF DMR-1523036.

9:36AM A09.00009: Collective modes in 2 dimensional fermionic superfluid near Pomeranchuk instability WEIHAN HSIAO (Presenter), University of Chicago — In this work we investigate order parameter collective modes in 2 dimensional fermionic superfluids in finite angular momentum pairing channels. We discover subgap bosonic excitations with finite mass analogous to order parameter collective modes in 3 dimensional superfluid 3He. We further investigate the effect of fermion vacuum on these modes and it is shown that some of these modes in the spectrum soften as the underlying Fermi liquid approaches Pomeranchuk instability, or the nematic critical point when considering a p-wave chiral superfluid.

9:48AM A09.00010: Fragile superconductivity in the presence of weakly disordered charge density waves YUE YU (Presenter), STEVEN KIVELSON, Stanford University — When superconducting (SC) and charge-density wave (CDW) orders compete, novel low temperature behaviors can result. From an analysis of the Landau-Ginzburg-Wilson theory of competing orders, we demonstrate the generic occurrence of a “fragile” SC phase at low temperatures and high fields in the presence of weak disorder. Here, the SC order is largely concentrated in the vicinity of dilute dislocations in the CDW order, leading to transition temperatures and critical currents that are parametrically smaller than those characterizing the zero field SC phase. This may provide the outline of an explanation of the recently discovered “resilient” superconducting phase at high fields in underdoped YBa2Cu3O6+δ.

10:00AM A09.00011: Study of the superconducting $T_c$ dome in the phase diagram of the two-dimensional Holstein model YAN WANG (Presenter), Departement de Physique, Universite de Sherbrooke, PHILLIP DEE, KEN NAKATSUKASA, STEVEN JOHNSTON, Department of Physics and Astronomy, University of Tennessee — $T_c$ dome, i.e., the nonmonotonic superconducting $T_c$ dependence as a function of parameters such as doping or pressure, is ubiquitous in the phase diagrams of unconventional superconductors, where the pairing interaction has a magnetic and electronic origin. By contrast, $T_c$ dome is rarely seen in conventional electron-phonon superconductors. We report the $T_c$ dome in the phase diagram of the two-dimensional Holstein model, where electrons and phonons interact through a local coupling. By solving the model using strong coupling Migdal-Eliashberg formalism and self-consistently renormalizing both the electrons and phonons, a $T_c$ dome as function of filling $n$ arises in the phase diagram, alongside a charge-density-wave phase around the half-filling. The dome is tied to the competition of three renormalized quantities as the filling increases: the increasing coupling constant $\lambda$, the decreasing $\omega_{\text{log}}$, and the nonmonotonically varying density of states at the Fermi-level. Interestingly, we also find the effective electron-electron interaction becomes nonlocal in $\mathbf{r}$-space and even repulsive at neighboring lattice sites. Our discovery could shed light on the high $T_c$ of the strongly electron-phonon coupled system such as the dense hydrogen-rich compounds and the monolayer FeSe on SrTiO3.

10:12AM A09.00012: Polaron, bipolaron and few-polaron states in the Peierls model of electron-phonon coupling* JOHN SOUS (Presenter), ALBERTO NOCERA, MONA INESA BERCIU, University of British Columbia — We consider the one-dimensional Peierls model of electron-phonon coupling describing the modulation of the electron hopping by phonons. We review recent results on single polarons and bipolarons, and extend our discussion to few-polaron states in the regime of competing phononic and electronic excitations. Single polarons experience a transition from weak coupling to strong coupling, while the Peierls coupling stabilizes strongly bound yet very light bipolarons. Few polarons, however, experience higher order interactions that result in the formation of multipolaron bound states. In the anti-adiabatic limit of large phonon frequencies, we find that bipolarons are stable against phase separation. We discuss the relevance of these ideas to superconductivity in higher dimensions.

*NSERC
Emergence of a Macroscopic Phase in an Isolated Electron-Phonon Superconductor*

WATARU KOHNO (Presenter), TAKAFUMI KITA, Hokkaido University — Within the number-conserving formalism introduced by Ambegaokar, we constructed a variational wave function of electron-phonon superconductors. The many-body correlations originated from electron-phonon coupling are incorporated in our variational wave function. Moreover, this wave function gives rise to a superposition over the number of condensed particles and the Cooper-pair wave function with a macroscopic phase can be defined naturally. Therefore, we conclude dynamical exchanges of phonons induce a well-defined macroscopic phase with emergence of superconductivity in an electron-phonon superconductor.

*Wataru Kohno is a JSPS Research Fellow, and this work was supported in part by JSPS KAKENHI Grant Number 18J13241.

Generalization of Anderson’s Theorem for Disordered Superconductors*

JOHN DODARO (Presenter), STEVEN KIVELSON, Stanford University, CATHERINE KALLIN, McMaster University — We show that at the level of BCS mean-field theory, the superconducting Tc is always increased in the presence of disorder, regardless of order parameter symmetry, disorder strength, and spatial dimension. This result reflects the physics of rare events - formally analogous to the problem of Lifshitz tails in disordered semiconductors - and arises from considerations of spatially inhomogeneous solutions of the gap equation. We discuss the relevance of these effects for short coherence length superconductors and compare them with an exact treatment of disorder within dirty d-wave BCS theory to describe superfluid stiffness results on the overdoped cuprates.

*supported in part by the Department of Energy, Office of Basic Energy Sciences, under contract no. DEAC02-76SF00515 at Stanford

Monday, March 4, 2019 8:00 AM - 10:36 AM

Session A10 DMP: Fe-based Superconductors I

8:00AM A10.00001: Orbital-selectivity in iron chalcogenide superconductors [Invited] MING YI (Presenter), Rice University — The electron correlation strength has a systematic spread across the material-base of iron-based superconductors. Near the most correlated end of the spectrum are the iron chalcogenides, where strong orbital-selective correlations are observed. In particular, the dxy orbital exhibits much stronger local behavior than the dxz and dyz orbitals, putting the material in close proximity to an orbital-selective Mott phase (OSMP). In this talk, I will first demonstrate the universality of orbital-selectivity amongst all iron chalcogenide superconductors including both Fe(Se,Te) and heavily electron-doped FeSe systems. For the second part of the talk, I will use the phase diagram of Fe(Se,Te) to illustrate that both Te-substitution and temperature increase act as effective pathways towards the OSMP. In the process, a dramatic increase of the dxy effective mass together with a redistribution of spectral weight on the Fermi surface strongly modify the low energy electronic states of this material family.

8:36AM A10.00002: A Neutron Total Scattering Study of the Nanoscale Structure of KxFe2−ySe2−zS

PANAGIOTIS MANGELIS, Institute of Electronic Structure and Laser, Foundation for Research and Technology—Hellas, HECHANG LEI, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, MARSHALL MCDONNELL, MIKHAIL FEYGENSON, Neutron Scattering Division, Oak Ridge National Laboratory, CEDOMIR PETROVIC, EMIL BOZIN, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, ALEXANDROS LAPPAS, Institute of Electronic Structure and Laser, Foundation for Research and Technology—Hellas, ROBERT KOCH (Presenter), Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — A Neutron Total Scattering Study of the Nanoscale Structure of KxFe2−ySe2−zS

Isovalent substitutions in alkali iron chalcogenides allow for selective tuning of electronic properties. For example, KxFe2−ySe2 is a superconductor (Tc = 32 K), while the sulfide analogue KxFe2−yS2 displays a spin glass semiconducting behavior. This change in behavior is accompanied by structural fluctuations both in the chalcogen and Fe sublattices. Motivated by such observations, the local atomic structure of the KxFe2−ySe2−zS compositional series was studied using neutron total scattering-based atomic pair distribution function (PDF) analysis at 5K. Aspects of the local structure are discussed in the context of electronic properties.


*Work at IESL FORTH was supported by the U.S. Office of Naval Research, NICOP grant award No. N62909-17-1-2126. Work at Brookhaven National Laboratory was supported by U.S. DOE-BES under contract DE-SC0012704 and in part by the Center for Emergent Superconductivity, an EFRC funded by the U.S. DOE-BES.
8:48AM A10.00003: Intertwined spin-orbit coupled orders in the iron-based superconductors  MORTEN HOLM
CHRISTENSEN (Presenter), University of Minnesota, JIAN KANG, National High Magnetic Field Laboratory, Florida State University, WILLIAM MEIER, ANDREAS KREYSSIG, Ames Laboratory & Department of Physics, Iowa State University, RAFAEL M FERNANDES, University of Minnesota — The phase diagram of the underdoped iron-based superconductors exhibits two electronically ordered phases, nematicity and stripe magnetism. Nematic order breaks the rotational symmetry of the lattice and can be seen as a vestigial phase of stripe magnetism. Here we discuss a similar phenomenon occurring for the tetragonal magnetic orders, the spin-vortex crystal and the charge-spin-density-wave phases. These vestigial phases break the glide-plane symmetry and render respectively the As/Se or Fe sites inequivalent. In materials with staggered FeAs/Se layers (e.g. 122), these have ordering vector \( Q = (0, 0, \pi) \) while in compounds with no staggering (e.g. 111) these are \( Q = 0 \) orders. We discuss how these vestigial phases couple to the lattice. Moreover, Kramers degeneracy is broken and Rashba- and Dresselhaus-like spin-orbit couplings are induced. Finally, we discuss the behavior under electromagnetic fields, including magneto-electric effects.

9:00AM A10.00004: Discovery of a strain-stabilized charge density wave in LiFeAs  CHI MING YIM (Presenter), CHRISTOPHER TRAINER, RAMA K P ALURU, University of St Andrews, SHUN CHI, WALTER N HARDY, RUIXING LIANG, DOUGLAS ANDREW BONN, Univ of British Columbia, PETER WAHL, University of St Andrews — In a number of high \( T_c \) superconductors, small orthorhombic distortions of the lattice structure result in surprisingly large symmetry breaking of the electronic states and macroscopic properties, an effect often referred to as nematicity. This nematicity has been studied extensively on materials with an orthorhombic crystal structure, where the lattice symmetry is already reduced from four-fold (\( C_4 \)) to two-fold (\( C_2 \)). To directly study the impact of symmetry breaking lattice distortions on the electronic states, we image at the atomic scale the influence of strain-tuned lattice distortions on the correlated electronic states in the iron-based superconductor LiFeAs, a material which in its ground state is tetragonal, with \( C_4 \) symmetry. Our experiments uncover a new strain-stabilized nematic phase that exhibits a unidirectional charge density wave (CDW) in LiFeAs, an electronic state which not only breaks rotational symmetry but also reduces translational symmetry. We follow the evolution of the superconducting gap from the unstrained material with \( C_4 \) symmetry through the new nematic phase with \( C_2 \) symmetry and CDW order to a state where superconductivity is completely suppressed.

9:12AM A10.00005: Evidence for multi-gap nodal superconductivity in FeS by penetration depth measurements.  SUJITH KUNNININYIL SUDHEESH (Presenter), Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore, TIANPING YING, State Key Laboratory of Surface Physics, Department of Physics and Laboratory of Advanced Materials, Fudan University, Shanghai, China, XIAOFANG LAI, School of Physics and Optoelectronic Engineering, Guangdong University of Technology, Guangdong, China, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, SHIYAN LI, State Key Laboratory of Surface Physics, Department of Physics and Laboratory of Advanced Materials, Fudan University, Shanghai, China, EE MIN CHIA, Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore — We report measurements of London penetration depth and magnetization on single crystals of FeS superconductor with a transition temperature of 4 K. From magnetization measurements, FeS was confirmed to be a type-II superconductor with \( H_{c1}(0) = 58 \pm 4 \) Oe, \( \lambda_{ab}(0) = 900 \pm 90 \) nm, and \( \xi(0) = 90 \pm 12 \) nm. The low temperature (\( T < 0.3T_c \)) behavior of penetration depth deviates from a conventional exponential predicted by BCS theory and fits well to a power law with an exponent \( n = 2.2 \pm 0.1 \) which suggests the presence of nodes in the system. The superfluid density was calculated and was found to fit best to a multi-gap s+d wave model with the d-wave gap having slightly larger weight (\( p = 0.6 \)). \( \Delta(0)/k_BT_c \) for the d-wave gap is higher than that of the BCS weak coupling model, implying superfluid density was calculated and was found to fit best to a multi-gap s+d wave model with the d-wave gap having a slightly larger weight (\( p = 0.6 \)). \( \Delta(0)/k_BT_c \) for the d-wave gap is higher than that of the BCS weak coupling model, implying superfluid density was calculated and was found to fit best to a multi-gap s+d wave model with the d-wave gap having a slightly larger weight (\( p = 0.6 \)). \( \Delta(0)/k_BT_c \) for the d-wave gap is higher than that of the BCS weak coupling model, implying superfluid density was calculated and was found to fit best to a multi-gap s+d wave model with the d-wave gap having a slightly larger weight (\( p = 0.6 \)).

9:24AM A10.00006: Influence of Spin-Orbit Coupling in the Iron-Based Superconductors  RYAN DAY (Presenter), GIORGIO LEVY, MATTEO MICHARDI, BEREND ZWARTSENBERG, MARTA ZONNO, SHUN CHI, Quantum Matter Institute, University of British Columbia, IVANA VOBORNIK, Elettra Synchrotron, WALTER HARDY, DOUGLAS BONN, ILYA ELFIMOV, ANDREA DAMASCHELLI, Quantum Matter Institute, University of British Columbia — In addition to the remarkable resilience of unconventional superconductivity, the iron-based superconductors (FeSCs) are characterized by a broad phenomenology across their phase diagram. This diversity has compounded the challenge of defining a minimal model for these complex materials. We explore the essential role of spin-orbit coupling (SOC) in the FeSCs via circularly-polarized spin- and angle-resolved photoemission spectroscopy (CPS-ARPES), a technique which provides direct access to both spin and orbital degrees of freedom [1]. Applying this technique to both LiFeAs and FeSe, we establish a strong momentum dependence of the spin-orbital entanglement near the Fermi surface imbedded by SOC. Influenced strongly by the details of the crystal field, the relevance of SOC to the states near the Fermi level, and consequently to superconductivity and magnetism is found to be strongly material-dependent. Furthermore, in the case of hole-like carriers in FeSe, SOC is observed to be of comparable strength to orbital order, allowing spin-orbit mixing to persist to the nematic phase.

9:36AM A10.00007: Infrared Spectroscopic Studies of the Phonon Dynamics in Iron-based Superconductors*  
XIANGGANG QIU (Presenter), RUN YANG, BING XU, ZIYANG QIU, Chinese Academy of Sciences, YAOMIN DAI, Nanjing University — The temperature dependent optical reflectivity has been measurement on iron-based superconductors of different families. The optical conductivity has been obtained by using the two-Drude components model. It has been found that the phonons show red- or blue-shift in different samples. Interestingly, the phonon conductivity exhibits a Fano lineshape, suggesting possible coupling between phonon and electrons. Based on the temperature evolution of the lineshape and peak shift, we discuss the possible role played by electron-phonon coupling and spin fluctuation in the occurrence of superconductivity in iron-based superconductors.

*This work is supported by MOST of China (Grant No. 2017YFA0302903) and NSFC of China (Grant No. 11774400).

9:48AM A10.00008: Spin anisotropy in the stoichiometric iron-based superconductor CaKFe$_4$As$_4$*  
TAO XIE (Presenter), HUIQIAN LUO, SHILIANG LI, National Lab for superconductivity, Institute of Physics, Chinese Academy of Sciences, Beijing, China — In the stoichiometric iron pnictide superconductor CaKFe$_4$As$_4$, we have discovered triple spin resonance modes with strong L-modulation by unpolarized neutron scattering experiments. The two odd modes appear around 9.5 meV and 13 meV, and the even mode locates around 18.3 meV. [1] To study the spin anisotropy of the three modes, we performed polarized inelastic neutron scattering experiments on the same CaKFe$_4$As$_4$ sample. Here, I will present our recent results. These results will give better understanding on the spin-orbit coupling in iron-based superconductors, which can also enlighten us about the nature of magnetism and its relation with unconventional superconductivity.


*We thank the funding supports from MOST of China, NSFC and CAS.

10:00AM A10.00009: Study of CaK(Fe$_{1-x}A_x$)$_4$As$_4$ ($A$ = Mn and Cr) single crystals*  
MINGYU XU (Presenter), WILLIAM MEIER, LI XIANG, SERGEY BUDKO, PAUL CANFIELD, Iowa State University and Ames Laboratory — Stoichiometric CaKFe$_4$As$_4$ is a Fe-based superconductor which has a critical temperature at 35 K. Substituting Fe with Ni or Co suppresses superconductivity and stabilizes an unusual hedgehog spin-vortex crystal magnetic structure [1]. There is a range of concentrations where superconductivity and magnetism coexist [2,3,4]. Having in mind different effect of [Fe, Co] and [Mn, Cr] substitutions in BaFe$_2$As$_2$, we grew single crystals of CaK(Fe$_{1-x}A_x$)$_4$As$_4$ ($A$ = Cr and Mn) and characterized them by magnetic and transport measurements. Phase diagrams of CaK(Fe$_{1-x}A_x$)$_4$As$_4$ ($A$ = Fe, Co, Mn, Cr) will be compared and the observed trends will be discussed in the context of Fe-based superconductors.


*We thank A. Kreyssig for insightful discussions. This work is supported by the US DOE, Basic Energy Sciences, Materials Science and Engineering Division under contract No.DE-AC02-07CH11358. W.R.M. was supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant No. GBMF4411. L. X. was supported, in part, by the W. M. Keck Foundation.

10:12AM A10.00010: The FFLO State in Unconventional Superconductors  
CHARLES AGOSTA (Presenter), RAJU GHIMIRE, CAMILLE E BALES, Clark University, MAKARIY A TANATAR, Ames Laboratory — Recent experiments suggest that inhomogeneous superconductivity (the FFLO state) exists in organic$^1$, pnictide$^2$, and heavy Fermion$^3$ superconductors. The FFLO state is a type of superconducting pair density wave, although unlike the proposed pair density wave in cuprates, the FFLO state is accompanied by a magnetized charge density wave (CDW) of the left over (un-condensed) quasiparticles. We will review the data from each of the families of superconductors above and present new data for the Ba$_4$K$_{1-x}$Fe$_2$As$_2$ family of pnictide superconductors via measurements of the rf penetration depth using a tunnel diode oscillator, down to 40 mK. We will also discuss early results of experiments to measure the q-vector of a CDW in organic conductors with x-rays. This CDW is known to compete with the superconducting state rather than coexist with the FFLO state referred to above. Additionally, this technique may be a way to measure the q-vector of the FFLO state directly. Understanding these competing and intertwined orders in unconventional superconductors will further our knowledge of quantum mechanical ground states in electronic materials.

Enhancement of $J_c$ at around $1/3B_\Phi$ in Iron-based Superconductors with Splayed Columnar Defects

TSUYOSHI TAMEGAI (Presenter), AYUMU TAKAHASHI, NOZOMU ITO, SUNSENG PYON, Department of Applied Physics, The University of Tokyo, ATSUSHI YOSHIDA, TADASHI KAMBARA, Nishina Center, RIKEN, SATORU OKAYASU, Japan Atomic Energy Agency, ATARU ICHINOSE, Electric Power Engineering Research Laboratory, Central Research Institute of Electric Power Industry — Columnar defects (CDs) are known to trap vortices very effectively, leading to a significant increase in the critical current density ($J_c$). In contrast to the case of parallel CDs along the c-axis, splaying the direction of columnar defects enhances $J_c$ even further due to the suppression of kink motions. In (Ba,K)Fe$_2$As$_2$ with splayed CDs introduced by irradiating 2.6 GeV U ions, we found a novel enhancement of $J_c$ at around $1/3B_\Phi$ ($B_\Phi$: matching field) for a range of splay angle of CDs. In the present study, we compare the enhancement of $J_c$ in (Ba,K)Fe$_2$As$_2$ with splayed CDs created by 2.6 GeV U ions with those created by 320 MeV Au ions. We find that the enhancement of $J_c$ always occurs at $\sim 1/3B_\Phi$, while the degree of enhancement and optimum splay angle depends on the morphology of splayed CDs. We also investigate the effect of the symmetry breaking of the two sets of splayed CDs, namely for the case where the average direction of two sets of CDs is different from the c-axis and another case where doses of two sets of splayed CDs are different.

*This work is partly supported by KAKENHI (17H01141) from JSPS.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A11 DMP DCOMP FIAP: Defects in Semiconductors -- 1D, 2D, and Layered Materials

8:00AM A11.00001: Nanoscale Conductivity Measurements of Biased Silicon Nanowires with Infrared Near-Field Optical Microscopy

CLAYTON CASPER (Presenter), EARL T RITCHIE, DAVID J HILL, TAYLOR S TEITSWORTH, Chemistry, University of North Carolina at Chapel Hill, SAMUEL BERWEGER, National Institute of Standards and Technology, JAMES F CAHOON, JOANNA M ATKIN, Chemistry, University of North Carolina at Chapel Hill — Vapor-liquid-solid (VLS) growth of Si nanowires (SiNWs) allows for precise control of dopant density and type. These encoded dopant superlattices have enabled microscopic diodes for a wide range of optoelectronic applications. However, performance of these diodes depends critically on the behavior of carriers at junctions, which is influenced by dopant activation, geometry, and defect states. Furthermore, junctions in SiNWs are abrupt (<100 nm), making it difficult to apply traditional characterization methods. Here we use mid-infrared scattering-scanning near-field optical microscopy (s-SNOM) to image the carrier distribution in axial p-i-n junction SiNWs in operando. The high spatial resolution (< 20 nm) allows us to directly measure the free-carrier concentration arising from not only the native doping, but also from band bending. Combined with finite element modeling, we can semi-quantitatively determine the local carrier concentration and mobility, and examine the effect of bias on junction lengths and space-charge regions. These measurements will demonstrate that s-SNOM can be used to study the I-V characteristics of SiNWs with unprecedented spatial resolution.

8:12AM A11.00002: Real space pseudopotential calculations for the Raman spectra of doped Si and C nanostructures

JOSHUA C NEITZEL (Presenter), JAMES CHELIKOWSKY, University of Texas at Austin — We use a real-space pseudopotential method implemented within density functional theory to calculate Raman spectra for doped Si and C nanostructures. We examine the role of dopant location, local structure, and quantum confinement on the Raman spectra. We contrast these nanoscale spectra with those of bulk crystals.

*Our work is supported by the U.S. Department of Energy under grant No. DE-FG02-06ER46286. Computational resources were provided by NERSC.
A comprehensive advanced solid-state NMR analysis reveals that approximately a third of carbon atoms reside in the partially saturated structures, the degree-4 nanotreads, with isolated double bonds retained in the recovered sample. Some enumerated degree-4 structures, like IV-12 and IV-18, have much smaller distances between the double bonds than that in normal materials due to the rigid sp³ backbone, which leads to very dispersive bands near the Fermi level and may make these threads feasible to be doped. We investigated such doping computationally, using jellium models, alkali intercalation, and nitrogen substitution on the carbon backbone in both pristine and partially fluorinated IV-12 and IV-18 threads. Under doping, the IV-12 thread collapses to fully saturated structures, probably due to the strongly overlapping of the double bonds. There is no clear evidence for charge transfer in the pristine IV-18 thread, but the partially fluorinated IV-18 thread can be doped; this system may constitute a new type of conductive polymer.

*This work is supported by DOE (DE-SC0001057) and NSF (CHE-1832471).
9:00AM A11.00006: Integrating quantum emitters in low-dimensional materials with nanocavities* [Invited] STEFAN STRAUF (Presenter), Stevens Institute of Technology — It was recently shown that low-dimensional materials such as 1D single-walled carbon nanotubes (SWCNTs) as well as 2D materials such as transition-metal dichalcogenides (TMDCs) and hexagonal boron nitride (hBN) can host 0D-confined quantum emitters. These quantum emitters hold great promise for future quantum technologies, particularly through covalent sidewall functionalization of SWCNTs resulting in quantum light emission at room temperature into telecom bands, through local strain-engineering in monolayer TMDCs providing spatial scalability, and via color centers in hBN that survive up to 800 K. Here we review our recent work integrating these quantum emitters into optical cavities. We will first focus on coupling to metallo-dielectric antennas and demonstrate near-unity light collection efficiency for SWCNTs [1,2] and hBN emitters. The second part of the talk focuses on reversible and deterministic coupling schemes of excitons with respect to nanoplasmonic gap-mode cavities in SWCNTs [3] and strain-induced excitons in TMDCs [4]. We will further discuss methods to increase the quantum emitter yield to near unity, ways to increase thermal stability for excitons in TMDCs, as well as discuss our latest work on indistinguishable single photon generation.

References

*We acknowledge financial support by the National Science Foundation (NSF) under awards DMR-1506711, DMR-1809235, ECCS-MRI-1531237, and EFRI-ACQUIRE-1641094.

9:36AM A11.00007: Deterministic Quantum Emitter Formation in Hexagonal Boron Nitride via Controlled Edge Creation* JOSHUA ZIEGLER (Presenter), RACHAEL KLAISS, ANDREW BLAIKIE, DAVID MILLER, University of Oregon, VIVA HOROWITZ, Hamilton College, BENJAMIN J ALEMAN, University of Oregon — Quantum emitters (QEs) in 2D hexagonal boron nitride (hBN) are extremely bright, stable under harsh conditions, and have the potential for strong coupling to hybrid devices due to their 2D host crystal. However, due to the difficulty of precisely creating these QEs, this potential for coupling into hybrid devices has been difficult to utilize. Motivated by recent studies showing that QEs in hBN tend to form at edges, we use a focused ion beam (FIB) to mill patterns in hBN. We optically characterize these milled hBN sheets and find that optimal FIB parameters create single QEs with a nearly Poisson-limited yield of 35%, and a 94% chance of creating at least one QE. We use atomic force microscopy to understand why these parameters are optimal and find that single QE yield is highest with a smooth milling profile on smooth hBN. This technique dramatically broadens the usefulness and convenience of hBN QEs – enabling facile integration into optoelectronic devices to fully take advantage of the appealing hBN QEs.

*We would like to acknowledge the use of the University of Oregon’s Rapid Materials Prototyping facility, funded by the Murdock Charitable Trust, and funding from University of Oregon and the National Science Foundation (NSF) under grant No. DMR-1532225.

9:48AM A11.00008: Quantifying the Effects of Sample Treatments on Quantum Emitters in Hexagonal Boron Nitride* STANLEY BREITWEISER (Presenter), Quantum Engineering Laboratory, Department of Electrical and Systems Engineering, University of Pennsylvania, ANNEMARIE L EXARHOS, Department of Physics, Lafayette College, RAJ PATEL, JENNIFER SAOUAF, BENJAMIN PORAT, LEE BASSETT, Quantum Engineering Laboratory, Department of Electrical and Systems Engineering, University of Pennsylvania — Hexagonal boron nitride (hBN) has emerged as a leading two-dimensional van der Waals material for next-generation quantum technologies. In particular, recent studies have identified spin-dependent quantum emission from defect states within the bandgap of hBN, making it a promising platform for quantum information processing and sensing applications. These optical-frequency emitters are among the brightest known, but they display heterogeneous properties and are poorly understood at the microscopic level. Confounding this, samples have undergone a variety of treatments in reported experiments - the two most common treatments being low-energy (keV) electron-beam irradiation and high-temperature (850°C) annealing in inert gas - with only a qualitative understanding of their effects. Here we systematically and quantitatively study the effect of these treatments using an analytical model which relates pixel intensity distributions from large-area confocal photoluminescence images to the density and brightness distributions of emitter ensembles. The results inform future efforts to control the formation and stabilization of quantum emitters in hBN.

*This work was supported by the Army Research Office (W911NF-15-1-0589).
10:00AM A11.00009: Stark shifts observed in single-photon emitters in hexagonal boron nitride  

GICHAN GOH (Presenter), DAEBOK CHOI, Physics and Energy Systems Research, Ajou University, JIN-HUN KIM, DONG-GIL IM, YOON-HO KIM, Physics, Pohang University of Science and Technology, HOSUNG SEO, JIEUN LEE, Physics and Energy Systems Research, Ajou University — Atomic defects, such as diamond NV-centers and SiC divacancies, have been widely studied as single-photon emitters, which are key ingredients of quantum information technology. Recently, two-dimensional (2D) materials are also found to host atomic defects that generate single-photons. Of particular interest is hexagonal boron nitride (h-BN) which possess single-photon emitters operating at room temperature. In this talk, we show the Stark-shift induced energy control of single-photon emitters in h-BN. By fabricating van der Waals heterostructures of h-BN with graphene gates, we observe linear Stark shifts as large as 7 meV induced by an out-of-plane electric field. We propose possible defect structures with out-of-plane dipoles, which are supported by theoretical calculations. We will also present other types of Stark shifts which have quadratic components. These Stark shifts are measured not only at low temperatures around 10 K, but also at room temperature. Our results demonstrating the on-demand energy control of atomic defects in h-BN show the potential of 2D-based single photon emitters for quantum information applications.


TAO JIANG (Presenter), VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, University of Central Florida — By employing density functional theory (DFT) and time-dependent DFT (TDDFT), we study the electronic and optical properties of monolayers of pure (h-BN) and defect-laden hexagonal Boron Nitride dh-BN (with boron vacancy (VB), nitrogen vacancy (VN), boron substitution for nitrogen (BN), nitrogen substitution for boron (NB), carbon substitution for boron (CB) and carbon substitution for nitrogen (CN)). The DFT analysis traces the defect-induced changes to the orbital- and spin-projected density of states of h-BN and their implications for the optical properties of the system. The TDDFT results show that the long-range nature of the exchange-correlation kernel significantly affects the excitation energy, and hence the absorption and emission properties of the systems. We demonstrate that experimental data on the emission in dh-BN can be explained by the VN defects only. Namely, the conduction band-to-VN electron transitions give the dominant contribution to the photoluminescence spectrum, observed experimentally [1]. We discuss possible applications of the results in optoelectronic single-photon emitting devices.


*Work is supported in part by DOE grant DE-FG02-07ER46354

10:24AM A11.00011: Dielectric environment effects on charged defects in 2D materials  

DAN WANG (Presenter), RAVISHANKAR SUNDARARAMAN, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute — Two-dimensional (2D) materials are the subject of significant ongoing research for technological applications in electronics, optoelectronics and quantum computing. These applications critically depend on the properties of charged defects, which has necessitated the development of computational methods to evaluate energies of charged defects in 2D materials. Such methods overcome the energy divergence from the Coulomb interaction of a charged defect with its periodic images and the compensating background charges. However, these methods do not easily account for the effects of substrates on charged defect properties, which is vital for realistic treatment of 2D materials that cannot be free-standing for most applications. We present a general technique for predicting properties of charged defects in 2D materials with substrates, bringing together accurate prediction techniques for free-standing charged defects with continuum solvation theories. Application of this method to defects in molybdenum disulfide (MoS2) on various substrates reveals how charge transition levels of these defects evolve with environmental screening effects and will guide the design of defects for 2D devices.
10:36AM A11.00012: Electrically tunable quantum emitters in an ultrathin graphene - hexagonal boron nitride van der Waals heterostructure  
ALESSIO SCAVUZZO (Presenter), SHAI MANGEL, Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany, JI-HOON PARK, SANGHYUP LEE, DINH LOC DUONG, CIFAP, IBS, DOES, SSKU, Suwon 16419, Korea, CHRISTIAN STRELOW, ALF MEWS, Institute of Physical Chemistry, University of Hamburg, 20146 Hamburg, Germany, MARKO BURGHARD, KLAUS KERN, Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — The recent discovery of solid-state single-photon emitters in two-dimensional host systems has unveiled a huge potential for quantum information processing and integrated nanophotonics.

In this context, hexagonal boron nitride (h-BN), owing to its unique optical properties, has emerged as a highly promising candidate for exploring atomic defect-related quantum emission. However, the presence of inhomogeneous energy distribution and spectral diffusion of the zero-phonon line (ZPL) makes it difficult to achieve the emission of indistinguishable photons as required for many applications. Stark effect-induced spectral tuning of the ZPL is able to compensate intrinsic local strain and electrostatic fields, which constitute the main sources of inhomogeneity and instability in the emission from individual h-BN defects.

Here, we investigate the Stark tuning of quantum emitters in few-layer h-BN sheets by means of low-temperature confocal photoluminescence spectroscopy. The required vertical electric field is implemented using a graphene top contact. The emitters can be effectively and reproducibly tuned, revealing a high robustness under repeated gate voltage sweep cycles. Moreover, we demonstrate an electric field-induced modulation of the emission intensity and fluorescence lifetime.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A12 DMP: Devices from 2D Materials -- Microscopy and Spectroscopy BCEC 153A - Kyle Seyler, Univ of Washington - Tag(s): Focus

8:00AM A12.00001: Band structure engineering of monochalcogenides and van der Waals heterostructures [Invited]  
SHUYUN ZHOU (Presenter), Tsinghua University — Two-dimensional (2D) materials provide an important playground for exploring fundamental physics and potential applications. In this talk, I will present our recent process on the band structure structure of 2D materials and heterostructures. In particular, I will present our recent work on the electronic structure of a few transition metal monochalcogenides - thermoelectric SnSe [1] and a charge density wave material CuTe [2]. I will also present our recent progress on the band structure engineering of two prototypical examples of van der Waals heterostructures, a commensurate graphene/BN heterostructure with Moiré pattern [3], and an incommensurate 30° twisted bilayer graphene which shows symmetries similar to a quasicrystal [4].

References:

8:36AM A12.00002: Visualizing and Controlling Coupled Graphene Quantum Dots  
FERESHTE GHAHARI (Presenter), DANIEL WALKUP, National Institute of Standards and Technology (NIST), KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, NIKOLAI BORISOVICH ZHITENEV, JOSEPH A STROSCIO, National Institute of Standards and Technology (NIST) — Recent progress in creating graphene quantum dots (QDs) with fixed build-in potentials has enabled visualizing the confined electronic states employing local probe measurements. In these nanometer-sized circular QDs, the Dirac quasiparticles are confined by Klein scattering from p-n junction boundaries. In this talk, I will present the scanning tunneling measurements (STM) of such double graphene QDs where the size and coupling between QDs can be tuned by varying the back-gate voltage. At high magnetic fields, Landau levels (LLs) inside each QD form a series of metallic rings separated by highly insulating incompressible rings where each LL shows its own charging characteristics. We used Coulomb blockade spectroscopy to probe and visualize the transition from the double dot system to a single large dot. The transition is reflected in distinct anticrossing patterns between charging lines corresponding to LL's electrons in different quantum dots.
Layered ferroelectric materials such as CuInP$_2$S$_6$ (CIPS) offer a huge potential for adding functionality in van der Waals heterostructures and domain dynamics. In graphene devices supported by hexagonal boron nitride (hBN), local charge pockets can be written by pulsing the bias voltage of a scanning tunneling microscope (STM) tip. In a strong magnetic field, discrete Landau levels (LLs) replace the continuous graphene density of states, and the charge pocket is characterized by a concentric series of compressible and incompressible rings, as successive LLs cross the Fermi energy. Here, Coulomb blockade peaks appear in the scanning tunneling di/dV spectra, revealing the addition of single electrons to the confined Landau island, and encoding the capacitances between it and the tip and back-gate electrodes. When two highly-gapped LLs cross the Fermi energy, two series of peaks appear, experiencing avoided crossings within the dot. The observed avoidance pattern of these anti-crossings is unusual and defies conventional explanation. We present a new phenomenological electrostatic model, taking into account the self-contained geometry of this double-quantum dot system, and are able to reproduce the most striking features of the experimental data.

Visualization and transport properties of complex graphene moiré superlattices. Graphene/hBN superlattices formed by a dual-alignment of graphene with respect to two hBN slabs. The atomic-scale phonon emitters that establish the dominant dissipation mechanism in graphene exhibit sharp peaks when the Fermi level comes into resonance with electronic quasi-bound states at such defects, a hitherto uncharted process. The atomic defects are very rare in the bulk but abundant at the edges, acting as switchable energy dissipation centers.

Energy dissipation is a fundamental process governing the dynamics of classical and quantum systems, even though direct imaging of dissipation in quantum systems remained out-of-reach experimentally until recently. We developed a scanning nanoSQUID with sub 50 nm diameter that resides at the apex of a sharp pipette acting simultaneously as nanomagnetometer with single spin sensitivity and as nano-thermometer providing cryogenic thermal imaging with four orders of magnitude improved thermal sensitivity of below 1 µK/Hz$^{1/2}$. Using this scanning nano-thermometry we visualize and control phonon emission due to inelastic electron scattering off individual atomic defects in graphene. The inferred electron-phonon “cooling power spectrum” exhibits sharp peaks when the Fermi level comes into resonance with electronic quasi-bound states at such defects, a hitherto uncharted process. The atomic defects are very rare in the bulk but abundant at the edges, acting as switchable atomic-scale phonon emitters that establish the dominant dissipation mechanism in graphene.


Two-dimensional ferroelectric van der Waals heterostructures and domain dynamics*. Layered ferroelectric materials such as CuInP$_2$S$_6$ (CIPS) offer a huge potential for adding functionality in van der Waals (vdW) heterostructures and furthermore the opportunity to investigate some fundamental physics related to confinement in two dimensions plus the effect of electrostatic doping through ferroelectric polarization modulation. In this study we investigate, through piezoresponse force microscopy (PFM), pure-phase CIPS flakes exfoliated by standard Scotch tape methods and incorporated into vdW stacks through a dry-transfer technique. We show that the vdW interface electrostatic environment has significant effects on the local domain structure. Local switching dynamics determined by PFM were also observed to depend on the exact device geometry.

*Swiss National Science Foundation grant no. P300P2_171433
9:36AM A12.00007: Sub-Micron Imaging of Encapsulated 2D layers of Graphene and Transition Metal Dichalcogenides by Conductive Scanning Probe Microscopy*  

MICHAEL ALTVATER (Presenter), TIANHUI ZHU, JUNXI DUAN, GUOHONG LI, EVA ANDREI, Rutgers University, New Brunswick — Encapsulation of 2D materials protects them from environmental disturbances and significantly improves their quality. However, these benefits are lost if impurities or structural defects become trapped within the encapsulating layers. It is therefore crucial to detect these prior to embarking on time-consuming device processing. While encapsulated flakes can be detected via post-processing of optical images or by confocal Raman microscopy, these techniques lack the sub-micrometer resolution to identify structural defects and charged impurities within the encapsulated layer. We demonstrate a facile technique to visualize charged contaminants within the heterostructure by measuring surface potential fluctuations using Kelvin probe force microscopy (KPFM). By applying a fixed tip bias larger than the surface potential fluctuations, the encapsulated flakes and their sub-micron structural defects, cracks, and bubbles can be detected through electrostatic force microscopy (EFM). We show that these methods, which are standard extensions of atomic force microscopy (AFM), are perfectly suited for imaging encapsulated conductors and their local charge environments.

*Work supported by NSF EFRI 1433307, DOE-FG02-99ER45742, and NSF DMR 1708158.

9:48AM A12.00008: Graphene-based Hall sensors for scanning magnetic microscopy*  

BRIAN SCHAEFER (Presenter), LEI WANG, ALEXANDER B JARJOUR, Cornell University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, PAUL L MCEUEN, KATJA NOWACK, Cornell University — Incorporating few-layer graphite gate electrodes and hexagonal boron nitride gate dielectrics into graphene devices provides an accessible route to create two-dimensional electron systems with extremely low charge inhomogeneity. Here, we fabricate micrometer-scale graphene Hall sensors that can be tuned to a carrier density of $\sim 2 \times 10^9$ cm$^{-2}$ at cryogenic temperatures. This translates to a Hall coefficient exceeding 300,000 $\Omega$/T, two orders of magnitude larger than previously reported in any other Hall sensor. The magnetic resolution of our devices is ultimately limited by low-frequency flicker (1/$f$) and random telegraph noise, and we reach a minimum magnetic field noise spectral density of 60 nT/$\sqrt{\text{Hz}}$ at 1 kHz. Together, our results suggest that these devices have the potential to outperform semiconductor-based Hall sensors. We will also discuss our progress towards fabricating submicron-scale graphene-based scanning Hall probes that function over a wide range of temperatures and magnetic fields.

*This work was primarily supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875). This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1650441.

10:00AM A12.00009: Inelastic Electron Tunneling Spectroscopy of Graphene/hexagonal Boron Nitride heterostructures  

ZHEHAO GE (Presenter), JOHN L DAVENPORT, FREDERIC JOUCKEN, EBERTH QUEZADA, JUNYAN LIU, Physics, University of California, Santa Cruz, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, DAVID LEDERMAN, JAIRO VELASCO JR., Physics, University of California, Santa Cruz — Inelastic Electron Tunneling Spectroscopy (IETS) has been used for several decades as an experimental probe to access the vibrational properties of low dimensional materials. Notably, the ability to investigate these properties could be leveraged to gain further insight into the recently reported unconventional superconductivity in twisted bilayer graphene. Currently, there exists several IETS measurements on heterostructures of graphene and hexagonal Boron Nitride (hBN). These studies employed different experimental approaches such as tunneling from an atomically sharp asperity with scanning tunneling spectroscopy (STS) and planar tunneling via tunneling field effect transistors (TFETs). Importantly, the IETS results from these different experimental approaches lack agreement. To address this disparity we provide a direct comparison between IETS measurements acquired from STS and TFETs on graphene/hBN heterostructures that underwent the same fabrication processes. Our work contributes towards benchmarking IETS of two-dimensional material heterostructures and will enable future application of this technique to the study of unconventional superconductivity in twisted bilayer graphene.
10:12AM A12.00010: Complete Strain Mapping of Nanosheets of Transition Metal Chalcogenides  YUE CAO
(Presenter), Argonne National Laboratory, TADESSE ASSEFA, Brookhaven National Laboratory, SOHAM BANERJEE, SIMON J L BILLINGE, JEDRZEJ WIETESKA, DENNIS WANG, ABHAY PASUPATHY, Columbia University, XIAO TONG, Brookhaven National Laboratory, YU LIU, WENJIAN LU, YUPING SUN, Institute of Solid State Physics, Chinese Academy of Sciences, YAN HE, Shanghai Synchrotron Radiation Facility (SSRF), Shanghai Institute of Applied Physics, Chinese Academy of Sciences, XIAOQING HUANG, HANFEI YAN, YONG S. CHU, IAN KEITH ROBINSON, Brookhaven National Laboratory — Holding promise for future electronics because of their unique band structures, quasi-two-dimensional (quasi-2D) materials host electronic and mechanical properties sensitive to crystal strains in all three dimensions. Quantifying the crystal strain is a prerequisite to correlating it with the performance of the relevant device, and calls for fast characterization methods compatible with the potential devices and applications. Here we bridge this knowledge gap using fly-scan nano X-ray diffraction with strain sensitivity below 0.001 over sub 100 µm length scales. Coherent diffraction patterns were collected from a thin sheet of 1T-TaS2 using an area detector by scanning across and rotating the sample. Reconstructing from the resulting five-dimensional datasets yields information on the morphology of and the strain distribution around micron and sub-micron ‘bubbles’ which form spontaneously in the quasi-2D plane. Our studies thus open way to experimentally quantify local strains in these quasi-2D materials and will allow better understanding of strains in tuning material properties.

10:24AM A12.00011: Reversible Nanoscale Control of the Charge Neutrality Point in Graphene Using LaAlO3/SrTiO3 Heterostructures* JIANAN LI (Presenter), QING GUO, JEN-FENG HSU, SHAN HAO, YANG HU, University of Pittsburgh, HYUNGWOO LEE, JUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin-Madison, BRIAN R D’URSO, Montana State University, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — The properties of graphene depend sensitively on doping with respect to the charge-neutrality point (CNP). Tuning the CNP usually involves electrical gating or chemical doping. Here, we describe a technique to reversibly control the CNP in graphene with extreme nanoscale precision, using LaAlO3/SrTiO3 (LAO/STO) heterostructures and conductive atomic force microscope (c-AFM) lithography. The conductivity of the LAO/STO interface can be tuned using a conductive AFM tip, even through graphene transferred on, affecting the LAO/STO interface conductive while shifting the position of graphene CNP. Here we demonstrate that edge state engineering can be achieved from this method using the quantum Hall effect. Clear quantized resistance at plateaus h/e2 and h/3e2 are observed in a split Hall device, demonstrating edge transport along the c-AFM written edge. This technique can be extended to many other device geometries.

*JL acknowledges a Vannevar Bush Faculty Fellowship, funded by ONR (N00014-15-1-2847). JL and BD acknowledge support from ONR (N00014-16-1-3152). C-BE acknowledges NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-4046).

10:36AM A12.00012: Probing band structure renormalization in 2D semiconductors induced by external dielectric screening through angle-resolved photoemission spectroscopy  LUTZ WALDECKER (Presenter), Stanford University and SLAC National Laboratory, ARCHANA RAJA, University of California, Berkeley, MALTE ROESNER, University of Southern California and CCQ, Flatiron Institute, CHRISTINA STEINKE, University of Bremen, ROLAND KOCH, AARON BOSTWICK, CHRIS JOZWIAK, Advanced Light Source, E. O. Lawrence Berkeley National Laboratory, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Tsukuba, ELI ROTENBERG, Advanced Light Source, E. O. Lawrence Berkeley National Laboratory, TIM WEHLING, University of Bremen, TONY F HEINZ, Stanford University and SLAC National Laboratory — We investigate the effect of dielectric screening by the external environment on the electronic states in the two-dimensional (2D) semiconductor WS2 using angle-resolved photoemission spectroscopy (ARPES). As has been previously reported from optical spectroscopy of monolayer WS2 [1], an increase in environmental screening from the presence of graphene can lead to a ~100 meV reduction of the bandgap. Our ARPES study of monolayer WS2 partially placed on h-BN and graphene, however, reveals that the dispersion of the valence band is essentially unchanged (< 10 meV shifts) when screening by graphene is present. Thus the screening-induced band renormalization appears to lead only to a rigid shift, rather than a restructuring of the valence band. We compare this experimental finding with theory based on GΔW calculations, including material-realistic frequency and momentum dependent screening due to the substrate. In agreement with experiment, theory predicts the primary effect of bandgap renormalization along with a scissor-like shift of all electronic states. We discuss the physical origin of this result and its implication for the use of controlled changes in the environment to tune the band structure of 2D semiconductors.

10:48AM A12.00013: Gating and superlattice effects in monolayer WSe2 devices in micro-ARPES* PAUL NGUYEN (Presenter), University of Washington, NATALIE TEUTSCH, ABIGAIL J GRAHAM, Physics, University of Warwick, MINHAO HE, University of Washington, VIKTOR KANDYBA, ALEXEI VICTOROVICH BARINOV, Elettra - Sincrotrone Trieste S.C.p.A, NEIL R WILSON, Physics, University of Warwick, XIAODONG XU, DAVID HENRY COBDEN, University of Washington — We investigate the effects of electrostatic doping and moiré superlattice potentials on monolayer WSe2 using micro-angle-resolved photoemission spectroscopy (micro-ARPES). By employing a local back gate of thin graphite under a hexagonal boron nitride dielectric support, we electrostatically populate the WSe2 conduction band during the photoemission measurements. We find the conduction band edge to be at the zone corner, or K point, confirming the direct gap nature of this material and yielding a measurement of the single-particle gap. As the electron doping is increased to a maximum of ~1.4E13 cm−2 the valence band shifts upwards towards the conduction band, corresponding to substantial band gap renormalization. At the highest doping levels, the conduction band minimum at the lower symmetry Q point is also populated, showing that it is within ~30 meV of the minimum at K. In some devices we also observe folded copies of the hBN and WSe2 bands with intensities often comparable to the original bands, yielding information about moiré superlattice effects.

*Supported in part by DoE awards DE-SC0002197, and DE-SC0018171, as well as NSF MRSEC award 1719797.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A13 DMP: 2D Materials (General) -- Transport BCEC 153B - Daniel Ralph, Cornell University - Tag(s): Focus

8:00AM A13.00001: First-principles studies of the electronic structure and photophysics of monolayer WS2 with point defects* JUN-HO LEE (Presenter), Lawrence Berkeley National Laboratory, University of California - Berkeley, SIVAN REFAELY-ABRAMSON, Weizmann Institute of Science, Lawrence Berkeley National Laboratory, University of California - Berkeley, DIANA QIU, University of California - Berkeley, Lawrence Berkeley National Laboratory, BRUNO SCHULER, KATHERINE COCHRANE, ALEXANDER WEBER-BARGIONI, Molecular Foundry, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, University of California - Berkeley, Lawrence Berkeley National Laboratory, JEFFREY B NEATON, Lawrence Berkeley National Laboratory, University of California - Berkeley, Kavli Energy NanoSciences Institute at Berkeley — Point defects in single-layer transition-metal dichalcogenides (TMDs) are common, and point defects in layered TMDs – including vacancies and chemical substitutions – have been reported to affect their electronic structure and photophysics. Here, we use first-principles density functional theory and the GW and GW-BSE calculations to explore the structure and the tunneling and optical properties of substitutional points defects in monolayer tungsten disulfide. Using a large supercell, we compute the atomic structure, quasiparticle band structure, defect states, and low-lying excitons for dilute defect concentrations. We compare our structure and quasiparticle excitation spectrum with state-of-the-art non-contact atomic force microscope and scanning tunneling spectroscopy measurements.

*This work was supported by the US Department of Energy. Computational resources are provided by NERSC.

8:12AM A13.00002: Dopant induced electronic inhomogeneity of epitaxial bilayer graphene in SiC* SHUAI ZHANG (Presenter), DI HUANG, LEHUA GU, YUAN WANG, SHIWEI WU, Department of Physics, Fudan University — Graphene has been a promising candidate for next-generation electronics due to its intriguing properties, particularly the high carrier mobility. Currently, wafer-scale single crystal graphene could be readily produced on silicon carbide (SiC) substrate by high-temperature annealing. But the mobility of epitaxial graphene is relatively lower than that by mechanical exfoliation. The underlying mechanism has not yet been resolved. Here we study the topography and electronic state of epitaxial graphene grown on 6H-SiC by scanning tunneling microscopy (STM) and spectroscopy (STS). We show that the nitrogen dopants inside SiC substrate result in the electronic inhomogeneity of epitaxial graphene, and give rise to electron-lack puddles. Our results provide the plausible microscopic mechanism for the low mobility in epitaxial graphene.

*The work at Fudan University was supported by the National Basic Research Program of China (Grant Nos. 2014CB921601, 2016YFA0301002), National Natural Science Foundation of China (Grant No. 11427902), and the Science and Technology Commission of Shanghai Municipality (Grant No. 16jC1400401).
8:24AM A13.00003: The Intrinsic Carrier Mobility in Two-Dimensional Semiconductors [Invited] YUANYUE LIU (Presenter), University of Texas at Austin — Two-dimensional (2D) semiconductors have attracted great interest for next-generation electronics and optoelectronics. However, they typically have a low mobility of electrons/holes, compared with Si/III-V semiconductors. Here I will discuss our recent theoretical understandings of the mobility-limiting factors in 2D semiconductors [1], and strategies of increasing the mobility. These results are based on the calculation of electron-phonon coupling matrix using density functional perturbation theory and the Wannier interpolation, as well as the Boltzmann transport theory. Moreover, I will also present a new approach for decoupling the entangled phonons to standard phonon modes [2], to analyze the electron-phonon coupling.


9:00AM A13.00004: Effect of current annealing to the transport properties of CVD graphene cooled with a biased gate voltage* U. KUSHAN WIJEWARDENA (Presenter), THARANGA NANAYAKKARA, RASANGA SAMARAWEERA, BINUKA GUNAWARDANA, C. RASADI MUNASINGHE, SAJITH WITHANAGE, ANNIKA KRIISA, RAMESH MANI, Georgia State University — Chemical vapor deposition of graphene is an excellent method for obtaining large area single-layer graphene. A topic of interest in this area is to characterize and reduce the impurity level in this material. In this experimental work, we investigate impurity effects on electron /hole transport in a graphene specimen by cooling down a graphene Hall bar device under different gate bias voltages. Further, we examine the impact of current annealing on the transport characteristics. Here we present results from the measurements carried out in a closed cycle refrigerator out over a broad temperature range (295K–15K), focusing on the charge neutrality point.

*This work was supported by National Science Foundation (Grant No: ECCS 1710302), U.S. Department of Energy (Grant No. DE-SC0001762), Army Research Office (Grant No: W911NF-14-2-0076 and W911NF-15-1-0433)

9:12AM A13.00005: Gateless and reversible carrier density tunability in epitaxial graphene devices functionalized with chromium tricarbonyl* ALBERT RIGOSI (Presenter), MATTIAS KRUSKOPF, HEATHER M. HILL, HANBYUL JIN, BI-YI WU, PHILIP E JOHNSON, SIYUAN ZHANG, MICHAEL BERILLA, ANGELA HIGHT WALKER, CHRISTINA HACKER, DAVID B NEWELL, RANDOLPH E ELMQUIST, National Institute of Standards and Technology — Monolayer epitaxial graphene (EG) has been shown to have clearly superior properties for the development of quantized Hall resistance (QHR) standards. One major difficulty with QHR devices based on EG is that their electrical properties drift slowly over time if the device is stored in air due to adsorption of atmospheric molecular dopants. The crucial parameter for device stability is the charge carrier density, which determines the energy spacing of the Landau levels and thus the magnetic flux density required for precise QHR measurements. This work presents one solution to this problem of instability in air by functionalizing the surface of EG devices with chromium tricarbonyl - Cr(CO)3. Observations of carrier density stability in air over the course of one year are reported, as well as the ability to tune the carrier density by annealing the devices. For low temperature annealing, the presence of Cr(CO)3 stabilizes the electrical properties and allows for the reversible tuning of the carrier density in millimeter-scale graphene devices close to the Dirac point. Precision measurements in the quantum Hall regime show no detrimental effect on the carrier mobility.

*Work performed as part of the duties of employees of the United States Government, including its guest researchers.

9:24AM A13.00006: Electronic properties of armchair transition metal dichalcogenides nanoribbons deposited with atomic chains.* CHI-HSUAN LEE (Presenter), CHIH-KAI YANG, National Chengchi University — Electronic properties of armchair transition metal dichalcogenides (TMD) nanoribbons bonded with atomic chains are studied using density-functional calculations. The pure armchair TMD nanoribbon with 15 dimer lines possesses non-magnetic band structures with a moderate energy gap. Their edge states near the Fermi level exhibit different kinds of behavior in accordance to the different elements. Energy bands of the deposited atomic chains hybridize with the edge states of the ribbon and induce various magnetic properties, with different locations of deposition taken into account. The results are useful for fabricating novel nanoelectronic devices.

*Supported by the Ministry of Science and Technology of the Republic of China under grant number MOST 105-2112-M-004-001-MY3.

9:36AM A13.00007: ABSTRACT WITHDRAWN
Tuning Charge Transport in Voltage-Reduced Graphene Oxide through Defect Control and Quantum Confinement* KEVIN SILVERSTEIN (Presenter), Department of Physics, Applied Physics, and Astronomy, Binghamton University, CHRISTIAN E HALBIG, Institute of Chemistry and Biochemistry, Freie Universität Berlin, AUSTIN C FAUCETT, JEREMY MEHTA, Department of Physics, Applied Physics, and Astronomy, Binghamton University, ANJU SHARMA, Small Scale Systems Integration and Packaging Center, Binghamton University, SIEGFRIED EIGLER, Institute of Chemistry and Biochemistry, Freie Universität Berlin, JEFFREY M. MATIVETSKY, Department of Physics, Applied Physics, and Astronomy, Binghamton University — Graphene oxide (GO) is a versatile two-dimensional nanomaterial that is being explored for its tunable electrical, optical, and chemical properties. This tunability is afforded by reduction which removes oxygen-containing functional groups, restores the sp² carbon lattice, and converts the electrically insulating material to one that is conducting. Here, we use voltage reduction, a simple and environmentally benign procedure, to manipulate the electrical properties of GO from insulating to conducting, and potentially semiconducting. A low-defect form of GO, oxo-G, was synthesized and voltage-reduced to produce a highly conductive graphene derivative. Variable temperature electrical resistance measurements reveal a transition from hopping transport to a temperature-stable resistance over a broad temperature range, making this material promising for use in sensors and other applications that require temperature-stable performance. Nanopatterning was also employed, by using a conductive atomic force microscope probe to initiate voltage reduction. Preliminary data suggests possible transport gap opening due to quantum confinement.

*This work was supported by the National Science Foundation (CMMI-1537648, CMMI-1429176)

The role of defects in the performance of graphene hot-electron devices.* A EL FATIMY, PEIZE HAN, LUKE ST. MARIE, Physics, Georgetown University, NICHOLAS QUIRK, Physics, Princeton University, MATTHEW T DEJARLD, RACHAEL MYERS-WARD, US Naval Research Laboratory, KEVIN DANIELS, Electrical and Computer Engineering, University of Maryland, SHOJAN PAVUNNY, DAVID KURT GASKILL, US Naval Research Laboratory, YIGIT AYTAC, THOMAS E MURPHY, Electrical and Computer Engineering, University of Maryland, PAOLA BARBARA (Presenter), Physics, Georgetown University — Defect-mediated electron-phonon collisions (supercollisions) play an important role in the cooling dynamics of hot electrons in graphene, but their impact on the performance of optoelectronic devices is still largely unexplored. Here we study supercollisions in hot-electron bolometers based on quantum dots of epitaxial graphene grown on SiC. We find that the fabrication process substantially affects the defect density and that a higher defect density greatly enhances the device performance, yielding faster response time and lower thermal conductance in a wide range of power and temperature.

*This work was supported by the US Office of Naval Research (N00014-16-1-2674) and the NSF (ECCS-1610953).

Incorporation of metallocene as n-dopant in vertical stacked van der Waals homostructure of atomically thin HfS₂* CHINEDU EKUMA (Presenter), SINA NAJMAEI, MADAN DUBEY, Sensors and Electron Devices Directorate, U.S. Army Research Laboratory, ALC, MD — Chemical or electrical doping is an efficient means of improving and controlling carrier transport and charge injection in materials. Using a combination of first-principles calculations and experiment, we tailor the properties of vertically stacked two-dimensional HfS₂ by intercalation of cobaltocene and chromocene (MC₅₂). Our data show that MC₅₂ behaves as pseudo-alkali metals, transferring electrons to the homostructure characterized by a shift of the Fermi level towards the empty states and an increase of the current density. The process of MC₅₂ evolving in the homostructure which led to the doping is due to charge transfer from the intercalant to the host material that induced ion pairing between the host and the dopant.

*This work has been supported by the U.S. Army Research Laboratory (ARL) and was accomplished under the Cooperative Agreement Number W911NF-11-2-0030 as an ARL Research [George F. Adams] Fellow.
Charge transfer in few-layer InSe/gas Interface*  
HANSIKA SIRIKUMARA (Presenter), MILINDA WASALA, ANANTH PANCHAMUKHI, PRASANNA DNYANESHWAR PATIL, ARON C WALBER, Department of Physics, Southern Illinois University Carbondale, SIDONG LEI, ROBERT VAJTAI, PULICHEL M AJAYAN, Department of Materials Science and Nano Engineering, Rice University, SAIKAT TALAPATRA, THUSHARI JAYASEKERA, Department of Physics, Southern Illinois University Carbondale — Few-layer InSe shows a strong potential for gas sensing applications primarily due to high sensitivity of electron lone pairs on Se to external gas molecules. Based on the results from first principles Density Functional Theory calculations, we carefully analyzed electronic band structures of few-layer InSe/Gas configurations. Our calculations show that charge transfer across few-layer InSe/gas system depends on the orientation and the type of the gas molecules. Therefore, it was seen that for certain gas molecules such as ethanol, the InSe layers are p-doped, while for other molecules such as methanol the InSe layers are n-doped. These results were verified through gas sensing experiments using few layer InSe FET devices. Further we show, while majority charge transfer happens through InSe/Gas interface, the polarity of external molecule can tune interlayer spacing through an induced dipole moment between the layers. The change in interlayer spacing is not monotonic, which results in pinning of impurity band with respect to valence band maximum. Fundamental understanding of charge transfer in few-layer InSe/gas interfaces at the atomic level is expected to pave the path for designing gas sensing devices based on few-layer InSe.

*U.S.Army Research Office MURI grant #W911NF-11-1-0362

Redox-Governed Charge Doping in WS2 and Graphene  
SUNMIN RYU (Presenter), KWANGHEE PARK, HA NEUL KANG, Pohang University of Science and Technology — Low dimensional materials often undergo spontaneous hole doping in the ambient conditions, the detailed mechanism of which has yet to be revealed. In this work, we propose a mechanism based on a redox couple of O2/H2O and verified it for two model systems: photoluminescence (PL) modulation in single-layer WS2 and thermally-activated phonon hardening in graphene with both supported on silica substrates. The PL modulation was directly correlated with the concentration of oxygen both in gaseous and aqueous states. Wide-field PL imaging, however, showed distinctively different spatial propagations of the modulation for the two states, revealing the microscopic picture of the charge doping in WS2. The mechanistic details and thermodynamic driving force for the charge doping will also be discussed in conjunction with the activated hole doping in graphene probed by Raman spectroscopy.

Monday, March 4, 2019 8:00 AM - 10:36 AM

Session A14 DMP: 2D Materials (Metals, Superconductors, and Correlated Materials) -- CDWs

Orbital- and k_z-selective hybridisation of Se 4p and Ti 3d states at the CDW transition of TiSe2*  
MATTHEW WATSON (Presenter), OLIVER J CLARK, FEDERICO MAZZOLA, IGOR MARKOVIĆ, VERONIKA SUNKO, School of Physics and Astronomy, University of St Andrews, St. Andrews KY16 9SS, United Kingdom, TIMUR KIM, Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, United Kingdom, KAI ROSSNAGEL, Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany, PHILIP KING, School of Physics and Astronomy, University of St Andrews, St. Andrews KY16 9SS, United Kingdom — We revisit the enduring problem of the 2×2×2 charge density wave (CDW) order in TiSe2, utilising photon energy-dependent angle-resolved photoemission spectroscopy (ARPES) to probe the full three-dimensional high- and low-temperature electronic structure. Our measurements demonstrate how a mismatch of dimensionality between the 3D conduction bands and the quasi-2D valence bands in this system leads to a hybridisation that is strongly k_z-dependent. This 3D momentum-selective coupling shifts the strongly hybridized states well away from the Fermi level, providing the energy gain required to form the CDW. However, we show how additional `passenger" states remain, and dominate the low energy physics in the ordered state. In particular we find that a branch of the conduction band with 3dz² character remains essentially unhybridised in the ordered phase, forming a coherent and ungepapped electron-like Fermi surface. We conclude by making a comparison to the 2x2 CDW of monolayer TiSe2, where k_z-selective effects are absent, but orbital-selective hybridisation persists. [1] Watson et al., arXiv:1808.07141 (2018).

*We gratefully acknowledge support from The Leverhulme Trust (Grant Nos. RL-2016-006 and PLP-2015-144) and The Royal Society.
Pairing induced by CDW fluctuations: the case of superconductivity in TiSe$_2$*  

CHUAN CHEN (Presenter), ANTONIO HELIO CASTRO NETO, VITOR PEREIRA, National University of Singapore — We theoretically studied the modes and spectrum of fluctuations of the CDW in TiSe$_2$ using a model that describes its CDW state as a result of the intrinsic excitonic instability in TiSe$_2$. The charge carriers are electrons within the CDW-renormalized conduction band (CDW quasiparticles). A calculation of the effective action for the CDW fluctuations shows the presence of gapless phase modes and gapped amplitude modes. Upon integrating out these fluctuations, we find that the amplitude fluctuations induce attractive pairing between the CDW quasiparticles resulting in s-wave superconductivity. A subsequent mean-field phase diagram of both CDW and superconducting critical temperatures as a function of doping reveals a dome-shaped superconducting phase coexisting with CDW in the near-commensurate regime, in agreement with the experimental phase diagram.

*Singapore Ministry of Education through grant MOE2015-T2-2-059, National Research Foundation of Singapore under its Medium-Sized Centre Programme

Electronic properties and charge density wave transition in single-layer VSe$_2$  

KIEN NGUYEN-CONG (Presenter), PAULA COELHO NETO, MATTHIAS BATZILL, IVAN OLEYNIK, University of South Florida — Single-layer VSe$_2$ has been recently attracted attention due to experimental observations of ferromagnetism and charge density wave (CDW) transition. There are controversies from both theory and experiment concerning ferromagnetism in both bulk and single layer VSe$_2$. In addition, CDW transition in VSe$_2$ is not well understood. In this work, structural, electronic, magnetic and CDW properties of this system are investigated using first-principle calculations. The calculated electronic structure is compared with recent APPRES measurements and conclusions concerning its magnetic state are made. The calculated phonon spectra are used in investigation of CDW transition mechanism. Crystal structure of the CDW state is determined using the evolutionary crystal structure prediction combined with lattice dynamics.

Unique gap structure and symmetry of the charge density wave in single-layer VSe$_2$  

PENG CHEN (Presenter), Physics, University of Illinois Urbana-Champaign, WOEI WU PAI, National Taiwan University, YANG-HAO CHAN, Academia Sinica, VIDYA MADHAVAN, Physics, University of Illinois Urbana-Champaign, MEI-YIN CHOU, National Taiwan University, SUNG-KWAN MO, ALEXEI V. FEDOROV, Lawrence Berkeley National Laboratory, TAI-CHANG CHIANG, Physics, University of Illinois Urbana-Champaign — Single layers of transition metal dichalcogenides (TMDCs) are excellent candidates for electronic applications beyond the graphene platform; many of them exhibit novel properties including charge density waves (CDWs) and magnetic ordering. CDWs in these single layers are generally a planar projection of the corresponding bulk CDWs because of the quasi-two-dimensional nature of TMDCs; a different CDW symmetry is unexpected. We report herein the successful creation of pristine single-layer VSe$_2$, which shows a (sqrt(7) x sqrt(3)) CDW in contrast to the (4 x 4) CDW for the layers in bulk VSe$_2$. Angle-resolved photoemission spectroscopy (ARPES) from the single layer shows a sizable (sqrt(7) x sqrt(3)) CDW gap of ~100 meV at the zone boundary, a 220 K CDW transition temperature twice the bulk value, and no ferromagnetic exchange splitting as predicated by theory. This robust CDW with an exotic broken symmetry as the ground state is explained via a first-principles analysis. The results illustrate a unique CDW phenomenon in the two-dimensional limit.
extendable to a broad set of two-dimensional materials with CDW order, including cuprates. Information includes orbital selectivity and electron-phonon coupling can explain both general and specific features and might be

CHOI, Physics, University of Seoul, Korea, CHRIS JOZWIAK, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source (ALS), E. O. Lawrence Berkeley National Laboratory, USA, JE-GUEN PARK, Center for Correlated Electron Systems, Institute for Basic Science (IBS), Korea, RAMAN SANKAR, Physics, Academia Sinica, Taiwan, KI-SEOK KIM, Physics, POSTECH, Korea, JUNGDae KIM, Physics, Ulsan University, Korea, YOUNG JUN CHANG (Presenter), Physics, University of Seoul, Korea — Although emergent phenomena driven by electronic reconstructions in oxide heterostructures have been intensively discussed, such interface-driven phenomena in shaping the electronic properties has not been well established in van der Waals heterointerfaces. By diminishing the material thickness and forming a heterointerface, we observed two types of charge-ordering transitions in monolayer VSe$_2$ on graphene substrates. Comprehensive combination of ARPES, STM, and renormalization group analysis enable us to reveal the low-dimensionality and the heterointerface play important roles in enhancing charge density wave temperature to 350 K contrasted to the 105 K in bulk VSe$_2$ and in driving the unexpected metal-insulator transition at 135 K in the family of monolayer transition metal dichalcogenides. We will discuss implications of our observations in comparison with the similar results reported by two other groups.

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9:00AM A14.00006: General and specific features of the charge density waves in transition metal dichalcogenides*

KAPILA WIJAYARATNE (Presenter), JUNJING ZHAO, Department of Physics, University of Virginia, CHRISTOS MALLIAKAS, Department of Chemistry, Northwestern University, DUCK YOUNG CHUNG, Materials Science Division, Argonne National Lab, GENDA GU, Condensed Matter Physics & Materials Science, Brookhaven National Lab, MERCOURI KANATZIDIS, Department of Chemistry, Northwestern University, JASPER VAN WEZEL, Institute of Theoretical Physics, University of Amsterdam, UTPAL CHATTERJEE, Department of Physics, University of Virginia — We report a series of elaborate Angle-Resolved Photoemission Spectroscopy (ARPES) studies on the charge density wave (CDW) phase in transition metal dichalcogenides (TMD) 2H-TaS$_2$, TaSe$_2$ and NbSe$_2$, analyzed above/ below the CDW transition temperature ($T_{\text{CDW}}$). Generally; i) On Fermi surface, CDW energy gap appears only in the vicinity of some symmetry points, while other momentum points are ungapped. ii) Gap is asymmetric in particles and holes. iii) Gap existed above $T_{\text{CDW}}$ beyond the CDW phase, (pseudogap). iv) Conventional Fermi surface nesting model is incapable of describing the CDWs in TMDs. v) phonon related band renormalizations were observed in 2H-TaS$_2$. Compound-specific features, due to different orbital orientations were; i) Size variation of some Fermi pockets are related to $T_{\text{CDW}}$ while other pockets were similar among compounds. ii) About a given symmetry point, in 2H-NbSe$_2$ the gap size varied upon momentum in contrast to 2H-TaS$_2$, where this variation was insignificant. A tight binding model that includes orbital selectivity and electron-phonon coupling can explain both general and specific features and might be extendable to a broad set of two-dimensional materials with CDW order, including cuprates.

*National Science Foundation and U.S. Department of Energy

9:12AM A14.00007: Ion intercalation tuned quantum transport, charge density waves, and superconductivity in atomically thin crystals of 2H-TaSe$_2$

YUESHEN WU (Presenter), Physics, Shanghai Jiao Tong University, CHAO-SHENG LIAN, Physics, Zhengzhou University, HUI XING, CHAO YAO, Physics, Shanghai Jiao Tong University, DUAN WENHUI, Physics, Tsinghua University, JINYU LIU, Physics, Shanghai Jiao Tong University, ZHIQIANG MAO, YING LIU, Physics, Pennsylvania State Univ — Quantum transport in an electronic system dealing with the quantum interference of diffusive electrons is influenced strongly by spin-orbital and electron-phonon interactions. Two-dimensional (2D) crystals of transition metal chalcogenides (TMCs) were found recently to show interesting behavior in quantum transport, which can be tuned, for example, by electric field effects. However, ion intercalation has not been used to tune quantum transport involving weak localization or weak antilocalization in 2D TMCs. We carried out magneto electrical transport measurements on atomically thin crystals of 2H-TaSe$_2$ intercalated by Li ions controlled by ionic gating. Gate voltage and temperature tuned crossovers from weak antilocalization to weak localization were observed. Meanwhile, ion intercalation was found to suppress charge density waves and enhance superconductivity at the same time. Band structure and phonon spectrum calculations show that the electronic density of states and the number of acoustic phonons available for scattering are reduced. Our observations suggest that the ion intercalation leads to an enhancement of the electron-phonon interaction and a simultaneous reduction in spin-orbital scattering.
Atomic-scale visualization of the low temperature charge density wave phase in 1T'-TaTe$_2$

Ismail El Baggari (Presenter), Nikhil Sivadas, Gregory Steihl, Daniel Ralph, Craig J Fennie, Lena F Kourkoutis, Cornell University — Many transition-metal dichalcogenides, such as TaS$_2$ and NbSe$_2$, exhibit charge density wave (CDW) instabilities which, by coupling to the lattice, induce complex periodic lattice displacement patterns. Tellurium-based TMDs further exhibit large electronic and structural anisotropy and significant interlayer correlations. Here, we use cryogenic scanning transmission electron microscopy (STEM) to probe in real space the high temperature (HT) and low temperature (LT) CDW phases in metallic 1T'-TaTe$_2$. We visualize Ta trimer states at room temperature and observe below the CDW transition temperature ($T_c \sim 170$ K) the formation of a superstructure arising from complex, periodic intensity modulations in STEM data. The modulations reflect longitudinal periodic lattice displacements that stack in a staggered fashion between the layers. Cross-sectional imaging, density functional theory calculations, and multislice image simulations further elucidate the nature of the HT and LT states. These atomically-resolved measurements reveal the complex role of lattice degrees of freedom in CDW transitions.

First principles description of Charge Density Waves in single-layer TiSe$_2$ and TiTe$_2$.

Bogdan Guster (Presenter), Roberto Robles, Miguel Pruneda, Catalan Institute of Nanoscience and Nanotechnology, Enric Canadell, ICMAB-CSIC, Pablo Ordejón, Catalan Institute of Nanoscience and Nanotechnology — We present some of our recent work on the understanding of the appearance of Charge Density Waves (CDW) in single-layer 2D transition metal dichalcogenides by means of first principles electronic structure calculations. This is done in connection with recent experimental studies that have been able to demonstrate the presence of CDS in several 2D single-layer materials like TiSe$_2$ and TiTe$_2$. The evolution of the CDW with external electrostatic doping, which has been achieved experimentally using field effect transistor setups, will be analyzed for the case of TiSe$_2$ [1]. For TiTe$_2$, we focus on the recently observed CDW in the single layer, which is not present in the bulk material [2].


*SWork supported by European Union H2020-EINFRA-5-2015 MaX Center of Excellence (Grant No.824143) and Spanish MINECO (Grant No. FIS2015-64886-C5-3-P). ICN2 is funded by the Severo Ochoa Centers of Excellence Program under Grant SEV-2013-0295 and the CERCA Program/Generalitat de Catalunya. Funding from Generalitat de Catalunya (Grant 2017SGR1506) is also acknowledged.

Spectroscopic signatures of many-body renormalizations in 1T-TiSe$_2$.

Utpal Chatterjee (Presenter), Physics, University of Virginia, Nandini Trivedi, Kyungmin Lee, Physics, Ohio State University, Goran Karapetrov, Physics, Drexel University, Junjing Zhao, Physics, University of Virginia — We have investigated the many-body renormalization of the single-particle excitations in 1T-TiSe$_2$ by employing high resolution angle resolved photoemission spectroscopy (ARPES) measurements. The energy distribution curves of the ARPES data reveal an intrinsic peak-dip-hump feature. The electronic dispersion extracted from the momentum distribution curves highlights, for the first time, multiple kink structures. These are canonical signatures of coupling between the electronic degrees of freedom and bosonic modes in the system. Theoretical modeling of electrons coupled to an Einstein mode provides insight into the peak-dip-hump features observed in the data. From a self-energy analysis of our ARPES data, we find a bosonic mode at 26 meV that correlates with ab-initio phonon-dispersion calculations and observation of Raman active shear (E$_g$) mode in Raman scattering experiments. The direct observation of band-renormalization due to such electron-boson coupling suggests that such modes could be important for driving charge density wave (CDW) and superconductivity in 1T-TiSe$_2$ like in many other transition metal dichalcogenides.

*National Science Foundation (NSF) under Grant No. DMR- 1629237
10:00AM A14.00011: Charge density wave order in a transition metal dichalcogenide probed by second harmonic generation*  
BRYAN FICHERA (Presenter), ANSHUL KOGAR, LINDA YE, JOSEPH CHECKELSKY, NUH GEDIK, Massachusetts Institute of Technology — Rotational anisotropy second harmonic generation (RA-SHG) is a nonlinear optical probe which has been used to study electronic order in solid state materials. Because the leading-order contribution to the second harmonic signal is zero in the bulk of centrosymmetric crystals, RA-SHG can be used to study the surface properties of ordered materials. We use RA-SHG to study electronic order on the surface of a transition metal dichalcogenide (TMD). We find that the symmetry-breaking character of ordered charge density wave (CDW) states in the TMD can be identified using RA-SHG, and that our technique can be used to differentiate surface CDW domains. We also posit a new framework for understanding RA-SHG data from crystal structures with incommensurate charge order.

*Financial support from the U.S. Department of Energy, the Gordon and Betty Moore Foundation, and from Shell is gratefully acknowledged.

10:12AM A14.00012: Dynamical slowing down in an ultrafast photo-induced phase transition* 
ALFRED ZONG (Presenter), ANSHUL KOGAR, Massachusetts Institute of Technology, PAVEL E DOLGIREV, Skolkovo Institute of Science and Technology, EMRE ERGECEN, MEHMET B YILMAZ, YA-QING BIE, TIMM ROHWER, Massachusetts Institute of Technology, I-CHENG TUNG, Argonne National Laboratory, JOSHUA STRAQUADINE, PHILIP WALMSLEY, Stanford University, XIAOZHE SHEN, JIE YANG, RENKAI LI, SUJI PARK, MATTHIAS C HOFFMANN, BENJAMIN K OFORI-OKAI, MICHAEL E KOZINA, SLAC National Accelerator Laboratory, HAIDAN WEN, Argonne National Laboratory, XJIE WANG, SLAC National Accelerator Laboratory, IAN R FISHER, Stanford University, PABLO JARILLO-HERRERO, NUH GEDIK, Massachusetts Institute of Technology — Complex systems, which consist of a large number of interacting constituents, often exhibit universal behavior near a phase transition. A slowdown of certain dynamical observables is one such recurring feature found in a vast array of contexts. This phenomenon, known as critical slowing down, is well studied mostly in thermodynamic phase transitions. However, it is less understood in highly nonequilibrium settings, where the time it takes to traverse the phase boundary becomes comparable to the timescale of dynamical fluctuations. Using transient optical spectroscopy and femtosecond electron diffraction, we studied a photo-induced transition of a model charge-density-wave (CDW) compound, LaTe3. We observed that it takes the longest time to suppress the order parameter at the threshold photoexcitation density, where the CDW transiently vanishes. This finding can be quantitatively captured by generalizing the time-dependent Landau theory to a system far from equilibrium. The experimental observation and theoretical understanding of dynamical slowing down may offer insight into other general principles behind nonequilibrium phase transitions in many-body systems.

*U.S. Department of Energy 
Gordon and Betty Moore Foundation 
Skoltech-MIT Joint Next Generation Program

10:24AM A14.00013: Superconductivity in Weyl semimetal Mo$_x$W$_{1-x}$Te$_2$ driven by high pressure  
RABIN DAHAL (Presenter), LIANGZI DENG, NARAYAN POUDEL, MELISSA GOOCH, ZHENG WU, CHING-WU CHU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204, USA — Tungsten ditelluride and molybdenum ditelluride have attracted tremendous attention due to recent discoveries of the Weyl semimetal state, large unsaturated magnetoresistance, and superconductivity in these materials. Mo$_x$W$_{1-x}$Te$_2$ is reported to be a Weyl semimetal with x = 0.25 and Weyl semimetal states are also predicted to exist in other doping. We carried out systematic high pressure measurements on Mo$_x$W$_{1-x}$Te$_2$ single crystals with doping via homemade BeCu clamp cells. High-quality single crystals of Mo$_x$W$_{1-x}$Te$_2$, with x = 0.25, 0.60, 0.90, were grown by chemical vapor transport method which were then characterized by X-ray diffraction and energy dispersive X-ray spectroscopy. In Mo$_{0.25}$W$_{0.75}$Te$_2$, a structural transition was observed under pressure 12.3 kbar with no signature of superconductivity at temperature down to 1.3 K and under pressure up to 17 kbar. In Mo$_{0.60}$W$_{0.40}$Te$_2$ and Mo$_{0.90}$W$_{0.10}$Te$_2$, structural transitions were observed at ambient pressure. Superconductivity appears in Mo$_{0.60}$W$_{0.40}$Te$_2$ with an onset T$_c$ of 1.7 K under 8.4 kbar and in Mo$_{0.90}$W$_{0.10}$Te$_2$ with an onset T$_c$ of 1.4 K under 3.9 kbar. T$_c$ continuously increases as pressure increases up to 17 kbar, the highest pressure we applied. Measurements under higher pressure range using diamond anvil cells are in progress.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A15 DMP: 2D Materials (Semiconductors) -- Monolayers BCEC 154 - Vinod Sangwan, Northwestern University
8:00AM A15.00001: Shortwave Coulomb excitations and local-field effects in monolayer transition-metal dichalcogenides.*  
HANAN DERY (Presenter), DINH VAN TUAN, University of Rochester, BENEDIKT SCHARF, Physics, university of Wuerzburg, IGOR ZUTIC, Physics, State University of New York at Buffalo — Many-body interactions in monolayer transition-metal dichalcogenides are strongly affected by local-field effects and their spin-split band structure. The former is caused by a strong contribution of umklapp processes to Coulomb excitations between the time-reversed valleys, where the effect is stronger for conduction-band electrons because of the nature of their atomic orbital. As a result, the blueshift of the neutral exciton, $X_0$, in electron-doped samples can be larger than 10 meV when the electron density increases from 0 to $5 \times 10^{12}$ cm$^{-2}$, while the blueshift in hole-doped samples is nearly absent. We develop an analytical theoretical model that elucidates the important role played by intervalley plasmons and local-field effects. We compute the energy shift of $X_0$ as a function of charge density and show that similar to experiment, the blueshift is evident only in electron-doped conditions, and that it is stronger in MoSe$_2$ than in WSe$_2$ due to differences in their band ordering and direct vs indirect exciton energies. In addition, the theory elucidates the observed emergence of exciton-plasmon peak in electron-doped WSe$_2$.

*This work is supported by the Department of Energy, Basic Energy Sciences (Grant No. DE-SC0014349), and the National Science Foundation (Grant No. DMR-1503601)

8:12AM A15.00002: Impact of dielectric environment on exciton binding energy in monolayer WS$_2$ and WSe$_2$*  
WEI-TING HSU (Presenter), JIAMIN QUAN, CHUN YUAN WANG, Department of Physics, The University of Texas at Austin, USA, LI-SHUAN LU, WEN-HAO CHANG, Department of Electrophysics, National Chiao Tung University, Taiwan, XIAOQIN (ELAINE) LI, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin, USA — The large exciton binding energy in monolayer transition metal dichalcogenides (TMDs) was determined recently. The robust excitons open a venue to explore the exciton physics such as Bose-Einstein condensation at room temperature. Recent reports further demonstrated the Coulomb engineering via dielectric environment based on a few-layer graphene. However, due to the conducting nature, quenching of optical transitions is often unavoidable. Thus, it is desirable to show the tunability using insulating dielectrics. Here we investigate the impact of dielectric environment on exciton binding energy and quasiparticle bandgap in monolayer WS$_2$ and WSe$_2$ by exciton Rydberg spectroscopy. The dielectric constant is systematically varied from $\kappa = 1.49$ to 3.82. We found that, with increasing $\kappa$, the exciton binding energy and quasiparticle bandgap exhibit significant reductions. We found the model using nonlocally-screened Keldysh potential captures the results very well. Our work validates the applicability of Keldysh model which can be used to design TMD-based optoelectronic devices in different dielectric media.

*Supported by Welch (F-1672), MRSEC (DMR-1720595), NSF (EFMA-1542747, DMR-1808751), AOARD (FA2386-18-1-4097). W.-T.H. acknowledges the support by MOST of Taiwan (107-2917-I-564-010).

8:24AM A15.00003: Band Symmetries in Two-Dimensional Materials*  
EDWARD ARIS FAJARDO (Presenter), ROLAND WINKLER, Northern Illinois University — The symmetries of the energy bands are of fundamental importance for understanding many properties of a material. Here we develop a general scheme to determine the irreducible representations of Bloch functions for a given wave vector. Using a tight-binding picture and exploiting the fact that the atomic orbitals are localized in the vicinity of the atomic sites, we demonstrate that this problem can be factorized into one characterizing the atomic orbitals times one characterizing the crystal-periodic plane waves. Each of these subproblems permits a universal classification, independent of the details of a particular crystal structure. We apply this general scheme to two-dimensional materials including transition metal dichalcogenides (such as MoS$_2$, WS$_2$, MoSe$_2$, and WSe$_2$) and few-layer graphene. We demonstrate that the irreducible representations characterizing the energy bands are not always uniquely determined by the symmetry of a crystal structure. However, we also show that this ambiguity does not affect observable physics such as selection rules or the effective Hamiltonians for Bloch states that can be derived by means of the theory of invariants.

*This work was supported by the NSF under Grant No. DMR-1310199.
8:36AM A15.00004: Direct observation and gate manipulation of dark trions in monolayer WSe$_2$  

CHUN HUNG LUI (Presenter), JEREMIAH VAN BAREN, University of California, Riverside, ZHENGGUANG LU, National High Magnetic Field Laboratory, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, DMITRY SMIRNOV, National High Magnetic Field Laboratory, CHUN HUNG LUI, University of California, Riverside — Dark trions, the bound states between a dark exciton and an electron (hole), are intriguing entities with novel applications, because their long lifetime and finite net charge allow us to efficiently control the excitonic dynamics by electric field. Detection of dark trions is, however, exceedingly challenging due to their optical inactivity. Prior research required indirect detection techniques, such as altering their spins with in-plane magnetic field and coupling to surface plasmons. Here we report the direct observation and gate manipulation of intrinsic dark trions in monolayer WSe$_2$. By using ultraclean WSe$_2$ devices encapsulated by boron nitride, we can directly resolve the weak photoluminescence of spin-forbidden dark trions and continuously tune between negative and positive charged dark trions with electrostatic gating. We also reveal their spin triplet configuration and distinct valley emission by their characteristic Zeeman splitting under magnetic field. The dark trions exhibit large binding energy (14-16 meV) and narrow line width (2.5 meV), signifying their high stability and long lifetime. Such robust and directly detectable dark trions provide a crucial component to realize electrically controllable trion transport in two-dimensional materials.

8:48AM A15.00005: Observation of trion Rydberg states in monolayer MoSe$_2$  

CHUN HUNG LUI (Presenter), ERFU LIU, JEREMIAH VAN BAREN, University of California, Riverside, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, HONGYI YU, WANG YAO, Department of Physics and Center of Theoretical and Computational Physics, University of Hong Kong, ZHENGGUANG LU, DMITRY SMIRNOV, National High Magnetic Field Laboratory — Trions in monolayer transition metal dichalcogenides (TMDs) attract much attention due to their large binding energy (20 ~ 50 meV). The high stability of trions makes them possible to form excited states. Here we report the observation of trion Rydberg states in monolayer TMD. By measuring the photoluminescence of ultraclean boron-nitride-encapsulated MoSe$_2$, we reveal the first and second excited states of trions. The excited-state trions exhibit much stronger interaction with the Fermi sea as well as higher valley polarization and coherence than the ground-state trions. The results reveal rich physics of few-body quantum states in two-dimensional systems.

9:00AM A15.00006: The Born-Oppenheimer approximation in graphene: A time-dependent perspective*  

VAIBHAV MOHANTY (Presenter), ERIC JOHNSON HELLER, Harvard University — In graphene, electron-phonon interactions are known to play an important role in the loss of electronic wavefunction character and relaxation processes following photoexcitation. We model electronic interactions with nuclear vibrations from a microscopic, time-dependent perspective. Utilizing a time-dependent tight-binding Hamiltonian for the electronic degrees of freedom, we numerically determine the time-evolved electronic wavefunction in the presence of classical nuclei vibrating along normal modes. We examine the solutions by comparing them to those predicted within the adiabatic Born-Oppenheimer (ABO) approximation. We find that, for electronic states on energetically isolated potential energy surfaces, the adiabatic Born-Oppenheimer (ABO) approximation offers an accurate picture of time-evolution. But, in the presence of avoided crossings, the ABO approximation quickly breaks down as the electronic wavefunction becomes a superposition of ABO basis states. Moreover, electronic character is preserved over several vibrational periods for a finite lifetime, indicating highly diabatic time-evolution.

*Research supported in part by the Harvard Program for Research in Science and Engineering and the Herchel Smith-Harvard Undergraduate Science Research Program.

9:12AM A15.00007: Transport and photoluminescent characterization of high-quality single layer WSe$_2$ devices  

KATERYNA PISTUNOVA (Presenter), LUIS JAUREGUI, ANDREW Y JOE, KRISTIAAN DE GREVE, ANDREY SUSHKO, Harvard University, DANIEL A RHODES, JAMES HONE, Columbia University, HONGKUN PARK, MIKHAIL LUKIN, PHILIP KIM, Harvard University — Single layer semiconducting transition metal dichalcogenides (TMD) are direct band gap semiconductors that exhibit a variety of novel phenomena, ranging from valley hall effect to highly correlated electron physic. However, the transport studies of many of these phenomena have been hindered by low mobility, defective TMD materials. While the defect density of commercially grown TMD can be higher than 0.1%, in this work we use flux grown TMD samples with defect density significantly reduced to 0.01%. We report unprecedentedly high hole mobility values of up to 30,000 cm$^2$/V.s in single layer (1L) WSe$_2$ encapsulated in between hBN single crystals. Unlike that of conventional semiconductors, mobility of flux grown WSe$_2$ devices increases with reduced carrier density, indicating that mobility is not dominated by charged impurities. We find the quantum scattering time, $\tau_q$, to be ~400 ps, similar to $\tau_q$ in graphene devices. Moreover, by preforming photoluminescence spectroscopy, we find extremely sharp exciton linewidth (>1 meV) and other optical features such as dark excitons and biexcitons.
The stable trion states in 2D WSe$_2$ monolayer

SHALVA TSIKLAURI (Presenter), Science, The City University of New York-BMCC, ROMAN KEZERASHVILI, Physics, City Tech and Graduate Center The City University of New York — We study the binding energies of negatively (two electron and one hole) and positively (one electron and two holes) charged trions in suspended two-dimensional monolayer of WSe$_2$ in the framework of effective-mass model by employing the method of hyperspherical harmonics in configuration space [1,2]. The binding energies of trions are calculated using the Ritova-Keldysh potential. Trion fine structure based on formation of intravalley trions in spin singlet (S=1/2) state and intervalley trions in triplet (S=3/2) state is addressed. Our calculations show that those state are stables. To understand the importance of dielectric screening on the formation of trions, we perform calculations of the binding energy for WSe$_2$ placed in three different dielectric environments: supported on an SiO$_2$ substrate, supported on an h-BN substrate, and encapsulated by h-BN, and compare these results with the case of suspended WSe$_2$ binding energy. The analysis and comparison of our results for the binding energies of trions with those calculated via different theoretical methods and experimental data are presented.


Revealing the Unusual Excitonic Complexes in BN Encapsulated Monolayer WSe$_2$

ZHIPENG LI (Presenter), TIANMENG WANG, Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, ZHENGUANG LU, Department of Physics, Florida State University, CHENHAO JIN, Physics Department, University of California, Berkeley, YANWEN CHEN, YUZE MENG, ZHEN LIAN, Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, TING CAO, Geballe Laboratory for Advanced Materials, Stanford University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, SHENGBAI ZHANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, DMITRY SMIRNOV, National High Magnetic Field Lab, SUFEI SHI, Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute — Strong Coulomb interactions in single-layer transition metal dichalcogenides (TMDs) result in the emergence of strongly bound excitons, trions and biexcitons. These excitonic complexes possess the valley degree of freedom, which can be exploited for quantum optoelectronics. However, in contrast to the good understanding of the exciton and trion properties, the binding energy of the biexciton remains elusive, with theoretical calculations and experimental studies reporting discrepant results. In this work, we present the high-quality low-temperature photoluminescence (PL) spectra of BN encapsulated monolayer WSe$_2$, which directly reveals the biexciton state only exists in charge neutral WSe$_2$ and one free electron binds to a biexciton and forms the trion-exciton complex, the binding energy is $\sim$17 meV and $\sim$49 meV for biexciton and trion-exciton complex, respectively. The magneto-PL also reveals unambiguous evidence of the dark exciton. The improved understanding of the biexciton, trion-exciton complexes and other excitonic complexes improve our understanding of the many-body interaction in TMDs, promising novel application in low-dimensional quantum optoelectronics.

*The Air Force Office of Scientific Research (Grant FA9550-18-1-0312);

Edge states of two-dimensional materials

GEORGIOS KOPIDAKIS (Presenter), GEORGIOS VAILAKIS, DAPHNE DAVELOU, IOANNIS N. REMEDIAKIS, Materials Science and Technology, University of Crete — Single layers of atomic thickness such as graphene, molybdenum disulfide and other transition metal dichalcogenides (TMDs) display unique electronic properties which depend on composition, dimensionality, strain, defects, chemical modification and nanostructurering, so that they may be engineered for specific applications. Intensive efforts to use two-dimensional (2D) materials in a wide range of technologies highlight the importance of edges in nanoribbons and nanoflakes. We will present theoretical results based on density functional theory calculations combined with simple models which clarify the effect of strain on TMD electronic and dielectric properties [1], the role of the metallic edge states in these otherwise semiconducting materials, especially in quasi-1D and 0D systems, and nanostructure stability [2]. The common origin of the edge states in TMD and graphene nanoribbons, as well as their main differences, will also be discussed.


*Financial support from the Research Committee of the University of Crete (KA 10120) is gratefully acknowledged.
10:00 AM A15.00011: Quasiparticle and optical properties of hexagonal boron nitride: from monolayer to bulk *
WEIYI XIA (Presenter), University at Buffalo, The State University of New York, WEIWEI GAO, Center for Computational Materials, University of Texas at Austin, PEIHONG ZHANG, University at Buffalo, The State University of New York — Hexagonal boron nitride (h-BN), an emerging building block for van der Waals heterostructures, has become a research focus in recent years. Interesting, some of the most fundamental aspects of this material are still not fully understood. For example, there are still debates on whether the fundamental band gap of bulk h-BN is direct or indirect, and, to the best of our knowledge, the quasiparticle band gap of monolayer h-BN has not been accurately determined. In this talk, we will present fully converged GW+BSE results for monolayer, bilayer and bulk h-BN, aiming to resolve some of the controversies and illustrate the effects of dielectric screening and interlayer interaction on the quasiparticle and optical properties of this material.

*This work is supported in part by the NSF (Grant No. DMR-1506669 and DMR-1626967) and NSFC (Grant No. 11328401 and 11628407).

10:12 AM A15.00012: Origins of spectral doublets from 2D semiconductors embedded in optical microcavities *
TREVOR LAMOUNTAIN (Presenter), Applied Physics Program, Northwestern University, Evanston, IL, United States, HONGFEI ZENG, Physics and Astronomy, Northwestern University, Evanston, IL, United States, PUFAN LIU, Materials Science and Engineering, Northwestern University, Evanston, IL, United States, NATHANIEL STERN, Physics and Astronomy, Northwestern University, Evanston, IL, United States — Recent progress embedding atomically-thin materials such as monolayer transition metal dichalcogenides (TMDs) in microcavities has enabled applications such as nanolaser devices as well as novel regimes of polarization-sensitive exciton-polaritons [1]. Compared to the highly optimized III-V semiconductors typically used in microcavities, TMDs exhibit significantly more spatial inhomogeneity as well as additional tears, strains, and chemical contaminants introduced by the mechanical layer transfer process. We show how the spatial inhomogeneity of WS2 and MoS2 can produce spectral doublets that mimic the upper and lower polariton branches. We identify common pitfalls for misidentifying these doublets, as well as more robust measurements that can be used to distinguish the anti-crossing feature of exciton-polaritons.


*Work supported by the U.S. Department of Energy (BES DE-SC0012130) and the NSF MRSEC program (DMR-1720139).

10:24 AM A15.00013: Quantum yield engineering of quantum emitters in WSe2 by deterministically coupling to plasmonic nanocavities
YUE LUO (Presenter), GABRIELLA D. SHEPARD, Stevens Institute of Technology, JENNY V. ARDELEAN, DANIEL A RHODES, BUMHO KIM, KATAYUN BARMAK, JAMES HONE, Mechanical Engineering, Columbia University, STEFAN STRAUF, Stevens Institute of Technology — Solid-state single-quantum emitters are important resources for on-chip photonic quantum technologies. Efficient cavity-emitter coupling is required to realize quantum networks application. Recent studies explored the scalability aspect via spatially defined stressors to create quantum emitters from monolayer transition metal dichalcogenide semiconductor. Yet the low quantum yield of those quantum emitters is a crucial challenge to any real applications. Here we present a deterministic approach to achieve Purcell-enhancement at lithographically defined locations using the sharp corners of a Au nanocube for both electric field enhancement and to deform a two-dimensional material. This nanoplasmatic platform allows for studying the same quantum emitter before and after coupling. We reached record high quantum yield to near-unity in combination with flux grown high quality material that has naturally low non-radiative defect centers1.

Reference:
10:36AM A15.00014: Electronic Dipole Spin Resonance of 2D Semiconductor Spin Qubits  MATTHEW BROOKS
(Presenter), GUIDO BURKARD, University of Konstanz — Monolayer transition metal dichalcogenides (TMDs) offer a novel two-
dimensional platform for semiconductor devices. One such application, whereby the added low dimensional crystal
physics (i.e. optical spin selection rules) may prove TMDs a competitive candidate, is quantum dots as qubits. The band
structure of TMD monolayers offers a number of different degrees of freedom and combinations thereof as potential
qubit basis, primarily electron spin, valley isospin and the combination of the two due to the strong spin orbit coulping
known as a Kramers qubit. Pure spin qubits in monolayer MoX$_2$ (where $X = S$ or Se) have been shown to be achievable by
energetically isolating a single valley and tuning to a spin degenerate regime within that valley by a combination of a
sufficiently small quantum dot radius and large perpendicular magnetic field. Within such a TMD spin qubit, we
theoretically induce and analyse single qubit rotations with an electric dipole spin resonance. We employ a rotating wave
approximation within a time dependant Schrieffer-Wolf approximation to derive analytic expressions for the Rabi
frequency of single qubit oscilations, and compare this result to more exact numerics, as to find optimal operational
regimes.

10:48AM A15.00015: Magneto-spectroscopy probe of exciton-electron interactions in monolayer MoSe$_2$
ZHENGGUANG LU (Presenter), National High Magnetic Field Laboratory, ZHIPENG LI, TIANMENG WANG, YUZE MENG, Rensselaer
Polytechnic Institute, YUXUAN JIANG, National High Magnetic Field Laboratory, SUFEI SHI, Rensselaer Polytechnic Institute, DMITRY
SMIRNOV, National High Magnetic Field Laboratory — Coulomb interaction driven many-body effects are expected to modify
significantly the quasiparticles properties in monolayer transition metal dichalcogenides at high carrier densities. Here we
report on low temperature magneto-photoluminescence and broadband reflection contrast measurements on high
quality monolayer MoSe$_2$ over a wide doping range. A valley g-factor around 4 is measured in the low-density regime,
which is consistent with the value deduced from the single particle picture. As the carrier density increases, one can access
the strongly interacting regime and observe a pronounced change of the valley magnetic response. The observed strong
modification of the valley g-factor in highly doped MoSe$_2$ will be discussed and compared to the previously reported
results on WSe$_2$ [1].

[1]. PRL 120, 066402 (2018)

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A16 DMP: Transport in Nanostructures -- Thin Films, Heterostructures and
Nanodevices  BCEC 155 - Jean Heremans, Virginia Tech - Tag(s): Focus

8:00AM A16.00001: Pascal-liquid phases in ballistic one-dimensional LaAlO$_3$/SrTiO$_3$ channels* [Invited]  JEREMY LEVY
(Presenter), MEGAN BRIGGEMAN, MICHELLE TOMCZYK, BINBIN TIAN, University of Pittsburgh, HYUNGWOO LEE, JUNG-WOO
LEE, University of Wisconsin-Madison, YUCHI HE, Carnegie Mellon University, ANTHONY TYLAN-TYLER, MENGCHEN HUANG,
University of Pittsburgh, CHANG-BEOM EOM, University of Wisconsin-Madison, DAVID PEKKER, ROGER MONG, PATRICK IRVIN,
University of Pittsburgh — The challenge of understanding strongly interacting composite fermionic phases of matter spans
many fields in physics, ranging from neutron stars to solid-state materials to quark-gluon plasmas. We report
experimental evidence of a new family of degenerate quantum liquids formed from bound states of $n = 2, 3, 4, ...$
 electrons, which are stabilized within quasi-one-dimensional electron waveguides formed at the LaAlO$_3$/SrTiO$_3$ interface.
The key signature of this phase is the existence of quantized conduction that follows a characteristic sequence within
Pascal's triangle: (1, 3, 6, 10, 15,...), where is the electron charge and is the Planck constant. The ability to create and
investigate composite fermionic phases opens new avenues for the investigation of strongly correlated quantum matter.

*This work is supported in part by a Vannevar Bush Faculty Fellowship ONR grant N00014-15-1-2847 (J.L.) and the Charles
E. Kaufman Foundation (D.P). The work at University of Wisconsin-Madison (design and synthesis of thin film
heterostructures) was supported by the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences,
under award number DEFG02-06ER46327.
YANG HU (Presenter), YUHE TANG, DENGYU YANG, YUN-YI PAI, JIANAN LI, University of Pittsburgh, HYUNGWOO LEE, JUNG-WOO LEE, CHANG-BEOM EOM, University of Wisconsin–Madison, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — The 2D electron gas at the LaAlO$_3$/SrTiO$_3$ interface can be patterned using conductive atomic force microscope (c-AFM) lithography [1], which has been used to create quantum dots and single electron transistors [2]. We aim to use this technique to create an on-demand single-electron source by sketching a linear array of quantum dots and applying out-of-phase excitation across the dot array. We will discuss both double-dot and triple-dot devices and their associated electron tunneling phenomenon and issues related to the individual tunabilities of the dots.


*JL acknowledges a Vannevar Bush Faculty Fellowship, funded by ONR (N00014-15-1-2847). C-BE acknowledges support from NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-4046).
9:24AM A16.00006: Stark Control of Electrons Across Interfaces*  ANTONIO GARZÓN-RAMÍREZ (Presenter), IGNACIO FRANCO, University of Rochester — We introduce a laser control scenario to transiently transform an insulating heterojunction into a conducting one on a femtosecond timescale. The scenario is based on opening Landau-Zener quantum tunneling channels for electron transfer between two adjacent semiconductors via Stark shifts induced by non-resonant lasers of intermediate intensity (non-perturbative but non-ionizing). Through quantum dynamics simulations we demonstrate the robustness of the approach and its utility for controlling electron dynamics at interfaces.


*This material is based on the work supported by the National Science Foundation under No. CHE-1553939.

9:36AM A16.00007: Photothermoelectric effects at and near individual grain boundaries in gold*  CHARLOTTE EVANS (Presenter), Physics and Astronomy, Rice University, RUI YANG, RACHEL TRAYLOR, Electrical Engineering, Stanford University, MAHDIYEH ABBASI, Electrical and Computer Engineering, Rice University, XIFAN WANG, Materials Science, Rice University, STEPHANIE BOHAICHUK, JONATHAN FAN, Electrical Engineering, Stanford University, DOUGLAS NATELSON, Physics and Astronomy, Rice University — Thermoelectricity is best known for thermocouples, where a voltage is generated when heating the interface of two materials with different Seebeck coefficients. In metals, the electronic Seebeck coefficient depends on the electrical conductivity which can be manipulated at the nanoscale to create single metal thermocouples. We will present scanning photothermoelectric measurements of the simplest single metal thermocouple: a single grain boundary between two single-crystal gold nanowires. Unlike a traditional thermocouple, where heating the grain boundary results in the largest voltage, the photovoltage as a function of laser position changes polarity at the grain boundary, varying on length scales much larger than the laser size. Modeling suggests that these results are consistent with long-scale Seebeck coefficient gradients within the crystals. Electron back-scatter diffraction relates the voltages to the relative crystallographic orientation across the boundary and x-ray probes provide insight of strain within the device. We propose how thermovoltages can probe areas of impurities, strain, and other intrinsic irregularities that may not otherwise be detected using traditional electronic transport measurements.

*Robert A. Welch Foundation award C-1636, and NSF ECCS-1704625

9:48AM A16.00008: Hierarchical Kinetics in 1/f Noise in Amorphous and Nanocrystalline Semiconductor Thin Films*  BRENDA KNAUBER (Presenter), School of Physics and Astronomy, University of Minnesota, MOHAMMAD ALI ESLAMISARAY, Department of Mechanical Engineering, University of Minnesota, JAMES KAKALIOS, School of Physics and Astronomy, University of Minnesota — We report studies of conductance fluctuations in hydrogenated amorphous germanium (a-Ge:H) that have an inverse frequency (1/f) spectral density with non-Gaussian statistics, as reflected in (1) histograms of the noise power per octave that are not described by Gaussian distributions, (2) strong correlations of the noise power in frequency-space and (3) power-law second spectra. In particular, histograms of the 1/f noise power per octave for a-Ge:H are well described by a log-normal distribution. The correlation coefficients across frequencies are non-zero and larger than expected for independently modulated fluctuators, and grow with averaging time with a logarithmic time-dependence. In contrast, the 1/f noise for polycrystalline Ge, and free-standing nanocrystalline thin films display Gaussian statistics. These results are discussed in terms of a model of filamentary conduction, where the conductance is modulated by hydrogen motion governed by hierarchical kinetics.

*This work was partially supported by NSF grants DMR-1608937 and PHYS-1344251, the NINN Characterization Facility, the Minnesota Nano Center and the University of Minnesota.
10:00AM A16.00009: Quantum dynamics of single-photon detection using functionalized quantum transport
electronic channels*  CATALIN SPATARU (Presenter), FRANCOIS LEONARD, Sandia National Laboratories California — Single photon detectors have historically consisted of macroscopic-sized materials, but recent experimental and theoretical progress opens new approaches based on nanoscale and molecular electronics. Here we present a theoretical study of photodetection in a system composed of a quantum electronic transport channel functionalized by a photon absorber. Notably, the photon field, absorption process, transduction mechanism, and measurement process are all treated as part of one fully-coupled quantum system, with explicit interactions. Using non-equilibrium, time-dependent quantum transport simulations, we reveal the unique temporal signatures of the single photon detection process, and show that the system can be described using optical Bloch equations, with a new non-linearity as a consequence of time-dependent detuning caused by the back-action from the transport channel. We compute the photodetector signal-to-noise ratio and demonstrate that single photon detection is possible for realistic parameters.

*This research was developed with funding from the Defense Advanced Research Projects Agency. Sandia National Laboratories is a multimission laboratory managed by NTI, a wholly owned subsidiary of Honeywell International, Inc., for the US DOE’s NNSA under contract DE-NA-0003525.

10:12AM A16.00010: Cross-plane thermal conductance of Au/graphene/Au heterojunction*  XIAOHUI QIU (Presenter), Chinese Academy of Sciences — Thermal management has become a critical issue for microelectronics, as the characteristic sizes of these devices shrink into the nanometer region. Interesting phenomena were observed for heat conduction through ultrathin interfacial layers, such as thickness dependent thermal boundary conductivity. Here, we use the Frequency Domain Thermoreflectance technique to investigate the heat conduction across the heterojunction composed of few-layer graphene as the interfacial layer between gold. By varying the graphene layer number to control the thickness of the interfacial layer, we measure the thickness dependent thermal conductance across this sandwiched structure. We found that electron transmission dominates the thermal conductance for monolayer graphene, and a two-orders of magnitude decrease in thermal conductance through bilayer graphene. For more layers graphene, phonon thermal conductivity is suggested to be the major contributor.

*This work was supported by the National Natural Science Foundation of China (Project No. 21425310) and CAS-PKU Pioneer Cooperation Team.

10:24AM A16.00011: Quantum oscillations under photoexcitation involve direct and indirect excitons and quantum photocapacitance in GaAs/AlAs/InAs p-i-n diode*  AMIT BHUNIA ( Presenter), Department of Physics, Indian Institute of Science Education and Research, Pune, India, MOHAMED HENINI, School of Physics and Astronomy, University of Nottingham, SHOUVIK DATTA, Department of Physics, Indian Institute of Science Education and Research, Pune, India — We explore the quantum dynamics at the interface of a single barrier GaAs/AlAs p-i-n device having InAs quantum dots embedded inside AlAs layer. We observe systematic quantum oscillations in photocapacitance measurements when the sample is optically excited at 10 K. Two sharp peaks in the photocapacitance spectra imply the presence of direct and indirect excitons formed inside the InAs quantum dot and at the interface of quantum dot and the triangular GaAs quantum well, respectively. Spectral peak shifts with increasing applied bias complies with the change of energy levels of triangular quantum well due to effective electric field. Presence of two-dimensional electron and hole gases near the GaAs/AlAs interface certainly point towards the involvement of quantum capacitance. In addition, we also discuss how the formation of excitonic dipoles affects such quantum capacitance. Moreover, periodic variation of negative differential resistance in photocurrent oscillations also correlate with photoconductance oscillations. Understanding the quantum dynamics of carriers involving quantum capacitance and negative differential resistance will help us to explain the many-body physics of these interfacial excitons and its applications.

*AB thankful to DST, India for Inspire PhD Fellowship.
non-classical noise and light emission of an ac-driven tunnel junction  HONGXIN ZHAN (Presenter), GIANLUCA RASTELLI, WOLFGANG BELZIG, Fachbereich Physik, Universitaet Konstanz — The non-symmetrized noise is crucial for the analysis of light emission in nanojunctions. The latter represent non-classical photon emitters whose description requires a full quantum approach [1]. It was found experimentally that light emission can occur with a photon energy exceeding the applied dc voltage [2], which intuitively should be forbidden due to Pauli principle. This overbias light emission cannot be described by the single-electron physics, but can be explained by 2-electron or even 3-electron process, correlated by a local antenna mode in analogy to the well-known dynamical Coulomb blockade (DCB) [3]. Here, we obtain the non-symmetrized noise for junctions driven by an arbitrarily shaped periodic voltage. We find that when the junction is driven, overbias light emission occurs and exhibits intriguing different features compared to the dc case. For example, multiple peaks appear at integers of the ac driving frequency. Our work generalizes the DCB theory to light emission in driven tunnel junctions and opens the avenue to engineered quantum light sources, which can be tuned purely by applied voltages.

References:
1. M. H. Devoret et al. PRL 1990
2. G. Schull et al. PRL 2009
3. F. Xu et al. PRL 2014, PRB 2016; P.-J. Peters et al. PRL 2018

Long-Range Frictional Drag in Coupled LaAlO3/SrTiO3 Nanowires*  YUHE TANG (Presenter), ANTHONY TYLAN-TYLER, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNG-WOO LEE, Department of Materials Science and Engineering, University of Wisconsin-Madison, MICHELLE TOMCZYK, MENGCHEN HUANG, Department of Physics and Astronomy, University of Pittsburgh, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — Frictional drag, where current in one nanowire induces a voltage across a nearby nanowire, is a powerful tool to study electron interactions. Here we investigate long-range electron interactions in coupled nanowires at the LaAlO3/SrTiO3 interface via frictional drag. In the normal state (B > 0.3T) regime, the antisymmetric drag resistance of double-wire devices is independent of their separation, ruling out the Coulomb interaction as the dominant coupling mechanism. In triple-wire devices this separation independence is corroborated. In the superconducting (B < 0.3T, T < 300mK) regime, a symmetric component is identified in the drag resistance and its separation independence also shows the coupling is predominantly non-Coulombic. These results provide strong evidence for a new long-range non-Coulombic electron interaction that must be accounted for in description of electron transport at oxide interfaces.

*Work at the University of Pittsburgh was supported by funding from the DOE Office of Basic Energy Sciences under award number DOE DE-SC0014417. Work at the University of Wisconsin was supported by funding from the DOE Office of Basic Energy Sciences under award number DE-FG0206ER46327. Theoretical portion of this work (AT-T) supported in part by ONR N0001415-1-2847.

Monday, March 4, 2019 8:00 AM - 10:24 AM

Session A17 DCOMP: Matter in Extreme Environments: Energetic Materials  BICEC 156A - Maosheng Miao, California State University, Northridge - Tag(s): Focus

Scalable Atomistic Simulations of Energetic Materials*  [Invited] AIICHIRO NAKANO (Presenter), RAJIV KALIA, PRIYA VASHISHTA, University of Southern California — We have developed an extension of the divide-and-conquer algorithmic framework called divide-conquer-recombine to make quantum molecular dynamics (QMD) and reactive molecular dynamics (RMD) simulations scalable on emerging exascale supercomputers and beyond. On today's supercomputing platform, for instance, the framework has achieved over 98% of the perfect speedup on 786,432 IBM Blue Gene/Q processors for 40 trillion electronic degrees-of-freedom QMD in the framework of density functional theory and 68 billion-atom RMD. Production simulations on energetic materials include: (1) dynamic phase transition, crossover in anisotropic mechanochemistry and multistage reaction pathways in energetic crystals; and (2) reaction dynamics and enhanced energetic performance of metallic-nanoparticle/graphene composites.

*Part of the work was supported by the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607.
Detonation on a tabletop in nitromethane: effects of sensitizers and desensitizers

MITHUN BHOWMICK (Presenter), ERIN J NISSEN, DANA DLOTT, University of Illinois at Urbana-Champaign — We have developed a method to study shock to detonation process on a tabletop with high temporal and spatial resolution. Here we present effects of additives on nitromethane (NM) detonation studied with optical pyrometry, photon doppler velocimetry, and high-speed video photography. Addition of ethylenediamine (EDA, 1% by wt.) reduces the detonation threshold from 20 GPa to 14 GPa of input pressures, while addition of acetone (up to 30% by wt.) inhibits the reaction and detonation is not at all observed for up to 20 GPa input pressure. With the help of optical pyrometry and high-speed videos, thermal properties of emission from the above mixtures were probed. Detonation experiments often measure the detonation shock wave using an optical window contacted to the explosive. We measured NM detonation in 9 different window materials and found that polycrystalline materials such as LiF are somewhat better than glasses, and both are much better than polymers, reported in earlier works.


Sub-nanosecond carbon condensation under ultrafast shock compression of cryogenic liquid carbon monoxide

MICHAEL ARMSTRONG (Presenter), REBECCA LINDSEY, NIR GOLDMAN, I-FENG W. KUO, TIAN LI, ELISSAIOS STAVROUL, JOSEPH MICHAEL ZAUG, SORIN BASTEA, Lawrence Livermore National Laboratory — The detonation of negative oxygen-balance explosives typically results in the formation of carbon condensates, including nano-onions and nano-diamonds. Although the production of carbon nano-condensates can occur via detonation, the carbon chemistry required to form such products does not require detonation chemistry per se: a negative oxygen-balance organic reactant and high pressure and temperature conditions are likely sufficient to condense nanocarbon. Furthermore, although carbon chemistry during detonation is thought to require 10-100s nanosecond time scales, simulations suggest that condensation of carbon can occur on nanosecond or sub-nanosecond time scales. To explore these fundamental issues, here we present the results of experiments and simulations of ultrafast shock compression of a simple negative oxygen-balance reactant, cryogenic liquid carbon monoxide.

Chemical behavior of strontium and magnesium oxalates at high-pressure

ISKANDER G BATYREV (Presenter), JENNIFER A CIEZAK-JENKINS, US Army Research Lab., Aberdeen Proving Ground, MD 21005, MICHAEL GOJKO PRAVICA, Department of Physicis, Univ. of Nevada Las Vegas, NV 89154 — We report theoretical and experimental investigations on the structure of strontium and magnesium oxalates at high-pressure. Both systems have shown progress in the generation of CO2 and in the synthesis of high-energy polymeric carbon monoxide after X-ray irradiation. It has been previously proposed that X-ray irradiation may facilitate photochemical reactions such as: SrC2O4 +hv -> SrCO3 +CO2 + poly-CO (MgC2O4 +hv -> MgO + CO2 + poly-CO) [1]. Density functional perturbation theory was used to calculate the zone center optical phonons and to identify the vibration modes in term of atomic displacements. The simulations were compared to previous EXAFS and IR spectroscopic studies [1] in an effort to elucidate the chemical structure. Additional calculations of the phonon dispersion and density of states, as well as the electronic band structure were performed to gain better insight into the phase behavior in strontium and magnesium oxalates.

Temperature evolution in plastic bonded explosives during impacts

NISHA MOHAN (Presenter), DARBY J LUSCHER, MARC CAWKWELL, KYLE J RAMOS, Los Alamos National Laboratory — The heterogeneous, polycrystalline structure of plastic-bonded explosives (PBX) leads to temperature localization under impacts. The thermo-mechanical responses of PBXs span processes from dislocation-mediated plasticity at small-scales to interfacial stress wave reflection and diffusion at higher scales. The thermal and deformation localization response under impact of a RDX/estane PBX have been studied using finite element simulations with ABAQUS. The modeling framework combines a dislocation-based, anisotropic, single crystal plasticity model with a visco-elastic constitutive model for estane. We systematically studied how heating arising from wave interactions and localized plasticity in the PBX depends on the impact velocity, slip resistance, grain orientation, position, and proximity to stress concentrators. The broadening of the shock front with increasing run distance by the microstructure of the PBX was found to play an important role in the evolution of temperature in the PBX. Grains with certain orientations produced higher temperatures and larger localized zones. Higher intrinsic resistance to slip restricts the dislocation density growth and thermal localization.
9:24AM A17.00006: Anisotropic Thermal Expansion of CL-20 Polymorphs from Ab initio Molecular Dynamics Simulations* IGOR SCHWEIGERT (Presenter), United States Naval Research Laboratory — Hexanitrohexaazaizowurtizane (CL-20) is a high-density nitramine compound with several known polymorphs. Anisotropic thermal expansion coefficients for different polymorphs are needed to model effects of polymorphic impurities during thermal cycling. In this presentation, I will describe density functional theory (DFT) based molecular dynamics simulations of temperature-dependent lattice constants of the epsilon and gamma polymorphs and compare the results to available experimental data as well as predictions from density functional tight binding and ReaxFF-based molecular dynamics simulations.

*This work was supported by the Office of Naval Research (ONR), both directly (project N0001416WX0003) and through the U.S. Naval Research Laboratory (NRL).

9:36AM A17.00007: High pressure structural study of TATB: Evidence of a structural phase transition.* ELISSAIOS STAVROU (Presenter), BRAD A STEELE, SAMANTHA CLARKE, JOSEPH MICHAEL ZAUG, MATTHEW KROONBLAWD, I-FENG W. KUO,SORIN BASTEA, LAURENCE FRIED, Lawrence Livermore Natl Lab, JESSE SMITH, HPCAT, X-ray Science Division, Argonne National Laboratory, VITALI PRAKAPENKA, ERAN GREENBERG, Advanced Photon Source - Sector-13, Argonne National Laboratory, OLIVER TSCHAUNER, Department of Geoscience, University of Nevada, Las Vegas — High pressure unreacted isothermal equations of state (EOS) for energetic materials are needed for accurate modeling of detonation and shock initiation. EOS determination through conventional powder X-ray diffraction (XRD) experiments is often problematic due to the low-Z of constituent elements (typically CHNO) and the low symmetry of the corresponding crystal structure. To overcome this barrier for TATB, we performed a concomitant powder and single crystal (SC) XRD study. Our SC XRD results reveal a structural phase transition, reported for the first time, towards a monoclinic C-centered structure above 4-5GPa. Experimental results are supported by calculations using the USPEX evolutionary crystal structure prediction algorithm. The phase transition involves a pressure-induced alteration of the stacking of the layers of the TATB molecules. This results to a higher crystal symmetry, from triclinic to monoclinic, without an abrupt change of the volume per formula unit.

*This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344. We thank the high explosives science campaign II research program at LLNL for supporting this study.

9:48AM A17.00008: WITHDRAWN ABSTRACT —

10:00AM A17.00009: Computational design of new fused heterocyclic energetic materials* MAIJA M KUKLA (Presenter), ROMAN TYSHEVSKIY, University of Maryland College Park, ALEKSANDR S. SMIRNOV, Bakhirev Scientific Research Institute of Mechanical Engineering — Linear oxadiazole-based energetic materials exhibit attractive performance and sensitivity characteristics compared to known conventional high energy density materials and are considered as appealing potential candidates to be used as explosives, propellants, and cast-melt ingredients in composite explosives. Despite all advantages of the oxadiazole-based compounds the improvements of their physical and chemical properties are bound by certain limits. It is impossible to create new material with significantly improved parameters by variation of oxadiazole rings within the linear molecule. A further step in enhancing explosive characteristics, i.e. higher performance and lower sensitivity, in heterocycles would be to probe a fused energetic molecules in which a stable (rigid) molecular core is functionalized with appropriate rings (or even combinations of rings). Here we report a systematic study that helps to reveal and optimize structure-property-function relationships in fused heterocyclic energetic materials. We show that arrangement of heterocyclic rings in fused molecules opens new opportunities for design new insensitive energetic materials with high performance.

*This work is funded by ONR (Grant N00014-16-1-2069). We used XSEDE, NERSC, MARCC and UMD supercomputing resources
Probing Equations of State and Novel Phases of Energetic Crystals via First Principles Simulations*  
BRAD A STEELE (Presenter), I-FENG W. KUO, Lawrence Livermore Natl Lab — Energetic crystals are widely used in military and industrial applications. Modeling the shock propagation and initiation of energetic materials rely on the unreacted equation of state which can vary greatly if there is a phase transition. Many current models do not include phase transitions which can be difficult to detect in experiment. Furthermore, most first-principles based models use density functional theory that gives a poor description of dispersion. In this work, pressure-induced phase transitions and equations of state of energetic crystals are investigated using first-principles based approaches ranging from density functional theory to post-Hartree-Fock perturbative methods that give a better description of dispersion. Novel high-pressure phases are probed using crystal structure prediction method USPEX. The feasibility of using perturbative and hybrid methods to predict phase transition pressures is investigated.

*This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344. Thanks to the Laboratory Directed Research and Development Program at LLNL for supporting this study under 18-SI-004.

Monday, March 4, 2019 8:00 AM - 10:24 AM

Session A18 DCOMP DCMP DAMOP: Machine Learning Material and Experimental Data I

8:00AM A18.0001: Unsupervised machine learning of single crystal x-ray diffraction data [Invited]  
JORDAN VENDERLEY (Presenter), MICHAEL MATTY, EUN-AH KIM, Cornell University — Data analysis has become a critical bottleneck in reciprocal spaces studies of single crystal x-ray diffraction. This is because while dramatic leaps in detector technology have enabled the collection of large amounts of data in short amounts of time, a parallel development in data analysis has been lacking. Current approaches for investigating this data often require highly devoted researchers to manually comb through it looking for evidence of new physics. This is time-intensive and increasingly infeasible as datasets continue to grow in size. Here we discuss an unsupervised machine learning approach to studying phase transitions in single crystal x-ray diffraction data. Our method leverages novel techniques for approximate Bayesian inference to identify contributions to the scattering intensity with distinct physical origins. It is highly scalable and employs recent developments in numerical linear algebra for memory efficiency and high speed on parallel computing hardware, such as graphical processing units.

8:36AM A18.0002: X-ray hyperspectral classification of the metal-insulator transition in NdNiO3  
WILLIAM ZHENG (Presenter), ALEXANDER SWINTON MCLEOD, Columbia University, KIRK W POST, University of California San Diego, MATTHIAS HEPTING, MARTIN BLUSCHKE, MATTEO MINOLA, ALEXANDER BORIS, EVA BENCKISER, Max Planck Institute Stuttgart, RAJESH V CHOPDEKAR, ANDREAS SCHOLL, LBNL Advanced Light Source, BERNHARD KEIMER, Max Planck Institute Stuttgart, DIMITRI BASOV, Columbia University — Rare-earth nickelates, such as NdNiO3, belong to a family of strongly correlated electron systems in which the electronic and magnetic properties are strongly coupled: NdNiO3 undergoes a temperature driven first-order Metal to Insulator phase transition (MIT) accompanied by charge-order and spin density wave-order phase transition. During the phase transition, the underlying evolution of the insulating domains are averaged out by the limited spatial resolution of conventional bulk probes but, soft X-ray photoemission electron microscopy (X-PEEM) can be applied in order to elucidate nanoscale heterogeneity. In this work we apply X-PEEM to image cooling and heating MITs and develop machine learning based analysis techniques, mainly Principle Component Analysis (PCA) and Independent Component Analysis (ICA) with k-means classification, to classify thermally evolving metallic and insulating domains. The performance of our suite of classifiers is evaluated in this novel application and we discuss their physical interpretation on the basis of charge ordering through the MIT. This class of tools can be applied to other experimental hyperspectral data to extract the characteristics of coexisting phases from otherwise intractably large datasets.
8:48AM A18.00003: Classifying Grazing Incidence X-ray Scattering Patterns via Convolutional Neural Networks*  
CHARLES MELTON (Presenter), Advanced Light Source, Lawrence Berkeley National Laboratory, SHUAI LIU, University of California Berkeley, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Laboratory, DANIELA USHIZIMA, Lawrence Berkeley National Laboratory — Nano-structured thin films have a variety of applications, such as antireflecting coatings for solar cells, waveguides, gaseous sensors, and piezoelectric devices. Grazing-incidence small-angle X-ray scattering (GISAXS) has become a key technique to determine the morphologies of such thin films. One of the main challenges is to determine the structure information encoded in the data based on scattering patterns alone. We propose a computational scheme that learns the structure of well-defined layers of nanoparticles from GISAXS patterns. We explore this class of thin-film materials in terms of physics-based simulation models and experimental data and apply convolutional neural networks to the simulated data to obtain the encoded information of the morphology. Our classification models categorize millions of simulated scattering patterns with success rates over 94%. In addition, we show how these data-driven models have the potential to decrease analysis time of real scattering patterns from experiment.

*Supported by the Center of Advanced Mathematics for Energy Research Applications (CAMERA) through the Office of Science, DOE, No. DE-AC02-05CH11231, and the National Energy Research Scientific Computing Center (NERSC), No. DE-AC02-05CH11231.

9:00AM A18.00004: Deep learning X-ray Absorption Near Edge Spectra  
LIANG LI (Presenter), MARIA CHAN, Center for Nanoscale Materials, Argonne National Laboratory — The interpretation of core-level spectroscopy data, such as x-ray absorption, has long been a challenging problem. In this talk, we will discuss the use of deep learning for the interpretation of x-ray absorption near edge spectra (XANES). In this work, computed spectra using a Bethe-Salpeter Equation-based approach, of transition metal oxides, are used as the training set. Corresponding experimental data of the system will be interpreted using the trained neural networks. We will discuss, in addition, the hyperparameter tuning and optimization for bias-variance tradeoff.

9:12AM A18.00005: Using machine learning to predict local chemical environments from X-ray absorption spectra*  
DEYU LU (Presenter), Brookhaven National Laboratory, MATTHEW CARBONE, MEHMET TOPSAKAL, Columbia university, SHINJAE YOO, Brookhaven National Laboratory — X-ray absorption spectroscopy is an element-specific technique for materials characterization. Specifically, X-ray absorption near edge structure (XANES) encodes important information of the local chemical environment (LCE, e.g. coordination number, symmetry and oxidation state) of the absorber atom that is key to the understanding of the electronic and chemical properties of materials. As such, unraveling the LCE from XANES spectra is akin to solving a challenging inverse problem. Existing methods rely on empirical fingerprints, which are often qualitative or semi-quantitative and not transferable. In this study, we present a machine learning-based approach to classify the LCE's of eight 3d transition metal families from the simulated K-edge XANES of a large number of compounds. The machine learning classifier can learn important spectral features in a broad energy range without human bias and once trained, can make predictions on the fly. We found that the machine learning classifier can achieve about 85% accuracy across the wide chemical space.

*This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

LUDWIG HOLLEIS, BELLAVE SHIVARAM, PRASANNA BALACHANDRAN (Presenter), University of Virginia — Single molecule magnets (SMM) are candidate materials for magnetocaloric applications, high-density information storage, magnetic qubits, and spintronic devices. These molecules are made of several lanthanide and/or transition metal ions coordinated by organic ligands. Despite the progress made in experimental and traditional first-principles modeling efforts, lack of predictive design guidelines hinder rapid design of SMM for targeted applications. Here, we develop a machine learning approach for predicting novel SMM for magnetocaloric applications. We construct a database from surveying the published literature on magnetocaloric effect in SMM and develop a representation scheme that include aspects related to dimensionality, structure, local coordination environment, ideal number of spins of magnetic ions, ligands, and linking chemistry. We train machine learning models to predict the entropy change. The models capture successfully the observed trends and identify key variables that contribute to the entropy. We also predict new SMMs and await experimental validation.
A Classifier for Metal-Insulator Transitions*  

NICHOLAS WAGNER (Presenter), JAMES M RONDINELLI, Materials Science and Engineering, Northwestern University — We have assembled the largest dataset of resistivity-temperature measurements on temperature-activated metal-insulator transitions (MITs) to date (45 unique compounds). We supplemented this dataset with additional entries on metals and insulators with known transport behavior, i.e., do not undergo temperature-driven MITs, for comparison. We then use the 147 compounds to formulate a machine-learning model using features we collected, which describe chemical composition (e.g. mean electronegativity, atomic radii, and elemental heat of fusion); overall and local atomic structure; and estimates of the on-site electron repulsion, charge transfer energy, and compound polarizability. From this data, we constructed a machine-learning classifier to predict whether a material would undergo a MIT or not. Our model achieves a cross-validation AUC score of 88.24 +/- 11.63 and a mean accuracy of 79.23 +/- 9.23%. We also conducted a survey of 51 graduate students, faculty, and staff scientists to estimate the ability of scientists to perform this classification. The mean accuracy for humans was 59.8%.

*This work was supported under National Science Foundation DMREF Award 1729303

Machine-learning model to predict adsorption energies in thiolated bimetallic nanoclusters  

GIHAN PANAPITIYA (Presenter), GUILLERMO AVENDANO FRANO, JAMES PATRICK LEWIS, West Virginia University — We developed a random forest based machine learning model to predict adsorption energies in Ag-alloyed thiolated gold nanoclusters. The features of this model are based only on the geometric properties of non-relaxed and adsorbate-free nanocluster. The features have been defined so that they can be applied to any nanocluster. Using Au_{25} system as a test case, we obtained prediction accuracies of 0.173 (RMSE) and 0.779 (R2). To show the applicability of our model to nanoclusters with different sizes and shapes, we also predicted adsorption energies in Au_{36} and Au_{133} nanoclusters. Our model can be used as a filtering tool to downselect nanoclusters with desired adsorption energies for further calculations.

Model Selection Based on Bayesian Inference that Uncovers Fundamental Dynamics of Desiccation Crack Patterns*  

SHIN-ICHI ITO (Presenter), The University of Tokyo, AKIO NAKAHARA, Nihon University, SATOSHI YUKAWA, Osaka University — We investigate dynamic properties of fragment size distribution in surface crack patterns observed on a thin layer of drying dense colloidal suspension experimentally and theoretically. The model selection analysis based on Bayesian inference reveals that the time-varying fragment size distribution observed in experiments exhibits a dynamic transition in its functional form from a lognormal distribution to a generalized gamma distribution. In order to explain this dynamic transition theoretically, we construct a statistical model based on an elastic theory that describes the dynamics of the shrinkage of the colloidal suspension owing to the desiccation. The statistical model predicts the existence of a characteristic length scale that determines the crossover of the dynamic transition, and reproduces the functional forms of fragment size distributions observed in experiments quantitatively.

*This work was supported by JSPS KAKENHI Grant Number 16K17779.

A machine-learning approach to magnetic neutron scattering  

ROBERT TWYMAN, STUART J. GIBSON, University of Kent, JAMES MOLONY, University of Durham, JORGE QUINTANILLA (Presenter), University of Kent — One of the benefits of magnetic neutron scattering (NS) is that it can constrain the parameters of a pre-existing model Hamiltonian. Here we propose an unbiased approach that can be used before a model has been formulated. It combines Principal Component Analysis (PCA) with an artificial neural network (ANN). The PCA algorithm extracts the essential variables describing a set of NS cross-sections in an unsupervised way. The ANN then uses that information to learn to predict the cross-sections under different conditions, with supervision. To test our method, we apply it to simulated diffuse NS cross-sections obtained by exact diagonalisation of a previously-studied model of molecular magnets [H. R. Irons et al., PRB 96, 224408 (2017)]. Our main result is that the PCA can efficiently "discover" the number of fundamental parameters in the problem. The principal component scores capture key elements of the Physics including entanglement transitions. The ANN can then accurately predict NS cross-sections, confirming the validity of the PCA-based description. We conclude that PCA of NS data from real materials can be a powerful tool, specifically one capable of placing severe constraints on possible model Hamiltonians.

Monday, March 4, 2019 8:00 AM - 11:00 AM  

Session A19 DCOMP DAMOP: Precision Many Body Physics | BCEC 156C - Tag(s): Focus
8:00AM A19.00001: Enhanced metrology using quantum-correlated matter* [Invited] ANA MARIA REY (Presenter), JILA, NIST and University of Colorado at Boulder — The best clock in the world has no hands, no pendulum, no digital display. It is made of ultra-cold atoms trapped in a crystal of light.

To date, this clock is the most precise table-top instrument built by humankind; had it begun ticking when the Earth first formed billions of years ago, it would not have gained or lost a second. Even so, current atomic clocks still use collections of independent atoms, and are fundamentally limited in precision by these atoms' intrinsic quantum noise. Here, I will discuss a simple protocol to break through this limit by entangling fermionic atoms in an optical lattice clock. The basic idea is to use atomic interactions to prolong inter-particle spin coherence, transforming the dephasing effect of spin-orbit coupling into a collective entangling process that generates spin squeezing. I will show squeezing can be further enhanced by driving the clock, and how even with realistic experimental imperfections our scheme can generate ~12-15 dB of spin squeezing with 10^2-10^3 atoms. I will also discuss how a generalization of this protocol can be used to generate high dimensional cluster states useful for one quantum computing. In addition to advancing the achievable precision of atomic clocks, our protocol showcases a new paradigm of employing driven, non-equilibrium systems to overcome current limitations in quantum metrology and for the development of the foundations necessary for the construction of a universal quantum computer.

*This work is supported by the AFOSR, AFOSR-MURI, DARPA and ARO, JILA-NSF-PFC-173400, and NIST.

8:36AM A19.00002: Algebraic Time Crystallization in a Two-dimensional Superfluid NIKOLAI PROKOF'EV, BORIS SVISTUNOV (Presenter), University of Massachusetts Amherst — Time crystallization is a hallmark of superfluidity, indicative of the fundamental fact that along with breaking the global U(1) symmetry, superfluids also break time-translation symmetry. While the standard discussion of the time crystallization phenomenon is based on the notion of the global phase and genuine condensate, for the superfluidity to take place in two dimensions an algebraic (topological) order is sufficient. We find that the absence of long-range order in a finite-temperature two-dimensional superfluid translates into an algebraic time crystallization caused by the temporal phase correlations. The exponent controlling the algebraic decay is a universal function of the superfluid-stiffness-to-temperature ratio; this exponent can be also seen in the power-law singularity of the Fourier spectrum of the AC Josephson current. We elaborate on subtleties involved in defining the phenomenon of time crystallization in both classical-filed and all-quantum cases and propose an experimental protocol in which the broken time translation symmetry--more precisely, temporal correlations of the relative phase, with all possible finite-size, dimensional, and quantum effects included--can be observed without permanently keeping two superfluids in a contact.

8:48AM A19.00003: Density dependence of the superfluid properties of superclimbing dislocation in solid 4He* ANATOLY KUKLOV (Presenter), Department of Physics and Astronomy, CSI of CUNY, NIKOLAI PROKOF'EV, BORIS SVISTUNOV, Department of Physics, UMASS — Dislocations with superfluid core [1,2] are the main candidates for the mechanism behind the observation of superflow through solid and the syringe effect [3]. The same features have been confirmed in Refs.[4,5], respectively. One of the unusual features observed in the experiment [4] is the exponentially strong suppression of the flow versus pressure (or crystal density). Our grand canonical ab initio simulations of the superclimbing dislocation by the Worm Algorithm [6] on samples containing about 1430 particles at T=0.25K find that Luttinger parameter K obeys the dependence K=exp (3.4 - 39 n), where n>0 stands for the fractional deviation of the density from the melting value, within the accuracy of 10-15%. Thus, by increasing the density by only about 10% the K-value drops by about two orders of magnitude. This qualitatively agrees with the observation [4].

[1] M. Boninsegni, et. al., PRL 99, 035301 (2007);

*We acknowledge support from NSF grants DMR 1720251 and 1720465.
9:00AM A19.00004: Numerical solutions of three-dimensional helium like atoms from the linear combination of their analogue one-dimensional wave functions*  
FAIZ UR RAHMAN, YANOAR PRIBADI SARWONO, RUIQIN ZHANG  
(Presenter), City University of Hong Kong — The solutions of Schrödinger wave equations for the ground state of three-dimensional helium atom and its isoelectronic series were obtained from the linear combination of one-dimensional helium-like wave functions. The result shows that the one-dimensional bases along the axes are good choices which facilitate easy numerical integration. The three-dimensional wave function was constructed from the linear combination of the bases and the result was further refined to converge to the exact value using the iteration technique. The resultant ground state energy for the helium atom is with deviation of from the exact value. The method developed is thus demonstrated to be an effective numerical approach to the many-body problem and could be extended to other atomic and molecular systems.

*This work was financially supported by grants from the Research Grants Council of the Hong Kong SAR (11305618) and from NSAF (U1530401).

9:12AM A19.00005: An integrable multi-channel sine-Gordon model with Josephson circuits*  
ANANDA ROY  
(Presenter), HUBERT SALEUR, Institut de Physique Theorique, CEA Saclay — Integrable field theories have always fascinated physicists. In particular, those which describe quantum impurity problems have been of much interest to both theorists and experimentalists. A prominent example is the boundary sine-Gordon (bSG) field theory. The latter describes a Luttinger liquid in the presence of an impurity. In this work, we propose an experimentally realizable, multi-channel generalization of the bSG model. We establish the classical and quantum integrability of the model by constructing a corresponding integrable bulk theory. We provide the first nontrivial conserved current of the bulk theory. Subsequently, we postulate the factorized scattering matrix describing the bulk theory and verify it using Bethe Ansatz computation of the ground state energy. Subsequently, we provide the factorized scattering matrix of the boundary field theory. Thermodynamic properties of both the bulk and boundary model are computed using the Thermodynamic Bethe Ansatz. Finally, we propose an experimental realization of the model with superconducting circuits, making use of the robust, tunable and dispersive Josephson nonlinearity. Our proposal can be realized with state-of-the-art system parameters.

*A.R. acknowledges the support of the Alexander von Humboldt foundation.

9:24AM A19.00006: Non-Equilibrium Transport in the Kondo Model: Strong and Weak Coupling*  
ADRIAN CULVER  
(Presenter), NATAN ANDREI, Center for Materials Theory, Rutgers University — We present an exact method of calculating the non-equilibrium current driven by a voltage drop across a quantum impurity. The system is described by the two lead Kondo model with non-interacting Fermi-liquid leads. We prepare the system in an initial state consisting of a free Fermi sea in each lead with the voltage drop given as the difference between the two Fermi levels. We quench the system by coupling the impurity to the leads at t=0 and following the time evolution of the wavefunction. In the long time limit, a steady state emerges provided that the size of the system is large compared to the time of evolution (the open system limit). We determine the wavefunction explicitly at any time and show, in particular, that the long time limit satisfies the Lippmann-Schwinger equation with the two Fermi seas serving as the boundary conditions. Using this wavefunction, we obtain an infinite series expression for the current as a function of voltage, either in powers of the antiferromagnetic Kondo coupling constant J or in powers of 1/J. Evaluating the first few terms, we find that a quench to small J reproduces known results while a quench to large J leads to a pre-thermalized regime of maximal conductance with ferromagnetic corrections.

*Research supported by NSF Grant DMR 1410583
9:36AM A19.00007: Strong and Weak Field Criticality of Liquid Gas Transition in 2D*  MAX YARMOLINSKY (Presenter), ANATOLY KUKLOV, Physics, College of Staten Island & the Graduate Center — Finite size scaling (FSS) analysis of the liquid gas criticality is complicated by the absence of any broken symmetry. This, does not allow a straightforward finding of the coexistence line and the critical point -- especially in 2D. The numerical flowgram (NF) method[1] is adapted for a controlled determination of the boundary between weak and strong field critical regions by applying classical Monte Carlo to the square well model. This boundary coincides with the coexistence line of the liquid-gas transition with respect to the leading scaling behavior. The NF method allows measuring the critical indices μ, ν within 1-2% of the total error. Furthermore, the NF allows testing the so called complete scaling theory of the critical point[2] without tuning the system into the coexistence line. This theory predicts linear mixing between the primary scaling operators and pressure. We show that the NF analysis should see corrections to scaling which are stronger than the standard ones of the 2D Ising model. It can also resolve the non analytical correction to the diameter.


*We acknowledge support by NSF under the Grant DMR1720251

9:48AM A19.00008: Emergent Symmetry U(1) and Tricriticality in a 2D Quantum Clock Model*  PRANAY PATIL (Presenter), Boston University, HUI SHAO, WENAN GUO, Physics, Beijing Normal University, ANDERS W SANDVIK, Boston University — We propose a quantum clock model on the square lattice built out of a q-state classical clock model with a quantum fluctuation (a generalization of a transverse field) added to it. We see evidence that this model is closely related to the 3D classical clock model through the standard quantum to classical mapping. For q=5, we see a continuous phase transition and for q=5,6 we show that, at the phase transition, an emergent U(1) symmetry appears, similar to the 3D classical clock models. We address the connection that this emergent symmetry has to a second length scale within the scenario of dangerously irrelevant perturbations of the XY model. We also demonstrate the existence of a tricritical point in the case of q=4, which can be tuned by changing the form of the quantum fluctuation operator.

*NSF Grant No. DMR-1710170

10:00AM A19.00009: Symmetry enhanced first-order phase transition in a two-dimensional quantum magnet*  BOWEN ZHAO (Presenter), ANDERS W SANDVIK, PHILLIP E WEINBERG, Boston University — Theoretical descriptions of quantum phase transitions have indicated the existence of critical points with higher symmetries than those of the underlying Hamiltonian. Here we present an example of such an emergent symmetry at a first-order transition, where coexistence of two ordered phases takes the form of higher rotational symmetry in the space of the two order parameters. Using quantum Monte Carlo simulations, we study a two-dimensional (2D) S = 1/2 quantum magnet hosting the antiferromagnetic (AFM) and plaquette-singlet solid (PSS) states recently detected in SrCu2(BO3)2. We observe that the O(3) symmetric AFM order and the Z2 symmetric PSS order form an O(4) vector at the transition. The control parameter (a coupling ratio) rotates the vector from the AFM sector to the PSS sector, with the length of the combined order parameter vector always remaining non-zero. This phenomenon should be observable in SrCu2(BO3)2.

*This work was supported by the NSF under Grant No. DMR-1710170 and by The Simons Foundation.

10:12AM A19.00010: Even-Odd effect of an Spin-S impurity coupled to a quantum critical system  KUN CHEN, YASHAR KOMIJANI, Department of Physics, Rutgers University, YUAN HUANG (Presenter), University of Massachusetts Amherst — We discuss an even-odd effect for an impurity with N degenerate internal states immersed in a two-dimensional superfluid--Mott-insulator quantum critical bath, which is described by a spin-S XY Bose Kondo impurity model with N = 2S + 1. Using a dimensionally and momentum-cut-off regularized renormalization group and an unbiased large-scale Monte Carlo numerical simulations, we establish the phase diagram of an S = 1 impurity with relevant terms included. We show that the impurity with N = 3-fold degeneracy is fully screened by the critical bath, which is qualitatively different from the N = 2 case where the impurity is only partially screened. We then argue that all even-N impurities share the same universal physics as the N = 2 case, and all odd-N impurities are as the N = 3 case. We validate our conjecture with unbiased Monte Carlo simulations up to N = 5.
10:24 AM A19.00011: Trapping Collapse: Generic weak traps localize an infinite number of repulsive bosons*  
NIKOLAI PROKOF’EV (Presenter), University of Massachusetts Amherst, KUN CHEN, Physics, Rutgers University, BORIS SVISTUNOV, University of Massachusetts Amherst — Weak potential wells (or traps) in one and two dimensions, and the potential wells slightly deeper than the critical ones in three dimensions, feature shallow bound states with localization length much larger than the well radii. We address a simple fundamental question of how many repulsively interacting bosons can be localized by such traps. We find that under rather generic conditions, for both weakly and strongly repulsive particles, in two and three dimensions—but not in one dimension!—the potential well will trap infinitely many bosons. For example, even hard-core repulsive interactions do not prevent this ``trapping collapse'' phenomenon from taking place. A quantum system acquires the phenomenon along with the universal (asymptotically exact) classical-field behavior at large distances, allowing generic description by the Gross-Pitaevskii equation. We also discuss the possibility of having a transition between the infinite and finite number of trapped particles when strong repulsive inter-particle correlations are increased.  
*National Science Foundation grant DMR-1720465
MURI Program  `Advanced quantum materials -- a new frontier for ultracold atoms'' from AFOSR

10:36 AM A19.00012: Two Temperature Scales in the Triangular Lattice Heisenberg Antiferromagnet*  
WEI LI (Presenter), BIN-BIN CHEN, LEI CHEN, HAN LI, DAI-WEI QU, Beihang University, JAN VON DELFT, University of Munich, ANDREAS WEICHSELBAUM, Brookhaven National Lab — The anomalous thermodynamic properties of the paradigmatic frustrated spin-1/2 triangular lattice Heisenberg antiferromagnet (TLH), has remained an open topic of research over decades, both experimentally and theoretically. Here we further the theoretical understanding using the recently developed, powerful exponential tensor renormalization group (XTRG) method on cylinders and stripes in a quasi one-dimensional (1D) setup, as well as a tensor product operator approach directly in 2D. The observed thermal properties of the TLH are in excellent agreement with two recent experimental measurements on the virtually ideal TLH material Ba8CoNb6O24. Remarkably, our numerical simulations reveal two cross-over temperature scales, at T₁/J ~ 0.2 and T₂/J ∼ 0.55, with J the Heisenberg exchange coupling, which are also confirmed by a more careful inspection of the experimental data. We propose that in the intermediate temperature range, the gapped roton-like excitations are activated with a strong chiral component and a large contribution to thermal entropies, which thus suppresses the incipient 120° order that emerges for temperatures below T₁.  
*This work was supported by the NSFC (No. 11504014 and 11834014), DFG (excellence initiative NIM, WE4819/3-1, and WE4819/2-1), and DOE DE-SC0012704.

10:48 AM A19.00013: Some Novel Applications and Interpretations of the Path Integral Formalism*  
JARETH BACA (Presenter), AJIT HIRA, JOSE PACHECO, Math and Physics, Northern New Mexico College, TOMMY CATHEY, Chemical Physics, Lockheed Information Systems, MATILDA FERNANDEZ, Math and Physics, Northern New Mexico College — Two important considerations which will be addressed in this presentation pertain to extending applications of the Feynman Path Integral Formalism (FPIF) to some important physical problems, and also to the role of this formalism in providing a generally acceptable view of the interpretation of Quantum Mechanics (QM). Of particular interest for our research is the extension of path integral quantization geometries other than spherical: namely parabolic, elliptic and hyperbolic geometries. We calculate perturbative expansions of various path integrals of interest, with a view to obtaining Conformal Field Theories (CFTs). We used a Python programming language interface, and Monte Carlo (MC) integrations in our computer codes. Our main results are in the field of plasma Physics, with some applications in fusion and Astrophysics.  
*Financial support from the New Mexico Alliance for Minority Participation (NM-AMP) program of the National Science Foundation (NSF)

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A20 DCOMP DMP: First-principles Modeling of Excited-state Phenomena in Materials I: Many-body Perturbation Theory (Techniques and Applications)  
BCEC 157A - Andre Schleife, University of Illinois at Urbana-Champaign - Tag(s): Focus
8:00AM A20.00001: Accurate Core-Level Spectra from GW* [Invited] DOROTHEA GOLZE (Presenter), PATRICK RINKE, Aalto University — We present an accurate method for computing X-ray photoelectron spectra based on the GW approximation that overcomes the limitations of density functional theory (DFT) approaches. The GW method is routinely used to predict charged valence excitations in molecules and solids. However, GW core-level spectroscopy has thus far been poorly explored. This in parts related to the fact that numerically very efficient techniques such as the analytic continuation, which treat the frequency dependence on the imaginary axis, break down for inner-shell excitations. We implemented a full-frequency approach on the real axis in the all-electron code FHI-aims [1] using a localized basis to enable the treatment of core levels in GW[2]. Our scheme is based on the contour deformation technique and facilitates precise and efficient calculations of the self-energy, which has a complicated pole structure for core states. We present benchmark studies for 1s excitations of small- and medium-sized molecules and discuss the optimization of the starting point as well as self-consistent approaches. We find that the absolute core-level binding energies deviate on average by less than 0.5 eV from experiment outperforming the DFT-based Delta Self-Consistent Field approach. Relative core excitations are also well reproduced with average deviations of less 0.2 eV from the experimental reference. Furthermore, our calculations reveal that the GW excitation spectrum exhibits satellite features in addition to the photoelectric peak, which might provide access to interesting many-body physics.


*The research is supported by Academy of Finland grant no. 316168.

8:36AM A20.00002: Time-dependent GW: Progress in Solving Kadanoff-Baym Equations with Dynamic GW Self Energy* DIANA QIU (Presenter), YANG-HAO CHAN, FELIPE DA JORNADA, STEVEN G. LOUIE, Lawrence Berkeley National Lab and University of California, Berkeley — The ab initio GW plus Bethe-Salpeter equation (GW-BSE) approach has achieved great success in describing the linear absorption spectra of materials in equilibrium. However, many important photo-processes and experiments of interest that involve ultrafast and high-intensity pulses of light fall well outside the regime of equilibrium and linear responses. One can generalize the Green's function formalism in many-body perturbation theory to nonequilibrium situations by solving the Kadanoff-Baym equations (KBE), but the presence of two time variables that need to be simultaneously evolved presents a significant computational challenge. In recent years, progress has been made in solving the KBE from ab initio in the static limit of the GW self energy, which greatly simplifies the time evolution. Here, we present progress on solving the KBE including dynamical effects in the self energy. We discuss time-evolution algorithms, memory effects, approximations to the dynamics, and convergence behavior.

*This work was supported by the Center for Computational Study of Excited State Phenomena in Energy Materials (C2SEPEM), which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231.

8:48AM A20.00003: Excitonic effects in shift currents of low dimensional materials from time-dependent GW approach* YANG-HAO CHAN (Presenter), Lawrence Berkeley National Lab, DIANA QIU, Physics, University of California, Berkeley, FELIPE DA JORNADA, Lawrence Berkeley National Lab, STEVEN G. LOUIE, Physics, University of California, Berkeley — We present first-principles studies on shift currents with excitonic effects in 2D materials using an adiabatic time-dependent GW approach. Shift current in a noncentrosymmetric semiconductor is a DC current generated by optical excitations from a nonlinear response processes. Using a newly developed real-time simulation method, we are able to include excitonic effects in the nonlinear responses from first principles, treating the complicated electron-hole interaction at the GW plus Bethe-Salpeter equation level for the first time. We applied this method to study shift currents in monolayer GeS and found strongly enhanced responses due to excitonic effects. Most interestingly, the dominant contributions to the shift currents here are generated at in-gap frequencies, which peaked at energies below the quasi-particle band gap by the exciton binding energies.

*This work was supported by the Center for Computational Study of Excited State Phenomena in Energy Materials (C2SEPEM), which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231.
Correlation satellites in optical and loss spectra

PIER LUIGI CUDAZZO (Presenter), Faculté des Sciences, de la Technologie et de la Communication, Université du Luxembourg, LUCIA REINING, Ecole Polytechnique — The coupling of excitations leads to intriguing effects in the spectra of materials. Current approximations to calculate spectra most often describe this coupling insufficiently. We propose a cumulant formulation for neutral electronic excitations which opens the way to describe effects such as double plasmon satellites or exciton-exciton coupling. Our approach starts from the widely used GW plus Bethe-Salpeter approximation to many-body perturbation theory which is based on a quasiparticle picture, and it adds coupling to other excitations through a consistent inclusion of dynamically screened interactions. We show that this requires to consider scattering contributions that are usually neglected. The result is formulated in a way that highlights essential physics, that can be implemented as a post-processing tool in widely used first principles codes, and that suggests which kind of materials and measurements should exhibit strong effects. This is illustrated using a model.

Faster and more accurate stochastic GW*

VOJTECH VLCEK (Presenter), Chemistry and Biochemistry, UC Santa Barbara, ERAN RABANI, College of Chemistry, UC Berkeley, ROI BAER, Chemistry, Hebrew University (Israel), DANIEL NEUHAUSER, Chemistry and Biochemistry, UC Los Angeles — I will present recent developments in stochastic approach to the GW approximation, which further accelerate the calculation of quasiparticle energies and increase their accuracy. A new concept of sparse stochastic compression is used to speed up stochastic approaches and leads to an overall decrease of statistical errors in large finite and periodic systems. Computation of quasiparticle energies and gaps for systems with up to $N_e > 10,000$ electrons is thus feasible with only small statistical fluctuation ($\pm 0.05$ eV) and consuming < 2000 core CPU hours. Further, I will present an efficient scissors-like GW self-consistency approach that can be implemented at zero additional cost. This result is a simple modification of the time-dependent G0W0 and enables an a posteriori self-consistency cycle applicable to large systems.

*This work was supported by the Center for Computational Study of Excited-State Phenomena in Energy Materials at the Lawrence Berkeley National Laboratory, which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DEAC02-05CH11231 as part of the Computational materials Sciences Program.

Calculations of Multiplet Splittings in Open Shell Systems within the GW approximation*

MEISAM REZAEI (Presenter), SERDAR OGUT, University of Illinois at Chicago — In open shell systems, the coupling of the orbital and spin angular momenta of electrons can result in multiple energy eigenstates of the electronically excited system leading to the characteristic multiplet structures observed in photoemission experiments. While DFT is not capable of determining the resulting multiplet splittings accurately, recent studies have shown that the GW approximation can describe the multiplet structure with reasonable accuracy. In this work, we investigate the multiplet splittings for open shell molecules such as NO$_2$, NF$_2$, O$_2$, ClO$_2$, and single atoms by applying the one-shot GW approximation. We compare predictions obtained with $G$ and $W$ computed with the same hybrid functional starting points containing varying amounts of Fock exchange with those where $G$ is still computed with a hybrid functional starting point but $W$ is computed within PBE. We show that it is possible to achieve excellent agreement with experimental results for molecular systems using both types of approaches, but the amount of exact exchange needed for quantitative accuracy depends on the molecule as well as the choice of the GW method employed.

*Work supported by DOE Grant No. DE-SC0017824.
9:36AM A20.00007: Electronic structure of 3d-transition-metal oxide clusters with partially filled d shells from GW calculations*  
YOUNG-MOO BYUN (Presenter), SERDAR OGUT, Department of Physics, University of Illinois at Chicago — The GW approximation using atom-centered localized basis sets is an emerging method for studying the excited properties of confined systems. However, G0W0@PBE, which is typically used for simple extended systems, fails to accurately describe the electronic excitations in 3d-transition-metal oxide clusters due to dimensionality and correlation effects, and suffers from exhibiting multiple solutions of the quasiparticle equation due to complex self-energy poles. G0W0 on top of exact exchange (EXX) is one way to overcome these problems, but the predictions depend on the amount of EXX and the method suffers from convergence errors in open-shell systems (e.g. due to spin contamination). In our previous work on early and late 3d transition metal oxide clusters, we showed that G0W0@PBE addresses all the above issues, and thus is an accurate and efficient GW method for these systems. In this work, we investigate various flavors of the GW method (one-shot, partially self-consistent, quasiparticle self-consistent) with different starting points for 3d transition metal oxide clusters, VO-, CrO-, MnO-, FeO-, CoO-, and NiO-, which display a number of high multiplicity states and exhibit moderate electronic correlation.

*This work was supported by DOE Grant No. DE-SC-0017824.

9:48AM A20.00008: Spin wave spectrum of 3d ferromagnet based on QSGW calculations  
OKUMURA HARUKI (Presenter), KAZUNORI SATO, Graduate School of Engineering, Osaka University, TAKAO KOTANI, Department of applied mathematics and physics, Tottori University — We have developed spin wave (SW) spectrum calculation code, combining quasi-particle self-consistent GW(QSGW) and maximum localized Wannier function (MLWF). With MLWF, we can overcome time-consuming calculations for large q-point SW spectrum. Since we adopt the linear response method for dynamical susceptibility,[1] our SW spectrum includes Stoner excitation, which causes the damping of spin SW. Stoner excitation is important in weak ferromagnet such as Fe, while not important in strong ferromagnet such as Ni. In the local density approximation (LDA), our SW energy in Fe is smaller than experimental result or other frozen SW calculation. In the QSGW calculations, due to the corrections of exchange splitting, the calculated SW stiffness constant of Ni (481 meV·Å in average) is in good agreement with inelastic neutron scattering experiment (483 meV·Å), while the LDA result (834 meV·Å) is almost twice as large as experimental one. In the fcc Co, our LDA result corresponds to frozen SW calculation because of weak Stoner excitation coupling in this strong ferromagnet. In the case of cubic FeCo in ordered state, we found acoustic and optical mode in the SW spectrum. [1] C. Friedrich, et al., First Principles Approaches to Spectroscopic Properties of Complex Materials pp 259-301 (2014).

10:00AM A20.00009: Tunable Low Temperature Phonon-induced Electronic Bi-stability in Vanadium Dioxide*  
MARK SCHILFGAARDE (Presenter), CEDRIC WEBER, SWAGATA ACHARYA, King's College London, MOSTAFA SHALABY, Beijing Normal University, Science Park, Beijing — We use a joint theory and experimental approach to clarify the nature of the Metal-insulator transition in VO₂, by QSGW calculations in the frozen phonon approach, and pump-probe ultra-fast spectroscopy with THz radiation. We first show that the insulating state is induced by a Peierls instability, that is responsible for the orbital selection that drives the material to its insulating state, and is associated with a degenerate two-orbital electronic valence band. At the same time, Peierls excitations driven by the lattice dynamics. A 5.7 THz phonon modes split the degeneracy, in a particular, which in turn induces a rapid metallization. This mode is observed in THz pump measurements, far below the critical temperature in the M₁ phase. Our combined approach sheds light in the nature of the transition, which is in our view mediated by a combination of the lattice dynamics and electronic excitations. Finally, we report a possibility in the theory for a novel mechanism to induce an electronic metal-insulator hysteresis via the electron-phonon coupling to the 6.5 THz phonon mode.

*This work was supported by the Simons Many-Electron Collaboration, and EPSRC (grants EP/M011631/1 and EP/M011038/1).
**Alternative approaches for calculations of exchange and correlation contributions to thermodynamic properties**

JOSHUA KAS (Presenter), JOHN REHR, University of Washington — The cumulant expansion of the one-electron Green's function has been found to be an improved method for calculations of excited states and spectra for a wide variety of systems [1]. Additionally, an extension of the cumulant Green's function approach to finite temperatures has yielded total energies and exchange correlation potentials in good agreement with quantum Monte-Carlo results [2]. Here we present an investigation of alternative thermodynamic pathways for properties such as the free energy, entropy, and heat capacity of the homogeneous electron gas. In addition we discuss approximate methods based on quasiparticle properties alone. These approximate methods improve the efficiency of the approach, and could be applied to real systems for which calculations of GW quasiparticle effects are computationally reasonable.


*Supported by DOE Office of Science BES Grant DE-FG02-97ER45623

**Electron Hydrodynamics of Graphene from a First-Principles GW Approach: Electronic Compressibility, Backflows and Transport Coefficients**

ANDREA CEPELLOTTI (Presenter), STEVEN G. LOUIE, Physics and Materials Sciences, University of California at Berkeley and Lawrence Berkeley National Laboratory — Doped graphene at low temperatures has experimental signatures of hydrodynamic behavior originating from the electron-electron interaction. Here, we use the GW approximation to study the electronic and thermal properties of graphene from first-principles within a Fermi liquid framework. We show how the electronic compressibility is modified by many-body contributions at finite temperature. Next, we solve the kinetic equation using an exact expression of the scattering matrix. We show how the commonly-used relaxation time approximation causes a severe underestimation of transport coefficients, and how a correct treatment of momentum dissipation is critical to the description of transport properties. We will present results for transport coefficients, including electrical conductivity, the electronic contribution to thermal conductivity and the viscosity coefficients, discussing corrections due to the interaction of carriers with the environment and the behavior of the electron liquid as a non-Newtonian fluid.

*Work supported by the Center for Computational Study of Excited-State Phenomena in Energy Materials at LBNL, as part of the Computational Materials Sciences Program, funded by the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources provided by NERSC.

**Cumulant Green's function approach for phonon satellites in resonant inelastic X-ray scattering**

KEITH GILMORE (Presenter), Brookhaven National Laboratory, ANDREY GEONDZHIAN, European Synchrotron Radiation Facility — Resonant inelastic X-ray scattering (RIXS) probes various excitations in materials, including plasmons, magnons and phonons. Calculating RIXS spectra is challenging since it is a second-order process involving the coupling of core-excited states to bosonic collective modes, and requires summation over virtual intermediate states. Using a cumulant expansion [1], we develop a tractable excitonic Green's function formulation of the RIXS cross section. We demonstrate our methodology by reproducing the phonon contribution to the RIXS spectrum of acetone [2]. The relative intensities of multiple phonon satellites are used to quantify the electron-phonon coupling strength. First, we show that RIXS actually probes exciton-phonon coupling, which can differ significantly from electron-phonon coupling. Second, we extend our numerical demonstration on acetone to the more challenging cases of quasi-1D Li$_2$CuO$_2$ and 3D SrTiO$_3$. This requires generalizing concepts of density functional perturbation theory to generate exciton-phonon coupling constants throughout the Brillouin zone. Comparison to experiment is made, resolving apparent anomalies in the spectra of Li$_2$CuO$_2$.

10:48AM A20.00013: Reexamining a local, real-space approach to screening  JOHN VINSON (Presenter), ERIC SHIRLEY, National Institute of Standards and Technology — Various many-body perturbation theory techniques for calculating electron behavior rely on $W$, i.e., the screened Coulomb interaction. The exact screening requires complete knowledge of the dielectric response of the electronic system. As a simplification, calculations often begin with the RPA or random phase approximation. However, even at the RPA level the calculations are costly and scale poorly with system size. A local approach has been shown to be efficient while maintaining accuracy [1]. We present improvements to this scheme, including reconstruction of the all-electron character of the pseudopotential-based wave functions, improved scaling with system size, and a parallelized implementation. We discuss applications to Bethe-Salpeter calculations of core and valence spectroscopies.


Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A21 DCOMP: Big Data in Physics 8CEC 157B - Hans Herrmann, Universidade Federal do Ceará - Tag(s): Careers, Focus, Undergraduate

8:00AM A21.00001: Big data in physics, biology and social science [Invited]  FLAVIANO MORONE (Presenter), City College of New York — In the digital age, we are creating 2.5 billion gigabytes of data every single day of our lives, and the 75% is unstructured, coming from texts, videos and opinions spread through online social networks. These data sets are so voluminous and complex that traditional data analytics methods are often inadequate to extract value from them. Here, I show how to extract summarized data by identifying an optimal set of network nodes, called influencers, with high predictive power in anticipating opinion trends and tracking the effectiveness of messages in massive social networks. I illustrate the theoretical framework to identify influencers using the concept of optimal percolation (OP). Big data analyses in social networks reveal that the set of influencers identified by OP theory is much smaller than the one predicted by heuristic centralities. Remarkably, a large number of previously neglected weakly connected nodes emerges among the optimal influencers.

I show that OP theory is also a powerful indicator of personal economic status. Said in very simple terms, we discovered that people located in positions of high influence have high financial levels. This result comes from the combined analysis of two large-scale datasets including telecommunication and financial data of 110 million people in Mexico. Finally, I also discuss applications of OP theory to brain networks. In particular, I show how OP theory identifies the essential nodes for integration of the memory network in a rat brain.

8:36AM A21.00002: AI Astrophysics [Invited]  KEVIN SCHAWINSKI (Presenter), Modulos AG — I present how some recent advances in artificial intelligence can help us explore astrophysical problems. Astrophysics faces a particular challenge from the fact that experiments with controlled variables are impossible. New approaches such as generative models can help us better constrain and understand the underlying processes governing the formation and evolution of galaxies and other objects. While cutting edge research from computer science can be helpful in many case, new tools abstracting AI/ML to a more user-friendly level also have a significant potential for advancing research in astrophysics, and other areas of the physical sciences.
9:12AM A21.00003: Insights into the world connectivity from aviation and tourism data* [Invited] NUNO ARAUJO (Presenter), University of Lisbon — The World Airline Network (WAN) is an infrastructure that reduces the geographical gap between societies, both small and large, and bring forth economic gains. With the extensive use of a publicly maintained data set that contains information about airports and alternative connections between these airports, we empirically reveal that WAN is a redundant and resilient network for long distance air travel, but otherwise breaks down completely due to removal of short and apparently insignificant connections [1]. These short-range connections with moderate number of passengers are the connections that keep remote parts of the world accessible. It is surprising, insofar as there exists a highly resilient and strongly connected core consisting of a small fraction of airports (around 2.3%) together with an extremely fragile star-like periphery. The core-periphery structure is also observed for a number of important transport networks. With a dynamic model for the evolution of transport networks, we show that core-periphery structures are (very likely) a product of a tug of war between connectivity and economic profit [2]. Finally, we will discuss how the mobility pattern of tourists around the world correlates with the underlying Airline Network [3].


*We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under Contract no. UID/FIS/00618/2019.

9:48AM A21.00004: Dynamics of Traffic Congestions from Large-Scale Data in the Taiwan Highway System* T. S. CHOI, YEE MAN TAI, YULIN XU, KWONG TAI SIU, Physics, Hong Kong University of Science and Technology, KI WING TO, Institute of Physics, Academia Sinica, K.Y. MICHAEL WONG (Presenter), Physics, Hong Kong University of Science and Technology — The Taiwan Highway System has the longest electronic toll collection (ETC) freeway mileage in the world. There are 300 sensors installed on the two North-South spanning highways. The collected data consists of the time information of individual vehicles passing through ETC sensors along their highway journeys. Highway segments are demarcated by successive sensors, enabling us to extract a tremendous volume of dynamical segment-wise data. We trace the evolution of the system on the so-called fundamental diagram with vehicle flux versus vehicle density during traffic congestions in segments, and show that congestions are characterized by loopy trajectories in the diagram. By considering the area enclosed by a loop, we find that there are two types of congestion dynamics -- moderate flow and serious congestion. They behave differently in terms of the area enclosed. Data extracted from the time delays of individual vehicles show that the area enclosed is a measure of the economic loss due to congestion.

*This work is supported by Research Grants Council of Hong Kong (grant numbers 16322616 and 16306817).

10:00AM A21.00005: How the brain transitions from conscious to subliminal perception FRANCESCA ARESE LUCINI (Presenter), City College of New York — We study the transition in the functional network that characterize the human brains’ conscious state to an unconscious subliminal state of perception by using k-core percolation. We find that the most inner core (ie, the most connected kernel) of the functional network in the state of consciousness (the visual cortex and the left middle frontal gyrus) is represented by the areas that remain active when the brain transitions to the subliminal unconscious state. That is, the inner core of the conscious network coincides with the unconscious state. Based on data analysis and mathematical modeling we interpret these results as a transition driven by k-core percolation, where the conscious state is inactivated by the disappearance of the peripheral shells in the k-shell decomposition structure. Thus, the inner core and most robust component of the brain seems to be the unconscious subliminal state. If this result were to be found valid for other states of the brain, it could set interesting constraints to models of consciousness and brain structure, in that the location of the core of the functional brain network is in the unconscious part of the brain rather than in the conscious state as previously thought.
10:12AM A21.00006: Super Resolution Convolutional Neural Network for Feature Extraction in Spectroscopic Data*

HAN PENG (Presenter), Department of Engineering, University of Oxford, XIANG GAO, Department of Chemistry, University of Florida, YU HE, Department of Applied Physics, Stanford University, YIWEI LI, Department of Physics, University of Oxford, YUCHEN JI, CHUHANG LIU, School of Physical Science and Technology, ShanghaiTech University, SANDY ADHITIA EKAHANA, DING PEI, Department of Physics, University of Oxford, ZHONGKAI LIU, School of Physical Science and Technology, ShanghaiTech University, ZHIXUN SHEN, Department of Applied Physics, Stanford University, YULIN CHEN, Department of Physics, University of Oxford — Two dimensional (2D) peak finding is a common practice in data analysis for physics experiments, which is typically achieved by computing the local derivatives. However, this method is inherently unstable when the local landscape is complicated, or the signal-to-noise ratio of the data is low. In this work, we propose a new method in which the peak tracking task is formalized as an inverse problem, thus can be solved with a convolutional neural network (CNN). In addition, we show that the underlying physics principle of the experiments can be used to generate the training data. By generalizing the trained neural network on real experimental data, we show that the CNN method can achieve comparable or better results than traditional derivative based methods. This approach can be further generalized in different physics experiments when the physical process is known.

*Acknowledgements to Mrs Chiying Liao for the financial support for the computing device. HP, YWL, DP thank the support of China Scholarship Council.

10:24AM A21.00007: A Library for Real Time Interactive High Performance Computing of 2D and 3D Physics Problems through GPU*

FLAVIO FENTON (Presenter), ABOUZAR KABOUDIAN, Georgia Institute of Technology — Many interesting and complex physics problems such as those that use large scale reaction-diffusion equations to study animal skin patterns, brain activity and cardiac arrhythmias require the use of supercomputers. Likewise is the case for systems displaying turbulent fluid dynamics, surface growth, and systems using heat and wave equations. We have developed a library using WebGL, which allows to code and run physics problems, that generally require supercomputers to run, in the GPU of a local PC and even a cellphone, which can run up to 7 billion differential equations per second. We have used this library not only for research but also with undergraduates in Computational Physics Courses at Georgia Tech and in workshops at RIT. In this talk we present the library and show interactive simulations of interesting problems in real time. 2D and 3D examples including Turing patterns, turbulent fluid flow, coral growth and fibrillation in the heart among others.

*NSF#1446675 NIH#143450

10:36AM A21.00008: A Robust Approach to Compressive Sensing by Shortest-Solution Decimation

MUTIAN SHEN (Presenter), University of Science and Technology of China, PAN ZHANG, HAIJUN ZHOU, Institute of Theoretical Physics, Chinese Academy of Sciences — Compressed sensing is an important problem in many fields of science and engineering, including computational physics. It reconstructs signals by finding sparse solutions to underdetermined linear equations. We propose a deterministic and non-parametric algorithm, shortest-solution guided decimation (SSD), to construct support of the sparse solution under the guidance of the dense least-squares solution of the recursively decimated linear equation. The most significant feature of SSD is its insensitivity to correlations in the sampling matrix. Using extensive numerical experiments, we show that SSD greatly outperforms $L_1$ -norm based methods, orthogonal least squares, orthogonal matching pursuit, and approximate message passing when the sampling matrix contains strong correlations. This nice property of correlation tolerance makes SSD a versatile and robust tool for different types of real-world signal acquisition tasks.
TBTK aims to solve this problem by providing general purpose data structures tailored for quantum mechanics. These data structures are intended to act as a layer between application developers that are interested in quickly developing code that answers specific physical questions and method developers that need high degree of low level control of the data representation in the most critical parts of their algorithms.

For further information, see the preprint (https://arxiv.org/abs/1808.02409), code (https://github.com/dafer45/TBTK), and documentation (http://www.second-quantization.com/).

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A22 DCOMP DMP DCMP DCP: Building the Bridge to Exascale: Applications and Opportunities for Materials, Chemistry, and Biology I

8:00AM A22.00001: Performance of Open-Source Real-Space Multigrid DFT Code on Pre-Exascale Architecture

EMIL BRIGGS (Presenter), WENCHANG LU, JERRY BERNHOLC, North Carolina State University — RMG (www.rmgdft.org) is an open-source suite of codes for performing large-scale, high-throughput electronic structure calculations. Designed for scalability, it discretizes the DFT equations on real-space grids that are distributed over the nodes of a massively parallel system via domain decomposition. The Kohn-Sham and Poisson equations are solved using multigrid techniques that dramatically accelerate convergence while only requiring nearest neighbor communications. In addition to the multigrid algorithms, the main parts of the calculations consist of dense matrix multiplications and iterative solutions of a partitioned eigenvalue problem that are particularly well suited for GPU accelerators. RMG makes very efficient use of GPUs, including multiple GPUs per node, if they are available. On the IBM/NVIDIA Summit supercomputer at ORNL, RMG utilizes all 6 GPUs per node and Cuda-managed memory to reach 83x performance improvement over the previous generation Cray XK7 Titan supercomputer at ORNL, which contains 1 prior-generation GPU per node. We will also discuss algorithmic improvements enabled by large-memory, high memory bandwidth nodes in view of future exascale architectures.

8:12AM A22.00002: Full-potential LSMS method for \textit{ab initio} electronic structure calculations at large scale

YANG WANG (Presenter), Pittsburgh Supercomputing Center, Carnegie Mellon University, XIANGLIN LIU, MARKUS EISENBACH, GEORGE MALCOLM STOCKS, Oak Ridge National Laboratory — The locally self-consistent multiple scattering (LSMS) method is a linear scaling \textit{ab initio} electronic structure calculation method in the framework of density functional theory with local density approximation. It is based on multiple scattering theory, which allows to use Green function and contour integration techniques for the calculation of electron density and density of states. With muffin-tin approximation, the LSMS method has demonstrated linear scaling and petascale performance at the scale of tens of thousands of atoms and has been applied to the study of nanostructures and random alloys. Recently, we have implemented full-potential capability in the LSMS method that enables the calculation of the Hellmann-Feynman force and also allows \textit{ab initio} investigation of materials with dislocations, interstitial defects, etc. In this presentation, we will show the scalability of the full-potential LSMS method on supercomputers, and discuss its applications in the study of mechanical properties of transition metal alloys.

*This work is supported by DOE, Office of Science, BES, MSE Division. This research used resources of the Oak Ridge Leadership Computing Facility, which is supported by the Office of Science of DOE under Contract No. DE-AC05-00OR22725.
8:24AM A22.00003: Application of full-potential LSMS method in high entropy alloys*  XIANGLIN LIU (Presenter), Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputing Center, CARNegie MELLon UNIVERSITY, MARKUS EISENBACH, GEORGE MALcolm STOCKS, Oak Ridge National Laboratory — The ability to treat large number of atoms from first principles is highly desired for the investigation of alloy systems. Here we demonstrate our latest implementation of the full potential LSMS method (FP-LSMS) that can accurately calculate systems with thousands of atoms. The acceleration is achieved by a parallelization of the FFT part of the Poisson solver for the electrostatic potential. We employed the code to investigate the elastic properties of high entropy alloys, which are a class of interesting new structural materials. Moreover, to demonstrate the power of the FP scheme, we used FP-LSMS to calculate the Hellman-Feynman forces.

*This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. This research used resources of the Oak Ridge Leadership Computing Facility, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

8:36AM A22.00004: Opportunities for exascale in the characterization of uranium materials*  ASHLEY SHIELDS (Presenter), ANDREW MISKOWIEC, JENNIFER NIEDZIELA, MARIE C KIRKEGAARD, ROGER KAPSIMALIS, BRIAN ANDERSON, Oak Ridge National Laboratory — Characterizing new materials or unknown polycrystalline solids is a long-standing challenge for chemists. This problem has new resonance with the nuclear forensics community, where polycrystalline and amorphous materials are regularly encountered. Further, prediction of crystal structures and the calculation of vibrational properties for actinide materials is computationally intensive, limiting the unit cell size and number of structures which can be calculated. By analyzing basic geometric configurations, we hope to isolate spectroscopic characterization of low-symmetry systems to fundamental units. We have performed an analysis of coordination geometries of over 4000 uranium oxide and uranium fluoride structures, generated by combining genetic algorithm searches for stable phases with density functional theory. Here we present progress toward correlating vibrational properties with the fundamental coordination environments, aiming to facilitate interpretation of experimental analytical data from spectroscopy to characterize complex uranium phases. We discuss the opportunities and challenges for exascale computing and actinide materials, with an emphasis on the impacts and importance to the field of nuclear forensics.

*A.E.S. is funded by a US DHS Postdoctoral Fellowship

8:48AM A22.00005: Moving the Effective Fragment Molecular Orbital method towards exascale*  ANASTASIA GUNINA (Presenter), Ames Laboratory, MARK S GORDON, Chemistry, Iowa State University — Steep computational scaling and significant memory requirements of conventional electronic structure methods both limit the size of systems that can be described and hinder transitioning towards exascale computing. One of the ways to overcome these problems is to use fragmentation approaches. Our approach of choice is the Effective Fragment Molecular Orbitals (EFMO) method, which combines advantages of the Fragment Molecular Orbital (FMO) and the Effective Fragment Potential (EFP) methods. The current implementation in the GAMESS program package, however, is not optimized nor fully parallelized.

In this study, a major effort is related to optimizing the bottleneck step of generating EFP parameters, called MAKEFP, which needs to be repeated for every new fragment geometry in the EFMO method. In addition, improvements implemented in other parts of the EFMO code include increasing accessible system sizes. The resulting performance is demonstrated using a ~1700-atoms piece of a mesoporous silica nanoparticle (MSN), which was inaccessible in the original implementation.

*Department of Energy Exascale Computing Project (ECP) grant

9:00AM A22.00006: Recent Advances in PARSEC for Performing Large-scale Electronic Structure Calculations in Real Space*  KAI-HSIN LIOU (Presenter), JAMES CHELIKOWSKY, University of Texas at Austin, CHAO YANG, Lawrence Berkeley National Laboratory — The electronic structure of various types of materials, including complex biomolecules, nanostructures, and interfacial systems can be obtained by solving the Kohn–Sham (KS) equations. PARSEC, a real-space pseudopotential density functional theory KS equation solver, can routinely tackle systems with thousands of atoms using a Chebyshev-filtered subspace iteration (CheFSI) method. We will present a number of recent advances made in PARSEC that allow users to tackle larger systems that contain tens of thousands of atoms. These new advances include new parallelization strategies that significantly improve the scalability of orthogonalization and the Rayleigh–Ritz steps in the CheFSI framework and a more efficient way to perform the previously proposed spectrum slicing method. We will demonstrate the scalability of both the CheFSI and spectrum slicing methods on modern high performance computers and discuss the remaining challenges.

*Our work is supported by an award from the U.S.Department of Energy under Contract No. DE-AC02-05CH11231
Towards Paradigm Shifts in Electronic Structure Calculation for Large Systems: Wavelets, Fragments and Advanced Treatments of Excited States* [Invited] LAURA RATCLIFF (Presenter), Department of Materials, Imperial College London, STEPHAN MOHR, Barcelona Supercomputing Center, THIERRY DEUTSCH, LUIGI GENOVESE, CEA Grenoble — The increasing power of massively parallel machines offers new opportunities for first principles materials simulations, providing software can be developed to effectively exploit new hardware. Density functional theory (DFT) has enjoyed widespread success for systems of up to a few hundred atoms, but is limited by the cubic scaling with the number of atoms of standard approaches. However, in recent years various linear scaling (LS) approaches have been developed, enabling simulations on tens of thousands of atoms. Since the parallel scalability is related to the number of atoms, such methods are also well suited to exploit supercomputers. One key factor influencing the accuracy and cost of DFT is the choice of basis set, where minimal, localized basis sets compete with extended, systematic basis sets. However, wavelets offer both locality and systematicity and are thus ideal for representing an adaptive local orbital basis which may be exploited for LS-DFT [1]. One may also make further approximations, e.g. dividing a system into fragments or exploiting underlying repetition of local chemical environments [2,3], where each approximation may be controlled and quantified. This ability to treat large systems with controlled precision offers the possibility of new types of materials simulations [4].

We will demonstrate the advantages of wavelets as a basis for large scale DFT calculations, as implemented in BigDFT. We will focus on the example of materials for organic LEDs, showing how our approach may be used to account for environmental and statistical effects on excited state calculations of disordered supramolecular materials [5].


*LER acknowledges an EPSRC Early Career Research Fellowship

Affordable and accurate large-scale hybrid-functional calculations on GPU-accelerated supercomputers* THIERRY DEUTSCH (Presenter), LUIGI GENOVESE, CEA Grenoble, LAURA RATCLIFF, Imperial College London — Since 2008, the BigDFT project consortium has developed an ab initio DFT code based on Daubechies wavelets. Performing high accuracy hybrid functional calculations for condensed matter systems containing a large number of atoms is at present computationally very demanding or even out of reach if high quality basis sets are used. We present a highly optimized multiple graphics processing unit implementation of the exact exchange operator which allows one to perform fast hybrid functional density-functional theory (DFT) calculations with systematic basis sets without additional approximations for up to a thousand atoms. With this method hybrid DFT calculations of high quality become accessible on state-of-the-art supercomputers within a time-to-solution that is of the same order of magnitude as traditional semilocal-GGA functionals. The method is implemented in a portable open-source library.

Laura E Ratcliff et al 2018 J. Phys.: Condens. Matter 30 095901

*This work was done within the MARVEL and PASC programs. We acknowledge computational resources from the Swiss National Supercomputing Center (CSCS) and research resources from the Argonne Leadership Computing Facility. Computer time was also provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.
At 10:00 AM A22.00009: Attacking the Strong and Weak Scaling Limits in Linear Scaling Hybrid Density Functional Theory

ROBERT DISTASIO (Presenter), Chemistry and Chemical Biology, Cornell University, HSIN-YU KO, Chemistry, Princeton University, JUNTENG JIA, Chemistry and Chemical Biology, Cornell University, BISWAJIT SANTRA, Physics, Temple University, ZACHARY SPARROW, Chemistry and Chemical Biology, Cornell University, ALVARO VAZQUEZ-MAYAGOITIA, Argonne National Labs, XIFAN WU, Physics, Temple University, ROBERTO CAR, Chemistry, Princeton University — Hybrid density functional theory (DFT) represents a quite favorable balance between accuracy and cost, and has therefore become the de facto standard in quantum chemistry. However, the steep computational cost associated with a cubic-scaling reciprocal-space evaluation of the exact-exchange energy has largely hindered the widespread use of hybrid DFT in the condensed phase. By utilizing a local representation of the occupied space, we have developed a formally exact and linear-scaling algorithm that exploits the real-space sparsity in the exact-exchange interaction by rigorously treating all overlapping orbital pairs. In this work, we present a series of theoretical developments and algorithmic improvements which drastically reduce the time to solution and take us one step closer to routine hybrid DFT-based ab initio molecular dynamics simulations of large-scale condensed-phase systems. In particular, we will focus on: (i) novel preconditioning techniques to speed up the computation, (ii) game and graph theoretical methods to improve the workload imbalance, (iii) sparse and asynchronous data transfer to mitigate the communication cost, and (iv) extensive code optimization/vectorization to efficiently utilize current- and next-generation architectures.

At 10:12 AM A22.00010: Large-Scale Benchmark of Electronic Structure Solvers with the ELSI Infrastructure*

VICTOR YU (Presenter), Department of Mechanical Engineering and Materials Science, Duke University, WILLIAM DAWSON, Center for Computational Science, RIKEN, Japan, ALBERTO GARCIA, Laboratorio de Estructura Electronica de Materiales, Institut de Ciencia de Materials de Barcelona, Spain, VILLE HAVU, Department of Applied Physics, Aalto University, Finland, BEN HOURAHINE, Department of Physics, University of Strathclyde, Scotland, WILLIAM P HUHN, Department of Mechanical Engineering and Materials Science, Duke University, MATHIAS JACQUELIN, Computational Research Division, Lawrence Berkeley National Laboratory, WEILE JIA, Department of Mathematics, University of California, Berkeley, MURAT KECELI, Argonne Leadership Computing Facility, Argonne National Laboratory, RAUL LAASNER, Department of Mechanical Engineering and Materials Science, Duke University, YINGZHOU LI, Department of Mathematics, Duke University, LIN LIN, Department of Mathematics, University of California, Berkeley, JIANFENG LU, Department of Mathematics, Duke University, JOSE ROMAN, Departament de Sistemes Informatics i Computacio, Universitat Politècnica de València, Spain, ALVARO VAZQUEZ-MAYAGOITIA, Argonne Leadership Computing Facility, Argonne National Laboratory, CHAO YANG, Computational Research Division, Lawrence Berkeley National Laboratory, VOLKER BLUM, Department of Mechanical Engineering and Materials Science, Duke University — Routine application of electronic structure theory to systems consisting of thousands of atoms is often hindered by the solution of an eigenproblem. We here present an update to the ELectronic Structure Infrastructure (ELSI), an open-source software interface to facilitate the implementation and optimal use of high-performance solver libraries covering cubic scaling eigensolvers, linear scaling density-matrix-based algorithms, and other reduced scaling methods in between. The ELSI interface has been integrated into four electronic structure code projects (DFTB+, DGDFT, FHI-aims, SIESTA), forming the foundation of our effort to rigorously benchmark the performance of the solvers on equal footing. This presentation will particularly focus on a systematic set of large-scale benchmarks for multiple solvers performed with Kohn-Sham density-functional theory and density-functional tight-binding theory. Factors that strongly affect the efficiency of the solvers are identified and analyzed, including system size and dimensionality, matrix sparsity, eigenspectrum width, number of MPI processes, etc. Based on these benchmarks, we discuss our strategy to automatically select a solver for an arbitrary problem.

*This work is supported by NSF under grant number 1450280.
Enabling Large-Scale Isobaric-Isothermal Hybrid Density Functional Theory Simulations in the Condensed Phase

HSIN-YU KO (Presenter), Chemistry, Princeton University, ROBERT DISTASIO, Chemistry and Chemical Biology, Cornell University, BISWAJIT SANTRA, Physics, Temple University, ROBERTO CAR, Chemistry, Princeton University — The combination of ab initio molecular dynamics (AIMD) and high-performance computing (HPC) has the potential to furnish an atomistic-level understanding of complex condensed-phase systems such as molecular liquids and crystals. Such a detailed understanding requires an accurate treatment of both the quantum mechanical interactions and statistical mechanical sampling under realistic experimental conditions (e.g., in the isobaric-isothermal (NpT) ensemble). However, the routine use of sophisticated quantum mechanical methods like dispersion-inclusive hybrid density functional theory (DFT) is hindered by the cubic-scaling cost of conventional reciprocal-space based approaches. With the use of localized occupied orbitals, we have developed a formally exact and linear-scaling algorithm that directly addresses this prohibitive cost. In this work, we derive and implement the exact-exchange contributions to the stress tensor, thereby enabling hybrid DFT-based AIMD simulations of arbitrary cell sizes and shapes in the NpT ensemble. As an application of this method, we will discuss the pyridine molecular crystal.


NWChemEx: Tackling Chemical, Materials, and Biochemical Challenges in the Exascale Era

WIBE A DE JONG (Presenter), Lawrence Berkeley National Laboratory, KRISTOPHER W. KEIPERT, RAYMOND A. BAIR, Computational Science Division, Argonne National Laboratory, RYAN RICHARD, JEFFREY S. BOSCHEN, THERESA L. WINDUS, Ames Laboratory, Iowa State University, ROBERT J HARRISON, Institute for Advanced Computational Science, Stony Brook University, THOMAS DUNNING, Northwest Institute for Advanced Computing, Pacific Northwest National Laboratory — Historically, the NWChem computational chemistry package has been adapted and optimized for supercomputer architectures as they emerged. While this strategy has been successful over the past two decades, adapting NWChem to the major changes in hardware and programming models anticipated at the exascale is infeasible without a revolutionary redesign of the code. The NWChemEx project is redesigning and re-implementing NWChem for exascale computers using C++ with the goal of dramatically improving upon the scalability, performance, extensibility, and portability of the original application. In the first portion of this talk, the limitations of NWChem will be described. Next, we will illustrate how the scalability limitations are addressed in the NWChemEx design via the implementation of novel reduced-scaling methods with a new high-performance tensor library. Finally, we will show how lossy compression and differenced checkpointing techniques are utilized in NWChemEx to address more general exascale challenges related to data volume and system resilience.

Fast Heat-Bath Configuration Interaction

JUNHAO LI (Presenter), MATTHEW OTTEN, ADAM HOLMES, Cornell University, SANDEEP SHARMA, Department of Chemistry and Biochemistry, University of Colorado Boulder, CYRUS JEHANGIR UMRIGAR, Cornell University — For many quantum mechanical systems the entire Hilbert space is enormous, but the important part is many orders of magnitude smaller. We have recently developed the semistochastic heat-bath configuration interaction (SHCI) method for efficiently calculating such systems. It is a systematically improvable selected configuration interaction plus perturbation theory method that is capable of giving essentially exact energies for larger systems than is possible with other such methods. I present recent advances we have made to the method that allow us to use 2 billion variational determinants and trillions of perturbative determinants. Details about the key data structures and the parallelization are presented. We use the algorithm to compute the potential energy surface of the very challenging chromium dimer in the cc-pVDZ-DK basis, correlating 28 valence and the semicore electrons. The Hilbert space has 5*10^29 determinants. At equilibrium our energy agrees with the recent p-DMRG energy, but is more precise. We also present results for the homogeneous electron gas.

Monday, March 4, 2019 8:00 AM - 10:12 AM
8:00AM A23.00001: Single Atom Scale Manipulation of Matter by Scanning Transmission Electron Microscopy [Invited]
STEPHEN JESSE (Presenter), Oak Ridge National Laboratory — tbd

8:36AM A23.00002: Automation of Atom-Scale Device Patterning using Machine Learning
JEREMIAH CROSHAW (Presenter), MOHAMMAD RASHIDI, KIERAN MASTEL, MARCUS TAMURA, Physics, University of Alberta — In recent years, research involving dangling bonds (DBs) patterned on hydrogen-terminated silicon (H-Si) has reached several significant benchmarks, including their applications as logic gates, binary wires¹ and rewritable memory². These newly developed devices show promise for the implementation of atom scale DB circuitry. As device applications become realizable, automation of device fabrication is necessary to facilitate the transition to commercial applications. We show that by incorporating a deep neural network in our patterning process, we can greatly reduce the amount of active user time needed for device fabrication. Semantic segmentation is used with a convolution-deconvolution network to properly map and label surface defects. By combining this neural network with libraries from a commercial scanning probe microscope controller and a previously implemented probe tip conditioning suite³, complete automation of the patterning process is realized.


8:48AM A23.00003: Reduced Damage Electron Microscopy with Conditional Sample Re-illumination*
AKSHAY AGARWAL (Presenter), Electrical Engineering and Computer Science, Massachusetts Institute of Technology, YURI VAN STAADEN, Technische Universiteit Delft, VIVEK GOYAL, Electrical and Computer Engineering, Boston University, KARL K BERGGREN, Electrical Engineering and Computer Science, Massachusetts Institute of Technology — We propose and theoretically analyze an electron microscopy scheme based on multiple sample illuminations with a very low current beam, in combination with Elitzur and Vaidman's interaction-free measurement scheme. Our analysis starts with a prior guess for the characteristic transparency of each pixel on the sample. We update these priors after each round of illumination based on the statistics at the imaging detectors. The re-illumination for a pixel ceases once a stopping criterion is met. This criterion could be based on either a minimum required signal-to-noise-ratio, or a maximum imaging time. We show that this scheme reduces the damage suffered by the sample during imaging, compared to a conventional imaging scheme without conditional re-illumination. We calculated the maximum resolution at a given sample damage and signal-to-noise ratio that could be obtained with this scheme. This resolution shows an improvement over that from conventional imaging. We are working towards implementing this scheme on a scanning electron microscope, modified to include bright- and dark-field transmission electron detectors, and a fast beam blanker to obtain extremely low-dose electron pulses.

*This work was funded by the Gordon and Betty Moore foundation, and the U.S. NSF under Grant 1422034.

9:00AM A23.00004: In situ observation of Sb₂S₃ single crystal formation in glass by micro x-ray diffraction *
COURTNEY AU-YEUNG (Presenter), Physics, Lehigh University, CAMELIA STAN, NOBUMICHI TAMURA, Lawrence Berkeley National Laboratory, HIMANSHU JAIN, Materials Science and Engineering, Lehigh University, VOLKMAR R G DIEROLF, Physics, Lehigh University — Single crystal architectures in glass can be formed by a solid-solid transformation via localized heating by a laser or x-ray beam. As a result of the confined environment and the asymmetry of the boundary conditions close to the surface new phenomena such as a rotating crystal lattice are observed. This novel form of a crystals can offer new functionalities in micro/nano-opto-electro-mechanical systems. To understand the process of lattice formation that proceeds via crystal growth, we have observed in situ Sb₂S₃ crystal formation under x-ray irradiation. In these experiments, an x-ray beam is used as the heating source to fabricate the crystal structures while Laue diffraction patterns are collected at the same time. We explore the earliest stages of crystallization in this model system wherein glass transforms into single crystal without any change in local composition or long-range diffusion. The implications of these observations for the origin of the lattice rotation and crystal growth in a confined medium will be discussed.

*This work is supported by the National Science Foundation Graduate Research Fellowship under Grant #DGE-1452783 and the U.S. Department of Energy, Basic Energy Science Division Award #DE-SC0005010
Characterization of stress induced by Si$_{1-x}$Ge$_x$ in the active epitaxial film on a SOI substrate via Scanning Surface PhotoVoltage Microscopy. JAMES SLINKMAN (Presenter), RF Technology Development, IBM Microelectronics (retired), DAMINDA DAHANAYAKA, PHILIP KASZUBA, LEON MOSZKOWICZ, RANDALL WELLS, SPM Laboratory, Globalfoundries, LLOYD BUMM, Dept. of Physics & Astronomy, University of Oklahoma — The mobility and breakdown voltage of field-effect transistors fabricated on a Silicon-on-Insulator substrate can be improved by embedding a Si$_{1-x}$Ge$_x$ layer in the active epitaxial silicon layer\textsuperscript{1}. The choice of the Ge fraction, $x$, dictates the mobility improvement due to band-bending proportionate to misfit strain. The thickness of the embedded Si$_{1-x}$Ge$_x$ layer, modulates associated stress relaxation, the density of extended defects, and degree of amorphization of the epitaxy. Techniques such as TEM and Raman spectroscopy are traditionally used to characterize the film stress state in such heterostructures. We present here a systematic study of the evolution of the stress state and relaxation as a function of the Si$_{1-x}$Ge$_x$ layer thickness in the active epitaxy on production SOI wafers using a novel technique, Scanning Surface PhotoVoltage Microscopy (SSPVM). These results are correlated with those obtained by Raman spectroscopy. Some advantages of the use of SSPVM are noted, as well other uses of it for semiconductor characterization.


Artificial Neural Networks for Analysis of Coherent X-Ray Diffraction Images* DANIEL ABARBANEL (Presenter), MARK SUTTON, HONG GUO, Physics, McGill University — We present an application of neural networks to the analysis of diffraction images produced via X-ray photon correlation spectroscopy (XPCS) experiments. The detection apparatus for these experiments is an array of charge-coupled devices (CCDs). Determining the incident location of each photon allows for estimation of the image contrast, which elucidates structural and dynamical properties of a measured system such as diffusion constant and particle radius. Photons incident on the detector in the same vicinity result in additive interference that obscures their individual locations. A neural network classifier was designed and trained on data from an artificial model to scan an image and determine a discrete probability distribution for the number of photons that have been incident within the area of each CCD. These distributions were fit to the contrast and were found to be in agreement with the true underlying value. We have thus demonstrated a promising method for accurately determining the contrast from experimental XPCS images.

*Supported by the Natural Sciences and Engineering Research Council (NSERC) and McGill University.

2-beam action spectroscopy for probing multiphoton absorption processes in semiconductors* NIKOLAOS LIAROS (Presenter), DANIEL JOVINELLI, JOHN T FOURKAS, University of Maryland, College Park — We recently introduced a new class of methods, called two-beam action (2-BA) spectroscopies for determining the order of effective absorptive nonlinearity in different materials. The 2-BA spectroscopy approach offers significant advantages over traditional logarithmic plots of an observable as a function of average excitation power, particularly when multiple orders of absorption are involved. In this work, we extend the 2-BA concept in a technique that we call 2-beam constant-amplitude photocurrent spectroscopy (2-BCAmP). We use this technique to study multiphoton absorption in wide-bandgap semiconductors. 2-BCAmP allows us for the measurement of the effective order of the absorption process at any desired value of the photocurrent or photovoltage, as opposed to traditional approaches that require data that span several orders of magnitude of average excitation power. Furthermore, the relative contributions of two different absorption orders can be extracted from non-integral 2-BCAmP exponents, and these data to validate the model of the absorption orders that are involved in photocurrent generation.

*This work was supported by the National Science Foundation, grant CMMI-1449309

High-Resolution Localization with Arbitrary Point Spread Functions ROHAN PARAB, Texas Tech University, CRAIG SNOEYINK (Presenter), Mechanical and Aerospace Engineering, University at Buffalo — We present a method of three dimensional localization of particles which is agnostic to point spread functions and which achieves high localization resolution. By learning the spatial variation of the imaging system’s point spread function using computationally efficient spline surfaces it is possible to utilize convex expectation-maximization localization methods with any imaging system. Perhaps more importantly, this methodology allows for the use of common localization point spread functions (Astigmatism, Double-Helix, Bessel Beam among others) but where strong aberrations might have precluded measurements. In addition to the method we will present experimental results comparing the resolution of this technique to localization where the point spread function is well known.
10:00AM A23.00009: Development of in-situ RF-enabled high-brightness femtosecond electron microscopy for complex material research*  
SHUAISHUAI SUN (Presenter), XIAOYI SUN, DANIEL BARTLES, ELLIOT D WOZNIAK, JOSEPH WILLIAMS, FARAN ZHOU, Department of Physics and Astronomy, Michigan State University, NELSON SEPULVEDA, Department of Electrical and Computer Engineering, Michigan State University, CHONG-YU RUAN, Department of Physics and Astronomy, Michigan State University — Correlated structural and electronic degrees of freedom in electronic materials help engineer macroscopic functional responses to external control parameters. Increasingly, new functionalities have been explored through integrating different electronic materials to form hybrid interfaces. Spatially and temporally resolved imaging and spectroscopy probe could provide a new perspective to study functionalities in ever increasing complexity in these new material platforms. However, significant challenges exist in reaching adequate sensitivities at the ultrafast timescale and nanometer spatial scale. Here we report a new development of ultrafast in-situ electron microscopy to address this limitation through active control of high-intensity femtosecond electron pulses, targeting the respective probe space using adaptive optics. An integrated system with compact DC gun, RF compression optics, and commercial TEM electron optics is established with the aim of nanometer-scale selected area imaging and core-level spectroscopy with combined ~100 femtosecond and ~1 eV resolution. We demonstrate our first application in studying the inhomogeneous phase transitions in VO₂ microelectronic devices.

*We acknowledge support by DOE Grant DE-FG02-06ER46309 and NSF MRI Grant DMR 1625181.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A24 DAMOP: Strongly Interacting Quantum Fermi and Bose Gases BCEC 159 - Bo Zhen, University of Pennsylvania

8:00AM A24.00001: Probing the many-body physics via measurement of the closed-channel fraction in a ⁶Li superfluid*  
QIJIN CHEN, Zhejiang University, XING-CAN YAO (Presenter), XIANG-PEI LIU, HAO-ZE CHEN, XIAO-QIONG WANG, YU-XUAN WANG, YU-AO CHEN, Department of Modern Physics, University of Science and Technology of China, KATHRYN LEVIN, University of Chicago, JIAN-WEI PAN, Department of Modern Physics, University of Science and Technology of China — Atomic Fermi gases provide an ideal platform for studying the pairing and superfluid physics, utilizing a Feshbach resonance between closed channel molecular states and open channel scattering states. The closed-channel fraction \( Z \) contains important many-body interacting effects. Here we probe the many-body physics of interacting Fermi gases of \( ^6\text{Li} \) by measuring \( Z \) in the entire system. We have observed a significant departure from two-body physics. Away from the deep BEC regime, the fraction \( Z \) is sensitive to the Fermi temperature \( T_F \). In particular, our data show \( Z \sim \sqrt{T_F} \) at unitarity, in good agreement with theory. Further more, we have found a progressive departure of our measured \( Z \) value from theory as the system enters the BCS regime, calling for further investigation in both theory and experiment.

*This work is supported by the National Key R&D Program of China (under Grant No. 2018YFA0306501), the NSFC of China (under Grant No. 11425417 and No. 11774309), the CAS, and the Fundamental Research Funds for the Central Universities (under Grant No. WK234000081), NSF of Zhejiang Province of China (Grant No. LZ13A040001), and NSF-DMR-MRSEC 1420709.

8:12AM A24.00002: Comparative Study of One-Dimensional Bose and Fermi Gases with Contact Interactions*  
YUTA SEKINO (Presenter), Department of Physics, Tokyo Institute of Technology, SHINA TAN, School of Physics, Georgia Institute of Technology, YUSUKE NISHIDA, Department of Physics, Tokyo Institute of Technology — One-dimensional spinless Bose and Fermi gases with contact interactions have the close relationship via Girardeau’s Bose-Fermi mapping, leading to the correspondences in their energy spectra and thermodynamics. However, correlation functions are in general not identical between these systems. We derive in both systems the universal relations for correlation functions, which hold for any energy eigenstate and any statistical ensemble of the eigenstates[1]. These relations include the large-momentum tails of static structure factors and of momentum distributions as well as energy relations, which connect the sums of kinetic and interaction energies to the momentum distributions. The relations involve two- and three-body contacts, which measure local two- and three-body correlations, respectively. We clarify how the relations for bosons and fermions differ and are connected with each other. In particular, we find that the three-body contact makes no contribution to the bosonic energy relation, but it plays a crucial role in fermionic one.


*The work was supported by JSPS KAKENHI Grants No. JP15K17727 and No. JP15H05855 and by the US National Science Foundation CAREER award under Grant No. PHY-1352208.
8:24AM A24.00003: Ultracold Gas of NaLi Molecules in the Triplet Ground State  JULIANA PARK (Presenter), Massachusetts Institute of Technology — Ultracold gases of molecules allow us to study short-range chemical reactions, novel quantum phases, and quantum information processing. The NaLi molecule, the lightest bi-alkali molecule, in the triplet ground state has permanent electric and magnetic dipole moments and is predicted to have a small universal loss rate leading to long collisional lifetime. This enables us to investigate the complexity of chemical reactions by finding links to scattering theory. Also, with the aid of tunable long-range interactions between the molecules, we can explore the possibility of quantum simulation of many-body physics. We have previously achieved the long-lived triplet ground state molecules in an optical dipole trap through a two-step process: formation of Feshbach molecules and stimulated rapid adiabatic passage. We report results of recent studies with our triplet state molecules including the observation of long lifetime of the molecules in a longer wavelength optical dipole trap.

8:36AM A24.00004: An improved Lieb-Robinson bound for many-body Hamiltonians with power-law interactions  FRANCISCO MACHADO (Presenter), University of California, Berkeley, DOMINIC ELSE, Massachusetts Institute of Technology and University of California, Santa Barbara, CHETAN NAYAK, University of California, Santa Barbara and Microsoft Research, Station Q, NORMAN YAO, University of California, Berkeley and Lawrence Berkeley National Laboratory, Materials Sciences Division — The Lieb-Robinson bound limits the velocity of the spread of information in non-relativistic short-range interacting quantum systems, inducing a notion of speed of light. More specifically, it proves that, under time evolution, any local operator remains confined (up to exponentially decaying tails) to a region whose radius grows linearly with time. Motivated by experimental platforms such as ion traps, Rydberg atoms and spin defects in solids, recent work has investigated such bounds in long-range interacting systems, where the interaction strength decays as a power-law of the distance. In these results, the extent of the time evolved local operator is characterized by power-law tails and one obtains a power-law light-cone. In this talk, we introduce a new notion of light-cone for power-law interacting systems that induces a more stringent definition of locality. We prove new Lieb-Robinson bounds for multi-body interacting systems which improve the spatial decay profile of the time evolved local operator and thus lead to a better light-cone. These improvements enable the proof of the existence of a long-lived prethermal regime in long-range interacting systems.

8:48AM A24.00005: Quantum phases of many-body dipolar system in one dimension*  NIRAJ GHIMIRE (Presenter), SUSANNE F YELIN, Department of Physics, University of Connecticut — We study the zero temperature quantum phases of dipoles in a quasi-one-dimensional zigzag chain. Since the dipole-dipole interaction is long-range, a dipolar many-body system is predicted to feature intriguing phases. We investigate the many-body effects in this model using the Density Matrix Renormalization Group (DMRG) method.

*This research project is supported by National Science Foundation.

9:00AM A24.00006: Efimov Enhanced Kondo Effect in Alkaline and Alkaline-Earth Atomic Gas Mixture  JUAN YAO (Presenter), HUI ZHAI, Tsinghua University, REN ZHANG, Xi'an Jiaotong University — Recent experiment has observed Feshbach resonances between alkaline and alkaline-earth atoms. These Feshbach resonances are insensitive to the nuclear spin of alkaline-earth atoms. Utilizing this feature, we propose to take this system as a candidate to perform quantum simulation of the Kondo effect. An alkaline atom can form a molecule with an alkaline-earth atom with different nuclear spins, which plays the role of spin-exchange scattering responsible for the Kondo effect. Furthermore, we point out that the existence of three-body bound state and atom-molecule resonance due to the Efimov effect can enhance this spin-exchange scattering, and therefore enhance the Kondo effect. We discuss this mechanism first with a three-body problem in free space, and then demonstrate that the same mechanism still holds when the alkaline atom is localized by an external trap and becomes an impurity embedded in the alkaline-earth atomic gases.

9:12AM A24.00007: Asymmetric Conductivity as a Manifestation of Kondo Effect in Cold Atom  YANTING CHENG (Presenter), XIN CHEN, Tsinghua University, ZHIGANG WU, Southern University of Science and Technology, REN ZHANG, Department of Applied Physics, School of Science, Xi'an Jiaotong University — Motivated by recent theoretical and experimental advances in the quantum simulation of alkaline earth(AE) atoms, we raise a proposal to detect the Kondo physics in cold atom system. It has been demonstrated that the intrinsic spin-exchange interaction in AE atoms can be significantly enhanced near a confinement-induced resonance(CIR), which facilitates the simulation of Kondo physics. Since the Kondo effect appears only for antiferromagnetic coupling, we find that the conductivity of such a system exhibits an asymmetry across a resonance of spin-exchange interaction. The asymmetric conductivity can serve as the smoking gun for Kondo physics in the cold-atom context. When an extra magnetic field ramps up, the spin-exchange process near Fermi surface is suppressed by Zeeman energy and hence the conductivity becomes more and more symmetric. Our results can be verified in the current experimental setup.
Variational methods are extensively used in quantum many-body problems to overcome the exponential growth of the Hilbert space with the system size. By focusing on a suitable submanifold of states, we can study properties of ground states and low excited states. Here, we will introduce a novel framework to approximate the low lying energy spectrum by studying the linearized Hamiltonian flow on the tangent plane to this manifold at the ground state.

Part I: After explaining our method, I will compare it with other tangent plane approaches and discuss key advantages in the context of the paradigmatic Bose-Hubbard model.

Variational methods are extensively used in quantum many-body problems to overcome the exponential growth of the Hilbert space with the system size. By focusing on a suitable submanifold of states, we can study properties of ground states and low excited states. Here, we will introduce a novel framework to approximate the low lying energy spectrum by studying the linearized Hamiltonian flow on the tangent plane to this manifold at the ground state.

Part II: I will focus on the underlying geometry and explain how the approximate ground state and the low energy spectra arise from invariant geometric structures of the variational manifold.

*This work is supported by the Max Planck Harvard Research Center for Quantum Optics.

I will present an experimental test of the new theory of Generalized HydroDynamics (GHD), introduced in 2016 to describe long wave-length dynamics of one-dimensional (1d) quantum integrable systems [1]. Integrable systems possess an infinite number of conserved quantities and GHD takes into account the conservation of all of them. We monitor the time evolution of the in situ density profiles of a single 1d cloud of bosonic atoms trapped on an atom chip after a quench of the longitudinal trapping potential. The weakly interacting atomic clouds lie at the crossover between the quasicondensate and the ideal Bose gas regimes. Predictions of GHD are in very good agreement with the experiment. Previously existing theories such as the "conventional" hydrodynamic approach, which relies on the assumption of local thermal equilibrium, described by a Gibbs ensemble, are unable to reproduce the experimental data. These results can be found in [3].


*MS acknowledges support by the Studienstiftung des Deutschen Volkes.
10:12AM A24.00012: Hydrodynamics of operator spreading and quasiparticle diffusion in interacting integrable systems (part I)* SARANG GOPALAKRISHNAN, Physics, The Graduate Center, CUNY, DAVID HUSE, Physics, Princeton University, VEDIKA KHEMANI, Physics, Harvard University, ROMAIN VASSEUR (Presenter), University of Massachusetts Amherst — We address the hydrodynamics of operator spreading in interacting integrable lattice models. In these models, operators spread through the ballistic propagation of quasiparticles, with an operator front whose velocity is locally set by the fastest quasiparticle velocity. In interacting integrable systems, this velocity depends on the density of the other quasiparticles, so equilibrium density fluctuations cause the front to follow a biased random walk, and therefore to broaden diffusively. Ballistic front propagation and diffusive front broadening are also generically present in non-integrable systems in one dimension; thus, although the mechanisms for operator spreading are distinct in the two cases, these coarse grained measures of the operator front do not distinguish between the two cases. Our results elucidate the microscopic mechanism for diffusive corrections to ballistic transport in interacting integrable models.

*This work was supported by NSF Grant No. DMR-1653271 (S.G.), DOE grant No. DE- SC0016244 (D.A.H.), US Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0019168 (R.V.). V.K. is supported by the Harvard Society of Fellows and the William F. Milton Fund.

10:24AM A24.00013: Hydrodynamics of operator spreading and quasiparticle diffusion in interacting integrable systems (Part II)* VEDIKA KHEMANI (Presenter), Harvard University, SARANG GOPALAKRISHNAN, City University of New York, DAVID HUSE, Princeton University, ROMAIN VASSEUR, University of Massachusetts Amherst — We address the hydrodynamics of operator spreading in interacting integrable lattice models. In these models, operators spread through the ballistic propagation of quasiparticles, with an operator front whose velocity is locally set by the fastest quasiparticle velocity. In interacting integrable systems, this velocity depends on the density of the other quasiparticles, so equilibrium density fluctuations cause the front to follow a biased random walk, and therefore to broaden diffusively. Ballistic front propagation and diffusive front broadening are also generically present in non-integrable systems in one dimension; thus, although the mechanisms for operator spreading are distinct in the two cases, these coarse grained measures of the operator front do not distinguish between the two cases. Our results elucidate the microscopic mechanism for diffusive corrections to ballistic transport in interacting integrable models.

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10:36AM A24.00014: Hydrodynamics with Spacetime-dependent Scattering Length* KEISUKE FUJII (Presenter), YUSUKE NISHIDA, Department of Physics, Tokyo Institute of Technology — Hydrodynamics provides concise but powerful description of long-time and long-distance physics of correlated systems out of thermodynamic equilibrium. Here we construct hydrodynamic equations for nonrelativistic particles with the spacetime-dependent scattering length and show that it enters constitutive relations uniquely so as to represent the fluid expansion and contraction in both normal and superfluid phases. As a consequence, we find that a leading dissipative correction to the contact density due to the spacetime-dependent scattering length is proportional to the bulk viscosity. Also, when the scattering length is slowly varied over time in a uniform system, the entropy density is found to be produced even without fluid flows in proportion to the bulk viscosity, which may be useful as a novel probe to measure the bulk viscosity in ultracold atom experiments.

*This work was supported by JSPS KAKENHI Grants No. JP15K17727 and No. JP15H05855. One of the authors (K.F.) was also supported by International Research Center for Nanoscience and Quantum Physics, Tokyo Institute of Technology and by RIKEN Junior Research Associate Program.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A25 DPOLY: Deformation, Flow and Relaxation of Melt and Glassy Polymers BCEC

160A - Robert Riggleman, University of Pennsylvania
8:00AM A25.00001: Dynamic Mechanical Spectrum of an Epoxy Polymer  JAMES M CARUTHERS (Presenter), YELIN NI, GRIGORI MEDVEDEV, Purdue University — Dynamic mechanical experiments were performed on an epoxy thermoset with a $T_g=101^\circ$C over a wide temperature range from -150$^\circ$C to 260$^\circ$C. Time-temperature superposition (TTS) is only observed at temperatures above $T_g+100^\circ$C where the network relaxation is the dominant relaxation process. At lower temperatures, both above and below $T_g$, TTS is clearly violated. The traditional representation of the relaxation spectrum as a sum of several broad empirical functions each with its own independent temperature dependence that are often designated as $\alpha$-, $\beta$-, etc. processes cannot describe the set of isotherms. Using a procedure that includes Tikhonov regularization with adaptive meshing, a relaxation spectrum consisting of discrete processes emerges. It is shown that determination of the spectrum is robust, resulting in a continuous spectrum at high temperatures and discrete peaks at lower temperatures. Each relaxation process has its own temperature dependence, which becomes stronger as $T_g$ is approached. Below $T_g$ the relaxation time of each process is affected differently by aging. The implications of a discrete spectrum of relaxation times vs. the more commonly assumed continuous distribution of relaxation processes for a theory of the amorphous state will be discussed.

8:12AM A25.00002: Different temperature dependence of nonlinear rheological responses in melt stretching*  JIANNING LIU, SHIQING WANG (Presenter), Department of Polymer Science, University of Akron — Decades of research in nonlinear polymer rheology [1] have not fully cleared all the confusion in the literature including one concerning the alleged difference in the rheological responses of entangled solutions and melts to fast extensional deformation. The idea of nematic interaction modification of chain friction has caused Huang et al. [2] to find support from the examination of three polystyrene solutions where the solvent is polystyrene of respective molecular weight equal 1 kg/mol (that has $T_g = 20^\circ$C), 2 kg/mol and 4 kg/mol with $T_g \sim 75^\circ$C. We refute this idea by investigating similar PS solutions to indicate a different interpretation by showing how a breakdown of the time-temperature superposition occurs in nonlinear responses of these solutions, causing the 1K solution to respond more strongly than a 5K solution where the 1K solution is examined at a lower temperature.


*This work is supported, in part, by NSF-DMR 1609977.

8:24AM A25.00003: Brittle-Ductile Transition of a polymer glass in the presence of a crack*  YEXIN ZHENG (Presenter), MESFIN TSIGE, SHIQING WANG, The University of Akron — Fracture behavior of polymer glasses under deformation has been widely studied in the experiment. However, molecular-level understanding of crack propagation in polymer glasses is still lacking. In this work, the standard bead-spring model based molecular dynamic simulation was modified to gain microscopic insights into the crack propagation in glassy polymers. In the presence of a pre-existing crack, the transition from brittle failure to shear yielding in extension was investigated by varying the temperature, the length of the pre-crack length and deformation rate. The results from the simulation are consistent with experiment. Our simulation results also show that the brittle-ductile transition temperature is strongly dependent on the strength of the pair potential.

*This work is supported, in part, by NSF-DMR 1609977.

8:36AM A25.00004: The relationship between unstable localized vibrational modes and dynamical heterogeneity in glass formers  WENGANG ZHANG (Presenter), JACK DOUGLAS, National Institute of Standards and Technology, FRANCIS STARR, Wesleyan University — The heterogenous dynamics of glass-forming materials is commonly characterized by the spatially correlated particles (clusters) with high and low mobilities, and are helpful for explaining the temperature dependence of the non-Arrhenius behavior of relaxation time. Due to the inherent difficulty to experimentally observe heterogeneous dynamical clusters, we consider the possibility that the localized unstable modes of the vibrational spectrum may be related to dynamical clusters. Specifically, we analyze the instantaneous normal modes (INMs) associated with the Hessian matrix of glass-forming liquids. We find that the particles that contribute most to the unstable, localized modes form spatially correlated clusters. We quantify the degree to which these clusters correlate to string-like cooperative motions and mobile clusters, and how polymer topology affects these clusters.
MASOUD RAZAVI (Presenter), SHIQING WANG, Department of Polymer Science, University of Akron — We borrow the insights that explain the molecular mechanism for the brittle-to-ductile transition in polymeric glasses [1] to study the mechanics of semicrystalline polymers. Polyesters such as poly(lactic acid) (PLA) and poly(ethylene terephthalate) (PET) are known to be brittle in their fully crystalline form. PLA is brittle in its amorphous state because of the rapid physical aging that cannot be avoided. Such poor mechanical properties are the bottleneck preventing the wider application of PLA to replace the petroleum-based polymers including PET. We demonstrate a strategy to make PLA tough and heat resistant with zero shrinkage at 100 °C along with a molecular picture detailing the structure-property relationship.

*This work is supported, in part, by NSF-DMR 1609977.

TREVOR BENNIN (Presenter), JOSHUA V RICCI, MARK EDIGER, University of Wisconsin - Madison — Polymer glasses are ubiquitous engineering materials, but their deformation is not well understood at a fundamental level. Here, the segmental dynamics of glassy poly(lactic acid) (PLA) were measured with a probe reorientation technique during constant strain rate tensile deformation at temperatures between T_g – 25 K and T_g – 15 K and local strain rates between 10^{-5} s^{-1} and 10^{-4} s^{-1}. The relaxation time of the undeformed PLA is about 10^4 s and decreases by up to a factor of 30 during deformation. The relaxation time in the plastic flow regime shows a temperature dependence of about 30 K/decade and is related to the local strain rate through a power-law relationship with an exponent near -1 for all investigated temperatures. We also find that the KWW β parameter for PLA increases during deformation from 0.42 to 0.60, indicating a narrowing of the distribution of relaxation times. These results are very similar to those previously reported on lightly crosslinked poly(methyl methacrylate) (PMMA) glasses, suggesting that these are universal effects of constant strain rate deformation on the segmental dynamics of polymer glasses.

*We thank the National Science Foundation (DMR-1708248) for support of this work

VALERIY GINZBURG (Presenter), Dow Chemical Company — The low-temperature behavior of glass-forming liquids is still poorly understood. Here, we propose a simple model with no divergence of relaxation time at any finite temperature. We hypothesize a “key degree of freedom” (KDF) associated with the Arrhenius-Andrade-Eyring transition state mechanism of the liquid flow. We then assume that the KDF energy levels are quantized in increments of ε (where ε can be an energy of a gauche-trans-gauche kink1 or another low-energy excitation). In that case, the “fictive temperature”, T_f, is proportional to the KDF internal energy, determined by the Planck-Bose-Einstein statistics, T_f = <u>/k_B = (ε/k_B)(exp(βε) – 1)^{-1}, where β = (k_B T)^{-1}. The temperature-dependent viscosity (or the shift factor) is then estimated in the standard fashion, ln(η) = const + (E_a/ε)(exp(βε) - 1) (where E_a is the Arrhenius activation energy). This expression is similar to the Mauro2 equation and is shown to agree very well with multiple experimental data sets for both polymers and organic liquids. The theory can be further extended to describe the behavior of random copolymers and miscible blends.


BRET SAVOIE (Presenter), GRIGORI MEDVEDEV, JAMES M CARUTHERS, Purdue University — Glass forming materials exhibit dramatic mobility decreases of up to ten orders of magnitude as their temperature approaches T_g. This slow-down exhibits a super-Arrhenian temperature dependence that is diagnostic for testing competing theories of glass formation. Using experimental data, it was recently shown that for 21 molecular glass formers a simple one-parameter model based on the excess enthalpy accurately predicts the super-Arrhenian behavior, whereas the traditional configurational entropy model of Adam-Gibbs shows significant deviations. Extending this analysis to polymeric materials is challenging since the requisite experimental data is limited. Here we present simulations on several common small molecules and polymers to explore the temperature dependence of the polymer dynamics in the supercooled regime, making comparisons with the new configurational enthalpy model and experimental data where available. We show that the configurational enthalpy model accurately describes the temperature and pressure dependence of the mobility slowdown in the studied polymers. Moving forward this provides justification for using simulations to investigate the molecular mechanisms responsible for the accurate predictions of the configurational enthalpy model.
9:36AM A25.00009: Chain-length dependent relaxation dynamics in glass-forming polymers*  DANIEL BAKER, Physics & Astronomy, University of Leeds, ROBIN MASUREL, University of Paris, Diderot, MATTHEW REYNOLDS, Physics & Astronomy, University of Leeds, PETER OLMSTED (Presenter), Georgetown University, JOHAN MATTSSON, Physics & Astronomy, University of Leeds — We present experimental and computational results on the effects of molecular size, monomer chemistry, and flexibility on the relaxation behaviour of glass-forming polymers. We show experimental data from broadband dielectric spectroscopy, calorimetry, and oscillatory rheology together with RIS computer simulation calculations. We discuss the length-dependence of molecular relaxation dynamics, chain conformation and shape; and relate these features to the glass transition temperature. We discuss the links between glass-formation in small molecules and oligomeric/polymeric glass-formers and the dependences on polymer chemistry and flexibility.

*Funding provided from Georgetown University, JS Ives Endowment, the UK Engineering and Physical Sciences Research Council.

9:48AM A25.00010: Dynamics of Viscoelastic Filaments based on Onsager Principle*  JIAJIA ZHOU (Presenter), MASAO DOI, Beihang University — When a polymer solution is uniaxially stretched and held fixed at both ends, the solution quickly separates into droplets connected by strings and takes the beads-on-string structure. The string then becomes thinner by capillary forces. Here we develop a theoretical framework on viscoelastic fluids based on Onsager principle, and apply it to the dynamics of viscoelastic filaments. We show that the beads-on-string structure is a thermodynamic quasi-equilibrium state, and derive an equation for the coexistence condition in the pseudo-equilibrium state. Using the condition, we solve the evolution equation analytically and show that the string radius and the tensile stress vary exponentially as predicted by the classical theory of Entov and Hinch [J. Non-Newtonian Fluid Mech. 72, 31 (1997)], but the prefactor for the tensile stress is different from their theory and agrees with the numerical solutions of Clasen et al. [J. Fluid Mech. 556, 283 (2006)].

*This work was supported by the National Natural Science Foundation of China (NSFC) through Grants No. 21504004 and 21774004.

10:00AM A25.00011: Visco-Elastic Property Reconstitution in Chain-Like Polymers*  MANON HEILI, JOHN KIEFFER (Presenter), University of Michigan — We investigate the elastic deformation and structural reorganization process in a chain-like polymer, e.g., polyvinylidene fluoride (PVDF) during straining and stress relaxation. Using a unique experimental setup in which a miniature tensile tester is placed into the optical path of a Brillouin light scattering (BLS) system, we simultaneously measure the adiabatic and isothermal elastic moduli of the polymer as a function of the strain history. Upon straining, elastic moduli of the polymer drop instantaneously, while during stress relaxation at constant strain both the static and adiabatic moduli reconstitute, tending towards the unstrained values. While such behavior is expected for the former, it is not for the latter. Although a detailed analysis allows us to identify a spectrum of relaxation rates, general visco-elastic theory (e.g., Maxwell-Wiechert model) is not adequate to describe the observed behavior, not even that of the static moduli. An improved description of material's visco-elastic response requires taking the structural rearrangements during straining and relaxation into account, and that the relaxation mechanisms, as well as the inherent elastic properties of the strained and unstrained polymer are indeed different.

*NSF-CBET-1402845
Tube models are not compatible with the slip-link model for entangled star polymers*  

JAY SCHIEBER (Presenter), KONSTANTIN TALETSKIY, Illinois Institute of Technology — The dynamics of entangled linear and star polymers have been described reasonably successfully by both the slip-link model and various tube models. Theory suggests that constraint dynamics plays a much larger role for star polymers than for linear chains, and has been essential in describing data even qualitatively. Experimentally, the role of constraint dynamics can be examined by blending star and linear chains. However, recent work has shown that the tube models are incapable of explaining these blends, whereas the slip-link model agrees well without any parameter adjustment.

These observations raise the question of whether slip-link models are capable of repairing the discrepancy of tube models with data. We have attempted to coarse grain the slip-link model to a tube level of description of stars. We find that the two models predict very different molecular weight dependence on the relaxation time of star arms without constraint dynamics. Moreover, we find that the tube level of description is incapable of capturing the physics in the slip-link model. We conclude that the two theories are incompatible, and at least one of them should be eliminated by comparison with data.

*NSF CBET 1438700

Thermal and viscoelastic properties of selectively hydrogenated poly(1,1-diphenylethylene-alt-butadiene)  

SUNGMIN PARK (Presenter), GAGAN KANGOVI, SANGWOO LEE, Rensselaer Polytechnic Institute — The synthetic utility of 1,1-diphenylethylene (DPE) to produce nearly perfectly alternating copolymers of DPE and vinyl monomers is well-established, but the physical properties of the alternating DPE copolymers have not been well documented. We characterized the thermal and viscoelastic properties of nearly perfectly alternating copolymer of 1,1-diphenylethylene (DPE) and butadiene and its selectively hydrogenated polymers. The entanglement molecular weights of the DPE-butadiene alternating copolymer and hydrogenated copolymers are measured 20 – 22 kg/mol. Interestingly, the glass transition temperatures of the DPE-butadiene copolymers decrease from 120 °C to 100 °C as the copolymer is selectively hydrogenated, and this behavior is opposite to the earlier report on the increasing glass transition temperature of hydrogenated DPE and styrene copolymers.

The Density Fluctuations of Polycarbonate under Deformation by Time-resolved small angle X-ray Scattering  

SHOTARO NISHITSUJI (Presenter), HIROSHI ITO, MASARU ISHIKAWA, TAKASHI INOUE, Yamagata University, MIKIHIITO TAKENAKA, Kyoto University — Polycarbonate(PC) in an excellent thermoplastic with high impact strength, good transparency and so on. However, PC becomes brittle by annealing below the glass transition temperature. The mechanism of this phenomenon, which is so-called physical aging, is not clarified. To understand this phenomenon, we focus on density fluctuations of PC. By using a strong X-ray source of synchrotron, this density fluctuations can be detected under deformation. In this study, the change with density fluctuations of PC under deformation is investigated by using time-resolved small angle X-ray scattering. PC sample used in this study is a commercial polymer (viscosity average molecular weight Mv=19,500). Time-resolved small angle X-ray scattering is carried out under a constant load at BL05XU, SPring-8, Japan. At steady state, the isotropic scattering pattern is detected. After applying a load, the scattering pattern become anisotropic and the scattering intensity is enhanced in the parallel direction of load. This means the density fluctuations are enhanced by deformation. After necking, the density fluctuations are enhanced at an accelerating rate. We will discuss the detailed change of density fluctuations in this presentation.

Accelerated and depressed aging of PS blocks under 3D nanoconfinement in diblock copolymers  

MINGCHAO MA (Presenter), YUNLONG GUO, Shanghai jiao Tong University — In this work, physical aging of polystyrene (PS) blocks in two representative diblock copolymers were investigated by a differential scanning calorimeter. Aging of PS blocks was remarkably accelerated in polystyrene-\textit{block}-poly(methyl methacrylate) (PS-b-PMMA), compared to the homo-PS. In addition, the enthalpy results demonstrate that the aging rate of PS blocks in PS-b-PMMA increases with larger PMMA/PS mole ratio. On the other hand, the aging rate of PS blocks in polystyrene-\textit{block}-poly(n-butyl methacrylate) (PS-b-PnBMA) is lower than the relaxation rate of corresponding neat PS. Together with morphology in these copolymers, the aging results imply that the hard three-dimensional confinement induced by the PMMA blocks accelerates the aging rate of relatively soft PS blocks in copolymer, while the sluggish aging of PS blocks in PS-b-PnBMA is attributed to the extremely soft confinement formed by PnBMA blocks, which was liquid in the aging process due to its low glass transition temperature.
8:00AM A26.00001: Measurement of GHZ and cluster state entanglement monotones in transmon qubits

AMARA KATABARWA (Presenter), MICHAEL GELLER, University of Georgia — Experimental detection of entanglement in superconducting qubits has been mostly limited, for more than two qubits, to witness-based and related approaches that can certify the presence of some entanglement, but not rigorously quantify how much. Here we measure the entanglement of three- and four-qubit GHZ and linear cluster states prepared on the 16-qubit IBM Rueschlikon (ibmqx5) chip, by estimating their entanglement monotones. We measure the decay of the monotones with time, and find in the GHZ case that they actually oscillate, which we interpret as a drift in the relative phase between the all zero and all one components, but not an oscillation in the actual entanglement. After experimentally correcting for this drift with virtual Z rotations we find that the GHZ states appear to be considerably more robust than cluster states, exhibiting higher fidelity and entanglement at later times. Our results contribute to the quantification and understanding of the strength and robustness of multi-qubit entanglement in the noisy environment of a superconducting quantum computer.

8:12AM A26.00002: Scalable generation of genuine multiparticle entanglement with superconducting qubits

MING GONG (Presenter), MING-CHENG CHEN, YARUI ZHENG, SHIYU WANG, CHEN ZHA, HUI DENG, ZHIGUANG YAN, HAO RONG, YULIN WU, SHAOWEI LI, FUSHENG CHEN, YOUWEI ZHAO, FUTIAN LIANG, JIN LIN, YU XU, CHENG GUO, LIHUA SUN, ANTHONY D CASTELLANO, Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, HAOHUA WANG, Department of Physics, Zhejiang University, CHENGZHI PENG, CHAO-YANG LU, XIAOBO ZHU, JIAN-WEI PAN, Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei — Solid state qubits by their nature are a scalable technology, but the number of entangled qubits still trails the size of state-of-the-art systems considerably. Producing large entangled states requires many different measures of processor quality to be high simultaneously: coherence times and tunability must be high; crosstalk and state leakage must be minimized. In addition, gate operations need to be specifically calibrated to create entanglement. In this work, based only on single-qubit gates and controlled-phase gates, we generated and verified the genuine multiparticle entanglement for more than 10 superconducting qubits. This gate-based approach to entanglement generation is directly scalable to larger systems. Our result is an important step towards achieving near-term quantum supremacy.

*This research was supported by the National Basic Research Program (973) of China under Grant No.~2017YFA0304300, the Chinese Academy of Science, Alibaba Cloud and Science and Technology Committee of Shanghai Municipality. Xiaobo Zhu is supported by NSFC under Grants No. 11574380. Haohua Wang is supported by NSFC under Grants No.11434008.

8:24AM A26.00003: Simple preparation of Bell and GHZ states using ultrastrong-coupling circuit QED

ANTON FRISK KOCKUM (Presenter), Chalmers University of Technology, VINCENZO MACRÌ, FRANCO NORI, RIKEN — The ability to entangle quantum systems is crucial for many applications in quantum technology, including quantum communication and quantum computing. Here, we propose a new, simple, and versatile setup for deterministically creating Bell and Greenberger-Horne-Zeilinger (GHZ) states between photons of different frequencies in a two-step protocol. The setup consists of a quantum bit (qubit) coupled ultrastrongly to three photonic resonator modes. The only operations needed in our protocol are to put the qubit in a superposition state, and then tune its frequency in and out of resonance with sums of the resonator-mode frequencies. By choosing which frequency we tune the qubit to, we select which entangled state we create. We show that our protocol can be implemented with high fidelity using feasible experimental parameters in state-of-the-art circuit quantum electrodynamics. One possible application of our setup is as a node distributing entanglement in a quantum network.
8:36AM A26.00004: Proposal to Generate and Characterize Quantum Entanglement using Coupled Metamaterial Resonators* FRANCISCO ROUXINOL (Presenter), Condensed Matter Physics Department, University of Campinas, FREDERICO BRITO, Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, MATTHEW LAHAYE, B.L.T. PLOURDE, Physics Department, Syracuse University — Entanglement is an underlying principle in quantum physics. Undoubtedly, the consequences of the correlations observed between measurements in spatially separated entangled systems has had a profound effect on our view of local realism of the world (EPR, Bell etc.). Using a left-handed metamaterial coupled to a nanomechanical resonator, we propose a new procedure to couple multiple microwave resonant modes and investigate entanglement in these limits. These investigation allow for the possibility to develop new techniques for characterizing entanglement in multi-mode systems. The potential of using these circuits in QED architectures is discussed.

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8:48AM A26.00005: Propagating Non-Gaussian States Generated by Degenerate 3-photon Downconversion CHUNG WAI SANDBO CHANG (Presenter), A. VADIRAJ, IBRAHIM NSANZINEZA, CHRISTOPHER WILSON, University of Waterloo — Nonclassical light sources have generated broad interest across a number of fields for their potential to enable novel quantum protocols. Spontaneous parametric downconversion (SPDC) processes have been widely adopted as an essential source of nonclassical light, generating various resource states. However, SPDC beyond second order has been an experimental challenge for decades. Here, with a superconducting parametric cavity designed for cubic interactions, we present experimental results for spontaneous three-photon downconversion when the cavity is flux pumped at three times the mode frequency. We measure propagating output states that are clearly non-Gaussian with a high degree of skewness in the quadrature amplitude distribution. Further, theory predicts that Wigner function negativity can persist for these states even after they escape from the cavity. With a linear detection scheme, we reconstruct the Wigner function of the propagating states from the directly measured moment matrix. We will present preliminary results on this reconstructed Wigner function.

9:00AM A26.00006: Multipartite entanglement mediated by shared microwave resonators* MARIE LU (Presenter), SYDNEY SCHREPPLER, University of California, Berkeley, LUKAS F BUCHMANN, FELIX MOTZOI, Physics, Aarhus University, IRFAN SIDDIQI, University of California, Berkeley — Developing highly connected networks of qubits is invaluable for implementing various quantum codes and simulations. Increased connectivity allows for entangling qubits with reduced gate depth. For example, the Mølmer-Sørensen gate generates high fidelity entanglement between multiple ions. We use shared coplanar waveguide (CPW) resonators to realize an analogous Mølmer-Sørensen gate between superconducting qubits. This talk describes how the CPW enables multipartite entanglement of all qubits coupled to the resonator as well as arbitrary subsets of qubits.

*This work was supported by the Army Research Office and the L’Oreal USA For Women in Science Fellowship Program.

9:12AM A26.00007: Probing the Tavis-Cummings level splitting with intermediate-scale superconducting circuits* MARTIN WEIDES (Presenter), University of Glasgow, PING YANG, JAN DAVID BREHM, JUHA LEPPAEKANGAS, Institute of Physics, Karlsruhe Institute of Technology, LINGZHEN GUO, Max Planck Institute for the Science of Light, MICHAEL MARTHALER, Institute for Theoretical Condensed Matter physics, Karlsruhe Institute of Technology, ISABELLA BOVENTER, Institute of Physics, University Mainz, ALEXANDER STEHLI, TIM WOLZ, ALEXEY USTINOV, Institute of Physics, Karlsruhe Institute of Technology — We demonstrate the local control of up to eight two-level systems interacting strongly with a microwave cavity. Following calibration, the frequency of each individual two-level system (qubit) is tunable without influencing the others. Bringing the qubits one by one on resonance with the cavity, we observe the collective coupling strength of the qubit ensemble. The splitting scales up with the square root of the number of the qubits, being the hallmark of the Tavis-Cummings model. The local control circuitry causes a bypass shunting the resonator, and a Fano interference in the microwave readout, whose contribution can be calibrated away to recover the pure cavity spectrum. The simulator's attainable size of dressed states is limited by reduced signal visibility, and -if uncalibrated- by off-resonance shifts of sub-components. Our work demonstrates control and readout of quantum coherent mesoscopic multi-qubit system of intermediate scale under conditions of noise.

*China Scholarship Council (CSC), European Research Council (ERC-648011), DFG project INST 121384/138-1 FUGG, Helmholtz IVF 'Scalable solid state quantum computing'
9:24AM A26.00008: Improving the fidelity of entangling gates via \textit{in situ} characterization of qubit control lines. ANATOLY KULIKOV (Presenter), MARKUS JERGER, ARKADY FEDOROV, ARC Centre for Engineered Quantum Systems — One of the factors limiting the fidelity of entangling gates are control signal distortions arising from non-trivial transfer functions of microwave lines. Distortions can be canceled, in principle, if the complex transfer function of the control line is known, by applying its inverse to the signal before it is transmitted. We have previously developed a method for \textit{in-situ} measurement of the system function using a qubit as a network vector analyser [1]. I will present the refinement of the method and its experimental application to improve the fidelity of CPHASE gate between two superconducting transmon qutrits. I will also show how our technique can be combined with other recently reported \textit{in-situ} methods to calibrate low-frequency response of control lines [2,3] to further enhance the fidelity of the two-qubit gates.


9:36AM A26.00009: \textbf{Fast Amplification and Rephasing of Entangled Cat States in a Qubit-Oscillator System} T. Fuse (Presenter), National Institute of Information and Communications Technology, Zhihao Xiao, Louisiana State University, Sahel Ashhab, Qatar Environment and Energy Research Institute, Fumiki Yoshihara, Kouichi Samba, Masahide Sasaki, Masahiro Takeoka, National Institute of Information and Communications Technology, Jonathan P Dowling, Louisiana State University — In this work [1], we study a qubit-oscillator system described by the quantum Rabi model with a time-dependent coupling coefficient, and present two schemes. We propose a scheme for the fast generation of entangled Schrödinger-cat states. We propose another scheme for protecting the cat states against dephasing caused by the nonlinearity in the system. We focus on the case where the qubit frequency is small compared to the oscillator frequency. We first present the exact quantum state evolution in the limit of infinitesimal qubit frequency, and then analyze the first-order effect of the nonzero qubit frequency. Our scheme works for systems with wide range of coupling strength, including the ultra-strong and deep-strong coupling regimes [2-5].


*T. F., Y., K. S., and M. T. would like to acknowledge support from JST CREST (Grant No. JPMJCR1775). Z.X and J.P.D. would like to acknowledge AFOSR, ARO, DARPA, NSF, and NGAS.

9:48AM A26.00010: \textbf{Ground-state cooling, Fock-state stabilization and photon-resolved thermalization dynamics in a hot 170 MHz resonator} M. Gely (Presenter), Marios Kounalakis, Christian Dickel, Jacob Dalle, Rémy Vatré, Mark D Jenkins, Gary Steele, Delft University of Technology — In order to observe coherent quantum effects, systems are usually cooled to their thermal ground states. Despite millikelvin temperatures being a dominant energy scale in a 170 MHz circuit QED mode, we show that quantum control of the mode can still be realized. This is achieved by coupling it to a cold mode at 5.9 GHz through the non-linearity of a Josephson junction shared between both modes. The resulting coupling leads to photon number splitting that allows reading out the state of the low frequency mode. Via four-wave mixing, we can sideband cool the low-frequency mode to its ground state, as well as stabilize one- and two-photon Fock states. In time-domain, we can then observe the photon-resolved thermalization dynamics of these stabilized states. Our platform could be used to resonantly interface quantum circuits with MHz frequency systems (e.g. mechanical elements) or enable further exploration of thermodynamical processes at the quantum scale.

*This work was supported by the European Research Council under the European Union’s H2020 program/ERC Grant Agreement 681476 - QOM3D
**10:00AM A26.00011: Probing the influence of many-body fluctuations on Cooper pair tunneling using circuit QED**

SÉBASTIEN LÉGER (Presenter), JAVIER PUERTAS, LUCA PLANAT, REMY DASSONVILLE, VLADIMIR MILCHAKOV, KARTHIK SRIKANTH BHARADWAJ, JOVIAN DELAFORCE, FARSHAD FOROUGHI, OLIVIER BUISSON, CECILE NAUD, WIEBKE GUICHARD, Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France, IZAK SNYMAN, Mandelstam Institute for Theoretical Physics, School of Physics, University of the Witwatersrand, Johannesburg, South Africa, SERGE FLORENS, NICOLAS ROCH, Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France —

Because of the value of the hyperfine constant (~ 1/137) observing many body effects in light-matter interaction is challenging. Reaching this regime is now possible using the tools of circuit Quantum ElectroDynamics (cQED) [1,2]. In this work we investigate the interactions between the plasma modes propagating in arrays of more than 4000 SQUIDs (which simulate the light) and a small Josephson junction (the matter). The first effect of these modes is to broaden the energy level of the Josephson junction [1,2]. More interestingly they can also induce strong phase fluctuations across the junction, which directly affects the Cooper pair tunneling. We will present our on-going experimental efforts aimed at observing this purely quantum many-body effect.


*This work was supported by the French Agence Nationale de la Recherche (ANR CLOUD project No. ANR-16-CE24-0005 and Investissement d’avenir” ANR-15-IDEX-02) and the Capital Fund Management.

**10:12AM A26.00012: Driving not so forbidden state transitions in a frequency-tunable transmon**

ALEXANDER OPREMCAK (Presenter), University of Wisconsin-Madison and Google, BEN CHIARO, BROOKS FOXEN, MATTHEW MCEWEN, Physics, University of California, Santa Barbara, ROBERT F MCDERMOTT, University of Wisconsin-Madison, JOHN M MARTINIS, Google — In a frequency-tunable transmon, transitions between the |0> and |2> states are nominally forbidden by selection rules, yet an experiment (Sank et al., PRL 117) observed that it is possible to drive these transitions. In this talk we explain that observation. We show that the apparent selection rule violation is a direct consequence of parametric modulation of the Josephson energy of the compound junction of the device. From a theoretical analysis of the dc SQUID, we derive a drive term that explains the violation. We validate our theory using experimentally measured Rabi oscillations and Ramsey interferometry on the |0> --> |2> transition. Surprisingly, the transition occurs for a transmon driven through a capacitor, indicating a modest degree of stray inductive coupling between the XY drive line and the compound junction of the transmon. These results identify a leakage channel and should inform efforts to integrate cryogenic control systems with arrays of frequency-tunable transmons.

*This work was supported by Google.

**10:24AM A26.00013: Perfect quantum state transfer in a superconducting qubit chain with parametrically tunable couplings**

XUEGANG LI (Presenter), Tsinghua University — Faithfully transferring quantum state is essential for quantum information processing. Here, we demonstrate a fast (in 84 ns) and high-fidelity (99.2%) transfer of arbitrary quantum states in a chain of four superconducting qubits with nearest-neighbor coupling. This transfer relies on full control of the effective couplings between neighboring qubits, which is realized only by parametrically modulating the qubits without increasing circuit complexity. Once the couplings between qubits fulfill specific ratio, a perfect quantum state transfer can be achieved in a single step, therefore robust to noise and accumulation of experimental errors. This quantum state transfer can be extended to a larger qubit chain and thus adds a desirable tool for future quantum information processing. The demonstrated flexibility of the coupling tunability is suitable for quantum simulation of many-body physics which requires different configurations of qubit couplings.

*This work was supported by the National Key R & D Program of China (Grants No. 2017YFA0304303 and No. 2016YFA0301803) and National Natural Science Foundation of China (Grants No. 11474177, No. 11874156, and No. 61771278). L. S. also thanks R. Vijay and his group for help on the parametric amplifier measurements.
Tunability and coherence are the desired properties of an ideal quantum computer. However, introducing tunability directly in the qubit often adversely affects its coherence. This tunability-coherence tradeoff can be optimized by using fixed frequency qubits coupled with a tunable coupler. This architecture has been widely used for demonstrating parametrically stimulated entangling gates. In previous theoretical studies of superconducting circuits, the coupler has always been assumed to be in the ground state and an examination of the temperature dependence of parametric gates has been lacking. Here we present the importance of thermalization of the tunable coupler, to the base temperature of a dilution refrigerator, for achieving a high-fidelity parametric gate. This talk is based on the work presented in "Suppression of Qubit Crosstalk in a Tunable Coupling Superconducting Circuit" (arXiv:1810.04182 [quant-ph]).

*This work is supported by IARPA under contract W911NF-10-1-0324.

Quantum entanglement dynamics due to dynamical Lamb effect

Mirko Amico (Presenter), Oleg Berman, Roman Kezerashvili, CUNY Graduate Center — We investigate the dynamics of a system of \( N \) qubits coupled to a common resonator with time-dependent coupling. The instantaneous switching on and off of the qubit/cavity coupling gives rise to the dynamical Lamb effect. The dynamical Lamb effect is the parametric excitation of the qubits, and the creation of cavity photons, due to the sudden change in Lamb shift of the qubit. In the absence of dissipation, the Schrodinger equation which describes the dynamics of the \( N \) qubits is solved within a perturbative approach. When dissipation is taken into account, the Lindblad equation for the system of \( N \) qubits is solved numerically. Different measures of entanglement compatible with pure and mixed states are adopted. The concurrence and the negativity are obtained in the two-qubit case; the three-\( \pi \) and the negativity are obtained in the three-qubit case. It is demonstrated that the different measures show different level of details of the entanglement between the qubits. We find that the dynamical Lamb effect can be used to create Greenberger-Horne-Zeilinger states even in presence of dissipation. Furthermore, the dynamical Lamb effect can be used as a fast entangling gate between two qubits.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A27 DQI: Quantum Simulation of Many-Body Physics

8:00AM A27.00001: WITHDRAWN ABSTRACT

8:12AM A27.00002: Hybrid quantum-classical algorithm for variational coupled cluster method

Sathyawageeswar Subramanian (Presenter), DAMTP, Cambridge University, Yudong Cao, Zapata Computing, Inc. — We present a hybrid quantum algorithm for the variational coupled cluster (vCC) method in quantum chemistry. We show that for a problem instance of \( n \) electrons described by \( m \) spin orbitals and a constant level \( \ell' \) of excitations, the energy expectation value of the vCC trial wavefunction can be estimated to precision \( \varepsilon \) in time proportional to \( \widetilde{O}(n^{3/2}m^{3/2}/\epsilon^2) \) on a quantum computer. Classically, computing the same expectation generally incurs a cost exponential in \( n \) and \( m \), implying that our quantum algorithm can yield a significant speedup over known classical methods. We envision that such capability combined with the framework of the variational quantum eigensolver (VQE) will add to recent quantum algorithms for unitary coupled cluster methods, enriching the toolset of quantum chemistry calculations beyond what is feasible on classical computers. We also illustrate a method for calculating analytical gradients for the vCC method, which can be used with gradient-free direct-search optimisation methods (such as the Nelder-Mead and COBYLA algorithms).

8:24AM A27.00003: Optical manipulation of entanglement in plasmonically coupled quantum dot qubits

Matthew Otten, Stephen K Gray, CNM, Argonne National Lab, German Kolmakov (Presenter), Physics, New York City College of Technology — We consider a system composed of two quantum dot qubits coupled with a common, damped surface plasmon mode; each quantum dot is also coupled to a separate photonic cavity mode. Cavity quantum electrodynamics calculations show that upon optical excitation by a femtosecond laser pulse, entanglement of the quantum dot excitons occurs, and the time evolution of the \( g(2) \) pair correlation function of the cavity photons is an indicator of the entanglement. We also show that the degree of entanglement is conserved during the time evolution of the system. Furthermore, if coupling of the photonic cavity and quantum dot modes is large enough, the quantum dot entanglement can be transferred to the cavity modes to increase the overall entanglement lifetime. This latter phenomenon can be viewed as a signature of entangled, long-lived quantum dot exciton-polariton formation. The preservation of total entanglement in the strong coupling limit of the cavity/quantum dot interactions suggests a novel means of entanglement storage and manipulation in high-quality optical cavities.
**8:36AM A27.00004: Simulating the t-J Model on a Quantum Computer**
BRIAN ROST (Presenter), JAMES FREERICKS, Georgetown University — Quantum computers are expected to give an exponential speed-up over classical computers for the simulation of strongly correlated quantum systems. Efficient implementation of these simulations is of great interest for many fields in the physical sciences. We consider algorithms for simulating the t-J model, a prominent model for high temperature superconductivity, on a quantum computer. Our approach focuses the computation on the low-energy projected phase space instead of taking the large interaction limit of the Hubbard model. We investigate trade-offs in noise, complexity, time and gate count in extracting the system's Green's function and self-energy, from which a wide variety of interesting physical quantities can be computed.

*This work was funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0019469. In addition, BR received supplemental support from the National Science Foundation under Award DMR-1747426 and JKF received supplemental support from the McDevitt bequest at Georgetown.*

**8:48AM A27.00005: Non-linear sigma model approach to many-body quantum chaos: regularized and unregularized out-of-time-ordered correlators**
YUNXIANG LIAO (Presenter), VICTOR GALITSKI, University of Maryland, College Park — In this work, we derive an extended version of Keldysh non-linear sigma model to investigate many-body quantum chaos in a 2D interacting fermion system subject to quenched disorder. This model provides a framework in which the regularized and unregularized out-of-time-ordered correlators with different arrangements of the thermal factors can be studied. The two types of correlators grow exponentially with different growth rates which can be extracted from the mass of the “inter-world” diffuson propagator. This should be compared with its “intra-world” counterpart that gives the dephasing rate corresponding to the phase relaxation of single-particle states. Our result for regularized exponent is consistent with the previous one obtained from the diagrammatic perturbation approach. Furthermore, the regularized (unregularized) exponent obeys (violates) the chaos bound 2πT. We note that the regularized exponent is entirely due to the inelastic collisions between particles, while the unregularized exponent contains an additional contribution from elastic scattering of particles off of the Friedel oscillations of the particle density. Therefore, we believe that the unregularized exponent cannot measure many-body quantum chaos which originates from interactions.

**9:00AM A27.00006: Information spreading in many-body systems and the out-of-time-ordered correlator**
SHENGLONG XU (Presenter), BRIAN SWINGLE, University of Maryland, College Park — The information spreading in quantum many-body systems under unitary real-time evolution is related to the growth of simple Heisenberg operators, which is quantified by out-of-order correlation (OTOC) functions. Using a time-dependent disordered Hamiltonian model, I will analytically show the emergence of hydrodynamics description of the OTOC arising from the unitary real-time dynamics. Corrections of quantum fluctuation are manifested as the diffusively broadened wavefront of the OTOC. This picture is supported by large-scale (~200 spins) real-time dynamics simulation on realistic spin Hamiltonians using our newly developed tensor-network method.

*This material is based upon work supported by the Simons Foundation via the It From Qubit Collaboration, by the Air Force Office of Scientific Research under award number FA9550-171-0180, and by the NSF Physics Frontier Center at the Joint Quantum Institute (PHY-1430094).*

**9:12AM A27.00007: Graph theory and bounds on operator growth**
ANDREW LUCAS (Presenter), Stanford University — Motivated by recent developments in many-body quantum chaos, I will present bounds on the growth of operators in k-local quantum many-body systems. These bounds can be interpreted as simple combinatorics problems in graph theory. I will give explicit examples of how these bounds can be parametrically stronger than Lieb-Robinson bounds.
Quantum codes for quantum simulation of Fermions on a square lattice of qubits*  
MARK STEUDTNER (Presenter), Lorentz Institute, STEPHANIE WEHNER, Delft University of Technology, QuTech — Quantum simulation of fermionic systems is a promising application of quantum computers, but in order to program them, we need to map fermionic states and operators to qubit states and quantum gates. While quantum processors may be built as two-dimensional qubit networks with couplings between nearest neighbors, standard Fermion-to-qubit mappings do not account for that kind of connectivity. In this work we concatenate the (one-dimensional) Jordan-Wigner transform with specific quantum codes defined under the addition of a certain number of auxiliary qubits. This yields a novel class of mappings with which any fermionic system can be embedded in a two-dimensional qubit setup, fostering scalable quantum simulation. Our technique is demonstrated on the two-dimensional Fermi-Hubbard model, that we transform into a local Hamiltonian. What is more, we adapt the Verstraete-Cirac transform and Bravyi-Kitaev Superfast simulation to the square lattice connectivity and compare them to our mappings.

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

Tripartite information and scrambling in quantum lattice models*  
OSKAR H. SCHNAACK, Max-Planck-Institute for Dynamics and Selforganization, SEBASTIAN PAECKEL, SALVATORE MANMANA (Presenter), STEFAN KEHREIN, University of Gottingen, MARKUS SCHMITT, UC Berkeley — For the characterization of dynamics in quantum many-body systems the question how information spreads and becomes distributed over the constituent degrees of freedom is of fundamental interest. The delocalization of information under many-body dynamics has been dubbed "scrambling" and out-of-time-order correlators were proposed to probe this behavior. In this work we investigate the time-evolution of tripartite information as a natural operator-independent measure of scrambling, which quantifies to which extent the initially localized information can only be recovered by global measurements. Studying the dynamics of quantum lattice models with tunable integrability breaking we demonstrate that in contrast to quadratic models a generic non-integrable system scrambles information irrespective of the chosen partitioning of the Hilbert space, which justifies the characterization as "scrambler."

*Funding through SFB/CRC 1073 (project B03) of the Deutsche Forschungsgemeinschaft (DFG) and by the Studienstiftung des Deutschen Volkes is gratefully acknowledged.

Realizing quantum Ising models in tunable two-dimensional arrays of single Rydberg atoms  
[Invited] ANTOINE BROWAEYS (Presenter), Institut d'Optique — tbd

Phase structure of Ising models at complex temperature*  
VADIM OGANESYAN, SANKHYA BASU (Presenter), Physics and Astronomy, CSI and GC, CUNY — This work explores continuation of phases and phase transitions in statistical sums of planar Ising models to complex couplings -- temperature and field. We use a combination of analytic and numerical techniques, based on tensor network formulations of renormalization group (TRG and SRG) to access the regimes of phase space displaying novel modulated correlations and entirely out of reach of standard monte carlo methods. We also study and improve convergence and stability properties of tensor renormalization methods.

*NSF DMR Grant No. 1508538

Quantum Feedback Protocol for Calculating Single-Particle Green's Functions at Finite Temperature*  
JAMES FREERICKS (Presenter), JEFFREY COHN, Georgetown University, FOREST YANG, Computer Science and Physics, University of California, Berkeley, KHADIJEH NAJAFI, Georgetown University, BARBARA JONES, IBM — Drawing on the eigenstate thermalization hypothesis, we present a quantum feedback algorithm that approximates single-particle Green's functions at finite temperature. Measuring a single-particle Green's function from a thermal state on a quantum computer is a well known procedure, but the challenges and resources needed for full Gibbs state preparation are generally too expensive for practical simulation in the near future. We examine how sampling from more easily prepared states yields accurate approximations to single-particle Green's functions at finite temperature. We employ an additional feedback mechanism, that tests for convergence and extracts the effective temperature of the system being simulated. We also compare the trade-offs of different approaches to make these techniques applicable on near term devices.

*This work was funded by the National Science Foundation under grants numbered PHY-1620555 and DMR-1659532. In addition, JKF was funded by the McDevitt bequest at Georgetown University.
MARCINIAK (Presenter), ROBERT WOLF, MICHAEL JORDAN BIERCUK, Univ of Sydney — We will present recent achievements in ultraviolet wavelengths required to cool and control $^{88}\text{Sr}^+$ trapped ion qubits. The combination of recently developed low-loss UV photonic waveguides made from Al$_2$O$_3$ with more typical SiN waveguides for IR and visible wavelengths within multiple layers of the chip enables integration of light at all the wavelengths required for ion control. We study the interaction of these new multi-wavelength photonics with a single ion qubit towards demonstration of a two qubit gate controlled via integrated technologies, a key component of a scalable trapped ion quantum information processor.

WAKS, University of Maryland-College Park — Time-multiplexed quantum random walk provides an efficient method to realize a quantum random walk via time delays and beam-splitters. Previously, researchers have demonstrated the control of random walk evolution based on photon's polarization degree of freedom. In this presentation, we propose adding synthetic gauge fields for controlling the evolution of the random walk which is important to simulate a broad class of physical effects. In this platform, varied lengths of optical fibers create the time delays and the gauge fields are implemented through phase modulations. We show how different gauge fields provide the possibility of opening band gaps in the band structure. The presence of these bandgaps leads to the pseudo magnetic confinement of the random walk distribution. We present the theoretical predictions and experimental observations of this confinement. We also demonstrate the possibility of creating edge states by applying different gauge fields to different regions of the synthetic space. The experimental results confirm the confinement of the evolution of the random walk around the boundary.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A28 DQI DAMOP: AMO Quantum Information

8:00AM A28.00001: Coherent control of large ion crystals in a Penning trap quantum simulator* CHRISTIAN MARCINIAK (Presenter), ROBERT WOLF, MICHAEL JORDAN BIERCUK, Univ of Sydney — We will present recent achievements towards building a quantum simulator for transverse-field Ising-type Hamiltonians based on laser-cooled Coulomb crystals of $^{9}\text{Be}^+$ in a Penning trap. We introduce the overall system design and describe key technical elements that have permitted site-resolved imaging of rapidly rotating 2D ion crystals with $> 70$ ions, stable over tens of seconds. Novel approaches to ion imaging using a room temperature APD-array-camera coupled to a microlens array are also presented as a means to achieve high-speed state detection with spatial resolution. In addition, we demonstrate coherent control over the ions' electron spin using millimeter waves near 55 GHz via a custom high-stability source and delivery system.

8:12AM A28.00002: Integrated multi-wavelength photonic addressing of trapped ion qubits ROBERT NIFFENEGGER (Presenter), JULES STUART, COLIN BRUZEWICZ, ROBERT MCCONNELL, MIT Lincoln Laboratory, GAVIN WEST, GARRETT SIMON, Physics, Massachusetts Institute of Technology, DAVE KHARAS, CHERYL SORACE-AGASKAR, SURAJ BRAMHAVAR, JEREMY SAGE, JOHN CHIAVERINI, MIT Lincoln Laboratory — Integrating quantum and classical technologies with systems like trapped ions is critical to enable the Moore's law like scaling of qubits necessary to develop practical quantum computers. For instance, individual addressing of trapped ion qubits typically requires bulky free space optics to tightly focus multiple laser beams onto single ions within linear chains, limiting scalability. Here we have designed and fabricated an ion trap chip with integrated photonic waveguides and grating out-couplers for integrated addressing in all of the infrared, visible, and ultraviolet wavelengths required to cool and control $^{88}\text{Sr}^+$ trapped ion qubits. The combination of recently developed low loss UV photonic waveguides made from Al$_2$O$_3$ with more typical SiN waveguides for IR and visible wavelengths within multiple layers of the chip enables integration of light at all the wavelengths required for ion control. We study the interaction of these new multi-wavelength photonics with a single ion qubit towards demonstration of a two qubit gate controlled via integrated technologies, a key component of a scalable trapped ion quantum information processor.

*We acknowledge Simons Foundation, Gordon and Betty Moore Foundation, NSF Grants PHY-1125565 and PHY-1125915.

BCEC 161 - Julian Leonard, ETH Zurich - Tag(s): Focus

This research was supported by the Australian Research Council Centre of Excellence for Engineered Quantum Systems (project ID CE170100009), and a private grant from H. & A. Harley.
Phase-modulated entangling gates robust against static and time-varying errors

INIGO ARRAZOLA (Presenter), Department of Physical Chemistry, University of the Basque Country, Bilbao, Spain, XIAO-HANG CHENG, Department of Physics, Shanghai University, Shanghai, China, JULEN S. PEDERNALES, Institute for Theoretical Physics and IQST, Universität Ulm, Ulm, Germany, LUCAS LAMATA, Department of Physical Chemistry, University of the Basque Country, Bilbao, Spain, XI CHEN, Department of Physics, Shanghai University, Shanghai, China, ENRIQUE SOLANO, Department of Physical Chemistry, University of the Basque Country, Bilbao, Spain — We study the nonlinear dynamics of trapped-ion models far away from the Lamb-Dicke regime. This nonlinearity induces a blockade on the propagation of quantum information along the Hilbert space of the Jaynes-Cummings and quantum Rabi models. We propose to use this blockade as a resource for the dissipative generation of high-number Fock states. Also, we compare the linear and nonlinear cases of the quantum Rabi model in the ultrastrong and deep strong-coupling regimes. Moreover, we propose a scheme to simulate the nonlinear quantum Rabi model in all coupling regimes. This can be done via off-resonant nonlinear red- and blue-sideband interactions in a single trapped ion, yielding applications as a dynamical quantum filter.


Characterizing Unwanted Motional Coupling in Mølmer-Sørensen Gates

LEONARDO ANDRETA DE CASTRO (Presenter), Electrical and Computer Engineering, Duke University, PAK HONG LEUNG, Department of Physics, Duke University, PAVITHRAN S IYER, Université de Sherbrooke, KENNETH R BROWN, Electrical and Computer Engineering, Duke University — Mølmer–Sørensen gates constitute an integral hardware component of an ion trap quantum computer. These gates entangle qubits to motional modes of the ions, generating phonons that manifest in errors on future gates. As a result, the analysis of fault tolerant quantum computation schemes becomes challenging. In this work, we quantify the impact of ignoring non-Markovian features in the noise model for Mølmer–Sørensen gates by developing numerical tools to compute the fidelity of a sequence of N Mølmer–Sørensen gates. Although completely ignoring non-Markovianity results in an overestimation of this fidelity, we present Markovian models that can reproduce the same scaling of fidelity as the true noise process. These accurate Markovian models rely on a heuristic assumption that the displacements of the motional modes resemble a random walk.

†ARO MURI W911NF-18-1-0258 and NSF Phy-1818914

Scalable Trapped Ion Architectures and Micromotion Enhancement

ALEXANDER RATCLIFFE (Presenter), JOSEPH HOPE, Department of Quantum Science, Australian National University — Quantum computing promises exciting new opportunities to answer currently intractable problems. To achieve this feat, a quantum architecture that is able to perform high fidelity operations and can be readily scaled to large numbers of qubits is required. The main obstacle to quantum computation being used as another computational tool is the limited scalability of current architectures. Trapped ions are presently one of the most promising platforms for large scale quantum computing, achieving high fidelity operations and long coherence times. Their current limitation lies in scalability. Most proposals to overcome this require coupling to many small trapped ion systems via an optical bus, or call for ions to be shuttled between segments of the system. Both of these proposals introduce new challenges and increase the complexity of the platform. Here, I demonstrate that a simple approach to scalability using microtrap arrays provides a feasible road to scalability. I show that this can be achieved without introducing any more complexity to the system than is required for trapping. Further, I show that this is realistically achievable with already demonstrated technology. Finally, I show that within this scheme, an old foe —micromotion —becomes an unlikely ally.
**9:12AM A28.00007: On-chip optical quantum memory using erbium ions**

IOANA CRAICIU (Presenter), MI LEI, JAKE ROCHMAN, JONATHAN KINDEM, JOHN BARTHOLOMEW, EVAN MIYAZONO, TIAN ZHONG, ANDREI FARAON, Caltech — Rare earth ion doped crystals provide an excellent solid state platform for optical quantum memories, which will enable long distance quantum communication and modular quantum computing. Among rare earths, erbium is appealing due to its long lived telecom wavelength resonance, allowing integration with silicon and with existing optical communication technology and infrastructure.

We present an on-chip all-optical quantum memory at telecom wavelengths using the atomic frequency comb protocol. By working at dilution fridge temperatures, we access a regime where the erbium ions have long optical coherence times and good spectral holeburning properties using only a moderate magnetic field, applied with permanent magnets. A nanobeam photonic crystal cavity etched directly in erbium-167 doped yttrium orthosilicate is used to enhance coupling to the ions. We store coherent pulses for memory times as long as 10 µs, albeit with limited efficiency. The memory has a high fidelity (>90%) and can be multiplexed in frequency and time. Ongoing work towards a higher efficiency device is discussed.

*We would like to acknowledge funding support from the Air Force Office of Scientific Research. Ioana Craiciu acknowledges support from Natural Sciences and Engineering Research Council of Canada.*

**9:24AM A28.00008: Probing amplified spontaneous emission to superradiance transition in cold Cs atoms inside a hollow-core photonic-crystal fiber**

ZHENGHAO DING (Presenter), Physics, Institute for Quantum Computing, University of Waterloo, TAE HYUN YOON, Electrical and Computer Engineering, Institute for Quantum Computing, University of Waterloo, JEREMY FLANNERY, PAUL ANDERSON, BRIAN DUONG, SHENG-XIANG LIN, FERESHTEH RAJABI, Physics, Institute for Quantum Computing, University of Waterloo, MARTIN HOUDE, Physics, University of Western Ontario, RUBAYET AL MARUF, MICHAL BAJCSY, Electrical and Computer Engineering, Institute for Quantum Computing, University of Waterloo — We investigate the critical conditions to realize the transition from amplified spontaneous emission (ASE) to superradiance (SR) with an ensemble of laser-cooled Cs atoms inside a hollow-core photonic crystal fiber (HCPCF). In our experiment, the Cs atoms, initially cooled using a magneto-optical trap (MOT), are guided and confined inside a short piece of HCPCF with a magic-wavelength dipole trap. This work constitutes the preliminary elements of our current experimental investigations towards realization of an ultra-narrow linewidth superriant laser. Additionally, we aim to study long range coherence in atomic ensembles and explore the symmetries governing atom-field couplings in the HCPCF platform.

*This works has been supported by Industry Canada, NSERC Discovery grant, Ontario’s Early Researcher Award, and by Transformative Quantum Technologies (TQT).*

**9:36AM A28.00009: Time/frequency high-dimensional entanglement via engineered parametric down conversion**

FRANCESCO GRAFFITTI (Presenter), PETER BARROW, MASSIMILIANO PROIETTI, ALEX PICKSTON, DMYTRO KUNDYS, Heriot-Watt University, AGATA M BRANCZYK, Perimeter Institute, ALESSANDRO FEDRIZZI, Heriot-Watt University — Photonic quantum technologies rely on the deterministic preparation of qubits encoded in single-photons degrees of freedom (DoF). While polarisation, orbital angular momentum and path have been routinely used since the early days of quantum information, the last few years have seen an increasing interest in the frequency-time encoding, due to the possibility of generating high-dimensional states combined with the compatibility of frequency modes with standard optical components. Here we present a new scheme for generating frequency-entangled photon pairs in parametric down-conversion (PDC) processes. By means of our novel non-linearity engineering technique, we deterministically choose the orientation of each ferroelectric domain of a poled crystal to tailor its phase-matching function as a multi-peaked function. The photons produced in such crystals emerge in a coherent superposition of an arbitrary number of orthogonal spectral Schmidt modes, allowing us to explore high-dimensional Hilbert spaces.

Our technique can easily be implemented as requires no additional components respect to a standard PDC setup, it’s highly compatible with other DoF encodings, and can be adapted to integrated waveguide sources.

*EPSRC Council (EP/N002962/1,EP/L015110/1).*
9:48AM A28.00010: Polarization-Independent Photon Storage System with Variable Time Delay* MICHELLE VICTORA (Presenter), FEDOR BERGMANN, University of Illinois at Urbana-Champaign, MICHAEL E GOGGIN, Truman State University, JIA JUN WONG, PAUL G KW IAT, University of Illinois at Urbana-Champaign — Quantum optical memories are a key component to a variety of quantum information applications, from extending quantum communication channels to building high-efficiency single-photon sources to synchronizing multiple protocols. However, most current broad bandwidth photon storage systems operate with somewhat shorter storage times (on the order of 10 ns), or require cryogenic operation. Here we develop a system with multiplexed free-space storage cavities, able to store single photons with high efficiency over variable delays [N x 12.5 ns, 1 ≤ N ≤ 999], and over several nanometers bandwidth. The system can store multiple photons simultaneously and can potentially store qubits encoded in various degrees of freedom, e.g., spatial modes, time-bin, and polarization. For the latter, we have demonstrated a memory fidelity >90% for storage times up to 500 ns. A future goal for this experiment is to achieve storage of hyperentanglement. While previous hyperentangled photon storage systems only achieved 5% efficiency, we have currently demonstrated a free-space transmission above 50% for delay times up to 5 µs.

*This work is supported in part by NSF grant No. 1521110.

10:00AM A28.00011: Efficient Two-Photon Interference with Pulse-Driven Quantum Emitters in Dynamic Environments HERBERT FOTSO (Presenter), Department of Physics, University at Albany, SUNY — The ability to achieve distributed entanglement across distant quantum nodes is essential for the construction of scalable quantum networks and other fundamental quantum information processing operations including quantum teleportation and Bell inequality tests[1, 2]. For solid-state spin qubits, it can be achieved through photon interference on a beam splitter. The efficiency of these interference operations rely on the indistinguishability of photons arriving from different emitters. However, for quantum emitters in dynamic environments, uncorrelated environment fluctuations lead to differences in temporal and spectral profiles of emitted photons resulting in reduced photon indistinguishability. We simulate the TPI operation in a Hong-Ou-Mandel-type experiment for two distant qubits in diffusion-inducing environments. We find that when the emitters are driven by appropriate pulse sequences, besides their emission spectra having little dependence on the environment[3, 4], photon indistinguishability can be restored to optimal values paving the way for improved efficiency in photon-mediated QIP operations.


10:12AM A28.00012: Universal Dynamics of Inhomogeneous Quantum Phase Transitions: Suppressing Defect Formation* FERNANDO GÓMEZ-RUIZ (Presenter), Physics, Universidad de Los Andes, ADOLFO DEL CAMPO, Physics, University of Massachusetts Boston — In the nonadiabatic dynamics across a quantum phase transition, the Kibble-Zurek mechanism predicts that the formation of topological defects is suppressed as a universal power law with the quench time. In inhomogeneous systems, the critical point is reached locally and causality reduces the effective system size for defect formation to regions where the velocity of the critical front is slower than the second-sound velocity, favoring adiabatic dynamics. The reduced density of excitations exhibits a much steeper dependence on the quench rate and is also described by a universal power-law, that we demonstrated in a quantum Ising chain.

*F. J. G.-R. acknowledges financial support from Facultad de Ciencias at Universidad de Los Andes. Funding support from the John Templeton Foundation and UMass Boston (project P20150000029779) is further acknowledged.

10:24AM A28.00013: Controlling Quantum Spin States and Dynamics with Light [Invited] MONIKA SCHLEIER-SMITH (Invited), EMILY J DAVIS, GREGORY BENTSEN, Stanford University, LUKAS HOMEIER, LMU Munich — Coupling many atoms to a single mode of light provides an efficient means of generating quantum correlations in an extended many-body system. I will report on experiments in which we harness photons in an optical cavity to mediate “flip-flop” interactions among distant spins in a millimeter-long cloud of atoms, as we directly observe by imaging quench dynamics. In our spin-1 system, these exchange interactions enable correlated pair creation in the m = ±1 Zeeman states, a process analogous to spontaneous parametric down-conversion or to collisional spin mixing in Bose-Einstein condensates. In contrast to direct collisional interactions, non-local light-mediated interactions offer unprecedented opportunities for engineering the spatial structure of spin-spin couplings and correlations. I will describe progress and prospects in tailoring atom-light interactions to enable new directions in quantum simulation and to generate new resources for quantum-enhanced sensing.
Cross-resonance gates applied to pairs of transmons satisfy this requirement with the added advantage of being fully controlled by microwave signals. However, applying these gates to a large transmon lattice is quite challenging. This is because cross-resonance gates set stringent requirements on the frequency landscape of neighboring qubits, which are difficult to satisfy with fixed-frequency transmons due to their relatively large frequency spread. To solve this problem, we realize a new flux-tunable qubit, compatible with cross-resonance gates, which can be tuned by less than 150 MHz. Such a weakly tunable qubit is useful for avoiding frequency collisions in a large lattice while limiting its susceptibility to flux noise. In this talk, we will introduce the qubit circuit and theory.

This work is funded by the IARPA Grant No. W911NF-16-1-0114-FE

Performing fast, high-fidelity two-qubit gates is an important requirement of quantum computers. Cross-resonance gates applied to pairs of transmons satisfy this requirement with the added advantage of being fully controlled by microwave signals. However, applying these gates to a large transmon lattice is quite challenging. This is because cross-resonance gates set stringent requirements on the frequency landscape of neighboring qubits, which are difficult to satisfy with fixed-frequency transmons due to their relatively large frequency spread. To solve this problem, we realize a new flux-tunable qubit, compatible with cross-resonance gates, which can be tuned by less than 150 MHz. Such a weakly tunable qubit is useful for avoiding frequency collisions in a large lattice while limiting its susceptibility to flux noise. In this talk, we will present some preliminary measurement results of these weakly tunable qubits.

This work is funded by the IARPA Grant No. W911NF-16-1-0114-FE

The quantization of magnetic flux in superconductors lies at the heart of realizing qubits using superconducting circuits. To construct a flux qubit, one must coherently couple the flux states of a superconducting ring, which requires breaking the rotational symmetry of the ring to introduce a phase-slip center. Established implementations guarantee an inherently broken symmetry by interrupting the ring with an insulating barrier; hence, forming a Josephson junction, giving rise to the flux qubit. However, these implementations are plagued by the variability of the fabrication process of the junction. Here, we theoretically propose a junctionless flux qubit consisting of a voltage-biased superconducting ring. The in-plane electric field, arising from the bias voltage, locally suppresses the density of superconducting electrons; hence, imitating the effect of interrupting the superconductor with an insulator. Furthermore, the proposed qubit could allow for electric-tunability of the transition frequency, a desired feature for multi-qubit systems since it renders the circuit less sensitive to magnetic noise. Realizing electrically-tunable flux qubits with long coherence times paves the road towards scaling up superconducting quantum computers.

We discuss a superconducting flux qubit whose sensitivity to low frequency flux is reduced through a null flux geometry consisting of one closed wire loop twisted into a “figure eight” shape composed of two open loops, each with opposite circulation. This protects against global flux noise in a similar way as the gradiometer qubit, but with only one loop degree of freedom instead of the two DOF of the gradiometer. This important difference opens several possibilities for dealing with the local flux noise that causes decoherence in the gradiometer qubit. We further show that the null flux shape increases the sensitivity to high frequency flux, making the system potentially useful for superconducting transduction.
8:48AM A29.00005: Symmetry Protected Qubits Through Fluxon Pairing* WEN TING HSIEH (Presenter), MATTHEW BELL, Department of Electrical Engineering, University of Massachusetts, WEN-SEN LU, WENYUAN ZHANG, PLAMEN KAMENOV, KONSTANTIN KALASHNIKOV, MICHAEL GERSHENSON, Department of Physics and Astronomy, Rutgers University — We present time-domain experiments with symmetry-protected qubits whose quantum states are encoded in the parity of fluxons in a superconducting loop. The qubit is composed of a Cooper pair box and a superinductor arranged in a superconducting loop [1]. The lowest-energy states of this qubit correspond to even/odd parity of fluxons in the loop. We will discuss proof-of-concept experiments that show how the qubit can be placed into a state protected against energy relaxation where the fluxon parity is preserved through the Aharonov-Casher interference. We will show that using fast gate pulses, the fluxon-pairing qubit can be adiabatically switched between the protected and unprotected states for quantum state initialization and readout. We will also discuss preliminary results on the implementation of fluxon-pairing qubits with superinductors fabricated from meandered nanowires made of strongly disordered Aluminum [2].


*The work at UMass (Boston) was supported by awards NSF ECCS-1608448, NSF DMR-1838979 and NSF DUE-1723511; the work at Rutgers was supported by awards NSF DMR 1708954, NSF DMR-1838979, and ARO award W911NF-17-C-0024.

9:00AM A29.00006: Breaking the trade-off between gate and relaxation times of a superconducting qubit with a Josephson quantum filter: Theory* KAZUKI KOSHINO (Presenter), College of Liberal Arts and Sciences, Tokyo Medical and Dental University, SHINGO KONO, YUTAKA TABUCHI, ATSUSHI NOGUCHI, DANY LACHANCE-QUIRION, YASUNOBU NAKAMURA, Research Center for Advanced Science and Technology, The University of Tokyo — When we couple a superconducting qubit strongly to a transmission line, the qubit completely reflects a weak resonant microwave field propagating through the line. On the other hand, the qubit becomes transparent to a stronger field due to the absorption saturation. This implies that a superconducting qubit functions as a nonlinear mirror, which we call a Josephson quantum filter (JQF). We theoretically investigate a setup in which a qubit (data qubit) to be controlled is coupled to an end of a semi-infinite control line and a JQF is placed at a distance of the order of the resonance wavelength of the qubit. An effective cavity is formed by the termination point and the JQF, and the radiative decay of the data qubit is suppressed if this effective cavity has a large detuning from the data qubit. Nearly complete suppression is achieved under the following conditions: the radiative decay rate of JQF is much larger than that of the data qubit, and the distance between the data qubit and the JQF is close to the half of the resonance wavelength.

*This work was supported in part by JST ERATO (Grant No. JPMJER1601), JSPS KAKENHI (No. 16K05497 and No. 26220601), JSPS Grant-in-Aid for JSPS Research Fellow, and ALPS, The University of Tokyo.

9:12AM A29.00007: Breaking the trade-off between gate and relaxation times of a superconducting qubit with a Josephson quantum filter: Experiment* SHINGO KONO (Presenter), The University of Tokyo, KAZUKI KOSHINO, Tokyo Medical and Dental University, YUTAKA TABUCHI, ATSUSHI NOGUCHI, DANY LACHANCE-QUIRION, YASUNOBU NAKAMURA, The University of Tokyo — The rapid development in designs and fabrication techniques of superconducting qubits is making coherence times of qubits longer and longer. In the near future, however, the radiation decay of the qubit (data qubit) into the control line will be a fundamental limitation, imposing a trade-off between the gate and relaxation times. Here, we successfully break the trade-off by strongly coupling another superconducting qubit, or a Josephson quantum filter (JQF), along the control line connected to the data qubit. The JQF prevents the data qubit from emitting a microwave photon and thus suppresses the relaxation, while transmitting faithfully large-amplitude control microwave pulses through the saturation of the quantum filter. In this talk, we will present the circuit design and demonstrate the effect of JQF on the qubit coherence.

*This work was supported in part by JST ERATO (Grant No. JPMJER1601), JSPS KAKENHI (No. 16K05497 and No. 26220601), JSPS Grant-in-Aid for JSPS Research Fellow, and ALPS, The University of Tokyo.
Theoretical analysis on the composite qubit approach to superconducting quantum computing

YUN-PIL SHIM (Presenter), Laboratory for Physical Sciences, DANIEL CAMPBELL, BHARATH KANNAN, RONI WINIK, Research Laboratory of Electronics, Massachusetts Institute of Technology, DAVID K KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, JONILYN L YODER, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, WILLIAM D OLIVER, Research Laboratory of Electronics, Massachusetts Institute of Technology, CHARLES TAHAN, Laboratory for Physical Sciences — Encoded qubit scheme [1] for superconducting qubit architecture could be a useful alternative to the conventional approach for simpler control of qubits. The composite qubit (CQB) defined in a two-dimensional subspace of a system of two physical transmon qubits can be manipulated using only base band control of each transmon qubit frequencies, allowing for microwave-free single- and two-qubit quantum gates. We present theoretical analysis of the optimal operating point (sweet spot) and the gate operations in a real device in the presence of various sources of noise and errors. The CQB computational subspace consists of excited states of the system and relaxation to the physical ground state is one of the main sources of error. We discuss the randomized benchmarking (RB) protocol in the presence of this leakage error.


Hamiltonian Quantum Computing with transmon qubits

ALESSANDRO CIANI (Presenter), RWTH Aachen University, BARBARA TERHAL, TU Delft, DAVID PETER DIVINCENZO, RWTH Aachen University — We discuss a possible implementation based on superconducting transmon qubits of the scheme for Hamiltonian Quantum Computing introduced in Ref. [1]. The scheme is completely passive and requires active control only for initialization and measurement. The scheme requires strong and negative cross-Kerr interactions and relatively weaker hopping interactions. We propose the implementation the strong of the cross-Kerr interactions with a newly designed direct coupler based on array of few Josephson junctions, which should allow to reach larger cross-Kerr coupling compared to other proposals, without causing any increase in the problem of cross-talk. The hopping interactions are responsible for the implementation of quantum gates, and can be implemented with simple capacitances or via indirect coupling mediated by resonators. In this way it is possible to obtain sufficient flexibility to achieve universality using only real gates. To this end, we also discuss explicitly how to implement a Toffoli gate. We finally discuss the main sources of errors in the model.


Low-Loss Dielectric Materials and the Merged Element Transmon

COREY RAE MCRAE (Presenter), National Institute of Standards and Technology Boulder, ANTHONY MCFADDEN, University of California Santa Barbara, MUSTAFA BAL, National Institute of Standards and Technology Boulder, XIAN WU, Lawrence Livermore National Laboratory, JUNLING LONG, National Institute of Standards and Technology Boulder, HSIANG-SHENG KU, Alibaba, JIANGUO WEN, JIE WANG, ILKE ARSLAN, Argonne National Laboratory, CHRIS PALMSTROM, University of California Santa Barbara, DAVID PAPPAS, RUSSELL LAKE, National Institute of Standards and Technology Boulder — Josephson junctions, a crucial component in quantum bits (qubits), are commonly composed of a pair of superconducting aluminum films separated by a thin layer of amorphous aluminum oxide. In order to avoid the high density of two-level states (TLS) in amorphous oxides, Josephson junctions are designed to be small, thus reducing the participation of the lossy material. However, the persistence of lossy materials in qubits leads to diminishing returns with this strategy. An alternative approach to TLS loss minimization in a transmon qubit junction is to combine the qubit’s nonlinear inductance and capacitance into a single trilayer junction with extremely low dielectric loss, i.e., a merged-element transmon. In this work, we characterize dielectric thin films within lumped-element resonators to determine microwave losses in the single-photon regime and to identify dielectric barrier materials for a merged element transmon. In addition to amorphous solid barriers, we measure microwave-frequency loss of single-crystal epitaxial superconductor-insulator-superconductor trilayers.

*Army Research Office
The design is highly hardware-efficient and eliminates the need for fast external measurement and feedback. Here, we discuss the theoretical model, highlighting features of experimental relevance. We present simulations results demonstrating coherence improvements of an order of magnitude against realistic noise models.


*This work was supported by NSERC, CMC Microsystems, and the Joint Waterloo-Technion Cooperation Program.

10:12 AM A29.00012: Engineering Sideband Interactions with the Very Small Logical Qubit (VSLQ) Device Part I*

GABRIELLE ROBERTS (Presenter), YAO LU, NELSON LEUNG, SRIVATSAN CHAKRAM, University of Chicago, ELIOT KAPIT, Physics, Colorado School of Mines, DAVID SCHUSTER, University of Chicago — Like most other architectures, superconducting quantum bits are extremely sensitive to unwanted interactions with the environment. Determining effective and hardware-efficient quantum error correction protocols is thus an urgent scientific priority. I will describe a simple circuit and protocol that autonomously implements the error correction process [1]. The circuit consists of two transmons connected to dissipative baths in the form of lossy cavities and driven by superconducting quantum interference device couplings. Autonomous error correction is achieved using resonances to coherently correct errored qubit states while leaving un-errored states unaffected. The design is highly hardware-efficient and eliminates the need for fast external measurement and feedback. Here, we discuss the theoretical model, highlighting features of experimental relevance. We present simulations results demonstrating coherence improvements of an order of magnitude against realistic noise models.


*This work was supported by NSERC, CMC Microsystems, and the Joint Waterloo-Technion Cooperation Program.

10:24 AM A29.00013: Engineering Sideband Interactions with the Very Small Logical Qubit (VSLQ) Device Part II*

YAO LU (Presenter), GABRIELLE ROBERTS, NELSON LEUNG, SRIVATSAN CHAKRAM, University of Chicago, ELIOT KAPIT, Colorado School of Mines, DAVID SCHUSTER, University of Chicago — We report our experimental progress towards implementing a VSLQ device for the autonomous quantum error correction. As a first step, we modify the original VSLQ superconducting circuit [1] and propose a new parametric modulation scheme for engineering the VSLQ Hamiltonian. The new scheme requires many fewer RF flux lines, which significantly reduces the device operational complexity and substantially mitigates cross-talks between the multiple flux loops. Next, in our experiment, we calibrate the static circuit parameters under DC flux biasing. We then further explore the dynamic behavior of the circuit under RF flux modulation, and demonstrate how to generate different types of sideband interactions from RF flux modulations with appropriately chosen frequencies and phases. These sideband interactions serve not only as critical components of the VSLQ protocol, but can also be used to realize instantaneous qubit interactions along arbitrary axes.


*This research work was supported by NEQST, ARO Grant No. W911NF-17-S-0001

10:36 AM A29.00014: Efficient characterization of correlated SPAM errors

MINGYU SUN (Presenter), MICHAEL GELLER, University of Georgia — State preparation and measurement (SPAM) errors limit the performance of gate-based quantum computers, but are partly correctable after a calibration step that requires, for exact implementation on a register of n qubits, 2n additional characterization experiments. Here we introduce an approximate but efficient method for SPAM error characterization requiring 2n(n − 1) measurements. The technique assumes that multi-qubit measurement errors are dominated by pair correlations, which are estimated with n(n − 1)/2 two-qubit experiments. We demonstrate this technique on the IBM and Rigetti online quantum computers, allowing comparison of their SPAM errors in both magnitude and degree of correlation. We find that the pair-correlation model is reasonably accurate on linear arrays of qubits. However qubits with more closely spaced two-dimensional geometries exhibit significant higher order (e.g., 3-qubit) SPAM error correlations.
8:00AM A30.00001: ‘Sideways’ and stable crack propagation in a silicone elastomer [Invited] MATT PHARR (Presenter), SEUNGHYUN LEE, Texas A&M University — This talk will describe a peculiar form of fracture that we have found in a highly stretchable silicone elastomer. Namely, under certain conditions a crack will deviate from its ‘standard’ trajectory and instead propagate perpendicular to that trajectory. The crack arrests stably, allowing the material ahead of the crack front to continue to sustain load, and thereby enabling enormous stretchabilities. We call this phenomenon ‘sideways’ cracking. To explain this behavior, we first perform finite element simulations that demonstrate a propensity for sideways cracking, even in isotropic elastomers. Next, we provide a hypothesis on the origin of sideways cracking that invokes microstructural anisotropy. To substantiate this hypothesis, we transversely pre-stretch samples to various extents prior to fracture testing, as to determine the influence of microstructural arrangement (chain alignment) on fracture energy. We conclude by describing how a number of loading conditions, such as sample geometry and strain rate affect this phenomenon. Overall, this talk aims to provide fundamental mechanical insight into basic phenomena associated with fracture of elastomers.

8:36AM A30.00002: How Supertough Gels Break* ITAMAR KOLVIN (Presenter), Physics, UC Santa Barbara, JOHN KOLINSKI, Mechanical Engineering, Ecole Polytechnique Federale de Lausanne,, JIAN PING GONG, Faculty of Advanced Life Science and Soft Matter Gi-CoRE, Hokkaido University, JAY FINEBERG, Hebrew University of Jerusalem — Fracture of soft materials typically takes place at large stretches. This condition challenges our view of how things break, which is based on small-strain linear elasticity. In this talk, I will show how we directly visualized rupture of tough double-network gels at >50% strain. During fracture, crack tip shapes obey a \( x \sim y^{1.6} \) power law, in contrast to the parabolic profile observed in low-strain cracks. A new length scale emerges from the power law that scales directly with the stored elastic energy and diverges when the crack velocity approaches the shear wave speed. Our results show that double-network gels undergo brittle fracture and provide a testing ground for large-strain fracture mechanics.

*J. F. and I. K. acknowledge the support of the Israel Science Foundation (Grant No. 1523/15), as well as the U.S.-Israel Binational Science Foundation (Grant No. 2016950). J. M. K. acknowledges the Fulbright-Israel postdoctoral fellowship for support. J. P. G. acknowledges the support of ImPACT Program of Council for Science, Technology and Innovation (Cabinet Office, Government of Japan).

8:48AM A30.00003: Quantitative Analysis of Spiropyran Mechanophore Activation in Multiple Network Elastomers* CHYI-HUEY YEH (Presenter), YINJUN CHEN, COSTANTINO CRETON, PPM, ESPCI — Multiple network elastomers (MNE) have been used as model systems to characterize the crack tip behavior in soft tough materials. These materials contain reinforcing swelled network chains that are largely responsible for the high fracture toughness of MNEs. By incorporating a spiropyran mechanophore as a chromatic force sensor in the swelled network, stress and energy density localization around a crack tip can be optically detected and quantified. Also, regions with a history of loading and unloading around a crack tip can be identified based on the reversible changes in absorbance of merocyanine isomers (spiropyran in its activated form) in the loading and unloading states. This allows for a more accurate identification of the onset of crack propagation, which occurs before reaching the peak stress. Based on the experimental results, a perspective can be constructed on how statistical molecular information, provided by the mechano-activation of spiropyran, can inform macroscopic modeling of soft tough materials.

*This project is funded by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement n° 695351 – Chemech).
9:00AM A30.00004: Depinning dynamics of crack fronts 
JULIEN CHOPIN (Presenter), Instituto de Fisica, UFBA, ADITYA BHASKAR, ATHARV JOG, LAURENT PONSON, Institut J. le Rond d'Alembert, UPMC/CNRS — Nacre, bones or rationally designed artificial materials are all heterogeneous solids with mechanical properties far exceeding those of their constitutive components. Understanding the role of microscale heterogeneities on the macroscale fracture behavior of solids remains a query, especially when toughness gradients are large. In this talk, I will present a combined experimental and theoretical study of the micro-instabilities of a crack front taking place in heterogeneous materials between two successive equilibrium positions. The instabilities are triggered by pinning the front by isolated tough obstacles of controlled strength and size. We show that the depinning dynamics is controlled by a nonlocal line elasticity and the rate dependency of the dissipative mechanisms taking place within the process zone. We model the behavior by an overdamped equation of motion involving a characteristic material speed and provide an analytical solution which captures quantitatively all our experimental observations. The implications of our results on the energy dissipated during fast fracture events and the fracture behavior of materials with randomly distributed obstacles will be discussed.

[Invited] WILLIAM STEINHARDT (Presenter), SHMUEL RUBINSTEIN, Harvard University — There is a disconnect between our theoretical understanding of brittle fracture, where 2D (effectively 1D) mathematical descriptions generate idealized fractures that are flat, smooth, and stable, and most brittle fractures we encounter in natural or manmade materials (rocks, bones, ceramics), which have significant 3D complexity. However, much of the basic physics that governs this complexity is not well understood. We have developed an experimental system to study 3D fracture mechanics by observing hydraulic fractures in brittle hydrogels. Heavily cross-linked hydrogels have been shown to be a good model system for brittle materials, with the benefits of highly tunable rheology, transparency, and low breakdown pressures. Studying hydraulic fractures allows us to match the refractive index of the interior of the fracture to the bulk, which combined with high speed photography and scanning laser sheet illumination, enables us to resolve the fracture dynamics in three dimensions at up to 1000 volumes per second. We observe that macro-scale roughness comes in the form of step-like perturbations of the fracture front, resulting from material heterogeneity, which leave in their wake a curved linear scar known as a step line. Our dynamic three-dimensional observations of these steps and their interactions allow us to understand the surprisingly elegant topological rules that govern their growth and interaction.

9:48AM A30.00006: Tearing path: instabilities for crack paths in thin sheets cut by blunt objects*
BENOIT ROMAN (Presenter), Physique et Mecanique des Milieux Heterogenes (PMMH), EUGENIO HAMM, Departamento de fisica, USACH, IRYNA SIVAK, Mathematics, EPFL — A thin sheet is a very soft object, which therefore undergoes very large deformation when torn. We found that a straight crack which propagates quasistatically in such a sheet when driven by a blunt object may become unstable in several configurations: oscillatory fracture when the object is displaced along a line, or spiraling when using a perforating cone. We wish to compare these two configurations and show how these instabilities compare in involving the very soft bending mode.

*ANR SMART

10:00AM A30.00007: The Virtual Frame Technique (VFT): direct imaging of fast cracks in soft elastomers*
SAMUEL DILLAVOU, SHMUEL RUBINSTEIN, SEAS, Harvard University, JOHN KOLINSKI (Presenter), IGM, Ecole polytechnique federale de Lausanne — Many phenomena of interest in nature and industry are rapid, making direct imaging both challenging and cost prohibitive. Dynamic cracks can propagate at the sound speed of a material and are ubiquitous in the earth sciences and engineering applications; thus fracture epitomizes such phenomena. In soft materials, the sound speed is of order several meters per second, and a dynamic crack will entirely rupture a cm-scale sample in about 10 msec requiring rapid imaging for direct visualization. Here we present the Virtual Frame Technique (VFT), a simple, useful, and accessible form of compressed sensing that leverages the dynamic range of the camera's sensor to increase the frame acquisition rate by up to 6 orders of magnitude. We discuss the requirements for use of the VFT and its performance when employed with several commercially available conventional and high-speed cameras. Even Modern cell phones can achieve imaging rates of over a million fps using the VFT.

*EMSI lab at EPFL
10:12AM A30.00008: Controlling fracture cascades through twisting and quenching  VISHAL PATIL (Presenter), Department of Mathematics, Massachusetts Institute of Technology, RONALD HEISSER, Sibley School of Mechanical and Aerospace Engineering, Cornell University, NORBERT STOOP, Department of Mathematics, Massachusetts Institute of Technology, EMMANUEL VILLERMAUX, IRPHE, Université Aix Marseille, JORN DUNKEL, Department of Mathematics, Massachusetts Institute of Technology — Fracture fundamentally limits the structural stability of macroscopic and microscopic matter, from beams and bones to microtubules and nanotubes. Despite substantial recent experimental and theoretical progress, fracture control continues to present profound practical and theoretical challenges. While bending-induced fracture of elongated rod-like objects has been intensely studied, the effects of twist and quench dynamics have yet to be explored systematically. Here, we show how twist and quench protocols may be used to control such fracture processes, by revisiting Feynman's observation that dry spaghetti typically break into three or more pieces when exposed to large pure bending stresses. Combining theory and experiment, we demonstrate controlled binary fracture of brittle elastic rods for two distinct protocols based on twisting and nonadiabatic quenching. Our experimental data for twist-controlled fracture agree quantitatively with a theoretically predicted phase diagram, and we establish novel asymptotic scaling relations for quenched fracture. Due to their general character, these results are expected to apply to torsional and kinetic fracture processes in a wide range of systems.

10:24AM A30.00009: Rifts in Rafts  KHA-I TO (Presenter), DANIEL HEXNER, VINCENZO VITELLI, SIDNEY ROBERT NAGEL, University of Chicago — Two-dimensional particle rafts are single-layers of aggregated sub-millimeter polydisperse particles floating at an air-fluid interface. The material failure of such rafts under an applied extensional load has a morphology that appears to be distinct from other known fracture modes. At higher extensional shear rates, numerous small-scale cracks are distributed diffusively throughout the entire system; at low strain rates, the distance between adjacent cracks increases. The characteristics of this distributed failure also depend on the surface tension and viscosity of the underlying fluid. To decrease the influence of secondary flows, we perform experiments by changing the liquid level in the tanks with inclined walls so that we are able to increase the area accessible to the rafts as the liquid height changes. This results in an expansion in quasi-1D (with and without boundaries) and isotropic 2-D expansion in the linear and cylindrical geometries respectively. We simulate this behavior with a model based on weak interparticle forces coupled to an expanding underlying metric.

10:36AM A30.00010: Cracking and self-healing in soft, shrinkable hydrogel packings  HAN-JAE JEREMY CHO (Presenter), MICHAEL P HOWARD, NANCY B LU, REBEKAH A ADAMS, SUJIT DATTA, Princeton University — We aim to better understand cracking in granular, shrinkable packings. Such packings are relevant to agriculture and CO2 sequestration; they also have potential uses in non-fouling films, biosensors, cosmetics, and drug delivery platforms. We use hydrogel particle packings as a model system and experimentally observed how these packings dry, shrink, and crack at an individual-particle level. Most remarkably, we observed a behavior where cracks can form but eventually self-heal. Furthermore, using discrete-element simulations that we developed, we found the precise range of individual-particle shrinkabilities, capillary forces, and contact forces needed to produce this self-healing behavior. Our results inform ways to control crack evolution, which could ultimately pave the way to engineering crack behavior for a wide variety of applications.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A31 DCP GMAG: Addressing Molecular Magnetic Qubits (QIS1) 8CEC 203 - Evelyn Goldfield, National Science Foundation - Tag(s): Focus

8:00AM A31.00001: TBD [Invited]  ALAN ASPURU-GUZIK (Presenter), University of Toronto — NA
First-principles studies of spin-electric coupling in frustrated triangular single molecule magnet qubits

FHOKRUL ISLAM, CARLO CANALI (Presenter), Linnaeus University, MARK PEDERSON, Johns Hopkins University — The efficient manipulation of the quantum states of single-molecule magnets (SMMs) by an electric field is highly desirable for using SMMs in molecular spintronics and quantum information processing. Frustrated triangular SMMs with antiferromagnetic exchange, such as Cu$_3$, are characterized by a doubly degenerate $S=1/2$ ground-state with opposite chirality. It has been proposed theoretically [1] and later verified by ab-initio calculations [2] that the lack of inversion symmetry in these triangular SMMs allows an external electric field to couple these two chiral spin states, even in the absence of spin-orbit interaction. The existence of such spin-electric coupling (SEC) has been observed only very recently in an experiment with a single crystal Fe$_3$ SMM [3]. In this talk, following this recent development, we consider the Fe$_3$ molecule and compare its SEC strength with the one of other triangular SMMs (Cu$_3$, V$_3$ and V$_{15}$), discussing their advantages and disadvantages.


Spin frustration, zero-field splittings, and Jahn-Teller effects in trinuclear copper SMMs: Insights from spin-flip calculations

PAVEL POKHILKO (Presenter), ANNA KRYLOV, University of Southern California — SMMs (single-molecule magnets) are molecules with several unpaired electrons that can be prepared in high-spin states and retain their magnetization for some time. From methodological point of view, SMMs are strongly correlated systems that require specially designed ab initio methods. In our group, we use spin-flip approach (SF). Starting from the highest spin state (usually triplet or quartet), SF treats in a balanced way lower-spin configurations, which is crucial for qualitatively correct description of SMMs. I will present the SF results for copper di- and triradicals. One of the systems has a spin-frustrated trinuclear copper structural motif. Natural orbital analysis indicates that the two lowest doublets and the quartet have purely covalent character thus validating Heisenberg-Dirac-van-Vleck model Hamiltonian. PBE50, a recommended functional from previous benchmarks, matches an experimental estimate for Jahn-Teller splitting of the doublets states – 19 cm$^{-1}$. A large zero-field splitting, previously explained through Dzyaloshinskii-Moriya interaction, originating from spin-orbit coupling (SOC). Validation of this idea will be done using our new SOC code within EOM-CC framework. Additional confirmation comes from El-Sayed rules, predicting a relative magnitude of SOC.

Generalized Hartree-Fock with Non-perturbative Treatment of Strong Magnetic Field: Application to Molecular Spin Phase Transition

XIAOSONG LI (Presenter), Chemistry, University of Washington — In this work, we present a framework of ab initio variational approach to effectively explore the spin phase space in the presence of a homogenous magnetic field. Complex generalized Hartree-Fock (C-GHF) in the spinor formalism is implemented with London orbitals. Recursive algorithms for computing one- and two-electron integrals of London orbitals are also provided. A Pauli matrix representation of the C-GHF is introduced to separate spin contributions from scalar part of the Fock matrix. The spin phase transition in the several molecular systems in the presence of a strong magnetic field is investigated. Non-collinear spin configurations are observed during the phase transition. The competing driving forces of exchange coupling and spin Zeeman effect have been shown to govern the spin phase transition and transition rate. The energetic contributions of the spin Zeeman, orbital Zeeman, and diamagnetic terms to the potential energy surface are also analyzed.

*US Department of Energy (DE-SC0006863)
National Science Foundation (CHE-1565520, OAC-1663636)
Molecular Magnets for Information and Sensing Applications: Response to Fields and Nuclear Spins*

KYUNGWHA PARK (Presenter), Virginia Tech — Recent advances have allowed the experimental realizations of quantum bits and quantum gates by using molecular magnets as active elements, as well as the experimental implementation of quantum algorithms within them. In particular, lanthanide-based molecular magnets are promising for such applications because of strong spin-orbit interaction, compatible molecular geometry to devices, and tunability of coupling between electron and nuclear spins via electric field. So far, there is a lack of ab-initio studies of such coupling and tuning corresponding magnetic properties for lanthanide-based molecular magnets. Nearly degenerate f-orbitals and strongly localized f-electrons suggest importance of calculations beyond density-functional theory. Here we investigate how magnetic properties of monometallic terbium-based molecular magnets are influenced by electric field and coupling to nuclear spin, using multireference quantum chemistry methods including scalar relativistic effects and spin-orbit interaction. We present effects of chemical environment and electric field on such coupling and magnetic anisotropy.

*Funded by the Department of Energy Basic Energy Sciences grant No DE-SC0018326. Computational support by Virginia Tech ARC.

Implementing high fidelity single and entangling two-qubit gates in multi-level systems*

KHADIJEH NAJAFI (Presenter), SOPHIA ECONOMOU, EDWIN BARNES, Physics, Virginia Tech — A recent experiment introduced a novel multi-level nuclear spin (3/2) of single molecule magnet TbPc2 as qubit or qudit. Due to the strong coupling of the nuclear spin to the electric field, this system exhibits simultaneously long coherence times and fast controllability. One of the important questions to address is how well one can implement quantum gates in these systems. By using a combination of analytically solvable two level dynamics and the Suzuki-Trotter product formula, we design z-rotations of high fidelity. We also investigate the implementation of two-qubit entangling gates mediated by a superconducting transmission line resonator coupling two TbPc2 qudits.

*This work is supported by the DOE (grant number DE-SC0018326).

Multireference ab initio studies of magnetic properties of TbPc2-type single-molecule magnets in different charge states*

RYAN PEDERSON, ALEKSANDER WYSOCKI (Presenter), Department of Physics, Virginia Tech, NICHOLAS MAYHALL, Department of Chemistry, Virginia Tech, KYUNGWHA PARK, Department of Physics, Virginia Tech — Lanthanide-based single-molecule magnets (SMMs) can have exceptionally large magnetic anisotropy due to interplay between the ligand crystal field and spin-orbit interaction. Among them, TbPc2 SMM was shown to be promising for quantum information science applications. Although a variety of TbPc2-type SMMs were synthesized in neutral and charged states under different chemical environment, there are no systematic theoretical studies of magnetic properties of such SMMs yet. Almost degenerate 4f orbitals demand multireference quantum chemistry calculations for the magnetic properties. Here, we investigate electronic structure and magnetic properties of TbPc2 and TbPcNc SMMs as a function of oxidation state, ligand type and distortion of molecular geometry, using first-principles relativistic multireference methods including spin-orbit interaction. By applying effective pseudospin Hamiltonian to the lowest multiplet, we examine how these chemical factors affect several important energy scales, such as tunnel splitting, exchange coupling between the Tb magnetic moment and the ligand spin, zero-field splitting, and magnetic anisotropy barrier.

*Funded by the Department of Energy Basic Energy Sciences grant No DE-SC0018326. Computational support by Virginia Tech ARC.
Towards magnetic resonance imaging of a single molecule.*

ALEXEI BYLINSKII (Presenter), Chemistry and Chemical Biology, Harvard University, ZIWEI QIU, SEAS, Harvard University, JEREMY AMDUR, LEI SUN, Chemistry, Northwestern University, DOMINIK BUCHER, OREN BEN DOR, DAVID GLENN, NITHYA ARUNKUMAR, Smithsonian - CFA, Harvard University, ELANA URBACH, TAMARA SUMARAC, BO DWYER, Physics, Harvard University, RONALD L WALSWORTH, Smithsonian - CFA, Harvard University, DANNA FREEDMAN, Chemistry, Northwestern University, MIKHAIL LUKIN, HONGKUN PARK, Physics, Harvard University — While magnetic resonance is an established tool for applications ranging from molecular structure determination to quantum computing, it typically requires large ensembles of molecules to detect the weak magnetic signals. In order to push magnetic resonance spectroscopy and control to the single-molecule limit, we magnetically couple spin-carrying metal-organic complexes to the electron spin of an individual nitrogen-vacancy (NV) defect in diamond, which can be optically initialized and read out. The electron spin on the coordinated metal acts as a reporter of the nuclear spin positions on the complex or a target of interest attached to it, promising to extend electron paramagnetic resonance spectroscopy (EPR) to the limit of single-molecule magnetic resonance imaging (MRI). In addition, the complex can be coherently controlled via the NV center and act as a molecular qubit, which can be assembled into desired quantum spin network architectures via chemical linking.

*Army Research Office (MURI program)
NSF-funded Center for Ultracold Atoms

Magnetic Anisotropy of a Tri-anionic Complex*

DER-YOU KAO (Presenter), SHAWN DOMAGAL-GOLDMAN, NASA Goddard Space Flight Center — The trivalent chromium tri-oxalate complex, \(\text{Cr}^{3+}\{(\text{C}_2\text{O}_4)^{2-}\}_3\)\(^3\) is known to exist as a tri-anion in water. Such systems are difficult to describe with standard DFT due to the fact the HOMO level of the complex solute is pushed to higher energies than the LUMO levels of the \(\text{H}_2\text{O}\) solvent. The mismatch in the solute/solvent Fermi-levels causes charge transfer from the tri-anion to the water as shown in earlier work. However, the spin of the solute complex is not affected by the unphysical charge transfer. The generalized gradient approximation gives a magnetic anisotropy for the isolated and solvated tri-anion \(\text{Cr}^{3+}\{(\text{C}_2\text{O}_4)^{2-}\}_3\)\(^3\)\(\{(\text{H}_2\text{O})_{24}\) of 0.83 and 0.82 Kelvin respectively. These values of magnetic anisotropy agree with 0.89 Kelvin (0.619 cm\(^{-1}\)), which is derived from measurement [1], and imply that the oxalates lose electrons. In this paper results on the electronic and magnetic structure of the tri-anionic complex in water are presented with and without a self-interaction corrected method as a function of cluster size.


*DK acknowledges the support by NASA Postdoctoral Program at Goddard Space Flight Center, administered by Universities Space Research Association.

NSF Quantum Leap Big Idea

EVELYN GOLDFIELD (Presenter), National Science Foundation — We are in the midst of the second quantum revolution which aims to exploit quantum phenomena such as superposition, entanglement, interference to enable major advances in quantum sensing, quantum communication, quantum computation and quantum simulation. These advances require a broad inter-disciplinary effort which includes physical scientists (including chemical physicists and chemists of all types), computer scientists, mathematicians and engineers. The NSF's Quantum Leap (QL) Big Idea draws from all these disciplines to engage in a transformative, high-risk-high reward enterprise to address fundamental questions such as how to prepare and manipulate complex or dynamic quantum states; how to control material-light interactions to create new quantum phenomena; how to design and engineer systems that use quantum effects to their fullest extent. In this talk, I will focus on opportunities for those engaged in chemical and molecular science to engage in NSF QL related initiatives.
8:00AM A32.00001: Catalytic CO oxidation by gas phase atomic clusters [Invited] SHENG-GUI HE (Presenter), Institute of Chemistry, Chinese Academy of Sciences — Oxidation of carbon monoxide (CO) into CO$_2$ is a major solution to removal of CO in air purification and this oxidation process also serves as a prototypical reaction in heterogeneous catalysis. Atomic clusters are ideal models of active sites in condensed phase systems and the elementary and catalytic oxidations of CO by gas phase metal clusters are being actively studied. I will report our recent research progress on catalytic CO oxidation by hetero-nuclear metal oxide clusters including M-Al-O, M-Ti-O, and M-V-O (M=Au, Pt, Cu, Ni, or others) species in the gas phase. The hetero-nuclear metal oxide clusters are generally more catalytic than their homo-nuclear counterparts. The electronic origins such as electro-negativity ladder effect have been proposed to account for the enhanced catalytic reactivity in the oxidation of CO by O$_2$.

References

8:36AM A32.00002: Computational studies of the properties and reactions of metal oxide clusters* [Invited] DAVID DIXON (Presenter), University of Alabama — Modern computational chemistry methods on advanced computer architectures are now capable of providing useful information, for example for catalytic reactions. Benchmarks of electronic structure methods for metal oxides will be described. Coupled cluster CCSD(T) theory has been used to provide benchmark values for the reactivity of metal oxide clusters including normalized clustering energies, Lewis acidities from fluoride affinities, and electron affinities for redox. The reactions of alcohols as models for biomass, the splitting of water, and splitting of hydrogen on transition metal oxide clusters will be described. Correlations with quantities such as Lewis and Brönsted acidities and redox properties will be described. New approaches for predicting the growth of nanoparticles of metal oxides will also be described.

*This work is supported by the U.S. DOE Office of Science, Basic Energy Sciences.

9:12AM A32.00003: Spectroscopy of metal oxide clusters using high resolution anion photoelectron spectroscopy and infrared photodissociation* [Invited] DANIEL NEUMARK (Presenter), University of California, Berkeley — Metal oxide clusters are important model systems for understanding a variety of catalytic processes. Here, the vibrational spectroscopy of size selected metal clusters is investigated with two complementary techniques: slow-electron velocity-map imaging of cryogenically cooled anions (cryo-SEVI) and infrared photodissociation spectroscopy (IRPD).

*This work is supported by the Air Force Office of Scientific Research under Grant No. FA9550-16-1-0097.

9:48AM A32.00004: Nanoparticles versus bulk materials: dramatic changes of ZrO$_2$ properties by nanostructuring GIANFRANCO PACCHIONI (Presenter), University of Milano - Bicocca — Materials in form of nanoparticles or clusters exhibit rather different properties compared to their bulk counterparts. This has been widely shown in the case of metals. Much less is known in the field of oxides. Here we report the results of first principles calculations on nanoparticles of ZrO$_2$ containing from a few tens to a few hundred of atoms. Zirconia is widely used in many technological applications for its wide gap, non-reducibility, low defects concentration, non-magnetic behaviour. We demonstrate that ZrO$_2$ in form of stoichiometric nanoparticles exhibits completely different properties: it becomes easily reducible (by oxygen removal or H$_2$ treatment), highly reactive (with charge transfer to supported metal species) and it turns from a non-magnetic material to a stable ferromagnet at room temperature. These results show the importance of preparing traditional materials in form of nm size particles to obtain new and unprecedented physical properties.
10:00AM A32.00005: Recent advances in THz/far-IR vibrational spectroscopy, synergy DFT-MD simulations and experiments* [Invited] MARIE-PIERRE GAIGEOT (Presenter), Physics, LAMBE UMR8587, Universite d'Evry val d'Essonne, Universite Paris-Saclay — We will present our most recent combined experimental (with the group of Dr A.M. Rijs, FELIX laboratory, Univ Nijmegen, The Netherlands; IR-UV ion dip IR spectroscopy) and theoretical investigations (our group at Univ Evry, Univ Paris-Saclay, France) in the 100-800 cm⁻¹ far-IR/THz vibrational domain for a series of Peptides, Phenol derivatives, beta-sheet Peptides. Finite temperature DFT-MD trajectories are employed in order to calculate anharmonic vibrational spectra of gas phase molecules and clusters.

Our emphasis is on the mapping of THz/far-IR vibrational motions and how to use such mapping to unveil 3D conformational structures in a systematic way. We will especially discuss localized/delocalized vibrational motions in the far-IR, anharmonic/harmonic modes, large amplitude motions, mode couplings and H-bonds signatures in the far-IR/THz spectral domain. We will also present our most recent methods development for extracting ‘effective modes’ from the DFT-MD trajectories and hence assign the vibrational modes.


*Acknowledgments: Collaborative works with Dr A.M. Rijs (The Netherlands), Prof M. Havenith (Germany) & PhD/Post-Doc students J. Mahé, D.J. Bakker, S. Jaaqx, A. Dey, Q. Ong, D.P. Tabor, D.R. Galimberti, S. Pezzotti. A CNRS-PICS 2018-2020 (Programme International de Coopération Scientifique) is acknowledged for supporting fund.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A33 FIAP: 2D Materials and Transition Metal Chalcogenides BCEC 204B - Akm Newaz, San Francisco State University

8:00AM A33.00001: Ultrafast nonlocal collective dynamics of Kane plasmon-polaritons in a narrow-gap semiconductor ALIAKSEI CHARNUKHA (Presenter), IFW Dresden, AARON STERNBACH, Department of Physics, Columbia University, H. TED STINSON, University of California, San Diego, CHRISTOPH BRÜNE, LAURENS W MOLENKAMP, Physikalisches Institut (EP3), University of Würzburg, DIMITRI BASOV, Department of Physics, Columbia University — The observation of ultrarelativistic Dirac, Weyl, and Kane fermions in condensed-matter systems has uncovered a cornucopia of novel phenomenology as well as a potential for effective ultrafast light engineering of novel states of matter. While the non-equilibrium properties of two- and three-dimensional (3D) hexagonal crystals have been studied extensively, our understanding of the photinduced dynamics in 3D singlevalley ultrarelativistic materials is lacking. Here, we employ ultrafast scanning near-field optical spectroscopy to access and control non-equilibrium finite-momentum plasmon-polaritons in thin films of a prototypical narrow-band-gap semiconductor Hg0.81Cd0.19Te. We demonstrate that these collective excitations exhibit distinctly non-classical scaling with electron density characteristic of the ultrarelativistic Kane regime and experience mode splitting due to the coupling of charge oscillations at the top and bottom surface of the thin film. Our observation and ultrafast control of Kane plasmon-polaritons in a semiconducting material using light sources in the standard telecommunications fiber-optics window open a new avenue towards high-bandwidth coherent information processing in next-generation plasmonic circuits.

8:12AM A33.00002: Quantum nonlinear Hall effect in two-dimensional materials with time-reversal symmetry JHIH-SHIH YOU (Presenter), Institute for Theoretical Solid State Physics, IFW Dresden, SHIANG FANG, Department of Physics, Harvard University, SUYANG XU, Department of Physics, Massachusetts Institute of Technology, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University, TONY LOW, Department of Electrical and Computer Engineering, University of Minnesota — We study the quantum nonlinear Hall effect in two-dimensional (2D) materials with time-reversal symmetry. When only one mirror line exists, a transverse charge current occurs in the second-order response to an external electric field, as a result of the Berry curvature dipole in momentum space. Candidate 2D materials to observe this effect are two-dimensional transition metal dichalcogenides (TMDCs). First, we use an ab initio based tight-binding approach to demonstrate that monolayer T_d structure TMDCs exhibit a finite Berry curvature dipole. In the 1H and 1T^* phase of TMDCs, we show the emergence of a finite Berry curvature dipole with the application of an electrical displacement field, respectively.

Quasiparticle Interference on a natural mineral: Mapping the bands of argentiferous Galena

CAROLINA DE ALMEIDA MARQUES (Presenter), CHRISTOPHER TRAINER, CHI MING YIM, School of Physics and Astronomy, University of St Andrews, TIMOTHY DAVID RAUB, School of Earth and Environmental Sciences, University of St Andrews, PETER WAHL, School of Physics and Astronomy, University of St Andrews — Galena (PbS) is the main ore of lead, and in the early days of wireless technology, it played a fundamental part in crystal radios. High-quality samples, that cleave perfectly, are common natural occurrences. It belongs to the lead chalcogenides PbX (X=Te, Se, S), narrow direct bandgap semiconductors which have high thermoelectric figures of merit and unusual semiconducting properties. Their electronic band structure has been studied theoretically and experimentally, revealing a bandgap which decreases with decreasing temperature and under pressure.

Previous Scanning tunnelling microscopy (STM) studies on PbS crystals reported atomically-resolved surfaces. In this study, a natural argentiferous PbS crystal (Ag impurities, p-doped) was cleaved in situ and measured at 20K, using a home-built low-temperature STM. We observe high-quality surfaces with a large variety of defects, surrounded by clear patterns due to quasiparticle interference (QPI). We will show results from QPI to map its electronic structure in the occupied and unoccupied states.

Emphanitic anharmonicity in PbSe at high temperature and anomalous electronic properties in the PbQ (Q=S,Se,Te) system

RUNZE YU, EMIL BOZIN, MILINDA ABYEYKOON, Brookhaven National Laboratory, BORIS SANGIORGIO, NICOLA SPALDIN, ETH Zurich, CHRISTOS MALLIAKAS, Northwestern University, MERCOURI KANATZIDIS, Argonne National Laboratory, SIMON J L BILLINGE (Presenter), Brookhaven National Laboratory — The temperature dependence of the local structure of PbSe has been investigated using pair distribution function (PDF) analysis of x-ray and neutron powder diffraction data and density functional theory (DFT) calculations. Observation of non-Gaussian PDF peaks at high temperature indicates the presence of significant anharmonicity, which can be modeled as Pb off-centering along [100] directions that grows on warming similar to the behavior seen in PbTe and PbS and sometimes called emphanisis. Interestingly, the emphanitic response is smaller in PbSe than in both PbS and PbTe indicating a nonmonotonic evolution with chalcogen atomic number in the PbQ (Q = S, Se, Te) series. The DFT calculations indicate a correlation between band gap and the amplitude of [100] dipolar distortion, suggesting that emphanisis may be behind the anomalous composition and temperature dependencies of the band gaps in this series.


Nonreciprocity in Thermal and Thermoelectric Transport of Electrons in Noncentrosymmetric Crystals

RYOTA NAKAI (Presenter), RIKEN, NAOTO NAGAOSA, University of Tokyo — A system with broken inversion symmetry shows direction-dependent conduction phenomena beyond linear response regime, which is referred to as nonreciprocal transport. In a single crystalline system, noncentrosymmetric crystal structure serves as a source of the nonreciprocal transport of the electrons. In this study, the nonlinear thermal and thermoelectric conductivities of electronic systems are calculated up to the second order in an electric field and a temperature gradient by using the Boltzmann equation with the relaxation time approximation. All the second-order conductivities are described by a small number of functions including the Berry curvature dipole. The second-order conductivities are estimated for the 1H monolayer of the transition metal dichalcogenides and a polar semiconductor BiTeX(X=I,Br).

WS2 atomically thin nanodot array via self-organized templates

ARCHANA KUMARI (Presenter), Slippery Rock University of Pennsylvania — Tungsten Disulphide (WS2) atomic layer nanodot arrays were fabricated with self-organized porous alumina templates as evaporation masks. First tungsten oxide (WO3) was deposited on sapphire substrates through the alumina template to create WO3 nanodot arrays, then WS2 nanodots were formed by the reaction of sulfur with WO3 using chemical vapor deposition (CVD) technique. The sizes of the observed two-dimensional WS2 nanodots varies from 45nm to 70nm. These nanodots exhibit a layer thickness ranging from monolayers to a few atomic layers. This is confirmed by atomic force microscopy (AFM) measurements. Monolayer dots dominated region produces characteristic Raman peaks and high intensity photoluminescence (PL) due to direct band gap transition. Also it has more edge sites which can increase the PL of WS2 dots. A region dominated by multilayer dots produces WS2 Raman peaks but negligible photoluminescence due to indirect transition in multilayers. These novel atomically thin nanodots are attractive for both fundamental studies and future device applications, for e.g. ultrasensitive and ultrafast sensors. Scanning Electron Microscopy and Atomic Force Microscopy of WS2 nanodots is shown in figure.
Piezochromism in the magnetic chalcogenide MnPS$_3$  
NATHAN HARMS (Presenter), University of Tennessee, HEUNG SIK KIM, Rutgers University, New Brunswick, KENNETH R O’NEAL, AMANDA CLUNE, AMANDA HAGLUND, University of Tennessee, DAVID GEORGE MANDRUS, Oak Ridge National Lab, ZHENXIAN LIU, Brookhaven National Lab, DAVID VANDERBILT, Rutgers University, New Brunswick, JANICE LYNN MUSFELDT, University of Tennessee — We bring together diamond anvil cell techniques, optical spectroscopy, and first principles electronic structure calculations to reveal the piezochromic properties of MnPS$_3$. Color changes (green - red - black) take place with pressure as the charge gap systematically redshifts across the visible regime and into the near infrared, moving toward closure at the rate of 0.05 eV/GPa. Strikingly, this extrapolated value for potential band gap closure (55 GPa) corresponds to the theoretically-predicted crossover to the dimerized phase.

Epitaxial growth and collective electronic states of monolayer 1T-NbSe$_2$*  
LIAN LI (Presenter), HUIMIN ZHANG, LIWEI LIU, ZHUOZHI GE, CHENHUI YAN, Department of Physics and Astronomy, West Virginia University, MICHAEL WEINERT, Department of Physics, University of Wisconsin — At the single layer limit, transition metal dichalcogenides (TMDs) can adopt two different structural variants, i.e., polymorphs, depending on the anionic environment around the metal ions: the anions arrange in trigonal prismatic fashion in the 1H polymorph, whereas in 1T the arrangement is octahedral. While bulk 1T NbSe$_2$ doesn't exist in nature, here we show that single layer 1T NbSe$_2$ polymorph can be grown by molecular beam epitaxy on epitaxial graphene/SiC(0001) substrates. A (Ö13xÖ13) Star-of-David charge density waves is observed by in situ scanning tunnelling microscopy, which persists above room temperature. A gap of 0.50 eV are further observed by tunnelling spectroscopy and angle resolved photoemission spectroscopy, indicating that this monolayer 1T phase of NbSe$_2$ is also a Mott insulator, similar to that of bulk 1T TaS$_2$. Our findings indicate that the presence of epitaxial constraints can generate structural configurations that are prohibited in fully-bonded TMD crystals. These findings and their implication on the collective electronic states of single layer 1T-NbSe$_2$ will be discussed at the meeting.

*This research is supported by NSF (DMR-1734017).

Low-Pressure Chemical Vapor Deposition Growth of Iron-Doped MoS$_2$ Monolayers*  
SHICHEN FU (Presenter), KYUNGNAM KANG, XIAOTIAN WANG, SIWEI CHEN, EUI-HYEOK YANG, Mechanical Engineering, Stevens Institute of Technology — Dilute magnetic semiconductors have drawn researchers' attention over the last decade, driven by the advent of spintronics. Transition metal dichalcogenides (TMDs) have demonstrated great potential for new generation spintronics owing to their unique structural and electronic properties. Experimental and theoretical efforts have been made to understand the role of magnetic impurities in TMDs, such as Mn, Fe, Co, and Ni.¹ Theoretical studies show that Fe-substitution in Mo site leads to spin-polarized states and can achieve room temperature ferromagnetic ordering and clustering.² Here, we demonstrate direct growth of Fe-doped monolayer (ML) MoS$_2$ via the chemical vapor deposition. We obtained Fe-doped ML MoS$_2$ with an average crystal size of 40 μm. We observed a PL peak at 1.78 eV, a 70 MeV eV redshift from 1.85 eV obtained from undoped ML MoS$_2$ synthesized in our lab. Scanning transmission electron microscopy images show Fe atoms substituted Mo atoms. X-ray photoelectron spectroscopy will be performed to quantitatively analyze the doping concentration. We will then correlate the growth recipe with its doping concentration for the optimized growth of Fe-doped MoS$_2$ monolayers.

1. C. Jia et al., RSC Adv., 2018, 8, 18837
2. Y. Wang et al., Mat. & Des., 2017, 121, 77

*CFN, BNL, DE-SC0012704.
9:48 AM A33.00010: Direct observation of ultrafast free carrier dynamics in InSe  XIAOQIAN ZHANG (Presenter), University of Missouri — The optical properties of semiconductors are specified by the dynamics of free carriers and bound excitons, both originating from dynamics of electron-hole pair excitations. However, the contribution of free carrier to the optical properties is masked by the excitons-related features. We overcome this issue by assessing the free carrier dynamics in bulk InSe with TR-ARPES measurements. Snapshots of conduction band pumped by 1.55 eV photons at different time delays is explored. The peak excitation is reached at $t = 0.2$ ps. The parabolic dispersion around the conduction band edges can be extracted from the peak intensity difference at $t = 0.2$ ps, where the full parabolic dispersions of the band extrema emerge due to the increased population of carriers. This then relaxes at later time delays. During interband excitons, a non-thermal distribution of excited electron-hole pairs is generated at the earliest time delays, relaxing into a quasi-equilibrium state with a temperature higher than that of the lattice. Our measurements provide a direct observation of population inversion occurs immediately after interband excitation. By directly measuring the band occupancy at all energies and times, we have made a quantitative evaluation of the carrier dynamics.

10:00 AM A33.00011: High harmonic anti-stokes upconversion in van der Waals heterostructure p-n junction photodidodes  FATEMEH BARATI (Presenter), NATHANIEL MONROE GABOR, VIVEK M AJI, University of California, Riverside — Here, we report phonon assisted antistokes absorption near the interlayer exciton edge of a van der Waals semiconductor heterostructure composed of tungsten diselenide and molybdenum diselenide. By carefully tuning the chemical potential of a WSe$_2$/MoSe$_2$ heterojunction, we find highly rectifying I-V characteristics of the device. We use photocurrent spectroscopy to show the system is depleted of charged excitons (trions) as we reach the charge neutrality point at the interface. At low photon energies near 1eV, we observe a strong photocurrent peak with several low energy echoes spaced by 30meV below this fundamental absorption feature. We attribute these highly unusual features to sub-gap antistokes absorption involving out-of-plane optical phonons. Multiple phonons are combined with a low energy photon to generate an electron-hole pair. This highly efficient process due to the alignment of the exciton dipole moment to the atomic displacement of the out-of-plane optical phonons marks the first and most critical step toward laser cooling of atomic layer semiconductors. The antistokes absorption process observed could enhance the efficiency of next generation photovoltaics, by converting vibrational energy into electronic excitations using photons with energies lower than band gap.

10:12 AM A33.00012: ReS$_2$ double gate field-effect transistors with h-BN as dielectric layers  JUNHEE CHOI (Presenter), Department of Physics, Ewha Womans University, KOOKJIN LEE, Electrical Engineering, Korea University, DONG HOON SHIN, Department of Physics, Ewha Womans University, GYU-TAE KIM, Electrical Engineering, Korea University, SANG WOOK LEE, Department of Physics, Ewha Womans University — Transition metal dichalcogenides (TMDs) are regarded as promising 2-dimensional materials for semiconducting devices and optoelectronic applications. Unlike group VI-TMDs, the rhenium-based dichalcogenides crystallize in a distorted triclinic (1T') structure due to an extra electron in the $d$ orbital. Because of this structure, the interlayer coupling effect is weaker than other TMDs. Here, we demonstrated electrical characteristics of double gate multilayer ReS$_2$ FETs, which is passivated with h-BN as gate dielectric layers. The device were measured in double gate mode by sweeping the bottom gate voltage with fixed the top gate bias. The field effect mobilities can be modulated from 26.1 to 40.2 cm$^2$V$^{-1}$s$^{-1}$. The second peak in transconductance ($g_m$) of bottom gate sweep is appeared depending on changing top gate potential indicating that conduction path separates in a multilayer system. Also, the threshold voltage shift of the bottom gate depends on the top gate voltage with two linear relationships due to top gate screening effect.

10:24 AM A33.00013: The thermoelectric and electron transport properties on the charge density wave(CDW) transition of (PbSe)$_n$(VSe$_2$)$_{1.2.3}$ heterostructure materials as well as 1-T VSe$_2$ 2D materials  YU WANG (Presenter), Materials Science, University of Southern California — A series of (PbSe)$_n$(VSe$_2$)$_n$ with $n = 1,2,3$ turbostratic disorder heterostructure materials were synthesized through modulated elemental reactants (MER) method. The in-plane and cross-plane Seebeck coefficient, as well as electron transport properties and Hall coefficient, were measured from 80K to 300K. At the charge density wave (CDW) transition, the Seebeck coefficient decrease by approximately two-fold when the material transforms from CDW state to normal state. And the Raman shift spectra dependence on the temperature of the materials were also measured. All those properties were also compared to the 1-T VSe$_2$ 2D materials.
10:36AM A33.00014: Structure and Electronic Properties of InSe and GaSe Polytypes  
MICHAEL BADAWI (Presenter), ANDREI POSTNIKOV, University of Lorraine, JULIANA SROUR, FOUAD EL HAJ HASSAN, Lebanese University — Equilibrium crystal structures, electron band dispersions, and bandgap values of layered GaSe and InSe semiconductors, each being represented by four polytypes, have been investigated within the density functional theory [1]. Several dispersion correction methods to the DFT, from empirical Grimme corrections to many-body dispersion schemes, have been assessed in comparison with experimental cell parameters [2]. Due to the high technical accuracy achieved, nearly degenerate energy-volume curves of different polytypes are resolved, and the conclusions concerning the relative stability of competing polytypes drawn [3]. The band structures are inspected using the modified Becke-Johnson (mBJ) scheme and hybrid HSE06 functional. Both methods nicely agree with the experimental results and with state-of-the-art GW calculations. Some discrepancies are identified in cases of close competition between the direct and indirect gap (e.g., in GaSe). The placement of bands are slightly different for mBJ and HSE06.


10:48AM A33.00015: Interplay between Rashba Spin-Orbit Coupling, Magnetic Field, and Topological Superconductivity in Monolayer NbSe_2  
DANIEL SHAFFER (Presenter), FIONA BURNELL, RAFAEL M FERNANDES, University of Minnesota, JIAN KANG, Physcis, Florida State University — The persistence of superconductivity above the Pauli limit in monolayer 1H-NbSe_2 is indicative of strong Ising spin-orbit coupling (SOC). It has been suggested that the interplay between Ising SOC and strong in-plane magnetic fields can lead to a topological nodal superconducting phase protected by a time reversal-like symmetry. An important ingredient not fully considered, however, is Rashba SOC. Not only is it expected to be significant due to substrate effects, but it is also tunable by electrostatic gating. In this talk, we present a microscopic model for superconductivity of NbSe_2 driven by repulsive electronic interactions as a function of magnetic field and Rashba SOC. For large enough magnetic fields, a small Rashba SOC lifts the nodes unless the magnetic field is aligned along certain directions, in which case a residual mirror symmetry protects some of the nodes and corresponding flat band edge modes. In the opposite limit of small magnetic fields, a topological chiral phase is found to be stabilized by large Rashba SOC.

Monday, March 4, 2019 8:00 AM - 10:24 AM

Session A35 DQI: Semiconducting Quantum Computing with Donors  
BCEC 205B - Ryan Jock, Sandia National Laboratories - Tag(s): Focus

8:00AM A35.00001: Modeling dopants in silicon: application to atomic-scale Si qubit systems.  
KEYI LIU (Presenter), Joint Quantum Institute, NIST/University of Maryland, College Park, GARNETT BRYANT, NIST, MICHAL ZIELINSKI, Nicholas Copernicus University — Dopants in silicon are strong candidates for qubits in scalable, atom-based, solid-state quantum systems due to their long decoherence times and Si nanofabrication infrastructure. In these devices, an impurity atom binds a donor electron at low temperatures and information is stored either in the electron or the dopant nuclear spin. Typically, tight-binding (TB) theory is expected to provide a good computational model with reasonable precision. However, calculations based on simple central cell potential cutoff failed to predict the well-established energy degeneracies for a variety of bulk Si tight-binding models, hinting missing corrections in the model. We present TB calculations using several new corrections including the induced nearest neighbor hopping, the varying screened potential, and the orthogonalization of the on-site wavefunctions. We also discuss the consequences of applying these atomic scale corrections on the dopant models, including effects on the hyperfine interactions and STM imaging of dopants. Finally, we discuss how these models can be potential guides for experiments in many-body physics using atom-based devices.
8:12AM A35.00002: Using multivalley effective mass theory to probe the phosphorus donor effective potential in silicon* LUKE PENDO (Presenter), XUEDONG HU, University at Buffalo, The State University of New York — Multivalley effective mass (MEM) theories combine physical intuition with an efficient use of computational resources. However, the most appropriate form of effective potential to use with MEM theory remains an open question. Here we develop an MEM theory for an electron confined to a phosphorous donor in Silicon, and explore the most useful form of effective potential that would allow us to accurately predict both spectrum and wavefunction of the electron. We employ a variational method with a freely extensible set of symmetrized Gauss- or Slater-type atomic basis states, with representatives from all five irreducible representations of the Td point-symmetry group. We employ stochastic optimization to complete both variational minimization and model parameter fitting, which allows for parameter spaces of large dimensionality. We consider an effective potential with tetrahedrally symmetric central cell corrections and a dynamic dielectric, as well as exchange-correlation effects, and we also explore effects of external perturbations such as an applied electric field. Our investigation here lays a solid foundation for studies of electronic states and interactions of multiple donors.

*We acknowledge financial support by US ARO via grant W911NF1710257.

8:24AM A35.00003: Quantum computation and simulation with dopants in silicon [Invited] SVEN ROGGE (Presenter), Univ of New South Wales — Bottom-up dopant engineering in silicon reached a level of control where devices can be reproducibly fabricated at the atomic scale with high yield. This talk focuses on the progress of single dopant atom placement in the context of quantum computation and simulation. Silicon offers a particularly interesting platform for quantum bits (qubits) because when isotopically purified it acts as a “semiconductor vacuum” for spins. This leads to extraordinary coherence that is used to realise donor atom based qubits. One and two qubit gates have been achieved with phosphorus qubits in silicon. High-bandwidth dispersive readout has been implemented and single-shot capability has been demonstrated with this technique. Spatially resolved tunnelling experiments that reveal the spectrum and quantum state image of single atoms and tunnel coupled arrangements of atoms will be discussed. This technique enabled the design and verification of a robust scheme to achieve exchange coupling of an two dimensional array of dopants that is immune to placement errors of the atoms. In addition, the fabrication of strongly coupled donor arrays that represent a hardware implementation of a Hubbard simulator will be presented. Quasi-particle tunnelling maps of spin-resolved states with atomic resolution reveal interference processes from which the entanglement entropy and Hubbard interactions are quantified. This represents a first stepping stone towards artificial quantum matter with up to 30 spins to implement complex highly correlated systems.

9:00AM A35.00004: Decoherence of donors in silicon at millikelvin temperatures* PATRICE BERTET (Presenter), VISHAL RANJAN, BARTOLO ALBANESE, SEBASTIAN PROBST, CEA-Saclay, GENGLI ZHANG, The Chinese University of HongKong, EMMANUEL FLURIN, DENIS VION, DANIEL ESTEVE, CEA-Saclay, REN-BAO LIU, The Chinese University of HongKong, JOHN MORTON, UCL London — Donors in silicon are model spin systems [1] and potential candidates for implementing solid-state quantum bits. In that perspective, a detailed understanding of their coherence properties is needed. I will present measurements of Bismuth donors spin relaxation and coherence times at millikelvin temperatures obtained with a homemade spectrometer working at the quantum limit of sensitivity based on superconducting micro-resonators and Josephson parametric amplifiers [2], and I will discuss the various mechanisms at play.


*Support of the European Research Council (grant 615767) and of the French Agence Nationale de la Recherche (projects QIPSE and NASNIQ) is acknowledged.

9:12AM A35.00005: Desorption and lithographic patterning of halogen-terminated Si(100)-(2x1) using STM K.J. DWYER (Presenter), University of Maryland, College Park, JENNIFER E. DEMELL, Laboratory for Physical Sciences, MICHAEL DREYER, University of Maryland, College Park, ROBERT E BUTERA, Laboratory for Physical Sciences — Scanning tunneling microscopy (STM)-based hydrogen depassivation lithography is a well-established technique used for fabricating atomic-scale devices in Si. Incorporation of donor atoms from PH3 into lithographic patterns in a Si surface allows for the formation of metallic wires, electrostatically defined quantum dots, and precise placement of donor atom qubits for quantum information (QI) research. However, interest in acceptor dopants and hole-based devices in QI and other fields necessitates the development of alternate precursor and/or resist chemistries for STM device fabrication. Here, we present results on the passivation and selective depassivation characteristics of halogen resists (Cl and Br) used for STM lithography on Si(100)-(2x1) at low and elevated temperatures (77 K, 300 K, 400 K). We explore STM tip-induced desorption and lithography as a function of tip bias, tunnel current, and electron dose. Through these studies, we demonstrate halogen lithography in an atomically precise mode where single Si dimer-wide features are depassivated, as well as a field emission mode for patterning larger areas of the halogen-terminated Si surface. This work moves us closer to realizing a resist and acceptor combination for fabricating atomic-scale, hole-based devices for QI.
Suppressing spectral diffusion in phosphorus-doped silicon via optical excitation in high magnetic fields* LIHUANG ZHU, Physics and Astronomy, Dartmouth College, JOHAN VAN TOL, National High Magnetic Field Laboratory, CHANDRASEKHAR RAMANATHAN (Presenter), Physics and Astronomy, Dartmouth College — The phosphorus donor impurity in silicon is a promising candidate for spin-based quantum devices. Recent experiments have shown that above-band gap optical excitation can result in strong hyperpolarization of the donor nuclear spins [1,2]. Here we show that low-power above-band-gap excitation can also extend the phase memory time of the donor electron spins in a low-concentration (\(\sim 3.3 - 3.5 \times 10^{15} \text{ cm}^{-3}\)) phosphorus-doped natural abundance silicon sample. A two-pulse Hahn echo experiment at 8.5T and 4K was used to measure the decay of the echo amplitude with time. The non-exponential decays (\(\sim \exp(-t/T_{SD})^n\)) suggest that the phase memory time is dominated by spectral diffusion due to the \(^{29}\text{Si}\) spins [3]. \(T_{SD}\) was measured to be 110 µs in the dark and with sub-bandgap excitation, rising to over 180 µs with 1050 nm laser excitation. With 980 nm excitation, \(T_{SD}\) was observed to increase with applied laser power, saturating at 200 µs.


Machine Learning approach to the inverse problem in STM imaging of dopant-based quantum devices* PIOTR T. RÀSKI (Presenter), MARTYNA PATERA, Institute of Physics, Nicolaus Copernicus University, GARNETT BRYANT, Atomic-Scale Device Group, NIST, MICHAL ZIELINSKI, Institute of Physics, Nicolaus Copernicus University — Atomic-scale solid-state qubits could be implemented using scanned-probe lithography to place two or more phosphorus dopants in silicon close to each other. Scanning tunnelling microscopy (STM) has been used to image individual dopants and to find dopant positions in the host silicon lattice based on that image. Determining the geometry of two-dopant based devices will be an essential step in device fabrication, however, double dopant-based devices will lead to a more challenging problem due to the complicated inter-valley wave-function interference patterns. Here we propose a theoretical solution to that problem. We utilize a multi-million atom tight-binding method, accounting for d-orbitals, surface passivation and surface reconstruction. Further, we use a machine learning approach to determine the positions of both dopants based on STM images generated with tight-binding simulations. From that we derive a set of rules for imaging two dopants and discuss possible generalizations for structures with a larger number of dopants.

*Support from the Polish National Science Centre based on decision No. 2015/18/E/ST3/00583 is kindly acknowledged.
10:00AM A35.00009: Investigating the impact of laser illumination upon coherence times of electron spin qubits bound to donors in silicon* DAVID WISE (Presenter), NAITIK PANJWANI, SIDDHARTH DHOMKAR, JOHN MORTON, London Centre for Nanotechnology, University College London — Donor spin qubits in silicon have long represented an attractive proposition for a qubit architecture. They have long coherence times, fast gate times and development can leverage techniques of the semiconductor industry. Another potential spin qubit, the optically active crystal defect - of which the NV centre in diamond is the most prominent example - has demonstrated exceptional single qubit properties particularly with regards to high fidelity single-shot read out.
An intriguing research question is whether these two different species of spin qubit could be employed in a hybrid architecture. To assess the potential for this an initial study is needed on the impact of laser illumination on coherence times of donor spin qubits in silicon to establish threshold wavelengths and powers at which coherence is negligibly affected. Here, we present an analysis of the impact of NIR illumination on the coherence of electrons bound to phosphorus donors in silicon.

*The authors gratefully acknowledge funding from EPSRC

10:12AM A35.00010: Electronic transport along atomically placed P ribbons in Si* BELITA KOILLER (Presenter), Universidade Federal do Rio de Janeiro, Brazil, AMINTOR DUSKO, CAIO LEWENKOPF, Universidade Federal Fluminense, Brazil — Atomically precise placement of dopants in Si permits creating P nanowires by design. High-resolution images show that these wires are few atoms wide with some positioning disorder with respect to the Si structure sites, which is expected to lead to electronic localization. Experiments, however, report good transport properties in quasi-1D P nanoribbons. We investigate their electronic properties using an effective single-particle approach based on a linear combination of donor orbitals (LCDO), keeping the ground state donor orbitals' oscillatory behavior due to interference among the states at the Si conduction band minima. Our model for the P positioning errors accounts for the presently achievable placement precision.

Transport properties are inferred from the calculated localization length $\zeta$ at the half-filling. For 1 to 3 atoms thick wires, $\zeta$ shows a rich non-monotonic behavior with respect to placement target parameters. We consider different systems widths and disorder scenarios to explore how transverse and longitudinal aimed interdonor distances can be chosen to optimize and control $\zeta$ for specific device applications.

*This work is partially supported by the Brazilian agencies CNPq and FAPERJ.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A36 DAMOP: Hybrid Quantum Systems BCEC 205C - Mukund Vengalattore, Cornell University - Tag(s): Invited

8:00AM A36.00001: Perfect bosonic quantum state transfer using imperfect transducers and interference* [Invited] AASHISH CLERK (Presenter), IME, University of Chicago — The ability to faithfully transfer quantum states between disparate quantum systems is a crucial functionality for quantum information processing. Quantum transducers are often limited by a weak overall coupling strength, or by unwanted spurious interactions. I will discuss recent theoretical work showing that such imperfect transducers can nonetheless be used to accomplish perfect transduction by harnessing interference effects. Unlike other recent approaches for mitigating transduction errors, our approach does not require the ability to inject squeezing at both source and receiver systems, and is applicable to a wide class of imperfect transducers. Our work has direct relevance to optomechanical microwave-to-optics transduction, and also to hybrid quantum memory schemes.

*This work was supported by the AFOSR MURI FA9550-15-1-0029 on quantum transduction.
Combined feedback and sympathetic cooling of a mechanical oscillator coupled to ultracold atoms* [Invited] PHILIPP CHRISTOPH, TOBIAS WAGNER, HAI ZHONG, ALEXANDER SCHWARZ, KLAUS SENGSTOCK, ROLAND MARTIN WISENDANGER, CHRISTOPH BECKER (Presenter), University of Hamburg — A promising route to novel quantum technologies are hybrid quantum systems, which combine the advantages of several individual quantum systems. We have realized a hybrid atomic-mechanical experiment consisting of a Si3N4 membrane oscillator cryogenically precooled to 500 mK and optically coupled to a cloud of laser cooled 87Rb atoms. Here, we demonstrate active feedback cooling of the oscillator to a minimum mode occupation of \( n = 16 \) corresponding to a mode temperature of \( T \approx 200 \mu K \). Furthermore, we characterize in detail the coupling of the membrane to the atoms by means of sympathetic cooling. By simultaneously applying both cooling methods we demonstrate the possibility of preparing the oscillator near the motional ground state while it is coupled to the atoms. Realistic modifications of our setup will enable the creation of a ground state hybrid quantum system, which opens the door for coherent quantum state transfer, teleportation and entanglement as well as quantum enhanced sensing applications.

*We gratefully acknowledge financial support by the DFG (grant No. BE 4793/2-1, SCHW 780/8-1, SE 717/9-1, WI 1277/29-1).

A Topological Source of Quantum Light [Invited] MOHAMMAD HAFEZI (Presenter), University of Maryland, College Park — TBD

Phonon networks with SiV centers in diamond waveguides [Invited] PETER RABL (Presenter), Atominstitut, TU Wien — Electronic and nuclear spins associated with defects in solids comprise a promising platform for various quantum technologies. Prominent examples are NV and SiV centers in diamond, for which many techniques for coherent manipulations and local entanglement operations are already available. However, despite the impressive progress in the local control of spin qubits in diamond and other materials, the next big step of coherently integrating many spin qubits into larger networks has not been achieved yet. In this talk I will discuss a new approach to reach this goal by using quantized mechanical vibrations to mediate interactions between distant spin qubits. Specifically, I will describe the implementation of phonon quantum networks, where multiple SiV centers are coupled to propagating phonon modes in a quasi-1D diamond waveguide. In this setting, quantum states encoded in long-lived electronic spin states can be converted into travelling phonon wave packets and be reabsorbed by a distant defect center in a fully controllable way. I will show that under realistic experimental conditions, this technique enables the implementation of high-fidelity, scalable quantum communication protocols within chip-scale spin-qubit networks.


Optical and mechanical properties of superfluid helium drops levitated in vacuum* [Invited] JACK HARRIS (Presenter), Yale Univ — Many of the goals of quantum optomechanics require a combination of low optical and mechanical loss, low temperature, and high-precision measurement. As a material, superfluid helium offers a number of potential advantages in these regards: vanishing optical absorption and viscosity, high thermal conductivity, and the ability to cool itself efficiently via evaporation. Superfluid optomechanical devices have made considerable advances in recent years, but their performance is often limited by the materials used to contain the superfluid. To avoid these limits we have proposed the use of magnetic levitation to suspend a drop of liquid helium in vacuum[1] with the goal of using the drop’s optical whispering gallery modes (WGMs) and its surface waves as an optomechanical system, while relying on the drop’s evaporation to maintain low temperature. Each of these individual components (i.e., magnetic levitation, WGMs, and evaporative cooling) has been previously demonstrated by other groups, but combining them in a single device should offer several intriguing possibilities. We will describe some of these possibilities, and will also present recent measurements of mm-scale superfluid drops that are magnetically levitated in high vacuum. Specifically, we will describe the formation and trapping of the drops, and their evaporative cooling in the trap to \( \sim 330 \) mK. We will also present measurements of the drops’ mechanical resonances, and of their optical Mie resonances.


*This work supported by W. M. Keck Foundation Grant No. DT121914, AFOSR Grants No. FA9550-09-1-0484 and No. FA9550-15-1-0270, DARPA Grant No. W911NF-14-1-0354, ARO Grant No. W911NF-13-1-0104, NSF Grant No. 1205861, the DARPA/MTO ORCHID Program (through a grant from AFOSR), the John Templeton Foundation, and the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1122492.
8:00 AM A37.00001: Gapless Visons and Emergent U(1) Spin Liquid in Kitaev’s Honeycomb Model* [Invited] CIARÁN HICKEY (Presenter), University of Cologne — In the field of quantum magnetism, the exactly solvable Kitaev honeycomb model serves as a paradigm for the fractionalization of spin degrees of freedom and the formation of $Z_2$ spin liquid ground states. An intense experimental search has led to the discovery of a number of spin-orbit entangled Mott insulators that realize its characteristic bond-directional spin interactions and, in the presence of strong magnetic fields, exhibit no indications of long-range magnetic order. Here, we map out the complete phase diagram of the Kitaev model in tilted magnetic fields and report the emergence of a distinct gapless quantum spin liquid at intermediate field strengths. Analyzing a number of static, dynamical, and finite temperature quantities using numerical exact diagonalization techniques, we find strong evidence that this phase exhibits gapless fermions coupled to a massless gauge field resulting in a dense continuum of low-energy states. Such a phase can be naturally understood within the framework of Abrikosov fermionic partons as a U(1) quantum spin liquid with a spinon Fermi surface, emerging via a superconductor-metal transition. Finally, we discuss its stability in the presence of perturbations, Heisenberg and off-diagonal symmetric exchange interactions, that naturally arise in spin-orbit entangled Mott insulators alongside Kitaev interactions.

*This work was supported by the DFG within the Transregio CRC 183 (project B01).

8:36 AM A37.00002: Ground State of the Spin-1/2 Honeycomb Γ Model: Zigzag Magnetic Order HAI-JUN LIAO (Presenter), RUIZHEN HUANG, YI-BIN GUO, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China, ZHI-YUAN XIE, Department of Physics, Renmin University of China, Beijing 100872, China, BRUCE NORMAND, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, TAO XIANG, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China — The off-diagonal symmetric interaction, $\Gamma ( S_i^\alpha S_{i+\gamma}^\beta + S_i^\beta S_{i+\gamma}^\alpha )$, has sprung to prominence as a competing term in the spin Hamiltonians of candidate Kitaev materials. We investigate the quantum ($S = 1/2$) $\Gamma$ model on the honeycomb lattice using the tensor-network method of infinite projected entangled pair states (iPEPS). We demonstrate that the ground state is a zigzag magnetically ordered state, rather than the spin liquid reported on the basis of density-matrix renormalization-group (DMRG) studies. By applying two quasi-one-dimensional numerical treatments, the infinite matrix-product-state (iMPS) and DMRG methods, we show that this contrast is a consequence of the system size considered. Thus the quantum $\Gamma$ model is quite different from its classical counterpart, which is a classical spin liquid due to its macroscopic ground-state degeneracy.

8:48 AM A37.00003: Nonlinear magnetic susceptibility in the Kitaev model YOSITOMO KAMIYA (Presenter), Department of Physics and Astronomy, Shanghai Jiao Tong University, JUNKI YOSHITAKE, YASUYUKI KATO, Department of Applied Physics, University of Tokyo, JOJI NASU, Department of Physics, Tokyo Institute of Technology, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo — We study the nonlinear spin susceptibility in the Kitaev model [1]. The model has been serving as a paradigmatic model for studying a quantum spin liquid and extensive experimental efforts are currently undertaken. While the Jackeli-Khaliullin mechanism [2] predicts the ferromagnetic Kitaev model, recent theoretical studies suggest that the antiferromagnetic Kitaev model may stabilize distinct spin liquids in a magnetic field. Since the determination of the sign of the Kitaev coupling can be experimentally problematic, we propose a convenient complementary experimental signature to distinguish the two cases. Here, in the gapped spin liquid phase, we derive an analytical expression in perturbation theory and find that the nonlinear spin susceptibility exhibits a characteristic sign change at finite temperature in the ferromagnetic Kitaev model. We also present results based on numerical simulations (exact diagonalization and quantum Monte Carlo simulations), with which we show that the characteristic sign change also appears in the gapless spin liquid phase with a ferromagnetic coupling [3].

9:00AM A37.00004: Ground-state phase diagram of the extended Kitaev-Heisenberg model on a honeycomb lattice


9:12AM A37.00005: Dynamical and Topological Signatures of the Kitaev-Model in a [111] Magnetic Field* [Invited]

MATTHIAS GOHLKE (Presenter), RODERICH MOESSNER, Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany, FRANK POLLMANN, Technische Universität München, 85747 Garching, Germany — Quantum spin-liquids represent exotic phases of matter that host emergent fractionalized excitations. The Kitaev model [1] is a two-dimensional model system in this context and relevant for recent experiments on putative quantum spin-liquid materials. Here, we present results for the Kitaev model coupled to a magnetic field along the [111] axis. Using infinite DMRG, we confirm three phases with vastly different transition fields depending on the sign of the Kitaev exchange [2]: A topological phase hosting non-abelian anyons at low fields, an intermediate regime only existing for antiferromagnetic Kitaev exchange, and a field-polarized phase hosting topological magnons [3].

For the topological phase, we numerically observe the expected cubic scaling of the gap and extract the quantum dimension of the non-abelian anyons.

A novel time-evolution based on matrix product operators enables to obtain the dynamical spin-structure factor, which in presence of a field behaves very differently compared to what is known for the three-spin exchange [4] obtained within a perturbation theory approach [1]. The magnetic field causes the flux degrees of freedom to become mobile. As a consequence the low-energy spectrum contains more structure and the gap in the dynamical spin-structure factor is reduced. Upon approaching the intermediate regime from high fields, the magnon modes reduce in frequency and simultaneously flatten. Near the transition, a broad continuum forms, that ranges down to zero frequency and merges with the single magnon branches. The spectrum appears to be gapless in the entire reciprocal space.


*This work was supported by DFG via SFB 1143.

9:48AM A37.00006: Field-induced neutral Fermi surface and QCD3 quantum criticalities in Kitaev materials

LIUJUN ZOU, Harvard University, YIN-CHEN HE (Presenter), Perimeter Institute — We perform both numerical and theoretical studies on the phase diagram of the Kitaev materials in the presence of a magnetic field. We find that a new quantum spin liquid state with neutral Fermi surfaces emerges at intermediate field strengths, between the regimes for the non-Abelian chiral spin liquid state and for the trivial polarized state. We discuss the exotic field-induced quantum phase transitions from this new state with neutral Fermi surfaces to its nearby phases. We also theoretically study the field-induced quantum phase transitions from the non-Abelian chiral spin liquid to the symmetry-broken zigzag phase and to the trivial polarized state. Utilizing the recently developed dualities of gauge theories, we find these transitions can be described by critical bosons or gapless fermions coupled to emergent non-Abelian gauge fields, and the critical theories are of the type of a $\text{QCD}_3$-Chern-Simons theory. We propose that all these exotic quantum phase transitions can be direct and continuous in the Kitaev materials. Therefore, besides being systems with intriguing quantum magnetism, Kitaev materials may also serve as table-top experimental platforms to study the interesting dynamics of emergent strongly interacting quarks and gluons in 2 + 1 dimensions.
10:00AM A37.00007: Formation of magnetic order in the Kitaev-Heisenberg model*
SHANG-SHUN ZHANG (Presenter), University of Tennessee, GABOR HALASZ, Oak Ridge National Laboratory, WEI ZHU, Los Alamos National Laboratory, CRISTIAN BATISTA, University of Tennessee — We compute the low-energy excitation spectrum and the dynamical magnetic spin structure factor of the Kitaev-Heisenberg model using a variational approach, that becomes exact at the exactly solvable Kitaev points. This approach reveals the physical origin of the asymmetry in the stability range of Kitaev spin liquid phases around the ferromagnetic and antiferromagnetic Kitaev points. We also show that bound states of fractionalized excitations appear in the proximity of a quantum phase transition between the ferromagnetic Kitaev spin liquid and the magnetically ordered states induced by ferro and antiferromagnetic Heisenberg interactions.

*S.~Z. and C.~D.~B. are supported by funding from the Lincoln Chair of Excellence in Physics and from the Los Alamos National Laboratory Directed Research and Development program. G.~B.~H. is supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant No.~GBMF4304. W.~Z. was supported by DOE National Nuclear Security Administration through Los Alamos National Laboratory LDRD Program.

10:12AM A37.00008: Quantum phases in spin-1 honeycomb antiferromagnets: application to Ni$_2$Mo$_3$O$_8$*
SHUYI LI (Presenter), VAIDEESH LOGANATHAN, WENJUN HU, ANDRIY NEVIDOMSKYY, Department of Physics and Astronomy, Rice University — Ni$_2$Mo$_3$O$_8$ is a recently synthesized material containing spin-1 moments on a honeycomb lattice [1]. Such systems are of interest due to their potential to exhibit topological magnons. According to the recent neutron scattering experiment [1], the two sub-lattices making up the bipartite honeycomb lattice each display a zig-zag antiferromagnetic order. Moreover, the order is non-coplanar with a non-trivial angle between adjacent spins due to competing interactions. In this work, we attempt to explain this spin ordering by the means of mean-field theory and Density Matrix Renormalization Group (DMRG) calculations. We use ab initio Density Functional Theory (DFT) calculations to extract the spin-exchange coefficients in the effective low-energy model. We propose that the Dzyaloshinskii-Moriya interaction is the most natural way to explain the observed magnetic ordering.


*Robert A. Welch Foundation Grant C-1818, NSF Grant DMR-1350237

10:24AM A37.00009: Three-dimensional chiral spin liquids in the Kitaev model on a hypernonagon lattice
PETR MISHCHENKO (Presenter), YASUYUKI KATO, Department of Applied Physics, The University of Tokyo, KEVIN O’BRIEN, Institute for Theoretical Physics, University of Cologne, TROELS BOJESEN, Department of Applied Physics, The University of Tokyo, TIM ESCHMANN, Institute for Theoretical Physics, University of Cologne, MARIA HERMANNS, Department of Physics, University of Gothenburg, SIMON TREBST, Institute for Theoretical Physics, University of Cologne, YUKITOSHI MOTOME, Department of Applied Physics, The University of Tokyo — Chiral spin liquids (CSLs) are exotic quantum states without magnetic order but with broken time-reversal symmetry. Recently, the ground-state and finite-temperature ($T$) behaviors of CSLs have been studied for the Kitaev models [1] on two and three-dimensional (3D) lattice geometries [2-4]. In this talk, we will present a comprehensive study of the ground state and thermodynamic properties of the Kitaev model on the 3D hypernonagon lattice, which has previously been explored in the limit of anisotropic interactions [4]. Our numerical simulations employ quantum Monte Carlo technique, which in combination with the Chebyshev polynomial expansion [5], allows us to study systems of up to 2600 spins. We find evidence for a first-order phase transition in the isotropic interactions case similar to the anistotopic limits, but into a different type of CSL ground state. We also present the ground-state phase diagram obtained by variational calculations.

10:36AM A37.00010: Nonlocal String Order Parameter in the S=1/2 Kitaev-Heisenberg Ladder*  ERIK SORENSEN  (Presenter), Physics, McMaster University, HAE-YOUNG KEE, ANDREI CATUNEANU, Physics, University of Toronto — We study the S=1/2 Kitaev-Heisenberg (KJ) model in a two-leg ladder. Without a Heisenberg interaction, the Kitaev phase in the ladder model has Majorana fermions with local Z2 gauge fields and is usually described as a disordered phase without any order parameter. Here we prove the existence of a non-local string order parameter (SOP) in the Kitaev phase which survives with a finite Heisenberg interaction. The SOP is obtained by relating the Kitaev ladder, through a non-local unitary transformation, to a one-dimensional XY chain with an Ising coupling to a dangling spin at every site. This differentiates the Kitaev phases from other nearby phases including a rung singlet. Two phases with non-zero SOP corresponding to ferromagnetic and antiferromagnetic Kitaev interactions are identified. The full phase diagram of the KJ model is determined using exact diagonalization and density matrix renormalization group methods, which shows a striking similarity to the KJ model on a two-dimensional honeycomb lattice.

*This research was supported by NSERC and CIFAR and enabled in part by support provided by (SHARCNET) (www.sharcnet.ca) and Compute/Calcul Canada (www.computecanada.ca).

10:48AM A37.00011: Ground-state phase diagram of the Kitaev-Heisenberg model on a kagome lattice  KATSUHIRO MORITA (Presenter), MASANORI KISHIMOTO, TAKAMI TOHYAMA, Tokyo University of Science Katsushika Campus — The Kitaev-Heisenberg model on the honeycomb lattice has been studied for the purpose of finding exotic states such as quantum spin liquid and topological orders. On the kagome lattice, in spite of a spin-liquid ground state in the Heisenberg model, the stability of the spin-liquid state has hardly been studied in the presence of the Kitaev interaction. Therefore, we investigate the ground state of the classical and quantum spin systems of the kagome Kitaev-Heisenberg model. In the classical system, we obtain an exact phase diagram that has an eight-fold degenerated canted ferromagnetic phase and a subextensive degenerated Kitaev antiferromagnetic phase. In the quantum system, using the Lanczos-type exact diagonalization and cluster mean-field methods, we obtain two quantum spin-liquid phases, an eight-fold degenerated canted ferromagnetic phase similar to the classical spin system, and an eight-fold degenerated q=0, 120° ordered phase induced by quantum fluctuation.


Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A38 GMAG DMP: Magnetoelectric and Multiferroic Effects in Molecular Systems
BCEC 206B - Janice Musfeldt, Univ of Tennessee, Knoxville - Tag(s): Focus

8:00AM A38.00001: Structure-property relations in multiferroic [(CH3)2NH2]M(HCOO)3 (M=Mn,Co,Ni)  KENDALL HUGHEY (Presenter), AMANDA CLUNE, MICHAEL O YOKOSUK, University of Tennessee, JING LI, Fudan University, NANDITA ABHYANKAR, Florida State University, XIAXIN DING, Los Alamos National Laboratory, NARESH DALAL, Florida State University, HONGJUN XIANG, Fudan University, DMITRY SMIRNOV, National High Magnetic Field Laboratory, JOHN SINGLETON, Los Alamos National Laboratory, JANICE LYNN MUSFELDT, University of Tennessee — We combine magnetization and infrared spectroscopy to unveil the B-T phase diagrams and vibrational properties of the [(CH3)2NH2]M(HCOO)3 (M=Mn,Co,Ni) family of multiferroics. While the magnetically-driven transition to Bc in the Mn analog takes place at 15.3 T, much higher fields are required to saturate the Ni and Co materials. Analysis of the infrared spectrum of the Mn and Ni compounds across Tc reveals splitting of the formate bending mode which functions as an order parameter of the ferroelectric transition. By contrast, the Co complex reveals a surprising framework rigidity where the ferroelectric state is driven solely by counterion freezing. With magnetic field, the Mn (and most likely, the Ni) materials engage the formate bending mode to facilitate the transition to the fully saturated magnetic states, whereas the Co complex adopts an alternate mechanism involving formate stretching distortions. Similar structure-property relations involving substitution of transition metal centers and control of the flexible molecular architecture are likely to exist in other molecule-based multiferroics.
8:12AM A38.00002: DFT Study of the Magnetic and Structural Properties of the DTN Molecular Crystal  

MAHER YAZBACK (Presenter), SHUANGLONG LIU, NEIL SULLIVAN, HAI-PING CHENG, University of Florida — DTN or dichloro-tetrakis-thiourea-nickel (NiCl₂ – [SC(NH₂)₂]₄) is a molecular crystal whose soft lattice structure allows it to more easily deform, allowing stronger magneto-electric coupling (ME) manifestations, compared to typical ME materials. At low temperatures and in moderate magnetic fields DTN exhibits exotic behavior including a quantum phase transition into a Bose-Einstein condensate/XY antiferromagnetic state. Moreover, the presence of disorder introduced by Br doping experimentally shows evidence for the existence of a Bose glass state. This system poses a challenge when trying to accurately model structural and mechanical properties due to its weak intermolecular interactions. Our work attempts to understand the nature of DTN and Br-DTN using density functional theory (DFT). By including the effects of Van der Waals interactions using the DFT-D3 correction we show that we can get accurate lattice constants, bond lengths and bond angles, which allows us to further probe the mechanism responsible for the magneto-electric phenomena present in DTN. We also report our calculation of the exchange coupling constants and zero-field splitting constants responsible for the behavior of DTN at low temperatures.

8:24AM A38.00003: Electron-Beam Patterning of the Low-Loss (High-Q) Ferrimagnetic Coordination Compound V[TCNE]ₓ₋₂ (Vanadium Tetracyanoethylene)*  

ANDREW FRANSON (Presenter), Physics, The Ohio State University, NA ZHU, Electrical Engineering, Yale University, SETH KURFMAN, MICHAEL CHILCOTE, EZEKIEL JOHNSTON-HALPERIN, Physics, The Ohio State University, HONG X TANG, Electrical Engineering, Yale University — Integrating patterned, low-loss magnetic materials into silicon-based devices and circuits presents many difficulties, from lattice matching requirements to extreme deposition conditions for traditional ferrite materials. Here we present the deposition, patterning, and characterization of the low-loss (α = 3.94 x 10⁻⁵), room-temperature ferrimagnetic coordination compound vanadium tetracyanoethylene, (V[TCNE]ₓ₋₂). Patterning of V[TCNE]ₓ₋₂ thin films from 100 nm to 1 µm thick is performed via electron-beam lithographic patterning using a poly(methyl methacrylate), poly(methyl methacrylate-methacrylic acid 8.5%) copolymer bilayer (PMMA/P(MMA-MAA)) on sapphire and silicon, and this process can be trivially extended to most inorganic substrates. The V[TCNE]ₓ₋₂ is deposited on the patterned PMMA/P(MMA-MAA) via chemical vapor deposition (CVD) at 30 mTorr and 50°C in an argon atmosphere. V[TCNE]ₓ₋₂ patterned in this method retains its low-loss characteristics down to feature sizes of 10s of µm, below which a non-conformal deposition regime leads to a non-trivial geometry. These results establish the versatility and potential of V[TCNE]ₓ₋₂ to be incorporated in future silicon-based electronic devices.

*NSF Grant No. EFMA–1741666

8:36AM A38.00004: Electric field modulation of magnetic exchange in molecular helices detected by Electron Paramagnetic Resonance*  

[Invited] MARIA FITTIPALDI, ALBERTO CINI, Department of Physics, University of Florence, Italy, GIUSEPPE ANNINO, Istituto per i Processi Chimico-Fisici - IPCF, CNR, Italy, ALESSANDRO VINDIGNI, Physics, ETH, Zurich, Switzerland, ANDREA CANESCHI, Department of Industrial Engineering, University of Florence, Italy, ROBERTA SESSOLI (Presenter), Department of Chemistry, University of Florence, Italy — The possibility to operate on magnetic materials through the application of electric rather than magnetic fields - promising faster, more compact and energy efficient circuits - continues to spur the investigation of magneto-electric effects. Beyond symmetry requirements, large spin-orbit coupling is generally considered a necessary ingredient. On the contrary, a control of the spin-spin interaction by an electric field, not relying directly on spin-orbit coupling but rather on the overlap of the electronic clouds of interacting centers, would be quite appealing in the emerging field of quantum materials. Here, we report the detection of a magneto-electric effect that we attribute to an electric field modulation of the magnetic exchange interaction theoretically predicted for molecular magnetic helices. On a Manganese(II)-radical helix, thus comprising spin centers with negligible orbital contribution, the application of an electric field (E) introduces an energy contribution, which is different in case of parallel or antiparallel alignment of neighboring spins along the helix. The E field effect on the intra-chain exchange interaction J has been here experimentally observed by exploiting the sensitivity of Electron Paramagnetic Resonance (EPR) spectroscopy under electric field modulation. It is in fact well known that one-dimensional spin correlation can induce a significant g-shift even when only a weak anisotropy of dipolar origin is present. By replacing the usual B-field modulation with the E-field modulation an EPR signal is induced by the shift of the resonance as a result of the electric field effect on J. The symmetry of the observed phenomenon unambiguously confirms its magneto-chiral nature. Our observation opens interesting perspectives, which may be relevant also for the investigation of multiferroic materials.

*Italian MIUR (PRIN 2015 HYFSRT project), European QuantERA (SUMO project), and Fondazione CR Firenze.
Together, this opens the door to further exploration of the high field phase using powered and pulsed magnets. Multiferroic materials with a cascade of transitions up to and including the 31 T transition to the fully polarized state. The phase diagram is different to other temperature phase diagram. Density functional theory and numerical simulations of the exchange interactions was measured using pulsed magnetic fields of up to 60 T and temperatures down to 0.6 K, to reveal the magnetic field-dependent electronic structure. The result implies a potential approach to realize spin injection and detection on SCs without using any magnetic material.


The zero-field effect of chirality-induced spin selectivity has been observed in a host of nanostructures involving chiral molecule monolayers on noble metals.1 However, there has been no report of similar experiments on semiconductor (SC) surfaces. Here, we report on a study of spin-selective electron transport across chiral polyalanine molecules in vertical junctions of (Ga,Mn)As/polyalanine/Au. The bottom electrode is an epitaxially strained (Ga,Mn)As film with perpendicular magnetic anisotropy. The junctions are formed in openings in a hardened PMMA layer on the (Ga,Mn)As defined by electron beam lithography. The native oxide on the exposed (Ga,Mn)As is removed by ion milling, followed immediately by polyalanine monolayer self-assembly in a solution. The top Cr/Au electrodes are thermally evaporated under liquid nitrogen cooling. The (Ga,Mn)As acts as a spin analyzer: Sweeping the perpendicular magnetic field at low temperatures, sharp jumps in the junction resistance are observed at the coercive fields, indicating spin filtering of electrons from the Au electrode by the polyalanine monolayer. The result implies a potential approach to realize spin injection and detection on SCs without using any magnetic material.

The interplay of magnetism and chirality with valley excitons SHUOFENG LAN (Presenter), XIAOZE LIU, SIQI WANG, HANYU ZHU, University of California, Berkeley, YAWEN LIU, University of California, Riverside, CHENG GONG, University of California, Berkeley, JING SHI, University of California, Riverside, YUAN WANG, XIANG ZHANG, University of California, Berkeley — Most biological molecules are chiral and exist in one of the two mirror-image enantiomers. The so-called homochirality of life is one of the most fundamental mysteries for human beings. Theory and experiments show that the magneto-chiral (MCh) effect albeit small may play a role in the molecular enantioselectivity of prehistoric life by simultaneously breaking both the parity-inversion and time-reversal symmetry. For the first time, we observe an excitonic MCh effect in artificially arranged van der Waals (vdW) crystals with an unprecedented giant MCh anisotropy more than 30 times larger than that in natural materials. Moreover, the observed excitonic MCh effect possesses a spectral splitting that is more than 50 times larger than that induced by the Zeeman effect. Such an excitonic MCh effect creates a link among magnetism, chirality, spin, and excitons, which has long been explored ever since the discovery of the natural optical activity by Arago and magnetically induced optical activity by Faraday in the early 19th century. Furthermore, the electronic nature of spins in two-dimensional vdW semiconductors makes the manipulation of enantioselectivity in magneto-chiral systems attractive for photochemical reactions, asymmetric synthesis, and chiral quantum optics.

Multiferroic Quantum Criticality AWADHESH NARAYAN (Presenter), ETH Zurich, ANDRES CANO, Institut Neel, CNRS & Univ. Grenoble Alpes, ALEXANDER BALATSKY, NORDITA, NICOLA SPALDIN, ETH Zurich — The zero-temperature limit of a continuous phase transition is marked by a quantum critical point, which can generate exotic physics that extends to elevated temperatures. Magnetic quantum criticality is now well known, and has been widely explored [1]. Ferroelectric quantum critical behavior has also been recently established [2], motivating a flurry of research investigating its consequences. In this talk, I will present the concept of multiferroic quantum criticality -- in which both magnetic and ferroelectric quantum criticality occur in the same system -- that we have recently proposed [3]. I will describe the phenomenology of multiferroic quantum critical behavior, its emergence in complex transition metal perovskite oxides and propose candidate materials in which it should be observable.


Magnetic field-temperature phase diagram of the molecule-based multiferroic (NH4)2FeCl3H2O AMANDA CLUNE (Presenter), University of Tennessee, JISOO NAM, Ulsan Natl Inst of Sci & Tech, KENDALL HUGHEY, University of Tennessee, MINSEONG LEE, Ulsan Natl Inst of Sci & Tech, WEI TIAN, JAIME FERNANDEZ-BACA, RANDY FISHMAN, Oak Ridge National Laboratory, JOHN SINGLETON, Los Alamos Natl Lab, JUN HEE LEE, Ulsan Natl Inst of Sci & Tech, JANICE LYNN MUSFELDT, University of Tennessee — The magnetization of a molecule-based multiferroic, (NH4)2FeCl3H2O and its deuterated analog, was measured using pulsed magnetic fields of up to 60 T and temperatures down to 0.6 K, to reveal the magnetic field-temperature phase diagram. Density functional theory and numerical simulations of the exchange interactions demonstrates the origin of non-collinearity and multiferroicity within the system. The phase diagram is different to other multiferroic materials with a cascade of transitions up to and including the 31 T transition to the fully polarized state. Together, this opens the door to further exploration of the high field phase using powered and pulsed magnets.
Spin dynamics in molecular multiferroic (ND₄)₂[FeCl₅(D₂O)]*  
WEI TIAN, HUIBO CAO, GABRIELE SALA, TAO HONG, RANDY FISHMAN, JAIME FERNANDEZ-BACA (Presenter), Oak Ridge National Laboratory — (ND₄)₂[FeCl₅(D₂O)] is a molecular magnet that exhibits extraordinary coupled magnetic and ferroelectric properties. Applying modest magnetic field induces successive magnetic transitions with distinct magnetoelectric (ME) coupling and the underlying mechanism is not fully understood yet. Knowing the microscopic interactions is essential to understand the complex coupled phenomena. We performed inelastic neutron scattering experiments to measure the spin dynamics in (ND₄)₂[FeCl₅(D₂O)]. We will present here some INS data analysis results using linear spin wave theory.

*Research conducted at ORNL's Spallation Neutron Source and High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

Giant Electrically Controlled Spinterface in Organic Ferroelectric Copolymer-based Multiferroic Tunnel Junctions  
HOANG LUONG (Presenter), RUGANG GENG, MINH PHAM, THO NGUYEN, Physics and Astronomy, University of Georgia — Controlling spin of electron by purely electrical means at high temperature is challenging and a long sought device in spintronics. In this APL (110, 053302, 2018), we report electrically controlled interfacial spin polarization, or the magnetoelectric effect in multiferroic tunnel junctions (MTJs) by employing organic ferroelectric copolymers, poly(vinylidene fluoride-trifluoroethylene) (P(VDF-TrFE)), as a tunneling barrier. First, we show that the spontaneous ferroelectric polarization of the P(VDF-TrFE) films can be formed in a thin interlayer. Next, the tunneling magnetoresistance in the unpolarized TMJ quenches from 21% at 20 K to 0.7% at 296 K. Remarkably, the interfacial spin polarization of the device, dubbed spinterface, can be gradually tuned by an applied electric field. Upon the electric polarization reversal, the tunneling electroresistance reaches about 30% at 200 K and the spinterface of the device significantly changes up to 100%. The interface between P(VDF-TrFE) and Co electrode might act as an electric-field-dependent spin filter causing the large magnetoelectric effect. The resistance of the MTJs can be controlled by either electric field or magnetic field, and therefore can potentially be used as a high density information storage element with four states.

Tunnel magnetoresistance in oligophenyl based magnetic tunnel junctions  
RICHARD MATTANA (Presenter), BENOIT QUINARD, SOPHIE DELPRAT, SOPHIE COLLIN, FRÉDÉRIC PETROFF, PIERRE SENEOR, Unité Mixte de Physique CNRS/Thales — Molecular spintronics, an emerging research field at the frontier between organic chemistry and spintronics, has opened novel and exciting opportunities in terms of functionalities for spintronics devices. Among those devices, molecular magnetic tunnel junctions have attracted a growing interest over the years. Indeed, it was shown that spin dependent hybridization at the metal/molecule interface could lead to a radical tailoring of spintronics properties. To achieve this, self-assembled monolayers appear to be very promising candidates thanks to their impressive molecular scale crafting properties and easy-processing. Previous works were done with basic molecules such as linear alkanethiols. We now focus on more complex molecules integrating aromatic moieties to study how the modification of the tunnel barrier impacts the magnetic and electronic behaviour of the devices. We will present spin dependent tunneling transport underlining the main similarities and differences between alkanethiols and oligophenyls MTJs.

Spin transport through graphene/molecules-based magnetic tunnel junctions*  
CLEMENT BARRAUD (Presenter), JACKO RASTIKIAN, PASCAL MARTIN, PHILIPPE LAFARGE, MARIA LUISA DELLA ROCCA, MPQ, Université de Paris, RICHARD MATTANA, UMR 137, CNRS, PIERRE SENEOR, UMR 137, Université Paris Saclay, FRÉDÉRIC PETROFF, BRUNO DLUBAK, UMR 137, CNRS — Spin transport through organic molecules is motivated by the ability to tune at the atomic scale the spin injection/detection properties. This property is barely achievable in inorganic systems and it is due to the possibility of designing molecules atoms by atoms. With this respct, ferromagnetic metal/molecules interfaces has focused most of the attention.

A common issue remains the quality of such complex interfaces. Ferromagnetic metals like Co, Fe, Ni are transition metals and are easily oxidizable. The presence of oxygen atoms is known to completely modify the magnetic and electronic properties of magnetic surfaces. The recently proposed Ni/graphene electrodes for spintronics applications is very appealing due to their protected character. Moreover, graphene is more and more viewed as a good platform for the absorption of molecules.

In this talk, I will describe the fabrication process of magnetic tunnel junctions made of Ni/graphene/nitrobenzene molecules/Co/Au. I will especially detail the electrografting procedure to attach molecules over the graphene surface. I will then present the magnetotransport measurements performed at low temperatures. I will also discuss the bias voltage dependence of the magnetoresistance.

*"2DSPIN" from the Emergence program (City of Paris)
Electronic Phase Separation induced dramatic enhancement of large magnetoresistance in Organic Spin Valves*  

WENTING YANG (Presenter), QIAN SHI, TIAN MIAO, QIANG LI, PENG CAI, HAO LIU, HANXUAN LIN, BAI YU, YINYAN ZHU, YANG YU, LINA DENG, WENBIN WANG, LIFENG YIN, Fudan University, DALI SUN, Department of Physics, North Carolina State University, XIAOGUANG ZHANG, Department of Physics, University of Florida, JIAN SHEN, Fudan University —  

Organic spin valves (OSVs) have been studied widely with respect to the long spin relaxation time of the carriers in the organic materials and their synthetic versatility, ease of manufacturing and pliability. Recent advances focused on the spin-interface and the multi-functionalities of OSVs. Here we employ LPCMO with high spin polarization and electronic phase separation (EPS) to tune the MR of the OSV, which depends strongly on the pre-set magnetic field, voltage and temperature due to the spin-flip scattering in LPCMO and the interface. An extremely high MR of 438% and the rangeability of 5.9 times are observed. Our findings point an alternative way for multistate of OSVs and controllable room temperature OSVs by using LPCMO with high Tc and electronic phase separation.

*National Key Research Program of China (2016YFA0300702), National Basic Research Program of China (973 Program) under Grants No. 2014CB921104, National Natural Science Foundation of China (11504053), the Program of Shanghai Academic Research Leader (18XD1400600) and the Shanghai Municipal Natural Science Foundation (18ZR1403200). D.S. and X.-G.Z. were supported by the start-up funding at the North Carolina State University and the US National Science Foundation DMREF-1534401.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A39 GMAG DQI DMP: Coherent Spins in Semiconductors  

8:00AM A39.00001: Spin–photon interface and spin-controlled photon switching in a nanobeam waveguide  
PETER LODAHL (Presenter), University of Copenhagen — Selected by FT organizers

8:36AM A39.00002: Off-Resonance Time-Resolved Kerr Rotation Spectroscopy*  
MEHMET NOYAN (Presenter), J. M. KIKKAWA, University of Pennsylvania — We show that time-resolved Kerr rotation (TRKR) is a quantitatively accurate tool to measure spin dynamics, even when conducted highly off resonance. We find that TRKR measurements have essentially identical temporal profiles when the probe energy is tuned far below, far above, and on resonance with a semiconducting band gap. We also present energy dependent TRKR spectra, and show they have an odd Lorenztian profile around the semiconducting band gap, at odds with the simplest theoretical model which predicts an even Lorenztian form. We show that this discrepancy is resolved if one accounts for a decrease in the transition linewidth as the optical energy increases above the band-edge transition.

*We gratefully acknowledge support from NSF DMR-1206270.

8:48AM A39.00003: Identification of multi-photon transitions between magnetic dipole states using electrically detected magnetic resonant excitation with variable drive-field helicities.*  
ADNAN NAHLAWI (Presenter), HANS MALISSA, Department of Physics and Astronomy, University of Utah, 115 South 1400 East, Salt Lake City, Utah 84112, USA, DANI STOLTZFUS, PAUL BURN, Centre for Organic Photonics and Electronics, School of Chemistry & Molecular Biosciences, The University of Queensland, Queensland 4072, Australia, TAMIM DARWISH, ANNA LEUNG, National Deuteration Facility, ANSTO, Lucas Heights, New South Wales 2234, Australia, JOHN LUPTON, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany, CHRISTOPH BOEHME, Department of Physics and Astronomy, University of Utah, 115 South 1400 East, Salt Lake City, Utah 84112, USA — For magnetic resonance conditions where the amplitude of the resonant driving field \( B_1 \) is close to the static magnetic Zeeman field \( B_0 \), quantum-optical effects linked to the two photon helicities, including the Bloch-Siegert shift [1,2] or multiple photon effects [3,4,5], emerge. In order to study the latter, we built a radio frequency domain electron spin resonance setup which allows for driving fields with arbitrary polarization. For the detection of magnetic resonance at \( B_0 \) in the mT-range where spin polarization is all but vanishing, we used spin-dependent recombination currents in a fully deuterated form of poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (d-MEH-PPV), in which proton-induced random hyperfine fields are minimized. We report results obtained for circularly, linearly, and elliptically polarized excitation states. [1] J. J. Sakurai, Modern Quantum Mechanics, Revised Edition. *Addison-Wesley* (1994); [2] J. Romhányi et al., *Phys. Rev. B* 92(5), 054422 (2015); [3] J. H. Shirley, *Phys. Rev.* 138 (4B), B979 (1965); [4] M. Göppert-Mayer, *Annalen der Physik*, 18(7-8), 466 (1931); [5] J. I. Kaplan and S. Melboom, *Phys. Rev.* 106(3), 499 (1957); [6] D. P. Waters et al., *Nature Phys.* 11(11), 910 (2015).

*We acknowledge support from the DOE under Award #DE-SC0000909.
A charge-tunable quantum dot strongly coupled to a nanophotonic cavity

ZHOUCHEN LUO (Presenter), EDO WAKS, University of Maryland, College Park — Quantum dots (QDs) integrated with photonic structures is a promising scalable platform for the development of quantum networks and distributed quantum computing. Probabilistic charging of the QDs with electron/hole spins by adding a doping layer suffers from low charging stability due to carrier tunneling. Sandwiching the QDs into a p-n junction, which allows deterministically changing the charging state of the QDs by changing the external gate voltage can resolve this problem. Many experiments that previously have been achieved in probabilistic charged QDs sample, like cavity assisted QDs spin manipulation, have been successfully demonstrated using those charge tunable p-n junction QDs sample. However, the strong coupling between QDs spin and a microcavity, which is the basis of many QDs-based quantum information processing protocols and quantum optics experiments, hasn’t been accomplished yet. Here, we report for the first time the realization of strong coupling between charge tunable QDs spin and a micro cavity, and the demonstration of spin population transfer via optical pumping. The strong coupling combined with deterministic charging paves way for applications of QDs in quantum optics.

Theory of the circulating current of a single magnetic impurity in a semiconductor

ADONAI RODRIGUES DA CRUZ (Presenter), Department of Applied Physics, Eindhoven University of Technology, MICHAEL FLATTÉ, Department of Physics and Astronomy, University of Iowa — The localized electron spin of a single impurity in a semiconductor is a promising system to realize quantum information schemes [1]. Coherent control of this spin depends on understanding the structure of the magnetic moment that couples the system with external fields. In this work we investigate the spin-orbit induced circulating current associated with the ground state of a single magnetic impurity in zincblende III-V semiconductor. This circulating current is dissipationless and represents an electron moving in a closed trajectory producing an orbital contribution to the magnetic moment [2]. We developed a formalism employing Green's functions obtained by the Koster-Slater technique [3,4] with a sp^3d^5s^* empirical tight-binding Hamiltonian to describe the host material.


Polarization-to-spin conversion and entanglement distribution via coherent interface with semiconductor double quantum dot

CHIEN-YUAN CHANG (Presenter), KAZUYUKI KUROYAMA, MARCUS LARSSON, SADASHIGE MATSUO, Department of Applied Physics, University of Tokyo, TAKAFUMI FUJITA, Institute of Scientific and Industrial Research, Osaka University, SASCHA R VALENTIN, ARNE LUDWIG, ANDREAS D. WIECK, Ruhr-Universität, AKIRA OIWA, Institute of Scientific and Industrial Research, Osaka University, SEIGO TARUCHA, Department of Applied Physics, University of Tokyo — Interfacing photonic qubits with a gate-defined spin qubit remains critical challenges in semiconductor devices. In this talk, we discuss the key properties of a coherent interface by two separate experiments, quantum state transfer, and entanglement absorption with a double quantum dot. We report polarization-to-spin conversion implemented with single-shot readout of a single electron spin generated in a GaAs quantum dot. The optical spin blockade effect requires in-plane magnetic field and photo-excitation associate to Zeeman-split light-holes, but not heavy-holes. This effect, following the optical selection rules, determines the generation efficiency depending on the photon linear-polarization and the electron number in the dot. Secondly, we discuss the experimental progress of entanglement absorption between an entangled photon pair to a single spin and a photon. With the temporal coincidences and the conditional probabilities of the polarized photon and the electron spin correlation, we plan to detect individual entanglement transferal events.

*This work is supported by Grant-in-Aid for Scientific Research, “Nano Spin Conversion Science” (No. JP15H01012, No. 26103004), and “Topological Materials Science” (No. JP16H00984) from MEXT, CREST (No. JPMJCR15N2).
9:36AM A39.00007: Observation of magnetoresistance effect in charge pumping measurements  MARK A ANDERS (Presenter), National Institute of Standards and Technology, PATRICK MICHAEL LENAHAN, Pennsylvania State University, JASON T RYAN, National Institute of Standards and Technology — We report on a new magnetoresistance effect based on spin dependent trapping events at MOSFET gate/substrate interfaces called near zero field spin dependent charge pumping (NZF SDCP). NZF SDCP involves the application of a trapezoidal gate voltage waveform which cycles the substrate Fermi level between the conduction and valence band edges. Interface defects are cyclically filled and emptied, generating a net substrate recombination current proportional to the number of defects. The change in current is measured as a function of magnetic field. We find that: (1) in most cases the NZF SDCP amplitude appears to saturate as a function of waveform frequency, and (2) the NZF SDCP spectrum broadens with increasing frequency. These observations may allow for experimental exploration of several magnetoresistance theories regarding interaction or exchange times between charge carriers and defect spin centers. (3) The addition of N to the 4H-SiC MOSFET interface can have a profound impact on the NZF SDCP response, and (4) we almost certainly resolve electron-nuclear hyperfine interactions from a H-complexed defect. These observations strongly suggest that NZF SDCP could be a powerful tool to obtain atomic-scale physiochemical information about MOSFET interface defects.

9:48AM A39.00008: Electrically Detected Magnetic Resonance in Silicon Nitride Thin Films of Widely Varying Stoichiometries*  RYAN WASKIEWICZ (Presenter), ELIAS B FRANTZ, PATRICK MICHAEL LENAHAN, Pennsylvania State University, SEAN KING, Intel Corporation — We utilize electrically detected magnetic resonance (EDMR) to identify defects responsible for electronic transport in thin films of silicon nitride. The EDMR response is detected via spin dependent trap assisted tunneling over a range of electric fields. The EDMR measurements are made at both high and low field/frequency combinations. These EDMR measurements are compared with near-zero field magnetoresistance (NZFMR) measurements in which no oscillating magnetic field is applied; we observe an NZFMR response related to the EDMR. A comparison between the EDMR and NZFMR allows us to draw conclusions with regard to the relative analytical power of NZFMR versus EDMR as well as aid in the development of the physical understanding of the NZFMR response.

*Funding provided by Intel and DTRA (grant no. HDTRA1-18-0012). The content and information do not necessarily reflect the position or policy of the federal government; no official endorsement should be inferred.

10:00AM A39.00009: Electrically Detected Magnetic Resonance Study of 4H-SiC/SiO2 Transistors with Barium Passivation*  JAMES ASHTON (Presenter), PATRICK MICHAEL LENAHAN, Pennsylvania State University, DANIEL J LICHTENWALNER, Wolfspeed, a Cree Company, AIVARS J LELIS, United States Army Research Laboratory, MARK A ANDERS, National Institute of Standards and Technology — We report on electrically detected magnetic resonance measurements on 4H-SiC/SiO2 metal oxide semiconductor field effect transistors. 4H-SiC/SiO2 based MOSFETs show great promise for high power and high temperature applications. However, the SiC/SiO2 interface has a high concentration of interface and near-interface traps which limits effective channel mobility. Passivation decreases the interface state density and thus increases the mobility. Passivation schemes typically including post-oxidation annealing in NO. Recent work suggests promise for a barium interfacial layer (IL) before oxidation1. We probe the atomic scale defects at the SiC/SiO2 in NO and barium treated devices and compare the results with those on unpassivated devices. Both the NO anneal and the barium IL greatly reduce the density of near-interface silicon vacancies, but yield somewhat different post-passivation defect structures.


*Funding was provided by the U.S. Army Research Laboratory
We report the tunneling current behavior in a nano-semiconductor structure of (Ga, Al) As / GaAs, which contains the Rashba spin orbital interaction in the presence of embedded InAs quantum dots of different geometries (lens, pyramid and ring) depending on the voltage, magnetic field, and different spin-orbit interaction values \( k_\text{gL} = \pi/4, \pi/2, 3\pi/4 \). These results show that the intensity of the current presents appreciable changes when the morphology of the quantum dot changes and also when the intensity of the bias voltage and magnetic field increase. For voltages less than or equal to 0.2 V and considering spin up we observed the appearance of the first peaks of current intensity according to the morphology of the following way: Pyramid, lens and ring. However, when the voltage is greater than 0.2 V a change in the current occurs due to the morphology of the quantum dots changing in its order: Ring, lens and pyramid. This phenomenon also occurs when the spin orbit coupling is changed, showing that as the value of the phase increases, a change in the domain of the morphology for similar voltages also occurs.

*The authors are thankful to vicerectoria de investigaciones-UIS

**10:24AM A39.00011: Zeeman-type spin splitting in non-magnetic three-dimensional compounds: Material prediction and electrical control** CARLOS MERA ACOSTA (Presenter), Center of Natural and Human Sciences, Federal University of ABC, Brazil, ADALBERTO FAZZIO, Brazilian Nanotechnology National Laboratory, Campinas, SP, Brazil, GUSTAVO DALPIAN, Center of Natural and Human Sciences, Federal University of ABC, Brazil — Besides the Rashba and Dresselhaus effects, another kind of spin discrimination phenomena in non-magnetic inversion asymmetry (IA) compounds is the so-called *Zeeman-type* spin splitting, which exhibits a spin-texture similar to the one observed in the magnetic Zeeman effect. Despite its potential for device application, this non-magnetic effect has only been predicted and observed in the two-dimensional WSe\(_2\) and MoS\(_2\) materials. Here, we demonstrate that three-dimensional compounds can also exhibit this splitting. The required conditions for this effect are: valence band maximum or conduction band minimum in a non-time-reversal-invariant \( k \)-point, inversion asymmetry, and zero magnetic moment. Using these conditions as filters, we perform a material screening and high-throughput *ab-initio* calculations to systematically search for these materials in the ICSD database. We find 20 candidates featuring this splitting. Our calculated spin splittings can be as large as 433, 510, and 491 meV for the compounds WN\(_2\) (\( P6m1 \)), WS\(_2\) (\( R3m \)), and SnTe (\( F43m \)), respectively. We also demonstrate that the spin splitting in slabs of these compounds depends on the growth direction and can be controlled by an external electric field.

*We thank FAPESP (grant 18/11856-7) and CNPq for financial support.

**10:36AM A39.00012: DETECTION OF STRONG MAGNETIC RESONANT DRIVE EFFECTS USING SPIN-DEPENDENT ELECTRONIC TRANSITION RATES IN ORGANIC SEMICONDUCTOR MATERIALS** SHIRIN JAMALI (Presenter), HANS MALISSA, Department of Physics and Astronomy, University of Utah, 115 South 1400 East, Salt Lake City, Utah 84112, USA,., DANI STOLTZFUS, PAUL BURN, Centre for Organic Photonics and Electronics, School of Chemistry & Molecular Biosciences, The University of Queensland, Queensland 4072, Australia., TAMIM DARWISH, ANNA LEUNG, The National Deuteration Facility, ANSTO, Lucas Heights, New South Wales 2234, Australia., JOHN LUPTON, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstrasse 31-93040 Regensburg, Germany., CHRISTOPH BOEHME, Department of Physics and Astronomy, University of Utah, 115 South 1400 East, Salt Lake City, Utah 84112, USA. — Spin-dependent recombination currents in \( \pi \)-conjugated polymers allow for the detection of charge carrier spin resonance at very weak applied static Zeeman fields \( B_0 \) [1]. We have used this effect to study magnetic resonance in the strong driving regime when the amplitude of the driving field \( B_1 \sim B_0 \). Technologically, these measurements were carried out by using monolithic thin-film device structures in which a polymer bipolar injection device [an organic light emitting diode] was fabricated directly on top of an RF microwire [2]. We used a fully deuterated form of poly [2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] as active device layer due to its low local hyperfine fields. Under strong-drive, spin collectivity set in [1,2] and a variety of strong drive effects could be observed, including the Bloch-Siegert shift and two photon transitions. The measured dependence of the former on \( B_1 \) confirmed theoretical predictions, suggesting that the monolithic nano-layer device stack used in these experiments could serve as probe for ultra-strong light-matter coupling of paramagnetic charge carriers in polymer materials. [1] Waters et al., *Nature Phys.*, **2015**, 11, 910; [2] Jamali et al., *Nano Lett.*, **2017**, 17, 4648.

*We acknowledge support from the DOE under Award #DE-SC0000909
Looking for new layered ferromagnetic semiconductor*  
TAI KONG (Presenter), KAROLINE STOLZE, Chemistry, Princeton University, JING TAO, Brookhaven National Laboratory, DANRUI NI, ROBERT CAVA, Chemistry, Princeton University — Layered magnetic semiconductors have attracted great attention recently since ferromagnetism was demonstrated to persist down to single-molecular-layer level. In this talk, we will show our recent effort in looking for new compounds under this category and report the discovery of a new layered ferromagnetic semiconductor with a van der Waals gap.

*Gordon and Betty Moore EPiQS initiative, Grant No. GBMF-4412

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A40 GMAG: Electric Field and Strain Control of Magnetism  
Virginia Commonwealth Univ - Tag(s): Focus

8:00AM A40.00001: E-field control of RKKY interaction in FeCoB/Ru/FeCoB/PMN-PT (011) multiferroic heterostructures  
XINJUN WANG (Presenter), YUYI WEI, NIAN-XIANG SUN, Northeastern University — E-field control of antiferromagnetic orders is promising for the realization of fast, compact, and energy-efficient AFM applications. However, because of the invisibility of AFM spins, the E-field control process is mainly based on the exchange bias regulation that usually confines at a low temperature. Here we explore a new magnetoelectric (ME) coupling mechanism for the modulation of AFM orders at room temperature. Based on the FeCoB/Ru/FeCoB/PMN-PT, the external E-field generates relative magnetization switching in the two ferromagnetic layers, leading the Ruderman–Kittel–Kasuya–Yosida interaction tuning. This voltage induced switching behavior can be repeated in a stable and reversible manner for various SAFs. We further quantify the voltage induced RKKY interaction changes by analyzing the dynamic optical and acoustic modes through the ferromagnetic resonance measurement, and with first principle calculations, we find that the distortion of the Fermi surface by the lattice reconstruction is the key of the relative magnetization switching and RKKY interaction modulation. This voltage control of RKKY interaction in ME heterostructures provides an easy way for the AFM coupling control and for achieving the next generation of AFM/FM spintronic applications.

8:12AM A40.00002: Voltage control of magnetic anisotropy of a FePt/MgO(001) heterostructure  
QURAT AIN (Presenter), Department of Physics, University of Ulsan, DORJ ODKHUU, Department of Physics, Incheon National University, SUNG-HYON RHM, SOON CHEOL HONG, Department of Physics, University of Ulsan — Control of magnetic properties by an external electric field can be a potential candidate to overcome the limitation of high-power consumption for non-volatile magnetoelectric random access memory (MeRAM). We predict a huge voltage control magnetic anisotropy (VCMA) coefficient \(1.77 \times 10^{-3}\) pJ/(V.m) of the Fe(Pt)-interfaced FePt/MgO heterostructure. The Fe-interfaced FePt/MgO film exhibits strain-induced magnetization reorientation instigated through second order magnetoelastic coupling along with extremely sensitive VCMA behavior. We anticipate a significant effect of the external field on the induced electric dipole that is formed in terms of charge accumulation or depletion at the metal/dielectric interface. These results are a step forward to achieve a full potential of MeRAM with write voltage below 1 V and switching bit energy below 1 fJ.

8:24AM A40.00003: Electric Field-Modulated Propagating Spin Wave Properties in Ultrathin CoFeB Film  
SAMIRAN CHOUDHURY (Presenter), S.N. Bose National Centre for Basic Sciences, BIVAS RANA, RIKEN-CEMS, ANJAN BARMAN, S.N. Bose National Centre for Basic Sciences, YOSHICHIKA OTANI, RIKEN-CEMS — One of the most promising magneto-electric effects is the recently discovered electric field controlled magnetic anisotropy (ECMA), generally observed at the interface between 3d-ferromagnets and oxide where CoFeB/MgO interface has attracted particular attention due to high TMR ratio at room temperature and low Gilbert damping. Interestingly, ECMA can be used to modulate SW properties at ultralow power consumption. We report a systematic experimental study on the modulation of propagating SW frequency in ultrathin CoFeB films by tuning interfacial perpendicular magnetic anisotropy (iPMA) by electric field applied through a top metal gate electrode. The magnetostatic surface SWs are excited and propagate along the waveguide. The SW signals are detected by measuring inverse spin Hall effect voltage across Ta layer underneath the CoFeB films. To modulate the SW frequency a dc gate voltage is applied from a voltage source. The resonance frequency either decreases or increases under the application of negative or positive gate voltages due to the increment or decrement of iPMA with gate voltages. We have also measured SW signals from CoFeB films of lower thicknesses and observed significant modulation of SW frequency with gate voltage due to higher magneto-electric coefficient.
Oxide heterostructures provide an exciting opportunity to engineer new artificial systems with unique properties that cannot be found in naturally occurring materials. Enabling the control of electronic properties of oxides that feature a metal-insulator transition (MIT) is a key requirement for developing a new class of electronics often referred to as “Motttronics” [1]. Although doping and radiation damage are effective tools to permanently change the MIT temperature in these materials, a simple method to switch the MIT properties in real-time is needed for practical applications. In this talk I will present the discovery of giant nonvolatile resistive switching ($\Delta R/R > 1000\%$) and strong modulation of the MIT temperature ($\Delta T_c > 30$ K) in a voltage-actuated $V_2O_3/PMN$-PT heterostructure. The control of the $V_2O_3$ electronic properties is achieved using the transfer of ferroelastic strain from the PMN-PT substrate into the epitaxially-grown $V_2O_3$ film. Strain can reversibly promote/hinder the structural phase transition in $V_2O_3$, thus advancing/suppressing the associated MIT. While oxide/ferroelectric hybrids had been studied in the past using other correlated materials, such as VO$_2$ [2], Fe$_3$O$_4$ [3], LaNiO$_3$ [4], NdNiO$_3$ [5], etc., the reported nonvolatile resistive switching was rather modest: $1.5\% < \Delta R/R < 110\%$. More than an order of magnitude larger resistive switching in $V_2O_3/PMN$-PT could enable practical implementations of voltage-controlled Mott devices and provide a new platform for exploring fundamental electronic properties of $V_2O_3$.


*The research was supported by the Vannevar Bush Faculty Fellowship program, funded by the Office of Naval Research through grant N00014-15-1-2848.
9:24AM A40.00006: Ultralow Voltage Control of Magnetism* YEN-LIN HUANG (Presenter), Lawrence Berkeley National Lab, BHAGWATI PRASAD, Department of Materials Science and Engineering, University of California, Berkeley, JAMES STEFFES, Department of Materials Science & Engineering, University of Connecticut, SAHAR SAREMI, LEI ZHANG, Department of Materials Science and Engineering, University of California, Berkeley, SASIKANTH MANIPATRUNI, Intel Corporation, BRYAN HUEY, Department of Materials Science & Engineering, University of Connecticut, IAN YOUNG, Intel Corporation, RAJESH CHOPDEKAR, Lawrence Berkeley National Lab, R RAMESH, Department of Materials Science and Engineering, University of California, Berkeley — The key to integrating the concepts of spintronics into conventional nanoelectronics lies with the ability to control the magnetic order in nanoscale devices. With the continuous shrinkage of integrated circuits, the energy efficiency required to control these tiny magnets as power dissipation becomes more and more important. Over the past decades, the oxide community has been exploring the materials that can provide the opportunities to control magnetism. Among the large investigated materials, multiferroics might be one of the most promising material family. Multiferroics are the materials which possess at least two order of parameters, particularly, the coexistence of ferroelectricity(P) and magnetism(M), and exhibit coupling from one to another. In this talk, I will demonstrate an ultra-low-voltage (<500 mV) and non-volatile manipulation of ferromagnetism at room temperature via the heterostructure of spin valves on a multiferroic layer, BiFeO3(BFO). Finally, I will conclude this talk with a summary of current challenges and future direction of multiferroics, especially BFO, toward the low-power electronics.

*Acknowledgments: R.R acknowledges support from the SRC-JUMP program through the ASCENT center. Y.L.H is supported by a grant from the DOE Advanced Manufacturing Office.

9:36AM A40.00007: Electric field manipulation of exchange bias in antiferromagnetic Cr2O3 thin films* WEI YUAN (Presenter), CLIFF CHEN, JUNXUE LI, YAWEN LIU, VICTOR ORTIZ, Physics and Astronomy, UC riverside, TANG SU, School of Physics, Peking University, PENG WEI, JING SHI, Physics and Astronomy, UC riverside — Cr2O3 is an interesting insulating antiferromagnetic material, which has been widely investigated recently, including in the studies of the spin Seebeck effect and the long spacing distance spin transport. Cr2O3 is also a well-known magneto-electric material, whose sublattice spins can be switched by an electric field. In this study, we first grow a 5 nm thick Pt layer on the substrate of (0001)-oriented Al2O3 using magnetron sputtering, and then the Cr2O3 thin films using high vacuum pulsed laser deposition. 1 nm Co is grown on top of Cr2O3 by molecular beam epitaxy or magnetron sputtering, followed by a 2 nm thick Pt capping layer deposited in-situ to prevent the oxidation of the ferromagnetic Co. The Co layer shows a very strong perpendicular magnetic anisotropy with exchange bias by anisotropy magnetoresistance measurements. The exchange bias can be reversibly manipulated by the gating electric field in Cr2O3 between the bottom and top Pt layers. The magneto-electric manipulation of Cr2O3 spins offers potential to switch the magnetization in high-density memory devices incorporating antiferromagnets with low energy consumption.

*Spins and Heat in Nanoscale Electronic Systems, funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences award NO. SC0012670

9:48AM A40.00008: Control over the ISHE in a platinum film by ionic gating SERGEY DUSHENKO (Presenter), University of Maryland, College Park/National Institute of Standards and Technology, MASAYA HOKAZONO, Department of Electronic Science and Engineering, Kyoto University, KOHJI NAKAMURA, Department of Physics Engineering, Mie University, TERUYA SHINJO, YUICHIRO ANDO, MASASHI SHIRAISHI, Department of Electronic Science and Engineering, Kyoto University — We report reversible modulation of the inverse spin Hall effect (ISHE) in Pt achieved through the careful control of Pt thickness and an ionic gating technique. The ISHE converts spin current into charge current, which allows easy detection of spin current and integration of spintronics and electronics. The effect is governed by spin-orbit interaction and is particularly strong in Pt, which has been widely used as the ISHE-based spin current detector. However, the gate tuning of the spin-orbit interaction in metals was considered out of reach because of high carrier density.

We fabricated Pt films, 1.5 nm to 20 nm thick, on top of the YIG ferrimagnetic layer and used spin pumping to inject spin current in the Pt layer. Using the the ionic gel (DEME-TFSI) top gate, the resistance of the Pt film was tuned up to 280%. Such control over the resistance and carrier density in Pt allowed us to gate tune the amplitude of the ISHE over two orders of magnitude—a result that can be used in spin-torque and other spintronics devices that use spin-charge conversion [1].

10:00AM A40.00009: Voltage control of magnetism in metal oxide/metal nanoislands and nanostripes*  MARTIN NICHTERWITZ (Presenter), SHASHANK HONNALI SUDHEENDRA, JONAS ZEHNER, KENNY DUSCHEK, Leibniz Institute of Solid State and Materials Research (IFW Dresden), Helmholtzstr. 20, 01069 Dresden, Germany, KORNELIUS NIELSCH, Leibniz Institute of Solid State and Materials Research (IFW Dresden), Helmholtzstr. 20, 01069 Dresden, Germany; Institute of Materials Science, Technische Universität Dresden, KARIN LEISTNER, Leibniz Institute of Solid State and Materials Research (IFW Dresden), Helmholtzstr. 20, 01069 Dresden, Germany — Voltage control of magnetism by ionic approaches presents a promising pathway to low-power magnetic devices. Up to now, magneto-ionic manipulation has been reported mainly for ultrathin films and nanoporous structures.[1-3] Since the mechanism is based on interfacial charge transfer, the morphology may be key to the magneto-ionic efficiency.

We investigate the influence of morphology on magneto-ionic changes during electrolytic gating of FeOx/Fe nanostructures. In FeOx/Fe nanoislands [4], the magneto-ionic changes are enhanced compared to continuous films and close to ON/OFF switching of magnetization is achieved.[5] The results are explained mainly by the higher surface/volume ratio of the nanoislands. Further, we investigate the transfer of magneto-ionic effects from extended thin film to nanostripe geometry. We present initial results on voltage-controlled magnetoresistance in FeOx/Fe stripes probed via in situ magneto-transport measurements.

[2] Quintana et al., Small, 2018, 14, 1704396

*Funding by the DFG (LE2558/2-1) is acknowledged.

10:12AM A40.00010: The Effect of Material Defects on Magneto-Elastic Switching*  DAVID WINTERS (Presenter), MD AHSANUL ABEED, SUPRIYO BANDYOPADHYAY, Electrical and Computer Engineering, Virginia Commonwealth University — Past experiments have shown that magneto-elastic switching phenomenon is extremely energy-efficient but error-prone. We have studied the effect of material defects (voids, thickness variations, etc.) on the switching probability of elliptical magnetostrictive nanomagnets subjected to uniaxial strain using micromagnetic simulations in the presence of thermal noise. Defects drastically increase the switching error rate. Curiously, there is a critical value of stress that results in the minimum error rate for both defective and defect-free nanomagnets. The critical stress is much higher for defective nanomagnets. Another interesting observation was that if the nanomagnet's thickness is different in two different halves, then stable magnetization states are spawned along the nanomagnet's hard axis. Above a certain thickness variation, the magnetization tends to get pinned along the hard axis when the nanomagnet is stressed and remains stuck there even after stress removal. These unexpected observations reveal some of the complexities associated with magneto-elastic switching, with important ramifications for practical applications of straintronics.

*National Science Foundation. Grant number ECCS-1609303.

10:24AM A40.00011: Ferroelectric control of magnetism in Pt/BaTiO3 thin films  QILONG SUN (Presenter), California State University, Northridge, JULIAN VELEV, Department of Physics, University of Puerto Rico at Rio Piedras, NICHOLAS KIOUSSIS, California State University, Northridge — The quest for artificial multiferroic heterostructures consisting of ferroelectric (FE) and ferromagnetic (FM) layers is of increasing interest. Because the optimizing interfacial magnetoelastic coupling between the magnetic and electric polarizations allows novel means of controlling magnetization or polarization in view of efficient, low-power spintronic devices. Using first principles calculations we predict the emergence of magnetism in ultrathin nonmagnetic Pt films induced by the ferroelectric polarization of BaTiO3 films, where the induced Pt magnetization depends on the polarization direction. More importantly, the calculations reveal that the Pt/BaTiO3 bilayer undergoes an in-plane to out-of-plane spin reorientation via ferroelectric polarization switching of the BTO, with a giant change of magnetic anisotropy from 1.15 to -0.49 erg/cm², indicating a huge magnetoelectric effect. These findings open interesting prospects for exploiting higher electric field efficiency of magnetic anisotropy for the next generation of magnetoelectric random access memory devices.
Strain and magnetic properties of antiferromagnetic NaNiF₃ thin films

SOPHIE MORLEY (Presenter), HUMBERTO MARQUEZ, DAVID LEDERMAN, University of California, Santa Cruz – Fluoro-perovskites have been proposed as an alternative candidate to the oxide perovskites for magneto-electric applications.¹,² It is therefore desirable to create thin film samples to integrate into devices. NaNiF₃ (NNF) is an antiferromagnet which has a distorted perovskite crystal structure that sustains weak ferromagnetism with a bulk TN = 156 K and a Pnma space group symmetry.³ We have grown NNF via molecular beam epitaxy on SrTiO₃ (100) to produce high quality epitaxial films in the thickness range of 5–50 nm. The films had the expected Pnma structure and were predominantly oriented along the [101] direction. The SQUID magnetometry displayed a temperature-dependent magnetization consistent with antiferromagnetic ordering and a weak ferromagnetic moment. We observe a thickness-dependent transition temperature, where the change is ΔTN = -7 K for decreasing thickness between 40 and 10 nm, which correlates with the increased tensile strain measured using x-ray diffraction.


*This work was supported by the MRPI program of the University of California under grant no. MRP-17-454963.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A41 GMAG DMP: Spin Transport and Excitations in Antiferromagnets

Fengyuan Yang, Ohio State University - Tag(s): Focus

8:00AM A41.00001: Spin Torque Switching of Antiferromagnet* [Invited] CHENG SONG (Presenter), XIANZHE CHEN, Tsinghua University, RICARDO ZARZUELA, YAROSLAV TSEKOVNYAK, University of California, Los Angeles, JIA ZHANG, Huazhong University of Science and Technology, FENG PAN, Tsinghua University — Antiferromagnets with zero net magnetic moment, strong anti-interference and ultrafast switching speed have potential competitiveness in high-density data storage. Electrical switching of antiferromagnets is at the heart of their device application [1,2]. The antidamping torque-induced switching of Néel order is attained in a biaxial antiferromagnetic insulator NiO, which is manifested electrically via spin Hall magnetoresistance in NiO (100)/Pt bilayers [3]. The antiferromagnetic moments are switched towards the current direction, different from the vertical configuration in the fieldlike torque scenario (e.g., CuMnAs and Mn₂Au) [4,5]. On the other hand, electric field is used to switch the magnetic moment of Mn₂Au films grown on piezoelectric Pb(Mg₁/₃Nb₂/₃O₃₋ₓTiO₃-x) (PMN-PT) (011) substrates. When the electric field is swept, the easy axis of Mn₂Au is switched between [100] and [01-1] directions of PMN-PT (011) at room temperature, exhibiting a butterfly-like switching feature. This feature indicates that the underlying mechanism is the electric field-induced ferroelastic strain. Such a transition of the easy axis leads to the change of threshold current for the field-like torque switching of Mn₂Au [6]. Electrical switching of antiferromagnetic moments pave the way for all-electrical writing and readout in antiferromagnetic spintronics.


*This work is supported by the National Key R&D Program of China (Grant No. 2017YFB0405704) and National Natural Science Foundation of China (Grant No. 51871130)

8:36AM A41.00002: Spin Dissipation Independent of Antiferromagnetic Order in IrMn BEHROUZ KHODADADI, YOUNGMIN LIM, DAVID A SMITH, RYAN W GREENING, Virginia Tech, YUANKAI ZHENG, ZHITAO DIAO, CHRISTIAN KAISER, Western Digital, SATORU EMORI (Presenter), Virginia Tech — We investigate the interaction of spin current with antiferromagnetic order in polycrystalline IrMn by resonant spin pumping. We use spin-valve-like multilayers (NiFe/Cu/IrMn/CoFe), in which no direct magnon coupling is present between the NiFe spin source and the exchange-biased IrMn/CoFe spin sink; the pumped pure spin current is mediated solely by electrons through the Cu spacer layer. We observe no anisotropic spin dissipation with respect to the exchange bias direction, nor do we observe any difference in spin dissipation for samples with and without pinned antiferromagnetic order. Moreover, although there is a pronounced resonance linewidth increase in NiFe that coincides with the switching of IrMn/CoFe, we show that this is not indicative of anisotropic spin dissipation in IrMn. Our results demonstrate that the dissipation of electron-mediated spin current is remarkably insensitive to the magnetization state of the antiferromagnetic IrMn spin sink.
8:48AM A41.00003: Two-Magnon Scattering Enhanced by Randomly-Distributed Antiferromagnetic Exchange Field
HIROTO SAKIMURA (Presenter), School of Materials and Chemical Technology, Tokyo Institute of Technology, AKIO ASAMI, Department of Applied Physics and Physico-Informatics, Keio University, TAKASHI HARUMOTO, YOSHIO NAKAMURA, JI SHI, School of Materials and Chemical Technology, Tokyo Institute of Technology, KAZUYA ANDO, Department of Applied Physics and Physico-Informatics, Keio University — We report a quantitative study of two-magnon scattering in Ni$_{81}$Fe$_{19}$/NiO bilayers with various NiO thicknesses. The magnetic damping of the Ni$_{81}$Fe$_{19}$/NiO bilayer was found to have strong dependence on NiO thickness. The amplitude of the two-magnon scattering is enhanced with increasing the thickness of the antiferromagnetic layer, which was evaluated from the out-of-plane-angular-dependent spectral linewidth of ferromagnetic resonance. The origin of this enhancement in the Ni$_{81}$Fe$_{19}$/NiO bilayer is the increase of randomly-distributed antiferromagnetic exchange fields. We have calculated the spin-mixing conductance by eliminating the effect of the two-magnon scattering, and found that the value is at 8.1 nm$^{-2}$ for the Ni$_{81}$Fe$_{19}$/NiO interface. Skipping this process leads to overestimation of spin-mixing conductance in ferromagnet/antiferromagnet bilayer structures. Our result gives further insight on the role of the two-magnon scattering in manipulating magnetic damping, which is crucial for generation and transmission of spin currents in widely-studied ferromagnet/antiferromagnet systems.

9:00AM A41.00004: An effective model of antiferromagnetic metal in the adiabatic region and its spin-motive forces*
JUNJI FUJIMOTO (Presenter), ICR, Kyoto University — Antiferromagnetic spintronics is one of the active research fields because of its potential advantages. Compared to ferromagnets, antiferromagnetic materials have favorable characteristics to spintronic applications; ultrafast dynamics, robustness against perturbation due to magnetic fields, and so on. Considering the connection to modern electronics, the effect of conducting electrons coupling with antiferromagnetic order parameters is a fundamental subject. However, it is hard to intuitively understand physics of the electrons even in the adiabatic region, where the antiferromagnetic texture is slowly varying, hence the conduction electrons staying bonding/antibonding states. These states are inherently different from the states of ferromagnetic metals in the adiabatic region.

Here, we derive an effective Lagrangian of electrons coupling to antiferromagnetic textures in the adiabatic region, from the tight-binding model in a general lattice with the exchange coupling to the antiferromagnetic order parameter depending on space and time. In the presentation, we show the effective model and discuss the spin-motive forces calculated using the linear response theory and the Green function method.

*This work is supported by JSPS KAKENHI (Grant Nos. JP15H05702 and JP17H02929).

9:12AM A41.00005: A Dirac nodal line metal for topological antiferromagnetic spintronics*
DING-FU SHAO (Presenter), GAUTAM GURUNG, University of Nebraska - Lincoln, SHUHUI ZHANG, Beijing University of Chemical Technology, EVGENY Y TSYMBAL, University of Nebraska - Lincoln — Topological antiferromagnetic (AFM) spintronics is an emerging field of research, which exploits the Néel vector to control the topological electronic states and the associated spin-dependent transport properties. A recently discovered Néel spin-orbit torque has been proposed to electrically manipulate Dirac band crossings in antiferromagnets; however, a reliable AFM material to realize these properties in practice is missing. Here, we predict that room temperature AFM metal MnPd$_2$ allows the electrical control of the Dirac nodal line by the Néel spin-orbit torque. Based on first-principles density functional theory calculations, we show that reorientation of the Néel vector leads to switching between the symmetry-protected degenerate state and the gapped state associated with the dispersive Dirac nodal line at the Fermi energy. The calculated spin Hall conductivity strongly depends on the Néel vector orientation and can be used to experimentally detect the predicted effect using a proposed spin-orbit torque device. Our results indicate that AFM Dirac nodal line metal MnPd$_2$ represents a promising material for topological AFM spintronics.


*This work was supported by NSF: DMR-1420645 and 1629270.
Antiferromagnetic Mn3NiN thin films supporting giant piezomagnetism

DAVID BOLDRIN, Blackett Laboratory, Imperial College London, ANDREI MIHAI, BIN ZOU, Department of Materials, Imperial College London, JAN ZEMEN, Faculty of Electrical Engineering, Czech Technical University in Prague, LESLEY COHEN (Presenter), Blackett Laboratory, Imperial College London — Controlling magnetism with electric field directly or through strain-driven piezoelectric coupling remains a key goal of spintronics. Here we demonstrate that giant piezomagnetism, a linear magneto-mechanic coupling effect, is manifest in antiperovskite Mn3NiN, facilitated by its geometrically frustrated antiferromagnetism opening the possibility of new memory device concepts. Films of Mn3NiN with intrinsic biaxial strains of 0.25% result in Néel transition shifts up to 60K and magnetisation changes consistent with theory [1]. Films grown on BaTiO3 display a striking magnetisation jump in response to uniaxial strain from the intrinsic BaTiO3 structural transition, with an inferred 44% strain coupling efficiency and a magnetoelastic coefficient approximately a 1000-fold increase over Cr2O3 as predicted previously by theory. Overall our observations pave the way for further research into the broader family of Mn-based antiperovskites where yet larger piezomagnetic effects are predicted to occur at room temperature [2]. In this talk we will review progress towards application of thin film piezomagnetism in Mn3NiN.


Spin Hall Effects in Antiferromagnets

SVERRE GULBRANDSEN (Presenter), CAMILLA ESPEDAL, ARNE BRATAAS, QuSpin Center of Excellence, Norwegian University of Science and Technology — Recent experiments demonstrate that antiferromagnets exhibit a spin Hall effect. Calculations also indicate that the intrinsic contribution is important in determining the magnitude of the spin Hall angle. However, we do not know how the mean free path, exchange interaction, and spin-orbit coupling govern these results and how these factors might influence our understanding of experiments. To address these questions, we consider a minimal model of an antiferromagnet. We numerically compute the spin Hall conductance as a function of impurity concentration, exchange energy, and spin-orbit coupling. We find that the spin Hall conductance is considerably larger in antiferromagnetic systems compared to normal metals. This opens yet another avenue of using antiferromagnets in spintronics devices.

Spin Orbit Torque Switching Mediated by Antiferromagnetic Insulators

HAILONG WANG (Presenter), JOSEPH FINLEY, PENGXIAO ZHANG, JIAHAO HAN, JUSTIN HOU, LUQIAO LIU, Massachusetts Institute of Technology — Spin transport and magnetic dynamics in antiferromagnetic (AF) insulators have attracted wide research interests recently. In contrary to the popular belief of AF being an inactive element for spin transport, recent experiments based on spin pumping, nonlocal spin transport and spin Seebeck effect suggest efficient spin current transmission can be realized in various antiferromagnetic systems, via the mediation of antiferromagnetic magnons. In this work, we show initial experimental evidences towards this direction, where by utilizing the current induced spin orbit torque in Pt layer, we achieved magnetic switching in CoxTb1-x free layer across a thin AF insulator NiO. In the ultrathin spacer thickness regime (1~2nm), we even observed an enhancement of the spin orbital torque efficiency compared with the Pt/CoxTb1-x bilayer film. The realization of magnetic switching in Pt/NiO/CoxTb1-x heterostructures provides an existence proof on AF insulator mediated spin orbit torque, enabling promising material platform and device structures for energy favorable spin manipulation.

Nonlocal Coupling between Antiferromagnets and Ferromagnets in Cavities

ØYVIND JOHANSEN (Presenter), ARNE BRATAAS, Norwegian University of Science and Technology — Microwaves couple to magnetic moments in both ferromagnets and antiferromagnets. Although the magnons in ferromagnets and antiferromagnets radically differ, they can become hybridized via strong coupling to the same microwave mode in a cavity. The equilibrium configuration of the magnetic moments crucially governs the coupling between the different magnons, because the antiferromagnetic and ferromagnetic magnons have opposite spins when their dispersion relations cross. We derive analytical expressions for the coupling strengths and find that the coupling between antiferromagnets and ferromagnets is comparable to the coupling between two ferromagnets. Our findings reveal a robust link between cavity spintronics with ferromagnets and antiferromagnets.

This work was supported by the Research Council of Norway through its Centres of Excellence funding scheme, Project No. 262633 “QuSpin” and Grant No. 239926 “Super Insulator Spintronics,” as well as by the European Research Council via Advanced Grant No. 669442 “Insulatronics.”
10:12AM A41.00010: Gigahertz frequency antiferromagnetic resonance and strong magnon-magnon coupling in the layered crystal CrCl₃  
JUSTIN HOU (Presenter), Electrical Engineering and Computer Science, MIT, DAVID MACNEILL, DAHLIA KLEIN, Physics, MIT, PENGXUANG ZHANG, Electrical Engineering and Computer Science, MIT, PABLO JARILLO-HERRERO, Physics, MIT, LUQIAO LIU, Electrical Engineering and Computer Science, MIT — Antiferromagnetic spintronics is an emerging field with the potential to realize logic and memory devices with high speed and bit density. Compared with well-studied ferromagnetic materials, the understanding on antiferromagnetic dynamics remains very limited, partly due to the ultrahigh intrinsic frequency, which often requires specialized terahertz techniques beyond the reach of facile device integration. Here we report broadband microwave magnetic resonance spectroscopy of the layered antiferromagnet CrCl₃. We observe a rich structure of resonances arising from quasi-two-dimensional antiferromagnetic dynamics. Due to the weak interlayer magnetic coupling in this material, we are able to observe both optical and acoustic branches of antiferromagnetic resonance in GHz frequency range. By breaking the rotational symmetry of the crystal, we further show that strong magnon-magnon coupling with large tunable gaps in orders of GHz can be induced between the two resonant modes. Our results therefore provide a versatile system for microwave control of antiferromagnetic dynamics.

10:24AM A41.00011: Electrical Signal Generation at Magnetic Resonance in Insulating Antiferromagnets  
PRIYANKA VAIDYA (Presenter), University of Central Florida, SOPHIE MORLEY, University of California, Santa Cruz, ENRIQUE DEL BARCO, University of Central Florida, JOHAN VAN TOL, National High Magnetic Field Lab, DAVID LEDERMAN, University of California, Santa Cruz — Antiferromagnetic materials, particularly antiferromagnetic insulators provide an alternative to present ferromagnetic spin-transfer torque based devices which suffer from limitations in terms of density and speed owing to their magnetic anisotropy dominated spin dynamics. In antiferromagnets spin dynamics are governed by the interatomic exchange interaction energies which are orders of magnitude larger than the magnetic anisotropy energy, leading to the potential for ultrafast information processing and communication in the THz frequency range. We will present studies of spin pumping at Manganese Difluoride(MnF₂) / Platinum (Pt) interfaces at temperatures below the MnF₂ Néel temperature (Tₐ = 67.34K). In particular, measurements of the inverse spin Hall Effect (ISHE) voltage arising from the interconversion of the dynamically injected spin currents into Pt will be reported. We observe clear electrostatic potential signals coinciding with the MnF₂ magnetic resonance positions including the spin-flop transition (Hₛₐₕ = 9T). The signals reverse by switching the polarity of the magnetic field, and display a marked dependence on the power of the microwave stimuli, as expected from the ISHE.

10:36AM A41.00012: Spin Nernst Effect in the Paramagnetic Regime of An Antiferromagnetic Insulator*  
YINHAN ZHANG (Presenter), Carnegie Mellon University, SATOSHI OKAMOTO, Oak Ridge National Lab, DI XIAO, Carnegie Mellon University — We theoretically investigate a pure spin Hall current driven by a longitudinal temperature gradient, i.e., the spin Nernst effect (SNE), in a paramagnetic state of a collinear antiferromagnetic insulator with the Dzyaloshinskii-Moriya interaction. The SNE in a magnetic ordered state in such an insulator was proposed by Cheng et al. [R. Cheng, S. Okamoto, and D. Xiao, Phys. Rev. Lett. 117, 217202 (2016)]. Here we show that the Dzyaloshinskii-Moriya interaction can generate a pure spin Hall current even without magnetic ordering. By using a Schwinger boson mean-field theory, we calculate the temperature dependence of SNE in a disordered phase. We also discuss the implication of our results to experimental realizations.

*Department of Energy, Basic Energy Sciences, Grant No.DE-SC0012509. S.O. acknowledges support by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:48AM A41.00013: Spin-torque control of the anomalous Hall effect in non-collinear antiferromagnets  
GAUTAM GURUNG (Presenter), DING-FU SHAO, EVGENY Y TSYMBAL, University of Nebraska - Lincoln — Non-collinear antiferromagnets have recently aroused significant interest due to the non-vanishing Berry curvature and the associated anomalous Hall effect sensitive to the magnetic ordering. In this work, we explore series of antiperovskite compounds Ga₁₋ₓNₓMn₃ with competing Γ₄g and Γ₅g phases, where the magnetic moments of Mn atoms are aligned in the (111) plane. An electric current flowing and polarized in the [111] direction produces a spin-transfer torque rotating the magnetic moments in the (111) plane. Based on the Landau-Lifshitz-Gilbert-Slonczewski equation, we explore spin dynamics in these non-collinear antiferromagnets and obtain conditions at which a pulse of the spin-polarized current can reverse the Néel vector and thus change the sign of the anomalous Hall conductivity. We find that the strength of the applied spin-polarized current density largely depends on the magnetocrystalline anisotropy energy controlling the stability of the Γ₄g and Γ₅g phases. Using density functional theory methods, we calculate the magnetocrystalline anisotropy energy in these antiperovskite compounds and find the optimum conditions for the current-induced reversal of the Néel vector.

Monday, March 4, 2019 8:00 AM - 11:00 AM
8:00AM A42.00001: A blueprint for demonstrating quantum supremacy with superconducting qubits [Invited]
CHARLES NEILL (Presenter), Google AI Quantum — Here, using nine superconducting qubits, we experimentally illustrate a blueprint for demonstrating quantum supremacy. We present data characterizing two basic ingredients required for any supremacy experiment: *complexity* and *fidelity*. First, we demonstrate that the qubits can uniformly explore the Hilbert-space, providing a direct measure of algorithm complexity. Next, we compare the measurement results with the expected behavior and show that the algorithm can be implemented with high fidelity. Experiments for probing complexity and fidelity provide a foundation for demonstrating quantum supremacy.

8:36AM A42.00002: Operating and Characterizing of a 72 Superconducting Qubit Processor “Bristlecone”: Part 1
JULIAN KELLY (Presenter), ZIJUN CHEN, Santa Barbara, Google, BEN CHIARO, BROOKS FOXEN, Physics, UCSB, JOHN M MARTINIS, Santa Barbara, Google — Quantum computing has recently entered a new regime where a number of quantum processors with tens of qubits are being built and operated around the world. With approximately 50 qubits and high performance, it is possible to outperform classical computers in limited cases, a feat known as “Quantum Supremacy.” However, achieving supremacy requires high-fidelity operations in all aspects of the algorithm, including single-qubit gates, two-qubit gates, and readout. While these milestones have been achieved in small scale devices, challenges in calibration, precision control, and reproducibility are amplified at scale. In this talk, we will discuss the 72 qubit “Bristlecone” processor we have been developing at Google, and our work towards calibrating, operating, and characterizing this device. Part 1 of 2.

8:48AM A42.00003: Operating and Characterizing a 72 Superconducting Qubit Processor “Bristlecone”: Part 2
ZIJUN CHEN (Presenter), JULIAN KELLY, Google Inc - Santa Barbara, BEN CHIARO, BROOKS FOXEN, Physics, University of California, Santa Barbara, JOHN M MARTINIS, Google Inc - Santa Barbara — Quantum computing has recently entered a new regime where a number of quantum processors with tens of qubits are being built and operated around the world. With approximately 50 qubits and high performance, it is possible to outperform classical computers in limited cases, a feat known as “Quantum Supremacy.” However, achieving supremacy requires high-fidelity operations in all aspects of the algorithm, including single-qubit gates, two-qubit gates, and readout. While these milestones have been achieved in small scale devices, challenges in calibration, precision control, and reproducibility are amplified at scale. In this talk, we will discuss the 72 qubit “Bristlecone” processor we have been developing at Google, and our work towards calibrating, operating, and characterizing this device. Part 2 of 2.

9:00AM A42.00004: Characterization and mitigation of noise and crosstalk in a five-qutrit transmon processor
VINAY RAMASESH (Presenter), MACHIEL BLOK, KEVIN P. O’BRIEN, DAR DAHLEN, JOHN MARK KREIKEBAUM, IRFAN SIDDIQI, University of California, Berkeley — The multi-level structure of the transmon circuit makes it an attractive choice for implementing multi-valued quantum logic, i.e. qudit-based protocols with d > 2. To date, while transmon levels outside of the qubit computational subspace have been used for control and sensing, experimental implementation of a quantum algorithm using multi-level transmons has not been demonstrated. Specifically, we address practical issues which arise when running a multi-qutrit algorithm. These include classical microwave crosstalk between the individual transmon control lines; an always-on ZZ interaction due to fixed off-resonant coupling between neighboring qutrits; conditionality of single-qutrit pulses due to the cross-resonance effect; and challenges due to the sensitivity of higher transmon levels to charge noise. For each of these issues, we present methods of characterization and mitigation, demonstrating their efficacy on our hardware and the future design choices they inform.

*This work was supported by the Department of Energy.

9:12AM A42.00005: Automatic calibration of arrays of superconducting qubits and couplers
KEVIN SATZINGER (Presenter), Google Inc - Santa Barbara, BROOKS FOXEN, BEN CHIARO, MATTHEW MCEWEN, University of California, Santa Barbara, JOHN M MARTINIS, Google Inc - Santa Barbara — High-fidelity operation of superconducting qubits requires fine-tuning numerous experimental parameters. As superconducting qubit systems scale up to large arrays, automatic calibration becomes essential, both for bringing up systems from scratch and for maintaining calibrations. These algorithms depend strongly on the qubit architecture. For example, consider arrays of qubits connected by adjustable couplers, where the coupling can be turned off to isolate qubits and turned on to facilitate fast interactions. These couplers substantially complicate automatic calibration. At the start, the coupling may inadvertently be very strong, which can disrupt qubit bringup, and we can only learn about the coupler configuration indirectly through qubit measurements. In this presentation, we describe algorithms and experiments to automatically calibrate superconducting qubits and couplers.
**9:24AM A42.00006: Coupler characterization of transmons for cross-resonance**

HANHEE PAIK (Presenter), JOSÉ CHAVEZ-GARCIA, MARTIN SANDBERG, OBLESH JINKA, JENG-BANG YAU, DONGBING SHAO, FIRAT SOLGUN, MARKUS BRINK, JERRY M. CHOW, IBM Thomas J. Watson Research Center — We characterize two-qubit cross-resonance gates and unintended residual coupling on various coupled qubit arrangements. Direct coupling versus coupling via a quantum bus are studied on the basis of cross-resonance gate rate and fall-off of non-nearest neighbor coupling. We experimentally extract coupling rates using Hamiltonian tomography methods, and compare with microwave simulations.

*We acknowledge support from IARPA under Contract No. W911NF-16-0114.

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**9:36AM A42.00007: Deletrious Effects of Spectator Qubits in Multiqubit Circuits**

XUAN WEI (Presenter), DAVID CHRISTOPHER MCKAY, SARAH SHELDON, EASWAR M MAGESAN, JAY GAMBETTA, IBM Thomas J. Watson Research Center — For a number of quantum technologies, such as superconducting qubits, multiqubit algorithms are performed by concatenating a series of one- and two-qubit gates. However, in such an architecture there will be no true one- and two-qubit gates because of spectator qubits, i.e., qubits which are connected, but should be idle during the gate. For drive activated two-qubit gates, such as the cross-resonance gate, the role of these spectator qubits can be non-trivial. Here we will discuss our studies on these spectator qubits, for example, by measuring the entanglement dynamics of the spectator qubit with the active qubits. Understanding spectator dynamics will lead to improved designs of multiqubit gates for quantum computing technologies.

*This work was supported by the Army Research Office under contract W911NF-14-1-0124

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**9:48AM A42.00008: Measuring and quantifying classical crosstalk in multi-qubit superconducting circuits**

PETAR JURCEVIC (Presenter), ABHINAV KANDALA, ANTONIO CORCOLES, EASWAR M MAGESAN, JERRY M. CHOW, JAY GAMBETTA, IBM Thomas J. Watson Research Center — In the most general sense, crosstalk is used to describe the unwanted interactions on elements of a quantum processor due to targeted drives on non-local elements. For superconducting circuits, we use “classical crosstalk” specifically to describe crosstalk that is a result of the microwave environment of the chip, and is not a direct consequence of the qubit frequency arrangement or the drive Hamiltonians. Such crosstalk can be an important source of gate infidelity. Here, we shall present techniques to measure and quantify classical crosstalk, and use them to probe the microwave environment of our chips. These techniques could serve as a useful guide for the design and packaging of large multi-qubit devices.

*We acknowledge support from IARPA under Contract No. W911NF-16-0114.

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**10:00AM A42.00009: Multi-qubit circuit characterization through physics-based statistical inference**

VADIM SMELYANSKIY (Presenter), SERGIO BOIXO, Google Inc., HRANT GHARIBYAN, Physics, Stanford, MURPHY YUEZHEN NIU, Physics, MIT, KOSTYANTYN KECHEDZHI, DVIR KAFRI, RAMI BAREND, ANDRE PETUKHOV, HARTMUT NEVEN, Google Inc. — We develop new physical models for realistic two-qubit gates in superconducting qubit architectures to account for specific shape of qubit control pulses and effects of noise and decoherence, including those induced by two-level defects prevalent in the fabrications of superconducting chip. We then formulate statistical inference method to efficiently estimate the physical model parameters for an ensemble of quasi-random circuits that contain non-Clifford gates. For a family of circuit ensembles, we are able to obtain analytically the circuit fidelities and their variances by averaging the log-likelihood distribution of the model parameters over Haar measure. Our inference method applies to quantum systems with arbitrary number of qubits and thus serves as valuable tools for characterizing large scale quantum circuit that will likely outperform the most powerful classical computers existing to date.
10:12AM A42.00010: Mode Hybridization Analysis of Bus Resonators for a Superconducting Multi-Qubit Chip*

NADIA HAIDER (Presenter), QuTech and Netherlands Organisation for Scientific Research (TNO), Delft, The Netherlands, JONATHAN GNANADHAS, QuTech, Netherlands Organisation for Applied Scientific Research (TNO) and Delft University of Technology, Delft, The Netherlands, MARC BEEKMAN, RENE VOLLMER, NANDINI MUTHUSUBRAMANIAN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands, ROMAN CAUDILLO, Components Research, Intel Corporation, 2501 NW 229th Avenue, Hillsboro, OR, 97124, USA, ALESSANDRO BRUNO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands, DAVID MICHALAK, Components Research, Intel Corporation, 2501 NW 229th Avenue, Hillsboro, OR, 97124, USA, FILIP MALINOWSKI, CORNELIS CHRISTIAAN BULTINK, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands, ADEL A ELSHERBINI, LESTER LAMPERT, Components Research, Intel Corporation, 2501 NW 229th Avenue, Hillsboro, OR, 97124, USA, ALEXANDER YAROVOY, Microwave Sensing, Signals and Systems, Delft University of Technology, Delft, The Netherlands, JIM CLARKE, Components Research, Intel Corporation, 2501 NW 229th Avenue, Hillsboro, OR, 97124, USA, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands.

— We present an effective numerical method to analyze the mode hybridization in a multi-transmon circuit QED chip. Surface code, a promising architecture for fault-tolerant quantum computing, requires qubits with connectivity to all nearest neighbors. This extensive interconnectivity together with strong coupling between qubits and resonators causes mode hybridization. A complete analysis of the chip is needed in these conditions to accurately predict the loaded frequency of the bus resonators and thereby also the two-qubit gate time. We present and experimentally verify a simulation method for analyzing the complete chip combining finite-element electromagnetic simulation with numerical circuit simulation for accurate and fast computation. This research is funded by Intel Corporation and IARPA (U.S. Army Research Office grant W911NF-16-1-0071).

10:24AM A42.00011: A many-body coupler for coherent 4-local interaction of superconducting flux qubits*

TIM MENKE (Presenter), Department of Physics, Harvard University; Department of Physics, MIT; Research Laboratory of Electronics, MIT, CYRUS F. HIRJIBEHDIN, STEVEN J. WEBER, MIT Lincoln Laboratory, GABRIEL O. SAMACH, Department of Electrical Engineering and Computer Science, MIT; MIT Lincoln Laboratory, SIMON GUSTAVSSON, Research Laboratory of Electronics, MIT, ALAN ASPURGUZIK, Department of Chemistry and Department of Computer Science, University of Toronto; Vector Institute for Artificial Intelligence, Toronto; Canadian Institute for Advanced Rese, WILLIAM D OLIVER, Department of Physics, MIT; Research Laboratory of Electronics, MIT; MIT Lincoln Laboratory, ANDREW JAMES KERMAN, MIT Lincoln Laboratory — Interactions of more than two bodies simultaneously rarely appear in nature. Even in dense systems, forces usually act pairwise. However, n-local terms with n>3 frequently arise when mapping physical or mathematical problems to an Ising spin Hamiltonian. Superconducting flux qubits have emerged as a promising, versatile platform to simulate such spin systems and find their ground state, but the implementation of n-local superconducting qubit couplers has so far proven elusive. Here we present a circuit that enables large 4-local interaction between four flux qubits without spurious 2-local terms and without relying on an effective low-energy description as in Hamiltonian gadgets. We demonstrate numerically how 4-local coupling of up to several hundred MHz arises from a coupler circuit with tailored spectral properties. These properties are engineered by combining known superconducting circuit physics with suggestions by an inverse design algorithm that we have developed previously. In addition, we show first experimental results probing a fabricated coupler prototype.

10:36AM A42.00012: Robust And Versatile Superconducting Coupler

CATHERINE LEROUX (Presenter), AGUSTIN DI PAOLO, ALEXANDRE BLAIS, Institut Quantique and Département de Physique, Université de Sherbrooke, Sherbrooke, QC, Canada, J1K 2R1 — Having access to a large collection of fast and high-fidelity two-qubit gates can significantly reduce the gate count of large-scale quantum computations. In this talk, we present a novel tunable superconducting dipole coupling element that enables a variety of strong two-qubit interactions by modulating external fields. The proposed device can realize both high-fidelity and fast SWAP and controlled two-qubit gates.
10:48AM A42.00013: Implementing optimized time-varying coupling and dissipation in small logical qubit architectures.* DAVID RODRIGUEZ PEREZ (Presenter), ELIOT KAPIT, Colorado Sch of Mines — Tunable couplings between high coherence quantum objects and lossy resonators is a promising approach to state stabilization. Using an additional lossy resonator to provide a mechanism for the fast reset of the first resonator, a steady state residual error scaling of about 1 / T1 can be achieved. While this technique has been demonstrated for a single qubit coupled to a single resonator, this work looks at applying the same resonator reset technique for an idealized three qubit bit flip code and the Very Small Logical Qubit (VSLQ), a promising route to passive error correction in superconducting architectures. Optimal device and signal parameters for the VSLQ are well understood for a numerically optimized, continuous coupling strength, so we explore the effects of using an optimized, time-varying coupling strength between the primary qubits and shadow resonators and report a best possible scaling logical qubit lifetime T_L that scales as T_1^2, where T_1 is the lifetime for a single primary qubit.

*This work was made possible by the NSF grant PHY-1653820 and ARO grant W911NF-18-1-0125.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A43 DCMP: 2D Materials Twistronics: Correlations and Moiré Physics BCEC 210B - Pablo Jarillo-Herrero, Massachusetts Inst of Tech-MIT - Tag(s): Invited

8:00AM A43.00001: Twisted Graphene Superlattices: Superconductivity, Electron Correlations and Beyond [Invited] YUAN CAO (Presenter), DANIEL RODAN LEGRAIN, ORIOL RUBIES-BIGORDA, VALLA FATEMI, Massachusetts Institute of Technology, SHIANG FANG, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, EFTHIMIOS KAXIRAS, Harvard University, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — The understanding of strongly-correlated quantum matter has challenged physicists for decades. Such difficulties have stimulated new research paradigms, such as ultra-cold atom lattices for simulating quantum materials. In this talk I will present a new platform to investigate strongly correlated physics, based on graphene moiré superlattices. In particular, when two graphene sheets are twisted by an angle close to the theoretically predicted ‘magic angle’, the resulting flat band structure near the Dirac point gives rise to a strongly-correlated electronic system[1]. These flat bands exhibit half-filling insulating phases at zero magnetic field, which we show to be a Mott-like insulator arising from electrons localized in the moiré superlattice[2]. Moreover, upon doping, we find electrically tunable superconductivity in this system, with many characteristics similar to high-temperature cuprates superconductivity[3]. These unique properties of magic-angle twisted bilayer graphene open up a new playground for exotic many-body quantum phases in a 2D platform made of pure carbon and without magnetic field. Since these discoveries, a large number of theoretical models have been proposed based on the magic-angle graphene superlattices and beyond. I will also discuss our data demonstrating nematic superconductivity as well as correlated states in other types of graphene superlattices. The easy accessibility of the flat bands, the electrical tunability, and the bandwidth tunability though twist angle may pave the way towards more exotic correlated systems, such as quantum spin liquids.


8:36AM A43.00002: Tuning flat bands in twisted bilayer graphene with pressure [Invited] MATTHEW YANKOWITZ (Presenter), Columbia University — Twisted bilayer graphene (tBLG) with rotational mismatch of ~1.1°, referred to as the “magic angle,” has emerged as an exciting new platform to host strongly correlated electronic states due to its very flat low-energy bands. The electronic bandwidth – and consequently the strength of the correlated states – is determined by an interplay between the separation of the Dirac cones of the two graphene layers in momentum space and the strength of the interlayer electronic coupling which hybridizes the bands. Here we demonstrate the capability to vary the bandwidth at fixed rotation angle by using hydrostatic pressure to modify the interlayer coupling [1]. For angles larger than the native magic angle, we can tune to the flat band condition with pressure, inducing correlated insulating states and superconductivity for both hole- and electron-type carriers. For a 1.27° twist angle, T_c increases above 3 K at ~1.3 GPa, and then diminishes with further pressure. This behavior is consistent with theoretical efforts to model the relationship between bandwidth and interlayer coupling strength, establishing layer compression as a viable route to engineering the energy scale of the superconductivity in this system. Improvements in device quality additionally allow us to resolve new sequences of quantum oscillations emerging from quarter-, half-, and three-quarters-filling of the moiré unit cell associated with the presence of new Fermi surfaces.

9:12 AM A43.00003: Topology and Correlations in Magic Angle Bilayer Graphene [Invited] ASHVIN VISHWANATH
(Presenter), Harvard University — The recent discovery of superconductivity and Mott insulators in twisted bilayer graphene and related materials points to the importance of correlation effects. An additional interesting and potentially crucial ingredient is band topology inherited from the Dirac fermion dispersion of graphene. We will discuss our theoretical efforts to derive faithful tight binding models that captures both the symmetry and topology of the flat bands, as well as their energetics. We then discuss aspects of the Mott and superconducting phases and find that key aspects of the physics differ from previously studied correlated superconductors.

Hoi Chun Po, Liujun Zou, Ashvin Vishwanath, T. Senthil

Liujun Zou, Hoi Chun Po, Ashvin Vishwanath, T. Senthil

Hoi Chun Po, Liujun Zou, T. Senthil, Ashvin Vishwanath

Yi-Zhuang You, Ashvin Vishwanath

9:48 AM A43.00004: Topologically Protected Helical States in Minimally Twisted Bilayer Graphene* [Invited] BRIAN LEROY (Presenter), University of Arizona — The ability to create arbitrary stacking configurations of layered two-dimensional materials has opened the way to the creation of designer band structures. Twisted bilayer graphene is one of the simplest examples of such a van der Waals heterostructure where the electronic properties of the composite material can be fundamentally tuned with twist angle. The angle between the two graphene layers in the heterostructure produces a moiré pattern which affects its electronic properties. Using scanning tunneling microscopy and spectroscopy, we have investigated these minimally twisted bilayer graphene heterostructures. As the twist angle between the layers decreases there are fundamental changes in the electronic properties. We have found that the degeneracy of the low energy bands increases at twist angles below about 1 degree. For even smaller twist angles, a series of domain walls form connecting the AA sites in the moiré pattern. When an electric field is applied to these very small twist angle samples, the AB and BA regions develop band gaps while topologically protected states emerge along the domain walls. In this talk, we will discuss the fabrication of these minimally twisted heterostructures as well as our latest scanning probe microscopy results.

*The work at the University of Arizona was partially supported by the U.S. Army Research Laboratory and the U.S. Army Research Office under Contract Grant No. W911NF-14-1-0653 and the National Science Foundation under Grant No. EECS-1607911.
Quantum Simulation and Many-Body Physics in Moiré Bilayers* [Invited]  FENGCHENG WU (Presenter), University of Maryland — Moiré superlattices form in van der Waals bilayers with a small lattice mismatch or misalignment. The moiré pattern produces spatial modulation and can dramatically alter electronic properties. I will present theoretical proposals of using moiré bilayers as a quantum simulation platform to realize model Hamiltonians, and discuss many-body effects that are magnified when the moiré bands are nearly flat. In semiconducting transition metal dichalcogenide (TMD) heterobilayers, isolated flat moiré bands can be used to simulate Fermi-Hubbard model on a triangular lattice [1], in which parameters such as bandwidth, interaction strength, and band filling are widely tunable. When the two layers are formed from the same TMD, holes in \( \pm K \) valleys move in a layer-pseudospin skyrmion texture in real space. The low-energy moiré bands then realize Kane-Mele model [2], providing a platform to study interplay between topology and correlation. Excitons in twisted TMD bilayers also experience moiré potential, which can be used to design topological exciton bands and to simulate Bose-Hubbard model [3]. Twisted bilayer graphene (TBLG) is a distinct example where the effective lattice theory does not simply map to any known model Hamiltonian. Motivated by the observed superconductivity, I will present a candidate theory of phonon-mediated superconductivity in TBLG [4]. Phonon fluctuations lead to both s-wave and d-wave pairings. New phenomena of the d-wave superconductivity in moiré pattern will be discussed.


*We acknowledge support by DOE.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A44 DCMP: Polariton Condensates at Room Temperature and Equilibrium BCEC 210C
- Peter Littlewood, University of Chicago - Tag(s): Invited

8:00AM A44.00001: Polaritons, a growing field of condensate studies* [Invited]  DAVID SNOKE (Presenter), University of Pittsburgh — In this talk I will review the physics of Bose condensation of polaritons, sometimes called “superfluids of light,” and review recent experimental results, such as equilibrium condensation, long-distance propagation to the global ground state of a system, phase locking of spatially separated condensates, evidence for superfluidity, measurement of correlation functions, and propagation in quasi-one-dimensional systems. I will end with a discussion of some of the challenges and promises of room-temperature condensation of polaritons.

*This work has been supported by the US Army Research Office under MURI award W911NF-17-1-0312.

8:36AM A44.00002: Room temperature polariton condensate using a biologically produced fluorescent protein [Invited]  MALTE GATHER (Presenter), School of Physics and Astronomy, University of St Andrews — Organic materials offer attractive properties for solid-state lasers, including large oscillator strength, high exciton binding energy, spectral tunability, and compatibility with low-cost fabrication processes. However, despite impressive proof-of-principle demonstrations and dramatic improvements in performance, important fundamental limitations remain. Particular challenges are concentration quenching and bi-molecular exciton recombination, which limit the available gain under practical pumping conditions. For electrical pumping, there are further restrictions, including the low charge carrier mobility of most organic materials. Recently, it has been suggested that lasers operating in the regime of strong exciton-photon coupling may address some of these challenges.

Here, we will summarize key results from two collaborations that both look at unconventional nano-scale organic materials for solid-state lasers: Biologically produced fluorescent proteins and single-walled carbon nanotubes. We found that the barrel-like molecular structure of fluorescent proteins prevents concentration-induced quenching of fluorescence and drastically reduces singlet-singlet annihilation at high exciton densities. This facilitates low-threshold lasing in various configurations and has recently enabled the realization of the first organic polariton laser that can be pumped in a quasi-continuous ns-regime.

In another collaboration, we have shown that the special photo-physical properties of polymer-sorted semiconducting single-walled carbon nanotubes render them well suited for strong light-matter coupling, possibly up to the ultra-strong coupling regime. Most recently, we found that the high charge carrier mobility and stability also enable efficient electrical generation of exciton polaritons. Using a light-emitting field-effect transistor geometry, we achieved current densities ~18,000 A/cm² while maintaining strong coupling conditions.
Zhang (KPZ) superfluid and the newly discovered rigid fluid phase, as well as the recently achieved equilibrium limit. I will discuss a few examples of novel non-equilibrium collective effects in polariton systems, such as the Kardar-Parisi-Zhang (KPZ) superfluid and the newly discovered rigid fluid phase, as well as the recently achieved equilibrium limit.

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This work was supported by EPSRC (Grant No. EP/K003623/2)

10:24AM A44.00005: Room Temperature Long-Range Coherent Exciton Polariton Condensate Propagation in Lead Halide Perovskites Microwire Cavity [Invited] RUI SU, Nanyang Technological University, CAROLE DIEDERICHS, Laboratoire Pierre Aigrain, Département de physique de l'ENS, Ecole normale supérieure, PSL Research University, Université Paris Diderot, Sorbonne Paris Cité, Sorbonne Unive, TIMOTHY LIEW, QIHUA XIONG (Presenter), Nanyang Technological University — Recent progress has shown that halide perovskites are promising optical gain materials towards room-temperature strong-light matter coupling leading to robust exciton polariton, due to large exciton binding energy and strong oscillator strength. Polariton condensates, exhibiting high speed coherent propagation and spin-based behaviour, attract considerable interest for implementing the basic elements of integrated optoelectronic devices: switching, transport, and logic. However, the implementation of such coherent polariton condensate flow is typically limited to cryogenic temperatures, constrained by small exciton binding energy in most semiconductor microcavities. Here, we demonstrate the capability of long-range non-resonantly excited polariton condensate flow at room temperature in a one-dimensional all-inorganic cesium lead bromide (CsPbBr3) perovskite microwire microcavity. The polariton condensate exhibits high speed propagation over macroscopic distances of 60 µm, while still preserving the long-range off-diagonal order. Our findings pave the way for utilizing coherent polariton condensate flow for all-optical integrated logic circuits and polaritonic devices operating at room temperature.

Monday, March 4, 2019 8:00 AM - 10:36 AM

Session A45 DCMP: Photophysics and Pattern Formation in Thin Films BCEC 211 - Radwan Elzein, University of South Florida - Tag(s): Focus

8:00AM A45.00001: Photosresponsive thin film based on photochromic diarylethene blended with thermoplastic elastomer: Structural and morphological analysis MAROUA LOUATI (Presenter), SOPHIE BARRAU, JEAN-FRANÇOIS TAISON, Unité matériaux et transformations, Lille University, France, STÉPHANE ALOISE, Laboratoire de Spectrochimie Infrarouge et Raman, Lille University, France, MICHINORI TAKESHITA, Advanced Technology and Fusion, Graduate School of Science and Engineering, Saga University, Japan — An increasing attention has been paid to photo-deformable polymeric materials that can convert light energy into mechanical energy without contact or electrical wires, using photosresponsive molecules. Diarylethenes known for their thermal stability and their fatigue resistance are one of the best studied compounds that exhibit photomechanical response. Upon alternating irradiation with UV and visible light, a change in molecular volume occurs between open- and close-ring during the photochromic reaction which induces photomechanical motions. In order to develop a light-driven polymer actuator, we investigate a novel system based on the mixture of a derivative diarylethene (Ureidopyrimidinone-functionalized diarylethene denoted UPy-DTE) and a thermoplastic elastomer (Ureidopyrimidinone -functionalized poly(ethylene-co-butylene) denoted UPy-PEB). In solution, the UPy-DTE/UPy-PEB system leads to a supramolecular assembly via quadrupole hydrogen bonding. The thin films are elaborated using different techniques such as drop casting or melt molding. Under illumination, a photomechanical response of the film is observed. Our strategy is to establish a correlation between the structural and morphological properties responsible for the macroscopic deformations.
8:12AM A45.00002: Singlet fission and exciton dynamics in vapor deposited rubrene films  DREW FINTON (Presenter), ELIZABETH DEJONG, VINCENT ZOUTENBIER, IVAN BIAGGIO, Physics, Lehigh University — In rubrene single crystals, singlet excitons can efficiently transition into two independent triplet excitons through a process called singlet fission. Photoluminescence in single crystals is a result of the singlet exciton’s radiative decay and both geminate and non-geminate triplet pair recombination. This process has been well documented, although a precise description of the intermediate steps is still an active area of research. In more disordered systems, such as amorphous films of rubrene, the singlet fission process is greatly hindered and the likelihood of non-geminate triplet recombination is effectively zero. As a result, photoluminescence measurements show only the radiative decay of the singlet exciton, as no singlet fission can occur. The effect of molecular ordering and the photoluminescence dynamics of amorphous rubrene samples will be addressed.

8:24AM A45.00003: Defect Engineering for Modulating the Trap States in Two-dimensional Photoconductor  JIE JIANG (Presenter), CHONGYI LING, TAO XU, WENHUI WANG, Southeast University, XIHANGONG NIU, Nanjing University of Posts and Telecommunications, AMINA ZAFAR, ZHENZHONG YAN, Southeast University, XIAOMU WANG, Nanjing university, YUMENG YOU, LITAO SUN, JUPENG LU, JINLAN WANG, ZHENHUA NI, Southeast University — Defect induced trap states are essential in determining the performance of semiconductor photodetectors. The de-trap time of carriers from a deep trap could be prolonged by several orders of magnitude as compared to shallow trap, resulting in additional decay/response time of the device. Here, we demonstrate that the trap states in two-dimensional ReS2 could be efficiently modulated by defect engineering through molecule decoration. The deep traps that greatly prolong the response time could be mostly filled by Protoporphyrin (H2PP) molecules. At the same time, carrier recombination and shallow traps would in-turn play dominant roles in determining the decay time of the device, which can be several orders of magnitude faster than the as-prepared device. Moreover, the specific detectivity of the device is enhanced (as high as ~1.89x10^13 Jones) due to the significant reduction of dark current through charge transfer between ReS2 and molecules. Defect engineering of trap states therefore provides a solution to achieve photodetectors with both high responsivity and fast response.

8:36AM A45.00004: Photothermoelectric detection of gold oxide non-thermal decomposition and related studies*  XIFAN WANG (Presenter), CHARLOTTE EVANS, MAHDIYEH ABBASI, DOUGLAS NATELSON, Rice University — Controlling morphology and composition via nanoscale structuring gives opportunities to improve the thermoelectric properties of materials for energy conversion and photodetection. In this study, we report the detection of the decomposition of metastable gold oxide via open circuit photothermoelectric voltage detection on thin-film Au nanowire devices as a function of the position of an optical heat source. A focused laser beam is used to locally heat the metal nanostructure. The first-scan enhanced photovoltage correlates with a reduction of the electrical resistance of the nanostructure back to pre-oxygen-exposure levels. These experiments demonstrate that combined optical and electronic measurements can provide a window on surface-sensitive photochemical processes. Besides the photothermoelectric voltage detection of gold oxide, we also report preliminary data on the thermoelectric properties of Au nanowires via other surface modification methods includes self-assembled monolayer formation.

*Acknowledge support from Robert A. Welch Foundation Grant C-1636. and support from NSF award ECCS-1704625.

8:48AM A45.00005: Formation of gold nanoparticles by laser annealing and enhanced terahertz beam by plasmonics  DONG HO WU (Presenter), Materials Science and Technology Division, United States Naval Research Laboratory — The plasmonic effect increases photocurrents substantially. There are considerable efforts to exploit this phenomenon for various applications, such as a high-efficiency photovoltaic cell, photodetector, etc. In this presentation, we will report gold nanoparticles on a photoconductive antenna and substantial terahertz power enhancement by the plasmonics. A laser annealing process creates the gold nanoparticles, and the plasmonic effect occurs when the gold nanoparticles interact with the femtosecond laser beam. The photoconductive antenna contains a pair of Schottky electrodes, which are fabricated by depositing shallow titanium-gold layers on a semi-insulating GaAs substrate. After the fabrication, the photoconductive antenna is exposed to a rather intense femtosecond laser beam exceeding 130 mW while applying a 70 V AC bias voltage to the electrodes. This laser annealing process generates about 1 mW of terahertz beam, which is nearly stable until the annealing time past 60 minutes when terahertz power abruptly jumps more than 20 -30%. This sudden power enhancement is coincident with the formation of gold nanoparticles and dendrites in a tiny area around the electrodes. We found that the plasmonic effect enhances the photocurrents of more than one order of magnitude.
9:00AM A45.00006: The Influence of Fractional Surface Coverage on Core-Core Separation in Monolayers of Thiol-Ligated Gold Nanoparticles*  
MORGAN REIK (Presenter), STUART A RICE, BINHUA LIN, MELANIE S CALABRO, SEAN GRIESEMER, SOPHIE MACFARLAND, University of Chicago — The way in which thiol-ligated gold nanoparticles self-assemble into ordered monolayers when deposited on a surface is contingent on the thiol's length and concentration. The influence of ligand composition on the properties of nanoparticle films is well-reported. However, the understanding of the molecular and structural origins of these properties is incomplete, particularly when examining the number of ligands on a nanoparticle surface. It has been assumed that the concentration of ligands in solution, within typical ranges, always generates the maximum possible nanoparticle surface packing. We demonstrate through Grazing Incidence X-Ray Diffraction and Transmission Electron Microscopy that the nanoparticle separation and correlation length of these films increases linearly with thiol concentration in solution, indicating that the bulk thiol is in equilibrium with thiol on the core surface. Our findings thus challenge the assumption that the free energy of binding of an alkanethiol to a gold nanoparticle is so large that its surface is consistently saturated with ligands.

*This work was supported by UChicago MRSEC, NSF-DMR-1420709, the Senior Mentor Grant from the Camille and Henry Dreyfus Foundation (Grant No. Sl-14-014), and NSF's ChemMatCARS (grant No. NSF/CHE-1346572).

9:12AM A45.00007: Laser-induced Detuning of Quartz Crystal Microbalances in Adsorbing and Non-adsorbing Environments*  
SAMUEL KENNY (Presenter), JACQUELINE KRIM, Physics, North Carolina State University — Light induced modifications in frictional behavior of films of adsorbed molecules constitute an area of current interest in nanotribology, and are potentially observable at room temperature by means of a quartz crystal microbalance (QCM). In order for such studies to be viable, the impact of laser light on a QCM must be established. We report here an investigation of the response of a QCM to green laser light in vacuum, nitrogen, and ethanol gas. Measurements of frequency and amplitude responses of the QCMs were performed, for samples with electrodes composed of AuNi alloys with varying degrees of Ni content. For the adsorbing ethanol films, we observed that the frequency response upon green laser irradiation initially strongly decreased with pressure, but recovered slowly up to the vapor pressure. This effect was more pronounced in electrodes with higher Ni content. QCMs exposed to non-adsorbing nitrogen produced responses of similar magnitude regardless of Ni content, however, we noticed marked changes in the initial response behavior upon illumination. The effects can be explained within the context of the effects of mass uptake, desorption and laser heating [1].


*Support of NSF-DMR1310456 is gratefully acknowledged.

9:24AM A45.00008: Interferometric Measurements of High Quality Acoustic Microcavities (MCs) on Anisotropic Surfaces*  
MADELEINE MSALL (Presenter), Bowdoin College, PAULO SANTOS, Paul Drude Institute for Solid State Electronics — Applications that couple high frequency surface acoustic waves (SAW) to quasi 0-D systems require high-Q acoustic MCs. We use optical interferometry to measure the surface displacement patterns between pairs of interdigital transducers (IDTs) configured to form resonant MCs with $Q \sim 1800$. Our focusing Al/Ti IDT with 0.6 rad (34°) aperture and wavelength $\lambda=5.6\,\mu$m emits a SAW beam along the [110] direction on GaAs with focusing comparable to the predicted 1.2$\lambda$ beam waist and 8$\lambda$ Rayleigh length. Reflections from the anisotropy corrected outer edges of the IDT fingers play an important role in performance. Previous assumptions of parabolic dispersion overcorrect for anisotropy and move the device focus closer to the IDT. Our resonant MC is created by placing additional floating fingers to form a 2.5$\lambda$ cavity around the focus. Since the inner cavity fingers are in the near field of the beam focus, their positions must also be adjusted to account for the Gouy phase shift. The resulting IDT + MC system shows highly localized elastic strain at frequencies within the electrical resonance band of the driving IDT. These 514 MHz, 5.6$\mu$m devices should scale well to the submicron wavelength and GHz frequency domain appropriate to quantum dot applications.

*Work supported by the DFG, Germany.
9:36AM A45.00009: Resonant Scattering as a Rapid and Site-Specific Spatiochemical Probe of Patterned Interfaces* ISVAR CORDOVA (Presenter), GUILLAUME FREYCHET, Lawrence Berkeley National Laboratory, CHRISTOPHER CHI, UC Berkeley, WEI XU, ALEXANDER HEXEMER, CHENG WANG, Lawrence Berkeley National Laboratory — The advent of highly precise nanofabrication tools has enabled the development of a new generation of mesoscale materials with potential across a variety of applications, but concomitant progress in the characterization techniques is also required.

In this presentation, we reveal a simple, yet powerful, patterning approach for sub-nm characterization that takes advantage of the physical processes intrinsic to small angle resonant X-ray scattering in order to 1) decouple the bulk from the interface scattering signal, 2) enhance the strength of the interfacial signal, and 3) collect a site-specific x-ray absorption spectra.

We demonstrate the potential of our approach by combining it with recently-developed in-situ/operando instrumentation compatible with a variety of soft and tender x-ray techniques. In particular, we highlight how the statistically-significant shape and electronic structure of a buried Ni(OH)2 interface can be monitored as it is charged/discharged under aqueous conditions with sub-nanometer spatial resolution and sub-millisecond time resolution. Moreover, we will show how this approach may be extended to a variety of materials relevant across a variety of fields including semiconductors, polymer science, energy conversion/storage, etc.

*US DoE Office of Science

9:48AM A45.00010: Effect of titanium adhesion layer on iridium thin film optical properties NICOLE PFIESTER, MARGARET STEVENS, THOMAS VANDERVELDE (Presenter), KEVIN GROSSKLAUS, Tufts University — The refractory metal iridium is useful for highly reflective mirrors for x-ray astronomy and high temperature plasmonic applications like selective emitters. However, the deposition conditions of the thin film can produce very different optical properties which will affect the final performance of the optical device. In this study, we report on the optical properties, crystal structures, and surface roughness of Ir thin films produced by dc magnetron sputtering. The chamber pressure was varied from 10 mTorr to 25 mTorr with a constant plasma power of 160 W. Films deposited on a titanium adhesion layer or directly on a silicon substrate will be compared.

10:00AM A45.00011: Pattern formation on a bubble: Capillary waves on surfactant-laden interfaces* LI SHEN (Presenter), Department of Mechanical Engineering, Imperial College London, FABIAN DENNER, Lehrstuhl fur Mechanische Verfahrenstechnik, Otto-von-Guericke-Universitat Magdeburg, NEAL MORGAN, Shell Global Solutions (UK), DANIELE DINI, Department of Mechanical Engineering, Imperial College London — On a surface-tension-driven liquid interface, the behaviour of the capillary wave is often a bellweather of the overall motion of the system. Consequently, understanding how capillary waves behave is crucial in various interfacial flows at the edge of instability, such as capillary-driven breakup, liquid bridges and pattern formation phenomena. Examining the dynamics of the capillary waves on a surfactant-laden interface, the role of critical wavenumber (at which the capillary wave transitions from the dispersive underdamped regime to the non-dispersive overdamped regime) is explored in the context of the onset behaviour of pattern formation instabilities observed experimentally. Moreover, we look at the effect of the convective-diffusive transport of insoluble surfactants along the interface on the critical wavenumber and the overall dynamics of the capillary waves.

*The authors acknowledge the financial support of the Shell University Technology Centre for fuels and lubricants.

10:12AM A45.00012: Active control of thin liquid film flows: beyond reduced-order models RADU CIMPEANU (Presenter), Mathematical Institute, University of Oxford, SUSANA N GOMES, Warwick Mathematics Institute, University of Warwick — A thin liquid film flowing down an inclined plane is a canonical setup in fluid mechanics and pertains to a wide range of industrial applications. In some cases it is desirable to maintain the liquid-gas interface flat (e.g. coating problems), whereas other contexts (e.g. heat transfer) benefit from increased interfacial area. Ultimately, there is a strong need to reliably manipulate the flow in this mathematically rich system. Control theory has recently been applied successfully by A.B. Thompson et al. (Physics of Fluids 28, 012107, 2016) for an extended range of long-wave models such as the Benney and weighted residual equations, forming a hierarchy of complexity in which the effect of the control is well understood. The subject of this talk relates to the transition from controls on reduced dimensional systems to full Navier-Stokes solutions of this setup. A state-of-the-art volume-of-fluid methodology is used for the direct numerical simulation of the target flow, with control techniques informed by the modelling framework. We study both distributed and localised controls and analyse the robustness of these strategies, bringing us closer to their integration into real-life engineering designs.
10:24AM A45.00013: How to control the morphology of a multiple-liquid system via direct mixing? TAO LI (Presenter), Institute of Physics, The Chinese Academy of Sciences — Arrested composites can be created via the stabilization of convoluted fluid-fluid interfaces, which applies to multiple immiscible liquid systems containing dispersed colloidal particles. Such systems can form various morphologies, including the conventional Pickering emulsions, multiple emulsions, Janus droplets and non-spherical droplets. Moreover, the jamming of interfacial particles provides a promising route to create even more elaborate arrested states. For instance, the bijels (bicontinuous interfacially jammed emulsion gels)! All these structures exhibit novel properties and can lead to numerous applications in drug delivery, food, energy conversion and functional materials. Part I of this talk will focus on the viscosity effect on the formed structures in a binary liquid system, which reveals the formation mechanism of bijels created by direct mixing, and fills an important gap between the phase behaviors in low molecular weight liquids and that in bulk polymers. When mixing three immiscible liquids, the morphology development becomes more complex. In Part II, I will introduce both the formation mechanism and the stability mechanism of Janus emulsions, which can be a combined effect of multiphase immiscibility, interfacial tensions and surface stabilization.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A46 DMP GMAG: 4d/5d Transition Metal Systems -- Perovskite and Honeycomb Iridates BCEC 212 - Feng Ye, Oak Ridge National Laboratory - Tag(s): Focus

8:00AM A46.00001: Anisotropic spin-orbit torque generation in epitaxial SrIrO3 by symmetry design [Invited]
TIANXIANG NAN (Presenter), University of Wisconsin Madison — Selected by Focus Topic Organizer (Gang Car and Jan Musfeldt)

8:36AM A46.00002: Electric Field Tuning of the Anomalous Hall Effect at the Oxide Interfaces: SrIrO3/SrMnO3 SASHI SEKHAR SATPATHY (Presenter), SAYANTIKA BHOWAL, University of Missouri — Using density-functional studies and appropriate models, we show that the anomalous Hall effect (AHE) at the magnetic oxide interfaces can be tuned by modifying the Rashba interaction with the application of an external electric field. Explicit density-functional calculations were performed for the recently grown SrIrO3/SrMnO3 interface in presence of an electric field to demonstrate the effect. Our model calculation indicates the importance of off-diagonal inter-orbital hopping in driving a non-zero Berry curvature, the central quantity that leads to the AHE. Furthermore, with the broken inversion symmetry by an applied electric field, the Rashba interaction comes into play, which enhances the AHE, providing a mechanism to manipulate the AHE. The observed results from the model calculations are corroborated by the first-principles studies, which yield an anomalous Hall conductivity in reasonable agreement with the available experiments in absence of an electric field. Our work has potential applications in spintronics with possible use of AHE as a novel electric field sensor.

8:48AM A46.00003: Role of non-local correlations for spectral properties of Sr2IrO4* BENJAMIN LENZ (Presenter), Centre de Physique Théorique (CPHT), Ecole Polytechnique, CYRIL MARTINS, Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier Toulouse, SILKE BIERMANN, Centre de Physique Théorique (CPHT), Ecole Polytechnique — The spin-orbit Mott insulator Sr2IrO4 has raised tremendous interest recently due to striking similarities to high-Tc superconducting copper oxides both in the pure and in electron-doped compounds. Here, we study the evolution of the spectral function of this 5d transition metal system as a function of doping by means of a combined ab-initio electronic structure and many-body quantum cluster approach. Thereby, important ingredients like spin-orbit coupling and distortions of the oxygen octahedra as well as Hubbard interactions and non-local charge fluctuations are taken into account. The spectral function of pure Sr2IrO4 is analyzed both in its high-temperature paramagnetic and in its low-temperature antiferromagnetic phase and the importance of non-local fluctuations is discussed. The spectra compare well with angular-resolved photoemission measurements and allow to study emerging changes under electron- and hole-doping. Special emphasis is placed on pseudogap features of the spectral function of electron-doped Sr2IrO4, which are found to be in good agreement with experiment.

*This work was supported by a Consolidator Grant of the European Research Council (CorrelMat-617196), the French Agence Nationale de la Recherche (ANR-15-CE30-0009-01) and IDRIS/GENCI Orsay (t2017091393).
9:00AM A46.00004: Broken in-plane rotational symmetry in the hidden order phase of Sr$_2$Ir$_{1-x}$Rh$_x$O$_4$  
SHIGERU KASAHARA, RYO KURIHARA, HINAKO MURAYAMA, YUKI SATO, YUICHI KASAHARA, YUJI MATSUDA, Kyoto University, DAVID HSIEH, California Institute of Technology, GANG CAO (Presenter), University of Colorado Boulder — The layered 5d transition metal oxide Sr$_2$IrO$_4$ hosts a $J_{\text{eff}} = \frac{1}{2}$ antiferromagnetic Mott insulating state, which strikingly resembles to the parent state of high-$T_c$ cuprate superconductors. Recently, great interest has been aroused in the series of Sr$_2$Ir$_{1-x}$Rh$_x$O$_4$, especially on the proposed hidden order phase above the antiferromagnetic ordering, which has been highlighted by optical second-harmonic generation and polarized neutron diffraction experiments [1, 2]. Here, by using exceptionally precise in-plane torque magnetometry [3-5], we provide thermodynamic evidence that nematicity, a spontaneous breaking of rotational symmetry of the underlying lattice, develops well above the antiferromagnetic transition in pure and doped Sr$_2$Ir$_{1-x}$Rh$_x$O$_4$. Our highly sensitive magnetic anisotropy measurements under in-plane field rotation reveal the growth of two-fold oscillations, which onset at the hidden order temperature $T^*$. The present results demonstrate striking similarities between the hidden order phase in Sr$_2$Ir$_{1-x}$Rh$_x$O$_4$ and the pseudogap phase in high-$T_c$ cuprates.


9:12AM A46.00005: Ultrafast control of antiferromagnetism in a Mott insulator by photo-doping  
ALBERTO DE LA TORRE (Presenter), Caltech, GUFENG ZHANG, University of California, San Diego, MICHAEL BUCHHOLD, YUVAL BAUM, NICHOLAS LAURITA, Caltech, JOHN W HARTER, University of California, Santa Barbara, LIUYAN ZHAO, University of Michigan, Ann Arbor, XIANG CHEN, University of California, Santa Barbara, RICHARD DOUGLAS AVERITT, University of California, San Diego, STEPHEN WILSON, University of California, Santa Barbara, GANG CAO, University of Colorado, Boulder, GIL REFAEL, DAVID HSIEH, Caltech — Ultrafast photo-doping provides a possible route to control antiferromagnetic order in Mott-Hubbard insulators out-of-equilibrium [1]. However, AFM order is notoriously challenging to probe by optical techniques [2]. Here, we demonstrate time-resolved nonlinear optical rotational anisotropy as a method to detect ultrafast transient changes of magnetic symmetry group. We leverage this technique to uncover the mechanisms by which photo-carriers suppress long range AFM order in the Mott insulator Sr$_2$IrO$_4$ and by which the AFM order is temporally restored.


9:24AM A46.00006: A time- and wavelength-resolved optical pump-probe reflectivity study of the Mott insulator Sr$_2$IrO$_4$  
ISABELLE PHINNEY (Presenter), ALBERTO DE LA TORRE, Caltech, XIANG CHEN, STEPHEN WILSON, UC Santa Barbara, DAVID HSIEH, Caltech — Photo-induced charge excitations in the copper oxide based antiferromagnetic Mott insulators are able to decay on extremely fast timescales owing to strong spin-charge coupling effects [1]. In recent years, the photo-carrier dynamics of the antiferromagnetic Mott insulator Sr$_2$IrO$_4$ has also become a subject of intensive study [2-4] owing to its similarity to the cuprates in terms of structural, electronic and magnetic properties. Here we examine how the photo-carrier relaxation dynamics of Sr$_2$IrO$_4$ vary with different excitation densities and excitation wavelengths, which access different inter-band transitions, using time-resolved optical reflectivity measurements. We will discuss our results in comparison to the cuprates.

9:36AM A46.00007: Novel Excitonic Condensate State with Block Magnetic Order at n=3.5 in Spin-Orbit Coupled Multiorbital Hubbard Model

NITIN KAUSHAL (Presenter), ALBERTO NOCERA, University of Tennessee, GONZALO ALVAREZ, CNMS, Oak Ridge National Lab, ADRIANA MOREO, ELBIO R DAGOTTO, University of Tennessee — Recent theoretical studies have established the condensation of spin-orbit excitons at momentum \( q = \pi \) for \( t_{2g}^{4} \) spin-orbit coupled three-orbital Hubbard models [1,2], but there is no consensus on experimental finding of this excitonic condensate for \( n=4 \) [3]. In parallel, materials with fractional valence states of Ir ions [4] have also attracted theoretical attention. In this work, we show numerical evidence for the existence of an excitonic condensation at the momentum \( q = \pi/2 \) for doping \( n=3.5 \), for intermediate Hubbard (U). We use the DMRG technique to study the one-dimensional multi orbital Hubbard model. We found an excitonic condensation between \( J_{\text{eff}} = 3/2 \) and \( J_{\text{eff}} = 1/2 \) bands in the triplet channel, together with a block magnetism. This new “block excitonic phase” is present even at large values of \( \lambda \) unlike the \( n=4 \) excitonic phase[2]. Our exact study can help to understand the magnetic phases of materials with the d3.5 valence and robust spin-orbit coupling.


9:48AM A46.00008: Symmetry-based analysis on Raman spectroscopy of two-magnon excitations in a spin-orbit coupled bilayer magnet \( \text{Sr}_3\text{Ir}_2\text{O}_7 \)

SIWEN LI (Presenter), WENCAN JIN, ROBERTO D MERLIN, KAI SUN, University of Michigan, ZACH PORTER, STEPHEN WILSON, University of California, Santa Barbara, LIUYAN ZHAO, University of Michigan — Layered perovskite iridates have been shown to realize a rare \( J_{\text{eff}} = \frac{1}{2} \) Mott insulating antiferromagnetic ground state. While the magnetic excitation dispersion of the single layer perovskite iridate \( \text{Sr}_2\text{IrO}_4 \) can be well explained by a classical spin wave modelof an isotropic Heisenberg magnet, the bilayer counterpart \( \text{Sr}_3\text{Ir}_2\text{O}_7 \) exhibits a giant magnetic excitation gap, ~90 meV, in the resonant inelastic X-ray scattering (RIXS) spectra whose origin is highly debated in literature. In this talk, we present our recent polarized Raman spectroscopy studies on magnetic excitations in \( \text{Sr}_3\text{Ir}_2\text{O}_7 \). Two continuums associated with magnetic excitations are observed, one centering around 170 meV and the other around 100 meV that is close to the magnetic gap reported in RIXS spectra. Through Raman selection rule measurements, we observe that the ~100 meV feature only shows up in the symmetric A1g channel, while the ~170 meV one is present in both A1g and B2g channels. We show that both features originate from two-magnon excitations, by performing symmetry analysis on the spin waves of a bilayer magnet. Our result provides a new insight to the origin of “the giant magnetic gap” in RIXS spectra.

*NSF CAREER Award No. DMR-1749774

10:00AM A46.00009: Unusual magnetic fluctuations in the hidden order phase of \( \text{Sr}_2(\text{Ir,Rh})\text{O}_4 \)

CHENG TAN (Presenter), ZHAOFENG DING, JIAN ZHANG, LEI SHU, Fudan University — Recently, hidden order was observed by L. Zhao et al. in Rhodium doped \( \text{Sr}_2\text{IrO}_4 \) at temperature \( T_{\Omega} \). As in the pseudogap phase of high \( T_{c} \) cuprates, this order breaks rotational symmetry and time reversal symmetry, while preserving translational symmetry. Using muon spin relaxation (MuSR) measurement, we found two types of dynamic magnetic order with different fluctuation rates in the hidden order phase of \( \text{Sr}_2(\text{Ir,Rh})\text{O}_4 \). We also found that the higher fluctuating magnetic field generated by the order setting in at the higher temperature slows its fluctuation rate on exiting the hidden order at \( T_{\Omega} \). A bump appears in the relaxation rate around \( T_{\Omega} \). The \( T_{\Omega} \) obtained by the MuSR measurements are consistent with those determined by second harmonic generation and polarized neutron scattering.
10:12AM A46.00010: Pseudospin-lattice coupling in the spin-orbit Mott insulator Sr$_2$IrO$_4$  JUAN PORRAS (Presenter), JOEL BERTINSHAW, HUIMEI LIU, GINIYATH KHALIULLIN, NAKHEON SUNG, Max Planck Institute for Solid State Research, JONG-WOO KIM, Advanced Photon Source, Argonne National Laboratory, SONIA FRANCOUAL, Deutsches Elektronen-Synchrotron DESY, PAUL STEFFENS, Institut Laue-Langevin, GUOCHU DENG, Australian Nuclear Science and Technology Organization, MARCO MORETTI SALA, ANNA EFIMENKO, European Synchrotron Radiation Facility, AYMÁN SAID, DIEGO M CASA, XIAN-RONG HUANG, THOMAS GOG, JUNGHO KIM, Advanced Photon Source, Argonne National Laboratory, BERNHARD KEIMER, Max Planck Institute for Solid State Research, BUMJOON KIM, Department of Physics, Pohang University of Science and Technology — Spin-orbit entangled magnetic dipoles, often referred to as pseudospins, provide a new avenue to explore novel magnetism inconceivable in the weak spin-orbit coupling limit, but the nature of their low-energy interactions remains to be understood. We present a comprehensive study of the static magnetism and low-energy pseudospin dynamics in the archetypal spin-orbit Mott insulator Sr$_2$IrO$_4$. We find that in order to understand even basic magnetization measurements, a formerly overlooked in-plane anisotropy is fundamental. In addition to magnetometry, we use neutron diffraction, inelastic neutron scattering and resonant elastic and inelastic x-ray scattering to identify and quantify the interactions that determine the global symmetry of the system and govern the linear responses of pseudospins to external magnetic fields and their low-energy dynamics. We find that a pseudospin-only Hamiltonian is insufficient for an accurate description of the magnetism in Sr$_2$IrO$_4$, and that pseudospin-lattice coupling is essential. This finding should be generally applicable to other pseudospin systems with sizable orbital moments sensitive to anisotropic crystalline environments.

10:24AM A46.00011: Bond ordering and phase transitions in Na$_2$IrO$_3$ under high pressure*  ZHIMOU ZHOU (Presenter), Peking University, KAIGE HU, Guangdong University of Technology, YI-WEN WEI, CHAO-KAI LI, JI FENG, Peking University — The Kitaev model of spin-1/2 on a honeycomb lattice supports degenerate topological ground states and may be useful in topological quantum computation. Na$_2$IrO$_3$ with a honeycomb lattice of Ir ions has been extensively studied as a candidate for the realization of this model, due to the effective $J_{\text{eff}} = 1/2$ low-energy excitations produced by the spin-orbit and crystal-field effect. As the eventual realization of the Kitaev model has remained evasive, it is highly desirable and challenging to tune the candidate materials toward such an end. It is well known that external pressure often leads to dramatic changes in the geometric and electronic structure of materials. In this work, the high-pressure phase diagram of Na$_2$IrO$_3$ is examined by first-principles calculations. It is found that Na$_2$IrO$_3$ undergoes a sequence of structural and magnetic phase transitions, from a magnetically ordered phase with space group $C2/m$ to two bond-ordered nonmagnetic phases. The low-energy excitations in these high-pressure phases can be well described by the $J_{\text{eff}} = 1/2$ states.

*The Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. XDB28000000), the 100 Talents Program for Young Scientists of Guangdong University of Technology (Project No. 220413139).

10:36AM A46.00012: Breakdown of magnetic order in the pressurized 3D Kitaev iridate β-Li$_2$IrO$_3$  RUDRA SEKHAR MANNA (Presenter), Department of Physics, Indian Institute of Technology Tirupati, Renigunta Road, Settipalli post, Tirupati - 517506, AP, India, M MAJUMDER, EP VI, EKM, University of Augsburg, 86159 Augsburg, Germany, G. SIMUTIS, ORAIN JEAN CHRISTOPHE, PSI, 5232 Villigen, Switzerland, T. DEY, F. FREUND, ANTON JESCHE, EP VI, EKM, University of Augsburg, 86159 Augsburg, Germany, RUSTEM KHASANOV, PSI, 5232 Villigen, Switzerland, P. K. BISWAS, ISIS, STFC Rutherford Appleton Laboratory, Didcot, Oxfordshire OX11 0QX, UK, E. BYKOVA, NATALIA DUBROVINSKAIA, Laboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, Germany, L. S. DUBROVINSKY, Bayerisches Geoinstitut, University of Bayreuth, 95440 Bayreuth, Germany, R. YADAV, L. HOZOI, S. NISHIMOTO, Institute for Theoretical Physics, IFW Dresden, 01069 Dresden, Germany, ALEXANDER TSIRLIN, PHILIPP GEGENWART, EP VI, EKM, University of Augsburg, 86159 Augsburg, Germany — Novel electronic and magnetic properties are found in honeycomb lattice iridates, having dominant Kitaev interactions, due to the presence of strong spin-orbit coupling and electronic correlations. We present the measurements of magnetization, thermal expansion, magnetostriction, muon spin resonance, single crystal x-ray diffraction under hydrostatic pressure of 3D hyperhoneycomb β-Li$_2$IrO$_3$. These measurements are complemented by the $ab initio$ calculations. The incommensurate magnetic order at 38 K initially increases as a function of hydrostatic pressure with a rate of 0.9 K/GPa, consistent with the thermodynamic Ehrenfest relation. The partial polarization at 2.5 T decreases with increasing pressure signifies the instability of the magnetic order. The ordered state breaks down upon a first-order transition at around 1.4 GPa, giving way to a new ground state marked by the coexistence of dynamically correlated and frozen spins. This partial spin freezing may indicate the classical nature of the resulting pressure-induced spin-liquid, expected for large-$\Gamma$ (nearest-neighbor off-diagonal exchange) limit [1].


Monday, March 4, 2019 8:00 AM - 11:00 AM
8:00AM A47.00001: Facet dependent cation segregation in layered lithium transition-metal oxide cathode materials  
HAKIM IDDIR (Presenter), JUAN GARCIA, Argonne National Laboratory, JAVIER BAREÑO, MIMSI Materials, GUOYING CHEN, Energy Storage and Distributed Resources Division, Lawrence Berkeley National Laboratory, JASON CROY, Argonne National Laboratory — The development of energy storage devices with enough power and energy density, long term stability, and extended cycle life that are capable of meeting environmental constraints is an important challenge for modern electrochemistry. Lithium-ion batteries are the primary energy storage devices for electric vehicles. However, there are still challenges for making this technology more competitive. Improving the understanding of the fundamental processes taking place in such materials is a prerequisite to accomplish any significant improvement. For example, the segregation of transition metals (TM) from the bulk to the surface of typical cathode-oxide particles plays a critical role in the formation and composition of surface reconstruction layers (SRL) that appear on pristine and cycled materials. Such layers have been indicated as the origin of cathode impedance rise with cycling, and hence, may significantly decrease the performance of batteries. The origin and thermodynamic driving force for such segregation processes are not clear yet. In the present work, we propose a facet dependent TM segregation/phase-change mechanism to explain observed experimental results.

8:12AM A47.00002: LiFePO4-Carbon Nanofiber Composite Cathodes for Li-ion Batteries*  
ADEWALE A. ADEPOJU (Presenter), QUINTON L WILLIAMS, Howard University — LiFePO4 offers interesting possibilities as a cathode material for Li-ion batteries because of its steady operating voltage, excellent structural stability, nontoxicity, and inexpensive source materials. However, its poor electronic conductivity is a major challenge for commercialization. Although different techniques have been developed to address this problem, we approach this challenge by incorporating carbon nanofibers (CNFs) as conductive additives in the LiFePO4 cathode material. CNFs have high electrical conductivity and high aspect ratio. The effect of adding different percentages of CNFs to LiFePO4 cathodes was investigated using scanning electron microscopy (SEM), four-point probe, and electrochemical measurements. Electrochemical testing showed the LiFePO4 with few percents CNFs added to the composite cathode exhibited excellent rate capability performance at 20C and higher cycling capacity with less fading over 200 cycles at 5C. This improved performance is attributed to the increase in electronic percolation pathways created by adding CNFs.

*This research was supported by the Howard University Partnership for Reduced Dimensional Materials via National Science Foundation PREM (Grant No. 1205608).

8:24AM A47.00003: First principles theory of unanticipated electron transfers in new organic energy-storage materials: application to phenothiazine-based polymer cathodes.*  
MARIEL TADER (Presenter), BRIAN PETERSON, HÉCTOR ABRUÑA, BRETT FORS, TOMAS ALBERTO ARIAS, Cornell University — Organic polymer cathodes have promise as low-cost, environmentally clean, lightweight alternatives to traditional inorganic battery cathodes, but are limited by their instability. To explain the observed limits to the charge capacity of PT-DMPD, a phenothiazine-based organic material, we utilize recently developed Joint Density Functional Theory (JDFT) methods to study electron transfer (redox) events. Comparing to experimental cyclic voltammetry (CV) data, we find that electron transfer from the primary PT-DMPD redox sites actually occurs at lower voltages than anticipated. As a consequence, batteries using this and related materials have been operated at voltages where some of the primary redox reactions have actually already occurred, so that, during operation, unexpected redox centers are accessed. These new centers weaken important structural bonds, perhaps explaining the observed loss of capacity of PT-DMPD cathode batteries with cycling. These findings suggest a pathway for design of more power dense, stable energy storage materials.

*This work was primarily supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875).
8:36AM A47.00004: Electrogenerated Hexacyanoferrate Thin Films for Battery Applications

ELSE AMANDA RENSMO, SCOTT D JOFFRE, JENNIFER R HAMPTON (Presenter), Hope College — Prussian Blue Analogues such as transition metal hexacyanoferrates (HCFs) have gained increasing interest as materials for energy storage applications, as they provide enhanced stability due to their open framework structure and potential for reduced cost by use of earth-abundant materials. Using Ni, NiCo and NiCu substrates, a variety of alloy HCF films were electrogenerated by cyclic in the presence of hexacyanoferrate. For NiCo- and NiCu-based HCF materials, the charge storage and transport properties were measured and compared to Ni-HCF to explore the effects of the addition of alloying metals. The addition of Co or Cu in the substrate results in a small increase in the total stored charge, but no observable trend in the transport kinetics. For Ni-HCF, the total amount of Fe in the resulting material was measured both electrochemically and with x-ray spectroscopic methods. Unexpectedly, the spectroscopic measurements were smaller than the electrochemical ones, indicating there must be additional electrochemical reactions occurring in the presence of the HCF.

*This research was made possible by the National Science Foundation under NSF-RUI Grant No. DMR-1608327, NSF-MRI Grant No. CHE-0959282, and NSF-MRI/RUI Grant No. PHY-0319523.

8:48AM A47.00005: Structural, Electronic, and Magnetic Properties of Li\(_{1+x}\)Mn\(_2\)O\(_4\) Based on First-Principles Calculations

JINSEON PARK (Presenter), Department of Physics and Astronomy, University of Tennessee, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Lab — Recent studies have focused on understanding the reaction mechanisms driven by the lithiation of Li\(_{1+x}\)Mn\(_2\)O\(_4\) spinels, in an effort to enhance the energy density of lithium-ion batteries. Experiments to characterize the spinels' fundamental properties during the reaction are challenging. Thus computational/theoretical modeling is highly desirable. In this study, we identified global/local minimum structures of Li\(_{1+x}\)Mn\(_2\)O\(_4\) spinels by using a global structure optimization algorithm coupled with first-principles calculations, and further characterized their basic electronic and magnetic properties, as well as their relative structural stabilities under external perturbations. Interestingly, the local Jahn–Teller distortion was found to play a governing role in determining spinels' relative stabilities, in comparison to other key factors such as charge states of the Mn ions, positions of the Li ions, and magnetic configurations. Feasible pathways for the experimental verification of lithiation are proposed.

9:00AM A47.00006: Structural mechanisms in complex oxides enabling high-rate lithium-ion energy storage

KENT GRIFFITH (Presenter), Northwestern University, KAMILA WIADEREK, Advanced Photon Source, Argonne National Laboratory, GIANNANTONIO CIBIN, Diamond Light Source, GIANNANTONIO CIBIN, Department of Chemical Engineering, Columbia University, LAUREN MARBELLA, Department of Chemistry, University of Cambridge — The maximum power output and minimum charging time of a lithium-ion battery depend on mixed ionic–electronic conduction. We show that complex niobium tungsten oxides with frustrated polyhedral arrangements and dense μm-scale particle morphologies can rapidly and reversibly intercalate large quantities of lithium. Analysis of high-rate and multi-electron energy storage will be discussed with insights from operando X-ray diffraction, solid-state nuclear magnetic resonance spectroscopy, and multi-edge X-ray absorption spectroscopy for the recently reported crystallographic shear structure and bronze-like oxide phases[1]. Materials and mechanisms that enable lithiation of μm particles in minutes have implications for high power applications, fast charging devices, all-solid-state batteries, and general approaches to electrode design and materials discovery.


*The Winston Churchill Foundation of the United States, a Herchel Smith Scholarship, and a Science and Technology Facilities Council Futures Early Career Award (KJG). EPSRC grant EP/M009521/1 (KJG, CPG). EU Horizon 2020/Marie Sklodowska–Curie grant 750294 and a Darwin Research Fellowship (LEM).
Study of Structural Transitions, Jahn-Teller Distortion, Cyclability, and Specific Energy in P2-type Na$_x$MO$_2$ Na-ion Battery Cathodes* WILLIAM REXHAUSEN (Presenter), UMA GARG, NATHANIEL SMITH, Department of Physics, University of Wisconsin Milwaukee, Wisconsin 53211, JOSHUA HARRIS, DEYANG QU, Department of Mechanical Engineering, University of Wisconsin Milwaukee, Wisconsin 53211, PRASENJIT GUPTASARMA, Department of Physics, University of Wisconsin Milwaukee, Wisconsin 53211 — Recent years have seen an interest in exploring the viability of Na-ion based battery cathode materials. Here, we report relationships between crystal structure and properties in the Na$_x$MO$_2$ (M=transition metal) family of layered metal-oxide battery cathodes. Using detailed Rietveld fitting, we characterize structural transitions that occur as a result of cycling. We further report the effect of these transitions on battery cyclability, and the effect of transition metal substitution in crystal structure and distortion in Na$_{2/3}$MnxFe$_{1-x}$O$_2$ (NMFO). Using specially designed transfer chambers, we have studied ex situ x-ray diffraction at different potentials in the charge-discharge cycle to examine the nature of the structural transitions both in the metal oxide planes and in the layering structure. We report specific energy, capacity, and cyclability of cells when cycling over several voltage ranges for different cathodes and find that substituents for Mn perform well when charged no higher than 4.0 V (vs. Na). Conversely, charging to 4.3 V degrades crystallinity.

*UWM

Modeling of 2D Materials for Sustainable Energy Storage: Opportunities and Challenges* VIDUSHI SHARMA, KAMALIKA GHATAK (Presenter), DIBAKAR DATTA, New Jersey Institute of Technology — In recent years, extensive research has been carried out on 2D materials to develop high-capacity anode materials for Li-ion batteries (LIBs). By first-principle calculations, we investigated the adsorption of Li on graphene with defects. We find that with controlled defect, we can achieve a maximum storage capacity of approximately 1675 for LIBs. However, despite enormous opportunities, we need to concern about several challenges such as adatom trapping at the defect sites, the effect of defects on adatoms diffusivity, microstructural changes, etc. In addition, our recent work shows that for the Si-based anode, we can achieve better electrochemical stability by coating the current collector surface with graphene sheets. Besides graphene, several other 2D materials such as graphene allotropes, Transition Metal Dichalcogenides (TMD), etc. have tremendous potential in energy applications. Moreover, by building heterostructures (stacking of different 2D materials), it is possible to combine the advantage and eliminate the disadvantages of the individual sheet. In this presentation, we will provide a detailed overview of opportunities and challenges of modeling of 2D materials and its heterostructures for the next-generation sustainable energy storage applications.

*XSEDE, DMR180013

Impact of Hybridization and Correlations on Transition-Metal Valence and Oxygen Redox in Li-ion Battery Cathode Materials ILKYU LEE (Presenter), CHUNJING JIA, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford University — Transition-metal oxide battery cathode compounds undergo distinct changes in their electronic distribution as one goes from a fully lithiated to a fully delithiated state. This would lead nominally to energetically unfavorable high valence states on the transition-metal, affecting overall energy capacity. Here, we analyze the influence of metal-to-ligand orbital hybridization and effective charge transfer using a configuration interaction cluster model to simulate different spectroscopic tools. We connect our observations to the framework of anionic redox, which prevents high transition-metal valency, and has been linked to increases in energy capacity of Li-ion batteries. By gaining insight into crucial features that are identified with such processes, we aim to have a greater understanding of the fundamental physics of Li-ion cathode materials, in the hopes of predicting novel, better performing Li-ion compounds.
Advanced characterization of high-capacity electrodes with x-ray Compton scattering

HASNAIN HAFIZ (Presenter), Mechanical Engineering, Carnegie Mellon University, Pittsburgh, PA, USA, BERNARDO BARBIELLINI, Physics, School of Engineering Science, Lappeenranta University of Technology, Lappeenranta, Finland, KOSUKE SUZUKI, Graduate School of Science and Technology, Gunma University, Kiryu, Gunma, Japan, GREGORY HOUCHINS, Mechanical Engineering, Carnegie Mellon University, Pittsburgh, PA, USA, HIROSHI SAKURAI, Graduate School of Science and Technology, Gunma University, Kiryu, Gunma, Japan, ARUN BANSIL, Physics, Northeastern University, Boston, MA, USA, VENKATASUBRAMANIAN VISWANATHAN, Mechanical Engineering, Carnegie Mellon University, Pittsburgh, PA, USA — Li-rich layered oxides (LRLOs) have been very promising cathode materials due to their exceptionally high capacity of ~300 mAh/g and energy density of ~1000 mWh/g. However, the reaction mechanism underlying their electrochemical operation is not fully understood. Recent work on pristine cathode materials shows that Compton scattering spectroscopy can provide a useful tool to unravel the relationship between the key battery characteristics and the nature of the electronic orbitals involved in Li intercalation reactions [1]. Here, we discuss high-energy x-ray Compton scattering spectra along with parallel first-principles computations from Li$_{1.2-x}$Ti$_{0.4}$Me$_{0.4}$O$_2$ (Me = Mn and Fe) for the purpose of developing advanced spectroscopic tools for characterizing LRLO battery materials. Our study gives insight into how we can obtain a faithful reconstruction of the redox orbitals using the Compton scattering technique. We also discuss the reversibility of the solid-state redox processes, and the related issues of lattice distortions, charge compensation, and the covalent mechanism of transition metal and oxide ions as a pathway to provide a new generation of insights into the mechanisms at play in LRLO battery materials.


Theoretical understanding of oxygen redox feature observed on RIXS map of battery cathode materials

IWNETIM ABATE (Presenter), Department of Materials Science and Engineering, Stanford University, CHUNJING JIA, BRIAN MORITZ, MICHAEL F TONEY, SSRL Materials Science Division, SLAC National Accelerator Laboratory and Stanford University, THOMAS DEVEREAUX, SRI CHAITANYA DAS PEMMARAJU, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory and Stanford University — High energy density rechargeable batteries are essential to meet the ever growing global energy demand. Recently, cathode materials which have redox activity of both transition metal and oxygen are found to be very promising in this regard. However, the exact mechanism for the oxygen redox is yet to be understood. Resonant inelastic x-ray scattering (RIXS) has been established as a reliable probe of the critical oxygen states involved in battery electrodes with oxygen redox activities. The interpretation of specific O -K RIXS features; however, has not yet been achieved. To this end, we have performed theoretical calculations using new algorithm we developed to understand the spectroscopic feature from first principle. We aim to shed light on the physics of cathode materials and suggest design schemes for cathodes with exceptional capacity.

Impact of Humidity on the Mobility of an Ionic Liquid Confined in Ti$_3$C$_2$T$_x$ MXene

NARESH OSTI (Presenter), Neutron Scattering Division, Oak Ridge National Laboratory, MATTHEW W THOMPSON, Department of Chemical and Biomolecular Engineering, Vanderbilt University, KATHERINE VAN AKEN, MOHAMED ALHABEB, Department of Materials Science and Engineering, Drexel University, MADHUSUDAN TYAGI, NIST Center for Neutron Research, JONG KEUM, Neutron Scattering Division, Oak Ridge National Laboratory, PETER THOMAS CUMMINGS, YURY GOGOTSI, Department of Chemical and Biomolecular Engineering, Vanderbilt University, EUGENE MAMONTOV, Neutron Scattering Division, Oak Ridge National Laboratory — MXenes are two-dimensional materials with a potential in energy storage applications, especially as electrode materials in supercapacitors. MXenes provide high volumetric capacitance, but still have some limitations affecting their power capabilities. On the other hand, high energy and power density can be achieved using room temperature ionic liquids (RTILs) as an electrolyte that withstands a high operational potential window. Here, as an effort to overcome the high voltage limitation, and to provide a guidance for the development of most robust energy storage systems in the future, we have investigated the microscopic dynamics of a RTIL, [EMIm$^+$$][\text{Tf}_2\text{N}^-]$, confined in a Ti$_3$C$_2$T$_x$ MXene. We have found that the ionic liquid was confined between the stacks rather than in between the layers of the MXene, thus showing a diffusion coefficient at about a half of the bulk value. This result is consistent with the unchanged c-lattice parameter revealed by X-ray diffraction measurement after the ionic liquid intercalation. An increase in the overall cation diffusivity after water vapor exposure, as revealed from quasi-elastic neutron scattering (QENS) and molecular dynamics simulations, will be presented.

*Department of Energy, Office of Science, Office of Basic Energy Sciences
10:24AM A47.00013: Symmetrical supercapacitors with α-MnO2 nanorods/carbon nanofiber (CNF) composite as electrode material  PRASADA RAO TALAKONDA (Presenter), AJAY KUMAR, Department of Physics & Astronomy, Wayne State University, VAMAN M NAIK, Department of Natural Sciences, University of Michigan-Dearborn, RATNA NAIK, Department of Physics & Astronomy, Wayne State University — α-MnO2 nanorods have been grown on the surface of CNF for enhancing the electrical conductivity of MnO2. α-MnO2/CNF (0-5 wt%) nanocomposites were synthesized using a co-precipitation method. The XRD results confirm the formation of a single phase α-MnO2 and SEM/TEM images reveal the formation of α-MnO2 nanorods. While α-MnO2/CNF(1.25 wt%) exhibits the largest surface area (381 m²/g) and only a slight increase in the electrical conductivity (0.05 S/cm), α-MnO2/CNF(5 wt%) shows the least surface area (131 m²/g) but an order of magnitude higher electrical conductivity (0.67 S/cm), compared to pure α-MnO2 nanorods. C-V measurements show improved performance in all α-MnO2/CNF supercapacitors compared to that of pure α-MnO2. Ragone plot shows that although α-MnO2/CNF(1.25 wt%) exhibits the highest specific capacitance (313 F/g at 1 A/g) and hence the highest energy density of 32.8 Wh/kg, it has a lower power density of 2720 W/kg. On the other hand, α-MnO2/CNF(5 wt%) shows the least energy density of 7.9 Wh/kg, but has a higher power density of 4640 W/kg. Results demonstrate that one can optimize both energy and power densities by controlling the amount of CNF in the nanocomposites.

10:36AM A47.00014: Flexible supercapacitors with vertically aligned multiwalled carbon nanotubes (MWCNT) directly synthesized on a metal foil.* THUSHANI DE SILVA (Presenter), COLE DAMERY, ROBINSON KARUNANITHY, RANA ALKHALDI, PRASANNA DNYANESHWAR PATIL, MILINDA WASALA, POOPLASINGAM SIVAKUMAR, SAIKAT TALAPATRA, Physics, Southern Illinois University Carbondale — We will present the results of our investigation on all solid-state flexible supercapacitors using MWCNT directly grown on ultrathin Inconel foil. A poly(vinyl alcohol)/phosphoric acid (PVA/H₃PO₄) polymer gel has been used as both the electrolyte and the separator. Since the aligned MWCNT has a higher effective surface area and the direct synthesis on a metal decreases the resistance at the interface, these supercapacitors display improved performance with the highest measured areal specific capacitance of 19.6 mF/cm². Key device parameters, measured and analyzed with standard electrochemical circuit modeling will also be presented. The flexibility of the devices was validated by testing them under different bending angles. These devices can withstand a large amount of such bending cycles, making them more durable and robust energy storage devices.

*Authors CD and ST acknowledge the support through the NSF REU Grant # 1757954 and DoD ASSURE programs. Partial support through NSF-CHE Grant # 1506277 is also acknowledged.

10:48AM A47.00015: Metal Organic Framework high performance supercapacitors fabricated by electrophoretic deposition* FATIMA AMIR (Presenter), DARIEN K. NGUYEN, Winthrop University — 2D ultrathin nanomaterials have attracted a significant interest because of their applications as energy storage devices. Metal organic frameworks (MOFs) a subset of these 2D nanomaterials are believed to be a key solution for energy storage devices such as electrochemical capacitors. In this work, we report the fabrication of the MOF Ni3(2,3,6,7,10,11-hexaaminotriphenylene)2 (Ni3(HITP)2) supercapacitor electrodes using electrophoretic deposition. The morphologies of the Ni3(HITP)2 electrodes were characterized using scanning electron microscopy, and transmission electron microscopy. The structure of the Ni3(HITP)2 electrodes was analyzed using x-ray diffraction. The MOF-based supercapacitor exhibited excellent capacitive performance in 0.5M Na₂SO₄ with an areal capacitance of 15.58mF/cm². Furthermore, the supercapacitor exhibited an outstanding cycling stability with a capacitance retention of 81% over 50,000 cycles indicating excellent long term electrochemical stability. These results pave a promising route for the design and manufacture of a new generation of devices for energy storage applications.

*NSF-EPSCoR award # OIA-1655740

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A48 DFD DBIO GSNC: Swimming, Motility and Locomotion  BCEC 251 - Amy Lang, University of Alabama
8:00AM A48.00001: Sperm motility in modulated microchannels*  SEBASTIAN RODE (Presenter), JENS ELGETI, GERHARD GOMPPPER, Institute of Complex Systems (ICS-2), Forschungszentrum Jülich —
Sperm cells swim through the fluid by a periodic wave-like beating of their flagellum [1-3]. At low Reynolds numbers and in confinement, the directed motion of sperm and other microswimmers is strongly influenced by steric and hydrodynamic surface interactions [1]. We model sperm motility in mesoscale hydrodynamics simulations by imposing a planar traveling bending wave along the flagellum [2]. Sperm are simulated swimming in curved, straight, shallow and zigzag-shaped microchannels. Changes in the sidewall modulations and the imposed beat pattern allow the identification of a strong dependence of the surface attraction on the beat-shape envelope of the sperm cell. The simulations reveal a strong dependence of the deflection angle on the orientation of the beat plane with respect to the channel sidewall, and thus deepen the understanding of sperm navigation under strong confinement. Detachment of sperm, while swimming along curved walls, is dominated by either the emergence of a nonplanar component of the flagellar beat with increasing wavelength or the strong confinement in shallow channels.


*DFG - SPP 1726 “Microswimmers”

8:12AM A48.00002: Development of a Microfluidic Device to Sort Sperm based on their Swimming Potential against the Flow  AFROUZ ATAEI (Presenter), ANDY W.C. LAU, WASEEM ASGHAR, Florida Atlantic University — The first step of in-vitro fertilization is to sort out the motile sperm from the non-motile ones. Currently, centrifugation based sperm swim-up and density gradient separation are common methods to sort sperm. However, these methods reduce sperm quality during the repetitive centrifugation steps and isolate sperm with high DNA fragmentation. In this work, we construct a microfluidic device based on the observation that motile sperm can swim against the flow within a specific range of flow rates. This sperm sorting device consists of two chambers, separated by a filter. After 45 minutes the sorted motile sperm are collected from the top retrieval chamber and is placed on a glass slide for visual inspection and data collection. We find that the most motile and functional sperm pass selectively through the micropores against the flow, showing that our device provide an efficient way to sort sperm.

8:24AM A48.00003: Varying pH influences the motility of Helicobacter pylori more strongly in porcine gastric mucin solutions than in broth.*  CLOVER TING-YI SU (Presenter), KATARZYNA BIENIEK, RAMA BANSIL, Boston University — Helicobacter pylori, a pathogen which inhabit the gastric mucus has to swim across the naturally occurring pH gradient in the mucus layer varying from 2-4 in the lumen to 7 on the epithelial surface. The mucus has a pH-dependent viscoelasticity forming a gel at low pH, whereas at higher pH it is solution-like. Previous studies have shown that H. pylori were immobile in porcine gastric mucin (PGM) below pH 4. How much of this effect is due to gelation of PGM and how much due to the effects of pH on the flagellar motors is unclear. To address this question we compared the translation and rotational motion of the bacteria in PGM versus broth at different pH. In broth, H. pylori swimming speed increased as pH was lowered from pH 7 to 4, followed by a drop in speed below pH4 indicating decrease of proton motive force, whereas in PGM the speed peaked at pH 5 and bacteria became immobile below pH3, indicating the increase in viscosity in PGM dominating the loss of motility. The body rotation rate is weakly dependent on pH in broth. in PGM the bacteria stuck in the low pH gel rotate much faster than the mobile bacteria at higher pH’s, indicating that bacteria can sense the environment’s mechanical properties and attempt to free themselves from being immobilized.

*Funded by NSF PHY1410798
8:36AM A48.00004: Experimental Evidence of Passive Separation Control by Shortfin Mako Shark Scale Bristling*  
AMY LANG (Presenter), LEONARDO SANTOS, ANDREW BONACCI, University of Alabama, PHILIP MOTTA, University of South Florida, MARIA LAURA HABEGGER, Florida Southern College, KEVIN DU CLOS, BRAD GEMMELL, University of South Florida, SEAN DEVEY, University of Alabama — The shortfin mako has scales (on the order of 0.2 mm in size) flexible to angles in excess of 40 degrees, but only in the direction of reversing flow and strategically placed on the body, such as flank and fins, for controlling flow separation to reduce pressure drag. Various experiments have been carried out to document the separation control capability of mako skin samples, including high-speed video evidence of passive, flow-actuated scale bristling. In water tunnel studies, a flat plate boundary layer was grown to Re > 10^5 and passed over flank skin samples whereon flow separation was induced by a controllable adverse pressure gradient produced by a rotating cylinder located above the test area. Velocity measurements, both instantaneous and time-averaged, were captured using Digital Particle Image Velocimetry (DPIV). Results confirm separation control was achieved under both laminar and tripped turbulent boundary layer conditions as quantified by backflow coefficient, or the percentage of time the flow was reversed. We hypothesize that the width of a single shark scale corresponds to the sizing of the reversing flow, which induces scale actuation, documented within the turbulent boundary layer case as occurring within a low speed streak.

*US Army and NSF

8:48AM A48.00005: How Hummingbirds Reorient Forces During Maneuvering Flight*  
BEN HIGHTOWER (Presenter), RIVERS INGERSOLL, DANIEL SHORR, DIANA D CHIN, DAVID LENTINK, Stanford University — Hummingbirds are among the most agile of birds with the unique ability to hover in flight. While their flight kinematics have been studied extensively, their aerodynamic forces have primarily been studied using indirect methods like inverse dynamics and particle image velocimetry, which are insufficient to capture the full weight support of the bird. Here we present in vivo force recordings of maneuvering Anna's hummingbirds feeding from a moving flower using a novel 3D aerodynamic force platform. The pressure field generated by the maneuvering bird travels to the boundaries of the flight arena, and the six instrumented plates mechanically integrate the resulting pressure and shear distribution at a high enough sample rate to record wingbeat-resolved forces. With these data, we can determine the tracking effectiveness of hummingbirds as well as the control methods they employ during feeding from moving flowers as well as in-flight prey capture. Unraveling how hummingbirds manipulate aerodynamic forces with their wings to maneuver has profound applications to the study of other flying animals and the development of more maneuverable aerial robots.

*The authors would like to thank the National Science Foundation and the Stanford Graduate Fellowship for support.

9:00AM A48.00006: DNS of squirmers (spherical microswimmers) with rotlet*  
RYOICHI YAMAMOTO (Presenter), FEDERICO FADDA, JOHN JAIRO MOLINA, Dept. Chemical Engineering, Kyoto University — The squirmer model introduced by Lighthill and later extended by Blake allows the description of microorganisms such as algae and bacteria. It consists in a spherical particle with a prescribed tangential surface velocity, neglecting the radial component, responsible for the self-propulsion. If the microorganism repels fluid along its axis and repels it to the sides it is called pusher (like the bacterium Escherichia Coli); in the opposite case it is called puller (like the alga Chlamydomonas Reinardti). In this study the squirmer model is incorporated into the Smoothed Profile Method, an efficient DNS scheme to simulate solid objects into a fluid taking fully into account the hydrodynamics, which has already been successfully used in the past to study collective motion and interactions of squirmers. Now the traditional squirmers (pusher and puller) are modified by introducing a rotlet term, an azimuthal component of surface velocity to give a more realistic description of the motion of microorganisms like bacteria whose flagellar and body rotate in the opposite direction.

*This work was supported by the Japan Society for the Promotion of Science (JSPS) KAKENHI (17H01083) grant, as well as the JSPS bilateral joint research projects.
From Single to Many: Swimming at Intermediate Reynolds Numbers*  THOMAS DOMBROWSKI (Presenter), SHANNON K JONES, UNC Chapel Hill, GEORGIOS KATSIKIS, Massachusetts Institute of Technology - MIT, AMNEET BHALLA, San Diego State University, BOYCE E. GRIFFITH, DAPHNE KLOTSA, UNC Chapel Hill — We propose a simple, self-propelled model swimmer which uses steady streaming flows for propulsion at intermediate Reynolds numbers (Re). Our model swimmer is composed of two unequal spheres that are tethered and oscillate in antiphase. For all Re>0, our reciprocal swimmer swims and interestingly, as Re increases, switches swimming direction from a small-sphere-leading to a large-sphere-leading regime. Varying a broad range of parameters (viscosity, amplitude, distance between the spheres, sphere radii and sphere-radii ratio), we identify a universal swimming transition at a critical Re. Flow fields are analyzed, and we determine that propulsion occurs as a result of the interfering steady streaming flows of the two spheres forced to oscillate close to one another. We also show that their bi-directional behavior is linked to their reversal in steady streaming flows. We continue by investigating interactions between multiple swimmers in both swimming regimes.

*This work is supported by NSF-CAREER DMR-1753148

Propulsion of asymmetric bodies through soft lubricated tubes  BHARGAV RALLABANDI (Presenter), University of California, Riverside, MARY-CASWELL STODDARD, Princeton University, JENS G EGGERS, University of Bristol, HOWARD A STONE, Princeton University — The motion of tightly fitting objects through soft tubes is a scenario that frequently arises in physiological processes. An example is that of avian egg laying, where observations across avian species suggest that eggs move through the oviduct pointy-end first, even though they are usually then laid blunt-end first. We investigate the mechanistic implications of this observation by considering the motion of fore-aft asymmetric intruders moving through lubricated elastic tubes. Using asymptotic theory, we find that the thickness of the lubricating fluid layer scales inversely with the square root of the slope of the intruder surface near its nose, in the direction of motion. Consequently, the force required to drive motion scales with the square root of this slope, and also depends on the translation velocity, the viscosity of the lubricant and the elasticity of the tube walls. Our findings show that asymmetric objects are more efficiently moved pointy-end-first through lubricated soft tubes, suggesting a mechanistic rationalization for the observed orientation of eggs moving in avian oviducts.

Hydrodynamic interactions between artificial swimmers and obstacles  FLORENCIO BALBOA USABIAGA (Presenter), Center for Computational Biology, Flatiron Institute, Simons Foundation, QUENTIN BROSSEAU, Courant Institute of Mathematical Sciences, New York University, YANG WU, Department of Chemistry, New York University, ENKELEIDA LUSHI, Department of Mathematical Sciences, New Jersey Institute of Technology, LEIF RISTROPH, JUN ZHANG, Courant Institute of Mathematical Sciences, New York University, MICHAEL WARD, Department of Chemistry, New York University, MICHAEL SHELLEY, Center for Computational Biology, Flatiron Institute, Simons Foundation — Bimetallic micro-rods swimming in hydrogen peroxide solutions are a standard example of self-propelled particles used in a large number of experiments. Here, we present how micro-rods can be designed to propel like pullers, pushers or symmetric swimmers.

We combine experiments and numerical simulations to investigate the dynamics of rods swimming around obstacles. We find that the characteristic residence time around an obstacle is longer for symmetric swimmers than for puller or pushers. When the obstacles form a lattice the swimmer speed and its residence time control the long time diffusion coefficient; for non-symmetric obstacles the displacement bias is different for each kind of rod. These differences suggest that microfluidic devices can be used to sort self-propelled particles with different swimming natures.
9:48AM A48.00010: A Robotic Fast-Start Fish Utilizing Post-Buckling Dynamics of Slender Column Under Compression to Passively Produce Rapid Underwater Locomotion  TODD CURRIER (Presenter), YAHYA MODARRES-SADEGHI, University of Massachusetts Amherst — An experimental study is conducted on a robotic fish designed to emulate the fast-start response. The fish body is constructed of 3D-printed materials and a light spring steel spine. The body is actuated using pressurized pistons. A total of two pistons are supplied with pressure through lightweight high-pressure service lines. The source of pressure is carbon dioxide with a 4.82 MPa peak operating pressure resulting in a body response that emulates a C-start maneuver in milliseconds. The motion of the fish is controlled using a programmable microprocessor. The buckling modes of a slender column in compression are used to produce organic movements in the body with only two sources of actuation. The interaction of the fluid with the underactuated structure results in a travelling wave in the body of the robotic fish that is kinematically similar to the live fish. The effect of the tail is considered using the model to test performance changes with various geometries.

10:00AM A48.00011: Rotation-translation coupling in a highly symmetric propeller at low Reynolds number* JOHANNES SACHS (Presenter), Micro Nano Molecular Systems, Max Planck Institute for Intelligent Systems, KONSTANTIN I MOROZOV, Department of Chemical Engineering, Technion, ODED KENNETH, Department of Physics, Technion, ALEXANDER LESHANSKY, Department of Chemical Engineering, Technion, PEER FISCHER, Micro Nano Molecular Systems, Max Planck Institute for Intelligent Systems — Nature has developed several strategies to generate locomotion at low Reynolds (Re) numbers. Ciliates and sperm cells beat cilia in a non-reciprocal way to overcome the scallop-theorem. Bacteria use the inherently symmetry-broken shape of a rotating helical flagellum to create translational motion. Artificial corkscrew propellers were successfully employed to mimic the rotation-translation coupling of the latter [Nanoscale, 3, 557-563 (2011)]. A long time ago Purcell stated: “Turn anything - if it isn't perfectly symmetrical, you'll swim.” [Am. J. Phys. 45, 3 (1977)]. All these examples inevitably indicate the close connection between an object's symmetry and its propulsion dynamics at low Re. In turn, this raises the question if all propellers have to be chiral to be propulsive? Can highly symmetrical, achiral shapes be propulsive too? We provide a rigorous symmetry analysis of an achiral, planar V-shaped object and experimentally prove that this shape can be indeed propulsive when driven by an external field. This is, to our knowledge, the first demonstration of a truly achiral micro-object that propels; showing that chirality is not prerequisite for propulsion at low Reynolds number.

10:12AM A48.00012: Maximum in density heterogeneities of active swimmers* FABIAN JAN SCHWARZENDAHL (Presenter), MARCO G. MAZZA, Dynamics of complex fluids, Max-Planck-Institute for Dynamics and Self-Organization — Suspensions of unicellular microswimmers such as flagellated bacteria or motile algae can exhibit spontaneous density heterogeneities at large enough concentrations. We introduce a novel model for biological microswimmers that creates the flow field of the corresponding microswimmers, and takes into account the shape anisotropy of the swimmer's body and stroke-averaged flagella. By employing multiparticle collision dynamics, we directly couple the swimmer's dynamics to the fluid's. We characterize the nonequilibrium phase diagram, as the filling fraction and Péclet number are varied, and find density heterogeneities in the distribution of both pullers and pushers, due to hydrodynamic instabilities. We find a maximum degree of clustering at intermediate filling fractions and at large Péclet numbers resulting from the competition of hydrodynamic and steric interactions between swimmers. We develop an analytical theory that supports these results. This maximum might represent an optimum for the microorganisms' colonization of their environment.

*Deutsche Forschungsgemeinschaft (SFB 937, project A20)
**10:24AM A48.00013: Experimental observation of catalytic Janus colloid microswimmer flow fields**

STEPHEN EBBENS (Presenter), ANDREW CAMPBELL, University of Sheffield, PIERRE ILLIEN, ESPCI Paris, PSL Research University, RAMIN GOLESTANIAN, Physics of Complex Systems, Max Plank Institute — A key current goal for micro-swimmer research is to understand and control collective behaviour. This has the potential to allow access to a wide range of dynamic, responsive non-equilibrium configurations and enable new applications. Hydrodynamic interactions play a significant role in determining collective behavior: however, the nature of the flow fields around synthetic micro-swimmers has to date largely been incorporated into simulations and theory based on assumed propulsion mechanisms. It is important to check how realistic these flow field approximations are for realizable systems. Here we address this by analysing the motion of tracer particles near to catalytic Janus colloids, a well-studied micro-swimmer system, in order to experimentally determine flow fields. The resulting data can be used to select the most appropriate far field description for swimmer hydrodynamics when modelling this system, and reveals additional near field details. We also use analytical theory to relate the flow fields to the micro-swimmer propulsion mechanism and slip velocity profile. Finally we report the ability to vary micro-swimmer flow field by geometric control of the colloids catalytic activity.

*S Ebbens acknowledges his EPSRC fellowship EP/N033736/1

**10:36AM A48.00014: No net motion for oscillating near-spheres**

KEVIN LIPPERA, Ladhyx, Ecole polytechnique, OLIVIER DAUCHOT, Gulliver, ESPCI, SEBASTIEN MICHELIN, MICHAEL BENZAQUEN (Presenter), Ladhyx, Ecole polytechnique — We investigate the hydrodynamics of oscillating nearly-spherical particles -- defined by their radius $r = 1 + e f(\theta, \phi)$ -- at low, yet non-vanishing, Reynolds numbers. In contrast with the results of [1], we analytically demonstrate that no net motion can arise up to order one in $\text{Re}$ and order one in the asphericity parameter $e$, regardless of the shape function $f$.


*This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme under Grant Agreement 714027 (SM).

**Monday, March 4, 2019 8:00 AM - 11:00 AM**

**Session A49 DPOLY GSOFT DFD GSNP: Additive Manufacturing of Soft Materials: Novel Characterization and Processing Strategies**

BCEC 252A - Jon Seppala, National Institute of Standards and Technology -

Tag(s): Focus

**8:00AM A49.00001: In-situ X-ray and thermal imaging of 3D printed PLA**

MIRIAM RAFAILOVICH (Presenter), YUVAL SHMUELI, JIAOLONG JIANG, YUCHEN ZHOU, Department of Materials Science and Chemical Engineering, Stony Brook University, GUANGCUI YUAN, SUSHIL K SATIJA, Center for Neutron Research, NIST, SUNGSIK LEE, APS, Argonne National Laboratory, TAEJIN KIM, Department of Materials Science and Chemical Engineering, Stony Brook University, GAD MAROM, Casali Institute for Applied Chemistry, Hebrew University of Jerusalem, DILIP GERSAPPE, Department of Materials Science and Chemical Engineering, Stony Brook University — In-situ WAXS together with FLIR imaging was performed during 3D FDM printing of PLA filaments. The results highlighted the importance of the temperature profiles during printing on the structure/property relationships of the samples. Printing along short axis resulted in increased thermal retention, higher degrees of crystallinity and mechanical strength relative to samples printed along the long axis. Neutron reflectivity used to construct a model of the interdiffusion between filaments as a function of time and temperature. Lattice Boltzmann calculations were used to determine the temperature of the filament as a function of nozzle temperature and extrusion speed. The thermal conduction between filaments in the vertical and horizontal direction was measured at four different nozzle temperatures and the interdiffusion was determined by scanning electron microscopy. The data showed large difference during printing between adjacent filaments. Fusion, was shown to occur when the diffusion length exceeded $R_g$ of PLA, occurred first in horizontal direction when the nozzle temperature exceeded 215°C and in the vertical direction when it exceeded 245°C.

*Support from the NSF (Inspire#1344267) and The Morin Foundation Trust is gratefully acknowledged
XPCS in operando Monitoring of Dynamic Recovery in 3D Printed Thermoset Nanocomposites

Additive manufacturing has made big strides in metals and polymer-based material processing applications; however, the processing of structural composites is still a challenge that requires a number of technical engineering and material improvements. State of the art, off the shelf, feedstock materials do not offer sufficient thermal and mechanical properties to compete with resin systems that are currently used in conventional polymer matrix composites. The goal of this work is to capture multiscale and temporal morphology and dynamics within thermosetting composite inks to get a better understanding of parameters that govern the printing process and establish a processing-structure-performance relationship that enables scientists and engineers to design optimal materials and processes to obtain additively manufactured parts with properties that, at minimum, come close to those known for conventional polymer matrix composites. Herein we use X-ray Photon Correlation Spectroscopy to reveal both morphology and dynamics of a thermoset composite ink composed of a rheology modifier (layered-silicate Cloisite 30B) and epoxy resin (EPON 826) during the printing process in real time and at critical locations along the print processing path.

Processing, Morphology, and Crosslink Network in Model Liquid Crystalline Thermosets for Additive Manufacturing

The additive manufacturing (AM) of high-temperature thermosetting resins would enable rapid functional prototyping and on-demand production of high-performance aircraft parts; however, limitations of current feedstock materials have prevented AM of such parts to date. The use of liquid crystalline thermosetting polymers could overcome several critical challenges in fused deposition modeling, such as tuning the rheology during print and cure and improving final mechanical properties. The shear-alignment of liquid crystal domains by the nozzle could also allow for the controlled design of anisotropic properties. Here, a model liquid crystal thermoset system based on epoxide chemistry is studied with respect to AM processing. We examine the effect of shear on morphology before, during, and after crosslinking, both in a controlled, uniform shear environment and at the printing nozzle. We explore how viscosity and final morphology (and therefore final properties) can be controlled by exploiting liquid crystallinity.

Feedstock development and in-operando experiments for 3D printing of polymer matrix composites for demanding defense applications [Invited]

Additive manufacturing, especially extrusion-based 3D printing, plays a critical role in areas where traditional composite manufacturing is too labor intensive, costly or even impossible. The ability to produce previously un-manufacturable designs combined with attractive economic and lead time benefits has led to significant interest in industry and government to invest in polymer-based 3D printing. Complexity enabled capabilities, part reduction and rapid prototyping are key drivers for DoD applications. While the current state-of-the-art in engineering solutions is progressing at a fast pace, the physics-based understanding of the process is lacking and at best poorly implemented in commercial machines. This inevitably leads to the issue of poor reproducibility with vastly different results from the same equipment conducted in different laboratories, between two pieces of the same equipment within a single laboratory and even between builds in different build plate locations of the same equipment. The fast, non-equilibrium processing space necessitates implementation of novel in-situ metrology controls. In addition, demanding applications that require materials to survive higher temperatures and survive extreme conditions with optimal thermo-oxidative stability are not available in commodity polymer feedstock. This presentation summarizes our efforts in designing and creating new feedstock materials for polymer matrix composite manufacturing via fused deposition modeling (high temperature thermosets) or direct write processes (carbon fiber reinforced epoxy thermosets), including advanced concepts for real-time, in-operando characterization of materials during the additive manufacturing process. The ultimate goal is to provide real-time data for closed-loop feedback control that leads to a sufficiently robust process.
9:12AM A49.00005: In-situ X-ray and thermal characterization of nanocomposites in FDM 3D printing*  YUVAL SHMUELI (Presenter), Department of Materials Science and Chemical Engineering, Stony Brook University, SUNGSIK LEE, APS, Argonne National Laboratory, TAEJIN KIM, Department of Materials Science and Chemical Engineering, Stony Brook University, GAD MAROM, Casali Institute for Applied Chemistry, Hebrew University of Jerusalem, DILIP GERSAPPE, MIRIAM RAFAILOVICH, Department of Materials Science and Chemical Engineering, Stony Brook University — In-situ synchrotron WAXS simultaneously with high resolution infra-red imaging were used to study the correlation between the extrusion parameters, the filaments deposition directionality and the internal structure of the nanocomposite in 3D printing by placing an “open-walled” FDM printer in the beamline. We used microbeam synchrotron SAXS to study the variance in the crystalline macrostructure formed as function of radial position in the filaments (from core to adjacent interfaces). We observed the effect of extrusion shear forces on the orientation of the nanoparticles and the influence of the particle/polymer interactions on the polymer crystallization. We show how thermal properties improved by directionality and transcrysallization. We used Raman, electron microscopy and rheological techniques to study the interactions between the polymer matrix and the nanoparticles.

*Support from the NSF (Inspire#1344267) and The Morin Foundation Trust is gratefully acknowledged.

9:24AM A49.00006: Molecular weight dependence of weld formation in material extrusion additive manufacturing JON SEPPALA (Presenter), National Institute of Standards and Technology — Material extrusion (MatEx) additive manufacturing (AM), after several decades of development, is now an established production method for small volume or highly complicated parts. While MatEx has transitioned from prototyping to end use production, little is known about the mechanisms that dominate strength development between layers. Previously we reported on a framework for determining weld time and weld strength of MatEx processed welds, comparing those results to traditional polymer-polymer weld formation. Here we extend that work by systematically varying the weight average molecular weight ($M_w$) of entangled bisphenol-A-poly carbonate (PC) MatEx filaments and measuring weld time and weld strength. The resulting weld formation will be discussed in the context of traditional polymer-polymer welding and weld thickness during the unique shear and thermal history produced by the MatEx process.

9:36AM A49.00007: Geometrical and Mechanical Characterization of Interlayer Bonding Quality in Fused Filament Fabrication* LI CHEN FANG (Presenter), YISHU YAN, OJASWI AGARWAL, KEVIN HEMKER, SUNG KANG, Johns Hopkins University — Fused filament fabrication (FFF) is one of the most popular additive manufacturing processes. However, advanced applications of FFF are still limited by the large variation of mechanical property and mesoscale structural geometry of printed parts. To develop a fundamental understanding of those issues, we focus on the interlayer bonding region of Polycarbonate FFF samples, and perform full 3D geometrical characterizations using X-ray micro computed tomography (Micro-CT). The result reveals large geometry variance brought by different printing conditions, including parameters like nozzle movement speed and layer thickness, and environmental factors like chamber temperature and humidity. The findings are further validated by mechanical peel/tear tests, showing the direct relationship between bonding zone geometry and bonding strength. The outcomes could guide printing parameter selections, as well as provide validations for future theoretical and simulation models.

*We would like to acknowledge the support of the National Science Foundation (DMREF-1628974), and the start-up fund from the Whiting School of Engineering at Johns Hopkins University.

9:48AM A49.00008: Effect of processing on semicrystalline morphology in the additive manufacturing of poly(lactic acid) ANTHONY KOTULA (Presenter), JONATHAN SEPPALA, National Institute of Standards and Technology, CLAIRE MCILROY, School of Mathematical Sciences, University of Nottingham — Material extrusion additive manufacturing processes force molten polymer through a printer nozzle at high (>100 s$^{-1}$) wall shear rates prior to cooling and crystallization. These high shear rates can lead to flow-induced crystallization in common polymer processing techniques, but the magnitude and importance of this effect is unknown for additive manufacturing. Of critical importance in semicrystalline polymer additive manufacturing is the semicrystalline morphology near the weld between extruded layers, which can affect mechanical properties. Here, we present a systematic study of printing conditions on the semicrystalline morphology of parts printed from poly(lactic acid) (PLA). The slow crystallization kinetics of PLA generate parts with low crystallinity, however a secondary annealing process at high temperatures (140 °C) generate a space-filled spherulitic texture, with smaller spherulites near the weld zone between the extruded layers. This spherulite size distribution is attributed to a higher nucleation density templated into the part by the temperature and deformation history of the printing process. We show that theoretical modeling of flow-induced crystallization processes can predict the spatial distribution of spherulites observed in experiment.
CLAIRE MCILROY (Presenter), University of Nottingham, ANTHONY KOTULA, JONATHAN SEPPALA, National Institute of Standards and Technology, RICHARD STEPHEN GRAHAM, University of Nottingham — The most common 3D printing method is known as fused filament fabrication (FFF). This process involves melting a thermoplastic, followed by layer-by-layer extrusion, cooling and re-solidification. The main concern with FFF is the strength at the welds between printed filaments; bulk strength is never achieved in these regions and the reason is currently unclear. Advancing FFF relies on a molecular understanding of how thermoplastics behave during the printing process. We employ a non-isothermal molecularly-aware model for FFF processing of a semi-crystalline polymer melt to show how typical FFF conditions can stretch the polymer molecules prior to cooling. Enhanced nucleation due to residual polymer stretch leads to accelerated crystallisation times at the surface of a deposited filament, whilst the bulk of the filament is governed by slower quiescent kinetics. Consequently we find a cross-sectional variation in the crystal morphology of single filament, with smaller spherulites forming in an outer skin layer. Furthermore, our model of a multi-filament walls reveals significant variations in crystal morphology from filament to filament.

*CM is grateful to the Royal Commission for the Exhibition of 1851 for funding. RSG gratefully acknowledges funding from the EPSRC (EP/P005403/1).

MEISHA SHOFNER (Presenter), EMILY FITZHARRIS, DAVID ROSEN, Georgia Institute of Technology — Among the additive manufacturing (AM) techniques available, material extrusion additive manufacturing (MEAM) has been widely researched due to its increased availability and relatively simple manufacturing method. This AM method has generally been limited to amorphous polymeric materials as feedstocks, but more recent research has investigated high performance semicrystalline polymers as potential feedstocks with varying levels of success. In this work, we have used two techniques to evaluate how the crystallization of a promising feedstock, polyphenylene sulfide (PPS), affects its use with MEAM. We have used fast scanning calorimetry (FSC) to more fully understand how the crystallization of PPS is affected by cooling rates relevant to MEAM. Additionally, we have used the Taguchi method to analyze the mechanical properties of printed parts when exposed to post-processing heat treatment steps. Overall, the results showed that PPS can be used effectively with MEAM and that its crystallization kinetics provide unique benefits to its processing with MEAM.

*The research described in this presentation was funded by the Kimberly-Clark Corporation.

NEIKO LEVENHAGEN (Presenter), MARK DADMUN, University of Tennessee — Minimizing anisotropy in parts prepared by fused deposition modeling (FDM) remains a key area of research in the development of robust and mechanically useful 3D printed objects. Due to the bulky nature of polymer chains and the complex thermal environment experienced by adjacent filaments, interaction of polymer chains in between layers is minimized. Weak interfaces and poor layer adhesion results. In recent years, our group has addressed these issues through the introduction of low molecular weight surface segregating additives (LMW-SuSAs). LMW-SuSAs are smaller than the polymer chains of the neat material and can more readily diffuse and entangle in adjacent layers. In the current research, we report, bimodal blends containing linear and 3-arm PLA LMW-SuSAs terminated with methacrylate groups and crosslinked by UV irradiation. In situ irradiation of the printed layers results in drastic increases in the transverse tensile stresses of the printed layers up to ~140% and ~200% for the linear and 3-arm LMW-SuSAs respectively. Additional experiments examine the effect of UV power on the process. By controlling the UV power, printed parts can be prepared with minimal interfilamentous voids and substantially robust interfaces.

*Honeywell Federal Manufacturing and Technologies LLC
10:36AM A49.00012: Axisymmetric Simulation of Viscoelastic Filament Thinning and Laser-Induced Forward Transfer with the Oldroyd-B Model* EMRE TURKOZ (Presenter), LUC DEIKE, CRAIG ARNOLD, Princeton University — A fundamental understanding of the filament thinning of viscoelastic fluids is important in practical applications such as spraying and printing of complex materials. Here, we present direct numerical simulations of the two-phase axisymmetric momentum equations using the volume-of-fluid technique for interface tracking and the log-conformation transformation to solve the viscoelastic constitutive equation. The numerical results for the filament thinning are in excellent agreement with the theoretical description developed with a slender body approximation. We show that the off-diagonal stress component of the polymeric stress tensor is important and should not be neglected when investigating the later stages of filament thinning. In addition, we use this numerical model to simulate the blister-actuated laser-induced forward transfer process, which is a nozzle-less laser-based printing technique. We reveal the effect of viscoelasticity on the ejected droplet size, derive criteria for optimum printing conditions, and compare the numerical results with experiments.

*This work is supported by National Science Foundation (NSF) through a Materials Research Science and Engineering Center program (DMR-1420541).

10:48AM A49.00013: Laser sintering of polymer particle pairs studied by in-situ visualization* PRAKHAT HEJMADY, RUTH CARDINAELS (Presenter), LAMBERT VAN BREEMEN, PATRICK D ANDERSON, Eindhoven University of Technology — A novel in-house developed experimental setup is used to perform laser sintering experiments on polystyrene (PS) particle doublets while performing in-situ visualization of the sintering dynamics. From the recorded images, the evolution of the growth of the neck radius formed between both particles is analyzed as a function of time. Sintering conditions such as heating chamber temperature, laser pulse energy and duration, laser spot size and particle size are precisely controlled and systematically varied. A non-isothermal viscous sintering model is developed that allows to qualitatively predict the observed effects of the various parameters. The sintering kinetics is determined by a complex interplay between the transient rheology caused by the finite relaxation times of the polymer and the time-dependent temperature profile which also affects the polymer viscosity. The combination of a full material characterization with sintering experiments under well-defined conditions has resulted in a general understanding of the effects of material and process parameters on laser sintering.

*Brightlands Materials Research Centre (BMC) is acknowledged for funding.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A50 DPOLY GSOFT DBIO: Chirality in Polymers and Soft Matter I: From Molecular to Hierarchical Scales BCEC 252B - Nicholas Kotov, University of Michigan - Tag(s): Focus

8:00AM A50.00001: Confinement-induced liquid crystalline transitions in amyloid fibril tactoids GUSTAV NYSTROM (Presenter), EMPA, MARIO ARCARI, RAFFAEOLE MEZZENGA, ETH Zurich — Chirality is ubiquitous in nature and plays crucial roles in biology, medicine, physics and materials science. Understanding and controlling chirality is therefore an important research challenge with broad implications. Unlike other chiral colloids, such as nanocellulose or filamentous viruses, amyloid fibrils form nematic phases but appear to miss their twisted form, the cholesteric or chiral nematic phases, despite a well-defined chirality at the single fibril level. In this contribution, I will report about our discovery of cholesteric phases in amyloids, using β-lactoglobulin fibrils shortened by shear stresses. The physical behavior of these new cholesteric materials exhibits a large structural complexity, with confinement-driven ordering transitions between at least three types of nematic and cholesteric tactoids. We use energy functional theory to rationalize these results and observe a chirality inversion from the left-handed amyloids to right-handed cholesteric droplets. These findings contribute to our understanding of cholesteric phases as well as their use in soft nanotechnology, nanomaterial templating and self-assembly.
experimental and simulation results point to the possibility of self-limitation by the spontaneous twisting of the assumption of bundles due to the build-up of the costs of geometric frustration with lateral diameter. Common to all these models is organogel fibers. Several theoretical models have shown that assembly twist can lead to a thermodynamic self-limitation. Chains are common architectures in a range of supramolecular materials, from protein filaments to self-stacking, (achiral filaments) should be expected only up to diameter of a few filaments wide. Of chiral bundles may reach mesoscopic (multi-filament) dimensions, while self-limitation of spontaneously twisting fibers evolution of pitch with lateral size as well as possible ranges of self-limitation. This analysis argues that self-limited fibers filament bundles of various states of order (e.g. columnar, solid, polymer nematic). I will contrast predictions for the evolution of pitch with lateral size as well as possible ranges of self-limitation. This analysis argues that self-limited fibers of chiral bundles may reach mesoscopic (multi-filament) dimensions, while self-limitation of spontaneously twisting fibers (achiral filaments) should be expected only up to diameter of a few filaments wide.

This work was funded by the NSF.

Twisted by fate, or screwing up purpose: self-limiting fibers from achiral vs. chiral filament assembly* GREGORY GRASON (Presenter), University of Massachusetts Amherst — Twisted bundles of cohesive filaments or chains are common architectures in a range of supramolecular materials, from protein filaments to self-stacking, organogel fibers. Several theoretical models have shown that assembly twist can lead to a thermodynamic self-limitation of bundles due to the costs of geometric frustration with lateral diameter. Common to all these models is the assumption of intrinsic chirality of the constituent filaments as the driving force for collective twist. However, recent experimental and simulation results point to the possibility of self-limitation by the spontaneous twisting of achiral fibers. In this talk, I describe a generic continuum elastic framework for comparing formation of twisted fibers of chiral vs. achiral filament bundles of various states of order (e.g. columnar, solid, polymer nematic). I will contrast predictions for the evolution of pitch with lateral size as well as possible ranges of self-limitation. This analysis argues that self-limited fibers of chiral bundles may reach mesoscopic (multi-filament) dimensions, while self-limitation of spontaneously twisting fibers (achiral filaments) should be expected only up to diameter of a few filaments wide.

*Supported by NSF DMR 1608862.

From Molecules to Helical Ribbons - Emergence of Elasticity* MINMING ZHANG, DORON GROSSMAN (Presenter), The Racah institute of Physics, The Hebrew University of Jerusalem, Jerusalem, Israel, DGANIT DANINO,Faculty of Biotechnology and Food Engineering, Technion - Israel Institute of Technology, Haifa, Israel, ERAN SHARON, The Racah institute of Physics, The Hebrew University of Jerusalem, Jerusalem, Israel — Self assembly of molecules into supramolecular structures is an important process through which no trivial structures are formed in nano-metric scale. The resulting structure depends on chemical and physical principles that govern the process, and may be sensitive to the exact condition in which they are formed. Typically, such self assembled structures are residually stressed, due to mismatch of the constituent element. Identifying the principles and way in which different structures are formed significantly affect the ability to control, guide and manipulate self assembly. In this research we relate chemical and physical properties of single (or few) molecules to the shape and mechanics of the resulting, residually stressed, elastic helical structure which is a common motif. We then continue to show the unique thermodynamics of the ribbons stemming from these residual stressed. Our predictions are quantitatively confirmed experimentally, suggesting a new framework for quantitative study of a large variety of self-assembled nanostructures.

This research was supported by the USA-Israel binational science foundation, grant # 2014310 (ES) and the Israel Science Foundation grant No. 1117/16 (DD). MZ was supported by the Hebrew University Post-doctoral scholarship (PBC).
9:00AM A50.00006: Mechanical basis for the morphology of fibrillar aggregates*  THOMAS MICHAELS (Presenter), L MAHADEVAN, Harvard University — The self-assembly of fibrillar aggregates is of importance in biology, biomedicine and materials science, yet understanding the range of possible shapes for these structures remains an open question. We propose a coarse-grained approach that averages over specific molecular details to suggest that the spatial complexity of self-assembling fibrillar structures is due to the competing effects of (the bending and twisting) elasticity of individual filaments and the adhesive interactions between them. We show that a theoretical framework accounting for this allows us to capture a number of diverse fibril morphologies observed in natural and synthetic systems, ranging from Filopodia to multi-walled carbon nanotubes, and leads to a phase diagram of possible fibril shapes. We also show how the extreme sensitivity of these morphologies can lead to spatially chaotic structures. Together, these results suggest a common mechanical basis for the micronscale fibril morphology as a function of the nanoscale mechanical properties.

*We acknowledge support from the Swiss National Science Foundation.

9:12AM A50.00007: Phase Behavior of Frustrated ABC2 Miktoarm Star Triblock Copolymer*  QI ZHANG (Presenter), WEI-HUA LI, Fudan University — The phase behavior of ABC triblock copolymer can be classified into “nonfrustrated” and “frustrated” cases according to the relative strength of the three Flory-Huggins interaction parameters. In the frustrated case, $\chi_{ACN}$ is much weaker than $\chi_{ABN}$ and $\chi_{BCN}$. Thus, the triblock copolymers prefer to form structures with $ABC$ interfaces. Under the competition of interfacial energy and the entropic energy, the phase behavior of ABC triblock copolymer is more complex, and it can form the phases of the Knitting pattern, double and triple helices on cylinders. However, stable single helical structure has not been reported yet. In order to get the stable single helical structure, we designed the molecule structure of ABC$_2$ miktoarm star triblock copolymer. Our design principle sheds light on the phase behavior of the frustrated case as well as the spontaneous curvature induced by the conformational asymmetry. Through the calculation of Self-Consistent Field Theory (SCFT), the triangular phase diagram shows the region of stable single helical structure as well as the knitting pattern phases.

* acknowledges the funding support by the National Natural Science Foundation of China (Grants Nos 21574026 and 21774025).

9:24AM A50.00008: Amplification of vibrational circular dichroism in chiral block copolymers driven by self-assembly  KAI-CHIEH YANG (Presenter), RONG-MING HO, National Tsing Hua University — Herein, various self-assembled phases including double gyroid (DG), double diamond (DD) and helical (H*) phases could be obtained from the self-assembly of chiral block copolymers with equivalent volume fraction of chiral segment, giving building blocks with equal contribution of the optical activities for self-assembly. Interestingly, with comparable chiral segment fraction as evidenced by electronic circular dichroism (ECD), significant enhancement of vibrational circular dichroism (VCD) signals could be found in the chiral H* phase while the VCD signals in the achiral phases of DD and DG remain after microphase separation for ordering, reflecting that the VCD enhancement is attributed to the formation of hierarchical helices with preferential handedness; the observed behaviors are represented as VCD enhancement by self-assembly. This finding provides a new concept to boost optical activities in the applications of chiroptic from self-assembly.

9:36AM A50.00009: Effects of Polymer Helical Chain Shape on Block Copolymer Self-Assembly*  BEIHANG YU (Presenter), SCOTT DANIELSEN, ANASTASIA PATTERSON, EMILY C DAVIDSON, GLENN FREDRICKSON, RACHEL SEGALMAN, University of California, Santa Barbara — While helical chain shapes in block copolymers have been shown to produce unique morphologies, the details of how chain shape influences the thermodynamics of self-assembly are unclear. Here, we utilize model coil–coil and coil–helix block copolymers based on polypeptoids, for which the chain shape can be tuned from helix to coil via monomer chirality with constant chemistry. This model block copolymer system is used to probe the effects of chain helicity on block copolymer self-assembly. With identical domain spacings in the lamellar morphology, the coil–helix block copolymer has a lower order–disorder transition temperature ($T_{ODT}$) than its coil–coil analogue. There is minimal difference in the enthalpic contribution to mixing. The most significant contribution in lowering the $T_{ODT}$ of the coil–helix block copolymer is the helical chain experiencing larger chain stretching penalties in the lamellar morphology, which leads to a larger entropic gain upon disordering. This yields insight into the importance of space filling and chain stretching of polymer chains in block copolymer self-assembly.

*NSF DMR-1608297
isotactic polypropylene*  

10:00AM A50.00011: Aligning stem orientation: confined chiral and epitaxial growth of the α-phase crystals of isotactic polypropylene*  

YAN CAO (Presenter), XINGMING ZENG, Institute for Advanced Study, Shenzhen University, HIROSHI JINNAI, Interdisciplinary Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, SHUAILIN ZHANG, Department of polymer science, The University of Akron —  

In the past, soft materials under soft or hard confinement have been extensively studied due to size effect at a small scale. Polymer nanorods confined to the anodic aluminum oxide (AAO) template have been examined in terms of crystal nucleation and orientation. So far, few molecular studies have been done on the polymer nanostructure under cylindrical confinement. In this research, we have fabricated isotactic polypropylene (i-PP) into a rod-shaped nanomaterial. We carried out 2D wide-angle x-ray diffraction (WAXD) and electron diffraction (ED) experiments of transmission electron microscopy (TEM) to analyze the chiral and epitaxial growth effect on hierarchical structure of i-PP nanorod. We found that stems of mother lamellae prefer to align with the rod long-axis (nanopore axis of AAO) and stems of daughter lamellar tilt 100 degree clockwise or counterclockwise with respect to the rod long-axis under 2D confinement.  

*This work was supported by the Foundation of Shenzhen Peacock Talent (827-000150), National Science Foundation of China (802-008992), Shenzhen Science and Technology Innovation Foundation (85135-000017) and Guangdong Natural Science Foundation (85118-000036).  

10:12AM A50.00012: Chirality Enabled Liquid Crystalline Physical Gels with High Modulus but Low Driving Voltage*  

HUAN RUAN, HAIYAN PENG, XIAOLIN XIE (Presenter), Huazhong University of Science and Technology —  

Liquid crystalline physical gels, which stabilize the fluidic liquid crystals by non-covalent three-dimensional fibrous network, are not only able to maintain the unique electro-optical response capability but also capable of affording the self-supporting function. In the past, soft materials under soft or hard confinement have been extensively studied due to size effect at a small scale. Herein, we report liquid crystalline physical gels with high modulus but low driving voltage. This behavior is enabled by chirality transfer from molecular level to three-dimensional fibrous networks during the self-assembly of 1,4-benzenedicarboxamide phenylalanine derivatives. Interestingly, the critical gel concentration is as low as 0.1 wt%. Our findings open doors to understanding and exploiting the role of chirality in organic gels.  

*NSFC (51433002, 51503045 and 51773073)  

10:24AM A50.00013: Universal Effects of Chirality on the Self-Assembly of Chiral Block Copolymers and Polymers* [invited]  

RONG-MING HO (Presenter), Chemical Engineering, National Tsing Hua University, Taiwan —  

Here, we aim to investigate the universal effects of chirality on the self-assembly of chiral block copolymers (BCPs*) and polymers. Poly(cyclohexylglycolide) (PCG)-containing BCPs* have been synthesized for self-assembly to give systematic comparisons with polylactide (PLA)-containing BCPs*. Opposite handedness of PCG helical chains in enantiomeric BCPs* were identified by the vibrational circular dichroism (VCD) results of carbonyl group (C=O) stretching due to intramolecular chiral interactions. By taking advantage of intermolecular chiral interactions as evidenced by the VCD results of C-O-C vibration, the self-assembly of the PCG-containing BCP* gave helical phase (H*) with preferential handedness as recognized by electron microscopy tomography, suggesting the chirality effect on BCP self-assembly and the homochiral evolution from molecular to hierarchical scales; the results are in line with theoretical prediction based on chiral orientational self-consistent field theory. For chiral polylactides, twisted lamellae in crystalline banded spherulite with preferred handedness could be formed, reflecting the homochiral evolution in crystallized chiral polylactides.  

*The authors thank the Ministry of Science and Technology, Taiwan, for financially supporting this research.
Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A51 DPOLY: Big Data, Polymers, and Soft Matter: New Developments in Machine Learning, Data Mining and High-Throughput Studies

BCEC 253A - Debra Audus, National Institute of Standards and Technology - Tag(s): Invited

8:00AM A51.00001: Machined-learned softness as a structural order parameter for understanding glassy systems*

[Invited] ANDREA LIU (Presenter), University of Pennsylvania — All solids flow at high enough applied stress and melt at high enough temperature. Crystalline solids flow and premelt via localized particle rearrangements that occur preferentially at structural defects known as dislocations. The population of dislocations therefore controls both how crystalline solids flow and how they melt. In disordered solids, there is considerable evidence that localized particle rearrangements induced by stress or temperature occur at localized flow defects but all attempts to identify them directly from the structure have failed. Here we describe an application of machine learning data mining methods to diagnose flow defects, or “soft” particles from their local structural environments. We follow the softness of each particle as it evolves under deformation or temperature. Our results show that machine learning methods can be used to gain a conceptual understanding of glassy dynamics and of plasticity that has not been achieved with conventional approaches.

*This work was supported by the UPenn MRSEC via National Science Foundation (NSF) Grant NSF-DMR-1720530, by US DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering Award DE-FG02-05ER46199 and the Simons Foundation Grant 327939.

8:36AM A51.00002: Accelerated Discovery in Polymer Materials Domain: Knowledge Extraction and Representation

[Invited] DMITRY ZUBAREV (Presenter), IBM Almaden Research Center — Acceleration of scientific discovery requires resolution of multiple bottlenecks along the flow connecting the perception of the available data, data analysis and hypothesis generation, and data acquisition via experiments. The challenges of a) ingestion of fast-growing volume of unstructured scientific data, and b) efficient generation of actionable hypotheses come from the limitations of human cognition. We investigate various approaches to the augmentation of the respective capabilities of human subject matter experts in the domain of polymer materials. Transition from curated datasets/databases to scientific knowledge graphs (sKGs) plays central role in this effort. In this talk, I discuss the technical aspects of the construction of sKGs from unstructured data in polymer materials domain, and utilization of sKGs for hypothesis generation, including human-in-the-loop approaches.

9:12AM A51.00003: Exploring Free Energy Landscapes with Neural Networks*

[Invited] JONATHAN WHITMER (Presenter), University of Notre Dame — The use of adaptive sampling algorithms is an indispensable part of modern molecular simulations. A wide array of techniques have been developed to accelerate the sampling of phase behavior and molecular conformations, with those exhibiting the proper mix of simplicity and power gaining wide acceptance within the simulation community. Here, we discuss recent efforts to incorporate machine-learning techniques, in particular, artificial neural networks, to drive sampling and efficiently obtain free energy landscapes from incomplete representations of the mean force and partition functions. We will discuss conceptual and numerical aspects of these approaches, presenting new improvements alongside applications of the algorithms to soft and biological materials.

*This work was supported by the Midwest Integrated Center for Computational Materials (MICCoM), as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy.
Text and Data Mining for Material Synthesis

ELSA OLIVETTI (Presenter), EDWARD KIM, Massachusetts Institute of Technology — Data has become a fundamental ingredient for accelerating and optimizing materials design and synthesis. Molecular synthesis planning, driven by advances in machine learning, has recently achieved human-level performance for the retrosynthetic design of organic molecules. The acceleration of data-driven synthesis planning and related analyses has, in part, been enabled by access to massive datasets which tabulate known chemical reactions. While macromolecule, polymer and inorganic materials databases also exist, the focus of these databases is primarily on materials structures and properties, rather than reactions and synthesis. Indeed, there is currently no comprehensive dataset which organizes the methods by which these materials are synthesized or even extensive property information. Comprehensively extracting the knowledge contained within written inorganic materials syntheses, without the use of significant human effort, is a key step towards reducing the overall discovery and development time for novel materials. This presentation will describe work to extract information from peer reviewed academic literature across a range of inorganic solid state materials synthesis approaches. We have demonstrated not only the potential of the natural language processing (NLP) approach to assemble materials data from the literature, but we have also shown that one can develop hypotheses for what synthesis conditions drive a particular target material outcome using learning approaches.

Data-driven learning of collective variables to understand and accelerate biomolecular folding

ANDREW L FERGUSON (Presenter), Institute for Molecular Engineering, University of Chicago — Data-driven modeling and machine learning have opened new paradigms and opportunities in the understanding and design of soft and biological materials. Nonlinear dimensionality reduction and deep learning present a powerful means to identify the underlying dynamical modes governing the assembly and folding of soft materials such as colloids, peptides, and polymers by direct analysis of molecular simulation data. Recovery of these modes, together with nonlinear collective variables with which to parameterize them, provides fundamental understanding of the microscopic forces and emergent dynamical motions governing the long-time evolution of the molecular system. We will discuss our use of diffusion maps, deep neural networks with novel topologies and loss functions, and enhanced sampling techniques to recover the high variance and/or slow collective variables from molecular dynamics simulations of protein folding, and our subsequent use of these coordinates to understand folding mechanisms and guide and accelerate sampling.

Session A52 DPOLY: Advanced Morphological Characterization of Polymers I: Imaging

8:00AM A52.00001: Topological Defects in Tubular Network Block Copolymers

EDWIN THOMAS (Presenter), HUA GUO, XUEYAN FENG, Rice University — Materials based on the double gyroid multicontinuous tubular structure can exhibit an array of exotic properties due to the unique 3D network structure. The nature, frequency and potential influence of topological defects present in the interpenetrating gyroid networks on various physical properties is an open question. We examined a polystyrene – polydimethylsiloxane copolymer possessing the double gyroid microdomain morphology in order to identify the types of topological defects present in high fidelity 3D reconstructions made by slice and view scanning electron microscopy tomography. Large volume tomograms were made by repeated sequentially ion beam milling of a thin section and then using a normal incidence electron beam to image the sample surface. We found node functionality “f defects” where the normal node functionality of 3 rose to 4 and to 5, broken network struts, bridging struts linking the two different networks as well as donut loops comprised of 5 or 6 node rings instead of the characteristic 10 node ring of the (10,3)-a gyroid network. We term the 5 node donut loops as 5-4,3 and 5-4,4,3 defects while the 6 node donut loop is termed a 6-4,3,4 defect to indicate, following Wells, the number of struts in the loop as well as the node functionality and sequence.
**Funding for this work was provided by the Soft Matter Electron Microscopy Program (KC11BN), supported by the Office of Science, Office of Basic Energy Science, US Department of Energy, under Contract DE-AC02-05CH11231.**

*Supported by DOE BES under award DE-SC0014549*

**NSF DMR-1609417, DOE SCGSR, and ALS.**
Three-dimensional morphological analysis of polymer blends through combined ToF-SIMS/AFM

HAO MEI, Chemical and Biomolecular Engineering, Rice University, ADELINE MAH, TRAVIS LAWS, Chemical and Biomolecular Engineering, University of Tennessee, WEI LI, Materials Science and Engineering, Northwestern University, TANGUY TERLIER, Shared Equipment Authority, Rice University, RAJEEV KUMAR, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, GILA E STEIN, Chemical and Biomolecular Engineering, University of Tennessee, RAFAEL VERDUZCO (Presenter), Chemical and Biomolecular Engineering, Rice University — Time-of-flight secondary ion mass spectroscopy (ToF-SIMS) enables three-dimensional compositional analysis using a focused ion beam along with an argon cluster beam for depth profiling. Combined with atomic force microscopy (AFM), topographical and compositional information can be acquired simultaneously. We apply ToF-SIMS to study the phase behavior of blends of bottlebrush polymers with linear polymers and generate a phase diagram for interfacial segregation. We quantify the composition of bottlebrush throughout the film by calibration of ion intensity ratios, and self-consistent field theory calculations elucidate the enthalpic and entropic contributions to segregation. We further analyze the three-dimensional morphology of phase-separation in thin film polymer blends using combined ToF-SIMS/AFM. ToF-SIMS/AFM is a powerful technique that enables analysis of unlabeled polymer blends, composites, and self-assembling systems.

The authors thank the National Science Foundation for financial support under CMMI-174045 and CMMI-1563008 and CBET-1626418 for the TOF-SIMS/AFM at Rice. Portions of the work were conducted at the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, which is a US Department of Energy Office of Science User Facility.

STM Characterization of Metallic Graphene Nanoribbons

DANIEL J RIZZO (Presenter), Physics, University of California - Berkeley, GREGORY VEBER, Chemistry, University of California - Berkeley, JINGWEI JIANG, CHRISTOPHER BRONNER, TING CHEN, STEVEN G. LOUIE, Physics, University of California - Berkeley, FELIX R FISCHER, Chemistry, University of California - Berkeley — Graphene nanoribbons (GNRs) are narrow strips of graphene that can host a wide range of 1-dimensional phenomena, including non-trivial topology and magnetism. The advent of molecule-based bottom-up synthesis techniques has enabled GNR properties to be tuned via the precise placement of individual carbon atoms. Realization of robust metallicity in bottom-up GNRs, however, remains elusive. The ability to engineer the frontier band structure of GNRs via hybridization of topologically-protected interface states suggests a strategy for inducing GNR metallicity by symmetrizing the hopping between adjacent interface states. Using this approach we have realized metallic GNR superlattices that are gapless by virtue of the symmetric placement of π-radical states along the GNR backbone. Scanning tunneling microscopy and spectroscopy (STM/STS) performed in conjunction with first-principles calculations confirms that these GNR superlattices possess a non-zero density of states (DOS) through EF, a hallmark of metallicity. Strategies for increasing the bandwidth of metallic GNRs will be discussed.

nano-FTIR nanoscopy based identification of polymers at the 10nm length scale

ANDREAS HUBER (Presenter), STEFAN MASTEL, TOBIAS GOKUS, ALEXANDER GOVYADINOV, neaspec GmbH — Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) employs the strong confinement of light at the apex of a sharp metallic AFM tip to create a nanoscale optical hot-spot. Analyzing the scattered light from the tip enables the extraction of the optical properties below the tip and yields nanoscale resolved images simultaneous to topography [1]. Recently, the technology has been advanced to enable FTIR-spectroscopy on the nanoscale (nano-FTIR) [2].

Applying nano-FITR near-field spectroscopy to measure the spectroscopic signature enables identification of i.e. polymers at a spatial resolution given only by the size of the AFM tip [3]. For example, nano-FTIR spectra of a phase-separated PS/LDPE polymer blend of only 50nm thickness enable to identify the samples polymer materials.

Results presented demonstrate that nano-FTIR can be an ideal analysis method to characterize complex material systems and to identify polymer materials at the nanoscale spatial resolution and unmatched sensitivity.

9:24AM A52.00008: Morphological Characterization of Well-Ordered Nanonetwork Materials via Real- and Reciprocal-Space Imaging  
POTING CHIU (Presenter), YUCHENG CHIEN, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University — The morphological evolution of network phases from templated electroless plating using block copolymer as a template was investigated as an exemplary system for the characterization of developing complex gyroid and diamond phases from self-assembly. By taking advantage of the nucleation and growth mechanism of templated electroless plating, network-structured Au could be successfully fabricated through the development of Au nanoparticle, tripod/tetrapod and branched tripods/tetrapods, finally network structure. Hence, the morphological evolution of each stage could be examined by combining real-space observation of transmission electron microscopy with reciprocal-space investigation using small-angle X-ray scattering. A simple approach for the fitting of the scattering results was established at which the fingerprint scattering profiles of the building block for network phases were fitted with the form factor of sphere (i.e., the nanoparticle) and the diffraction results of final morphology (i.e., the network phases) could be well addressed by combined scattering of the form and structure factors, revealing the difference between the curvatures of gyroid and diamond phases from self-assembly.

9:36AM A52.00009: Recent developments of morphological characterization in nano-composite materials by electron microscopy [Invited] 
HIROSHI JINNAI (Presenter), Tohoku University — In order to truly understand various interesting properties of soft materials, it is crucial to directly visualize their morphologies both in quiescent state and under deformation. The interfacial region between fillers and polymer matrix, the interphase region for short, is believed to be one of the key morphological elements in nanocomposite materials. Direct visualization of such interphase region has been a subject for many years. Although transmission electron microscopy (TEM) is a powerful tool to visualize nano-scale polymeric morphologies, however, because the interphase region consists of the same polymeric species as the matrix, it is invisible under TEM. Atomic force microscopy (AFM), on the other hand, clearly demonstrates regions with higher elastic modulus (than the matrix) around the fillers, indicating the existence of the interphase region. However, because the mechanical properties can be easily affected by the structures underneath the measurement points, the high elastic regions around the fillers may not truly reflect the interphase region. Thus, we used transmission electron tomography, a nano-scale three-dimensional (3D) visualization method, to investigate the internal 3D structure of rubber nano-composite at exactly the same places as the AFM force measurements. In doing so, it became possible to accurately determine the interphase regions for the first time.

Morphological characterization under deformation is another crucial factor for fundamental understanding of mechanical properties of nano-composites. We have developed a tomography holder for in-situ tensile deformation. Because both ends of specimen are stretched simultaneously at the same stretching rate in this new holder, drifting of field of view for TEM observations becomes minimum. The newly-developed holder was used to observe deformation processes of a rubber nano-composite. Details of the structural deformation will be discussed at the conference time.

10:12AM A52.00010: Construction of 3D Models From USAXS on Aggregate Structures*  
ALEX MCGLASSON (Presenter), ANDREW J MULDERIG, GREG BEAUCAGE, KABIR RISHI, Chemical and Materials Engineering, University of Cincinnati, VIKRAM K KUPPA, University of Dayton Research Institute — An accurate 3D model of aggregate structures is desirable for comparison with TEM micrographs and as an input to computer simulations of aggregate transport and growth. For example, we have used such 3D models for polymer nanocomposites with carbon black and silica. Ultra-small angle X-ray scattering was coupled to a hierarchical scattering model, the unified scattering function, to obtain topological parameters that describe 9 average features of aggregates including details of the branched structure. A simple diffusion limited aggregation model was simulated and used to generate aggregates using two free parameters, the degree of aggregation, z, and the sticking probability, p [1]. USAXS measurements resulted in z for input to the simulation and the single parameter p was varied from 0 to 1 until a value that could reproduce the 8 remaining USAXS aggregate descriptors was found. The simulated average aggregates agreed well with TEM micrographs of the same samples. This approach can be used to depict complex morphological differences in ceramic oxide and carbon black aggregates and has the potential to be applied to a wide range of other aggregated materials.


*NSF grants CMMI-1635865 and CMMI-1636036.
10:24AM A52.00011: Self-Assembled Morphologies of Poly(styrene-b-1,4-butadiene) Confined within Cone-Shaped Templates

YOUNGKEOL KIM (Presenter), Seoul National University, TAKESHI HIGUCHI, Tohoku University, SUNGYOUL HWANG, Seoul National University, ANCHANG SHI, McMaster University, BAOHUI LI, Nankai University, HIROSHI JINNAI, Tohoku University, KOOKHEON CHAR, Seoul National University — Block copolymers (BCPs) self-assembled under nanoscale confinement have distinctive nanostructures, which do not appear in bulk state. Especially, depending on different dimensionality of confinement spaces, shape and morphology of block copolymers and their optical properties are affected. In this study, we report phase-separated morphologies of polystyrene-block-1,4-polybutadiene (PS-b-PB) confined in conical templates with various size, shape and surface properties. Based on experimental observation using transmission electron microscopy (TEM) and theoretical calculation of simulated annealing method, we found that phase separation of PS-b-PB in the conical confinement system are competitively affected by three thermodynamic factors; (1), (2) the interfacial energy between two different block and surrounding environment (air and substrates) and (3) the entropic penalty associated with large curvature at the vertices of conical pores. In addition, 3D imaging of TEM tomography were also performed in an attempt to identify internal nanostructures of BCP thoroughly.

*Nuclear Radiation Research Program through the National Research Foundation of Korea (NRF) grant

10:36AM A52.00012: The distinctive microstructures in bitumen and their indication of bitumen’s phase stability

XIAOKONG YU (Presenter), NANCY BURNHAM, Worcester Polytechnic Institute, SERGIO GRANADOS-FOCIL, Chemistry, Clark University, MINGJIANG TAO, Worcester Polytechnic Institute — Bitumen, similar to some amorphous polymeric systems, display diverse microstructures that are related to bitumen's bulk physical and rheological properties; yet the chemical-microstructural-mechanical relationships for bitumen have been very challenging to establish due to bitumen's complicated molecular interactions. To tackle this challenge, we chose two pristine bitumen (i.e., ABD and AAD), separated them into their asphaltene and malthene fractions, and prepared derivative bitumen by remixing their corresponding asphaltenes and maldenes at different ratios. We studied the microstructures of the two pristine bitumen and their derivatives using atomic force microscopy (AFM), and their phase stability using differential scanning calorimetry and their rheology using dynamic shear rheometry. Our results suggest that AAD-based derivatives had phase separation; in contrast, ABD-based samples were phase stable. The difference in phase stability between the two groups of bitumen is largely relevant to the aggregation behavior of their respective asphaltene fraction that was measured via NMR.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A53 GSNP: Geophysical Applications of Granular Flows

8:00AM A53.00001: Geophysical applications of granular flows: probing earthquakes applying machine learning

[Invited] PAUL JOHNSON (Presenter), BERTRAND ROUET-LEDUC, Earth and Environmental Sciences, Los Alamos, CLAUDIA HULBERT, Laboratoire de Géologie, l'Ecole normale supérieure — The influence of granular flows is widespread in geophysics, from the physics of earthquakes, avalanche and landslide, to debris flow to the effects of strong ground motion due to earthquakes. In this presentation I focus on earthquakes and the influence of the granular core of the fault—the fault gouge. Earthquakes take place when two juxtaposed fault blocks are stressed sufficiently to overcome the frictional force holding them in place and they abruptly slip relative to each other. Earthquake faults exhibit a continuum of behaviors ranging from stick slip associated with strong shaking, to slow slip which is primarily aseismic, to very slow slip that is essentially aseismic and can take place over hours to months. The different slip behaviors appear to be controlled by the combined elasticity of the fault gouge the adjacent fault blocks. As faults slip, the fault core emits elastic waves. We analyze these waves applying machine learning continuous acoustic data streams in the laboratory and continuous seismic data streams in Earth. We use as labels characteristics of the measured fault slip behavior in the laboratory such as the fault friction, shear displacement and fault thickness. In Earth, we use surface displacement as determined by Global Positioning Systems (GPS). We find that the laboratory acoustic data and the Earth seismic data are a type of Rosetta Stone revealing fault characteristics at all times and fault displacements. This is a surprising observation because previously we believed most or much of the signal was noise. Here we describe an overview of recent work in this area and also describe recent efforts on parallel problems such as volcanoes and geysers.

*Institutional Support (LDRD) and Los Alamos and the DOE Office of Science, Geosciences Program
8:36AM A53.00002: Incipient Motion in Granular Beds Driven by Shear Flows* [Invited] NICHOLAS OUELLETTE
(Presenter), Stanford University — Granular packings on Earth's surface are regularly subjected to shear flows, as they are typically exposed either to moving water or air. These flows agitate the packings, and may erode them by removing grains given sufficient flow strength. Incipient motion of the packings (that is, the point in parameter space when a nonzero net downstream flux of grains appears) is typically thought to occur at a critical value of the Shields number, which balances the shear stress delivered to the grains with the weight of a grain. However, such a simple framework cannot directly account for additional but common physics, including granular packing effects, turbulent flow fluctuations, or the stress delivered to the bed by other mobile grains. I will discuss both simple numerical models and laboratory experiments aimed at elucidating the consequences of these effects on describing incipient motion, with particular application to the armoring phenomenon observed in gravel-bedded rivers.

*This work was supported by the Army Research Office under grants W911NF-14-1-0005 and W911NF-17-1-0164.

9:12AM A53.00003: Shear jamming in packings of frictional disks* [Invited] MARK SHATTUCK (Presenter), The City College of New York, FANSHENG XIONG, PHILIP WANG, Yale University, ABE CLARK, Naval Postgraduate School, NICHOLAS OUELLETTE, Stanford University, COREY SHANE O’HERN, Yale University —
The mechanical properties of geotechnical structures depend on the history that generated them. Examples include riverbed hardening and delta formation. Similar history or protocol dependence also occurs on the particle scale. For example, the seminal experiments by D. Bi, et al. in Nature 480 (2011) 355, showed that simple and pure shear can generate jammed packings of thin cylinders whose properties are different from those generated via isotropic compression. In our recent computational studies, we showed that for frictionless disks, shear- and isotropically jammed packings possess the same packing fraction. However, shear-jammed packings possess nonzero stress anisotropy, whereas isotropically jammed packings possess zero anisotropy in the large-system limit. Here, we describe discrete element modeling simulations to prepare jammed packings of frictional disks via isotropic compression and simple shear. We compare the contact number and packing fraction at jamming onset versus the friction coefficient for packings generated via isotropic compression and simple shear. We also address whether the ensemble of jammed packings generated via simple shear and that generated via isotropic compression are the same.

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9:48AM A53.00004: Yielding in granular materials: from riverbeds to renormalization group [Invited] ABE CLARK (Presenter), Naval Postgraduate School — Granular media, like many other amorphous materials, possess a yield stress. The nature of yielding in granular materials is relevant to many industrial and geophysical problems, such as the onset of sediment motion in riverbeds or near-shore environments. When the applied shear stress $\Sigma$ is below the yield stress $\Sigma_c$, grains move temporarily, but only until finding a mechanically stable (MS) configuration that is able to resist the applied shear stress. When $\Sigma > \Sigma_c$, the material is no longer able to find MS configurations. However, the geometrical reasons why MS states vanish at the yield stress is not well understood. In this talk, I will show evidence from molecular dynamics simulations, both in a riverbed-like geometry as well as simple shear, that yielding in granular materials is akin to a second-order critical point, where the behavior near the yield stress is dominated by a correlation length $\xi$ that diverges at the yield stress as $\xi \sim |\Sigma - \Sigma_c|^{-\nu}$. MS states exist above the yield stress for finite systems, but they vanish as the system size becomes large according to a critical scaling function. The packing fraction and coordination number for MS states are independent of the applied shear stress, implying that the critical behavior we observe is distinct from the jamming scenario. Additionally, the critical behavior persists for overcompressed systems, confirming that jamming and yielding are distinct. Instead, we observe that MS states at nonzero shear stress possess anisotropic force and contact networks, suggesting that the yield stress is set by the maximum anisotropy that can be realized in the large-system limit.
Naturalistic Granular Flows: Using Experiments to Apply Granular Physics to Geophysical Shear Systems* 

EMILY BRODSKY (Presenter), STEPHANIE E TAYLOR, University of California, Santa Cruz, SHALEV SIMAN-TOV, Geological Survey of Israel — Granular flows are ubiquitous in nature and deviate in potentially important ways from idealized systems. Shearing in fault zones, landslides and debris flows involve water-saturated, rough particles of varying composition and particle size accelerating through a range of velocities while abutting stationary grains. In addition, the types of observations that can be made in nature also differ from laboratory and experimental situations. Here we present a range of experiments that attempt to isolate these naturalistic features and elucidate their implications. Specifically we find that: (1) Natural, rough particles emit acoustic energy during shear, which can affect the flow behavior at intermediate velocities, (2) The acoustic energy observed in the lab depends on the particle diameter cubed, (3) Mineralogy affects the intermediate to high velocity flow behavior primarily through the combination of elastic, fracture and plastic material properties captured by the critical slip distance required for fracture nucleation, (4) high and low shear rate regions of the flow are coupled through acoustic waves, creating a non-trivial boundary condition at the base of a landslide or other natural shear system, (5) Fluid-saturation can result in dilation at high velocities regardless of the initial compaction state and therefore dilatary drainage is expected even in repeated activation of the same shear flows, and (6) preserved, fine-grained apparent shear bands in the geological record can be indicative of fine grains migrating at high velocities. These experimental observations suggest important directions for theoretical development in order to bring granular physics to bear on natural systems.

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Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A54 DPOLY GSOFT DBIO: Smart and Responsive Polymers and Soft Materials I: Micro-Length Scale Phenomena

Mechanochromic Polycarbonate: Seeing Plasticity with Color* 

STEVEN YANG (Presenter), YUVAL VIDAVSKY, MEREDITH SILBERSTEIN, Mechanical and Aerospace Engineering, Cornell University — We use force-driven chromism to detect plasticity in polycarbonate. We create this functionality by embedding spiropyran, a mechanochromic compound, in the polymer backbone. While there are many examples of force-driven functionality in elastomers, there are few for glassy polymers. In prior experiments, the activation of spiropyran in glassy polymers was limited to tests near Tg, or with an added plasticizer. With glassy polycarbonate, we demonstrate tensile activation at room temperature. Spiropyran activation begins after yield and increases with hardening during plastic flow. For monotonic tensile tests, the activation is inversely related to the strain rate, while the stress is comparable. These results suggest that for glassy polymers, the activation of mechno-responsive compounds is coupled with stress, plastic flow, and time. Understanding how these factors contribute to activation will enable using mechano-responsive polymers for quantitative sensing.

*A statistical mechanical model for the electrostriction of polymers* 

MATTHEW GRASINGER (Presenter), KAUSHIK DAYAL, Carnegie Mellon University — Dielectric elastomers (DEs) are soft materials that polarize in the presence of an electric field. Using statistical mechanics, the thermodynamics of a DE chain subject to electrical loading and kinematic constraints is investigated. The equations of the monomer orientation density and the approximate chain free energy are derived. Solutions are presented in the small chain stretch limit and near the fully stretched limit. A closed-form approximation for the free energy of a DE chain is developed using asymptotic matching and shown to agree well with the numerical solutions. Next, averaging over chain orientations, the chain-scale response is built up to an electromechanically coupled DE constitutive model. Some preliminary results from the constitutive model are presented, which includes a contribution, at the macromolecular scale, to the electrostriction of DEs. The contribution to electrostriction is shown to be dependent on the lengths and orientations of chains in the DE network.

*The authors acknowledge the Army Research Office, Office of Naval Research, and Air Force Office of Scientific Research for funding this work.
8:24AM A54.00003: Simulating Polymeric Microstructures With Encoded Pre-Determined Deformability  JAMES WATERS (Presenter), University of Pittsburgh, JOANNA AIZENBERG, Harvard University, ANNA CHRISTINA BALAZS, University of Pittsburgh — Biological systems are able to translate stimuli into meaningful actions, reshaping themselves in response to changes in their environments. Liquid crystalline elastomers (LCE’s) represent a synthetic means of achieving this type of behavior, undergoing large deformations when nematic-isotropic phase transitions occur within the material. We use a finite element simulation method to predict the thermal response of LCE microplates, in a particular instance of this phenomenon. The shape changes are dictated by the director orientation in the nematic state, programmed in by a magnetic field present during cross-linking. After calibrating our simulation parameters against experimental results, we are able to accurately predict the observed experimental response of LCE microplates with a range of initial nematic orientations.

8:36AM A54.00004: Rational Design of Strain-Adaptive Elastomers through Polymer Architectures*  HEYI LIANG (Presenter), Department of Polymer Science, University of Akron, MOHAMMAD VATANKHAH-VARNOSFADERANI, SERGEI SHEIKO, Department of Chemistry, University of North Carolina at Chapel Hill, ANDREY DOBRYNIN, Department of Polymer Science, University of Akron — Designing materials capable of mimicking the mechanical properties of soft biological tissues is important for tissue engineering, soft robotics, and wearable electronics. The biological tissues show a unique combination of the mechanical softness and strong strain-stiffening, which make it difficult to replicate in synthetic elastomers composed of linear polymers. Using a combination of theoretical calculations and molecular dynamics simulations, we have developed a universal materials design strategy which encodes the stress-strain curve of soft materials into the molecular architecture of graft polymer networks. Such networks can be made either by chemical crosslinking of graft polymer strands or by self-assembly of linear-bottlebrush-linear triblock copolymers. The mechanical response of such networks is controlled by the architectural parameters (i.e. network strand length, side chain length, grafting density, and composition of triblock copolymers). Our approach is verified by synthesizing PDMS networks of combs and bottlebrushes with mechanical properties of jellyfish, lung, and arterial tissue. This technique lays the foundation for computationally driven design of soft materials.

*NSF DMR 1436201, 1407645, 1624569

8:48AM A54.00005: Detecting Bond Breakage and Fracture in Tough Hydrogels Using Mechanoluminescence*  GABRIEL SANOJA (Presenter), ESPCI, RINT SIJBESMA, TU Eindhoven, COSTANTINO CRETON, ESPCI — Synthetic hydrogels are soft materials composed of 3-D polymer networks swollen with water. They are promising synthetic analogues of tissues but their excessive brittleness remains an important limitation. Though there have been advances in the design of tough hydrogels, it is not yet possible to quantitatively predict toughness from molecular design. A promising strategy towards this endeavor is based on the incorporation of mechanoluminescent probes in these materials. Upon force-induced bond breakage, emission of visible light allows for spatio-temporal mapping of molecular bond scission during failure. We have incorporated a mechanoluminescent probe based on bis(adamantyl)-1,2-dioxetane into a model double-network hydrogel composed of stiff PAMPS and soft PAAm. Due to the low quantum yield of the emitter ketone resulting from force-induced ring-opening, we explored a range of FRET agents to detect bond scission during deformation. This information serves not only to establish a relation between polymer network structure and fracture energy, but also to develop multi-scale physical models of fracture in soft materials.

*This project has received funding from the ERC under the European Union's Horizon 2020 Research and Innovation Program (Grant Agreement N° 695351 – Chemch)

9:00AM A54.00006: Light-Actuated Liquid Crystal Elastomer Waveguides*  ALEXA KUENSTLER (Presenter), RYAN HAYWARD, University of Massachusetts Amherst — The ease with which light can be spatially and temporally modulated makes it an attractive stimulus for the actuation of soft materials. However, many devices require direct line-of-sight access for deployment, severely compromising their utility in confined geometries where remote control is required. One way to circumvent these limitations is to employ actuators that act as waveguides to deliver light over distances that make flood illumination impractical. To this end, we present a method to fabricate liquid crystal elastomer fibers that can adopt defined 3D conformations in response to waveguided visible light due to localized photothermal deformation. By exploiting the photo-mediated reduction of gold salt, spatially-defined regions of nanoparticles are patterned in aligned fibers to define the location and direction of bending. Fibers are demonstrated to bend simultaneously in orthogonal directions on a characteristic time scale of seconds. Furthermore, these fibers are shown to waveguide light, thereby removing the need for line-of-sight access to achieve complex shape change.

*NSF EFRI-ODISSEI 1332271
Fracture of soft materials involves large deformations before eventual macroscopic failure occurs and the damage to the material is much less localized at the crack tip than in stiff and brittle materials such as inorganic glasses. Although fracture of simple elastic networks made of flexible polymers connected by covalent bonds, obeys relatively well the classical Lake and Thomas theory, fracture of complex soft materials is much harder to predict from knowledge of the molecular structure and architecture. Organic chemists have recently developed new molecules that can be incorporated in networks and give an optical signal (fluorescence, luminescence or change in absorption) in response to the application of a force. These optical signals can then be used to obtain quantitative information about bond scission and energy dissipation during a macroscopic fracture event. Previous work\(^1\) has shown that it is possible to toughen and stiffen soft materials by incorporating a minority percolating filler into a stretchable matrix. Using model interpenetrated networks we demonstrate here, by incorporating mechanophore molecules in the filler or in the matrix network, how such materials break in two stages, by first softening the stiff filler network, losing mechanical percolation, and then breaking the stretchable matrix. Such mechanisms active at the crack tip are responsible for the much higher toughness of these stiffened materials and should be widely generalizable to elastomers and hydrogels reinforced by particles forming a percolating network.


**This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement n° 695351), from the Chinese Scholarship Council through the fellowship of YC, and from Royal DSM through the fellowship of PM.**

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**Electric field induced bending of Ionic polymer electrolyte membrane**

CHATHURANGA PRAGEETH RAJAPAKSHA (Presenter), Department of Physics, Kent State University, Kent, OH 44240, USA, CHENRUN FENG, Liquid Crystal Institute, Kent State University, Kent, OH 44240, USA, CAMILO PIEDRAHITA, JINWEI CAO, THEIN KYU, Department of Polymer Engineering, University of Akron, OH 44325, USA, ANTAL ISTVAN JAKLI, Department of Physics, Kent State University, Kent, OH 44240, USA — Electroactive polymers (EAPs) are promising candidates for future soft robotics due to their light weight, low cost and ease of fabrication. Among different kinds of EAPs Ionic electroactive polymers (IEAPs) are more attractive, since they are low voltage driven. Here we report about electric field induced studies of solid-state ionic polymer electrolyte membranes (IPEMs). Three different kinds of electrodes (gold, carbon and PEDOT: PSS based) were tested to optimize performance. Highly ionic conductive IPEMs were prepared by using Poly (ethylene glycol) diacrylate (PEGDA), thiosiloxane and ionic liquid(1-Hexyl-3-methylimidazolium hexafluorophosphate) as described by Piedrahita et al \(^1\). Different ionic liquid concentrations were tested to achieve large bending displacements. In addition to the reversible short-term low voltage (<3V) responses, we also studied responses up to 20V ac and dc voltages in wide-range of time scales. Not only non-linearity and hysteresis, but also a so far not understood inversion of displacement was also observed at large voltages and large time scales. These studies will provide important information on electrode effects and applicability limits of IEAPs.


**Programmable Assembly of Responsive Capillary Multipoles**

JINHYE BAE (Presenter), University of California, San Diego, NAKUL P BENDE, ARTHUR A EVANS, JUNHEE NA, CHRISTIAN SANTANGELO, RYAN HAYWARD, Univ of Mass - Amherst — The ability to program inter-particle interactions with well-defined selectivity, directionality, strength, and range remains a central challenge in efforts to realize complex materials by self-assembly of simple building blocks. Capillary attraction or repulsion owing to the geometrical distortion of the three-phase contact line by non-spherical particles has emerged as a powerful means to program two-dimensional assembly. To date, however, the focus has been almost exclusively on assembling rigid particles having shapes of limited complexity, restricting both the types of assemblies and their reconfigurability. We take advantage of the stimuli-responsiveness and the low-energy bending deformation of hydrogel particles, to show stimulus-controlled modulation of shape-induced capillary assembly. We anticipate that such surface tension-driven modification of the capillary interaction will suggest a rich area for fundamental studies and opportunities to further tailor the inter-particle interactions.

\*This research was funded by the Army Research Office through grant W911NF-16-1-0119, with additional support from the National Science Foundation MRSEC at UMass (DMR-0820506).
10:12AM A54.00010: Structure Dependent Ice Inhibition in Physically Crosslinked Hydrogels by Crystallization of Hydrophobic Crosslinks*  

PABLO SEPULVEDA-MEDINA (Presenter), Polymer Engineering, University of Akron, CHAO WANG, Chemical & Biomolecular Engineering, University of Delaware, BRYAN VOGT, Polymer Engineering, University of Akron — 

Confined water at the nanoscale can enable significant supercooling that is not possible in bulk water, but common strategies to confine water lead to low water content. We have recently demonstrated near complete ice inhibition in physically crosslinked hydrogels that use the hydrophobic association of perfluorinated moieties to crosslink and confine the water. However, the confining structure and water content in these hydrogels are coupled, which leads to some questions about the underlying physics. Here we demonstrate a similar route to modulate the nanostructure of a physically crosslinked hydrogel based on 2-hydroxyethyl acrylate (HEA) and n-octadecyl acrylate (ODA) without changing the copolymer composition and water content by crystalline crosslinks. Crystallization in the dry state leads to sheets of crystalline ODA, while melting and re-crystallizing the ODA in a hydrated copolymer leads to spherical nanodomains. The temperature-dependent structure was probed by SAXS, WAXS and SANS. DSC revealed that crystallization in the state leads to significantly more unfrozen water inside the hydrogel (10 to 15 wt%). The hydrogel morphology appears to control the unfrozen water content in these hydrogels under cryogenic temperatures.

*Work funded by NSF grant CBET-1606685.

10:24AM A54.00011: Rheological Signature of a Thermally-Gelling Nanoemulsion*  

MEYSAM HASHEMNEJAD (Presenter), ABU ZAYED MD BADRUDDOZA, Chemical Engineering Department, Massachusetts Institute of Technology, BRADY ZARKET, L’Oréal Research and Innovation, Clark, Nj, PATRICK DOYLE, Chemical Engineering Department, Massachusetts Institute of Technology — We report the rheological behavior of a new thermoresponsive oil-in-water nanoemulsion system. The nanoemulsion undergo a transition to a gel at elevated temperature. The gelation mechanism is entirely different from previous reports and nanoemulsion droplets play a major role in thermoresponsive behavior. The formulation contains FDA approved amphiphilic triblock copolymer as gelling agents. Nanoemulsions were also prepared using a low-energy process. The thermogelling formulation exhibits unique rheological behaviors. The power-law shear thinning behavior at sol and gel states were observed. Yielding behavior of the nanoemulsion gels was characterized using large amplitude oscillatory shear (LAOS) experiments. These gels display strain-softening behavior under application of large shear-deformation prior to failure of the material. The material turn back to the initial state simultaneously after cessation of applied high shear stress/strain.

*We acknowledge L’Oréal for financial support of the work.

10:36AM A54.00012: Oscillating chemo-mechanical Belousov-Zhabotinsky (BZ) hydrogels*  

BAPTISTE BLANC (Presenter), Physics, Brandeis University, NING ZHOU, Chemistry, Brandeis University, ERIC LIU, Chemical and Biological engineering, Tufts University, S.ALI AGHVAMI, Physics, Brandeis University, BING XU, Chemistry, Brandeis University, HYUNMIN YI, Chemical and Biological engineering, Tufts University, SETH FRADEN, Physics, Brandeis University — 

Yoshida [JACS 1996] developed a gel that undergoes cyclic swelling and deswelling without external stimuli. This self-oscillating gel undergoes an oxidation-reduction cyclic reaction, leading to a cyclic change of solubility of the gel. We present a new synthesis technique, offering high modularity in the gel composition and shape. We present simple experimental techniques to characterize the properties of the spherical BZ gels, such as their elasticity, timescale of swelling, density and catalyst content. Moreover, we find that a single spherical BZ gel needs to be larger than a critical size to chemically oscillate, thereby limiting the amplitude of its mechanical oscillation. We finally show how the remarkably high sensitivity of the BZ gel to its chemical environment can be harvested to enhance its actuation.

*We acknowledge financial support from the NSF DMREF-1534890 and the microfluidics facility of the NSF MRSEC DMR-1420382.
10:48AM A54.00013: The Effects of Mesogen Spacer and Linker on the Actuation of Liquid Crystal Elastomers — JAN-MICHAEL CARRILLO (Presenter), BOBBY G SUMPTER, Oak Ridge National Laboratory, SUK-KYUN AHN, Pusan National University — Experiments have shown that the actuation temperature of thermo-responsive main-chain liquid crystal elastomers (LCE) can be controlled by adjusting the spacer length ($N_L$) of reactive mesogen (i.e., LC monomer). Actuation occurs when the order parameter of LC mesogens changes at the nematic-isotropic transition temperature ($T_{NI}$). The precursor LC oligomers, which are connected LC units via linking thru an alkyl diamine chain extender, exhibits an increasing $T_{NI}$ as $N_L$ is increased. This behavior is opposite to what is observed in LC monomers. To elucidate this behavior, we performed isothermal-isobaric (NPT) ensemble coarse-grained molecular dynamics simulation of stiff-chains that are connected to flexible spacers at different temperatures, where $T_{NI}$ is determined when the smoothly decaying orientational correlation function, $g_2(r)$, transitions to an oscillating decay function. Simulations show that increasing $N_L$ decreases $T_{NI}$ for both monomers and oligomers. However, the dangling beads ($N_D$), representing the alkyl length of the diamine linkers in the experiments, amplifies the decrease of $T_{NI}$ when the linker length ($N_L$) is short. We infer that the combination of $N_L$ and $N_D$ changes the shape anisotropy of the LC mesogen, affecting its ability to transition to the nematic phase.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A55 DPOLY GSOFT: Broadband Dielectric Spectroscopy of Polymers and Soft Matter

8:00AM A55.00001: Broadband dielectric spectroscopy on miscible polymer blends in the bulk and in nanometer thick films - Comparison of the different confinement situations* [Invited] ANDREAS SCHOENHALS (Presenter), PAULINA SZYMONIAK, SHERIF MADKOUR, Department 6.6, Federal Institute of Materials Research and Testing — Broadband dielectric spectroscopy in the frequency range from $10^{-1}$ to $10^9$ Hz is employed to revisit the segmental dynamics of the miscible blend system of poly(vinyl methyl ether)/polystyrene (PVME/PS) in dependence on the composition first in the bulk state. Here, the case of high polystyrene concentrations is considered especially. It is important to note that the dipole moment of polystyrene is negligible, thus only the molecular dynamics of PVME segments, as affected by PS, is observed. Three relaxation processes are found, which are due to fluctuations of differently constrained or confined PVME segments. The degree of the confinement of PVME segments due to PS is discussed in dependence on the composition. Secondly, a spatial confinement is considered by investigating thin films of the PVME/PS blend, where the film thickness varies from 100 nm down to 5 nm. Two concentrations of PVME/PS (50/50 wt% and 25/75 wt%) are investigated. To measure nanometer thick films a novel electrode system based on nanostructured electrodes was employed. Nanostructured electrodes can be considered as a cut-edge technology in dielectric spectroscopy. The relaxation spectra of the films showed multiple processes, which are discussed in dependence on the film thickness.

*German Science Foundation DFG Grant number SCHO 440/20-2

8:36AM A55.00002: Thin supported polymer films: Modified mobility at the interfaces* EMMANUEL MAPESA (Presenter), NOBAHAR SHAHIDI, EMMANOUIL DOXASTAKIS, JOSHUA SANGORO, Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — Using a nanostructured electrode arrangement that effectively offers two different interfaces to the thin polymer layers under study, Broadband Dielectric Spectroscopy (BDS) is employed to characterize interfacial dynamics in thin supported poly(vinyl acetate) (PVAc) films. By analyzing the dielectric loss peak due to the dynamic glass transition, it is demonstrated that although the mean relaxation times for thin films remain bulk-like, there are indeed layers at the polymer/substrate and polymer/air interfaces that exhibit modified mobility in dependence on both overall film thickness and temperature. Preliminary molecular dynamics simulations corroborate these findings.

*E.M. and J.S. are grateful for support from the National Science Foundation, Division of Materials Research, Polymers Program, award DMR-1508394.
8:48AM A55.00003: The Cooperative Free Volume Rate Model: Applications to Pressure Dependent Dynamics and Dynamics under Confinement*  
RONALD WHITE (Presenter), JANE E LIPSON, Dartmouth College — In this talk we discuss our recent work in modeling and predicting alpha relaxation times (τ) using the cooperative free volume rate model (CFV), an approach where the system's free volume determines the molecular cooperativity, and thus the activation energy. The term "free volume" carries some historical baggage, having been ill-defined and, at times, over-enthusiastically applied. However, our definition of free volume is grounded in analysis of experimental volumetric information (PVT data) using our locally correlated lattice (LCL) model equation of state. We have shown, for both polymers and small molecules, that the LCL predicted free volume is very effective in representing a system's volume-based contribution to dynamics. Another essential feature (ignored in historical models) is that the CFV model incorporates an independent temperature-based contribution. We have shown this contribution acts in a product form together with an inverse $V_{\text{free}}$ dependence, a result that follows mechanistically from the rate model. This presentation will summarize some of our applications of the CFV $\tau(T,V_{\text{free}})$ form to experimental systems, with a particular focus on pressure dependent dynamics and dynamics under confinement.

*This work is supported by NSF, DMR-1708542.

9:00AM A55.00004: Dielectric Phenomena in Polymers and Multilayered Dielectric Films*  
LEI ZHU (Presenter), Case Western Reserve University — High dielectric constant and low dielectric loss are desirable electrical properties for next-generation polymer dielectrics that show promise for applications in pulsed power, power electronics, and printable electronics. Unfortunately, the dielectric constant of polymers is often limited to 2-5, much lower than that of inorganic dielectrics, because of the nature of hydrocarbon covalent bonds for electronic and atomic polarizations. It is essential to understand the fundamental physics of different types of polarization and the associated loss mechanisms in polymers. In this presentation, we discuss the characteristics of each polarization and explain how to enhance the polarization using rational molecular designs without causing significant dielectric losses. Among various approaches for high dielectric constant and low loss polymers, the multilayer film technology is of particular interest because a multilayer film is a unique one-dimensional system with tailored material choices, layer thicknesses, and interfaces. By minimizing the disadvantageous polarizations and enhancing the advantageous polarizations, multilayer films hold promise as advanced dielectrics for future polymer film capacitors.

*This research is supported by Office of Naval Research (N00014-16-1-2170).

9:12AM A55.00005: Deciphering Relaxation Spectra of Amorphous Polymers through Dielectric Spectroscopy of an Epoxy  
DANIEL WILCOX (Presenter), GRIGORI MEDVEDEV, YELIN NI, AKASH PATIL, BRETT SAVOIE, BRYAN BOUDOURIS, JAMES M CARUTHERS, Purdue University — In contrast to the crystalline solid and gaseous phases, the mechanism behind the behavior of liquids and amorphous solids remains a significant challenge, where current descriptions of relaxation behavior in these materials are highly empirical with tenuous physical significance. Recently, we have found that the dynamic mechanical relaxation behavior of an epoxy resin is better described using a small, finite number of discrete relaxation processes instead of the continuous spectrum of relaxation times that are typically employed. In this work, the broadband dielectric spectroscopy of the same epoxy material is investigated, where isotherms were measured from liquid nitrogen temperatures to well above the glass transition temperature. By comparing the loss spectra between the two techniques, we observe that the same discrete set of relaxation times unifies the description of both mechanical and dielectric data. Each of the discrete relaxation processes exhibits its own temperature dependence that is the same for mechanical and dielectric experiments, although the strength of the individual spectral components is different. The implications of the existence of discrete relaxation spectrum for developing theory of amorphous materials will be discussed.
Rigid Amorphous Phase in Polymer Nanocomposites as Revealed by Dielectric Relaxation Spectroscopy and Fast Scanning Calorimetry

Paulina Szymoniak (Presenter), Andreas Schoenhalts, Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — For inorganic/polymer nanocomposites a so-called Rigid Amorphous Phase (RAF) is formed in the interfacial region by adsorption of polymer segments onto the nanoparticles. The segmental dynamics of RAF is expected to be altered, as compared to the pure matrix, which might percolate into the entire system, affecting the overall nanocomposite properties. A combination of two relaxation spectroscopy techniques (Broadband Dielectric Spectroscopy (BDS) and Specific Heat Spectroscopy (SHS)), as well as Fast Scanning Calorimetry (FSC) was employed to investigate the structure and molecular mobility of nanocomposites based on Epoxy and Layered Doubled Hydroxides.

First, BDS investigations proved the existence of a process, which is present only for nanocomposites, assigned to the dynamics of polymer segments within RAF. Second, the amount of RAF was quantified by analyzing the change of specific heat capacity step of nanocomposites, comparing to the pure material.

Thirdly, the glass transition of nanocomposites was studied with FSC, applying high heating rates (500-10 000 K/s). Considering that all techniques probe the same molecular process, an activation plot was constructed, delivering a complete picture of the molecular mobility and structure of the polymer nanocomposites including RAF.

Network dynamics in hydrogen-bonding telechelic polymers: associate lifetime, structural relaxation and phase separation

Martin Tress (Presenter), Kun Yue Xing, Department of Chemistry, University of Tennessee, Knoxville, Peng-fei Cao, Chemical Sciences Division, Oak Ridge National Laboratory, Shi Wang Cheng, Department of Chemical Engineering and Material Science, Michigan State University, Tomonori Saito, Chemical Sciences Division, Oak Ridge National Laboratory, Vladimir Novikov, Alexei P Sokolov, Department of Chemistry, University of Tennessee, Knoxville — Supra-molecular networks formed by reversible bonds between polymer chains exhibit extraordinary properties, e.g. extreme toughness and elongation at break, self-healing. We study short telechelic polymers with different H-bonding end-groups and backbone flexibility [1]. The H-bonds increase the glass transition temperature (Tg), though in flexible polydimethyl siloxanes (PDMS) it does not vary with H-bond strength whereas in much stiffer telechelic polypropylene glycol (PPG) Tg varies significantly. In contrast, viscosity strongly depends on the H-bond strength in PDMS while it remains similar in PPG. Complementary measurements of shear modulus and dielectric relaxation indicate that this can be explained by competing lifetimes of the supra-molecular associations and the chain relaxation. Only if the former exceeds the latter, viscosity increases. Furthermore, the viscoelastic properties can be enhanced tremendously by phase separating ends, controlled primarily by Tg of the aggregations. Our analysis reveals that the concept of bond lifetime renormalization [2] describes the results qualitatively but fails on a quantitative level.


Dynamics of freeze-dried proteins embedded in organic glasses revealed by broadband dielectric spectroscopy

Simone Capaccioli (Presenter), Physics, University of Pisa, Maria Pachetti, Physics, University of Trieste, Gaia Ciampalini, Physics, University of Pisa, KIA L. Ngai, Elpidio Tombari, IPCF-CNR Pisa, Alessandro Paciaroni, Physics, University of Perugia — We present extensive broadband dielectric spectroscopy (BDS) studies of dynamics in freeze-dried, de-hydrated, binary mixtures of proteins and excipients. The latter have been selected among hydrogen bonding glass-formers, with different viscosity and molecular mass, spanning more than 150 K in glass transition temperatures Tg. Apart from interfacial relaxation and Maxwell-Wagner polarization effects we found the ubiquitous presence of three relaxation processes: one has a Vogel-Fulcher-Tamman temperature behavior, it is strongly influenced by the type of solvent and it share the same timescale of the process, revealed by calorimetry, bringing the system to vitrify; the other two processes are faster and active also in the glassy state. The intermediate process shows activated dynamics independent on the excipient but it appearing to evolve on ageing.

Combining BDS data with calorimetry and neutron scattering experiments a complex scenario emerges, where some dynamic processes of proteins appear to be coupled to solvent dynamics in the range from ns to ks, as predicted also for faster dynamics by the “slaving” assumption, but other processes seem to have a more peculiar behavior. In particular, their dynamics is not suppressed in the glassy state of freeze-dried proteins.
10:00AM A55.00009: Hard versus soft confinement effects on molecular dynamics of 4-hexyl-4′-isothiocyanatobiphenyl liquid crystals* MALGORZATA JASIUKOWSKA-DELAPORE (Presenter), TOMASZ ROZWADOWSKI, Department of Soft Matter Research, The Henryk Niewodniczanski Institute of Nuclear Physics, Polish Academy of Sciences, ANNA BARANOWSKA-KORCZYC, Faculty of Chemistry, University of Warsaw, EWA EWA JUSZYNSKA-GALAZKA, MARIA MASSALSKA-ARODZ, Department of Soft Matter Research, The Henryk Niewodniczanski Institute of Nuclear Physics, Polish Academy of Sciences — The purpose of this work is to examine the dynamic properties of 4-hexyl-4′-isothiocyanatobiphenyl (6BT) experiencing different forms of confinement. Hard confinement was achieved by the infiltration of LCs into nanoporous aluminium oxide (AAO) templates with non-intersecting, cylindrical, channels. Soft confinement derived from the interactions between polymer and guest liquid crystalline molecules was investigated on an example of electrospun polymer/liquid crystal composite fibres. We prepared composite fibres for three different mass ratios of polycaprolactone (PCL) and 6BT. The formation of liquid crystalline domains in fibres was confirmed by polarizing microscope observations and their distribution was illustrated by Raman. The intra-molecular interactions in composite fibres were revealed by analysis of the temperature dependencies of specific infrared (IR) absorption bands. By a combination of broadband dielectric spectroscopy with the other spectroscopic methods, the microscopic picture of role of soft and hard confinement on molecular dynamics and a crystallization process in liquid crystals is obtained.

*M. J-D acknowledges the National Science Centre (Grant SONATA11: UMO-2016/21/D/ST3/01299) for financial support.

10:12AM A55.00010: On the Fragility of Hydroxypropyl Methylcellulose as Measured via Broadband Dielectric Spectroscopy WILLIAM WOODWARD (Presenter), MICHAEL LESNIAK, TIRTHA CHATTERJEE, KEVIN O’DONNELL, ROBERT SAMMLER, TRAVIS MCINTIRE, YONGFU LI, MARK RICKARD, DAVE MEUNIER, Dow Chemical Company — A special class of hydroxypropyl methylcellulose polymer (HPMC) has been developed for the production of amorphous solid dispersions of active pharmaceutical ingredients by hot-melt extrusion. This has produced the opportunity to acquire frequency-dependent Tg measurements of HPMC via broadband dielectric spectroscopy (BDS). Our study revealed that the fragility (m) of this polymer is very low (m = 16.9 ± 0.4). Although the measurements herein are limited to this type of HPMC, it is hypothesized that this low fragility is not unique to this particular grade of HPMC.

10:24AM A55.00011: Role of α and β relaxations in Collapsing Dynamics of a Polymer Chain in Supercooled Glass-forming Liquid MRINMOY MUKHERJEE (Presenter), JAGANNATH MONDAL, SMARAJIT KARMAKAR, Tata Institute of Fundamental Research Hyderabad — Understanding the effect of glassy dynamics on the stability of bio-macromolecules and investigating the underlying relaxation processes governing degradation processes of these macromolecules are of immense importance in the context of bio-preservation. In this work we have studied the stability of a model polymer chain in a supercooled glass-forming liquid at different amount of supercooling in order to understand how the dynamics of supercooled liquids influence the collapse behavior of the polymer. Our systematic computer simulation studies find that apart from long time relaxation processes (α relaxation), short time dynamics of the supercooled liquid, known as β relaxation plays very important role in controlling the stability of the model polymer. These observations are in stark contrast with the common belief that only long time relaxation processes are the sole players (vitrification hypothesis). We also show that anti-plasticizing effect found in this context can be rationalized using the β-relaxation process. We believe that our results will lead to understand the primary factors in protein stabilization in the context of bio-preservation.

10:36AM A55.00012: Insights into the role of dynamic heterogeneity in reorientational and translational dynamic measurements from simulations in the isoconfigurational ensemble* DANIEL MAURICIO DIAZ VELA (Presenter), Polymer Engineering, The University of Akron, DAVID SIMMONS, Chemical and Biomedical Engineering, University of South Florida — A major question in the study of the glass transition over the last 50 years has been the origin of stretched exponential relaxation and its connection to the observations of non-Gaussian dynamics and decoupling phenomena such as Stokes-Einstein breakdown. The proposition that these phenomena all emerge from averaging over spatial dynamic heterogeneity has emerged as a major view of the common origin of these phenomena. However, significant questions remain, such as the frequent observation that stretching exponents obtained from dielectric spectroscopy commonly do not exhibit the pronounced temperature dependence expected to accompany growing dynamic heterogeneity on cooling. Here we employ molecular dynamic simulations of glass-forming dimers and bead-spring polymers in the isoconfigurational ensemble to quantify the extent to which each of these phenomena emerge from spatial averaging vs locally anomalous dynamics. Results point to important differences between the role of dynamic heterogeneity in reorientational and translational dynamic quantities such as those measured by dielectric spectroscopy and neutron scattering respectively.

*This material is based in part on work supported by the National Science Foundation NSF Career Award grant number DMR1554920.
Recently we reported [1] that the super-Arrhenian temperature dependence of the relaxation time for 21 molecular glass formers is quantitatively described by a single-parameter model based on the excess enthalpy, where the excess entropy based model of the Adam-Gibbs form fails to describe the data. For these molecular glass formers the liquid/crystalline enthalpy/entropy were obtained by straightforward integration of the heat capacity data, where excess enthalpy/entropy was obtained by subtracting the crystalline value from the liquid value and the independently measured heat of fusion fixes the value of integration constant. For polymeric glass formers the crystalline values are unavailable; consequently, the glassy heat capacity was used in place of the crystalline heat capacity to obtain the configurational (vs. excess) enthalpy/entropy, and the glassy PVT surface is used to determine these quantities at elevated pressures. We show that the resulting configurational enthalpy model describes the mobility data for 12 amorphous polymers, including both the temperature and pressure dependence of the relaxation time above Tg. The configurational entropy model in the Adam-Gibbs form fails to describe the mobility data.

**8:48AM A56.00003: Discovering the genes mediating the interactions between chronic respiratory diseases in the human interactome**

ENRICO MAIORINO (Presenter), Harvard Medical School, ALBERT-LASZLO BARABASI, Northeastern University, SCOTT WEISS, BENJAMIN A. RABY, AMITABH SHARMA, Harvard Medical School — Biological networks are powerful resources for the discovery of potential candidate genes and for the investigation of the mechanisms underlying human complex disease like asthma and chronic obstructive pulmonary disease (COPD). Recent network-based computational studies have shown that disease genes encoding proteins have a strong tendency to interact with each other and to agglomerate in specific ‘disease modules’ identified as connected localized neighborhoods in the network [1]. In this scenario, perturbations originating within one disease module can diffuse through the network and affect other close diseases [2].

Recognizing the genes mediating such perturbations is crucial for understanding the biological pathways responsible for the comorbidity of similar diseases such as asthma and COPD. In this work, we identify the topological modules of these two diseases in the protein-protein interaction network and determine their mediators by defining a variant of betweenness centrality measure, called ‘flow centrality’. The biological role of the observed flow central genes sheds light on the hypothesized common genetic origin of asthma and COPD [3].


**9:00AM A56.00004: The New Field of Network Physiology: Mapping the Human Physiolome**

PLAMEN IVANOV (Presenter), XIYUN ZHANG, FABRIZIO LOMBARDI, Physics Department, Boston University — The human organism is an integrated network where complex physiological systems continuously interact to optimize and coordinate their function. Organ-to-organ interactions occur at multiple levels and spatiotemporal scales to produce distinct physiologic states. Disrupting organ communications can lead to dysfunction of individual systems or to collapse of the entire organism. Yet, we do not know the nature of interactions among systems and sub-systems, and their collective role as a network in maintaining health. The new field of Network Physiology aims to address these fundamental questions.

Through the prism of concepts and approaches from statistical and computational physics and nonlinear dynamics, we will present a new framework to identify and quantify dynamic networks of organ interactions. We will demonstrate how physiologic network topology and systems connectivity lead to integrated global behaviors representative of distinct states and functions.

The presented investigations are initial steps in building a first Atlas of dynamic interactions among organ systems and the Human Physiolome, a new kind of BigData of blue-print reference maps that uniquely represent physiologic states and functions under health and disease.

*We acknowledge support from W M Keck Foundation.

**9:12AM A56.00005: Complex statistical interactions in biology**

ISTVAN KOVACS (Presenter), ALBERT BARABASI, Department of Physics, Northeastern University — Although each individual carries dozens of deleterious mutations, each of which should have a dramatic impact on our health, life carries on due to extensive genetic buffering. Therefore, interpreting genetic information requires the understanding of not only the impact of individual mutations but also their interactions. Genetic interactions occur when the combined impact of two mutations results in an unexpected phenotype, for example a positive interaction in the case of genetic buffering. Negative interactions are even more striking, such as synthetic lethality, where two individually mild mutations lead to cell death. Understanding and predicting (even higher order) genetic interactions is a key to better understand complex traits, missing heritability and genetic buffering in humans. In the talk we will overview the major sources of data and recently developed statistical methods to analyze and predict it. Our results enable us to better understand the emergence of biological function under both healthy and pathological conditions and directly contribute to improved disease module identification, drug target prediction, and drug combination design.

*This work has been supported by the Burroughs Wellcome Fund 2018 Collaborative Research Travel Grant.
Reconstructing model humans from observed health data*  SPENCER FARRELL (Presenter), ANDREW RUTENBERG, Dalhousie University — Human aging can be understood as a stochastic process of damage accumulation. This stochasticity is evident in the heterogeneity of health trajectories and lifespans of individuals. Measurements of health “deficits” can be used to quantify an individual's state of health. We model human aging using a network of interacting health deficits with stochastic damage/repair. Our model incorporates both “observed” nodes, corresponding to observed deficits, and “hidden” nodes, representing the large amount of health aspects that are not measured. We use maximum likelihood techniques to estimate parameters with observed human data of deficits and death ages. We then generate individuals from our model using these estimated parameters, so that they have health trajectories distributed approximately the same as the data. This lets us extrapolate from observed data to future health trajectories and lifespans.

*This research was funded by a Nature Sciences and Engineering Research Council (NSERC) Doctoral Award. Computational resources were provided by ACENET and Compute Canada.

Emergence of Laplace-Distributed Growth Rates in Network Dynamics  CHIA-HUNG YANG (Presenter), Network Science Institute, Northeastern University, SEAN CORNELIUS, Center of Complex Network Research, Northeastern University — The dynamical state of a complex network is rarely stationary in time, often exhibiting sufficiently erratic fluctuations so as to seem random. Previous observational studies on annual fish catches, flock sizes of migrating birds, and company sales have revealed that the growth rates follow a Laplace (double exponential) distribution, which is characterized by a higher probability of large increases/decreases relative to the Gaussian growth statistics predicted by typical null models. Yet despite the prevalence of Laplacian growth rates in disparate systems, their mechanistic origin has remained elusive. Here we show that Laplacian growth statistics emerge generically from the interplay between two ubiquitous features in real complex systems — multistability and noise. Under specific conditions, these factors combine to allow frequent transitions between the underlying attraction basins, which broadens tails of the growth distribution relative to that produced by a random walk. Our results suggests that “boom and bust” behavior may be the rule rather than the exception in networks with nonlinear dynamics, with implications for problems ranging from sustainable ecosystem management to financial system stability.

Spreading dynamics of forget-remember mechanism*  SHENGFENG DENG (Presenter), Department of Physics, Virginia Tech, WEI LI, College of Physical Science and Technology, Central China Normal University — We study extensively the forget-remember mechanism (FRM) for message spreading, originally introduced in [Eur. Phys. J. B 62, 247 (2008)]. The freedom of specifying forget-remember functions governing the FRM can enrich the spreading dynamics to a very large extent. The master equation is derived for describing the FRM dynamics. By applying the mean field techniques, we have shown how the steady states can be reached under certain conditions, which agrees well with the Monte Carlo simulations. The distributions of forget and remember times can be explicitly given when the forget-remember functions take linear or exponential forms, which might shed some light on understanding the temporal nature of diseases like flu. For time-dependent FRM there is an epidemic threshold related to the FRM parameters. We have proven that the mean field critical transmissibility for the SIS model and the critical transmissibility for the SIR model are the lower and the the upper bounds of the critical transmissibility for the FRM model, respectively.

*This work was partially supported by the Programme of Introducing Talents of Discipline to Universities under Grant No. B08033.

Measuring and Modeling the Flow of Information Online and on Networks*  JAMES BAGROW (Presenter), University of Vermont, LEWIS MITCHELL, University of Adelaide — We propose a model for the flow of information in the form of symbolic data. Nodes in a graph representing, e.g., a social network take turns generating words, leading to a symbolic time series associated with each node. Information propagates over the graph via a quoting mechanism, where nodes randomly copy short symbolic sequences from each other. We characterize information flows from these data via information-theoretic estimators, and we derive analytic relationships between model parameters and the values of these estimators. We explore and validate the model with simulations on small network motifs and larger random graphs. Tractable models such as ours that generate symbolic data while controlling the information flow allow us to test and compare measures of information flow applicable to realistic data. In particular, by choosing different network structures, we can develop test scenarios to determine whether or not measures of information flow can distinguish between true and spurious interactions, and how topological network properties relate to information flow.

*This material is based upon work supported by the National Science Foundation under Grant No. IIS-1447634
Complex contagion and network structure*  
JULIAN KATES-HARBECK (Presenter), MICHAEL DESAI, Physics, Harvard University — Social networks provide the grounds for the spread of physical infections, ideas, memes, behaviors, or opinions. Socially spreading information and ideas can represent "complex contagions" where, in contrast to physical infections, the probability of the contagion spreading to a new individual on the network need not be a linear function of the fraction of affected neighbors. Here we explore the relationship between complex contagions and the underlying structure of interaction networks, and show that nonlinear adoption produces qualitatively novel spreading behaviors that are strongly affected by network structure. In particular, we demonstrate the effects of network sparsity, community structure, and degree distributions on the contagion. Finally, we demonstrate that complex contagions can undergo a phase transition where sufficiently cohesive community structures and sufficiently sparse networks can allow for global epidemics even for very large networks.

*This work was supported by the Department of Energy Computational Science Graduate Fellowship Program of the Office of Science and National Nuclear Security Administration in the Department of Energy under contract DE-FG02-97ER25308.

Scale-free Networks Well Done*  
IVAN VOITALOV (Presenter), PIM VAN DER HOORN, Department of Physics and Network Science Institute, Northeastern University, REMCO VAN DER HOFSTAD, Department of Mathematics and Computer Science, Eindhoven University of Technology, DMITRI KRIOUKOV, Department of Physics, Department of Mathematics, Department of Electrical and Computer Engineering, and Network Science Institute, Northeastern University — We bring rigor to the vibrant activity of detecting power laws in empirical degree distributions in real networks. We first provide rigorous definitions of scale-free and power-law distributions, the latter equivalent to the definition of regularly varying distributions in statistics. These definitions allow the distribution to deviate from a pure power law arbitrarily but without affecting the power-law tail exponent. We then identify three estimators of these exponents that are proven to be statistically consistent - that is, converging to the true exponent value for any regularly varying distribution - and that satisfy some additional niceness requirements. Finally, we apply these estimators to a representative collection of synthetic and real data to find that real scale-free networks are definitely not as rare as one would conclude based on the popular but unrealistic assumption that real data comes from power laws of pristine purity, void of noise and deviations.

*This work was supported by NSF Grant No. IIS-1741355, ARO Grants No. W911NF-16-1-0391 and No. W911NF-17-1-0491, NWO VICI Grant No. 639.033.806, and the Gravitation Networks Grant No. 024.002.003.

Network architecture of energy landscapes in mesoscopic quantum systems  
ABIGAIL N. POTESHMAN, EVANGELIA PAPADOPOULOS (Presenter), University of Pennsylvania, EVELYN M TANG, Max Planck Institute for Dynamics and Self-Organization, DANIELLE BASSETT, LEE BASSETT, University of Pennsylvania — Mesoscopic quantum systems exhibit complex many-body phenomena. Even simple, non-interacting theories display a rich landscape of energy states, where many-particle configurations are linked by spin- and energy-dependent transition rates. This collective energy landscape is difficult to characterize, especially in regimes of frustration. Here, we use network science to quantify the organization of these state transitions. Using a computational model of electronic transport through quantum antidots, we construct networks where nodes represent energy states and edges represent allowed transitions. We explore how current and conductance, which measure transport, are reflected in the network topology in response to changes in external voltages. We find that the state-transition networks exhibit Rentian scaling, which is characteristic of efficient computer and neural circuitry, and which measures the interconnection complexity of a network. Remarkably, networks corresponding to points of frustration in transport exhibit enhanced complexity relative to networks not experiencing frustration. Our results demonstrate that network-based analyses can capture salient properties of quantum transport, and motivate future efforts using network science to understand complex quantum systems.
8:00AM A57.00001: Ab initio molecular dynamics, machine learning and complex liquids* [Invited] ROBERTO CAR (Presenter), Princeton University — Using liquid water as an example I will show that deep neural networks allow us to greatly accelerate ab-initio molecular dynamics simulations without loss of accuracy. The approach naturally leads to models with different levels of coarse-graining both for the electronic ground-state and the atomic structure information. The basic procedure was outlined in two recent papers [1,2].


*Supported from the DOE-BES under grant DE-SC0019394

8:36AM A57.00002: A viscoelastic hydrodynamic theory of density fluctuations in liquids ZHIKUN CAI (Presenter), YANG ZHANG, University of Illinois at Urbana-Champaign — Long-wavelength longitudinal phonons can propagate in liquids, but whether transverse phonons exist in liquids has been long debated. Moreover, according to the classic hydrodynamic theory, it was believed that the transverse modes have no causal relation to the density fluctuations. However, these points of view are challenged by the recent data measured in the generalized hydrodynamic regime from computer simulations and scattering experiments. Hence, in this work, a viscoelastic hydrodynamic approach is proposed to describe the density fluctuations of supercooled liquids in the generalized hydrodynamic regime. Based on the generalization of the Navier-Stokes stress-strain constitutive relation, viscoelastic temporal response and spatial anisotropic effect are integrated into the framework of the hydrodynamic theory using a time-dependent relaxation tensor. As a result, it is found that liquids may exhibit either transverse excitations or transverse kinetic relaxations, depending on specific viscoelastic responses. Moreover, it is demonstrated that anisotropy naturally leads to a hybrid contribution of longitudinal dynamics and transverse dynamics to the density and current correlation functions.

8:48AM A57.00003: Study of the Correlated Molecular Dynamics in D₂O using Inelastic Neutron Scattering* YADU KRISHNAN SARATHCHANDRAN (Presenter), University of Tennessee, YUYA SHINOHARA, WOJCIECH DMOWSKI, University of Tennessee/Oak Ridge National Laboratory, DOUGLAS L ABERNATHY, Oak Ridge National Laboratory, TAKESHI EGAMI, University of Tennessee/Oak Ridge National Laboratory — We report the real-space correlated molecular dynamics in heavy water (D₂O). Dynamic structure factor, S(Q, E), obtained from high-resolution inelastic neutron scattering data over large Q (momentum transfer) and E (energy transfer) is double-Fourier transformed to obtain the Van Hove function, which is a time-dependent pair-correlation function. A two-step relaxation is observed in the intermolecular dynamics of D₂O. Its relaxation time and amplitude depends on the temperature. By comparing the results with classical MD simulations of D₂O and inelastic x-ray scattering measurements of H₂O[1][2], correlated dynamics of water molecules in ps time-scale is discussed.

References

*Supported by the US Department of Energy, Office of Science, Basic Energy Science, Materials Science and Engineering Division.

9:00AM A57.00004: Elucidating the role of vapor-liquid interfaces on ice nucleation SARWAR HUSSAIN (Presenter), AMIR HAJI-AKBARI, Chemical and Environmental Engineering, Yale Univ — Vapor-liquid interfaces are known to accelerate heterogeneous ice nucleation at their vicinity, in a phenomenon known as contact freezing [1]. Their impact on homogeneous nucleation, however, is more ambiguous, as the experimental evidence for surface freezing [2], or enhancement of homogeneous nucleation at free interfaces, is not conclusive. Computational investigations of surface freezing also predict conflicting qualitative behaviors for different water models [3-4]. It has, however, been suggested that contact and surface freezing are related, as if a free interface can enhance heterogeneous nucleation, it must also have the same effect on homogeneous nucleation. In this work, we use forward-flux sampling [5] to explore this relationship, and observe that tetrahedral liquids undergoing surface freezing will also exhibit accelerated heterogenous nucleation kinetics when the crystal-nucleating agent is very close to the free interface. We attribute this finding to instabilities induced at a free interface due to the proximity of the nucleating surface.

9:12AM A57.00005: Transient Structured Fluctuations in a 2D Liquid* ZACH KREBS, ARI ROITMAN, LINSEY NOWACK (Presenter), CHRISTOPHER M LIEPOLD, BINHUA LIN, STUART A RICE, University of Chicago — Using the Aperture Cross Correlation Function as diagnostic, we find the existence of transient structured fluctuations in the liquid phase of a two-dimensional system with a repulsive, core-softened pair potential [1]. This system supports several hexagonal solid phases, a square solid phase, liquid and hexatic phases, and a quasi-crystalline phase with 12-fold symmetry. Our computer simulations suggest the surprising results that deep within the liquid region and approaching transition boundaries, the structured fluctuations favor only the same symmetries supported in the ordered phases of the system, i.e. three-fold, four-fold, and twelve-fold. To our knowledge, no theory to date suggests why such a system would not display local fluctuations of other symmetries well within the liquid phase.


*We thank the University of Chicago MRSEC, NSF Grant No. DMR-1420709, the Senior Mentor Grant from the Camille and Henry Dreyfus Foundation (Grant No. SI-14-014), NSF's ChemMatCARS (grant No. NSF/CHE-1346572), and the Jeff Metcalf Internship Program for their financial support.

9:24AM A57.00006: A new scenario describing `water-like` thermodynamic anomalies - the double liquid-liquid critical point scenario* DOMAGOJ FIJAN (Presenter), MARK WILSON, Department of Chemistry, University of Oxford — Thermodynamic `water-like` anomalies in liquids have been a long unsolved problem in terms of origin and implications for nature of the liquid (and other similar states). The widely accepted thermodynamic scenario that describes this behaviour in water models and Stillinger-Weber (SW) potential silicon is the second (liquid-liquid) critical point (LLCP) scenario. In this work we present simulation evidence for a novel scenario in wide range of SW liquids. In this scenario the locus of liquid density anomalies (the density minimum and maximum) encloses a region of thermodynamic space with two liquid-liquid critical points connected by a first order transition. We scan the parameter space of the SW potential (tetrahedrality and ideal bond angle parameter) and observe limiting instances where density anomalies disappear. We observe the interactions of density anomaly with the compressibility anomaly, heat capacity anomaly and spinodal line and confirm they show thermodynamically consistent behaviour.

*Domagoj Fijan acknowledges financial support from Clarendon scholarship, St Edmund Hall (University of Oxford), Japan Society for Promotion of Science Short-Term Fellowship and EPSRC Centre for Doctoral training - Theory and Modelling in Chemical Sciences, under grant EP/L015722/1.

9:36AM A57.00007: Molecular Dynamics Simulations for Optical Kerr Effect of Liquid and Supercooled Water* TENG-MING WU (Presenter), Inst. of Physics, National Chiao Tung University — The optical Kerr effect (OKE) spectroscopy measured with heterodyne detection (HD) is a useful tool to provide information regarding intermolecular vibrations and structural relaxations in liquid water. Recently, the measurements of the OKE spectroscopy have been extended to supercooled water [1]. Though the measured results can be well described by using a phenomenological model, the time-resolved OKE spectroscopy of liquid and supercooled water still need a comprehensive understanding. In this paper, we investigated the OKE nuclear response functions for a novel scenario in wide range of SW liquids. In this scenario the locus of liquid density anomalies (the density minimum and maximum) encloses a region of thermodynamic space with two liquid-liquid critical points connected by a first order transition. We scan the parameter space of the SW potential (tetrahedrality and ideal bond angle parameter) and observe limiting instances where density anomalies disappear. We observe the interactions of density anomaly with the compressibility anomaly, heat capacity anomaly and spinodal line and confirm they show thermodynamically consistent behaviour.


*This work is supported by Ministry of Science and Technology, Taiwan R.O.C.

9:48AM A57.00008: Systematic investigations of Infrared spectra of liquid water by first-principles methods JIANHANG XU (Presenter), MOHAN CHEN, XIFAN WU, Temple University — The infrared spectroscopy (IR) is a powerful experimental technique to probe the dynamic dipole fluctuations of water molecules, which are strongly correlated through the H-bond network of liquid water. Here, we compute the infrared spectra of liquid water based on ab initio molecular dynamics simulations by using maximally localized Wannier functions as basis, in which both the generalized gradient approximations (GGA) level exchange-correlation (XC) functional and meta-GGA level strongly constrained and appropriately normed (SCAN) XC functionals are employed. For comparison, the vibration frequencies of the water vapor are computed as well. Our theoretical studies show that the theoretical predictions of spectral features are systematically improved by better liquid water structural predictions through the more physical description of H-bond strengths as well as the capture of intermediate range van der Waals interactions by the SCAN meta-GGA functional.
Emergence of local slow dynamics of water molecules induced by sodium chloride* YUYA SHINOHARA (Presenter), WOJCIECH DMOWSKI, University of Tennessee, Knoxville, TAKUYA IWASHITA, Oita University, DAISUKE ISHIKAWA, JASRI/SPring-8, ALFRED Q R BARON, RIKEN, TAKESHI EGAMI, University of Tennessee, Knoxville — We report on the real-space correlated motion of water molecules in sodium chloride aqueous solution. Measurements of high-resolution inelastic X-ray scattering spectra, \( S(Q, E) \), over wide energy transfer (\( E \)) and momentum transfer (\( Q \)) enabled us to determine the Van Hove function, \( G(R, t) \), by Fourier transform of \( S(Q, E) \) over \( Q \) and \( E \). The results show that the addition of sodium chloride induces the emergence of a slow decay component at the first neighbor peak in the Van Hove function. The intensity of the slow decay and that of the fast decay are proportional and inversely proportional to the salt molality, respectively, whereas their decay time is independent of the molality. This indicates that the slowed correlated dynamics of water molecules is localized in the hydrated shell around ions whereas the dynamics of bulk water is not influenced by the salt.

*Work supported by the US Department of Energy, Office of Science, Basic Energy Science, Materials Science and Engineering Division.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A58 GSOFT: Self-Assembly I

8:00AM A58.00001: Bundling of Rod-Like Colloids via Depletion Forces* JONATHAN ADAMS (Presenter), HENDRICK W DE HAAN, Modelling and Computational Science, University of Ontario Institute of Technology — Self assembly of rod-like colloids in to bundles can be driven by entropic processes. We use Coarse Grained Molecular Dynamics simulations to investigate using depletion forces to induce bundling in a suspension of rod-like colloids. The colloids are approximated as bead-spring polymers, with persistence lengths much larger than the length of the polymer. Depletion forces are an effective attractive force between colloids due to the presence of particles significantly smaller than the colloids, called depletants. Depletion forces are modelled as an implicit entropic force between colloids. Bundling begins to occur when the occupied volume fraction occupied by depletants is above a critical value. This volume fraction is dependent on the length and stiffness of the rod-like colloids. We investigate using this property to induce bundling only in rods above a certain length or certain persistence length.

*NSERC Discovery Grant

8:12AM A58.00002: Self Assembly of Colloidal Polymers Using Isotropic Potentials DEBAPRIYA BANERJEE (Presenter), BETH A LINDQUIST, RYAN B JADRICH, THOMAS TRUSKETT, University of Texas at Austin — Self-assembly of spherical colloids into fluidic chains with no directional bonding or external perturbation promises to be a facile approach to engineer “designer” materials for enhanced surface transport, catalysis, optics, etc. Employing an Inverse Design technique (Relative Entropy optimization), we discern radially-symmetric pair potentials that result in the formation of fluidic, single-stranded, polydisperse colloidal strings (“colloidomers”). Comparing these potentials with those that form size-selective, compact, isotropic colloidal clusters, we find that the ranges of attraction (\( \delta_A \)) and repulsion (\( \delta_B \)) between the two are distinctly different. The energetics combined with the ranges determine the resulting structural motifs. A simple universal potential form is proposed whose morphological phase diagram predicts a gamut of microstructures as a function of \( \delta_A \) and \( \delta_B \) at fixed energetics and packing fraction. Four main broad classes of structures are observed - (i) dispersed monomeric fluid, (ii) ergodic, short chains as well as porous, space-spanning, one-monomer diameter thick, percolated strings, (iii) clusters and (iv) thick cylindrical structures including the tri-helical Bernal spirals.
Encapsulation of circular DNA and non-organic particles inside virus-Like DNA origami icosahedrons.  

S. ALI AGHVAMI (Presenter), Physics, Brandeis University, CHRISTIAN SIGL, ELENA MARIE WILLNER, HENDRIK DIETZ, Physics, Technical University of Munich, SETH FRADEN, Physics, Brandeis University — The principle of quasi-equivalence, announced by Caspar and Klug in 1962, articulates how icosahedral viruses can be constructed using a minimal number of distinct sub-units. Following this scheme, we used DNA origami to construct 5MDa monomers of 3-fold symmetry, which interact through base stacking and shape complementarity and self-assemble into icosahedrons. We encapsulated cargo by functionalizing the interior facing portion of the monomers with single stranded DNA that was complementary to strands on cargo. Two categories of cargo were utilized. The first type of cargo were gold colloids, which were functionalized with complementary ssDNA to the monomers. These colloids were smaller than a monomer and did not bridge between monomers. The second type of cargo was 2.5 MDa circular ssDNA, which could bridge between monomers. The assembly yield was studied as a function of the monomer concentration, interaction strength, and amount of encapsulated cargo.

*We acknowledge financial support from NSF MRSEC DMR-1420382

Nucleation rate in a heterogeneous quartic system

SARAH DAWSON (Presenter), ANCHANG SHI, McMaster University — The nucleation of a stable phase from a metastable phase is studied using the string method applied to a model Ginzburg-Landau system with a quartic potential. A temperature-like parameter is varied in order to move the system between its binodal and spinodal points. A heterogeneity is added to the system in the form of a wedge-shaped substrate. The effect of the heterogeneity on the nucleation barrier height is obtained from the string method. The results are compared with those of the classical nucleation theory. Our results highlight the value of the string method, as well as the validity and limitations of the classical theory.

Light controlled crystallization of DNA coated particles

ETIENNE DUCROT (Presenter), New York University, ILJA VOETS, Eindhoven University of Technology, DAVID J PINE, New York University — DNA coatings have been proposed and successfully applied as a versatile tool for programming the self-assembly of micrometer size particles into numerous crystalline structures. The DNA-mediated interaction is highly temperature dependent. For given buffer conditions, a set of complementary DNA-coated particles present a melting temperature Tmelt that marks the transition between aggregated and melted states. Without a change of environment, one has no further control over Tmelt and a local control of the interaction is challenging.

Here we present a strategy that uses the combination of DNA coatings and an azobenzene photo-switch to access fine control of the interaction between particles, independently from temperature. Azobenzenes reversibly switch between trans and cis conformations, an exposure to UV or blue light shifts the population towards the cis or trans respectively. Once attached to the backbone of a DNA sticky-end, the flat trans form can intercalate in the double helix and stabilize the duplex. On the contrary the kinked cis azobenzene disrupts the hybridization. We harvest this molecular behavior to modulate the melting temperature of DNA-coated particles, pattern their melting or aggregation, correct defects on the crystals and switch between crystal structures.

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Exploring nucleation pathways and solid-solid transitions in two-dimensional binary colloidal crystallization

HUANG FANG (Presenter), STEFAN PAQUAY, MICHAEL F HAGAN, WILLIAM B ROGERS, Brandeis University — Crystals are prevalent in many natural and manmade systems, including metals, minerals, proteins, and colloids. Although the crystal structures themselves are often well understood, the microscopic pathways by which crystals form are difficult to observe or predict. We use a combination of simulations and microscopy experiments to investigate the crystallization pathways of DNA-coated colloids. We observe a rich diversity of behaviors, including one-step and two-step nucleation pathways, as well as a spontaneous solid-solid phase transition during the crystallization of two-dimensional binary mixtures. In this talk, I will present the results of free energy calculations which indicate that the two-step nucleation transition arises from a competition between the free-energy landscapes of two different structures. I will also explore the possibility that the critical size governing this transition can be tuned by changing the relative strengths of interactions. These results may help shed light on fundamental aspects of nucleation, as well as provide new methods for controlling the self-assembly of materials made from colloids.

*We acknowledge support from the National Institute of General Medical Sciences (R01GM108021,) the NSF (DMR-1710112,) and the Brandeis MRSEC (DMR-1420382.)
Entropy Driven Assembly of Truncated Colloidal Tetrahedra into Diamond Lattice

ZHE GONG (Presenter), STEFANO SACANNA, New York University — Building blocks with non-trivial shape are thought to bear invaluable information that largely determines both pathway and final product in self-assembly system. Packing of polyhedra leads to a large diversity of hierarchical structures, among which tetrahedra with various degrees of truncation have been of particular interest due to its unique symmetry. However, the experimental realization of colloidal tetrahedra remains challenging. Here for the first time, surface tension assisted by geometric constraints is used to synthesize truncated colloidal tetrahedra via colloidal fusion, with high size and morphology regularity. The entropy driven assembly of truncated tetrahedral particles was carefully studied via depletion interaction and sedimentation. In both cases, particles exhibit strong face-to-face contact tendency induced by directional entropic force, leading to hexagonal and cubic diamond structures. This study provides information about shape-structure relationship in the packing of truncated tetrahedra, and may further enhance the understanding of crystallization of diamond and its stacking hybrid.

Stochastic Yield Catastrophes and Robustness in Self-Assembly

FLORIAN M GARTNER, ISABELLA R GRAF (Presenter), PATRICK WILKE, PHILIPP M GEIGER, ERWIN FREY, Ludwig Maximilian University of Munich — A guiding principle in macromolecular self-assembly is that, for high production yield, nucleation of structures must be significantly slower than their growth. However, details of the mechanism that impedes nucleation are broadly considered irrelevant. Here, we analyze a generic stochastic model for self-assembly into finite-sized target structures, and investigate two key scenarios to delay nucleation: (i) by introducing a slow activation step for the assembling constituents and, (ii) by decreasing the dimerization rate. These scenarios have widely different characteristics. While the dimerization scenario exhibits robust behavior even in the limit of small particle numbers, the activation scenario is highly sensitive to stochastic effects, which can completely suppress yield. Our results reveal that stochasticity is an important limiting factor for self-assembling systems and, in general, details of the nucleation process play a significant role for the final yield.

Measuring crystal nucleation and growth of DNA-grafted colloidal particles

ALEXANDER HENSLEY (Presenter), WILLIAM B ROGERS, Brandeis University — Grafting DNA onto microscopic colloidal particles can `program' them with information that tells them how to self-assemble into a variety of interesting crystal structures. However, the dynamic pathways by which these crystals self-assemble are largely unknown. In this talk I will present progress on an experimental study of the nucleation and growth of colloidal crystals due to DNA hybridization. Specifically, I will describe a microfluidics-based approach in which we produce hundreds of monodisperse, isolated droplets filled with colloidal particles and then track the formation of crystals within each drop as a function of time. We find that the initial nucleation of crystals from a supersaturated solution involves overcoming a free-energy barrier, and that the height of this barrier decreases dramatically with decreasing temperature. We also find that once nucleated, the crystals grow at a rate that is limited by the diffusive flux of colloidal particles to the growing crystal surface. These findings may help us to devise strategies to tune the nucleation rates and crystal growth kinetics independently, which will be helpful as we try to engineer higher quality or more complex self-assembled structures.

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Nanoparticle superlattice self-assembly via interpolymer complexation

NATHAN HORST (Presenter), ALEX TRAVESSET, Iowa State University — Controlled self-assembly of nanoparticles into ordered structures is an auspicious strategy for fabricating novel devices in nanotechnology. As the number of successful strategies for synthesis increases, emphasis shifts to those that are general, versatile, inexpensive and scalable. To this end, nanoparticle superlattices formed via interpolymer complexation offer a promising route towards a stable, usable class of materials. Understanding the interactions that drive these systems to equilibrium is a primary goal of the theoretical and computational community, as we develop models that capture the configurational characteristics of the system and ultimately predict experimental results. Making use of molecular dynamics simulations, we present our efforts towards understanding nanoparticle superlattices created via interpolymer complexation.

*U.S. Department of Energy (DOE), Office of Science, B.E.S., Materials Science and Engineering Division and performed at the Ames Laboratory, operated for the US DOE by Iowa State University under contract number DE-AC02-07CH11358.

*We acknowledge support from the NSF, DMR-1710112.
10:00AM A58.00011: Aqueous Electrostatic Colloidal Crystallization  THEODORE HUECKEL (Presenter), New York University, JEREMIE PALACCI, Physics, University of California, San Diego, STEFANO SACANNA, New York University — The complementarity demonstrated by atomic ions is an effective strategy to form a range of complex structures from relatively simple building blocks. Due to van der Waals forces, however, mixtures of oppositely charged colloids in water only form disordered aggregates. Consequently, formulating sets of complementary particles has required intensive surface chemistry, despite the availability of these naturally charged starting materials. Here we employ a straightforward technique to stabilize and tune the bonds between oppositely charged colloids to promote ordered self-assembly. After introducing surfactants that can reliably hold particles physically separated, the long-range electrostatic attraction is tuned via charge screening until particles spontaneously crystallize. Single crystals on the centimeter scale are produced in solution that become permanently fixed when introduced to deionized conditions, after which they become robust enough to survive drying for SEM analysis and further processing.

10:12AM A58.00012: Understand Janus particle assembly assisted by surface active molecules*  SHAN JIANG (Presenter), AYUNA TSYRENOVA, KYLE MILLER, MUHAMMAD FAROOQ, JARED ANDERSON, Iowa State University — Janus particles assemble into remarkable superstructures due to different chemistry on the two sides of a single particle. The directional interactions between particles can lead to clusters, chains and stripes, which present new structures and physics of colloidal systems. However, how Janus particles assemble in the presence of surface active molecules has not been systematically studied. On the contrary, most of the previous studies have focused on purified Janus particles in the absence of surface active species. In our experiment, surface active molecules have drastically changed the assembly behavior of Janus particles. Using real time imaging and particle tracking algorithm, we studied the dynamics the Janus particles. We also observed intriguing new crystal structures with highly correlated orientation formed by amphiphilic Janus particles assembled with ionic liquid molecules.

*Startup fund from Iowa State University and 3M Non-Tenured Faculty Award.

10:24AM A58.00013: Phase behavior of hard colloidal bipyramid family  YEIN LIM (Presenter), SANGMIN LEE, SHARON GLOTZER, Chemical Engineering, University of Michigan — Colloidal particles with bipyramidal shape are experimentally obtainable today, and some of them are known to self-assemble into highly complex crystals such as clathrates and quasicrystals by maximizing face-to-face alignment, e.g. via DNA-programmable assembly or via entropy maximization. We present a study of the effect of shape variation on the self-assembly of hard bipyramids using Monte Carlo simulation. We report the phase behavior as a function of the number of vertices in the base polygon and the aspect ratio. From geometric and thermodynamic analysis, we identified over 10 different crystalline structures with varying complexity and symmetry. Our results offer guidance to experiments by providing information about entropically driven self-assembly in the bipyramidal shape family.

10:36AM A58.00014: Crosslinking 2D gold nanoparticle assembly at the air-water interface*  BINHUA LIN (Presenter), IREM KOSIF, University of Massachusetts, Amherst, SIHENG YOU, Harvard University, MRINAL K BERA, University of Chicago, BRIAN LEATHY, Harvard University, TODD EMRICK, University of Massachusetts, Amherst, KA YEE C LEE, University of Chicago — We report the results of crosslinking of two-dimensional gold nanoparticle (Au-NP) assemblies at the air-water interface in situ. We introduce an aqueous soluble ruthenium benzylidene catalyst into the water subphase to generate a robust, elastic two-dimensional network of nanoparticles containing cyclic olefins in their ligand framework. The most striking feature of the crosslinked Au-NP assemblies is that the extended connectivity of the nanoparticles enables the film to preserve much of its integrity under compression and expansion, features that are absent in its non-crosslinked counterparts. The crosslinking process appears to “stitch” the nanoparticle crystalline domains together, allowing the crosslinked monolayers to behave like a piece of fabric under lateral compression.

*This work was supported by The University of Chicago MRSEC under grant no. NSF DMR-1420709, the UMass Amherst MRSEC DMR-0820506, and the Materials Research Facility Network (MRFN). K.Y.C.L. acknowledges the support from the NSF through grant MCB-1413613. All X-ray measurements were carried out at NSF’s ChemMatCARS 15-ID-C, which is supported by the NSF through grant NSF/CHE-1346572.
10:48AM A58.00001: Linker-mediated binding of DNA-grafted colloids: how competition affects phase behavior*
JANNA LOWENSOHN (Presenter), Physics, Brandeis University, BERNARDO OYARZÚN, Physics, Université Libre de Bruxelles, GUILLERMO NARVAEZ PALIZA, Physics, Brandeis University, BORTOLO MATTEO MOGNETTI, Physics, Université Libre de Bruxelles, WILLIAM B ROGERS, Physics, Brandeis University — DNA is a promising tool for programming the self-assembly of new materials: its interactions are chemically specific, tunable, and predictable. In principle, DNA can be grafted to colloids to favor the formation of a predetermined aperiodic structure. In this talk, I promote linker-mediated binding of DNA-coated colloids as an experimental system that could create these hundreds of specific interactions in practice. Here, DNA-coated particles interact through DNA linker strands dissolved in solution. Using optical microscopy, we study the melting transition of our linker system as a function of linker concentration, grafting density, and DNA sequences. We find a phase diagram different from that of directly hybridizing DNA-coated colloids, featuring a reentrant melting transition at high linker concentrations and a region of stable coexistence between solid and fluid. We also examine how the introduction of hundreds of competing linker strands might affect linker-mediated interactions and show that the system can accommodate many interacting linkers simultaneously. These results show the tunability and capacity of our linker-mediated system, and demonstrate how it might expand the design space for aperiodic and adaptive structures.

*NSF grant No. DMR-1710112.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A59 GSOFT GSNP: Rheology and Flow of Particulate Matter I

8:00AM A59.00001: Toward General Rheological Models of Dry and Fluid-Saturated Granular Media [Invited] KEN KAMRIN (Presenter), Mechanical Engineering, Massachusetts Inst of Tech-MIT — Dry and fluid-saturated granular media display multiple modeling challenges from a continuum perspective. Foremost is the search for quantitative and robust constitutive models, in order to robustly predict the flow and stress fields in a flowing body. However, a major challenge is also to find methods to implement these theories in non-trivial geometries up to huge deformations. Methods able to do this are needed not just to implement models in realistic settings of practical interest, but also to test the versatility and correctness of any proposed model, especially models that employ higher-order effects. In this talk we will discuss various continuum modeling approaches for dry and for fluid-saturated granular media. We will also present two numerical techniques for running these models in general geometries. Key challenges on the modeling front include the importance (or lack thereof) of grain size, the various influences of an interstitial fluid phase, and modeling the granular “phase transition” between solid-like, dense-flowing, and disconnected gas-like regions of material.

8:36AM A59.00002: Continuum modeling of flow and size-segregation in dense, bidisperse granular mixtures*
DAREN LIU, DAVID HENANN (Presenter), Brown University — Dense granular systems, consisting of particles of disparate sizes, segregate based on size during flow, resulting in complex, coupled segregation and flow patterns. In this talk, we study size-segregation in three dense granular flow configurations: (1) gravity-driven flow down a long vertical chute with rough parallel walls, (2) annular shear flow with rough inner and outer walls, and (3) planar shear flow with gravity. We perform two-dimensional discrete element method (DEM) simulations of flow of dense, bidisperse granular systems in all three configurations, while varying system parameters, such as the flow rate, flow configuration size, fraction of large/small grains, and grain-size ratio, and we study the effects of these parameters on the segregation dynamics. Our simulations inform continuum constitutive equations for both the size-segregation flux as well as the diffusion flux. When coupled with the nonlocal granular fluidity model - a nonlocal continuum model for dense granular flow - we show that both the flow field and segregation dynamics may be simultaneously captured using this closed, coupled, continuum system of equations.

*This work was supported by funds from NSF-CBET-1552556.
Near-contact dynamics of a sphere-wall collision in a viscous medium

SUMIT KUMAR BIRWA (Presenter), International Centre for Theoretical Sciences, Bangalore, NARAYANAN MENON, Physics, University of Massachusetts Amherst, RAMA GOVINDARAJAN, International Centre for Theoretical Sciences, Bangalore — As a sphere falling under gravity through a viscous medium approaches a wall, there is a large increase in the pressure in the thin layer of fluid being squeezed out between the sphere and wall. At low enough Stokes number, this leads to settling, and above a threshold Stokes number, the sphere bounces. Our earlier experiments have shown that even near this threshold, bouncing involves direct mechanical contact with the bottom plate [SK Birwa et al., Physical Review Fluids, 3(4), 044302, (2018)]. This is in contradiction with lubrication theory (LT) which says that the pressure diverges in the fluid and contact is not made in finite time. To study this difference, we conduct experiments to measure optically and interferometrically the dynamics of a sphere until the micrometer scale preceding the normal collision. The sphere is found to be decelerating slower than predicted by LT. We present an attempt to go beyond LT by accounting for the inertial terms neglected while making the boundary layer approximation, and by defining an appropriate non-orthogonal coordinate system. We obtain a single parametric differential equation which provides us with the time-evolution of the velocity profiles at different radii.

Normal Stresses in Steady-State and Transient Frictional Granular Flows

ISHAN SRIVASTAVA (Presenter), JEREMY LECHMAN, GARY GREST, Sandia National Laboratories, LEONARDO SILBERT, School of Math, Science and Engineering, Central New Mexico Community College — Steady flow of sheared frictional granular matter is well-described by a plastic yield criterion along with a rate-dependent viscoplastic rheology. However, existing constitutive formulations focus exclusively on steady-state simple shear rheology. Using stress-controlled discrete element simulations, we highlight that normal stresses are crucial in the rheology of granular matter, both in steady flow above yield stress and transient creep flow below yield stress. The evolution of shear and normal stress components with strain rate is described in terms of friction-dependent viscometric flow functions, and the effect of friction on the directionality of stress and strain rate tensors is assessed. Additionally, correlations between the evolution of bulk stress tensor and granular fabric—both in transient and steady-state flows—are also described. These results provide important inputs toward formulating rheological constitutive equations that predict stresses during arbitrary deformations of frictional granular matter.

Dynamics of the granular fluidity field

SEONGMIN KIM (Presenter), School of Engineering and Applied Sciences, Harvard University, KEN KAMRIN, Department of Mechanical Engineering, Massachusetts Institute of Technology — A collection of densely-packed solid grains such as sand, rice, and sugar can flow like liquids. A key issue for dense granular flows is rheology: what is the relation between stress and strain rate? The mu(I) rheology postulates a local rheology for steady-state inertial flows. Modified from the local rheology, the non-local granular fluidity (NGF) model has been proposed to explain non-local phenomena due to finite grain size. In the NGF model, an order parameter called ‘granular fluidity’ diffuses away following a partial differential equation in a form of the reaction-diffusion equation. This PDE, however, has only been verified in steady-states. Using the discrete element method, we observe dynamics of the order parameter in different configurations and verify the PDE of the NGF model in transient states.

Fluid-driven transport of spherical sediment particles: from discrete simulations to continuum modeling

QIONG ZHANG (Presenter), KEN KAMRIN, Massachusetts Institute of Technology — Empirical bedload transport expressions commonly over- or underpredict sediment flux by more than a factor of two, even under controlled laboratory conditions. In this work, the discrete element method and lattice boltzmann method are coupled together to simulate 3D fluid-driven transport problems of spherical particles. After comparisons with flume experiments are made to test the numerical simulations, the grain-scale physics is studied, such as the flow field around individual particles and higher order descriptions of the granular motion. A more robust continuum model, unifying empirical models under various conditions and in different regimes, is further proposed based on the new grain-scale understanding of the mechanisms.
Dynamics of ultrasonically levitated granular rafts

MELODY LIM (Presenter), University of Chicago, ANTON A SOUSLOV, Physics, University of Bath, VINCENZO VITELLI, HEINRICH M JAEGGER, University of Chicago — Macroscopic particles in an acoustic trap can self-assemble into close-packed granular rafts consisting of hundreds of particles. These rafts are formed and stabilised due to a sonic depletion force mediated by scattering, which establishes short-range attractions between the constituent particles [1]. We show that this cohesive granular material displays fluid-like behaviour, forming circular “granular droplets” with an emergent surface tension and viscosity. These droplets interact with the acoustic field, inducing forces and torques that drive the droplets to merge, deform, and break-up. We focus on a rotational instability that provides a persistent torque to objects moving in the acoustic field. As the angular momentum of a granular droplet is increased, it deforms from a circle to an ellipse, eventually pinching off into two separate droplets. We use hydrodynamic models for rotating liquid drops to describe the granular dynamics and extract the droplet surface tension.

References:

Material stability and localization in the nonlocal granular fluidity model for dense granular flow∗

SHIHONG LI (Presenter), Brown University — A common and successful continuum model for steady, dense granular flows is the inertial rheology. Recent work has shown that under certain conditions, the inertial rheology displays a linear instability in which short wavelength perturbations grow at an unbounded rate - i.e., a Hadamard instability. This observation indicates that the inertial rheology is capable of describing strain localization; however, it also raises concerns regarding the robustness of numerical solutions. It has been shown that the inclusion of higher-order velocity gradients into the rheology can suppress the Hadamard instability, while not precluding the modeling of strain localization into diffuse shear bands. In this talk, we consider the nonlocal granular fluidity (NGF) model - which also involves higher-order flow gradients and has been shown to quantitatively describe a wide variety of steady, dense flows - and show that the NGF model successfully regularizes the Hadamard instability of the inertial rheology. We further apply the NGF model to the problem of strain localization in quasi-static plane-strain compression using nonlinear finite-element simulations in order to demonstrate that the model is capable of describing diffuse strain localization in a mesh-independent manner.

*NSF-CBET-1552556

Suspension clogging fronts in a leaky pipe

JEREMY S. YODH (Presenter), Department of Physics, Harvard University, L MAHADEVAN, SEAS, Physics, OEB, Harvard University — A particle suspension flowing through a leaky microfluidic channel forms clogs that propagate backwards against the incident flow direction indefinitely. We study the speed and shape of clogs in such situations and show how we can control them. Further, we show that the particulate order in the clog can be controlled by tuning the geometry of the leaky walls. Time permitting, the implications of this for flow through parallel channels will also be addressed.

On the reversibility of granular rotations and translations∗

ANTON PESHKOV (Presenter), IREAP, University of Maryland, College Park, MICHELLE GIRVAN, Departments of Physics, IPST and IREAP, University of Maryland, College Park, DEREK C. RICHARDSON, Department of Astronomy, University of Maryland, College Park, WOLFGANG LOSERT, Departments of Physics, IPST and IREAP, University of Maryland, College Park — We analyze reversibility of both displacements and rotations of spherical grains in three-dimensional compression experiments. Using transparent acrylic beads with cylindrical holes and index matching techniques, we are not only capable of tracking displacements but also, for the first time, analyze reversibility of rotations. We observe that for moderate compression amplitudes, up to the bead diameter, the translational displacements of the beads after each cycle become mostly reversible after an initial transient. By contrast, granular rotations are largely irreversible. We find a weak correlation between translational and rotational displacements, indicating that rotational reversibility depends on more subtle changes in contact distributions and contact forces between grains compared with displacement reversibility.

*This work was supported by National Science Foundation grant DMR-5244620.
10:24AM A59.00011: Drag and interactions of rigid bodies moving through submerged granular beds

BENJAMIN ALLEN (Presenter), RAUSAN JEWEL, ARSHAD KUDROLLI, Clark University — We discuss experimental investigation of the forces encountered by a rod moving through a fluid-saturated granular medium to understand the dynamics of intruders and organisms in sedimentary beds at the bottom of lakes and oceans. By dragging vertically oriented rods through a granular bed of glass spheres, immersed in a fluid, we probe the observed transition from a quasi-static granular-like response to a viscous fluid-like behavior of the medium with speed. The relative importance of inertia, gravitational, and viscous forces is probed in terms of the dimensionless Stokes number, inertial number, and viscous number by varying the rod speed, rod depth, rod diameter, and the viscosity of the fluid. We find that the measured drag is best scaled with the integrated hydrostatic pressure along the rod and the Stokes number at low drag speeds corresponding to the quasi-static region. The transition between the quasi-static and fluid behavior scales with the viscous number, which is the ratio of viscous stress and gravity. We further discuss the interaction of two intruders as a function of the distance of separation compared with their diameter and length.

*Supported by NSF-CBET 1805398.

10:36AM A59.00012: Transition to Steady State in Sheared Dense Granular Materials

HAN-HSIN LIN (Presenter), MELANY HUNT, Caltech — Jamming and shear-thinning are interesting, time-dependent behaviors found in granular materials; however, most prior research has focused on the steady-state behavior under different shear rates. We study the transition phenomenon from unsteady to steady state by using a Couette cell and controlling the torque and speed of the inner cylinder. When controlling the torque, the system cannot reach a steady state when it is below a critical stress. When controlling the speed of the boundary, the shear stress at the wall increases slowly over a period of time that depends on the initial state of the bed, wall friction, shear rate, and flow along the free surface. At steady state, the stress decreases at the highest rotation speeds. Simulations show a recirculation cell driven by gravity and the free surface, which results in the increasing stress observed in the measurements. The effective friction of the inner wall matters. When using the smooth cylinder, the system needs more time to reach a steady state than using the rough cylinder. At steady state, its wall stress decreases more significantly at the highest rotation speeds compared to the rough cylinder.

*The authors acknowledge support from Caltech's Otis Booth Endowment Fund and NSF Grant 1706166.
High thermoelectric performance, or ZT, necessarily depends on achieving the contradictory combination of low thermal conductivity $\kappa$ and high electrical conductivity (along with a large Seebeck coefficient). However, for ultralow $\kappa$ materials (defined here as $\kappa < 1$ W/m-K at 300 K) the electrical conductivity requirement is proportionally reduced. There may therefore exist a new opportunity for such materials in the thermoelectric arena. Examples of such materials are Tl$_3$VSe$_4$ [1], AgBiSe$_2$ [2], and SnSe [3].

However, there are several scientific issues that must resolved prior to usage of any of these materials in an actual application. Ultralow $\kappa$ materials tend to occur near to a ferroelectric transition or other structural instability, due primarily to the large anharmonicity near such an instability. This usually renders materials such as PbTe [4,5,6] unsuitable for device applications due to unfavorable mechanical properties. Is proximity to a structural instability a necessary condition for ultralow $\kappa$? Similarly, another ultralow $\kappa$ route to high ZT is the use of mobile cations, such as Cu in Cu$_2$Se [7], which presents another hurdle for device applications. Can one create a robust thermoelectric device using a material with a structural instability, or mobile structural disorder, in the operating temperature range? The author will discuss these issues.

References


*This work supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Energy supply by fossil fuels only has a limited lifetime and is responsible for an increasing environmental pollution, influencing also climate change. A rapid transition to more sustainable solutions is thus also in the focus of modern research. Renewable fuels are meant to circumvent supply fluctuations arising from energy sources like PV and wind, at the cost of infrastructural adaptations. Direct renewable energy storage is thus highly desirable, but expansive and complicated.

Herein, we report an earth-abundant polymeric material, which for the first time enables the synergistic coupling of two key functions of energy conversion within one single material: visible light harvesting and electrochemical energy storage. The “solar battery” anode material, a 2D cyanamide-functionalized polyheptazine imide (NCN-PHI), is the first of its kind being capable of storing large amounts of photogenerated electrons, operating even in aqueous conditions. Charge compensation and stabilization is realized by pseudocapacitive effects enabled by various aqueous alkali metal ions. Energetically, this occurs at energies well above the reversible hydrogen electrode, allowing for stable aqueous batteries with increased cell voltages.

Limitations arise from low conductivity and hole shuttling to a suitable cathode material. We herein present approaches that address these issues and present our work on hybrid material solutions for full aqueous solar batteries. As such, we aim to provide a sustainable and cheap, earth abundant solution to overcome the intermittency of solar irradiation and other renewable electrical energy sources at a time.


*B.V.L. acknowledges financial support by an ERC Starting Grant (project COFLeaf, Grant No. 639233)
Power generation from direct conversion of infrared radiation from a thermal source.*

PAUL DAVIDS (Presenter), JOSHUA SHANK, JARED KIRSCH, ANDREW STARBUCK, ROBERT JARECKI, DAVID PETERS, Sandia National Laboratories — In this talk, we will describe a new photo-thermoelectric conversion device that consists of a large-area nanoantenna-coupled metal-oxide-silicon (MOS) tunnel diode that directly converts infrared radiation into electrical power. This infrared photonic device needs only view a moderate temperature thermal source to generate a direct photocurrent. A resonant photonic frequency selective surface and a polar oxide material with longitudinal optical phonon resonance are arranged to spectrally overlap and enhance transverse field confinement in an extreme sub-wavelength MOS tunnel barrier. The enhanced field confinement is shown to drive photon-assisted tunneling resulting in large infrared photocurrent in the room temperature device. The measurement of photon-assisted tunneling photocurrent across a matched load impedance is shown to arise due to direct rectification of infrared radiation and a new radiative micropower supply will be described.

*Funding for this work was provided by Sandia's Laboratory Directed Research and Development (LDRD) program. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, a wholly owned subsidiary of Honeywell International Inc., for the United States Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Advanced Materials for Energy Storage*

GEORGE CRABTREE (Presenter), Joint Center for Energy Storage Research (JCESR) — Batteries are central to fundamental changes in transportation through electric vehicles, in the electricity grid through renewable energy integration, replacement of natural gas peaker plants and customized electricity service, and in electric flight through drones, air taxis, package delivery and short-haul passenger service. Next generation batteries to meet these diverse applications require new high-performance materials for anodes, cathodes, electrolytes and interfaces. Using new approaches for simulation and characterization at the atomic and molecular level, these materials can now be designed from the bottom up, atom-by-atom and molecule-by-molecule, where each atom or molecule plays a prescribed role in producing targeted overall materials behavior. Examples will be given for advanced materials for several beyond-lithium-ion batteries.

*This talk is supported by the Joint Center for Energy Storage Research (JCESR), an Energy Innovation Hub funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES).

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A61 GSOFT GSNP: Nonequilibrium Statistical Mechanics of Driven Systems and Pattern Formation I

Phase Coexistence in a 2D System of Granular Self-propelled Particles*

ZHEJUN SHEN (Presenter), NARAYANAN MENON, University of Massachusetts Amherst — We study a system of vibrated self-propelled granular particles on a horizontal plate within a circular boundary covered by an acrylic top. The particles are square and designed to have polar activity along one body diagonal. With fixed particle size, we find that the activity of particles (quantified by the persistence length of motion along the mobility direction) can be controlled by varying the gap between top cover and bottom base. We then study the phase behaviour of the particles as the total number of particles in the system is varied. For a fixed value of activity, particles are uniformly distributed in the system at low density. As the density is increased, particles separate into a high-density ordered region at the boundary of the system, while the remaining particles remain uniformly distributed in the in the central area. Thus the system shows phase coexistence between a mobile, liquid phase and a dense, low-mobility ordered phase.

*We acknowledge financial support through NSF DMR1507650
**8:12AM A61.00002: Calculation of Critical Nucleation Rates by the Persistent Embryo Method: Application to Quasi Hard Sphere Models**

SHANG REN (Presenter), Department of Physics and Astronomy, Iowa State University, YANG SUN, FENG ZHANG, Ames Laboratory, ALEX TRAVESSET, Department of Physics and Astronomy, Iowa State University, CAI-ZHUANG WANG, Ames Laboratory, KAI-MING HO, Department of Physics and Astronomy, Iowa State University — We study crystal nucleation of the Weeks-Chandler-Andersen (WCA) model, using the recently introduced Persistent Embryo Method (PEM). The method provides detailed characterization of pre-critical, critical and post-critical nuclei, as well as nucleation rates that compare favorably with those obtained using other methods (umbrella sampling, forward flux sampling or seeding). We further map our results to a hard sphere model allowing to compare with other existing predictions. Implications for experiments are also discussed.

*Work at Ames Laboratory was supported by the US Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division, under Contract No. DE-AC02-07CH11358, including a grant of computer time at the National Energy Research Supercomputing Center (NERSC) in Berkeley, CA. The Laboratory Directed Research and Development (LDRD) program of Ames Laboratory supported the use of GPU-accelerated computing.

**8:24AM A61.00003: Magnetotactic bacteria droplets: a controllable motor**

BENOIT VINCENTI (Presenter), PMMH Laboratory - ESPCI Paris, GABRIEL RAMOS, MARIA-LUISA CORDERO, Departamento de Física, FCFM - Universidad de Chile, CARINE DOUARCHE, Laboratoire de Physique des Solides - Université Paris-Sud, RODRIGO B SOTO, Departamento de Física, FCFM - Universidad de Chile, ERIC CLEMENT, PMMH Laboratory - ESPCI Paris — We confine magnetotactic bacteria in spherical droplets suspended in oil. The application of a uniform and constant magnetic field induces a focusing of the bacteria at the North and South poles of the droplets due to both alignment with the magnetic field and confinement by the droplet curvature. The focusing of the bacteria at these particular points can eventually create a vortex when the bacteria are densely packed. The spatial characteristics of the vortex flow are extracted with PIV analysis. The dependences of the vortex flow with respect to the magnetic field strength and the droplets radii are quantitatively analyzed and correlated to the flow created outside the droplet by the collective rotation of bacteria. The outstanding applications allowed by such a system are finally discussed in terms of energy harvesting.

*We acknowledge the support of the ANR-2015 BacFlow under Grant No. ANR-15-CE30-0013, Franco-Chilean EcosSud Collaborative Program No Ecos-C16E03, and Millenium Nucleus Physics of Active Matter of the Millenium Scientific Initiative of the Ministry of Economy, Development and Tourism (Chile).

**8:36AM A61.00004: Boosted Annealing of Colloidal Monolayers using Active Dopants**

SOPHIE RAMANANARIVO (Presenter), University of California, San Diego, ETIENNE DUCROT, Department of Physics, NYU, JEREMIE PALACCI, University of California, San Diego — Active particles are microscopic particles, which can inject energy locally and made available by recent progress in colloidal science. They are ideal “pump-probes” to explore the emergent properties in non-equilibrium soft systems and control the behavior of soft matter and self-assembly at the microscale.

In this talk, we will demonstrate how active particles added to a material to regulates its activity internally and boost the annealing of a colloidal monolayer. It opens a broad range of novel opportunities to thermal treatments, where the properties of matter are not controlled macroscopically but microscopically and in real time by active dopants.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1554724. J.P. thanks the Sloan Foundation for support through grant FG-2017-9392. E.D. acknowledges support of the US National Science Foundation under Award Number DMR-1610788, as well as the NYU IT High Performance Computing resources, services, and staff expertise.

**8:48AM A61.00005: Rectification in non-equilibrium gyroscopic networks**

ZHENGHAN LIAO (Presenter), WILLIAM T. M. IRVINE, SURIYANARAYANAN VAIKUNTANATHAN, University of Chicago — One of the goals of molecular engineering is to find design principles for rectification in microscopic conditions, which could lead to the fabrication microscopic motors. Past studies have successfully achieved rectifications in few-body or terminal systems, however, the extension to many-body system is not straightforward. We study energy rectification in a many-body model that combines the active bath and the gyroscopic metamaterials, and numerically and theoretically show that spontaneous heat rectification is achieved at the steady state. We then focus on understanding two issues: the mechanism of this rectification, and the relationship between the network geometry and the flow pattern. Given the knowledge of chiral eigenmodes in isolated gyroscopic networks, the rectification mechanism can be understood as a result of the weighted excitation of these modes. By expanding the heat flux as a summation over paths in the weak interaction regime, we can understand the flow pattern in a complex network from simple paths, which in turn enables us to control the rectification by the design of the network geometry.
Characterizing elusive correlation lengths by computable information density

**STEFANO MARTINIANI (Presenter), Center for Soft Matter Research, New York University, YUVAL LEMBERG, Physics, Technion - IIT, PAUL M CHAIKIN, Center for Soft Matter Research, New York University, DOV LEVINE, Physics, Technion - IIT** — The analysis of computable information density (CID) has recently been introduced as a general approach to quantifying order in equilibrium and non-equilibrium many-body systems, both discrete and continuous, even when the underlying form of order is unknown. The approach has been shown to reliably identify phase transitions, determine their character, and to quantitatively predict certain dynamical critical exponents without prior knowledge of the order parameters. A natural question is whether CID may also inform us on the existence of diverging correlation lengths, and their exponents, in the proximity of phase transitions. We study the CID flow under a renormalization group transformation, and show how this can be exploited to extract correlation lengths and their critical exponents without knowledge of the system's specific correlation functions. To demonstrate the greater generality of the approach, we consider a system for which a simple analysis based on pair-correlation functions cannot detect the diverging correlation length. Hence, with this work, we introduce a new approach for the identification of elusive correlation lengths.

*This work was primarily supported by the NSF Physics of Living Systems Grant 1504867.

Surfactant effect on collective dynamics of surface-associated bacterial particles

**MINGFEI ZHAO (Presenter), XIN YONG, Binghamton University** — Bacteria exhibit collective behavior on moist agar surface to expand and acquire new territories. Self-produced surfactant could entail a significant surface activity due to the reduction of the interfacial friction between moving bacteria and substrates. The bacteria density determines surfactant concentration, so that surface motility will vary locally. The contribution of the density-dependent motility to the collective behavior of bacteria communities remains unclear. We use a discrete self-propelled particle model to simulate an ensemble of rod-like bacteria without the background fluids. The self-propulsion speed is coupled with the local surfactant concentration, solved by a diffusion equation that describes the surfactant production and transport. Simulations between constant self-propulsion speeds will serve as the comparison to test the influence of surfactant. Our investigation will provide a deep understanding of how surfactant influence the collective behavior of bacteria, and further inspire new designs of active materials.

*Financial support for this research was provided by the U.S. National Science Foundation under Grant No. CMMI-1538090.

Transverse Temperature Interfaces in the Katz-Lebowitz-Spohn Driven Lattice Gas

**RUSLAN MUKHAMADIAROV (Presenter), PRIYANKA , UWE CLAUS TAUBER, Virginia Tech** — We explore the intriguing spatial patterns that emerge in a two-temperature Katz-Lebowitz-Spohn (KLS) model in two dimensions, a driven lattice gas with attractive nearest-neighbor interactions and periodic boundary conditions. The domain is split into two regions with hopping rates governed by different temperatures $T > T_c$ and $T_c$, respectively, where $T_c$ indicates the critical temperature for phase ordering, and with the temperature boundaries oriented transverse to the drive. In the hotter region, the system behaves like the (totally) asymmetric exclusion processes (T)ASEP, and experiences particle blockage in front of the interface to the critical region. We argue that transport in the subsystem is impeded by the lower current in the cooler region, which tends to set the global stationary particle current value. We observe the density profiles in both high-and low-temperature subsystems to be strikingly similar to the well-characterized coexistence and maximal-current phases in (T)ASEP models with open boundary conditions. If the lower temperature is set equal to $T_c$, we instead detect the corresponding critical power law density decay.

*Research was sponsored by the Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.

Dynamical fine-tuning to external forcing in disordered networks of bistable springs

**HRIDESH KEDIA (Presenter), DENG PAN, JEREMY L ENGLAND, Physics, Massachusetts Institute of Technology** — A driven many-body system can absorb energy from an external drive quite differently depending on the system’s internal configuration. Thus, the nonequilibrium exploration of configuration space can be strongly biased by the matching between external drive and system response properties. We demonstrate such emergent, adaptive fine-tuning in simulations of an externally forced, disordered mechanical network of bistable springs under a variety of driving conditions.

*This work was funded by AFOSR grant FA9550-17-1-0136
9:48AM A61.00010: Ordering and Synchronization in Driven Systems  PRASHANT SHARMA (Presenter), Suffolk University — Active matter systems display a rich phenomenology of ordered phases and dynamic pattern formation that can be described by models of self-propelled particles with interactions. We introduce a class of models relevant for studying magnetic nanoparticles (and magnetotactic bacteria) in a fluid at low Reynolds number, and explore the different ordered structures observed in these models and their relevance to experimental systems. We analyze the stability of the ordered structures using ideas of stochastic thermodynamics and discuss how this approach solves the problem of general stability analysis of non-stationary ordered states of active matter.

10:00AM A61.00011: Chemical oscillators on star graphs, theory and experiment*  MICHAEL NORTON (Presenter), NATHAN D P TOMPKINS, BAPTISTE BLANC, MATTHEW CAMBRIA, JESSE HELD, SETH FRADEN, Brandeis University — Oscillator networks represent a large class of physical systems in both the natural and engineered worlds. Here we present experimental data for chemical oscillators on star graphs with inhibitory coupling. We examine dynamics as a function of star-degree (number of nodes coupled to a central hub) and coupling strength. We control both by loading a water-in-oil Belousov-Zhabotinsky emulsion (drops ∼100μm) into etched-Si wafer wells. We observed three dynamical attractors: (1) a phase locked state in which the arm-nodes form a synchronized cluster, (2) center-silent dynamics in which the hub well is inhibited by the arm nodes and (3) unlocked dynamics. We developed theory at two levels: a chemically realistic discrete reaction-diffusion model and a phase model; we found excellent agreement to experiment. In particular, in the locked state, we find non-trivial dependence of the locking angle between the arm nodes and the hub as a function of star degree. Finally, we demonstrate that the system can be dynamically reconfigured through photo-inhibition of targeted drops.

*We acknowledge financial support from the U. S. Army Research Laboratory and the U. S. Army Research Office under contract/ grant number W911NF-16-1-0094, and the microfluidics facility of the NSF MRSEC DMR-1420382.

10:12AM A61.00012: Control of a microfluidic three-ring chemical oscillator network*  MARIA ELENI MOUSTAKA (Presenter), MICHAEL NORTON, CHRIS SIMONETTI, SETH FRADEN, Brandeis University — Inspired by the collective behavior and synchronization patterns, which are a common phenomenon in nature, our work focuses on studying the non-linear dynamics of microfluidic networks of Belousov-Zhabotinsky (BZ) chemical oscillators. In our experiments, the auto-catalytic, light-sensitive, BZ reaction is confined to micro-fabricated wells constructed from the elastomer PDMS. Using soft lithography, PDMS networks are arranged into wells with controlled topology. Each well can be regarded as a single network node that sends and receives inhibitory signals. We are particularly interested in the dynamics of a 3-node ring network. This network exhibits spontaneous chiral behavior. In theory, control over the chirality can be achieved by exploiting the light sensitivity of the BZ catalyst, which can modulate the frequency of a node. In experiment, we perturb the network by changing the light intensity and duration in each of the three BZ wells. This technique provides a model of gait switching in central pattern generators and a dynamic method of information storage.

*We acknowledge financial support from the U. S. Army Research Laboratory and the U. S. Army Research Office under contract/ grant number W911NF-16-1-0094, and the microfluidics facility of the NSF MRSEC DMR-1420382.

10:24AM A61.00013: Minimal Model for an Energy Cascades in Driven Nonequilibrium Systems*  GURAM GOGIA (Presenter), JUSTIN BURTON, Emory University — Complex systems that are fed energy at their constituent-level frequently exhibit self-organizational and emergent properties. The external driving can be periodic, but more commonly it comes in the form of noise. Here we show how a spatially extended layer of charged particles exhibits intermittent switching between crystalline and gas-like states. The particles are driven by individual charge fluctuations which feed energy into one vibrational degree of freedom. A small amount of disorder leads to recurrent energy cascades (melting) in the system. Using normal mode analysis, we show that the fraction of vertical vibrational modes with low participation ratio determine the response of the system to the noisy driving. We propose a minimal model of the transfer of the kinetic energy between vertical and horizontal degrees of freedom using modified Lotka-Volterra equations. The model reproduces all of the salient features of the energy cascades observed in the experiment and simulation. Similar to the Reynolds number in fluid flow, we characterize a dimensionless number that is the ratio of the energy input and dissipation. Intermittent energy cascades are observed for a narrow range of this number, in striking resemblance to transition to turbulence in pipe flow.

*NSF DMR 1455086
10:36AM A61.00014: Thermodynamic Efficiency in Dissipative Chemical/Supramolecular Processes*  EMANUELE PENOCCHIO (Presenter), RICCARDO RAO, MASSIMILIANO ESPOSITO, University of Luxembourg — Out-of-equilibrium chemistry is not anymore a prerogative of nature. In recent years, fuel-driven self-assembly became a paradigmatic example of how chemists were able to access the realm of nonequilibrium processes. In the meantime, theoretical physicists achieved a deep understanding of these phenomena, which resulted in rigorous formulations of nonequilibrium thermodynamics for chemical systems. In this work, we crossbreed experimental and theoretical cutting edge research by building a quantitative thermodynamic description for two classes of chemical dissipative processes: energy storage and dissipative synthesis, which boast experimental examples in supramolecular chemistry. The former consists in storing chemical energy in the form of high-energy molecules, whereas the latter in synthesizing molecules by consuming fuel species. As nascent thermodynamics did for heat engines, we treat these systems as chemical engines and develop a quantitative framework for evaluating their efficiency. In doing so, we set the foundation for performance analysis of generic dissipative chemical processes.

*This work was funded by the European Research Council project NanoThermo (ERC-2015-CoG Agreement No. 681456).

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A62 DCMP: Undisguised View of the Mott Transition  BCEC 258C - Martin Dressel, University of Stuttgart - Tag(s): Invited

8:00AM A62.00001: Inequivalence of the zero-momentum Limits of Transverse and Longitudinal Dielectric Response in the Cuprates*  [Invited]  CHANDAN SETTY (Presenter), BIKASH PADHI, KRIDSANAPHONG LIMTRAGOOL, ALI HUSAIN, MATTEO MITRANO, PETER ABBAMONTE, PHILIP PHILLIPS, Physics, University of Illinois at Urbana-Champaign — In this talk, I will address the question of the mismatch between the zero momentum limits of the transverse (optical conductivity) and longitudinal (momentum resolved EELS) dielectric functions observed in the cuprates. This question translates to whether or not the order in which the longitudinal and transverse momentum transfers are taken to zero commute. While the two limits commute for both isotropic and anisotropic Drude metals, I will argue that a scaleless vertex interaction is sufficient to achieve non-commutativity of the two limits even for a system that is inherently isotropic.

*1) Center for Emergent Superconductivity, DOE EFRC, Grant No. DE- AC0298CH1088.
2) NSF DMR-1461952
3) EPiQS program of the Gordon and Betty Moore Foundation, grant GBMF4542
4) Alexander von Humboldt Foundation: Feodor Lynen Fellowship program.

8:36AM A62.00002: Quasi-Continuous Mott Transition from a Spin Liquid to a Fermi Liquid at Low Temperatures  [Invited]  TETSUYA FURUKAWA (Presenter), Department of Applied Physics, Tokyo University of Science — For a long time, the Mott transition has been believed to be the first-order transition with a clear discontinuity at low temperatures, as shown by various experiments and the celebrated dynamical mean-field theory. Recent theoretical works, however, suggest that the transition can be continuous if the Mott insulator carries a spin liquid with a spinon Fermi surface[1,2]. Indeed, recent several experimental studies have suggested the existence of such spin liquids[3]; an organic triangular-lattice system κ-(ET)$_2$Cu$_2$(CN)$_3$ is one of the spin-liquid candidates with a spinon Fermi surface. In the present study, we demonstrate the case of a quasi-continuous Mott transition from a Fermi liquid to a spin liquid in κ-(ET)$_2$Cu$_2$(CN)$_3$[4]. We performed electric transport experiments under fine pressure tuning and found that as the Mott transition is approached, the Fermi-liquid coherence temperature continuously falls to the scale of kelvins, with a divergent quasi-particle decay rate on the metal side, and the charge gap gradually closes on the insulator side. A Clausius-Clapeyron analysis of the pressure-temperature phase diagram provides thermodynamic evidence for the extremely weak first-order nature of the Mott transition. These findings provide additional support for the existence of a spinon Fermi surface, which becomes an electron Fermi surface when charges are delocalized.

9:12AM A62.00003: Coherent Spin Excitations and Correlated Fermi Liquid in Genuine Mott Systems [invited] ANDREJ
PUSTOGOW (Presenter), 1. Physikalisches Institut, Universität Stuttgart — Recent success in determining the electronic
Correlation strength in Mott insulators by means of optical spectroscopy [1] enables a quantitative comparison among (i)
different materials and (ii) between experiment and theory. We identify frustrated molecular conductors as ideal
realizations of the single-band Hubbard model in contrast to transition-metal oxides with a more complicated band
structure, such as the charge-transfer insulator Herbertsmithite [2]. This finally allows us to selectively probe specific
regions in the unified phase diagram and unveil exotic phenomena in absence of magnetic order [1,3]. Deep in the
insulating state of a quantum spin liquid, coherent spin excitations show up in the optical conductivity when the charge
degrees of freedom are sufficiently suppressed within the Mott gap [3,4]. Turning to the correlated metallic state, we can
unambiguously identify the spectral features of coherent and bad-metallic transport. We observe a pronounced quadratic
temperature and frequency dependence of the scattering rate in the Fermi-liquid state. All data collapse on a generalized
energy scale in excellent agreement with the theoretical framework of Landau and Gurzhi from the 1950’s. We monitor the
effective mass enhancement as correlations increase and infer that the Fermi liquid retains its intrinsic properties towards
the Mott transition.

9:48AM A62.00004: A unified perspective on cuprates and layered organic superconductors* [invited] ANDRE-MARIE
TREMBLAY (Presenter), CHARLES-DAVID HÉBERT, Institut quantique, RQMP, Université de Sherbrooke, PATRICK SEMON,
Brookhaven National Laboratory — Layered organic superconductors of the BEDT family are model systems for
understanding the interplay of the Mott transition with magnetic order and frustration, ingredients that are essential to
understand superconductivity also in cuprate high-temperature superconductors. Cellular Dynamical Mean-Field Theory
yields a unified theoretical perspective on the corresponding phase diagrams containing superconducting,
antiferromagnetic and spin-liquid phases. In particular, the superconducting dome is tied to the Mott transition and its
continuation as a transition (Sordi transition) separating pseudogap phase from correlated metal in doped BEDT
compounds, as in the cuprates. Contrary to heavy fermions, the maximum of the dome is not attached to an
antiferromagnetic quantum critical point. The experimental superfluid stiffness shows highly non-BCS behavior that can
also be explained. A few experimental predictions follow. In particular, destroying superconductivity with a magnetic field
in the doped compounds should reveal the normal state transition between pseudogap and correlated metal.
Collaborators: C-D Hébert, P. Sémon, G. Sordi

*Sponsored by NSERC RGPIN-2014-04584, CIFAR, FRQNT, Compute Canada/Calcul Québec, Canadian Foundation for
Innovation, MESR (Québec), Research Chair in the Theory of Quantum Materials

Transistor* [invited] YOSHITAKA KAWASUGI (Presenter), RIKEN, KAZUHIRO SEKI, SISSA, JIANG PU, TAISHI TAKENOBU, Nagoya
University, SEIJI YUNOKI, RIKEN, HIROSHI YAMAMOTO, Institute for Molecular Science, REIZO KATO, RIKEN — Yoshitaka
Kawasugi: The electron correlation in solids, or the Mott physics, offers intriguing phenomena in materials such as
unconventional superconductivity. The key parameters for controlling the Mott physics are the electronic band filling and
bandwidth. However, the simultaneous control of these parameters has been lacking so far, leaving a comprehensive
phase diagram of correlated materials inaccessible. By combining electrostatic doping and bending-strain techniques, we
are able to control the band filling and bandwidth of an organic Mott insulator κ-(BEDT-TTF)2Cu[N(CN)2]Cl in a single
sample. As a result, doping-asymmetric ambipolar superconductivity has been observed in the proximity of the Mott
transition.

*This work was supported by MEXT and JSPS KAKENHI (Grant Nos. JP16H06346, JP15K17714, JP26102012 and JP25000003),
JST ERATO, MEXT Nanotechnology Platform Program (Molecule and Material Synthesis), and MEXT HPCI Strategic Programs
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time of the HOKUSAI GreatWave and HOKUSAI BigWaterfall supercomputer at RIKEN Advanced Center for Computing and
Communication (ACCC), and the K computer at RIKEN Center for Computational Science (R-CCS). K.S. acknowledges
support from the Overseas Research Fellowship Program of the Japan Society for the Promotion of Science.

Monday, March 4, 2019 8:00 AM - 11:00 AM
8:00AM A63.00001: The role of tolerance in the evolution of antibiotic resistance: from mathematical analysis to observations in the clinic* [invited] NATHALIE BALABAN (Presenter), Physics, Hebrew University of Jerusalem — The evolution of antibiotic resistance is a fascinating example of the versatility of bacterial evolution, as well as a burning health issue. Resistance mechanisms include efflux pumps that directly lower the intracellular drug concentration, mutations that reduce binding affinity of the drug to its target, enzymes that degrade the drug, etc. These mechanisms result in a decrease of the effective concentration of the antibiotic. However, bacteria were shown to be able to cope with antibiotic treatments that are supposed to kill them also using a different strategy termed "tolerance". Tolerant bacteria are not able to reduce the concentration of the antibiotic, but to make the duration of the treatment less effective. For example, bacteria that remain transiently dormant during the antibiotic treatment can survive because many different types of antibiotics require active growth to be able to kill. We developed a mathematical and experimental framework to characterize and measure the evolution of tolerance in vitro(1) and in vivo(2). By following the evolution of tolerance and resistance closely, we show that tolerance evolves fast and promotes the subsequent evolution of resistance.

Mathematical analysis of the way tolerance promotes the evolution of resistance reveals unexpected routes by which tolerance acts as a stepping stone for the subsequent evolution of resistance.

(2) Liu Jiafeng et al., Submitted

*European Research Council
Israel Science Foundation
Minerva Foundation

8:36AM A63.00002: Enzyme Evolution and Emergence of Novel Catalytic Functions ADITYA BALLAL (Presenter), Physics, Rutgers Univ, PAUL O'MAILLE, Stanford Research Institute, ALEXANDRE V MOROZOV, Physics, Rutgers Univ — Enzyme evolution underlies major expansions of metabolic complexity with profound biological implications. In this talk, I will discuss emergence of cyclization reactions catalyzed by terpene synthases. Cyclic terpenes mediate numerous biological functions in modern plants and provide bioactive compounds for human use, including artemisinin, the most effective treatment for malaria currently available. Guided by the available structural, kinetic, and sequence data, we have constructed mutant libraries which include combinations of amino acids responsible for inducing cyclization reactions in an enzyme that produces E beta-farnesene, a linear hydrocarbon chain. We have used measurements of kinetic rates and mass spectrometry in order to assess catalytic efficiency and specificity of the mutant enzymes. Inspired by spin glass models adapted from statistical physics, we have developed a model which predicts properties as a function of enzyme sequence. Using this model we have inferred evolutionary patterns of enzyme energetics. We have also developed a bio-physical model on fitness of an enzyme based on its catalytic properties. Our studies provide quantitative insights into evolutionary dynamics of a major enzyme family, and highlights the importance of epistasis.

8:48AM A63.00003: Nonlinear dispersal and growth change the phylogenetic structure of expanding populations GABRIEL BIRZU (Presenter), Physics, Boston University, OSKAR HALLATSCHEK, Physics and Integrative Biology, University of California, Berkeley, KIRILL KOROLEV, Physics, Boston University — Range expansions have shaped the evolutionary history of many organisms, from microbes to humans. Here, we study how the specifics of growth and dispersal affect the genealogical structure of expanding populations. The genealogical structure plays an important role in fixation of alleles, maintenance of genetic diversity, and genomic inference. Previous studies suggest that genealogies of expanding populations could be nontrivial because organisms at the expansion edge are expected to have an unusually large number of descendants. Indeed, we find these structures can be described by a family of Λ-coalescents, controlled by a single parameter: the ratio between the expansion velocity and the geometric mean of the dispersal and growth rates at low densities. For high values of this ratio, which occur when populations grow or disperse cooperatively, the genealogies are described by a Kingman coalescent. For low values—when the velocity is determined by growth and dispersal at the edge—we find a family of coalescents in which many lineages can merge simultaneously, including the Bolthausen-Sznitman coalescent at one end. These findings show that genealogies in expanding populations have a much richer structure than previously thought.
9:00AM A63.00004: Coevolution of multiple growth traits in microbial populations under serial dilution  JIE LIN (Presenter), School of Engineering and Applied Science, Harvard University, MICHAEL MANHART, Institute of Integrative Biology, ETH Zurich, ARIEL AMIR, School of Engineering and Applied Science, Harvard University — The relative fitness of mutants in a microbial population depends on multiple cellular traits. In the most widely-used evolution experiment protocol, serial dilution (where cells grow, enter stationary phase, and are diluted into a fresh medium), three major traits determining fitness are the growth rate, lag time (the duration of time cells do not grow when exiting stationary phase), and yield (number of cells per unit resource). Here we investigate how these traits coevolve in laboratory evolution experiments using a minimal model of population dynamics, where the only interaction between cells is competition for a single resource. We find that the fixation probability of a beneficial mutation depends on a linear combination of its growth rate and lag time relative to the background strain. The relative selective pressure on growth rate and lag time is set by the dilution factor; for example, a larger dilution factor favors adaptation of growth rate over the adaption of lag time. This result applies equally to the regime of large populations and high mutation rate, where there is abundant clonal interference, as well as the regime of sequential mutations. Moreover, we find an emergent correlation between growth rate and lag time even if mutations have uncorrelated effects.

9:12AM A63.00005: Rugged landscapes and evolutionary paths to variations in extreme size  THOMAS DAY (Presenter), SHANE JACOBEEN, COLIN BRANDYS, Physics, Georgia Institute of Technology, WILLIAM RATCLIFF, Biology, Georgia Institute of Technology, PETER YUNKER, Physics, Georgia Institute of Technology — The evolutionary transition to multicellularity transformed life on earth, allowing for the evolution of large, complex organisms. While multicellularity can be strongly advantageous, its earliest stages bring unique physical challenges, including the need to mitigate internal and external stresses. Previous work (Jacobeen et.al. *Nature Physics* 2018 and Jacobeen et.al. *PRE* 2018) used the model experimental system “snowflake yeast”, a baker's yeast (*S. cerevisiae*) genetically modified to remain attached via uncut chitin bonds during mother-daughter budding. However, so far these studies have focused on unimpeded directional selection for large size. Here, we varied the selection protocol to probe the effects of a more complex and rugged fitness landscape on the evolutionary trajectory of nascent multicellular clusters by subjecting the population to external compression prior to selection for larger size. We find that despite this challenge, the maximum cluster size achieved over eight weeks of experimental evolution is unchanged by the presence of compression. This indicates that significant evolutionary changes are possible even under harsh environmental conditions, and that very different selection environments can yield similar phenotypic variation.

9:24AM A63.00006: Protein evolution under multiple opposing selective forces*  ERDAL TOPRAK (Presenter), Green Center for Systems Biology, University of Texas Southwestern Medical Center — Evolution on a multidimensional adaptive landscape is the rule, not an exception in biological systems. When multiple opposing selection factors are simultaneously present or rapidly fluctuating in an environment, evolution is a genetic search on a convoluted fitness landscape with several pitfalls due to incompatibilities between genetic changes. Using a bacterial membrane protein as a model system, I will address (i) how evolutionary constraints on multiple fitness conditions arranged in a protein sequence and, (ii) how the rate and mechanism of protein evolution can vary under different (opposing or overlapping) selection conditions.

*This work was partially funded by National Institutes of Health (R01GM125748).

9:36AM A63.00007: Plastic tradeoffs in evolution: a simple theoretical model*  MIKHAIL TIKHONOV (Presenter), Physics, Washington University, St. Louis, SHAMIT KACHRU, Physics, Stanford University, DANIEL S FISHER, Applied Physics, Stanford University — Performance tradeoffs are fundamental to evolutionary thinking, but in most models, are simply postulated. This approach is justified for tradeoffs enforced by rigid biophysical or biochemical constraints; unsurprisingly, the best-understood examples are in this class. However, experimental results suggest that many relevant tradeoffs are not rigid, but can themselves evolve. We propose a simple theoretical framework for studying how an evolving tradeoff structure both shapes and is shaped by the evolutionary trajectory. We show that this feedback loop naturally leads to non-intuitive behaviors. For instance, although strongly diverging tasks might be expected to result in stronger tradeoffs, evolution can reverse this trend. We also show that within our model, pre-evolving a genome in one environment can predictably impede or facilitate its subsequent speed of adaptation in another. Our results extend previous work relating modularity and "evolvability" to a more general discussion of flexible tradeoff architectures and their impact on evolutionary dynamics.

*This work was supported by the National Science Foundation grants PHY-1607606, PHY-1720397, and by the Simons Foundation Investigator Award to SK.
9:48AM A63.00008: Homologous recombination rates of bacteria  EDO KUSSELL (Presenter), New York University —
Bacteria can take up DNA from their environment and incorporate it into their genomes using various recombination mechanisms. To quantify recombination rates in different environments requires a robust method that operates efficiently using large scale sequencing datasets. In this talk, I present such a method, based on exact solutions of population genetic models, and apply it in a wide range of bacteria.

10:00AM A63.00009: Tuning Spatial Profiles of Selection Pressure to Modulate the Evolution of Drug Resistance*
MAX DE JONG (Presenter), Physics, University of Michigan, KEVIN WOOD, Biophysics, Physics, University of Michigan — Spatial heterogeneity plays an important role in the evolution of drug resistance, but relatively little is known about resistance in complex spatial profiles of selection pressure. Here we use a toy model of stochastic microbial dynamics to investigate how different spatial profiles of selection pressure impact the time to fixation of a resistant allele. Using mean first passage time calculations, we show that spatial heterogeneity accelerates resistance evolution when the rate of spatial migration is sufficiently large relative to mutation but slows fixation for small migration rates. We also demonstrate that optimal tuning of the spatial profile can dramatically slow the spread and fixation of resistant subpopulations, even in the absence of a fitness cost for resistance. Finally, we incorporate a fitness cost associated with the resistant allele and observe that the intermediate regime in which spatial heterogeneity can speed or slow resistance is much larger and the effect of heterogeneity can be greatly amplified. Our results may lay the groundwork for optimized, spatially resolved drug dosing strategies for mitigating the effects of drug resistance.

*This work is supported by NSF No. 1553028 and NIH No. 1R35GM124875-01.

10:12AM A63.00010: Evolutionarily stable strategies in dynamic population models with applications to bird migration*  SAMUEL CHO (Presenter), SIMON LEVIN, Princeton University — Dynamic state variable models have been widely used to understand individual animal behaviors.1 However, when a population is studied, frequency-dependence and density-dependence often provide incentives to switch strategies, which are not captured in traditional dynamic models. In the discrete states and discrete time problem, we have a coupled forward-backward system, solution of which gives the evolutionarily stable policies determining the strategies for a given state. With the recent development of mean field game theory2, we can find general ecological conditions under which evolutionarily stable policies exist, and can be numerically found. We will also apply the results to understand various strategies during bird migration, such as choice of intermediate sites, foraging rates, and timing of arrival.

References:


*This work was supported by NHGRI pre-doctoral training grant of NIH and by NSF grant DMS-1514606: “Mathematical Methods for Water Problems”.

10:24AM A63.00011: Environmental heterogeneity limits the action of selection  MATTI GRALKA (Presenter), OSKAR HALLATSCHEK, University of California, Berkeley — Evolutionary dynamics is fundamentally shaped by stochastic processes: mutations enter populations randomly, and the fate of a mutant lineage is determined by the competition between (random) genetic drift and (deterministic) selection. In populations undergoing range expansions, fluctuations in the reproductive process and the local motion of individuals are enhanced within a small subpopulation at the edge of the population. Geographical heterogeneities could therefore have a dramatic impact on evolutionary dynamics if they shape the local advance of the population front.

To test this, we track the dynamics of spontaneous mutations with a tunable fitness effect in colonies of E. coli grown on randomly disordered surfaces and find that environmental heterogeneity can dramatically reduce the efficacy of selection. Time lapse microscopy and computer simulations suggest that this effect is a general consequence of a local "pinning" of the expansion front, whereby stretches of the front are slowed down on a length scale that depends on the structure of the environmental heterogeneity. This pinning focuses the range expansion into a small number of individuals with access to expansion paths, increasing the importance of chance and thus limiting the efficacy of selection.
The Replicator Dynamics for Multilevel Selection in Evolutionary Games

DANIEL COONEY (Presenter), Princeton University — We consider a stochastic model for evolution of cooperation in the Prisoner's Dilemma played in group-structured populations. Selection operates at two levels: individuals compete with individuals in their group, while groups compete with other groups. In the limit of infinite population size, we derive a non-local PDE describing the probability distribution of groups in the population. We characterize the long-time behavior of our system, with an emphasis on understanding the most frequent group compositions at steady state.

When average payoff of groups is maximized by all-defector groups, steady state composition ranges from all-defector groups when individual-level selection dominates to all-cooperator groups when group-level selection dominates. When group payoff is maximized by a mix of cooperators and defectors, then the steady state features a fewer cooperators than required for the optimal mix, even in the limit where group-level selection is infinitely stronger than individual-level selection. In such cases, the conflict between the two levels of selection cannot be decoupled, and cooperation cannot survive when between-group competition favors perfect coexistence of cooperators and defectors.

*I acknowledge support from NSF grants DMS-1514606 and GEO-1211972.

Evolution of weak cooperative interactions for biological specificity

ANG GAO (Presenter), KRISHNA SHRINIVAS, PAUL LEPEUDRY, HIROSHI I SUZUKI, PHILLIP SHARP, ARUP K CHAKRABORTY, Massachusetts Institute of Technology — A hallmark of biological systems is that particular functions and outcomes are realized in specific contexts, such as when particular signals are received. One mechanism for mediating specificity is described by Fisher's "lock and key" metaphor, exemplified by enzymes that bind selectively to a particular substrate via specific finely tuned interactions. Another mechanism relies on multivalent weak cooperative interactions. Its importance has recently been illustrated by the recognition that liquid-liquid phase transitions underlie the formation of membraneless condensates that perform specific cellular functions. Based on computer simulations of an evolutionary model, we report that the latter mechanism likely became evolutionarily prominent when a large number of tasks had to be performed specifically for organisms to function properly. We find that the emergence of weak cooperative interactions makes organisms more evolvable. Specificity mediated by weak cooperative interactions results in some useful cross-reactivity, but also increases susceptibility to mis-regulation.

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Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A64 DBIO: Physics in Synthetic Biology

Synthetic Biology: Physical Biology by Design [Invited] JAMES COLLINS (Presenter), Massachusetts Institute of Technology — Synthetic biology is bringing together physicists and biologists to model, design and construct biological circuits out of proteins, genes and other bits of DNA, and to use these circuits to rewire and reprogram organisms. These re-engineered organisms are going to change our lives in the coming years, leading to cheaper drugs, rapid diagnostic tests, and synthetic probiotics to treat infections and a range of complex diseases. In this talk, we highlight recent efforts to create synthetic gene networks and programmable cells, and discuss a variety of synthetic biology applications in biophysics, biotechnology and biomedicine.

Designing Physical Synthetic Biology [Invited] CHRIS VOIGT (Presenter), MIT — TBD
9:12AM A64.00003: Multiscale Effects of Temperature on Synthetic Gene Circuits  
DANIEL CHARLEBOIS (Presenter), KEVIN HAUSER, Laufer Center for Physical and Quantitative Biology, Stony Brook University, SYLVIA MARSHALL, Laufer Center for Physical and Quantitative Biology, Department of Biochemistry and Cell Biology, Stony Brook University, GABOR BALAZSI, Laufer Center for Physical and Quantitative Biology, Department of Biomedical Engineering, Stony Brook University — Synthetic gene circuits are rationally designed gene networks that perform predefined functions, and have promising applications in many areas including agriculture, bioenergy, and biomedicine. However, synthetic gene circuits are built and characterized in laboratory settings where extracellular variables, such as temperature, are maintained at optimal levels. To study how nonoptimal temperatures (as in real-world conditions) affect the function of synthetic gene networks, we combined multiscale computational modeling with experiments in genetically engineered budding yeast Saccharomyces cerevisiae. We discovered that nonoptimal temperatures induce a cell fate choice between stress resistant and growth arrested phenotypes. Overall, we found that four key effects are required to fully predict the effect of nonoptimal temperatures across different biological scales: 1) cell fate choice between arrest and resistance, 2) slower growth rates, 3) Arrhenius dependence of reaction rates, and 4) changes in protein structure. These findings advance our understanding of how temperature affects living systems and enable more robust genetic engineering for real-world applications.


9:24AM A64.00004: On the noise of gene expression in membrane-bound picolitre biochemical reactors  
ZIANE IZRI (Presenter), BYUOTA SAKAMOTO, Kyushu University, VINCENT NOIREAUX, Physics and Nanotechnology, University of Minneapolis, YUSUKE T. MAEDA, Kyushu University — A clonal population, sharing exactly the same genetic information, eventually displays variability in its observed metabolic properties, such as protein concentrations. In this presentation will be shown a new microfluidic setup that allows the screening of gene expression in a large number (N>1000) of identical picolitre microwells sealed by a biological membrane.

Gene expression of GFP using a cell-free transcription-translation system is performed in picolitre microreactors sealed by a membrane made of a mixture of phospholipids. Each experiment stands for a model clonal population. Although the kinetics of gene expression follows the same master curve for all the microwells, the end-points of the gene expression revealed a variability in the amount of protein produced, with a long right-tail distribution. This observation holds regardless of the composition of the outer phase, emphasizing this intrinsic property of the artificial cells.


9:36AM A64.00005: CRISPRgates: Programmable and Orthogonal Gene Circuit Elements  
DAVID SPECHT (Presenter), GUILLAUME LAMBERT, Cornell University — While CRISPR may be better-known as a gene editing tool, it can also be used as a tool for selective repression of genes using a catalytically-dead CRISPR nuclease. Here, we exploit both the freedom in the CRISPR identification region as well as the freedom in promoter design to create a set of 128 synthetic ‘barcoded’ promoters in E. coli, each of which is keyed to a specific CRISPR guide RNA. These synthetic promoters can then be used to drive chosen genes in modular fashion. We take a multiplexed approach using ‘randomized’ promoter barcodes to demonstrate orthogonality of the ‘CRISPRgates’ on a large scale. This method is immediately transferrable to many different CRISPR nucleases, including Cas9, Cas12a, Cas13a, and CasX, and we use it to study and contrast the behavior of these different systems and probe their properties, including the crRNA structure and PAM site sequence. We then explore how these orthogonal circuit elements can be exploited to create complex genetic circuits. These gates function as transcriptional NOT gates but are Boolean-complete and can in principle be assembled to produce time-dynamic gene circuits.

9:48AM A64.00006: Development of a new measurement standard for synthetic circuit design*  
BIN SHAO (Presenter), CHRIS VOIGT, Department of Biological Engineering, MIT — Large-scale engineering of biological circuits requires reliable measurements of genetic parts and a deep understanding of interactions between synthetic circuits and the host cell. However, the widespread adoption of non-physical units of measurement makes it difficult to parameterize synthetic parts and cellular context, which hinders the efforts to model multi-component synthetic circuits in a predictable way. Here we present a new measurement standard in which DNA- and RNA- binding proteins fused with spectrally well-separated fluorescent proteins are used to visualize plasmid and mRNA simultaneously. By combining quantitative fluorescence microscopy with a customized image processing pipeline, we are able to quantify promoter copy number, RNA production and protein abundance at the single cell level. This allows us to determine biophysical parameters of genetic devices, such as the RNA polymerase flux of a standard promoter. We also show that the new measurement standard can be further applied to investigate the transcriptional power of bacteria cells.

*NIST award 70NANB16H164
10:00AM A64.00007: Quantification of randomized programmable CRISPR-based toggle switches in Escherichia coli

YASU XU (Presenter), GUILLAUME LAMBERT, Cornell University — Recent developments and advances in CRISPR-Cas (Clustered regularly interspaced short palindromic repeats and CRISPR-associated proteins) systems have ushered a new generation of powerful genetic engineering tools in synthetic biology. In particular, a catalytically 'dead' version of CRISPR-Cas proteins that lack nuclease activity can essentially function as a logic NOR gate by selectively binding to a promoter sequence and preventing initiation of transcription by RNA polymerase. In this work, we create programmable and compact genetic toggle switches using pairs of mutually repressible orthogonal CRISPR-based NOR gates and measure the strength of these toggle switches in parallel using a next-generation sequencing method called “Cross-Seq”. Pairs of tandem positioned CRISPR toggle switch with randomized target barcode are inserted into plasmid and transformed into E. coli cells. Each toggle switch output controls a selectable or counter-selectable marker and, by the positively and negatively selecting for bacteria survival, we are able to measure the output of co-repressing NOR gates in all possible combinations and simultaneously quantify the relative strength and stability of dozens of toggle switches in parallel.

10:12AM A64.00008: Out-of-equilibrium microcompartments for the bottom-up integration of metabolic functions in population of artificial microsystems*

THOMAS BENEYTON, CRPP, CNRS, Univ. Bordeaux, DOROTHEE KRAFFT, CLAUDIA BEDNARZ, CHRISTIN KLEINBERG, CHRISTIAN WOELFER, IVAN IVANOV, TANJA VIDKOVIC-KOCH, KAI SUNDMACHER, Process Systems Engineering, Max Planck Institute for Dynamics of Complex Technical Systems, JEAN-CHRISTOPHE BARET (Presenter), CRPP, CNRS, Univ. Bordeaux — Self-sustained metabolic pathways in microcompartments are the corner-stone for living systems. From a technological viewpoint, such pathways are a mandatory prerequisite for the reliable design of artificial cells functioning out-of-equilibrium. We develop microfluidic platforms for the miniaturization and analysis of metabolic pathways in man-made compartments formed of water-in-oil droplets [1]. In a modular approach, we integrate a nicotinamide adenine dinucleotide (NAD)-dependent enzymatic reaction and a NAD-regeneration module as a minimal metabolism. We show that the functionalized microcompartments sustain a metabolically active state until the substrate is fully consumed. Reversibly, the external addition of the substrate reboots the metabolic activity of the microcompartments back to an active state. We therefore control the metabolic state of thousands of independent monodisperse microcompartments, a step of relevance for the construction of large populations of metabolically active artificial cells. The next challenges would be the coupling of our chemical functionalization with mechanical functions to design active micro-systems with life-like properties.


*MaxSynBio, IUF, ERC (306385), 'Région Aquitaine' and ANR-10-IDEX-03-02

10:24AM A64.00009: Synthetic Gene Circuits Controlling Precise Biological Pattern Formation in Multicellular-Mammalian Systems*

TYLER GUINN (Presenter), GABOR BALAZSI, Stony Brook University — Small molecules offer a diverse range of tools for probing fundamental principles of biological organization and hierarchy in biological physics. Yet, despite their strengths for controlling temporal biological functions, they are limited in exploring questions relevant to biological pattern formation. To address this need for studying spatiotemporal phenotypes in multicellular systems, we have created a toolbox of multiple light-inducible gene circuits that can tune gene expression and control levels of transcriptional noise at the single cell level. We accomplish this by engineering the tetracycline gene-expression system to convert light stimuli information into cellular response proteins in a spatiotemporal context with single-cell resolution. These circuits are built using the light responsive proteins LOV2 & VVD, a small peptide synthesized by the cell, and a light-inducible degradation tag. The resulting tools provide a platform for robust gene expression control in a spatiotemporal fashion, allowing easy exchange for genes of interest and probing physical biology questions in the context of cell-to-cell communication.

*We acknowledge the NIH MIRA grant #R35GM122561 and Laufer Center for Physical & Quantitative Biology for funding.
10:36AM A64.00010: Drop chemostats on a chip  ELAD STOLOVICKI (Presenter), LLOYD UNG, ROY ZIBLAT, DAVID A WEITZ, Harvard University — The adaptation process of biological system to novel challenge has a lot of variability. To investigate the spectrum of possible adaptation trajectories requires large ensemble of identical twin population. To address this challenge, we are developing a drop-based microfluidic device with hundreds of chemostats on a single chip. The chemostat is a continuous-culture apparatus that enables growth of cells in a well-controlled environment. The controlled conditions of the chemostat enable the measurement of population response to specific factor by varying only one environmental factor at a time. In the drop microfluidic approach, the chemostat vessel is ~1µL media drop surrounded by inert oil. Every population in every drop is an independent chemostat population. Each chemostat droplet is continuously diluted with fresh media. The flow of the chemostat drop insure the mixing of nutrient and suspension of the cells. The surrounding oil reduce the fouling of cells to the channel walls. The measurements can be done on the whole chemostat drop or only on the subtracted fraction. The subtracted fraction from the chemostat can be used to monitor the cells and environment in the drop using variety of distractive assays without interfering the chemostat experiment.

10:48AM A64.00011: Nanoelectronic lab-on-a-chip sensors to detect and monitor DNA hybridization  DELPHINE BOUILLY (Presenter), CLAUDIA MARCELA BAZAN, MADLINE SAUVAGE, MOHAMED OUQAMRA, AMIRA BENCHERIF, Université de Montréal — Nanoelectronic circuits are emerging as a promising technology for lab-on-a-chip, molecular-scale biosensors. In this presentation, I will present the design of such sensors using functionalized nanocarbon materials and their principle of operation to detect and monitor the hybridization of DNA sequences. Carbon nanotubes or graphene ribbons are immersed in a microfluidics platform and functionalized with single-stranded DNA. Hybridization of the tethered DNA with its complementary sequence induces a specific change in the electrical conductance of the devices. First, I will present recent experiments based on this design to detect specific DNA sequences. Second, I will describe the miniaturization of this approach to the single-molecule scale, and its application to monitor DNA hybridization dynamics with single-molecule resolution. Finally, I will discuss applications of this emerging technique for lab-on-a-chip biomedical technology.

Monday, March 4, 2019 8:00 AM - 10:48 AM

Session A65 DBIO: Physics of Behavior t BCEC 260 - Greg Stephens, Vrije Universiteit - Tag(s): Focus

8:00AM A65.00001: Reading the mind of the worm: Brain-wide neural dynamics predict behavior in C. elegans  [Invited]  MONIKA SCHOLZ (Presenter), ASHLEY N LINDER, FRANCESCO RANDI, ANUJ K SHARMA, XINWEI YU, JOSHUA SHAEVITZ, ANDREW M LEIFER, Princeton University — We record calcium activity from the majority of head neurons in freely moving C. elegans to reveal where and how natural behavior is encoded in a compact brain. We find that a sparse subset of neurons distributed throughout the head encode locomotion. A linear combination of these neurons’ activity predicts the animal’s velocity and body curvature and is sufficient to infer its posture. This sparse linear model outperforms single neuron or PCA models at predicting behavior. Among neurons important for the prediction are well-known locomotory neurons, such as AVA, as well as neurons not traditionally associated with locomotion. We compare neural activity of the same animal during unrestrained movement and during immobilization and find large differences between brain-wide neural dynamics during real and fictive locomotion.

8:36AM A65.00002: Root Circumnutation Facilitates Effective Subterranean Surface Exploration  ERIN N MCCASKEY (Presenter), Georgia Institute of Technology, KEVIN R LEHNER, ISAIAH TAYLOR, Biology, Duke University, YASEMIN OZKAN AYDIN, ENES AYDIN, Georgia Institute of Technology, PHILIP BENFEY, Biology, Duke University, DANIEL GOLDMAN, Georgia Institute of Technology — Circumnutation is the oscillatory movement first described by Darwin of a variety of plant organs including roots. A number of root traits have been suggested to improve tip penetration in environments where soil mechanical impedance is a limiting factor in growth, though little is known about the roles of circumnutation. After observing a root coiling phenotype on flat surfaces in non-circumnutating mutant rice roots, we hypothesized that root tip circumnutation facilitates effective root-surface exploration. To model a surface environment of a compact soil horizon with biopores we used plates with 2mm holes equally spaced at different densities. Mutant and wild-type (WT) rice were grown in a clear gel-based media and an automated high-throughput system acquired images to visualize the root growth. As hole density decreased mutants showed reduced success in finding a hole. WT roots had higher success indicating WT roots are more effective in flat surface exploration and less affected by sparse hole density, providing a plausible mechanism to buffer against environmental uncertainty inherent in soil exploration. We propose circumnutation provides a mechanism to break the intrinsic root coiling pattern seen in mutants, and that this movement consequently promotes root exploration.
Worm blob dynamics under thermal stress  YASEMIN OZKAN AYDIN (Presenter), DANIEL GOLDMAN, SAAD BHAMLA, Georgia Institute of Technology — Aggregate formation and clustering are common behaviors observed from bacteria to humans, and can facilitate the survival of the collective [Allee, 1978]. Here we discuss aggregation behavior in aquatic worms and its potential biological function. We first show how aquatic worms can be induced to aggregate into ensembles of thousands of worms that knot together, forming an active viscoelastic ‘blob’. This worm blob can be modulated from an elastic solid-like state to a viscous liquid-like state by changing the surrounding temperature. To establish how this complex transition occurs, we measure both the dynamics of individual worms and the collective. In single worms, we find that activity of an individual worm increases with temperature and reaches a peak value (0.05 cm/s) around 32°C. Thus, in groups at lower temperature (10°C), individual worms are less active and entangle together, while at higher temperatures (35°C), individual worms are more active and disentangle. More specifically, the steady-state density of the cluster decreases from 75% to 33% as temperature increases from 15 to 35°C, respectively. Our results suggest that worm's aggregates may serve as a robust survival strategy of the collective against environmental thermal stresses.

Dynamics of lateral undulation in legged terrestrial locomotion*  FABIO GIARDINA (Presenter), L MAHADEVAN, SEAS, Harvard — Although undulatory locomotion is commonly associated with limb-less animals such as snakes, there exist instances of slender multi-legged animals where undulation is also observed. In centipedes, for example, lateral body undulations emerge when they move fast, although the causes for the appearance of undulations have not been unequivocally clarified. A key unresolved question is whether undulation in myriapod locomotion arises due to the natural dynamics of the organism or if it is neurally enforced. To answer this question, we developed and studied a dynamical model that accounts for biologically plausible leg kinematics and morphologies. The insights obtained from the model analysis will be presented together with their implications for the evolution of locomotor morphology in many-limbed organisms, the principles of propulsion in terrestrial locomotion, and the design of robotic locomotion systems.

Inertial Tail-like Appendage Use in Quadrupeds Improves Stability in Diagonal Sequence Walking Gaits  HAOSEN XING (Presenter), Carnegie Mellon University, BAXI CHONG, Georgia Institute of Technology, GUILLAUME SARTORETTI, JULIAN WHITMAN, Carnegie Mellon University, YASEMIN OZKAN AYDIN, DANIEL GOLDMAN, Georgia Institute of Technology, HOWIE CHOSET, Carnegie Mellon University — There are two main sequences of footfall patterns for quadrupedal walking: lateral, adopted by most quadrupedal animals, and diagonal, preferred by quadrupedal primates. We observe that, compared with the lateral sequence (LS) gait, the diagonal sequence (DS) gait produces a larger stride displacement (i.e., higher average speed) but at the cost of decreased body stability. This work aims to increase the stability of the DS gait by investigating the use of an inertial tail-like appendage. We model this actuated tail as a multi-link manipulator whose dynamics describe how the system moves in response to joint torques. Employing a Lagrangian analysis, we derive tail oscillations that can resist the gravitational torque that drives the system off-balance. We validate our approach on a servo-based quadruped robot with an actuated tail, and compare the stride displacements of the LS and stabilized DS gaits. There, we experimentally show that with the help of an actuated tail, such a quadruped can take advantage of the higher stride displacement (larger) of the DS gait while maintaining stability. Future work will consider the use of an actuated tail to stabilize locomotion on unstructured terrain, as well as to balance dynamic trotting gaits.

Active sensing of particles suspended in unsteady flow*  DAISUKE TAKAGI (Presenter), Mathematics, University of Hawaii at Manoa, J. RUDI STRICKLER, Biological Sciences, University of Wisconsin Milwaukee — Animals can generate highly unsteady flow around their body. We explore how the flow on their mechanical sensors may help in remotely detecting and locating particles suspended in the surrounding fluid. A simple analytical model demonstrates the basic physical principle, which is analogous to active sonar except with flow instead of sound. The model shows that particle-induced fluctuations in pressure or shear on the sensors can be used to reconstruct a hydrodynamic image revealing the size and position of the particle. Our findings suggest that a variety of organisms and devices may actively agitate their surroundings to enhance their sensory range.

*We acknowledge support from the US Army Research Office (W911NF-17-1-0442) and the National Science Foundation (CBET-1603929).
### Kuramoto Model of Weakly Conformed Oscillators

**Presenter:** HUNG-YI LY, KUO-AN WU, National Tsing Hua University, HUAN-YU KUO, University of California San Diego — Conformity is a common phenomenon which is observed in social psychology, group decision making, and animal behavior. Inspired by the experiments of Moiseff and Copeland, in which they found that the response of female *Photinus carolinus* to computer flashes depends grossly on the synchrony of flashes, we consider a Kuramoto model with weakly conformed oscillators to study the effects of conformity on synchronization. In our model, the tendency of individual oscillator catching up each other varies with the degree of synchronization that mimics the conformity effect. While considering unimodal frequency distribution, a hysteresis loop emerges in the bifurcation diagram and the branch of unstable fixed points corresponds to the threshold, or "quorum", over which systems move toward more synchronized states. This result is similar to quorum response of consensus decision making, which a consensus decision is finally reached by entire group (oscillators reach synchronized states) once the population supporting it exceeds a quorum (once the degree of synchronization exceeds the threshold).

### Geometric mechanics and locomotion in dissipative environments

**Presenter:** JENNIFER RIESER, Physics, Georgia Institute of Technology, HENRY ASTLEY, Biology, University of Akron, JOE MENDELSON, Zoo Atlanta, CHAOHUI GONG, JIN DAI, Carnegie Mellon University, BAXI CHONG, Georgia Institute of Technology, PERRIN SCHIEBEL, YASEMIN OZKAN AYDIN, Physics, Georgia Institute of Technology, ALEX M HUBBARD, Georgia Institute of Technology, JEFFREY W RANKIN, KRIJN MICHEL, Royal Veterinary College, ALFREDO NICIEZA, Universidad de Oviedo, JOHN R HUTCHINSON, Royal Veterinary College, ROSS L HATTON, Oregon State University, HOWIE CHOSET, Carnegie Mellon University, DANIEL GOLDMAN, Physics, Georgia Institute of Technology — Sustained movement through complex terrain arises from the coupling of environmental interactions with cyclic self-deformation patterns generated by animals. Using both biological experiments and mathematical modeling, we explore the importance of body coordination and morphology for both limbless and limbed animals moving though a widely-encountered environment: on and within sand. Given the highly-dissipative nature of sand, we model environmental forces using granular resistive force theory (RFT) and use geometric mechanics (GM) to map local body deformations to body-frame displacements. We find that undulatory snakes and lizards swimming within sand use waveforms that produce near-maximal displacements per undulation cycle. Recently, we have found that granular RFT also applies to movement at the surface of dissipative materials, even when contact is intermittent. We apply surface granular RFT and GM to animals with cyclic ground contact patterns (e.g., legged locomotors). We find that the coordination between foot placement and spinal flexion observed in walking salamanders produces near-maximal displacements per gait cycle. These results highlight the broad applicability of these tools to understand coordination and self-deformation patterns in dissipative environments.

### Behavioral pattern transitions and habituation to pulsed mechanical vibration in crawling Drosophila larvae

**Presenter:** ALEXANDER BERNE, University of Miami, TOMOKO OYHAMA, McGill University, MASON KLEIN, University of Miami — How the brain receives, stores, and deploys information to create an adaptive response depends on external stimuli. Mechanical vibrations affect animal behavior, and are useful tool for understanding the correlation between neuron function and response. Using the Drosophila larva model system, a slow-moving animal with readily quantifiable behavior, we elicit a discrete set of observable avoidance responses: pause, turn, and reversal (strong) with vibration. We characterize in detail how each response type depends on vibration timing (pulse spacing and duration) and intensity (frequency and amplitude). Through precise larva tracking, we find that intensity above a threshold value increases the frequency of the reverse crawl behavior. Stimulus timing affects the probability of the each behavior: both prolonged and repeated vibration bursts over time reduce the proportion of animals reverse crawling (habituation). Additionally, memory deficient fly mutants show altered responses to repeated and sustained vibrations, suggesting the possible mechanism underlying habituated response. Drawing an analogy to a capacitor charging circuit, we model the possible relationship between biological mechanisms and habituated behavior in general.
10:12AM A65.00010: A minimal reaction-diffusion neural model generates *C. elegans* undulation  
HAROLD HASTINGS (Presenter), Bard College at Simon’s Rock, JENNY MAGNES, Physics, Vassar College, SIMON ELLIS, Computer Science, Vassar College, KATHLEEN SUSMAN, Biology, Vassar College, CHERIS C CONGO, MIRANDA R HULSEY-VINCENT, RIFAH TASNIM, Physics, Vassar College — The small (1 mm) nematode *Caenorhabditis elegans* has become widely used as a model organism; in particular the *C. elegans* connectome has been completely mapped (c.f. Jabr 2012) and *C. elegans* locomotion has been widely studied. The purpose of this paper to describe a minimal reaction-diffusion model for the *C. elegans* central pattern generator (CPG) (c.f. Xu et al. 2018, Wen et al. 2012). We use simulation methods to show that a small network of FitzHugh (1961)-Nagumo (et al.1962) neurons (one of the simplest neuronal models) based on a skeleton model of the *C. elegans* CPG can reproduce key features of *C. elegans* undulation (c.f. Magnes et al. 2017) and thus locomotion, compare the neuromechanical model of Izquierdo and Beer (2015). We also investigate dynamics and stability of the model. See Stephens et al. (2011) for the role of simple models in analyzing neurons and behavior.

References
Stephens Gj et al. 2011. PNAS USA 108 (Suppl 3), 15565
Xu T et al. 2018. PNAS USA 115 E4493.

10:24AM A65.00011: Comparative undulatory locomotion in complex environments  
KELIMAR DIAZ (Presenter), PERRIN SCHIEBEL, School of Physics, Georgia Tech, JIMMY L DING, Department of Bioengineering, Georgia Tech, HANG LU, Department of Chemical and Biomolecular Engineering, Georgia Tech, DANIEL GOLDMAN, School of Physics, Georgia Tech — Despite the difference in size, slithering animals from mm scale nematodes to m scale snakes are resistive-force dominated systems. These animals press lateral body bends against heterogeneities in their surroundings to overcome drag on the elongate, limbless body. To search for general principles of control in undulatory locomotion we studied the desert-specialist *C. occipitalis* and the nematode *C. elegans* traversing sparse lattices of rigid cylindrical posts, a model heterogeneous terrain. We challenged *C. occipitalis* to move through square arrays of 0.64 cm diameter posts embedded in a low-friction substrate and *C. elegans* with fluid filled PDMS lattices of comparable size. Both animals used a waveform which was largely preserved throughout a trial resulting in bouts of locomotion-when the body contacted an opportune obstacle-interspersed with large-slip-when the substrate alone provided propulsion. *C. elegans'* performance was comparable to *C. occipitalis*; when the animals did not contact posts they moved at ~0.2 body lengths per cycle (BL/cyc) while when they were in contact with the posts they moved at ~0.35 BL/cyc by bouts of motion. This suggests the strategies employed by both animals were similar despite the difference in size.

10:36AM A65.00012: Accurate quantification of bumblebee foraging  
DAVID HOFMANN (Presenter), AHMED ROMAN, DONNA ROSA MCDERMOTT, BERRY BROSI, ILYA NEMENMAN, Emory University — Bumblebees have been shown to learn simple forms of tool use and to transmit these skills to other members of the colony. They are thus an excellent animal model system to study learning and social interactions. However, such studies are complicated by the difficulty of precisely quantifying bumblebee behavior and interactions with the environment even in simple tasks, such as foraging. To address this, we designed a flight chamber with 3D printed artificial flowers to accurately quantify individual and collective bumblebee foraging. A radio frequency identification (RFID) system is employed to identify the individual foragers and detect their presence in flowers. A microfluidic system releases carefully controlled sucrose solution droplets of varying sizes in each flower in response to the presence of specific bees, and we then detect when the droplets are consumed. We quantify individual foraging behavior of naive bees exposed to two flowers with different reward probabilities in the course of multiple days. This mimics the setting of the well studied two-armed bandit problem in behavioral economics. We analyze the operant learning of the relation between a flower and a reward probability by the bees, and we compare the observations to predictions of various theoretical models.
8:36AM A66.00002: Hierarchical “buckling without bending” and cerebellar shape* MAHESH CHANDRASEKHAR
GANDIKOTA (Presenter), JM SCHWARZ, Syracuse University — While studies of brain shape development have focused on the cerebrum, the cerebellum, otherwise known as the little brain, typically houses more neurons than the cerebrum. Mammalian cerebella have 8-10 primary lobes which subsequently branch into smaller lobes. Recently, a “buckling without bending” model has been introduced to quantify the onset of shape change in the developing cerebellum and other brain organs/organoids. It consists of an inner incompressible core of cells and an outer fluid-like cortical layer of dividing cells encased by a pia membrane. Additionally, there are two types of fibrous cells - ones spanning the cerebellum and ones spanning the cortical layer. The onset of shape change is a consequence of mechanical constraints on the outer fluid-like cortical layer as it proliferates. Predictions of the model have been recently supported by experimental studies of the developing mouse cerebellum. Here, we generalize the model beyond the onset of shape change to predict shape development at later stages. We implement a hierarchical version of the above model to predict subsequent branching of the smaller lobes. Predictions are compared with various mammalian cerebella exhibiting varied counts of branching generations.

*NSF Grant #: 1507938

8:48AM A66.00003: Wrinkles on Tori XIAOXIAO ZHANG, Mechanical and Aerospace Engineering, Syracuse university, PATRICK MATHER, Chemical Engineering, Bucknell University, MARK BOWICK, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, TENG ZHANG (Presenter), Mechanical and Aerospace Engineering, Syracuse university — Wrinkling patterns in soft materials have been extensively studied due to their important roles in determining surface morphologies in biological structures and developing multifunctional devices. Most existing work focuses on relatively simple geometries, such as flat structures and curved structures with constant curvature such as the cylinder and 2-sphere. In this talk we discuss wrinkling patterns on a torus, the Gaussian and mean curvatures of which vary along the poloidal direction. We observe eight different wrinkling patterns from large-scale finite element simulations and construct a phase diagram for these patterns. We further show that the non-uniform curvature and anisotropic deformation play critical roles in determining the formation and evolution of these wrinkling patterns. The anisotropic deformation along the toroidal and poloidal directions controls pattern transitions from stripes to hexagons and the non-uniform curvatures determine the nucleation sites of the wrinkling patterns. Our results show that global deformations of a torus lead to strong coupling between elasticity and curvature which may enlarge the design space as well as the dynamically control of wrinkling patterns.

9:00AM A66.00004: Pattern formation in elastic bilayer systems through substrate pre-stretching FRANCISCO LOPEZ JIMENEZ (Presenter), University of Colorado, Boulder, RASHED A AL-RASHED, Massachusetts Institute of Technology, JOEL MARTHELOT, Princeton University, PEDRO REIS, Ecole polytechnique federale de Lausanne — Compressing a thin film bonded to an elastic substrate beyond a critical stress results in an elastic instability, often referred to as wrinkling or ruga, that generates complex surface deformation. Although the best-known example is the sinusoidal wrinkling that appears under uni-axial compression of the film, other loading conditions and actuation mechanisms result in a diverse range of self-organized patterns. We will present experiments in which the substrate is pre-stretched prior to the adhesion of the film, which when released results in film compression. We will show that with only moderate variations in the system and control parameters we can transition between a wide range of patterns, with a well-defined phase diagram spanning periodic wrinkles, creases, folds, and high aspect ratio ridges. We will also explore the dynamics that control the pattern formation, as well as the effect of repeated unloading and reloading, in an effort to rationalize how the specific details of the pattern are determined.

9:12AM A66.00005: Mechanical Principles Underlying Development of Bacterial Biofilm Morphology CHENYI FEI (Presenter), SHENG MAO, JING YAN, RICARD ALERT, HOWARD A STONE, BONNIE BASSLER, ANDREJ KOSMRILJ, NED WINGREEN, Princeton University — Surface-attached bacterial communities called biofilms display diverse morphologies. Our recent experiments demonstrated that growth-induced mechanical instabilities – including wrinkling and delamination – underlie the morphogenesis program of biofilms growing at the air-solid interface, and determine the characteristic wavelength of surface undulations. Yet, how the interplay between mechanics and biofilm growth determines colony expansion and morphogenesis remains unclear. Here, we define the physical mechanism underlying biofilm mecano-morphogenesis by combining microscopic and continuum models. We show that surface friction affects the thickness and edge propagation angle of colony biofilms. Moreover, this friction, along with a non-uniform pattern of growth due to nutrient depletion at the biofilm center, gives rise to anisotropic stress patterns. Interestingly, we also find that the combination of active exponential growth near the edge and linear increase of contour length contributes to a constant accumulation of tangential stress. This residual stress can be relaxed by subsequent mechanical instabilities. Finally, we propose a coarse-grained model to characterize the post-wrinkling/delamination expansion of biofilms.
Mechanical Feedback in Gut Looping

ADITI CHAKRABARTI (Presenter), SEAS, Harvard University, CLIFFORD J TABIN, Genetics, Harvard Medical School, LAKSHMINARAYANAN MAHADEVAN, SEAS, Physics, OEB, Harvard University

The midgut of most organisms consists of a long coiled tube that is dorsally attached to a thin sheet called the mesentery. Previous work has established that the physical foundations of the looping patterns arise from the differential growth between the gut tube and the mesentery in the context of their respective geometric and elastic properties, and that these looping patterns are evolutionarily modulated, at least in part, through species-specific variation in BMP2 levels, affecting the growth rates within the developing mesentery. However, how BMP2 signaling itself is modulated in an endogeneous setting remains unknown. We explore the possibility that tension in the mesentery feedbacks onto the tissue to regulate levels of BMP2, thereby controlling looping morphogenesis, using in-ovo and explant experiments. Quantifying this idea closes the feedback loop linking molecular signaling and gut morphogenesis in the chick embryo, and suggests an evolutionary pathway for exploring gut looping across organisms at a mechanistic level.

Modeling bio-inspired morphing mechanisms in hydrogel micro capsules

PAOLA NARDINOCCHI (Presenter), Sapienza University of Rome

We study changes in shape and size triggered by external stimuli in structures made of soft active materials. In particular, we consider morphing mechanisms driven by hydration and dehydration processes in capsule-like bodies which can hydrate and dehydrate causing the lateral collapse of the capsule body and the change of shape of the capsule. Typical examples come from Nature. In fern sporangium, the cells in the crest to one side of a spherical capsule enclosing the spores lose water by evaporation, so determining tension building up within them, and lateral walls collapsing internally [1,2]. In Sphagnum Moss, dehydration of the capsules cause them to change shape from spherical to cylindrical and to increase the internal air pressure [3].

In both the examples, the coupling between the dehydration process and the change in internal pressure determines a fast mechanism which allows to realize spore dispersal.

The goal of our study is to identify the mechanical determinants of the mechanism and investigate the role of the key geometrical and material parameters.


We acknowledge Sapienza Università di Roma for funding

Stress-Free Morphing

LUCIANO TERESI (Presenter), Mathematics & Physics, University Roma Tre, Italy

We study the morphing of soft materials within the framework of non-linear elasticity with large distortions: a distortion field induces a target metric, and the configuration which is effectively realized by a body is the one that minimizes the distance, measured through the elastic energy, between the target metric and the actual one.

Deformations due to distortions, in contrast to those generated by forces, can have a peculiar feature: they can be stress-free; if this is the case, the distortions field is called compatible.

We maintain that the morphing through compatible distortions is a key strategy exploited by many soft biological materials, which can exhibit very large shape-change in response to distortions controlled by chemicals or by temperature changes, while keeping their stress state almost null.

Thus, the study of compatible distortions, and of the related shape-changes, is quite important. Here, we show how the notions of metric tensor and of Riemannian curvature can be used to assess the compatibility of a distortion field.
10:00AM A66.00009: Modeling hemodynamic fluctuations: the brain vasculature as an excitable network  
MIGUEL RUIZ GARCIA (Presenter), ELENI KATIFORI, University of Pennsylvania — Multiple studies have examined blood oxygen level dependent (BOLD) signals of functional magnetic resonance imaging (fMRI) showing spontaneous fluctuations when the brain is at rest, sleeping or even anesthetized. These fluctuations are found at lower frequencies (around 0.1 Hz) than respiratory or cardiac functions. In addition, recent experimental works seem to rule out their relation with neural activity, suggesting a non-neural origin.

We propose a minimal model for microcirculation that only assumes a nonlinear relation between the current supported by each vessel and the pressure drop between its starting and final nodes, and a dispersive relation for volume accumulation. This simple approach qualitative reproduces the main characteristics of the observed behavior. The fluctuations emerge spontaneously under constant boundary conditions as self-sustained oscillations, forming different patterns depending on the topology of the network.

We expect that this model can shed light on the nature of spontaneous fluctuations on brain vasculature and its interplay with the properties of the network. Finally, the simplicity of the model makes it suitable for its use with different nonlinear flow networks exhibiting complex dynamical behavior.

10:12AM A66.00010: A simple developmental model recapitulates complex insect wing veination patterns (A wingkle in time)*  
JORDAN HOFFMANN (Presenter), Harvard University, SETH DONOUGHE, University of Chicago, KATHY LI, Columbia University, MARY SALCEDO, CHRISTOPHER RYRCROFT, Harvard University — Geometric patterns in nature have long been a matter of fascination and intrigue. Veins bifurcate insect wings into a diverse and complicated menagerie of shapes. For many insect species, even the left and right wings from the same individual have veins with unique topological arrangements, and little is known about how these patterns form. We present a quantitative study of the fingerprint-like “secondary veins.” We compile a dataset of wings from 232 species and 17 families from the order Odonata (dragonflies and damselflies), a group with particularly elaborate vein patterns. We characterize the geometric arrangements of veins and develop a simple model of secondary vein patterning. Last, we show that our model is capable of recapitulating the vein geometries of species from other, distantly related winged insect clades.

*US Department of Energy (DOE) Computational Science Graduate Fellowship, National Science Foundation Graduate Training Fellowships, the Applied Mathematics Program of the US DOE Office of Advanced Scientific Computing Research under Contract DE-AC02-05CH11231.

10:24AM A66.00011: Self-organization of tubular networks by fluid flows  
JEAN-DANIEL JULIEN, KAREN ALIM (Presenter), Max Planck Institute for Dynamics and Self-Organization — Long-ranged dynamic patterns are important for development and functioning of large-scale organisms. In the tubular networks of plasmodial slime molds the tubes’ periodic contractions organize in a traveling wave on scales of up to several centimeters. What drives communication across the network? What drives the self-organization of the tube’s cortex to form long-wavelength patterns? Searching for the mechanism of signal propagation we find that flows are hijacked by signals to propagate through the network. Signals promote their own transport by invoking a propagating front of increased flow. This mechanism is sufficient to explain complex dynamics of the organism like finding the shortest path through a maze. Importantly, we find that distant parts within the tubular network communicate by fluid flow. We investigate the mechanism behind the self-sustained contractile waves by developing a minimal model, coupling the mechanics of a cell’s cortex to a contraction-triggering chemical. The chemical itself is spread with the fluid flows that arise due to the cortex contractions. Through theoretical and numerical analysis, we find that the oscillatory component of the flows can give rise to robust scaling of contraction waves with system size—much beyond predicted length scales.
10:36AM A66.00012: Patterned smooth muscle constrains and constricts the airway epithelium during branching morphogenesis* KATHARINE GOODWIN (Presenter), ANDREJ KOSMRLJ, CELESTE NELSON, Princeton University — During branching morphogenesis, a simple tube of cells gives rise to an arborized epithelial network. In the mouse lung, the airway epithelium develops concomitantly with a layer of smooth muscle, which is derived from the surrounding mesenchyme and wraps circumferentially around the airways. We examined the role of smooth muscle in shaping domain branches that establish the underlying architecture of the lung. We found that branches begin as wide buds that thin at their bases as they extend. At the same time, there is an increase in the amount of smooth muscle wrapped around the parent bronchus at the base of each nascent domain branch. Perturbing the pattern of smooth muscle differentiation causes abnormal epithelial branching. Loss of smooth muscle results in ectopic branching events and slows branch thinning. Enhanced smooth muscle differentiation suppresses branch initiation and extension. Combining experiments with computational modeling revealed that patterned smooth muscle wrapping constrains and constricts the growing epithelium to properly position and physically sculpt domain branches.

*HHMI Faculty Scholars Award; NIH/NHLBI R01 HL120142; NSF CMMI-1435853

10:48AM A66.00013: Smooth Muscle Mechanically Sculpts the Airway Epithelium in Birds and Reptiles MICHAEL PALMER (Presenter), CELESTE NELSON, Princeton University — The reptilian lung, with its basic sac-like structure, is considered to be the most evolutionarily basic among amniotes. In comparison, mammalian and avian lungs are much more complex and finely branched. Smooth muscle (SM) is required for branching in the early mouse lung but to date this tissue remains uninvestigated in other amniotes. The respiratory system of birds contains a network of connected airways that begin as terminal structures but fuse as embryonic development progresses. We found that prior to airway fusion in the domestic chicken, Gallus gallus, the airways initiate branches in the direction of their target, which will make the first contact. These new branches occur in regions devoid of SM, implying a role for it in shaping the airway epithelium prior to fusion. We have also examined early development of reptile lungs using the brown anole, Anolis sagrei, as a model organism and found that SM is present in a mesh-like arrangement and regulated by the same signaling pathways as in the murine lung. Contraction of SM defines the shape of the epithelium. Despite the fact that the tissue forms at different periods in development and in varying patterns, these data suggest an evolutionarily conserved mechanism for SM as a physical force in airway morphogenesis.

Monday, March 4, 2019 8:00 AM - 11:00 AM

Session A67 APS/SPS: Undergraduate Research I BCEC 050 - Brad Conrad, American Institute of Physics - Tag(s): Undergraduate

8:00AM A67.00001: In-Operando Characterization and Investigation of Individual Defects in GaAs Solar Cells* SUNNY Y ZHANG (Presenter), QIONG CHEN, University of North Carolina at Charlotte, CHANG-KUI HU, Wuhan University of Technology, TIMOTHY HURLEY GFROERER, Davidson College, MARK W WANLASS, National Renewable Energy Laboratory, YONG ZHANG, University of North Carolina at Charlotte — The ultimate constraint for a solar cell to reach its theoretical efficiency limit is the quality of the absorber material. It is common knowledge that the existence of structural defects degrades device performance. However, in a real device, it is unclear (1) how individual defects affect performance via different cell parameters, (2) how the impact depends on the operation conditions, and (3) how the impact varies from one defect to another. This work answers these questions through investigating individual dislocation defects in GaAs solar cells under different illumination conditions. An array of correlative and spatially-resolved techniques, including electroluminescence, photoluminescence, Raman, and current-voltage (I-V) characteristics, is used to identify and characterize the defects. By comparing the I-V characteristics with the laser beam focused at the defect and defect-free site, the adverse impact of the defects is quantitatively measured through changes in the key device parameters, including short-circuit current, open-circuit voltage, fill factor, energy-conversion efficiency, and shunt resistance. This study provides insights for both a fundamental understanding of defect physics and practical knowledge of defects in the single defect level.

*ARO Electronics
8:12AM A67.00002: Charge-transfer-state energy reduction at various donor/acceptor interfaces*  
SARA ANJUM (Presenter), Physics, Princeton University — Organic solar cells have several properties that make them desirable over inorganic solar cells such as cost-effectiveness, flexibility, and lightweight. While organic solar cells tend to exhibit energy losses due to the need to break up charge-transfer (CT) states, a phenomenon that does not exist in its inorganic counterparts, highly-crystalline rubrene is a donor that has been shown to allow for delocalized CT states. This project aimed to examine the effects of the acceptor choice in the delocalization of charge transfer states by examining the energies of these states in the acceptors Cl6-subPc-Cl and Cl12-subPc-Cl. We found that the CT state energy dropped by 0.38 eV when going from amorphous to crystalline rubrene with Cl12-subPc-Cl as the acceptor. The CT state energy dropped by 0.38 eV when going from amorphous to crystalline rubrene with Cl12-subPc-Cl, which compares to the energy drop of 0.38 eV observed with C60 as the acceptor. This indicates that the choice of acceptor does have an impact on the CT-state energies.

*I would like to thank Prof. Rand and his lab for providing the funding necessary for my project.

8:24AM A67.00003: Determining the Interface Conductivity of Nb-SrTiO3 (Nb-STO) with Various Electrodes*  
GILLIAN HAGEN (Presenter), Physics, Mount Holyoke College, DAEHEE LEE, RUIYUN HUANG, SOSSINA HAILE, Materials Science and Engineering, Northwestern University — Solid oxide fuel cells have the potential to function within efficient systems of energy infrastructure. Nb-doped SrTiO3 (Nb-STO) (001) is an n-type semiconductor which has the potential to provide electrical contact for application in solid oxide fuel cells. We study the interface conductivity of Nb-STO with various metal and oxide contacts as a function of temperature (200°C-550°C) and oxygen partial pressure (10^-5 - 0.2 atm). We consider the interface of Nb-STO with metal contacts of Cr and oxide contacts of vertically aligned STO (100) and Sm-doped ceria (SDC) (100) through the fabrication of symmetric electrode devices. This presentation examines the interface electrical characteristics of Nb-STO with the two electrode materials studied. Overall, we demonstrate that Cr metal can provide contact to Nb-STO without resulting in a Schottky barrier, while vertically aligned STO (100) and Sm-doped ceria (100) nanocolumns cannot provide contact at elevated temperatures. The results of this study have implications on the use of single crystal Nb-STO as a conductive substrate for electrolyte materials in solid oxide fuel cells.

*This project was supported by the Northwestern University Materials Research Science and Engineering Center under NSF grant DMR #1720139.

8:36AM A67.00004: Ultrafast Carrier Dynamics of Exfoliated Transition Metal Dichalcogenides with Optical-Pump Terahertz-Probe Microscopy*  
KENNETH LIN (Presenter), Department of Physics, University of Massachusetts Amherst, SATOSHI KUSABA, TAKASHI ARIKAWA, Department of Physics, Kyoto University, FRANÇOIS BLANCHARD, Department of Electrical Engineering, École de technologie supérieure, KOICHIRO TANAKA, Department of Physics, Kyoto University — Atomically thin two-dimensional transition metal dichalcogenides (TMD) exhibit extraordinary properties similar to graphene but features an intrinsic bandgap, opening vast potential applications in photonics and optoelectronics as semiconductors. The characterization of these materials is essential for developing such technologies and the emerging technique of terahertz (THz) microscopy enables contactless probing that directly reveals the carrier dynamics of TMDs. We employ a unique, optical-pump THz-probe microscope to measure the electric field response of mechanically exfoliated bulk TMD MoS2. We measure the decay lifetime of bulk MoS2 electron carriers with a temporal resolution of approximately 500 femtoseconds in the 1 THz range. We observe the relaxation of free carriers to be uneven on a single sample and the decay constant was found to vary with position from 36.9 ps to 82.5 ps. Using atomic force microscopy, we demonstrate a correlation between the thickness of a given position on the MoS2 sample with the decay rate, where a thinner region or sample edge position corresponded to a faster decay. We attribute this nonuniform carrier relaxation rate to the edge state and surface defect effects.

*This work was supported by the Nakatani Foundation and Rice University.

8:48AM A67.00005: Development of Low Cost Room Temperature STM for the Preliminary Analysis of 2D Materials and Twisted Graphene Bilayers*  
PARAM PATEL (Presenter), MICHAEL ALTVATER, GUOHONG LI, EVA ANDREI, Physics, Rutgers University — Scanning tunneling microscopy (STM) is a valuable tool for studying atomic positions, electronic energy properties of materials, and distributions of electrons at the surface of a material. Using 3D printing, we developed a cost-effective room temperature STM for the analysis of 2D materials. After noise reduction and calibration, we can examine Moiré patterns in CVD-grown twisted bilayer graphene to efficiently identify the relative angle between the bilayers. This work demonstrates how modern tunneling microscopes can be used as a cost-effective preliminary diagnostic tool for studying atomic positions and electronic superlattices at material surfaces.

*Work supported by NSF EFRI 1433307, DOE-FG02-99ER45742, NSF DMR 1708158
Thermal and Structural Properties of Alkali Modified TeO2 Glasses

MARTHA JESUIT (Presenter), MICHAEL JOSEPH PACKARD, Coe College — The structural and thermal properties of lithium, sodium, and potassium tellurite glasses, written as JM2O-TeO2 where M is an alkali metal, were studied. Raman spectra were measured on all glasses along with the glass transition onset (Tg), crystallization (Tx), and melting (Tm) temperatures. All thermal measurements were measured on a Perkin-Elmer DSC-7. The thermal measurements were compared to the coordination of the tellurium. Coordination data was found by deconvoluting Raman spectra using Igor Pro to find the percent of Q4 and Q3 units in the glass.

Pure amorphous TeO2 was made using the water-quenching method then thermally tested against time to see how the glass transition onset and crystallization changed. We measured Tx and Tg every 30 minutes on glassy TeO2. Since TeO2 has a strong crystallization tendency, the samples were prepared in a nitrogen glovebox to minimize the effect that water could have on the recrystallization.

*NSF Grant DMR 1746230

Effect of varying the gate voltage scan rate in a MoS2/ferroelectric polymer field effect transistor

LUIS RIJOS (Presenter), NICHOLAS PINTO, Physics and Electronics, University of Puerto Rico at Humacao, MENGQIANG ZHAO, WILLIAM PARKIN, ALAN T JOHNSON, Physics and Astronomy, Univ. of Pennsylvania — A ferroelectric field effect transistor (FE-FET) using chemical vapor deposition (CVD) grown monolayer MoS2 as the semiconductor was fabricated and tested at room temperature. Ferroelectric poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE was used as the gate insulator, and the effects of varying the gate voltage scan rate from 200 mV/s to 4 mV/s on device performance were investigated. Prior to the device switching on, a negative trans-conductance was observed for all scan rates. It was followed by a rapid increase in the channel current to the on state, corresponding to the polarized down configuration of the FE. This effect was independent of the drain-source voltage. Our results revealed a narrowing in the memory window width, an increase in the mobility (μ) from 0.02 – 10 cm²/V-s, and a decrease in the sub-threshold voltage swing (SS) as the scan rate was lowered. These parameters appeared to stabilize at slower scan rates suggesting an asymptotic limit to their values. A model based on nucleation and unrestricted domain growth was used to explain these results. By lowering the gate voltage scan rate, the performance of polymer based FE-FET's can therefore be improved.

*This work was supported by NSF grants DMR PREM 1523463, DMR RUI 1800262 and EFRI 2DARE EFMA1542879.

Fabrication of planar tunnel junctions on bulk Pb1-xSnxSe

RAKIN BATEN (Presenter), DERRICK VANGENNENP, TIFFANY PAUL, JAMES HAMLIN, Department of Physics, University of Florida — The topological crystalline insulator Pb1-xSnxSe can undergo a trivial to non-trivial transition as a function of temperature or pressure. Angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling spectroscopy (STS) are both useful measurements for studying the nature of these topological transitions. However, ARPES and STS are incompatible with high pressure conditions. Planar tunneling spectroscopy (PTS) can provide similar information as STS but can be deployed at high pressure. I will discuss our efforts to fabricate Pb-alumina-Pb1-xSnxSe planar tunnel junctions and will present the results obtained thus far.

*This work was supported by National Science Foundation (NSF) CAREER award DMR-1453752.
REBELLO SOUSA DIAS, Physics, University of Richmond — Despite previous investigations on the fabrication and optical sheet resistance as low as 19.8 Ω for a composition of Zn_{0.25}Cd_{0.75}O. Moreover, the thin films have an average increasing Cd concentration, we notice a nonlinear red-shift. Also, we find that most of our films were conductive with a range. We show that the optical band gap of ZnO is in the ultraviolet region of the electromagnetic spectrum, and while samples through spectroscopy ellipsometry and transmittance measurements in the [300 nm – 3200 nm] wavelength range. In this work, we deposited Zn_{1-x}Cd_{x}O alloyed thin films via the spray pyrolysis method. We optically characterized the quality of (BixSb_{1-x})_{2}Te_{3} films. With RHEED and XRD we obtained information about different aspects of the crystal structure and how they were correlated. Further, we made devices of these films and measured their transport properties allowing us to correlate their structural and electronic properties.

*This work was supported by NSF grant 1560090 and NSF grant DMR-1557434.

OMAR AGUILAR (Presenter), Physics, University of Richmond, SUELEN DE CASTRO, MARCIO P. F. GODOY, Physics, Federal University of Sao Carlos, MARIAMA REBELLO SOUSA DIAS, Physics, University of Richmond — Despite previous investigations on the fabrication and optical characterization of Zn_{1-x}Cd_{x}O thin films spanning the whole composition range, the permittivity has yet to be determined. In this work, we deposited Zn_{1-x}Cd_{x}O alloyed thin films via the spray pyrolysis method. We optically characterized the samples through spectroscopy ellipsometry and transmittance measurements in the [300 nm – 3200 nm] wavelength range. We show that the optical band gap of ZnO is in the ultraviolet region of the electromagnetic spectrum, and while increasing Cd concentration, we notice a nonlinear red-shift. Also, we find that most of our films were conductive with a sheet resistance as low as 19.8 Ω for a composition of Zn_{0.25}Cd_{0.75}O. Moreover, the thin films have an average transmittance of 0.8 over a wide range of the electromagnetic spectrum. Understanding the optoelectronic properties of Zn_{1-x}Cd_{x}O thin films can pave the way to a more efficient Transparent Conducting Oxide (TCO).

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

AHMAD MATAR ABED (Presenter), Physics and Electronics, University of Puerto Rico at Humacao, TIMOTHY PILLSBURY, RUN XIAO, ANTHONY RICHARDELLA, NITIN SAMARTH, Physics, Pennsylvania State University — Topological insulators are in the focus of research due to their unique characteristics. Their unusual metallic surface states allow the spin of electrons moving through them to be controlled and used for spintronics and even potentially quantum computing. Here we present a structural analysis of bismuth antimony telluride (Bi_{x}Sb_{1-x})_{2}Te_{3} thin films grown using molecular beam epitaxy. The films were analyzed using the in-situ characterization technique reflection high-energy electron diffraction (RHEED) as they were grown and afterward using ex-situ x-ray diffraction (XRD). The work focused on having a better analysis for understanding the crystal quality of (Bi_{x}Sb_{1-x})_{2}Te_{3} films. With RHEED and XRD we obtained information about different aspects of the crystal structure and how they were correlated. Further, we made devices of these films and measured their transport properties allowing us to correlate their structural and electronic properties.

*The Penn State REU program in Interdisciplinary Materials and Materials Physics; supported by the Penn State Department of Physics, the Center for Nanoscale Science (NSF-MRSEC) and the National Science Foundation (DMR1460920 and DMR 1420620).
10:24AM A67.00013: Cassie-Baxter Transition: Gibbs Energy Analysis and CFD Simulations Using Newly Developed, Validated Algorithms  CHAE ROHRS (Presenter), PING HE, ARASH AZIMI, Lamar University — A liquid droplet on a textured substrate equalizes into either the Cassie-Baxter, or Wenzel state. In addition, metastable states between these conditions are reported in the literature. The Cassie-to-Wenzel transition has been understood as the intersection of the Cassie-Baxter and Wenzel equations, which are functions of the Young's angle; however, a major issue exists: the texture shape and dimensions are not considered. What's more, the transition point of the Young's model has not been experimentally verified. Because changing texture dimensions will also cause the droplet to transit from one state to another, we plan to build a new transition model through a Gibbs energy analysis of a liquid-gas-solid system. The Young's angle is held constant and the wetting phenomena are computed as a function of texture dimensions. Each dimension set will have an equilibrium state identified by its penetration depth and apparent contact angle. Lastly, the energy barrier describing the obstacle to a droplet moving from a meta-stable state toward the stable state can simultaneously be computed. Our newly developed, experimentally validated CFD method will be used to confirm our Gibbs energy analysis, and to explore the dynamic behaviors of a droplet during the Cassie-to-Wenzel transition.

10:36AM A67.00014: Magnetic vortex disks for magneto-mechanotransduction*  GEORGIA NELSON (Presenter), MEREDITH XU, XIAO WANG, ANDY CLARK, Department of Physics, Bryn Mawr College, DAVID KEAVNEY, The Advanced Photon Source, Argonne National Laboratory, RALU DIVAN, DAFEI JIN, Center for Nanoscale Materials, Argonne National Laboratory, XUEMEI CHENG, Department of Physics, Bryn Mawr College — A magnetic vortex, the ground state existing in micron- and submicron-sized ferromagnetic disks, is a three-dimensional spin structure that consists of a circulating in-plane magnetization and an out-of-plane vortex core. Magnetic vortex disks are promising mechanotransduction toolkits due to their capabilities in spatiotemporal manipulation of mechanical forces via the magnetic field. Here we report fabrication and magnetic imaging of patterned magnetic vortex disks. An array of Fe80Ni20 (Py) disks 3 um in diameter and 40 nm in thickness were fabricated using the photolithography, sputtering deposition, and lift off process. Element-specific photoemission electron microscopy imaging at the Ni L3 edge, performed at Beamline 4-ID-C of the Advanced Photon Source of Argonne National Laboratory, confirmed that the magnetic configuration of these Py disks are indeed magnetic vortices as expected. In the future, these fabricated magnetic vortex disks will be used as force or torque transducers in biomedical systems.

*This research was supported by the Center for Engineering MechanoBiology through a grant from the National Science Foundation's STC program (CCMI): 15-48571. Work at Argonne National Laboratory is supported by US-DOE, Office of Science, BES (No. DE-AC02-06CH11357).

10:48AM A67.00015: Thermoelectric Effects in a Double Mushroom Phase Change Memory Cell*  NOAH DEL CORO (Presenter), Electrical Engineering and Computer Science and Engineering, University of Connecticut, JAKE SCOGGIN, ALI GOKIRMAK, Electrical and Computer Engineering, University of Connecticut — Phase change memory (PCM) is a non-volatile memory that uses crystalline (set) and amorphous (reset) states to hold information. We use a finite-element PCM model1,2 to demonstrate thermoelectric effects in a cell with a novel “double mushroom” geometry. We analyze the impact of thermoelectric power (Peltier and Thomson heating) on device performance. We also compare the double and single mushroom cell write (reset and set) requirements and find better performance in the double mushroom due to enhanced thermal isolation.


*NSF REU EEC 1560098

Monday, March 4, 2019 8:00 AM - 10:24 AM

Session A69 FHP: The Author in Dialogue: David Kaiser's "How the Hippies Saved Physics"  BCEC 052A - Paul Cadden-Zimansky, Bard College - Tag(s): Invited, Undergraduate

8:00AM A69.00001: How the Hippies Saved Physics: Adventures with Bell's Theorem, Then and Now [invited]  DAVID KAISER (Presenter), Massachusetts Institute of Technology — In this talk I will describe the historical questions that led me to write my book, "How the Hippies Saved Physics". I will summarize some of the main findings, with a focus on how topics like Bell's theorem, and research on the foundations of quantum theory more broadly, moved from the margins to the mainstream of physics research. I will also reflect on the catalytic role that the historical project has played in my own, more recent research, including the recent "Cosmic Bell" experiments.
(Presenter), Williams College — John Wheeler arrived at the University of Texas at Austin in 1976. A year later he introduced a new graduate seminar, "Theory of Measurement," which, in addition to covering well-established topics such as the Wigner-Araki-Yanase theorem, also addressed more speculative concepts such as backward-in-time causation. Students were encouraged to try out their own ideas toward resolving some of the questions raised by quantum theory. This course, mentioned in David Kaiser's book, How the Hippies Saved Physics, provides an example of imaginative thinking about foundational issues within the mainstream physics community in the 1970's.

9:12AM A69.00003: Groovy Physics [Invited] PATRICK MCCRAY (Presenter), University of California, Santa Barbara — If the 1960s represented a boom time for physics, the 1970s presented something totally different. From a general backlash against Cold War-fueled research to the collapse of the job market for physicists, the Me Decade was mean decade. Despite these challenges – or perhaps because of them – a new ensemble of ideas and communities emerged. This talk provides a historical frame for appreciating David Kaiser's book How the Hippies Saved Physics while offering some observations on the various ways new kinds of physics emerged in response to changes in American values, society, and the economy.

9:48AM A69.00004: Embarking on a PhD to test Bell's inequalities in 1974: the most exciting subject I had ever encountered* [Invited] ALAIN ASPECT (Presenter), Laboratoire Charles Fabry — When I read Bell's paper[1] in 1974, it was like love at first sight. I immediately decided that this would be the subject of my PhD thesis. The paper clearly explained that one could experimentally settle the debate on the interpretation of Quantum Mechanics, between Einstein's position, which was totally convincing, and Bohr's point of view, which was the mainstream. A young professor at Institut d'Optique, Christian Imbert, allowed me to perform a Bell's test it in his lab. At that time, two pioneering experiments, one in Harvard (Holt and Pipkin) and one in Berkeley (Clauser and Freedman) had provided opposite results.

Beyond settling that contradiction, my goal was to work out an improved experimental scheme, in which the tension between quantum mechanics and relativity would be tested[3]. After some time, it was clear that this tension was subtle: even if standard quantum mechanics would be vindicated, it did not mean that one could use quantum non-locality to transmit "operational" information faster than light[4]. It had become clear to the physicists interested in that question, and I was one of them, that this "no signaling" was linked to the fundamental randomness of each individual quantum measurement and to the impossibility to duplicate a photon without perturbing its state.

[2] For a general review of the tests of Bell's inequalities, see for instance A. Aspect, Viewpoint: Closing the Door on Einstein and Bohr's Quantum Debate, Physics, 8 (2015) 123. 10.1103/Physics.8.123

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Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B01 DCMP: Defects in Topological Materials BCEC 106 - Jennifer Cano
transport characterization. We have demonstrated this method by carving a 2μm x 5μm x 10μm piece of SmB6 and placing
methods due to the inability to grow macroscopic crystalline samples. However, using standard TEM sample preparation
exist a large number of new quantum materials that are difficult to characterize using standard electrical transport
quantities and to understand the role of magnetization due to vacancies in the electronic propagation. The last is responsible for spin-flip processes. We use a self-consistent recursive Green's functions technique to calculate the
transport of graphene in the QSH phase in the presence of those magnetic vacancies. We use an unrestricted Hubbard mean field
Hamiltonian to model the electron-electron interaction, which enables both out-of-plane and in-plane magnetization.

For a monolayer graphene device, there exists one topological kink state, and the oscillation of the transmission
coefficients has a single period. The π Berry phase and the linear dispersion relation of kink states can be extracted from the
transmission data. For a bilayer graphene device, there are two topological kink states with two oscillation periods.
Our proposal provides an experimentally feasible route to manipulate and characterize the valley-polarized topological
kink states in classical wave and electronic graphene-type crystalline systems. The realization of the proposal in photonic
graphene is also discussed.

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BK20160007.

Partial lattice defects in higher order topological insulators  RAQUEL QUEIROZ, Department of Condensed Matter Physics, Weizmann Institute of Science, ION COSMA FULGA, Institute for Theoretical Solid State Physics, IFW Dresden, NURIT AVRAHAM, HAIM BEIDENKOPF, Department of Condensed Matter Physics, Weizmann Institute of Science, JENNIFER CANO (Presenter), Department of Physics and Astronomy, Stony Brook University, and the Center for Computational Quantum Physics, Flatiron Institute — Non-zero weak topological indices are thought to be a necessary condition to bind a single helical mode on lattice dislocations. In this work we show that higher-order topological insulators (HOTIs) can, in fact, host a single helical mode along screw or edge dislocations (including step edges) in the absence of weak topological indices. This helical mode is necessarily bound to a dislocation characterized by a fractional Burgers vector, locally detected by the existence of a stacking fault. The robustness of a helical mode on a partial defect is demonstrated by an adiabatic transformation that restores translation symmetry in the stacking fault. We present two examples of HOTIs, one intrinsic and one extrinsic, that show helical modes at partial dislocations. Since partial defects and stacking faults are commonplace in bulk crystals, the existence of such helical modes can in principle significantly affect the expected conductivity in these materials.

Honey, I Shrunk the Transport Geometry, or Carving Micro-Crystals of Topological Insulators for Transport Experiments  DMITRI MIHALIOV (Presenter), ALEXA RAKOSKI, SHRIYA SINHA, CAGLIYAN KURDAK, Physics, University of Michigan, PRISCILA ROSA, Los Alamos National Laboratory, ZACHARY FISK, Physics and Astronomy, University of California, Irvine, BOYOU N KANG, MYUNG-SUK SONG, BEONGKI CHO, Gwangju Institute of Science and Technology — There exist a large number of new quantum materials that are difficult to characterize using standard electrical transport methods due to the inability to grow macroscopic crystalline samples. However, using standard TEM sample preparation methods, it is possible to carve 10s of microns size crystalline pieces and place them on an insulating substrate for transport characterization. We have demonstrated this method by carving a 2μm x 5μm x 10μm piece of SmB6 and placing it on a Si substrate. The Hall bar was subsequently wired using Pt contacts deposited via FIB. We are also developing more demanding transport structures, such as double-sided Corbino rings with the goal of studying transport through individual threading dislocations. We will present challenges associated with sample preparation at the micro crystalline scale.

*CNpq and FAPERJ, Brazil
12:03PM B01.00005: Topological gravity, defects, and topological phases protected by both spatial and internal symmetries*  
BO HAN, university of illinois, HUAJIA WANG, UCSB, PENG YE (Presenter), Sun Yat-sen University — A substantial attention of quantum gravity has been paid in different areas of physics, from high energy physics, condensed matter physics to quantum information science. In this paper, we explore the topological quantum gravity from the perspective of symmetry-protected topological (SPT) phases. To be specific, we study the gravitational effect on the classification and response of 3+1d topological phases protected simultaneously by both spatial and internal symmetries from the topological response theory. The latter describes how geometric defect (e.g. disclination) and internal symmetry defect (e.g. domain wall) are topologically entangled. New topological terms involving nontrivial geometries are proposed, which are extensions of purely internal topological theories discussed before. Physical observables derived from these response theories are discussed and compared with their analogs in 2+1d systems, some of which have been well-studied in quantum Hall (QH) systems, like the Wen-Zee (WZ) term. Generalizations to symmetry-enriched topological (SET) phases are also discussed (arXiv:1807.10844).

*DARPA YFA program (D15AP00108), NSF DMR 1408713 and DMR 1725401, and Gordon and Betty Moore Foundation

12:15PM B01.00006: Kondo Signatures of a Quantum Magnetic Impurity in Topological Superconductor*  
XIAOQUN WANG (Presenter), RUI WANG, Shanghai jiao tong University, WEI SU, Nanjing University, JIAN-XIN ZHU, Los Alamos National Laboratory, CHIN-SEN TING, HAI LI, University of Houston, CHANGFENG CHEN, University of Nevada, BAIGENG WANG, Nanjing University — We study the Kondo physics of a quantum magnetic impurity in two-dimensional topological superconductors (TSCs), either intrinsic or induced on the surface of a bulk topological insulator, using a numerical renormalization group technique. We show that, despite sharing the p + ip pairing symmetry, intrinsic and extrinsic TSCs host different physical processes that produce distinct Kondo signatures. Extrinsic TSCs harbor an unusual screening mechanism involving both electron and orbital degrees of freedom that produces rich and prominent Kondo phenomena, especially an intriguing pseudospin Kondo singlet state in the superconducting gap and a spatially anisotropic spin correlation. In sharp contrast, intrinsic TSCs support a robust impurity spin doublet ground state and an isotropic spin correlation. These findings advance fundamental knowledge of novel Kondo phenomena in TSCs and suggest experimental avenues for their detection and distinction.

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12:27PM B01.00007: Impurity-induced bound states as a signature of chiral p-wave superconductivity in Pb_{1-x}Sn_xTe*  
SARBAJAYA KUNDU (Presenter), VIKRAM TRIPATHI, Tata Institute of Fundamental Research — The recent observation of surface superconductivity on the (001) surface of the topological crystalline insulator Pb_{1-x}Sn_xTe is intriguing, but the nature of the superconducting order is yet to be ascertained. In this context, we have recently proposed that a chiral p-wave superconducting order can be realized on the (001) surface of Pb_{1-x}Sn_xTe, in the presence of weak electronic correlations. In this talk, I will discuss impurity-induced subgap bound states as a possible experimental signature of the chiral p-wave order. In particular, I will introduce two parameter regimes: the normal band gap regime where the subgap bound states are smoothly connected to impurity states in semiconductors, and the inverted band gap regime, where they nontrivially depend on the existence of chiral p-wave superconductivity. I will further discuss properties of the analytically obtained bound state wavefunctions that are peculiar to the chiral p-wave order. For a point defect, these include the quasi-localized nature of the bound-state wavefunctions, and an internal SU(2) rotational symmetry of the zero-energy bound states that enables their use as a possible quantum qubit.

*DST for a Swarnajayanti grant (No. DST/SJF/PSA-0212012-13)
**12:39PM B01.00008: Fractional Chern insulator edges and layer-resolved lattice contacts**  
CHRISTINA KNAPP  
(Presenter), ERIC SPANTON, ANDREA YOUNG, CHETAN NAYAK, University of California, Santa Barbara, MICHAEL ZALETEL, Physics, UC Berkeley — Fractional Chern insulators (FCIs) realized in fractional quantum Hall systems subject to a periodic potential are topological phases of matter for which space group symmetries play an important role. In particular, lattice dislocations in an FCI can host topology-altering non-Abelian topological defects, known as genons. Genons are of particular interest for their potential application to topological quantum computing. In this work, we study FCI edges and how they can be used to detect genons. We find that translation symmetry can impose a quantized momentum difference between the edge electrons of a partially-filled Chern band. We propose layer-resolved lattice contacts, which utilize this momentum difference to selectively contact a particular FCI edge electron. The relative current between FCI edge electrons can then be used to detect the presence of genons in the bulk FCI. Recent experiments have demonstrated graphene is a viable platform to study FCI physics. We describe how the lattice contacts proposed here could be implemented in graphene subject to an artificial lattice, thereby outlining a path forward for experimental detection of non-Abelian topological defects.

*C.K. acknowledges support from the NSF GRFP under Grant No. DGE 114085.*

**12:51PM B01.00009: Quasiparticle interference and nonsymmorphic effect on a floating band surface state of ZrSiSe**  
ZHEN ZHU (Presenter), Shanghai Jiao Tong University, FENGQI SONG, Nanjing University, HSIN LIN, Academia Sinica, WEI KU, HAO ZHENG, JINFENG JIA, Shanghai Jiao Tong University — Nonsymmorphic crystals are generating great interest as they are commonly found in quantum materials, like iron-based superconductors, heavy-fermion compounds, and topological semimetals. A new type of surface state, a floating band, was recently discovered in the nodal-line semimetal ZrSiSe, but also exists in many nonsymmorphic crystals. Little is known about its physical properties. Here, we employ scanning tunneling microscopy to measure the quasiparticle interference of the floating band state on ZrSiSe (001) surface and discover rotational symmetry breaking interference, healing effect and anomalous half-missing Umklapp scattering. Using simulation and theoretical analysis we establish that the phenomena are characteristic properties of a floating band surface state. Moreover, we uncover that the half-missing Umklapp process is derived from the glide mirror symmetry, thus identify a nonsymmorphic effect on quasiparticle interferences. Our results may pave a way towards potential new applications of nanoelectronics.

**1:03PM B01.00010: Topological 0D defect states in 3D insulators**  
FRANK SCHINDLER, STEPLAN TSIRKIN (Presenter), TITUS NEUPERT, Department of Physics, University of Zurich, ANDREI B BERNEVIG, BENJAMIN WIEDER, Department of Physics, Princeton University — There has been intense interest in relating the electronic states bound to crystal defects to the bulk electronic structure of pristine crystals. By mapping the momentum-space Hamiltonians of Brillouin zone surfaces to the real-space surfaces between crystal defects, we develop a general formulation of topological (crystalline) defect states. We introduce topological invariants for these states using (nested) Wilson loops and Topological Quantum Chemistry. Our framework captures all previous results, including fractional charges bound to point defects in inversion-symmetric Chern insulators and helical modes bound to screw dislocations in weak topological insulators (TIs). However, we also discover new examples. In particular, we show that screw dislocations and edge disclinations in 3D higher-order TIs (HOTIs) can bind anomalous 0D higher-order “end states,” which are equivalent to the fractionally charged corner modes of 2D “fragile” TIs and obstructed atomic limits, and persist under the relaxation of particle-hole symmetry, which is not present in real materials. Using density functional theory and tight-binding calculations, we demonstrate the presence of higher-order defect end states in the HOTI and topological crystalline insulator SnTe.

**1:15PM B01.00011: Complete description of symmetry-protected topological properties of Sn_xPb_1-xTe_ySe_1-y topological crystalline insulators with a step edge**  
WOJCIECH BRZEZICKI, MARCIN WYSOKINSKI, TIMO HYART (Presenter), International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences — Surfaces of multilayer semiconductors typically have regions of atomically flat terraces separated by atom-high steps. Here we investigate the properties of the low-energy states appearing at the surface atomic steps in Sn_xPb_1-xTe_ySe_1-y. We identify the important approximate symmetries and use them to construct relevant topological invariants. We calculate the dependence of mirror- and spin-resolved Chern numbers on the number of layers and show that the step states appear when these invariants are different on the two sides of the step. Moreover, we find that a particle-hole symmetry can protect one-dimensional Weyl points at the steps. Since the local density of states is large at the step the system is susceptible to different types of instabilities, and we consider an easy-axis magnetization as one realistic possibility. We show that magnetic domain walls support a pair of zero-energy states because the regions with opposite magnetization are topologically distinct in the presence of non-symmorphic chiral and mirror symmetries, providing a possible explanation for the zero-bias conductance peak observed in the recent experiment [Mazur et al., arXiv:1709.04000].

*The work is supported by the Foundation for Polish Science through the IRA Programme co-financed by EU within SG OP.*
1:27PM B01.00012: Dynamically Induced Topology in the Fermi Sea* DANIEL DAHAN, EYTAN GROSFELD, Ben Gurion University of the Negev, BABAK SERADJEH (Presenter), Indiana University Bloomington — We study the dynamics of topological bound states following their coupling to the Fermi sea of a topologically trivial, gapless lead. Specifically, we study the quench dynamics of solitons in the Su-Schrieffer-Heeger model and of Majorana zero modes of Kitaev model. Remarkably, we find bound states propagate through the lead preserving their topological nature, such as fractional charge and exchange statistics. We explain this phenomenon as a manifestation of dynamically induced topology in the Fermi sea arising from the entanglement between the topological and gapless systems. We obtain, both analytically and numerically, topological features of propagating bound states, including their fractional charge, charge fluctuations, entanglement entropy, and fractional statistics. This allows us to characterize the coherence time over which these topological features relax. We also study the effects of interactions and disorder in the lead on the integrity of the topological bound states and the coherence time of dynamically induced topology.

*Supported by ISF grants 401/12 and 1626/16, the EU Seventh Framework Programme (FP7/2007-2013) grant 303742, BSF grant 2014345, and NSF grants PHY-1607611 and DMR-1350663.

1:39PM B01.00013: The influence of 1D topological states on the thermoelectric properties of Bi₂Te₃ from the perspective of coupled Tomonaga-Luttinger liquids (TLLs).* PIOTR CHUDZINSKI (Presenter), Queen's University Belfast — Bi₂Te₃, the first discovered strong 3D topological insulator is also one of the best known thermoelectric materials at ambient conditions. It has been recently discovered that in such 3D topological insulator each skew dislocation will host a pair of 1D topological states – a helical TLL. Any 1D state gives rise to huge Seebeck coefficient, a fact that is used in thermoelectricity enhancement by engineering of low dimensional nano-structures. One could then ascribe the outstanding thermoelectric properties of Bi₂Te₃ to these 1D topological states. However, in order to achieve a non-zero Seebeck coefficient, a mechanism that will induce curvature and backscattering of the 1D states is needed. One also needs a good description of 3D electronic states within a dense network of dislocations and proof that a large overlap with the 1D states is possible. In this study we show how to overcome these obstacles and then derive an exact analytic formula for Seebeck coefficient within a framework of coupled TLLs. Our study is applicable either to the regime of an extremely weakly n-doped material or to the case where the transport is activated by photo-excitations.

*Research supported by SFI-DfE Investigators Programme Partnership, Grant Number 15/IA/3160.

1:51PM B01.00014: Probing the Topological Classification of Bismuth with Topological Defects NURIT AVRAHAM (Presenter), ABHAY K NAYAK, JONATHAN REINER, RAQUEL QUEIROZ, HUIXIA FU, Weizmann Institute of Science, CHANDRA SHEKHAR, CLAUDIA FELSER, Max Planck, Dresden, BINGHAI YAN, HAIM BEIDENKOPF, Weizmann Institute of Science — The growing diversity of topological classes may lead to ambiguity in the classification of materials. Such is the case of Bismuth. While most theoretical models indicate that Bismuth possesses a trivial topological order, other theoretical and experimental studies suggest other classifications such as a strong, a weak, and a higher order topological insulator (TI), all of which host helical modes on their boundaries. We use scanning tunneling microscopy to investigate the response of the topological edge mode, in Bismuth, to a topological defect in the form of a screw dislocation. We find that the edge mode extends over a wider energy range than previously thought, and withstands crystallographic irregularities, without showing any signs of backscattering and gapping. Moreover, it seems to bind to the bulk screw dislocation, as expected for a TI with non-vanishing weak indices. These observations disfavor its recent identification as a hinge mode of a high order TI. We argue that the small scale of the bulk $L$ gap positions Bismuth within the critical region of a topological phase transition to a strong TI with non-vanishing weak indices. Consequently, the observed boundary modes are approximately helical already on the trivial side of the topological phase transition.

2:03PM B01.00015: Static analogues of driven phases of matter IAN MONDRAGON (Presenter), Department of Physics, Yale University, BRAHYAM RIOS, BORIS RODRIGUEZ, Instituto de Fisica, Universidad de Antioquia, MENG CHENG, Department of Physics, Yale University — Driven phases of matter are often said to arise only in nonequilibrium conditions. We here show that analogues of driven phases can be created as time-independent eigenstates of matter interacting with quantum light. These phases are characterized by a hidden geometric phase, referred to here as optical Berry phase, which is related to the average photon number of the system. We illustrate our results by studying an analogue of a driven topological state, the so called Anomalous Floquet Anderson Insulator. We show that the optical Berry phase manifests itself as a topological pumping of photons at the boundary equal to the bulk invariant. Finally, we discuss how the tools of cavity QED systems can be brought to bear in the study of these phases of light and matter.
11:15AM B02.00001: Clamped-ion flexoelectricity from first principles [Invited] CYRUS DREYER (Presenter), Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA; and Center for Computational Quantum Physics, Flatiron Institute, New York, NY, USA, ANDREA SCHIAFFINO, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra, Spain, MASSIMILIANO STENGEL, ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain; and Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra, Spain, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, USA — The flexoelectric (FxE) effect, where polarization is induced by a strain gradient, is universal in all insulators. As devices shrink to the micro and nano scale, large strain gradients can occur, and therefore the FxE effect can play a significant role in their electrical and mechanical properties. Also, the FxE effect can be exploited for novel device design paradigms such as piezoelectric "meta-materials" constructed from nonpiezoelectric constituents, or mechanical switching of ferroelectric polarization. One of the crucial limitations to understanding and exploiting the FxE effect is the lack of an efficient first-principles methodology to calculate all of the components of the bulk FxE tensor; the clamped-ion transverse and shear components in particular are problematic. In this work we develop such a methodology based on density functional perturbation theory to calculate the full bulk, clamped-ion FxE tensor from a single unit cell, by calculating the current-density response to the adiabatic displacement of atoms from a long wavelength acoustic phonon. In this talk I will outline our methodology, including recent developments relating to the implementation of a “metric wave” formalism, and apply it to calculate the clamped-ion flexoelectric constants in the context of cubic and distorted perovskite oxides.

11:51AM B02.00002: Spatial dispersion effects in ferroic oxides: Dynamical quadrupoles and flexoelectric tensor MASSIMILIANO STENGEL, ICMAB-CSIC and ICREA, MIQUEL ROYO (Presenter), ICMAB-CSIC — In condensed-matter physics, spatial dispersion refers to the dependence of many material properties on the wavevector $q$ at which they are probed, and is ultimately due to the nonlocality of the response to a given external field (electric, magnetic, strain). A remarkable example is the flexoelectric tensor, describing the polarization response to a gradient of applied strain, or equivalently the electrical current that is produced by an acoustic phonon at second-order in $q$. Density-functional perturbation theory (DFPT) appears as the ideal framework to compute these effects from first principles, but the general computational tools to deal with the long-wavelength limit are currently missing. Here we present a general formalism, based on the analytical long-wavelength expansion of the second-order DFPT energies, that enables the direct calculation of spatial dispersion quantities at a computational cost that is comparable to that of a uniform-field response calculation. We present results for the clamped-ion flexoelectric tensor in SrTiO$_3$ and the dynamical quadrupoles (the higher-order multipolar counterpart of the Born effective charges) in tetragonal PbTiO$_3$. The quadrupoles relate to the clamped-ion piezoelectric tensor as predicted by R. Martin in his 1972 seminal paper.

12:03PM B02.00003: Flexoelectricity and Twins in LaAlO$_3$* CHRISTOPHER MIZZI (Presenter), BINGHAO GUO, LAURENCE MARKS, Materials Science, Northwestern University — Flexoelectricity in complex oxides has recently garnered much interest due to its ubiquity, intrinsic scaling at the nanoscale, and device applications. Although this has resulted in a dramatic increase in the number of publications on this phenomenon, an abundance of fundamental questions persists. In particular, the role of microstructure on the flexoelectric response of oxides is scanty considered in the existing literature. Twinned oxides are well-posed to elucidate this question because they naturally bridge the gap between single crystals and polycrystalline ceramics. In this work, a dynamic mechanical analyzer in a three-point bending configuration was used to study the flexoelectric response of $\{100\}_{pc}$-LaAlO$_3$ with lamellar twin microstructures as a function of temperature. We found the flexoelectric response of LaAlO$_3$ is dominated by its twinned microstructure and tunable by two orders of magnitude via changing the number of twins, domain wall orientation, and domain wall mobility.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under award no. DE-FG02-01ER45945.
12:15PM B02.00004: Ferroelectric Materials for Photocatalytic Water-Splitting – Strained Mixed Anion Perovskites*
NATHALIE VONRÜTI (Presenter), ULRICH ASCHAUER, University of Bern — Polarity, for example in ferroelectric materials, can significantly increase a catalyst's performance by improving charge-carrier separation. However, polar distortions also increase the band gap as shown for epitaxially strained SrTiO\textsubscript{3} (1). While this band-gap increase is small for oxides, our density functional theory calculations show a much larger increase for oxynitrides: The enhanced covalency due to reduced electronegativity of nitrogen compared to oxygen results in larger strain-induced polar distortions and therefore more strongly increased band gaps by up to 1.5 eV. The reduced electronegativity, which leads to a higher valence band in oxynitrides and therefore a band gap in the visible that is attractive for photocatalysis, thus also has a detrimental effect on photo absorption when polar distortions are present. This results in a trade-off between small band gaps and polarity. We will discuss different strategies on how to overcome this trade-off with mixed anion perovskite compounds, which have not yet been considered for photocatalytic water-splitting.


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12:27PM B02.00005: Bulk- and Flexo-Photovoltaic effects*
[Invited] MARIN ALEXE (Presenter), MING-MIN YANG, DONG-JIK KIM, ZHENGDONG LUO, University of Warwick — Two years after the invention of modern prototype solar cells, it was found that BaTiO\textsubscript{3} exhibits a photovoltaic effect distinct from that of \textit{p-n} junctions, later called the bulk photovoltaic (BPV) effect. Under uniform illumination, a homogeneous ferroelectric material gives rise to a short-circuit current and produces an anomalously large photo-voltage well exceeding the bandgap energy. The microscopic origins of this effect supposed to originate from the asymmetric distribution of photoexcited non-equilibrium carriers in \textit{k}-space, caused by absence of centrosymmetry. The talk will present a short history and the basics of the bulk photovoltaic effect, tip enhancement, as well as the electronic origin of the anomalous BPV in some materials such as BiFeO\textsubscript{3}. Potential applications such as energy harvesting or light-induced reversible switching of ferroelectric polarization at room temperature will be addressed. I will show how the BPV effect may be used in optical switching tunnel junctions or other similar devices. Finally, I will discuss a new photovoltaic effect which turns the BPV effect into a universal effect allowed in all semiconductors by mediation of the flexoelectric effect. [M.-M. Yang D. J. Kim, & M. Alexe, Flexo-Photovoltaic Effect, Science 360, 904 (2018)]

*The work was partly supported by the EPSRC (UK) through Grant Nos. EP/M022706/1, EP/P031544/1 and EP/P025803/1

1:03PM B02.00006: Complex chalcogenides as highly-polarizable semiconductors*
STEPHEN FILIPPONE, Massachusetts Institute of Technology, SHANYUAN NIU, Department of Chemical Engineering and Materials Science, University of Southern California, KRISTOPHER WILLIAMS, WILLIAM A TISDALE, Massachusetts Institute of Technology, YI-YANG SUN, Shanghai Institute of Ceramics, Chinese Academy of Sciences, JAYAKANTH RAVICHANDRAN, Department of Chemical Engineering and Materials Science, University of Southern California, RAFAEL JARAMILLO (Presenter), Massachusetts Institute of Technology — Ternary sulfides and selenides in the distorted-perovskite and related structures ("complex chalcogenides") are predicted to be semiconductors with band gap in the visible-to-infrared, and may be useful for optical, electronic, and energy conversion technologies. The crystal structures familiar to complex oxides, together with larger chalcogenide anions, suggest that complex chalcogenides will be highly polarizable semiconductors.

We will report theoretical and experimental progress towards establishing the fundamentals of highly-polarizable complex chalcogenide semiconductors. We use computational thermodynamics to predict the phase diagrams for select materials, highlighting windows of equilibrium between solid and vapor phases – relevant to growing films by molecular beam epitaxy (MBE). We then report on progress towards MBE growth of complex chalcogenide films, focusing on control of H\textsubscript{2}S and H\textsubscript{2}Se gas precursors. We will also report experimental results on complex chalcogenides in the Ba-Zr-S system, including time-resolved photoluminescence suggesting slow minority carrier recombination, and impedance spectroscopy providing evidence of highly-polarizable materials with band gap below 2 eV.

*NSF DMR-1751736 "CAREER: Fundamentals of complex chalcogenide electronic materials"
Understanding Negative Thermal Expansion in Layered Perovskites
CHRIS ABLITT (Presenter),
Department of Materials, Imperial College London, NICHOLAS C BRISTOWE, School of Physical Sciences, University of Kent, MARK S SENN, Department of Chemistry, University of Warwick, ARASH A MOSTOFI, Department of Materials and Department of Physics, Imperial College London — Negative thermal expansion (NTE) is an unusual phenomenon where a material shrinks rather than expands with increasing temperature. We will present recent results showing that in layered perovskites there is a significant enhancement of elastic anisotropy due to symmetry breaking that results from the combined effect of layering and frozen rotations of oxygen octahedra. This feature, unique to layered perovskites of certain symmetry, is what allows uniaxial NTE to persist over a large temperature range [1]. Since the structure of this phase facilitates cooperative strains in-plane and along the layering axis without necessitating the deformation of stiff nearest neighbour bonds, it has been possible to derive a mathematical description of this mechanism in an idealised system using simple geometrical models [2]. This insight has allowed us to investigate how changing structural features, such as the layer thickness [3]; physical features, such as temperature [1]; and chemistry, by substitutional doping [4] may all be used to control the thermal expansion of the material.


Reduction of the thermal conductivity in PbTiO3 thin-films by ferroelectric domain walls.*
ERIC LANGENBERG, Materials Science and Engineering, University of Cornell, DAVIG BUGALLO-FERRÓN, University of Santiago de Compostela, DIPANJAN SAHA, Mechanical Engineering, Carnegie Mellon University, ELAS FERREIRO-VILA, University of Santiago de Compostela, JONATHAN A MALEN, Mechanical Engineering, Carnegie Mellon University, DARRELL G. SCHLOM, Materials Science and Engineering, University of Cornell, FRANCISCO RIVADULLA (Presenter), University of Santiago de Compostela — The development of materials with switchable thermal conductivity have been limited to small low/high thermal conductivity ratios. We experimentally demonstrate that the thermal conductivity of PbTiO3 films can be significantly reduced through ferroelectric domain wall engineering. Ferroelectric domain walls (DWs) are effective phonon scattering sites, whose density and spacing can be controlled by an electric field, and therefore offer a unique opportunity to modulate the thermal conductivity by an external stimulus. In our experiments, we significantly reduced thermal conductivity by engineering the type and configuration of the DWs, as well as the DW density, through epitaxial strain and impurity doping.

*We acknowledge support from MINECO (Spain), Proj. MAT2016-80762-R, Xunta de Galicia (Centro singular de investigación de Galicia accreditation 2016-2019, ED431G/09) and the European Regional Development Fund.

Intrinsic Piezoelectricity above Curie temperature in BaTiO3*
SERGEI PROKHORENKO (Presenter),
YOUSRA NAHAS, Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, IGOR KORNEV, Laboratoire Structures, Propriétés et Modélisation des Solides, CentraleSupélec, DARIUSZ KAJEWSKI, Institute of Physics, Institute of Silesia, DANIEL RYZT, Forschungsinstitut für mineralische und metallische Werkstoffe, Edelsteine/Edelmetalle (FEE) GmbH, KRISTIAN ROLLEDER, Institute of Physics, Institute of Silesia, LAURENT BELLAICHE, Physics Department and Institute for Nanoscience and Engineering, University of Arkansas — Barium titanate, a classical ferroelectric compound, is known to exhibit non-trivial precursor properties above the Curie temperature that directly point to the polar character of its “paraelectric” phase. In this study we combine theoretical analysis, large scale effective Hamiltonian simulations and experiments performed on high quality single crystals to revisit the origins of precursor effects in BaTiO3. Our results demonstrate that the non-trivial piezoelectric response at temperatures far above Tc is an intrinsic feature of BaTiO3 not related to structural defects or sample fabrication conditions but rather a consequence of complex high-temperature dipolar structure and strong order-disorder nature of local ionic potential of this material.

*S.P and L.B. acknowledge the DARPA Grant HR0011-15-2-0038 (MATRIX program). Y. N. and L.B. thank the ARO Grant No. W911NF-16-1-0227, S.P., Y.N. and L.B. also acknowledge the DARPA Grant No. HR0011727183-D18AP00010 (TEE Program), and are grateful for support provided by NVIDIA GPU Grant program. K.R. thanks the National Science Centre, Poland, for support through the project 2016/21/B/ST3/02242. Computations were possible thanks to the use of the Arkansas High Performance Computing Center and the Arkansas Economic Development Commission.
First-principles study on piezoelectricity in Bi(Fe,Co)O₃

HIROSHI KATSUMOTO (Presenter), KUNIHIKO YAMAUCHI, TAMIO OGUCHI, The Institute of Scientific and Industrial Research, Osaka University — The perovskite solid solution BiFe₁₋ₓCoₓO₃ (BFCO) is composed of BiFeO₃ and BiCoO₃, which have rhombohedral and tetragonal structure, respectively. BFCO is a promising lead-free piezoelectric material, since the morphotropic phase boundary (MPB) was discovered around 0.2 < x < 0.4 region at room temperature, where monoclinic phase is present [1]. A typical multiferroic material, BiFeO₃ shows ferroelectricity and G-type antiferromagnetic order at room temperature. On the other hand, BiCoO₃ shows high tetragonality and C-type antiferromagnetic order. The enhancement of piezoelectric coefficients and polarization rotation can be expected in a vicinity of the MPB as in PZT. The monoclinic crystal structure is √2×√2×1 perovskite cell which accommodates the antiferromagnetic configuration. The spontaneous polarization and the piezoelectric coefficients have not been measured in the bulk system so far, owing to the large leakage current. In this context, we performed first-principles calculations of the spontaneous polarization and the piezoelectric response of a Fe/Co chemically ordered model of BFCO. Based on the results, we discuss the ferroelectric distortion and the microscopic mechanism of the piezoelectric effect in BFCO.


Lithium niobate single crystal as a novel host for persistent luminescence

SHAO PENG LIN (Presenter), HUASHAN LI, CHEN WEI XIONG, DECAI MA, Sino-French Institute of Nuclear Engineering and Technology, Sun Yat-sen University, BIAO WANG, School of Physics, Sun Yat-sen University — LiNbO₃ (LN) is one of the most versatile and widely used materials in photonics with broad applications such as holographic storage, electro-optical modulator, optical switch, on-chip waveguide circuit, harmonic generator and micro-electro-mechanical system, etc. In the past decades, LN has presented various mysterious optical properties based on ions-doping engineering. However, persistent luminescence (PersL) has not been reported so far. In this study, bright red PersL was found in Mg²⁺ and Pr³⁺ co-doped congruent LiNbO₃ single crystal excited with ultraviolet at room temperature. Photoluminescence, photoluminescence excitation, thermoluminescence glow curves and afterglow decay curves have been investigated. Accordingly, a transition mechanism based on energy level distribution has been proposed to describe PersL, wherein both Mg²⁺ and Pr³⁺ ions play essential roles. Given the outstanding ferroelectric, piezoelectric, electro-optical, and mechanical properties of host material, our findings open an opportunity to couple various responses to external stimuli, and thus to develop novel applications based on multifunctional persistent luminescence phosphors.


Session B03 DCMP: Novel Excitations in Topological Systems

Splitting the hinge mode of higher-order topological insulators

RAQUEL QUEIROZ (Presenter), Condensed Matter Physics, Weizmann Institute of Science — We study the effect of the coupling of a helical mode in a two-dimensional topological insulator without inversion symmetry — focusing at the surface of a higher order topological insulator (HOTI) — to a proximate ferromagnet and to a proximate s-wave superconductor. We find that in contrast to the helical modes of inversion symmetric systems, which are gapped by these couplings, when inversion is broken the helical modes generically remain gapless and spatially split. The ferromagnet turns the helical mode into a chiral mode that surrounds the magnetized region, and the superconductor, when strong enough, turns that mode to two helical Majorana modes that surround the superconducting region. The enclosed superconductor comprises a two dimensional, time-reversal invariant, topological superconductor. We propose that this state can be measured in electrical transport by an extension of previously proposed interferometry experiments.
11:27AM B03.00002: Magneto Optic Kerr Effects of an Antiferromagnet - Topological Insulator Heterostructure*
TONMOY BHOWMICK (Presenter), AMRITANAND DE, ROGER LAKE, University of California, Riverside — We investigate the magneto-optic memory applications of a topological insulator proximity coupled to an anti-ferromagnet. We find that this gives rise to a high figure of merit magneto optic Kerr effects. The optical dielectric tensor elements are calculated using the Kubo formula and are based on a tight-binding electronic structure model. We calculate the Fermi level dependence of the MOKE signature and explore the AFM-TI optical phase diagram. This system can lead to applications such as a topologically protected high density antiferromagnetic magnetic optic memory device with ultra-low error rates.

*This work is supported by the NSF ECCS-1408168 and by SHINES an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0012670.

11:39AM B03.00003: Glide-resolved photoemission spectroscopy: measuring topological invariants in nonsymmorphic space groups*
ARIS ALEXANDRADINATA (Presenter), Yale University, ANDREI B BERNEVIG, ZHIJUN WANG, Princeton University, MICHAEL ZALETEL, University of California, Berkeley — The two classes of 3D, time-reversal-invariant insulators are known to subdivide into four classes in the presence of glide symmetry. Based on ab-initio calculations, we predict materials that realize all three, nontrivial insulating phases. We further elucidate the smoking-gun experimental signature of each class in the photoemission spectroscopy of surface states. Measuring the Z_4 invariant relies on identifying the glide representation of the initial Bloch state before photo-excitation -- this is accomplished with relativistic dipole selection rules, combined with standard spectroscopic techniques to resolve both momentum and spin. As an orthogonal by-product of our method, we propose how to generate a source of 100% spin-polarized photoelectrons, which have diverse applications in solid-state spectroscopy.

*AA: Yale Postdoctoral Prize Fellowship. BAB and ZW: Department of Energy de-sc0016239, Simons Investigator Award, the Packard Foundation, the Schmidt Fund for Innovative Research, NSF EAGER grant DMR-1643312, ONR - N00014-14-1-0330, ARO MURI W911NF-12-1-0461, and NSF-MRSEC DMR-1420541.

11:51AM B03.00004: Bulk-edge correspondence in 1D non-Hermitian systems
KAZUKI YOKOMIZO (Presenter), SHUICHI MURAKAMI, Tokyo Institute of Technology — Recently, the role of the topology in non-Hermitian systems is attracting much attention. It is known fact is that the conventional bulk-edge correspondence breaks down in non-Hermitian systems if the Bloch wavevector $k$ is set to be real. Here, to restore the bulk-edge correspondence, the non-Bloch factor $\beta=\exp(ik)$, $k\in \mathbb{C}$ is introduced in the SSH model with the asymmetric hopping [1]. In this case, one can show the bulk-edge correspondence by defining the winding number by using $\beta$. However, it is not obvious how to systematically calculate $\beta$ in general case. In this talk, we show how to calculate $\beta$ in general 1D models for constructing the continuum bulk-bands. It is non-trivial because the states in the continuum bulk-bands do not extend over the bulk, unlike those in the Hermitian systems. We also discuss the bulk-edge correspondence in general cases by defining the generalized Brillouin zone in terms of $\beta$. [1] S.Yao, et al., Phys. Rev. Lett. 121, 086803 (2018)

12:03PM B03.00005: Quantum Control of Current Partition at Trifurcating Topological Channels*
TAO HOU (Presenter), Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, YUJIE QUAN, YAFEI REN, Department of Physics, University of Science and Technology of China, JEIL JUNG, Department of Physics, University of Seoul, WEI REN, Physics Department, Shanghai University, ZHENHUA QIAO, Department of Physics, University of Science and Technology of China — Topological channels can emerge a network along the domain walls that separate AB and BA stacking regions in minimally twisted bilayer graphene, which have been imaged by using scanning tunneling microscope recently. Here, we design a six-terminal graphene device to study how the incoming valley-polarized current will partition at the topological crossing point. We find that the incoming current not only can be partitioned into the two adjacent topological channels, but also goes straight along the incoming topological channel, which together form a trifurcating beam splitter. We provide a further systematic study on how to externally tune the trifurcating current partition by means of manipulating the system size, Fermi-energy, magnetic field, relative masses.

*National Key Research and Development Program (Grant No. 2016YFA0301700) National Key Research and Development Program (Grant No. 2017YFB0405703) National Natural Science Foundation of China (Grant No. 11474265)
12:15PM B03.00006: Metallicity at the Ioffe-Regal limit in a topological insulator thin film*  ILAN ROSEN (Presenter), Stanford University, INDRA YUDHISTIRA, GIRISH SHARMA, National University of Singapore, MARYAM SALEHI, JISOO MOON, DEEPTI JAIN, SEONGSHIK OH, Rutgers University, MARC KASTNER, Stanford University, SHAFFIQUE ADAM, National University of Singapore, DAVID GOLDHABER-GORDON, Stanford University — The topological surface states of time-reversal invariant 3D topological insulators have applications for spintronics, metrology, and the realization of topological superconductivity. Initial excitement around these surface states, however, focused on the prediction that they should be robust against Anderson localization, even under strong disorder. This prediction has never been directly confirmed by transport measurements. We present low-temperature transport measurements of a gate-tunable Sb$_2$Te$_3$ topological insulator thin film that features high mobility and low carrier density. We find that metallicity is preserved at conductivities well below $e^2/h$, where two dimensional electron systems conventionally scale to an insulating state. Near the charge neutrality point, we observe an unusual magnetoconductance response, which we associate with known weak localization/anti-localization behavior, but beyond the Ioffe-Regal limit $k_F l \sim 1$.

*This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.

12:27PM B03.00007: High order band topology and fractional charges of vortex bound states*  EUNWOO LEE (Presenter), BOHM-JUNG YANG, Physics and Astronomy, Seoul National University — In a one-dimensional system described by the SSH model, a half-integer electric charge can be localized at the domain wall between topological and trivial systems. A similar phenomenon can also occur in certain two dimensional systems in which fractional electric charge can be localized at a vortex core. We show that the origin of the zero-mode bound to a vortex comes from the higher order topological physics. Considering several concrete examples, we show that vortex bound states can generally be understood as a spatial charge pump between higher order topological phase and trivial phase. In particular, when PT symmetry exists, we show that the pumping of the second Stiefel-Whitney invariant $w_2$ corresponds to the number of zero modes localized at the vortex core.

*E.L is supported by IBS-R009-D1. This work is supported in part by the U.S. Army Research Office under Grant Number W911NF-18-1-0137.

12:39PM B03.00008: Topological phases of non-Hermitian systems*  FLORE KUNST, Stockholm University, VATSAL DWIVEDI (Presenter), University of Cologne — Non-Hermitian fermionic systems are known to exhibit features strikingly different from their Hermitian counterparts, a quintessential example being the lack of a bulk-boundary correspondence in the conventional sense. In this talk, I will describe a transfer matrix approach to these systems. The algebraic structure of the transfer matrix and a Riemann surface associated with the complex energies provide a clear and intuitive picture of various topological aspects of these systems.

*VD was funded by the Deutsche Forschungsgemeinschaft (DFG) within the CRC network TR 183 (Projects No. B01 and No. B03). FK was funded by the Swedish Research Council(VR) and the Knut and Alice Wallenberg Foundation.

12:51PM B03.00009: Many-Body Invarinats for Electric Multipoles in Higher-order Topological Insulators  BYUNGMIN KANG (Presenter), HYUNWOONG KWON, KWON PARK, Physics, Korea Institute for Advanced Study, GIL YOUNG CHO, Physics, Pohang University of Science and Technology — According to the modern theory of polarization, the electric polarization in solids is defined via Berry phase, which definition is fundamentally different from the classical definition of polarization involving charge distribution. In certain classes of crystalline topological insulators, the electric polarization is known to take quantized value due to underlying crystalline symmetries. Recently, the theory of multipole moments in crystalline insulators was developed where the quadrupole moment and higher-order multipole moments can be defined quantum mechanically. Although crystalline symmetries are useful they are not essential in understanding multiple moments, and so far the theory is only applicable to non-interacting crystalline band insulators. In this talk, I will introduce a many-body order parameter for quadrupole moment which provides a way to extend the quantum theory of multipole moments to the most general setting including interacting case. I will also discuss the bulk-boundary correspondence for quadrupole moment, relating seemingly unrelated quantities from the bulk and from the boundary.
1:03PM B03.00010: Spin Transport in Topological Material - Graphene Heterostructures

DMITRII KHOKHRIAKOV, ANDRE DANKERT, SAROJ DASH (Presenter), Chalmers University of Technology — Topological insulators are known to have unique electronic and spintronic properties [1]. On the other hand, graphene and h-BN are proven to be excellent materials for long distance spin transport [2] and a large tunnel spin polarization [3], respectively. Here, we combine graphene with topological materials and semiconductors in van der Waals heterostructures to demonstrate the emergence of a strong proximity-induced spin-orbit interaction in graphene [4,5]. By performing spin transport and precession measurements, we discover a strong tunability and suppression of the spin signal and spin lifetime due to a strong hybridization of their electronic bands [4,5]. The enhanced spin-orbit coupling strength is estimated to be nearly an order of magnitude higher than in pristine graphene. These findings in 2D materials heterostructures could open interesting opportunities for exploring exotic physical phenomena and new spintronic device functionalities.


1:15PM B03.00011: Dynamical Phase Transitions in Topological Insulators

NICHOLAS SEDLMAYR (Presenter), Department of Physics and Medical Engineering, Rzeszow University of Technology, MICHAEL FLEISCHHAUER, Technical University of Kaiserslautern, JESKO SIRKER, University of Manitoba — The traditional concept of phase transitions has, in recent years, been widened in a number of interesting ways. The concept of a topological phase transition separating phases with a different ground state topology, rather than phases of different symmetries, has become a large widely studied field in its own right. Additionally an analogy between phase transitions, described by non-analyticities in the derivatives of the free energy, and non-analyticities which occur in dynamically evolving correlation functions has been drawn. Here we focus in particular on the way in which these dynamical phase transitions themselves can be used to shed light on topological phase transitions and topological phases. We consider, firstly, the effect of the topologically protected edge states, which are one of the interesting consequences of topological phases, on dynamical phase transitions. Secondly we consider what happens in the experimentally relevant situations where the system is either in a thermal state rather than the ground state, or connected to an external environment.

1:27PM B03.00012: Spin Stiffness and Domain Walls in Dirac-Electron Mediated Magnets*

SAHINUR REJA, HERBERT FERTIG (Presenter), Indiana University Bloomington, LUIS BREY, Instituto de Ciencia de Materiales de Madrid — We consider the problem of ordering of classical magnetic impurities which are indirectly coupled by two-dimensional Dirac electrons, as might be present in graphene or at the surface of a topological insulator. For chemical potential at a Dirac point, the magnetic order parameter develops an emergent long-range form of the spin stiffness, becoming truly long-range as the magnetization density becomes very small. It is demonstrated that this leads to screened Coulomb-like interactions among domain walls. A transfer matrix analysis demonstrates that the interaction takes this form from a subtle cancellation between energy contributions from in-gap bound states and phase shifts of scattered electrons. Detailed studies of graphene and a topological crystalline insulator surface are used to illustrate the behavior. The non-analytic behavior of the stiffness on magnetization density is shown to have interesting consequences for the phase diagram of these systems.

*Supported by the NSF, BSF, and MEyC-Spain.
1:39PM B03.00013: Topological tunability from even-odd order parameter mixing of monolayer 1T-TaSe₂ charge density wave*  
MING-CHIEN HSU (Presenter), SHIN-MING HUANG, Department of Physics, National Sun Yat-sen University, 
BAHADUR SINGH, College of Optoelectronic Engineering, Shenzhen University, CHUANG-HAN HSU, Department of Physics, National University of Singapore, SUYANG XU, Department of Physics, Massachusetts Institute of Technology, Cambridge, HSIN LIN, Institute of Physics, Academia Sinica, CHENLIANG SU, SZU-NUS Collaborative Center and International Collaborative, Laboratory of 2D Materials for Optoelectronic Science & Technology, Engineering Technology Research Center for 2, ARUN BANSIL, Department of Physics, Northwestern University — Monolayer 1T-TaSe₂ has been found to have charge density wave (CDW) experimentally. The primary CDW order parameter takes the M₁⁻ symmetry having odd parity and will change parity of electronic states of the system. Due to the coexistence of three q vectors from the primary order parameter, a secondary order parameter of even parity is induced inevitably. The mixture of the two opposite-parity order parameters will break inversion symmetry, which fails connection between symmetry and topology. Here we propose a method to decouple the parity-odd and parity-even CDW gaps, so that we can perform continuously the inversion-asymmetric CDW state into an inversion-symmetric one. In this way it helps to understand topological phase transitions in inversion asymmetric systems from the inversion-symmetry point of view.

*The project is supported by the Ministry of Science and Technology (MoST) in Taiwan under grant No. 105-2112-M- 110-014-MY3 and also by the NCTS of Taiwan.

1:51PM B03.00014: Spectral weight suppression as a gap-like feature in the non-magnetic states of topological insulators*  
TURGUT YILMAZ (Presenter), University of Connecticut, ANNA PERTSOVA, Nordita, WILLIAM HINES, University of Connecticut, ALEXANDER BALATSKY, Nordita, BORIS SINKOVIC, University of Connecticut — Here, we present an answer to one of the much debated questions in the topological insulator research, i.e., the opening of an energy gap-like feature at the Dirac point without long range ferromagnetic order. This is in sharp contrast to the topological protection of the surface states against non-magnetic perturbations. We carried out a systematic photoemission study on Cr-doped Bi₂Se₃ films grown on pristine Bi₂Se₃ films which allow us to monitor the evolution of the topological electronic structure. Our angle-resolved photoemission spectroscopy experiments revealed a gap-like feature appears just below the Dirac point leaving the Dirac point unaffected by the doping. Furthermore, the Dirac point is buried under the bulk conduction band which prevented it from being resolved in previous photoemission experiments. The spectral weight suppression just below the Dirac point leads to the gap-like feature being mistakenly identified as an energy gap at the Dirac point.

*This work was funded by the University of Connecticut under the UCONN-REP (Grant No. 4626510) and also by the Institute for Materials Science and LDRD XWNK at Los Alamos National Laboratory.

2:03PM B03.00015: Anomalous dielectric response in insulators with a topological π Zak phase*  
SHUICHI MURAKAMI (Presenter), YUSUKE AIHARA, Dept. of Physics, Tokyo Institute of Technology, MOTOAKI HIRAYAMA, CEMS, RIKEN — In the topological phase of the Su-Schrieffer-Heeger model, the Zak phase is equal to π. While it corresponds to the e/2 polarization, there is no electric dipole moment because of inversion symmetry. We find that an external electric field gives rise to an abrupt rise of the dipole moment, close to e/2. This sudden uprise of the dipole moment is attributed to the midgap state at the two ends of the system. We also extend this idea to two- and three-dimensional insulators with the π Zak phase over the whole Brillouin zone, and show that similar sudden uprise of the polarization by an external electric field happens also in these cases, if the midgap boundary states due to the π Zak phase has sufficiently flat dispersions. Finally, we discuss possible candidate materials for this behavior, including the (111) surface of Si and the (111) surface of a topological electride Sc₂C.

*This work was supported by Grant-in-Aid for Scientific Research from MEXT (Grant No.18H03678), by CREST, JST (Grant No. JPMJCR14F1), and by MEXT Elements Strategy Initiative to Form Core Research Center (TIES).

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B04 DMP GMAG: Dirac/Weyl Semimetals -- Magnetic Topological Semimetals BCEC
107C - Zhiqiang Mao - Tag(s): Focus
11:15AM B04.00001: Magnetic Weyl Semimetal in Quasi Two-dimensional Half Metallic Co$_3$Sn$_2$S$_2$  QIUNAN XU (Presenter), Max Planck Institute for Chemical Physics of Solids, ENKE LIU, Institute of Physics, Chinese Academy of Sciences, WUJUN SHI, School of Physical Science and Technology, ShanghaiTech University, LUKAS MUECHLER, Chemistry, Princeton University, JACOB GAYLES, CLAUDIA FELSER, YAN SUN, Max Planck Institute for Chemical Physics of Solids — A Weyl semimetal can exist in a time reversal or inversion symmetry breaking system. Since the Berry curvature is odd under time reversal, the Berry curvature from Weyl points are expected to generate a large anomalous Hall effect in time reversal symmetry breaking Weyl semimetals. In this work, we find a Weyl semimetal phase in half metallic ferromagnet Co$_3$Sn$_2$S$_2$ with Weyl points only 60 meV away from the Fermi level, which derive from nodal lines that are gapped by spin-orbit coupling. Therefore, the Weyl-related physics should be easy to detected by both ARPES and bulk transport measurements. Due to the Berry curvature deriving from the gapped nodal lines and Weyl points, its anomalous Hall conductivity can reach up to 1200 S/cm. Substituting S by Se, Co$_3$Sn$_2$Se$_2$ shows very similar property. Moreover, since Co$_3$Sn$_2$S$_2$ is easily grown quasi two-dimensional compound, it provides an ideal platform for the study of magnetic Weyl physics and its future application in topological material based spintronic devices.

11:27AM B04.00002: Topological Weyl semimetals in Full Heusler Co$_2$MnX (X = Si, Ge, Sn)*  ABHISHEK SHARAN (Presenter), University of Delaware, FELIPE CRASTO DE LIMA, Instituto de Física, Universidade Federal de Uberlândia, SHOAIB KHALID, ANDERSON JANOTTI, University of Delaware — Topological semimetals exhibit band crossing in the bulk and exotic surface states, called Fermi arcs, which are protected by topology of the associated wavefunctions. These states are characterized by their connectivity and dimensionality in the momentum space. Using first-principles calculations we show that ferromagnetic full Heusler compounds Co$_2$MnX (X = Si, Ge, Sn) belong to the category of topological semimetals called Weyl semimetals. Based on electronic structure calculations, we show that these materials show multiple nontrivial band crossings called Hopf links or entangled nodal lines and chain-like nodal lines, in absence of spin-orbit coupling, which are protected by mirror symmetry of the lattice. On breaking the time-reversal symmetry, we find that these band crossings are protected along multiple zero-dimensional Weyl points with different chiralities. We further explore the possibility of identifying non-trivial Fermi arc surface states connecting projection of these Weyl points on surface of opposite chiralities.

*This work was supported by the U.S. Department of Energy Basic Energy Science program (DE-SC0014388).


*DOE/BES (DE-FG-02-05ER46200) and GBMF4547 (EPIQS initiative)
12:15PM B04.00004: Inelastic Neutron Scattering in Semimetallic YbMnBi2* TIMOTHY REEDER (Presenter), WESLEY T FUHRMAN, Department of Physics and Astronomy, Johns Hopkins University, QUINN GIBSON, Department of Chemistry, Princeton University, JOSE A RODRIGUEZ, YIMING QIU, NIST Center for Neutron Research, National Institute of Standards and Technology, MATTHEW BRANDON STONE, ALEXANDER I KOLESNIKOV, Spallation Neutron Source, Oak Ridge National Laboratory, ROBERT CAVA, Department of Chemistry, Princeton University, COLLIN BROHOLM, Department of Physics and Astronomy, Johns Hopkins University — Layered pnictide AMnBi2 (A=Eu, Sr, Ca, Yb) compounds host quasi-2D square antiferromagnetic layers with alternating Bi square nets responsible for relativistic Dirac bands. Novel transport and peculiar optical conductivity that could be brought on by the coupling of these Dirac bands to the square-lattice antiferromagnetic Mn has garnered further interest in these materials, with the hopes of achieving the magnetically ordered Weyl semimetallic phase. We show that the magnetic lattice in YbMnBi2, fits to a frustrated J1-J2 model with antiferromagnetic J1 and J2 interactions, and J2/J1 less than the critical value, 1/2. While we rule out an ordered ferromagnetic coupling that would give rise to a Weyl Semimetal, we explore the relation between relativistic electronic band structure and anisotropic magnetic degrees of freedom.

*This work was supported by the US Department of Energy, office of Basic Energy Sciences, Division of Material Sciences and Engineering under grant DE-FG02-08ER46544

Access to MACS was provided by the Center for High Resolution Neutron Scattering, a partnership between NIST and the NSF under Agreement No. DMR-1508249

12:27PM B04.00005: Complicated magnetic phases interplayed with charge density waves in a new topological semimetal SHIMING LEI (Presenter), Princeton University, JÜRGEN NUSS, VIOLA DUPPEL, BETTINA LOTSCH, Max Planck Institute for Solid State Research, LESLIE SCHOOP, Princeton University — Topological semimetals have attracted a lot of attentions as they provide a new platform for studies of quantum matter as well as offer a new paradigm for next-generation electronics. Within these discovered topological materials, there is a class of materials that share the same structural motifs—sheets of square-arranged atoms, such as that in ZrS1S, CeSbTe and SrMnBi2. Within these materials, CeSbTe stands out as one unique system that offers the opportunities to study its tunable Weyl and Dirac states due to the existence of field-induced magnetic phase transitions. Here in this work, we present the synthesis and characterizations of a new series of square-net-based magnetic topological semimetals. Based on a comprehensive structural characterization by powder x-ray diffraction, single crystal x-ray analysis, and transmission electron microscopy on this series of compounds, we observed a crystal symmetry evolution from an orthorhombic phase to a tetragonal one, in accompany with a tunable charge density wave (CDW) modulation. Besides the structural characterizations, we have also performed a comprehensive study on the magnetic properties. The impact of crystal symmetry evolution and CDW on the linear crossing band is also discussed.

12:39PM B04.00006: Creating Weyl Nodes and Tuning Their Energy by Magnetization Rotation in a Metallic Ferromagnet* MADHAV PRASAD GHIMIRE (Presenter), Central Department of Physics, Tribhuvan University, JORGE FACIO, JHIH-SHIH YOU, Institute for Theoretical Solid State Physics, IFW Dresden, LINDA YE, JOSEPH CHECKELSKY, Massachusetts Institute of Technology, SHIANG FANG, EFTHIMIOS KAXIRAS, Harvard University, MANUEL RICHTER, JEROEN VAN DEN BRINK, Institute for Theoretical Solid State Physics, IFW Dresden — Weyl nodes are robust topological features of the electronic structure that can occur at any momentum and energies. To observe the large anomalous effects Weyl nodes need to be close to or at the Fermi-level. However, most materials Weyl nodes are observed slightly away from the Fermi-level. Here we propose a novel strategy to tune the Weyl node energy close to or even precisely at the Fermi energy that relies on the interplay between the magnetism and the energy dispersion in the time-reversal symmetry breaking Weyl semimetals. We show that magnetization effect is strong enough to create new Weyl nodes close to the Fermi surface and, vice versa annihilate other Weyl pairs. We focus on Co3Sn2S2, a ferromagnet recently found to be a Weyl semimetal and to display a large anomalous Hall effect. Performing ab initio density-functional calculations we show that canting the magnetization away from the easy axis leads to large displacements of the Weyl points in energy and in momentum space such that, at different orientations, Weyl fermions can be placed exactly at the Fermi surface.

*M.P.G. thanks the Alexander von Humboldt Foundation for financial support through the Georg Forster Research Fellowship Program.
12:51PM B04.00007: Hole Doping and Antiferromagnetic Correlations above the Néel Temperature of Topological Semimetal SrMnSb₂⁺

YONG LIU, FARHAN ISLAM, Ames Laboratory, Iowa State University, WEI TIAN, Oak Ridge National Laboratory, THOMAS HEITMANN, The Missouri Research Reactor, University of Missouri, BENJAMIN UELAND, ANDREAS KREYSSIG, ALAN IRA GOLDMAN, ROBERT J. MCQUEEN, DAVID VAKNIN (Presenter), Ames Laboratory, Iowa State University —

Neutron diffraction and magnetic susceptibility studies of orthorhombic single crystal SrMnSb₂ and hole doped Sr₀.₉₇K₀.₀₃MnSb₂ confirm the three dimensional antiferromagnetic (AFM) ordering of the Mn²⁺ moments at $T_N = 297(3)$ K for SrMnSb₂ and $T_N = 305(3)$ K for the hole doped compound. Neutron scattering show strong quasi two-dimensional AFM correlations that persist to almost twice $T_N$. In conjunction with susceptibility measurements, this observation seems to rule out a recently suggested ferromagnetic phase above $T_N$ in SrMnSb₂. We also report detailed analysis of de-Haas van- Alphen oscillations observed on the parent and doped compounds.

*This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No.—DE-AC02-07CH11358.

1:03PM B04.00008: Impact of antiferromagnetic order on Landau level splitting of quasi-two-dimensional Dirac fermions in EuMnBi₂

HIDETOSHI MASUDA (Presenter), University of Tokyo, HIDEAKI SAKAI, Osaka University and JST-PRESTO, MASASHI TOKUNAGA, University of Tokyo, MASAYUKI OCHI, Osaka University, HIDEFUMI TAKAHASHI, KAZUTO AKIBA, ATSUSHI MIYAKE, University of Tokyo, KAZUHIKO KUROKI, Osaka University, YOSHINORI TOKURA, University of Tokyo and RIKEN-CIMS, SHINTARO ISHIWATA, University of Tokyo and JST-PRESTO —

Dirac fermions in solids have been of current interest for their unique transport properties. The interplay of Dirac fermion with magnetism in magnetic Dirac materials is recently of particular interest. Among them, EuMnBi₂ is a rare compound that exhibits quantum transport of Dirac fermions coupled with the field-tunable magnetic order. However, it remains elusive how and to what extent the Dirac-like band dispersion is affected.

In this study, we report spin-split Landau levels of quasi-two-dimensional Dirac fermions in EuMnBi₂, as revealed by interlayer resistivity measurements in a tilted magnetic field up to ~35 T. The amplitude of Shubnikov–de Haas (SdH) oscillation in interlayer resistivity is strongly modulated by changing the tilt angle of the field, i.e., the Zeeman-to-cyclotron energy ratio. The effective g factor estimated from the tilt angle, where the SdH oscillation exhibits a phase inversion, differs by approximately 50% between two antiferromagnetic phases. This observation signifies a marked impact of the magnetic order of Eu sublattice on the Dirac-like band structure. The origin may be sought in strong exchange coupling with the local Eu moments, as verified by the first-principles calculation. [H. Masuda, H. Sakai et al., Phys. Rev. B 98, 161108(R) (2018)]

1:15PM B04.00009: Observation of Magnetic Bubble Domains in the Quasi-2D Kagomé Ferromagnetic Weyl Semimetal Co₃Sn₂S₂

PAUL SASS (Presenter), WEIDA WU, Rutgers University, New Brunswick, LINDA YE, JOSEPH CHECKELSKY, Department of Physics, Massachusetts Institute of Technology —

The Co-based shandite, Co₃Sn₂S₂, is a Weyl³ semi-metal hosting an itinerant ferromagnetic quasi-2D Kagomé lattice of Co ions. This system exhibits strong c-axis anisotropy with a curie temperature ~ 174 K and a spontaneous moment of ~ 0.3 μB/Co.² Low-field magnetization and AC susceptibility measurements have revealed an anomalous magnetic phase above ~ 126 K and below ~ 40 mT, indicating a possible skyrmion phase. To this end, we carried out variable-temperature magnetic force microscopy studies on Co₃Sn₂S₂ single crystals. MFM images under zero-field cooling revealed fingerprint-like magnetic domains, while low-field cooling through $T_C$ resulted in seemingly periodic magnetic bubble domains, which is consistent with the quasi-2D nature of the magnetic ordering. Detailed temperature and cooling field dependence of the magnetic domain patterns will be presented.


*¹This work is supported by DOE BES under award DE-SC0018153.
ANH PHAM (Presenter), PANCHAPAKESAN GANESH, Oak Ridge National Laboratory — Materials that can host a magnetic-Weyl semimetallic phase represent a novel platform for fundamental physics studies and can also be potentially applicable for quantum computing. The search for such magnetic-Weyl semimetals is ongoing given the recent discovery of Weyl semimetals which show absence of time reversal or inversion symmetry [1, 2]. In our study, we demonstrate a new pathway to engineer magnetic Weyl semimetals by doping topological crystalline insulators (TCI) such as SnTe with a magnetic transition metal element, such as Cr. The magnetic dopant breaks both time reversal and inversion symmetry while maintaining the band inversion between Sn-p and Te-p orbitals, thus resulting in Weyl nodes in the bulk. These Weyl nodes were characterized through chirality calculation, large intrinsic anomalous Hall conductivity (AHC), and presence of Fermi arcs in the surface. Furthermore, the Weyl semimetallic phase is maintained even under dilute dopant concentrations, suggesting experimental feasibility of realizing this system.


*This research was funded by ORNL-LDRD (Project ID: 8988).

CUNEYT SAHIN (Presenter), Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, DUNG VU, Department of Mechanical and Aerospace Engineering, The Ohio State University, WENJUAN ZHANG, NANDINI TRIVEDI, Department of Physics, The Ohio State University, JOSEPH P C HEREMANS, Department of Mechanical and Aerospace Engineering, The Ohio State University, MICHAEL FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa — Bi and Sb alloys exhibit novel physical phenomena depending on the antimony concentration, such as semimetal-semiconductor transitions, giant spin Hall conductivities, and topologically protected phases including Weyl semimetal phases. Although the band structures of Bi and Sb are well studied in terms of k.p or tight-binding Hamiltonians, it is still a challenge to predict the behavior of the band edges as a function of the alloy concentration. Simple linear virtual crystal approximations lack the correct symmetries of the electron and hole pockets; on the other hand, alternative VCA approaches are insufficient to describe band crossings at different Sb concentrations. In this work, we introduce a new VCA parametrization describing the symmetries and crossing of the band edges using a 16 band tight-binding Hamiltonian. Then, from that Hamiltonian, we derive and calculate g-tensors of the electrons and holes and show that the large spin-orbit couplings of Bi and Sb result in giant effective g-factors whose axes of symmetry differ from the crystallographic axes. We also show that the band gap between symmetric and antisymmetric bands at the L point can be closed by a moderate magnetic field due to large g-factors. The closing of this gap produces a Weyl state.

*NSF DMR-1420451

RISHI BHANDIA (Presenter), BING CHENG, Department of Physics and Astronomy, Johns Hopkins University, TOBIAS L BROWN-HEFT, SEAN HARRINGTON, SHOUVIK CHATTERJEE, CHRIS PALMSTROM, Materials Department, University of California, Santa Barbara, PETER ARMITAGE, Department of Physics and Astronomy, Johns Hopkins University — Weyl semimetals are a class of topological materials that been the subject of intense research in the past few years. While there have been definitive examples of inversion symmetry breaking Weyl semimetals, good examples of time-reversal symmetry breaking Weyl semimetals remain elusive. In addition to being of great interest to the spintronics community due to its half-metallicity, the Heusler alloy Co2TiGe has attracted interest recently due to theoretical predictions suggesting it hosts time-reversal symmetry breaking Weyl semimetal states. Recently, MBE-grown thin films of Co2TiGe have become available, allowing for time-domain THz spectroscopy (TDTS) measurements. We present results of the low frequency optical conductivity of Co2TiGe and discuss our results in the context of prevailing theories.
Zeeman Splitting Induced Topological Nodal Structure in ZrTe$_5$*

YICHL CHOI (Presenter), Physics, Virginia Tech, JOHN VILLANOVA, Physics, University of Arkansas, KYUNGLWA PARK, Physics, Virginia Tech — When time-reversal symmetry is broken by an external Zeeman field in a Dirac semimetal or small-gap insulator, rich nodal structures can be induced, including Weyl nodes or nodal lines. ZrTe$_5$ is known to be located near the phase boundary between strong and weak topological insulator, and recent experiments showed intriguing magnetic transport properties including anomalous Hall effect and the chiral magnetic effect. This indicates that Weyl nodes are developed in ZrTe$_5$ due to Zeeman splitting. However, a concrete theoretical study of the nodal structure of ZrTe$_5$ under Zeeman splitting covering the full Brillouin zone is still missing. We construct a Wannier-function based tight-binding model from first principles to investigate the effect of Zeeman splitting in ZrTe$_5$ and to fully explore the nodal structure near the Fermi level. We calculate the topological character of induced band crossings and examine the importance of magnetic field direction effect on the nodal structure.

*This work is supported by the Virginia Tech ICTAS Fellowship with computational support by SDSC under DMR060009N and VT ARC.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B05 DCMP: General Talks BCEC 108

Mechanics of Rugby Union Scrums: stability and collective production of force* CAROLINE COHEN (Presenter), CORENTIN REISS, DAVID QUERE, LadHyX, Ecole polytechnique, ANETTE E. HOSOI, MIT, CHRISTOPHE CLANET, LadHyX, Ecole polytechnique — Rugby Union is a contact sport played by two 15-players teams. During scrummaging, two 8-players groups called packs confront each other in a 3-4-1 configuration. The objective of each team is to push the opponent backwards while staying stable. A surprising fact is that there is a loss in collective force produced by the pack : 8 international level players in the pack able to generate together only 75% of the sum of forces produced individually.

We study experimentally both the stability of the scrum with a simple beam analogy, and the origin of the loss in collective force produced by players of Racing 92, a top level team of Top 14, the French national championship. We perform experiments at the « Atelier de la mêlée », the Rugby French Federation training tool to measure the forces produced by players and packs. By coupling forces measurements with a Particle Image Velocimetry (PIV) analysis of videos taken from above, we show that there is a correlation between force fluctuations and the lack of synchronization of the 8 players pushing together.

*Racing 92 Federation Francaise de Rugby

Theory of Direction KAUSTAV B. ARYA (Presenter), Assam Jatiya Bidyalay — The law of gravitation indicates that every object of the universe attracts each other. On the other side we determine our earth’s magnetic poles as north and south. The magnetism describes that different poles attract each other. Therefore, the connection points of any two objects always face with different directions (poles) because they have attraction. Otherwise without this principle of nature the system may will be collapsed. So, in this way the author tries to find the procedure of different directions causing the gravitation. This journey propells the path of all moving objects and their neighbor matters in which they create attraction by opposite poles. Before all, the main thing is the final decision will be relative as the universe is still out of reach fully. Here, mentioned theory will be based on either rotatory or annual motion of the objects or both in space. Finally, the whole method will explain how the gravitation works by opposite directions in space. The research shows that like earth’s magnetic poles north and south it may possible to have poles with the directions west and east in the universe. In this huge universe it is always possible to have such objects which rotate vertically from north to south in their rotatory motion.

Sources of Biconformal Gravity* WALTER MUHWEZI (Presenter), Physics, Utah State University — Biconformal gravity is a 2n-dimensional conformal gauge theory with a curvature linear action that has been shown to reproduce scale invariant general relativity on the cotangent bundle of n-dimensional spacetimes. We explore Yang-Mill's sources for biconformal gravity. The questions we seek to clarify are whether the augmented field equations reduce the Yang-Mill's sector to n-dimensional Yang-Mill's theory and yield the appropriate energy momentum tensor as the gravitational source.

*Keith Taylor Award, Utah State University.
Gravity and electromagnetism are two sides of the same coin, which is the clue of this unification. Gravity and electromagnetism are represented by two mathematical structures, symmetric and antisymmetric respectively. Einstein gravitational field equation is the symmetric mathematical structure. Electrodynamics Lagrangian is three parts, for electromagnetic field, Dirac field and interaction term. The definition of canonical energy momentum tensor was used for each term in Electrodynamics Lagrangian to construct the antisymmetric mathematical structure; symmetric and antisymmetric gravitational field equations are two sides of the same Lagrangian.

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The authors of a neutron interferometer experiment published in Physical Review in 1992 said that neither they, nor quantum mechanics could not explain their data. It is unusual to find an experiment that QM cannot explain. If we follow that trail of evidence, where does it lead? It leads to the Elementary Wave hypothesis, according to which Schrödinger waves convey probability amplitudes that particles follow backwards. Should we put so much emphasis on one peculiar finding? This hypothesis explains the double slit experiment in a logical and coherent way; something that QM has been unable to do. It indicates that wave function collapse occurs when a particle is emitted, not when it is detected. That profoundly changes the measurement problem.

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In shooting sports, champions develop an aiming strategy in order to maximize the precision of their shot. We study experimentally the aiming dynamics of different shooting sports such as archery, rifle and laser-run, with international level athletes. We observe that the movement of the arm exhibits notable differences among the shooting sports, according to the particular constraints of the sport. We build a simple mechanical model for the control of an aiming movement. This model shows that the movement naturally chosen by the athletes corresponds to an optimal trajectory for their sport. In shooting sports where athletes have to shoot fast, such as laser run or speed shooting, it minimizes the shooting time. In contrary, in archery where the force needed to lengthen the bow string is quite large, it minimizes the energy spent in the movement.

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We propose to investigate the mechanism of cosmological inflation and expansion through the physical properties of space-time [1]. We demonstrate that a cosmological inflation scenario occurs when the bulk modulus of space-time $K=1.64 \times 10^{109} \text{N.m}^{-2}$, and show that the dark energy density is decreased by a factor of $10^{122}$ while the scaling factor expands from $10^{-60}$ to $10^{-32}$ during a time of the order of $10^{-42} \text{s}$. At the end of the presentation, we discuss a microscopic interpretation of the inflation mechanism and future investigations on longitudinal waves.


There is an active quest to discover new topologically quantized physical properties of topological quantum states of matter, similar to the quantized Hall conductance in quantum Hall states. The motivation is to discover not only new fundamental physics in exotic materials, but also technologically desirable robust physical properties which are unaffected by modest disorder and manufacturing variations. We establish that a novel topological response is found in a wide variety of topological quantum states — we term this the topological gravitational response — and comment on the still-unknown topological physics underlying the quantization of the corresponding response coefficient, the gravitational coupling constant.
The interface of Internet-connectivity and automotive technology promises to dramatically improve transportation. However, with these known benefits come unknown risks, especially since Internet-connected vehicles have become targets for computer hacking. Vehicles, unlike sensitive data, can collide or physically interact when their systems become compromised, and there is a broad class of scenarios generically leading to Internet-connected vehicles being suddenly and simultaneously disabled. Here, we investigate how large-scale hacking affects traffic flow using agent-based simulations, and discover the critical relevance of percolation for predicting outcomes on a multi-lane road. Inspired by this discovery, we develop and validate an analytic percolation-based model to rapidly assess the effect of hacking. We then apply our analytic model to investigate the outcomes on the street network of Manhattan (NY, USA), revealing a latent risk. A small number of disabled vehicles can gridlock the city and substantially reduce access to emergency services. By discovering percolation as the phenomenological driver of city-wide disruption, we simultaneously uncover a strategy for risk-mitigation.

*GeorgiaTech Soft Matter Incubator
GeorgiaTech Institute for Robotics and Intelligent Machines

**Five dimensional rotating regular black holes and shadow**

We present a five-dimensional ($5D$) rotating regular black hole metric, with a deviation parameter $k \geq 0$, that interpolates between the $5D$ Kerr black hole ($k = 0$) and $5D$ Kerr-Newman ($r \gg k$), and is an exact solution of general relativity coupled to nonlinear electrodynamics. Interestingly, for a given value of parameter $k$ there exits a critical value of rotation parameter $a = a_E$ which corresponds to extremal rotating regular black hole with degenerate horizons, while for $a < a_E$, one has non-extremal rotating regular black hole with outer and inner horizons. Owing to the correction factor ($e^{-k/r^2}$), due to nonlinear electrodynamics, the ergoregions and black hole shadows get modified.

**Reconciliation of the Rosen and Laue theories of special relativity in a linear dielectric medium**

We show that the incompatible Laue and Rosen treatments of special relativity in a dielectric are both correct but have different regimes of applicability. The Laue theory has a fundamental physical basis in Einstein's special relativity and the relativistic velocity sum rule. The Rosen version of dielectric special relativity was derived heuristically. Consequently, the Rosen theory and its consequences are almost completely ignored in the scientific literature and there is little to no discussion about the incompatibility of the two theories of relativity in a dielectric. We derive both versions of relativity using inertial reference frames moving at constant velocity along the interface between a simple linear dielectric medium and the vacuum. We show that the Rosen theory applies to relativistic physics in the interior of a simple linear dielectric medium and the Laue theory is used to relate these physics to a Laboratory Frame of Reference in the vacuum where measurements can be performed.

**A Novel Interpretation of the Lorentz Transformations**

While 'interpretations of a theory' are most commonly associated with quantum mechanics, they can become important in other branches of physics as well. Here we present a novel interpretation of the Lorentz Transformations in which length contraction is re-conceptualized as the abatement of a body's dimensionality, and time dilation as the abatement of its duration of existence within a given coordinate time interval. The re-interpretation of length contraction makes it possible to understand the invariance of the speed of light and the relationship between classical electric and magnetic fields at a deeper level. The re-interpretation of time dilation makes it possible to integrate the heretofore purely philosophical concept of existence into physics. Together, they lead to a recognition of the importance of two invariance principles and two corresponding spacetime symmetries which are under the prevailing paradigm so obvious that it usually goes unnoticed, and thereby set the stage for recognizing new fundamental relationships in other areas of physics, in particular quantum mechanics.
1:39PM B05.00013: Synchronization of human network  MOTI FRIDMAN (Presenter), Bar-Ilan University, NIR DAVIDSON, Physics of Complex Systems, Weizmann Institute of Science — The synchronization of human networks is essential for our civilization and understanding the motivations, behavior, and basic parameters which govern the dynamics of human networks are important for many aspects of our lives. We studied complex human networks in different configurations with full control over the network connectivity, the coupling strength of each connection and the delay between coupled individuals. Our system is based on coupling violin players in different configurations and measuring the synchronization of their phase, period, frequency and volume. In our system, each player is connecting it's violin output to our computer system and has headphones for the input.

We found that humans tend to find a non-trivial solution for frustration situations and spontaneously change the connectivity of the network in order to reach a stable solution. We also found that out-of-phase synchronized state is highly stable and usually is preferable by the entire network. Our results are important for understanding the dynamics of human networks in different conditions and are the first experiments in which human networks are investigated with full control over the network parameters.

1:51PM B05.00014: On the origin of kinetic energy in The Physical Universe including the Godforsaken area of turbulence  SIMON BERKOVICH (Presenter), George Washington University — There is a popular parable attributed to W. Heisenberg: "When I meet God, I am going to ask him two questions: Why relativity? And why turbulence? I really believe he will have an answer for the first." Answers to diverse problems in physics can be obtained with a Cellular Automaton (CA) Model (see our recent minireview [1], with pertinent references) CA model combines divergent functionalities that otherwise difficult to imagine. The CA generates steady relocating formations - corresponding to the basic stable constituents of the physical world: electrons, protons, photons, and neutrinos, they exist only in continuous motion. Quantum behavior of micro-objects results from the specifics of the CA measurements.. As to macro bodies, they are split into fragments dragged by conflicting velocities. In seismology, this leads to rifts of tectonic plates causing abrupt mechanical impacts. Similar rifts occur in turbulence lamina, although they are far away from cosmic phenomena. Emulated in closed cycles such laminar cracks can lead to extraction of heat from the fragments dragged by of the CA Universe.


2:03PM B05.00015: Quantum materials research at the upgraded CHESS-U facility: Introducing <QM>2*  JACOB RUFF (Presenter), CHESS, Cornell University — The recent CHESS-U project comprised a significant upgrade of the Cornell High Energy Synchrotron Source. CHESS-U enables running with a single, lowered-emittance 6 GeV positron beam in CESR, and has also funded the construction of 6 new hard x-ray undulator beamlines. One of these is the <QM>2 beamline, dedicated to high-precision studies of quantum materials in reciprocal space. In this talk, I will (i) introduce the <QM>2 beamline; (ii) identify the scientific questions that motivated its construction; (iii) explain the design decisions that enable its function; and (iv) highlight the unique new capabilities that it offers to users in the quantum materials community.

*Research conducted at CHESS is supported by the NSF under award DMR-1332208.
The CHESS-U project was supported by New York State via the Upstate Revitalization Initiative.

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B06 DCMP: Cuprates and Related  BCEC 109A - Jasminka Terzic, National High Magnetic Field Laboratory - Tag(s):
Focus

11:15AM B06.00001: Magnetic-field-tuned superconducting quantum phase transition in highly overdoped Bi2+xSr2-xCuO6+δ*  JASMINA TERZIC (Presenter), PAUL G. BAITY, BAL K POKHAREL, LILY STANLEY, DRAGANA POPOVIC, Department of Physics and National High Magnetic Field Lab, Florida State University, SHIMPEI ONO, Central Research Institute of Electric Power Industry, Japan — The conventional picture of overdoped cuprates as BCS d-wave superconductors has been recently challenged, with the roles of disorder and quantum fluctuations under debate. To address these questions, we focus on the highly overdoped regime, which we have explored via measurements of linear transport and voltage-current characteristics on the hole-doped, La free, Bi2+xSr2-xCuO6+δ (Bi2201) single crystals with zero-resistance transition temperatures Tc ~ 5 K. Measurements were performed in magnetic fields (H) up to 45 T and temperatures (T) down to 17 mK. We discuss the nature of the H-field-tuned superconducting quantum phase transition and the high-field ground state, and present the T-H phase diagram for the highly overdoped Bi2201.

*Supported by NSF DMR-1707785 and NHMFL via NSF DMR-1644779 and the State of Florida.
11:27AM B06.00002: Scale-Invariant transport in high-temperature superconductors* ARKADY SHEKHTER (Presenter), National High Magnetic Field Laboratory, BRAD RAMSHAW, Laboratory of atomic and solid state physics, Cornell university, KIMBERLY MODIC, Max Planck Institute for chemical physics of solids, LAUREL WINTER, National High Magnetic Field Laboratory, SEIKI KOMIYA, SHIMPEI ONO, CRIEPI, FEDOR BALAKIREV, JONATHAN B BETTS, GREGORY SCOTT BOEBINGER, ROSS MCDONALD, National High Magnetic Field Laboratory — We report high-magnetic-field (up to 93T) Hall measurements in LSCO cuprates superconductor near critical doping (x=0.20). The observed Hall behavior exhibits a crossover from a low-field to high-field behavior in a broad range of temperatures. Such Hall behavior is incompatible with Fermi surface quasiparticle transport in the strange metal state.

*National High Magnetic Field Laboratory is supported through the National Science Foundation Cooperative Agreement numbers DMR-1157490 and DMR-1644779, The United States Department of Energy, and the State of Florida.

11:39AM B06.00003: Optical Thermal Diffusivity Measurement in Bad Metals* JIECHENG ZHANG (Presenter), ERIK KOUNTZ, AHARON KAPITULNIK, Physics, Stanford University, RICHARD L. GREENE, Physics, University of Maryland — Local measurements of thermal diffusivity are used to analyze the transport of heat in the bad metallic regime of several strongly correlated materials. Thermal diffusivity DQ was measured for several cuprate systems in their so-called bad metal regime, including both electron and hole doped cuprates. The temperature dependence of normal state resistivity of these systems are either linear or close-to-quadratic, while the overall magnitudes exceed the Mott-Ioffe-Regel limit at approximately 250K, indicating failure of the conventional quasiparticle transport picture. We found that the various doping of (Nd/Pr/Sm)1-xCe_xCuO_4 all have T-linear DQ^-1. We interpret our results through a strong electron-phonon scattering picture where both electron and lattice system saturates a quantum scattering time bound of ~h/kBT, and the slope of the T-linear DQ^-1 is associated with a characteristic intermediate speed between the speed of sound and the Fermi velocity. Our results suggest that neither well-defined electron nor phonon quasiparticles might be present in these systems, and that thermal transport is carried out by a collective “soup” of strongly coupled electrons and phonons.

*Supported by the Gordon and Betty Moore Foundation through the EPiQS Initiative, Grant GBMF4529.

11:51AM B06.00004: High Temperature Electrical Transport in Electron-Doped Cuprates* NICHOLAS PONIATOWSKI (Presenter), TARAPADA SARKAR, PAMPA MANDAL SARKAR, RICHARD L. GREENE, Department of Physics, University of Maryland, College Park — Although the origin of high-temperature superconductivity in the cuprates has eluded the community for decades, the normal state of these materials is similarly enigmatic. The universal T-linear electrical resistivity observed in hole-doped compounds such as YBCO and LSCO, persistent to high temperatures, is thought to violate the Mott-Ioffe-Regel (MIR) limit on the scattering rate, where traditional Boltzmann theories of transport break down. Consequently, the normal state of these and other strongly correlated materials are now considered a new phase of matter, the “strange metal.” We report resistivity and magnetoresistivity (MR) measurements of the electron doped cuprate La_{2-x}Ce_xCuO_4 (LCCO) from 100K to above room temperature and relate our findings to the hole-doped side of the phase diagram. By studying slightly underdoped samples (x=.08, .10) in proximity to the antiferromagnetic phase (without a field), we are able probe the strange metallic regime in the vicinity of the MIR bound without having to resort to excessively high temperatures. For other dopings, we report new MR data.

*This work is supported by the NSF under Grant No.DMR-1708334.
12:03PM B06.00005: Hall coefficient in two-dimensional metals with spiral magnetic order and application to cuprate high-\(T_c\) superconductors  
Johannes Mitscherling (Presenter), Walter Metzner, Max Planck Institute for Solid State Research — Charge transport measurements in high magnetic fields recently shed new light on the non-superconducting ground state in cuprate high-\(T_c\) superconductors [1]. In particular, Hall measurements yield a drop of the Hall number indicating a phase transition associated with a Fermi surface reconstruction. On the theoretical side, spiral magnetic order (or quasi-order) remains a hot candidate for the Fermi surface reconstruction mechanism.

The electromagnetic response of spiral magnetic states has already been analyzed by Voruganti et al. for small relaxation rates [2]. However, the relaxation rate in the cuprate samples studied experimentally is sizable. We have, thus, derived, for the first time, a complete formula (including all interband contributions) for the Hall conductivity in the low field limit \(\omega_c \tau \ll 1\). [3]

We use the complete expressions to study the importance of a sizable relaxation rate and show that the observed Hall number drop in cuprates can be fitted with realistic parameters.


12:15PM B06.00006: Correlation between scale-invariant normal state resistivity and superconductivity in an electron-doped cuprate*  
Tarapada Sarkar (Presenter), Pampa Mandal Sarkar, Nicholas R. Poniatowski, University of Maryland, College Park, Mun Keat Chan, Los Alamos National Laboratory, Richard L. Greene, University of Maryland, College Park — An understanding of the normal state in the high-\(T_c\) superconducting cuprates is crucial to the understanding of the long-standing problem of the origin of the superconductivity itself. This so-called “strange metal” state is thought to be associated with a quantum critical point (QCP) hidden beneath the superconductivity. In electron-doped cuprates, it is possible to access the normal state at very low temperatures and low magnetic fields to study this putative QCP and to probe the \(T \to 0 \) K state of these materials. We report measurements of the low temperature normal state magnetoresistance (MR) of the n-type cuprate system (LCCO) and find that it is characterized by a linear-in-field behavior, which follows a scaling relation with applied field and temperature, for doping \(x\) above the putative QCP \((x=0.14)\). This unconventional behavior suggests that magnetic fields probe the same physics that gives rise to the anomalous low-temperature linear-in-T resistivity. The magnitude of the linear MR decreases as \(T_c\) decreases and goes to zero at the end of the superconducting dome \((x \sim 0.175)\) above which a conventional quadratic MR is found. we discuss the correlation between Linear-in-T and Linear-in-H resistivity with the superconductivity.

*NSF-DMR-1708334 and AFOSR-FA9550-14-1-0332.

12:27PM B06.00007: short-range pair density wave in cuprates  
Zhehao Dai (Presenter), Yahui Zhang, Senthil Todadri, Patrick Lee, Massachusetts Institute of Technology — We analyze recent STM results on period-8 density wave in the cuprate vortex halo and provide a theory of short-range pair density wave to explain quantum oscillation above \(H_c^2\) and the electron gap in the anti-nodal region in underdoped cuprates.

12:39PM B06.00008: Gauge theory for the cuprates near optimal doping*  
Subir Sachdev, Harley Scammell, Matthias Scheurer (Presenter), Grigory Tarnopolsky, Department of Physics, Harvard University — We propose a SU(2) gauge theory with fermionic low-energy excitations as an effective field theory for the cuprate high-temperature superconductors. For the hole-doped compounds, the theory describes fluctuating incommensurate spin-density waves. While we recover the conventional Fermi-liquid state as the confining phase of the theory at large doping, there is a quantum phase transition to a Higgs phase corresponding to the pseudogap at low doping. Depending on details of the theory, the Higgs phase shows one or more of charge-density wave, Ising-nematic, scalar spin chirality, and \(Z_2\) topological order. For the electron-doped systems, we assume commensurate spin-density wave fluctuations and there is only a crossover between the confining and the Higgs regime, with an exponentially large confinement length deep in the Higgs regime. For both the electron- and hole-doped systems, the electronic spectral function shows small Fermi surfaces at scales shorter than the confinement length. Finally, we present a large-N analysis of the deconfined quantum criticality of the Higgs transition.

*Research supported by NSF Grant No. DMR-1360789, by the National Academy of Sciences Leopoldina through grant LPDS 2016-12, by the MURI grant W911NF-14-1-0003 from ARO, and by DOE grant de-sc0007870.
12:51PM B06.00009: Normal-state optical conductivity and linear resistivity of the cuprates from tightly bound pre-formed pairs  LONG ZOU (Presenter), SHENTAO JIANG, WEI KU, Shanghai Jiao Tong University — We investigate anomalous normal-state in-plane resistivity and optical conductivity of cuprates by using multi-orbital bose-liquid model. Specifically, we assume that the charge carriers in cuprate are tightly bound pre-formed pairs. We show the low-energy optical spectrum involving both intra- and inter-band excitation. While inter-band excitation explain the continuous spectrum and its contribution around the van-Hove singularities of the pre-formed pairs can reproduce the experimental observed onset near 1000 cm\(^{-1}\), the intra-band excitation will mainly contribute to low frequency conductivity and gives rise to linear behavior originate from the continuously decreasing height of low-frequency peak since its weight transfers to high energy region with temperature. Our study reveals the bosonic nature of the low-energy carriers and provides a strong support for the picture of tightly bound preformed pairs in describing the high-temperature superconductivity and other low-energy physics of the cuprates.

1:03PM B06.00010: Slow magnetic fluctuations in the pseudogap phase of YBa\(_2\)Cu\(_3\)O\(_y\)† JIAN ZHANG (Presenter), State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, People's Republic of China, DOUGLAS E. MACLAUGHLIN, Department of Physics and Astronomy, University of California, Riverside, Riverside, CA 92521, USA, ZHAOFENG DING, CHENG TAN, State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, People's Republic of China, OSCAR BERNAL, Department of Physics and Astronomy, California State University, Los Angeles, CA 90032, USA, PEI-CHUN HO, Department of Physics, California State University, Fresno, CA 93740, USA, GERALD D MORRIS, TRIUMF, Vancouver, British Columbia V6T 2A3, Canada, AKIHIRO KODA, Muon Science Laboratory and Condensed Matter Research Center, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), ADRIAN HILLIER, STEPHEN P. COTTRELL, PETER J. BAKER, P. K. BISWAS, ISIS Facility, Science and Technology Facilities Council Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, Didcot OX11 0QX, UK, YANXING YANG, ZHAO ZHU, State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, People's Republic of China, JUN QIAN, YAN WAN, XIN YAO, State Key Lab for Metal Matrix Composites, Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Department of Physics and Astronomy, Shanghai, LEI SHU, State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, People's Republic of China. — We report broken time-reversal symmetry in the pseudogap state of underdoped single crystalline YBa\(_2\)Cu\(_3\)O\(_y\) using muon spin relaxation technique. Slow magnetic fluctuations are observed below the characteristic pseudogap onset temperature T\(^*\), signaled by the Redfield relation between the Lorentzian relaxation rate of the positive muons and the applied field along the muon initial spin polarization. We measured the temperature dependence of the local field and compared it with the order parameter measured by neutron scattering. The slow frequency scale of the fluctuations, 5 orders of magnitude below the energy scale of the pseudogap energy, implies that time-reversal symmetry is broken for properties intermediate between the two scales, but raises the question of the nature of the quantum fluctuations responsible for time-reversal not being absolutely broken.

†This research was supported in part by the National Key Research and Development Program of China (Nos.-2017YFA0303104 and 2016YFA0300503), the National Natural Science Foundation of China No. 11774061.

1:15PM B06.00011: Imaging Domains and Domain Walls in High-Temperature Superconductor* TADESSE ASSEFA (Presenter), Brookhaven National Laboratory, YUE CAO, ROSS HARDER, Argonne National Laboratory, IAN KEITH ROBINSON, JOHN TRANQUADA, GENDA GU, Brookhaven National Laboratory — Phase transition, Symmetry breaking and recovery in condensed matter systems are closely related to the exotic physical properties of strongly correlated materials such as superconductivity, magnetism, ferroelectricity, etc. A key signature of broken symmetry is the formation of structural domains of few nanometer size. Bragg coherent X-ray diffraction techniques can enable novel experimental opportunities to directly visualize symmetry changes in these materials through domain structure. We have pushed Bragg Coherent Diffractive Imaging (BCDI) into the cryogenic regime where most phase transitions in quantum materials reside. Utilizing coherent photons at 34-ID-C beamline of the Advanced Photon Source, we image the structural domain evolution of La\(_{2-x}\)Ba\(_x\)CuO\(_4\), x=1/8 sample during the low-temperature-orthorhombic (LTO) to high temperature tetragonal (HTT) phase transition. These phases break the local four-fold rotational symmetry of its high temperature tetragonal (HTT) structure and our preliminary data suggests the low-temperature-orthorhombic (LTO) phase is not pinned to local crystal disorder or defects.

*Research was sponsored by the US Department of Energy (DOE) Basic Energy Sciences (BES), by the Materials Sciences and Engineering Division.
1:27PM B06.00012: What happened at 19% doping in Bi2212: an ARPES perspective

SUDI CHEN (Presenter), Applied physics, Stanford University, MAKOTO HASHIMOTO, SLAC National Accelerator Laboratory, YU HE, Applied physics, Stanford University, DONGJOON SONG, National Institute of Advanced Industrial Science and Technology, KEJUN XU, JUNFENG HE, Applied physics, Stanford University, DONGHUI LU, SLAC National Accelerator Laboratory, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, ZHIXUN SHEN, Applied physics, Stanford University — In the hole-doped cuprate superconductors, the special doping p = 0.19 has attracted considerable research interest. Various anomalies have been observed at this doping and associated with fascinating physics, for example the change from small to large Fermi surface, the termination of the pseudogap, the recovery of coherence, and the possibility of a quantum critical point. In this talk we present a systematic ARPES study across 84 temperature-doping points in Bi2212 near p = 0.19. The results provide important insights about the nature of this special doping and the phenomenology of the cuprates.

*Supported by the DOE Office of Basic Energy Sciences, Division of Material Science under Contract #DE-AC02-76SF00515.

1:39PM B06.00013: Anomalous Dimensions for Conserved Currents from Holographic Dilatonic Models to Superconductivity

PHILIP PHILLIPS (Presenter), KRIDSANAPHONG LIMTRAGOOL, GABRIELE LA NAVE, University of Illinois at Urbana-Champaign — Anomalous Dimensions for Conserved Currents from Holographic Dilatonic Models to Superconductivity

It is well known that the dimension of conserved currents is determined simply from dimensional analysis. However, a recent proposal is that what is strange about the conserved currents in the strange metal in the cuprate superconductors is that they carry anomalous dimensions. The basic model invoked to exhibit such behaviour is a holographic dilatonic one in which the field strength couples to the radial coordinate. I will show that the anomalous dimension in such cases arises from a fractional electromagnetism[1] that can be thought of as a general loop-hole in Noether's second theorem. The general mechanism operative is a mass term in the IR that couples to the UV current. I will also show that even the Pippard kernel invoked to explain the Meissner effect in traditional low-temperature superconductors is a special case of the non-local action found here.


*NSF DMR-1461952

1:51PM B06.00014: A novel solution of the 2D Hubbard model within a 4-pole approximation: electronic dispersion and Fermi surface evolution

ANDREA DI CIOLO (Presenter), ADOLFO AVELLA, Dipartimento di Fisica “E.R. Caianiello”, Università degli Studi di Salerno, I-84084 Fisciano (SA), Italy — We present and characterize a novel solution of the 2D Hubbard model within the Composite Operator Method [1,2] in a 4-pole approximation [3]. We have chosen a basis of four fields: the two Hubbard operators plus two fields describing the Hubbard transitions dressed by nearest-neighbor spin fluctuations, which play a crucial role for strong correlations. This 4-pole solution performs very well once compared with advanced (semi-)numerical methods for all relevant values of interaction, doping and temperature, being considerably less computational-resource demanding. By carefully treating spin fluctuations and featuring momentum selectivity, this solution can address the underdoped-cuprate puzzle (Fermi arcs, pseudogap, non-Fermi liquid behavior, ...). We adopt this approximation to study the single-particle properties of the model in the strong coupling regime, where spin fluctuations are responsible for anomalous features in the analyzed properties. We focus on the investigation of the electronic dispersion and of the Fermi surface, studying their evolution with doping and temperature.


Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B07 DCMP GMAG: Correlated Magnetism and Other Ordered Phases

Wei, Florida State University
**11:15 AM B07.00001: Enhanced Magnetic Ordering in Sm Metal under Extreme Pressure**

YUHANG DENG (Presenter), JAMES S SCHILLING, Physics, Washington University, St. Louis — The dependence of the magnetic ordering temperature $T_0$ of Sm metal was determined through four-point electrical resistivity measurements to pressures as high as 127 GPa. A strong increase in $T_0$ with pressure was observed above 40 GPa. In this pressure range Sm ions alloyed in dilute concentration with superconducting Y exhibit giant Kondo pair breaking. Both results suggest that for pressures above 40 GPa Sm enters a highly correlated electron state, likely related to a Kondo lattice, with an unusually high value of $T_0$. Similar results were found previously for Nd [1], Tb [2], and Dy [3] and their dilute magnetic alloys with superconducting Y. Both Y(Sm) and Y(Nd) alloys display record-high pair breaking $\Delta T_c$ as large as 40 K/at.%.  


*Work at Washington University is supported by NSF grant DMR-1104742/1505345 and CDAC through NNSA/DOE DE-FC52-08NA28554.

**11:27 AM B07.00002: Superparamagnetic clusters in antiferromagnetic Eu$_{0.52}$Ca$_{0.48}$B$_6$ seen by Small Angle Neutron Scattering (SANS)**

GABRIELLE BEAUDIN (Presenter), ANDREA BIANCHI, Universite de Montreal, MARK LAVER, ROBERT ARNOLD, School of Metallurgy and Materials, University of Birmingham — Since the term was introduced by Pekar in 1946, polarons have been thought to underpin a range of prominent phenomena from high-$T_c$ superconductivity to colossal magnetoresistance. Polarons are quasiparticles consisting of charge carriers “dressed” by lattice distortions. Similarly, magnetic polarons are charge carriers dressed with spins. In the europium chalcogenides, magnetic polarons are thought to be formed as a spin polarization of the mobile charge carriers by the localized 4f moments. This leads to the formation of magnetic “bubbles” and the localization of charge carriers within them. Here we report on experiment which extends an earlier experiment on EuB6 where SANS indicated the presence of magnetic polarons. The experiment was carried out at the Institut Laue Langevin (ILL) in Grenoble. It shows the presence of superparamagnetic clusters well above the critical temperature in 48% Ca doped-EuB6. Unlike EuB6, Eu$_{0.52}$Ca$_{0.48}$B$_6$ does not undergo an insulator to metal phase transition, and its resistivity grows rapidly below 10 K. A metallic state can be obtained through the application of a magnetic field greater than 2 T. In Eu$_{0.52}$Ca$_{0.48}$B$_6$, the charge carrier stay trapped inside the magnetic polarons, leading to an increasing resistivity at lower temperature.

**11:39 AM B07.00003: NMR Studies of TmVO$_4$**

ZHIPAN WANG (Presenter), ZIWEN MEI, University of California, Davis, PAULO MENEGASSO, Instituto de Física “Gleb Wataghin”, UNICAMP, TANAT KISSIKOV, University of California, Davis, PIERRE MASSAT, IAN R FISHER, Stanford University, NICHOLAS CURRO, University of California, Davis — TmVO$_4$ undergoes a tetragonal to orthorhombic structural phase transition below 2.2K due to a cooperative Jahn-Teller distortion. The Tm ions experience a crystal-field effect with a non-Kramers ground state doublet. We have performed $^{51}$V NMR in a single crystal to investigate the role of magnetic and quadrupolar fluctuations. We find that the spin lattice relaxation rate varies strongly with field orientation, which reflects the role of quadrupolar(nematic) fluctuations near the critical temperature. We have also observed strong angular dependence of the $^{51}$V NMR Knight shift.

**11:51 AM B07.00004: NMR Studies of Nematicity in TmVO$_4$ and TmAsO$_4$**

ZIWEN MEI, ZHIPAN WANG, University of California, Davis, PAULO MENEGASSO, Physics, Campinas State University, PIERRE MASSAT, IAN R FISHER, Physics, Stanford University, NICHOLAS CURRO (Presenter), University of California, Davis — The crystal field ground state of Tm ions in certain crystal symmetries is a non-Kramers doublet, with a vanishing g-factor. In such cases strain can couple to the quadrupolar moment of the Tm ions, and a cooperative Jahn-Teller effect leads to Ising orbital-nematic order of the Tm moments. Application of a magnetic field along the $c$-axis suppresses the nematic order continuously and gives rise to a nematic quantum critical point. We have studied the critical nematic fluctuations via $^{51}$V and $^{75}$As NMR in TmVO$_4$ and TmAsO$_4$. These nuclei have quadrupolar moments that couple to the nematic degrees of freedom of the Tm. Fluctuations of both the Tm magnetic moments and the quadrupolar moments contribute to the spin-lattice relaxation of the nuclei, and we demonstrate how both the dynamical magnetic and dynamical nematic susceptibilities can be extracted from the spin-lattice relaxation rate.

*We acknowledge support from the NSF Grant number DMR-1807889.*
ANNA GALLER (Presenter), LEONID POUROVSKII, SILKE BIERMANN, Centre de Physique Théorique, Ecole Polytechnique — Designing new materials for permanent magnet applications is currently a very active field of research. While, at present, the best permanent magnets are based on the expensive rare-earth elements Nd, Sm or Dy (e.g. Nd$_2$Fe$_{14}$B), efforts are made to replace them with more available elements like Ce, with the hope to discover compounds with even better performance and lower production costs. Theoretical efforts to assist this quest encounter challenges related to the correlated nature of the rare-earth 4f states. In particular, in the family of potential Ce-based permanent magnet materials a key question is the localized vs. heavy-fermion behavior of the Ce-4f electrons. In this context, we investigate the role of electronic correlations in CeFe$_2$, CeFe$_{12}$ and CeFe$_{11}$Ti from first principles by using combined density functional and dynamical mean-field theory. We solve the corresponding quantum impurity problem by means of a continuous-time Quantum Monte Carlo solver and analyze the resulting electronic structure focusing on the degree of localization of the Ce-4f states as well as the magnetic properties of the compounds.

*DFG - Deutsche Forschungsgemeinschaft
ANR - Agence Nationale de la Recherche
FWF - Fonds zur Förderung wissenschaftlicher Forschung
ERC - European Research Council

RYOSUKE YAMAMURA (Presenter), TAKASHI HOTTA, Tokyo Metropolitan University — In recent decades, multipole ordering in f$^2$-electron systems such as Pr and U compounds have attracted continuous attention in the research field of condensed matter physics. In fact, peculiar modulated antiferro non-Kramers $\Gamma_3$ quadrupole ordering in PrPb$_3$ has been reported in 2005 [1], but the mechanism has been still under debate. To understand such incommensurate $\Gamma_3$ quadrupole ordering in PrPb$_3$, we develop a microscopic theory of multipole ordering in f$^2$-electron systems from an itinerant picture on the basis of a j-j coupling scheme [2]. For the purpose, we introduce the $\Gamma_7$-$\Gamma_8$ Hubbard model on a simple cubic lattice with the effective interactions which induce local $\Gamma_3$ states. By evaluating multipole susceptibility in a random phase approximation, we find that the hybridization between $\Gamma_7$ and $\Gamma_8$ orbitals plays a key role for the emergence of $\Gamma_3$ quadrupole ordering. We propose that $\Gamma_3$ quadrupole ordering can be explained from a combined concept of “multipole nesting”, which contains a couple of pieces of information about nesting properties and multipole density distribution on the Fermi surfaces.


ELLIOTT ROSENBERG (Presenter), IAN R FISHER, Stanford University — Electronic nematicity, in which the electronic degrees of freedom break the rotational symmetry of the lattice, has been exhibited by many materials including various high-temperature superconductors. A local realization of electronic nematicity is also seen in 4f intermetallic materials undergoing ferroquadrupolar order. In these materials the lattice of local 4f electronic multiplets collectively and spontaneously break the rotational symmetry of the point group of the lattice. Here we measure the quadrupole-strain (nematic) susceptibility of TmAg$_2$, which exhibits a ferroquadrupolar phase transition at 5.0K. We implement an elastoresistivity technique previously used in probing another 4f intermetallic, YbRu$_2$Ge$_2$, and extend this technique to investigate the nematic behavior of TmAg$_2$ while applying a “transverse” magnetic field to suppress the ferroquadrupolar phase transition to 0K.

*Funded by the Moore Foundation
12:39PM B07.00008: Ferromagnetic spin correlations in the filled skutterudite SrFe$_4$As$_{12}$ revealed by $^{75}$As NQR-NMR studies*  
YUJI FURUKAWA (Presenter), QING-PING DING, KHUSBOO RANA, Iowa State University, KOHEI NISHINE, JUN-ICHI HAYASHI, YUKIHIRO KAWAMURA, CHIHIRO SEKINE, Muroran Institute of Technology — Recently new filled-skutterudite compounds Sr$_3$T$_{4}$As$_{12}$ ($T$ = Fe, Ru, Os) have been synthesized, which provides a new opportunity of systematic studies of the effects of different d electron of 3d, 4d and 5d in the systems. In this study, as the first step for the systematic studies, we have carried out nuclear quadrupole resonance (NQR) and nuclear magnetic resonance (NMR) measurements on the filled skutterudite SrFe$_4$As$_{12}$ in order to investigate the magnetic properties from a microscopic point of view. Using the NQR spectra under small magnetic field, we have succeeded in determining Knight shift $K$. The temperature dependences of both $K$ and the nuclear spin-lattice relaxation rate divided by temperature, $1/T_1T$, have been reasonably explained by the simple model in which a concave-shaped band structure near the Fermi energy is assumed. The Korringa ratio parameter is found to be much smaller than unity, indicating the existence of ferromagnetic fluctuations. These NMR/NQR results evidence that SrFe$_4$As$_{12}$ is a metal with ferromagnetic spin correlations.

*USDOE under Contract No. DE-AC02-07CH11358.

12:51PM B07.00009: Antiferromagnetic order in Sr(Co$_{1-x}$Ni$_x$)$_2$As$_2$ revealed by single-crystal neutron diffraction*  
JOHN WILDE (Presenter), ANDREAS KREYSSIG, DAVID VAKNIN, SANGEETHA N. S., BING LI, BENJAMIN UELAND, DAVID C JOHNSTON, ROBERT MCQUEENEY, ALAN IRA GOLDMAN, Ames Laboratory, Iowa State University — SrCo$_2$As$_2$ has the same tetragonal lattice as the 122 Fe-based high Tc superconductors. It does not order magnetically, but inelastic neutron scattering experiments find antiferromagnetic (AF) fluctuations found in many of the 122 superconductors. Here we show results from neutron diffraction and magnetization experiments on single-crystals of Sr(Co$_{1-x}$Ni$_x$)$_2$As$_2$. However, the AF order is not stripe-type. Instead, the AF structure consists of ferromagnetic layers (with moments in the layer) that are stacked along c with an incommensurate propagation vector (0, 0, $q_z$). The propagation vector is doping dependent, suggesting spin density wave order. Using high-energy x-ray diffraction, we also find no evidence for a structural phase transition accompanying the AF order.

*Work at Ames Lab was supported by US DOE, BES, DMSE under DE-AC02-07CH11358. This research used resources at Oak Ridge National Laboratory and Argonne National Laboratory, both DOE BES user facilities.

1:03PM B07.00010: Electronic Structure and the Origin of the Phase Transition in BaAg$_2$As$_2$ Revealed by ARPES and REXS Studies  
XIA LOU (Presenter), Physics, Fudan University — Transition metal pnictides in 122 families are rich with fantastic quantum phenomena such as spin density wave (SDW) in BaFe$_2$As$_2$[1], superconductivity (SC) and charge density wave (CDW) in SrP$_2$As$_2$[2] and BaP$_2$As$_2$[3]. In the meanwhile, BaP$_2$As$_2$ and SrP$_2$As$_2$ shares CaBe$_2$Ge$_2$-type structure while BaFe$_2$As$_2$ crystallizes in ThCr$_2$Si$_2$-type structure. Studying the interplay among SDW, SC and CDW and their relationship with crystal structure and structural transition is of wide interests. BaAg$_2$As$_2$, as a newly-discovered transition metal pnictide adopted to ThCr$_2$Si$_2$-type structure, possess a phase transition at 138K in resistivity whose origin is still unknown[4]. To study the mechanism, we applied systematic angle-resolved photoemission spectroscopy (ARPES) combined with resonant elastic soft X-ray scattering (REXS) and identified the exact structural transition and density-wave-like transition in it for the first time.

propagation vector of (0, 0, 0.5) for both samples. The ordered moment lies along with present and discuss quantitative results from neutron and high-energy x-ray diffraction experiments on single crystals.

No structural phase transitions accompany the AFM transitions. Current and magnetic field configurations. Its possible origin will be discussed.

CaMn2Bi2 forms a hexagonal structure, consisting of alternately stacked Ca and Mn2Bi2 layers. Instead of ferromagnetic ordering seen in MnBi, CaMn2Bi2 orders antiferromagnetically below TN ~ 150 K, as reflected in the magnetization, specific heat, and electrical resistivity. Although it is considered as a narrow-gap semiconductor, our resistivity shows metallic behavior with a sharp drop at TN and a little bump at Tp ~ 20 K. Below Tp, large positive magnetoresistance with non-monotonic field dependence is observed in all current and magnetic field configurations. Its possible origin will be discussed.

Recent research are focused on perovskite materials because of their interesting properties. Among others, double perovskites La2-xNa1+x+xMnMoO6 shows magnetocaloric effect and large magnetoresistance making it appropriate substance for magnetic refrigeration applications at room temperature. Here, we investigate the electronic and magnetic properties of this recently synthesized material. We found that consistent with the experiment, for x~1.5, a ferromagnetic (FM) ground state is observed. With increase in La concentration, the charge transfers to Mn and Mo sites with increasing moment. It is interesting to note that magnetic phase transition occurs when doping concentration varies for x≤1. The electronic behavior shows metallic with major contribution from Mo-4d on Fermi level. The calculated net magnetic moment is 5.78 Bohr magneton which is in good agreement with the experimental value of 5.55 Bohr magneton. Our results reveals that interaction between the nearest neighbor and next nearest neighbor among Mn3+(t2g3eg1) and Mo5+(t2g1eg0) ions on the octahedral sites shows ferromagnetic coupling for x>1.

*Work at the Ames Laboratory was supported by the U.S. DOE, BES, DMSE under Contract No. DE-AC02-07CH11358. This research used resources at the High Flux Isotope Reactor and Advanced Photon Source, which are U.S. DOE Office of Science User Facilities.
2:03PM B07.00015: Band structure induced electronic correlations in nickel and iron: van-Hove singularities vs. Earth’s core conditions

ANDREAS HAUSOEL (Presenter), MICHAEL KAROLAK, Department for theoretical physics, University of Wuerzburg, Germany, ERSOY SASIOGLU, Institute for Physics, University of Halle, Germany, ALEXANDER I. LICHTENSTEIN, Institute for theoretical physics, University of Hamburg, Germany, KARSTEN HELD, Institute of Solid State Physics, TU Vienna, Austria, ANDREY A. KATANIN, Ural Federal University Ekaterinburg, Russia, ALESSANDRO TOSCHI, Institute of Solid State Physics, TU Vienna, Austria, GIORGIO SANGIOVANNI, Department for theoretical physics, University of Wuerzburg, Germany — Some Bravais lattices have a particular geometry and can slow down the motion of Bloch electrons: a 'pre-localisation' due to band structure properties. Another known source of electronic localisation in solids is the Coulomb repulsion in partially-filled d- or f-orbitals, which leads to the formation of local magnetic moments. The combination of these two effects has been viewed so far as mainly an academic issue. Here we show with ab-initio calculations of unprecedented accuracy and model studies, that their synergy represents instead the underlying physical mechanism in two of the most important ferromagnets: nickel and iron. Furthermore in nickel, the van-Hove singularity is essential for ferromagnetism to appear. Nickel's electron-electron scattering rate is linear in temperature, in violation of the conventional Landau theory of metals. This is true even at Earth's-core conditions, at which iron is instead a good Fermi-liquid. The importance of nickel in models of geomagnetism may therefore be reconsidered.

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B08 DCMP: Superconductivity: Copper Oxide - ARPES

11:15AM B08.00001: Three observations on the ARPES data of the cuprate superconductors - what the AF spin fluctuation can do and what it cannot Tao Li Renmin University of China, Beijing, China

TAO LI (Presenter), Physics, Renmin University of China — We discuss the origin of the pseudogap phenomena in the cuprate superconductors from the perspective of the spin-Fermion model. We find that the vanishing of the pseudogap around (\pi,0) as observed recently in Pr_{1.3-x}La_{0.7}Ce_{x}CuO_{4} is consistent with the AF band folding picture of the pseudogap in the electron-doped cuprates, if we assume a strongly momentum dependent quasi-particle scattering rate on the Fermi surface[1,4]. However, we find that the pseudogap in the hole-doped cuprates is unlikely an AF band folding gap. In particular, we show that electron pairing is indispensable to eliminate the Fermi level crossing along (\pi,0)-(\pi,\pi) in a way consistent with the ARPES observation on the underdoped Bi-2201 system around T*[2,4]. Nevertheless, we find that the AF spin fluctuation in the hole-doped cuprates is responsible for the high energy hump structure, the mismatch between the hump back-bending momentum and the bare Fermi momentum, and in particular, the extremely flatness of the anti-nodal quasi-particle dispersion in the superconducting state [3,4].


11:27AM B08.00002: Temperature Dependence of the Anisotropic Gap in YBa_{2}Cu_{3}O_{7}∗

GUANG-LIN ZHAO (Presenter), Southern University — Due to the complexity of the material structures, the experimental results for high Tc cuprates, including YBa_{2}Cu_{3}O_{7} (YBCO), are far more difficult to understand than those for conventional low Tc superconductors of simple structures. It is our view that many experimental results cannot be understood without careful first-principles calculations to include realistic electronic structures and electron-phonon (e-ph) interaction effect in these materials. We present the results of first-principles calculations for the electronic structure, e-ph interaction, and the temperature dependence of the anisotropic superconducting gap in YBCO. Our calculations show that the smaller gaps at some k-points on the Fermi surface of YBCO collapse earlier than the larger ones as the temperature increases, that leads to gapless state on the Fermi surface of YBCO even below Tc. The work was funded in part by NSF (Award # HRD 1736136 ) and ARO (Award # W911NF-15-1-0483).

*The work was funded in part by NSF (Award # HRD 1736136 ) and ARO (Award # W911NF-15-1-0483).
11:39AM B08.00003: Study of the interplay between pseudogap and antiferromagnetic correlations in electron-doped cuprates via TR-ARPES MARTA ZONNO (Presenter), FABIO BOSCHINI, ELIA RAZZOLI, MATTEO MICHIAIRD, RYAN P DAY, BEREND ZWARTSENBERG, PASCAL NIGGE, Department of Physics & Astronomy, University of British Columbia, EDUARDO DA SILVA NETO, Department of Physics, University of California Davis, ANDREAS ERB, Walther-Meissner-Institute for Low Temperature Research, SERGEY ZHDANOVICH, GIORGIO LEVY, Department of Physics & Astronomy, University of British Columbia, CLAUDIO GIANNETTI, Universita’ Cattolica del Sacro Cuore, DAVID J JONES, ANDREA DAMASCELLI, Department of Physics & Astronomy, University of British Columbia — In recent years, various angle-resolved photoemission spectroscopy (ARPES) studies focused on electron-doped cuprate superconductors to explore the similarities and differences between the two sides of the cuprates phase diagram. The pseudogap (PG) is a well-known phenomenon in the physics of high-temperature superconductors but despite numerous theoretical and experimental works, the origin of the PG in the cuprates is still under debate. Contrary to the hole-doped counterpart, antiferromagnetic (AF) correlations in the electron-doped side are stronger, offering the unique opportunity to explore the close interplay between AF, superconductivity, PG and other underlying phases. By exploiting time-resolved ARPES, we investigate the transient evolution of the low-energy density of state of the optimally doped Nd$_{2-x}$Ce$_x$CuO$_4$ (NCCO, x=0.15). In particular, by studying the temperature-dependence of the PG spectral features, we demonstrate the direct relation between PG and spin correlation length and provide evidence for the primary role of AF correlations in determining the PG in electron-doped cuprates.

11:51AM B08.00004: Strong electron-phonon coupling in Hg1201* MING YI, Physics and Astronomy, Rice University, JAYITA NAYAK, Physics, University of California, Davis, ZACHARY ANDERSON, YANG TANG, MARTIN GREVEN, Physics and Astronomy, University of Minnesota, ROBERT J BIRGENEAU, Physics, University of California Berkeley, INNA VISHIK (Presenter), Physics, University of California, Davis — Among single-layer cuprate high temperature superconductors, some materials have maximum $T_c$ ($T_{c,\text{max}}$) near 40K while others have $T_{c,\text{max}}$ near 100K, and the origin of this discrepancy is still unsettled. We present doping-dependent angle-resolved photoemission spectroscopy (ARPES) studies on HgBa$_2$CuO$_{4+\delta}$ (Hg1201), a single-layer cuprate with higher $T_{c,\text{max}}$ with a focus on spectral features which differ from more commonly studied single layer cuprates with lower $T_{c,\text{max}}$. Our studies indicate two different aspects of enhanced electron-phonon coupling in this system with distinct momentum dependence.

*JN and IV supported by Air Force Office of Scientific Research grant #FA9550-18-1-0156.

12:03PM B08.00005: Micro-ARPES study on the cuprate superconductor YBCO HIDEAKI IWASAWA (Presenter), Graduate School of Science, Hiroshima University, NIELS SCHRÖTER, Paul Scherrer Institut, Swiss Light Source, TAKAHIKO MASUI, Department of Physics, Kindai University, SETSUKO TAJIMA, Department of Physics, Osaka University, TIMUR KIM, Diamond Light Source, MORITZ HOESCH, Photon Science, Deutsches Elektronen-Synchrotron — Utilizing angle-resolve photoemission spectroscopy with several tens of microns spot size (micro-ARPES), we disentangled surface electronic inhomogeneity of the high-$T_c$ cuprate superconductor YBa$_2$Cu$_3$O$_y$. Two surface terminations consisting of either a CuO or BaO layer are identified through a chemical-states-specified core-level intensity distribution. This enables us to perform termination-selective ARPES measurements that uncover the different charge fillings and electronic configurations depending on the surface termination. By combining the real-space and electronic information, we propose a simple model to explain the termination-dependent surface electronic reconstruction. Further, we will also present new observations of peculiar superconducting states as well as zero-energy surface states on the heavily overdoped BaO surface.

12:15PM B08.00006: Hidden Spin-Momentum Texture in High $T_c$ Cuprate Superconductor CHIU-YUN LIN (Presenter), KENNETH GOTLIEB, University of California, Berkeley, MAKSYM SERBYN, Institution of Science and Technology Austria, WENTAO ZHANG, Shaqihai jiao Tong University, China, CHRISTOPHER L SMALLWOOD, San Jose State University, CHRIS JOZWIAK, Lawrence Berkeley National Lab, Berkeley, USA, HIROSHI EISAKI, Electronics and Photonics Research Institute National Institute of Advanced Industrial Science and Technology, Japan, ASHVIN VISHWANATH, Havard University, ZAHID HUSSAIN, Lawrence Berkeley National Lab, Berkeley, USA, ALESSANDRA LANZARA, University of California, Berkeley — Spin-orbit coupling (SOC) in cuprate superconductors was not a focus of condensed matter research due to the negligible SOC value of the conducting orbitals comparing with the strong electronic correlations and its centrosymmetric crystal structure. By using spin- and angle-resolved photoemission spectroscopy, we unveiled a nontrivial spin-momentum locking pattern in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$. The asymmetry of the spin-up and spin-down channel suggests the strength of SOC is in the same order of the bilayer interaction. This poses an intriguing question of how the high temperature superconducting state emerges in the presence of SOC.
**12:27PM B08.00007: Fermi Surface Topology and Energy Gap of Heavily Underdoped Bi2212 Studied by Laser ARPES**

QIANG GAO (Presenter), PING AI, JING LIU, CHENG HU, GUODONG LIU, XINGJIANG ZHOU, The Chinese Academy of Sciences, Institute of physics — The high temperature cuprate superconductors exhibit a number of exotic properties especially in the underdoped region. Here we have carried out high resolution angle-resolved photoemission (ARPES) measurements on heavily underdoped Bi2Sr2CaCuO8 (Bi2212) superconductors by using our new laser-based ARPES system equipped with angle-resolved time-of-flight analyzer and 7 eV and 11 eV laser sources. We have synthesized high quality heavily underdoped Bi2212 single crystals with different dopings by Dy substitution of calcium and vacuum annealing. Taking advantage of our high resolution laser-ARPES, we have systematically studied the Fermi surface topology, the energy gap and the many-body effects in these heavily underdoped Bi2212. Implications of these results will be discussed.

*This work is supported by the National Key Research and Development Program of China (Grants No. 2016YFA0300300 and No. 2017YFA0302900).

**12:39PM B08.00008: ARPES study of the phase diagram of superconducting BSCCO-2212 with in-situ control of surface doping**

ILIYA K DROZDOV (Presenter), CMPMSD, Brookhaven National Laboratory — In high-Tc cuprates, the doping of carriers into the parent Mott insulator induces unconventional superconductivity. In most materials, including the widely studied Bi-2212, the doping level p cannot be determined from the chemical composition but is rather derived from the superconducting transition temperature, Tc, which is, in turn, measured in transport, relying on the assumption that Tc dependence on doping is universal across all the cuprate families. I will present angle-resolved photoemission studies of Bi2Sr2CaCu2O8+δ single crystals cleaved and annealed in ultra-high vacuum or in ozone to reduce or increase the doping on-demand. Such in-situ annealing technique allows mapping of a wide doping range, covering not only the superconducting dome but also previously experimentally inaccessible for this material family, metallic, non-superconducting phase on the overdoped side (OD0K). Evolution of the Fermi surface with doping shows surprisingly smooth dependence across the superconducting dome while the evolution of spectroscopic features corresponding to electron-boson coupling can be continuously tracked across the entire phase diagram including the extreme overdoped region.

*US DOE BES contract # DE-AC02-98CH10886; BNL Gertrude and Maurice Goldhaber Distinguished Fellowship

**12:51PM B08.00009: Co-substitution effect on electronic structure of high-Tc cuprate superconductor, Bi2Sr2Ca(Cu1-xCox)2O8**

TAKEO MIYASHITA (Presenter), WUMITI MANSUER, HITOSHI TAKITA, TAKUYA KUBO, SATOSHI ISHIZAKA, HIDEAKI IWASAWA, Graduate School of Science, Hiroshima University, EIKE F SCHWIER, KENYA SHIMADA, MASASHI ARITA, Hiroshima Synchrotron Radiation Center, Hiroshima University, YOSHINORI NUMATA, TATSURO UTO, AZUSA MATSUDA, School of Advanced Science and Engineering, Waseda University, AKIHIRO INO, Faculty of Engineering, Kurume Institute of Technology — Conventional superconductivity occurs when electron pairs are formed. However, the pairing mechanism of high-Tc superconductivity is still controversial. One may expect that experimental clues to this problem can be obtained from the behavior of superconducting gap, which represents the binding energy of an electron pair. It has previously been reported that the decrease in critical temperature, Tc, of Bi2Sr2Ca(Cu1-xCox)2O8 is proportional to Co substitution, x. Thus, it gives us a good opportunity to investigate the relation between Tc and the energy gap. Here, we report a high-resolution angle-resolved photoemission study of Bi2Sr2Ca(Cu1-xCo0.4)2O8 by using ultraviolet laser and synchrotron radiation. Even though Tc decreases from 91 K to 55 K with 4 % substitution of Co for Cu, almost no decrease in the superconducting gap has been observed. We also measured the residual intensity within the gap as a function of temperature. We have found that the residual intensity for Co 4% samples is larger than that for pristine samples. These results suggest that the Co substitution results in reduction of the density of the electron pairs rather than the change in the binding energy of the electron pairs.
1:03PM B08.00010: Deviation between magnetic quantum- and Lifshitz- critical point in electron doped cuprate $Pr_{1-x}La_{x}CuO_{4-δ}$

DONGJOON SONG (Presenter), IBS-CCES, Seoul National University, SUHEON LEE, Physics, Chung-Ang University, WOOBIN JUNG, IBS-CCES, Seoul National University, SEUNG-RYOUNG PARK, Physics, Incheon National University, SHIGEYUKI ISHIDA, YOSHIYUKI YOSHIDA, HIROSHI EISAKI, AIST, KWANG-YONG CHOI, Physics, Chung-Ang University, CHANGYOUNG KIM, IBS-CCES, Seoul National University — Since high-$T_{c}$ superconductivity in copper oxide (cuprate) and Fe-based material arises near the anti-ferromagnetic (AF) order phase boundary, relation between the magnetic quantum criticality and superconductivity has attracted extensive interest. On the other hand, there is an argument in many novel superconductors that the key role in inducing superconductivity is played by Lifshitz transition which leads to Fermi surface transformation without symmetry breaking.

We performed systematic doping and temperature dependent muon spin rotation ($\mu$SR) measurement and angle resolved photoemission spectroscopy (ARPES) on the electron-doped cuprate $Pr_{1-x}La_{x}CuO_{4-δ}$ in order to resolve the interplay among the magnetic quantum criticality, Lifshitz criticality, and superconductivity. Surprisingly, while the long-range AF order phase boundary is located around heavily under doped regime, the Lifshitz transition associated with nodal hole pocket takes place in the vicinity of optimal doping concentration. In this talk, we will present the magnetic and electronic phase diagram of electron doped cuprate $Pr_{1-x}La_{x}CuO_{4-δ}$ and discuss the implication of our results on the generic phase diagram of high-$T_{c}$ superconductors.

1:15PM B08.00011: Doping Evolution of Energy Gaps in Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ superconductors studied by Laser-based ARPES

PING AI (Presenter), QIANG GAO, LIU JING, JIANWEI HUANG, YING DING, GUODONG LIU, GENDA GU, XINGJIANG ZHOU, Chinese Academy of Sciences — The energy gap is a key quantity in understanding the high temperature superconductivity mechanism in cuprate superconductors. We have carried out comprehensive angle-resolved photoemission (ARPES) measurements on Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ (Bi2212) superconductors by utilizing our high resolution laser-based ARPES system equipped with an angle-resolved time-of-flight (ARToF) electron energy analyzer and lasers with 7 and 11 eV photon energies. With high instrumental resolution (~1 meV) and wide coverage of the momentum space, we will report detailed doping, momentum and temperature dependences of the energy gap (superconducting gap and pseudogap) in Bi2212. Implications of these results will be discussed.

1:27PM B08.00012: Doping evolution of kink from the contionously doped cuprate surface

YIGUI ZHONG (Presenter), JIANYU GUAN, JIN ZHAO, Chinese Academy of Sciences, JIANHAO ZHANG, ZHENG-YU WENG, Tsinghua University, GENDA GU, Brookhaven National Laboratory, YIJIE SUN, HONG DING, Chinese Academy of Sciences — We present the doping evolution of the kink dispersion at node by in-situ ARPES measuring on a continuously doped surface of Bi2212 using our recently pronounced surface treating technique of ozone/vacuum annealing [1]. We demonstrate the Fermi velocity (<5meV) decreases and the band velocity of middle energy (25~55 meV) is a constant when doping decreases. However, the band velocity beyond ~70 meV is larger and larger when goes to UD region. We propose a splendid scenario as a possibility to explain these exotic velocities of kink dispersion. We speculate there is an additional renormalisation to the Fermi velocity for the reason that the kink at ~ 10 meV comes from the coupling to boson modes like phonons. The band at middle energy constitutes by the "bared electron", so its band velocity is independent with doping due to the rigid-band shift nature of Bi2212 [2]. However, for band dispersion higher than the ~70 meV, the electrons are fractionalized then they acquire a greater velocity. And this fractionalized effect becomes stronger when comes to more and more UD, so the band velocity becomes bigger and bigger.

Ref:
1:39PM B08.00013: Fermi surface reconstruction in electron-doped cuprates without antiferromagnetic long-range order  JUNFENG HE (Presenter), Physics, University of Science and Technology of China, COSTEL R. ROTUNDU, Stanford University, MATHIAS SCHEURER, Harvard University, YU HE, MAKOTO HASHIMOTO, KEJUN XU, Stanford University, YAO WANG, Harvard University, EDWIN HUANG, TAO JIA, SUDI CHEN, BRIAN MORITZ, DONGHUI LU, YOUNG SANG LEE, THOMAS DEVEREAUX, ZHIXUN SHEN, Stanford University — Fermi surface (FS) topology is a fundamental property of metals and superconductors. In electron-doped cuprate Nd_{2-x}Ce_xCuO_4 (NCCO), an unexpected FS reconstruction has been observed in optimal- and over-doped regime (x=0.15-0.17) by quantum oscillation measurements (QOM). This is all the more puzzling because neutron scattering suggests that the antiferromagnetic (AFM) long-range order, which is believed to reconstruct the FS, vanishes before x=0.14. To reconcile the conflict, a widely discussed external magnetic field-induced AFM long-range order in QOM explains the FS reconstruction as an extrinsic property. Here, we report angle-resolved photoemission (ARPES) evidence of FS reconstruction in optimal- and over-doped NCCO. The observed FSs are in quantitative agreement with QOM, suggesting an intrinsic FS reconstruction without field. This reconstructed FS, despite its importance as a basis to understand electron-doped cuprates, cannot be explained under the traditional scheme. We discuss the possible origin.

1:51PM B08.00014: In situ angle-resolved photoemission spectroscopy measurements of cuprate thin films grown by molecular beam epitaxy  ZHUOYU CHEN (Presenter), SLAVKO REBEC, TAO JIA, GLAM, Stanford University, MAKOTO HASHIMOTO, DONGHUI LU, SSRL, SLAC, ZHIXUN SHEN, GLAM, Stanford University, ROBERT G MOORE, SIMES, SLAC — Utilizing the oxide molecular beam epitaxy (MBE) in situ connected to beam-line angle-resolved photoemission spectroscopy (ARPES) in Stanford Synchrotron Radiation Lightsource (SSRL), high-quality cuprate films grown atomic-layer-by-layer enable measurements of electronic structure tuned by various parameters, such as epitaxial strain and surface termination, which have not been possible before with bulk materials. With the in situ connected scanning tunneling microscopy (STM), we are able to further resolve electronic properties of these films in spatial dimensions. In this talk, the newest results coming from this interconnected system will be presented.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B09 DCMP: Superconductivity: Theory/Computational

BCEC 151A - Brian Moritz, SLAC National Accelerator Laboratory

11:15AM B09.00001: Pairfield fluctuations in the 2D Hubbard Model*  THOMAS MAIER (Presenter), Computational Sciences and Engineering Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, DOUGLAS J SCALAPINO, Physics Department, University of California, Santa Barbara — The nature of the pseudogap phase out of which superconductivity emerges in the cuprates remains an open problem. Pairfield fluctuations above the superconducting transition temperature provide information on the nature of this phase. Here we report numerical calculations of the d-wave pairfield susceptibility of a 2D Hubbard model for dopings which have a pseudogap and for dopings which do not. One knows that in both cases there will be a region of Kosterlitz-Thouless fluctuations as the transition at TKT is approached. Above this region, we find evidence that the pseudogap limits the growth of the local pairfield and provides an environment in which phase fluctuations determine the temperature dependence of the pairfield susceptibility. In contrast, in the overdoped regime where there is no pseudogap, the temperature dependence of the pairfield is consistent with Ginzburg-Landau amplitude fluctuations. We discuss an experiment that can be used to measure this characteristic difference.

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

11:27AM B09.00002: Superconducting symmetry of the extended Hubbard model below Tc  FRANK MARSIGLIO (Presenter), JOEL HUTCHINSON, University of Alberta — The two-dimensional extended Hubbard model on a square lattice is known to host s-wave, d-wave and p-wave superconducting phases depending on the values of the on-site and nearest-neighbour interactions. By examining the free energy functional of the gap in this model, we find that these symmetries are often dependent on temperature. The critical points of this functional are highly constrained by the lattice symmetry and allow us to formulate stringent conditions on the temperature profile of the gap function, applicable to other models as well. In this talk, we discuss the finite temperature phase diagram of the extended Hubbard model, and point out the existence of first and second order symmetry transitions below Tc. Understanding such transitions may be important for assessing the symmetry of some unconventional superconductors such as UPt_3.
11:39 AM B09.00003: An accurate indicator for unconventional superconductivity using charge-spin coupling

RODRIGUES (Presenter), LUCAS WAGNER, Department of Physics, University of Illinois at Urbana Champaign — A data-based prediction model for unconventional superconductivity is constructed, which has three ingredients: a layered crystal structure, stable local magnetic moments and an intermediate spin-orbital (as opposed to spin-orbit) coupling. This classifier is sufficiently specific to clearly distinguish cuprate and iron-based superconductors from other materials in the same structural class. We discuss some of the putative false positives and whether they might be good candidates for new unconventional superconductors.

*This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DEAC0298CH1088. The computational resources used in this work were provided by the University of Illinois Campus Cluster and the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Superconducting Applications. All data will be available through the Materials Data Facility.

11:51 AM B09.00004: Ground state phase diagram of doped Hubbard model on 4-leg cylinders

YIFAN JIANG (Presenter), THOMAS DEVEREAUX, HONG-CHEN JIANG, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory and Stanford University — We report a large-scale density-matrix renormalization group study of the lightly doped Hubbard model on 4-leg cylinders in the presence of next-nearest hopping t'. By keeping a large number of states for long system sizes, we are able to reveal a rich phase diagram consisting of a variety of distinct phases, including (1) The Luther-Emery (LE) liquid with quasi-long-range superconductivity (SC) and charge-density-wave (CDW) order, but with a gap in the spin sector; (2) Insulating phase with "filled" charge stripe and long-range CDW order but no long-range SC, and (3) Luttinger liquid phase with dominant single-particle correlation and subdominant SC and CDW correlations. In particular, at δ=12.5% doping concentration, we found that a tiny t'∼-0.01t is enough to drive the system out of the insulating state at t'=0 to the LE phase. Aside from t', the effect of Coulomb repulsion and doping concentration has also been explored. Our results indicate that a route to robust long-range superconductivity involves destabilizing insulating charge stripes in the doped Hubbard model.

*This work was supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.

12:03 PM B09.00005: Study of nodal gap in t-J model via renormalized mean field theory

YIHSUAN LIU (Presenter), WEI-LIN TU, Institute for Solid State Physics, The University of Tokyo, TING-KUO LEE, Institute of physics, Academia Sinica — Angle-resolved photoemission (ARPES)[1] and scanning tunnelling microscopy (STM) [2] results show that Bi$_2$Sr$_{2-2y}$La$_y$CuO$_{6+δ}$ exhibit a gap, instead of a node, near the nodal region for x < 0.1. A similar gap has also been found in lightly doped La$_{2-x}$Sr$_x$CuO$_4$[3]. All these experiment results indicated that spin density wave (SDW) and nodal gap(NG) are closely related. However, why the NG close when the insulator-superconductor transition occurs remains unclear.

From the theoretical point of view, various degenerate intertwined order states have been investigated via renormalized mean field theory(RMFT) [4]. Among these states, we found that only the states accompanied by SDW open the nodal gap. Otherwise, there is either node or arc near nodal region. In this work, we will discuss the mechanism of the gap formation and show the gap evolution upon doping.


*The authors are grateful for the support of the Taiwan Ministry of Science and Technology Grant MOST 106-2112-M-001-020 and MOST 107-2112-M-001-034.
CHEN SHUAI (Presenter), Tsinghua University — We study a ground-state ansatz for the single hole doped t-J model in two dimensions via a variational Monte Carlo method. Such a single hole wavefunction possesses a composite structure with a finite angular momentum associated with hidden spin currents, which gives rise to a novel ground state degeneracy in agreement with recent ED and DMRG results. We further show that the wavefunction is composed of a quasiparticle component and an incoherent momentum distribution in excellent agreement with the DMRG results up to an 8×8 lattice. But the quasiparticle spectral weight determined by the VMC vanishes in a power-law fashion, indicating that the doped hole becomes a non-Landau quasiparticle in the large sample-size limit. Here the bare hole propagator decays much faster as compared to the composite hole over a spatial distance, supporting the picture that a bare hole must be turned into a “twisted” quasiparticle in order to propagate more coherently in an antiferromagnetic background. However, by turning on the phase string induced by the hole hopping in the t-J model, a normal Bloch-wave wavefunction with a finite quasiparticle spectral weight and conventional quantum numbers can be simply recovered in the so-called σt-J model, again well agreeing with the ED and DMRG results.

HONG-CHEN JIANG (Presenter), SLAC National Accelerator Laboratory — We report a large-scale density-matrix renormalization group study of lightly doped t-J-type model on the square lattice, which hosts a quantum paramagnetic state at half-filling. We observe an interesting interplay between d-wave superconductivity and spin and charge density wave (CDW) order. Despite the tendency of CDW order on thinner cylinders is strong, our results on wider systems suggest that the CDW order may disappear in the thermodynamic limit. The spin correlations are found to decay exponentially, on the contrary, the superconducting pair-field correlations decay power-law with an exponent significantly smaller than the spatial dimension. Our results suggest that a uniform d-wave superconductivity emerges in doping the quantum paramagnet on the square lattice. The connection of our results to two dimensions is also discussed.

MASON PROTTER (Presenter), RUFUS BOYACK, FRANK MARSIGLIO, University of Alberta — The standard BCS approach to superconductivity considers only particle-particle pairing interactions, meaning that Cooper pairing arises as an instability of an otherwise well-defined Fermi surface. In a more generic situation, other interactions can compete with the Cooper instability and lead to a breakdown in the formation of a Fermi surface, which as a result changes the properties of the ground state. We explore a functional-integral method for rigorously incorporating particle-hole fluctuation corrections to the BCS theory of superconductivity. These corrections arise naturally as the result of a multi-channel Hubbard-Stratonovich decomposition of an attractive Hubbard interaction. Differences between this approach and previous models of particle-hole corrections to BCS theory are considered.

YONGYOU ZHANG (Presenter), FAN YANG, School of Physics, Beijing Institute of Technology — Superconductivity in quasicrystal has been discovered in experiments [1] for Al–Zn–Mg quasicrystal with \( T_c \approx 0.05 \) K. In this presentation, we systematically studied the quasicrystal superconductor properties on Penrose lattices. Within two-particle approximation the negative U Hubbard model shows that the Cooper binding energy is proportional to exp(−1/U) and Anderson Law works well. Besides, the negative U Hubbard model was studied by the mean-field method with which the superconductor gap, superconductor density of states, entropy, specific heat, and current density are analyzed. The superconductor gap decreases to zero when the temperature is larger than \( T_c \), simultaneously the lines entropy and specific heat show the superconductor phase by their discontinuities. The paramagnetic and diamagnetic superconductor currents also have discontinuities at \( T_c \) and cancel each other when \( T>T_c \). Different from periodical lattices the superconductor current has a finite value when \( T = 0 \), which shows the difference of the superconductor behavior between the quasicrystals and common crystals.

Proximity induced superconductivity in quasicrystal-superconductor hybrid rings

Gautam Rai (Presenter), University of Southern California, Anuradha Jagannathan, Laboratoire de Physique des Solides, L’université Paris Sud, Stephan Wolfgang Haas, University of Southern California — Quasicrystals with their exotic long range spatial order are expected to host an exotic superconducting state. As a first step to understanding these new kinds of superconducting systems, we have studied proximity-induced superconductivity in a hybrid 1D chain. The hybrid system is modeled using the Bogoliubov-de Gennes approach, consists of a non-interacting Fibonacci chain coupled to a periodic superconductor. This quasiperiodic chain has topological properties which have been explored in a number of experimental/theoretical works. We show that an inhomogeneous superconductivity is induced in the normal chain, and, in particular, how edge states affect the induced pairing amplitudes.

Bond disproportionation and electron-phonon driven oxygen-bismuth hybrid hole pairing in bismuth perovskites

Kateryna Foyevtsova (Presenter), Arash Khazraie, Ilya Elfimov, George Albert Sawatzky, Stewart Blusson Quantum Matter Institute — In this talk, we will present the recently developed theory describing the bismuth perovskites ABIO₃ (A = Sr or Ba) as bond- (as opposed to charge-) disproportionated insulators where Bi-O hybridization and the presence of oxygen holes lead to formation of molecular orbitals and strong polaronic effects, which might be the prime mechanism driving these materials towards superconductivity upon doping. In particular, we will first use electronic structure methods to demonstrate that oxygen holes indeed condense into A₁g molecular orbitals centered at collapsed BiO₆ octahedra and then to derive an appropriate tight-binding (TB) model, as well as to estimate electron-phonon coupling and an effective attraction between the two holes in the A₁g symmetry in this collapsed “BiO₆ molecule”, emphasizing that these two parameters are strong enough to sustain polaronic superconductivity. We will also explore the parameter space of the TB model, finding a cross-over from the bond- into the charge-disproportionated insulating phase, as well as a metallic phase with a non-bonding character of the oxygen holes.

Pressure-enhanced high temperature superconductivity in XH₃ (X=As, Se, Br, Sb, Te and I)

Po-Hao Chang (Presenter), Swabir Silayi, Dimitrios A Papaconstantopoulos, George Mason University, Michael Mehl, US Naval Academy — The discovery of high critical temperature Tc superconductivity in highly compressed H₃S has opened up the question of searching for strong electron-phonon coupling in the hydrides outside the transition metal series. In this work, we performed linearized augmented plane wave (LAPW) calculations for many different volumes in the Im3m structure for XH₃ (X=As,Se,Br,Sb,Te and I), We then applied the multiple scattering-based theory of Gaspari and Gyoorffy to obtain the Hopfield parameters and the McMillan-Allen-Dynes theory to estimate λ and Tc. Based on our analysis, all considered materials share similar trends of Tc enhancement under increasing pressure. H₃Se in particular, could potentially go to a Tc well over 200 K. Finally, in addition to pressure enhanced electron-phonon coupling, by applying rigid band model we predict that a small amount of alloying with a neighboring element could lead to even further increase of Tc.
1:39PM B09.00013: First-principles evolutionary structural searches for new high-pressure phases of Nb3Al*
JIANJUN MAO (Presenter), YUE CHEN, The University of Hong Kong — High cost and poor stability have inhibited the large-scale applications of high-temperature cuprate superconductors. Intermetallic niobium compounds such as Nb3Sn and Nb3Al attract significant research interest due to their potential superconducting applications. Herein, we have combined evolutionary algorithms with density functional theory to perform structural searches for ground-state crystal structures of Nb3Al under high pressures. At ambient pressure and low temperature, a new phase with distorted Nb atomic chains is found to be energetically more stable than the well-known A15 phase. Because the Nb atomic chains are believed to be closely related to the superconducting properties, the electron-phonon coupling of this new phase has been further studied using density functional perturbation theory. Moreover, we identify a pressure-induced structural phase transition of Nb3Al under high pressures. Base on ab-initio molecular dynamics simulations, the temperature effects on the structural phase transitions of Nb3Al have also been investigated.

*This work is supported by the Research Grants Council of Hong Kong under project numbers 27202516, 17200017 and 17300018, and the National Natural Science Foundation of China under project number 51706192.

1:51PM B09.00014: Magnetism of the low-dimensional orbital-selective Mott insulators
JACEK HERBRYCH (Presenter), University of Tennessee, JONAS HEVERHAGEN, MARIA DAGHOFER, University of Stuttgart, GONZALO ALVAREZ, Oak Ridge National Laboratory, ADRIANA MOREO, ELBIO R DAGOTTO, University of Tennessee — The magnetic properties of low-D iron-based superconductors belonging to the 122 (Rb_xFe_ySe_2) and 123 (BaFe_2Se_3) families [1-2] proved to be a challenge for the theoretical description. Investigation of the orbital-selective Mott phase in 1D (relevant for 123 family) [3,4] revealed the existence of an exotic block spin order, namely AFM coupled FM spin islands. In parallel, inelastic neutron scattering experiments on quasi-1D BaFe_2Se_3 [2] and 2D Rb_xFe_ySe_2 [1] confirmed the relevance of these spin-block phases. The theoretical description of the latter requires long-range interaction and strong dimerization if within spin-wave models. In our work [4,5] we show that the magnetic properties of the orbital-selective Mott phase can be properly described by (short-range) multiorbital Hubbard models. Furthermore, we argue that the electronic correlations of itinerant orbitals are important for block-magnetism and that the minimal model which properly captures such a physics is the generalized Kondo-Heisenberg model.


BOQUN SONG (Presenter), MANH CUONG NGUYEN, CAI-ZHUANG WANG, PAUL CANFIELD, KAI-MING HO, Physics, Iowa State University — The recently discovered 1144-phase [1-2] suggests a new type of composite alloys, namely hetero-crystals. The author will present its definition and demonstrate wide existence. The hetero-crystals consist of the layered skeleton and hetero-cations alternatively located on both sides of the skeleton. Tuning cation species leads to significant modifications to structures, granting an exceptional chance to manipulate the emerging phases. The 1144-phase is examined as a case study of hetero-crystals. Various 1144-arsenide and phosphides are examined by combining first principle calculation and ideal solution approximation, wherein configurational, vibrational and electronic degrees of freedom are fully considered. Remarkably, the seemingly random occurrence of the 1144 phases is governed by a rule that involves two factors: elastic distortion and charge balance. Derived from 1144-phosphides, the rule, nevertheless, is heuristic and generic, which leads to an outlook of other hetero-crystals promising to be stabilized. [1] B. Q. Song, et. al. Physical Review B 97 (9), 094105 (2018). [2] B. Q. Song, et. al. Physical Review Materials 2 (10), 104802 (2018)

*The work was performed at Ames Laboratory, operated for U.S. DOE by Iowa State University under contract DE-AC02-07CH11358.

**Monday, March 4, 2019 11:15 AM - 1:51 PM**

Session B10 DMP: Fe-based Superconductors II BCEC 151B - Vitalii Vlasko-Vlasov, Argonne National Laboratory - Tag(s): Focus
11:15AM B10.00001: Elastoresistive and elastocaloric anomalies in iron pnictides* [Invited] MATTHIAS IKEDA
(Presenter), Geballe Laboratory for Advanced Materials, Stanford University — Electronic nematicity is a prominent feature in Fe-based superconductors, but is also present in at least some cuprates, and heavy fermion superconductors. Being a possible common thread for unconventional superconductivity, the role of nematic fluctuations for superconductivity needs to be assessed. This calls for new techniques that allow for tuning nematicity continuously towards quantum criticality. In the first part of this talk I will discuss how to disentangle the response of nematicity to strain components of different symmetry, and will show that both symmetric (A1g) and antisymmetric (B1g) strain are suitable means to tune the critical temperature of the nematic phase transition in Fe based superconductors. In the second part of the talk, I will outline recent experimental advances exploring the thermoelastic properties of these materials. In particular, the finite response of nematicity to strain causes anomalies in the elastocaloric effect as well as in the elastoresistivity which can be measured via an AC technique. These anomalies are proportional to the corresponding heat capacity anomalies and are understood to be a direct consequence of the strain dependence of the nematic and the antiferromagnetic transition temperatures. A similar mechanism should more generally be expected for any phase transition tunable by strain.

*This work was supported in part by the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4414 and by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DEAC02-76SF00515.

11:51AM B10.00002: Suppression of T_C in an underdoped iron-based superconductor through uniaxial strain*
PAUL MALINOWSKI (Presenter), SHUA SANCHEZ, JOSHUA Mutch, QIANNI JIANG, University of Washington, JONG-WOO KIM, PHILIP RYAN, Advanced Photon Source, Argonne National Labs, JIUN-HAW CHU, University of Washington — The iron-based superconductors generically have been shown to host the electronic nematic phase which competes with superconductivity. Previous work has also shown that anisotropic strain is particularly well suited as a tunable, symmetry breaking field that can couple to the nematic order parameter. In this work, we present electrical transport, magnetic susceptibility, and single crystal x-ray diffraction measurements demonstrating that the superconducting transition in an underdoped iron-based superconductor is efficiently tuned towards zero temperature through the application of large, uniaxial strain that enhances the orthorhombic distortion. This demonstrates that application of mechanical strain is a novel external parameter that is able to tune a superconductor to metal transition in a three-dimensional system.

*AFOSR Grant No. FA9550-17-1-0217

Gordon and Betty Moore Foundation's EPiQS Initiative, Grant GBMF6759

12:03PM B10.00003: Elastoresistivity measurements in a 65 T pulsed magnet on Fe-based superconductors*
JOSHUA STRAQUADINE (Presenter), JOHANNA PALMSTROM, PHILIP WALMSLEY, ALEXANDER T HRISTOV, Stanford University, FRANZISKA WEICKERT, FEDOR F. BALAKIREV, MARCELO JAIME, ROSS MCDONALD, IAN R FISHER, Pulsed Field Facility, National High Magnetic Field Laboratory — One of the most striking signatures of the nematic transition in the underdoped iron-based superconductors is a diverging elastoresistivity, which is the linear response of the resistivity anisotropy to the corresponding symmetry-breaking strain. Elastoresistivity, however, cannot be measured in the superconducting state; tracking the nematic fluctuations down to the putative quantum critical point near optimal doping necessitates the use of extreme magnetic fields to suppress superconductivity. We report the first elastoresistivity experiments in pulsed magnetic fields up to 65 T on near-optimally-doped Ba(Fe1-χCoχ)2As2 at temperatures down to 1.3 K, and discuss the technical advances required to make such a measurement possible within the few millisecond window when the field is above Hc2. These new techniques expand the applicability of elastoresistivity measurement for disentangling the role of nematic fluctuations in strongly correlated systems.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-76SF00515. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation Cooperative Agreement No. DMR-1644779 and the State of Florida.
12:15PM B10.00004: Changing nature of superconductivity in tetragonal FeS under pressure  MAKOTO SHIMIZU, Department of Physics, Okayama University, NAYUTA TAKEMORI, Research Institute for Interdisciplinary Science, Okayama University, DANIEL GUTERDING, Fachbereich Mathematik, Naturwissenschaften und Datenverarbeitung, Technische Hochschule Mittelhessen, HARALD JESCHKE (Presenter), Research Institute for Interdisciplinary Science, Okayama University — Tetragonal FeS is an iron chalcogenide superconductor with similarities to FeSe but without nematic phase and with weaker electronic correlations. In contrast to pure FeSe, however, FeS shows two superconducting domes under pressure. We use electronic structure and spin fluctuation theory calculations for tetragonal FeS in order to study the nature of the superconducting order parameter [1]. In the random phase approximation, we find a gap function with d-wave symmetry at ambient pressure which is in agreement with several reports of a nodal superconducting order parameter in FeS. We find that, as a function of pressure, the superconducting pairing strength decreases until a Lifshitz transition takes place at 4.6 GPa. As a hole pocket with a large density of states appears at the Lifshitz transition, the gap symmetry is altered to sign-changing s-wave. At the same time the pairing strength is severely enhanced and increases up to a new maximum at 5.5 GPa. Therefore, our calculations explain the occurrence of two superconducting domes in FeS without any structural phase transition.


12:27PM B10.00005: Specific heat measurements of the high-temperature magnetic superconductor RbEuFe4As4* KRISTIN WILLA, ROLAND WILLA, JINKE BAO, ALEXEI E KOSHELEV, DUCK YOUNG CHUNG, Argonne National Laboratory, MERCOURI KANATZIDIS, Department of Chemistry, Northwestern University, WAI-KWONG KWOK (Presenter), ULRICH WELP, Argonne National Laboratory — We report specific heat measurements on the newly discovered magnetic superconductor RbEuFe4As4. We investigated the superconducting transition at Tc = 38K and extracted the phase boundary for in and out of plane magnetic fields and obtained an anisotropy ratio of 1.8. At small fields near the magnetic transition temperature Tm ~ 14.9K, we resolved a cusp-like behavior in the temperature dependence of the specific heat curve that shifts to lower temperatures for fields along the c-axis and a broad shoulder that shifts to higher temperatures for in-plane fields. We can reproduce our measured calorimetry data quantitatively by Monte-Carlo simulations of an anisotropic easy-plane 2D Heisenberg model that suggests that the cusp in specific heat is due to a BKT transition and the high temperature hump at higher fields marks a crossover from a paramagnetically disordered to an ordered state.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. K. W. and R. W. acknowledge support from the Swiss National Science Foundation through an Early Postdoc Mobility fellowship.

12:39PM B10.00006: Superconducting phase diagram of magnetically ordered superconductor RbEuFe4As4 in pulsed fields up to 65 T* MATTHEW SMYLIE (Presenter), Physics and Astronomy, Hofstra University, KRISTIN WILLA, JINKE BAO, ROLAND WILLA, ALEXEI E KOSHELEV, WAI-KWONG KWOK, DUCK YOUNG CHUNG, Argonne National Laboratory, MERCOURI KANATZIDIS, Northwestern University, JOHN SINGLETON, FEDOR BALAKIREV, Los Alamos National Laboratory, PRASHANTA NIRAULA, EIMAN BOKARI, ASGHAR KAYANI, Western Michigan University, ULRICH WELP, Argonne National Laboratory — The superconducting phase diagram of single-crystal RbEuFe4As4 (Tc ~ 36.5 K), which has long-range Eu magnetic order at Tm ~ 15 K, has been measured in pulsed magnetic fields up to 65 T using a proximity diode oscillator technique. Upon decreasing temperature, the anisotropy Hc2ab/Hc2c decreases from 1.8 near Tc towards unity indicating significant Pauli paramagnetic limiting effects for both H // (110) and H // (001). This is born out in theoretical fits for a Fermi surface in the form of warped cylinders, yielding a high in-plane Maki parameter of ~2.4, suggesting that a low temperature FFLO state may exist above 65 T. Irradiation with 5 MeV protons to a dose of 5x1016 p/cm² suppresses Tc by ~ 3K, a substantial increase in vortex pinning and a reversal in anisotropy at temperatures below 15K.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. K. W. acknowledges support from the Swiss National Science Foundation through an Early Postdoc Mobility fellowship. Part of this work is supported by the US DoE BES FWP Science in 100 T, and carried out at the National High Magnetic Field Laboratory, which is funded by NSF Cooperative Agreement DMR-1157490, the State of Florida and U.S. DoE.
DING HU (Presenter), PENGCHENG DAI, Rice University, ZHIPING YIN, Department of Physics, Beijing Normal University — Superconductivity in BaFe2(As1−xPx)2 iron pnictides emerges when its nematic phase and stripe AF order at TN (Ts = TN) are gradually suppressed with increasing x, reaching optimal superconductivity around x = 0.30 with Tc ≈ 30 K. We show that a moderate uniaxial pressure along the c-axis in BaFe2(As0.70P0.30)2 spontaneously induces a 3D collinear antiferromagnetic order with TN = Ts > 30 K, while only slightly suppresses Tc. Furthermore, c-axis pressure pushes the underdoped BaFe2(As0.72P0.28)2 to optimal superconductivity with Tc = 30K without AF order firstly, then AF order emergences at higher pressure region. We find that a c-axis pressure compresses the c-axis lattice while expanding the in-plane lattice and increasing the nearest-neighbor Fe–Fe distance, it barely changes the average iron-pnictogen height in BaFe2(As0.70P0.30)2. Therefore, the pressure-induced antiferromagnetic order must arise from a strong in-plane magnetoelastic coupling, suggesting the universal phase diagram under c-axis pressure in BaFe2(As1−xPx)2.

*U.S. NSF-DMR-1700081 (P.D.) and Robert A. Welch Foundation Grant no. C-1839 (P.D.).

MARTA CIEPLAK (Presenter), IRYNA ZAYTSEVA, IRINA ABALOSZEWA, KATARZYNA KOSYL, DARIUSZ GAWRYLUK, Polish Academy of Sciences — The structural disorder, frequently present in crystals of iron chalcogenides, sometimes leads to unexpected improvement of superconducting properties, as reported in the case of FeTe0.65Se0.35 crystals [1]. In an effort to find the origin of such behavior, here we study the structure, the Hall effect, and the angle-dependent magnetoresistance (AMR) of the Fe1−yNiyTe0.65Se0.35 crystals, with y in the range from 0 to 0.08, grown by Bridgman's method with different cooling rates, slow (S) and fast (F). The S crystals with single, tetragonal phase show inferior superconducting properties to these shown by F crystals, in which an admixture of monoclinic phase is found. The Hall effect of crystals with y>0.03, in which superconductivity is suppressed, confirms the electron doping of both types of crystals, while the AMR is an order of magnitude larger in F crystals, with y-dependent anisotropy at low temperatures (T < 8K), which disappears on warming. The analysis of the AMR suggest that it may originate in the magnetism of monoclinic inclusions, most likely of the type Fe3(Se-Te)4. The relation of these findings to superconductivity will be discussed.


*Supported by Polish NSC Grant No. 2014/15/B/ST3/03889.

NIKOLA MAKSIMOVIC (Presenter), IAN M HAYES, VIKRAM NAGARAJAN, University of California, Berkeley, JOHN SINGLETON, FEDOR BALAKIREV, Los Alamos National Laboratory, JAMES G. ANALYTIS, University of California, Berkeley — The "strange metal" parent phase of high-temperature superconductors displays a resistivity that scales linearly with temperature. Recent experiments reveal that the resistivity of these compounds also increases linearly with applied magnetic field, and is characterized by a striking scaling law between magnetic field and temperature. It has been suggested that this behavior is governed by physics beyond the standard quasiparticle picture of metals, but it is necessary to determine to what extent conventional transport theory is applicable; for example, elastic scattering from lattice imperfections typically has a well-defined effect on magnetotransport. In this study, we measure high-field transport of systematically disordered samples of a high-Tc iron-pnictide superconductor near an antiferromagnetic instability. Our data suggest that antiferromagnetic fluctuations dominate at low temperatures, producing robust transport scaling between temperature and magnetic field which is intimately tied to the onset of superconductivity.

*This work was Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4374, and by the NHMFL-PFF at Los Alamos National Laboratory through NSF Cooperative Agreement No. DMR 1157490 and the DoE.
1:27PM B10.00010: Precision Controlled Detwinning of Orthorhombic Twin Domains in Underdoped BaFe$_2$As$_2$

SHUA SANCHEZ (Presenter), JIUN-HAW CHU, University of Washington, PHILIP RYAN, JONG-WOO KIM, Argonne National Labs — Underdoped BaFe$_2$As$_2$ exhibits an orthorhombic structural phase transition driven by electronic nematic ordering. In the past, the relation between lattice distortion and electronic anisotropy above the phase transition has been studied comprehensively by the technique of elastoresistivity. In contrast, the relation between spontaneous orthorhombicity ($(a-b)/(a+b)$) and spontaneous resistivity anisotropy ($(R_a - R_b)/(R_a + R_b)$) below the phase transition has never been measured to the same level of precision. Several previous detwinning experiments have used samples under a constant uni-axial stress, which results in additional lattice distortion especially close to phase transition. Here we present x-ray diffraction data on a crystal sample in which in-situ tunable uniaxial stress is used to precisely control the detwinning of domains. Lattice constant data showing both the relative domain populations and the elastic response to stress are matched with simultaneous resistivity measurements to yield a precise determination of the domain resistivity anisotropy. Elastoresistivity tensor coefficients are also computed in the fully detwinned single domain state, which cannot be inferred from macroscopic strain measurements alone.

1:39PM B10.00011: Post annealing effect on Ca(Fe$_{1-x}$Co$_x$)$_2$As$_2$ and AeFe$_2$As$_2$ (Ae = Ca, Sr, Ba) single crystals

SHUYUAN HUYAN (Presenter), LIANGZI DENG, YANFENG LYU, ZHENG WU, HANMING YUAN, FEI TIAN, The Texas Center for Superconductivity, University of Houston, YUANYUAN ZHAO, School of Physics and Optoelectronic Engineering, Nanjing University of Information Science and Technology, KUI ZHAO, Advanced Micro-Fabrication Equipment Inc., JINGYING SUN, MELISSA GOOCH, JAMES K MEEN, SHUO CHEN, ZHIFENG REN, CHING-WU CHU, The Texas Center for Superconductivity, University of Houston — Through post annealing & quenching process, we could induce superconductivity in the non-superconducting single crystals of Ca(Fe$_{1-x}$Co$_x$)$_2$As$_2$ and AeFe$_2$As$_2$ (Ae = Ca, Sr, Ba) grown by self-flux solution method, with onset-$T_c$ below 15 K, 16 K, 22 K and 24 K, respectively. A series of experiments were designed in order to look for the differences between as-grown samples and post annealed samples. By systematical characterization, including resistivity, Hall coefficient, magnetization, X-ray diffraction and wavelength dispersive spectroscopy results, the possible cause for the superconductivity in these samples is discussed. These experimental results help to shed light on the underlying mechanism for the repotted superconductivity in Fe-based 122 system.

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B11 DMP DCOMP FIAP: Defects in Semiconductors -- Device Materials

Peelaers, University of Kansas - Tag(s): Focus

11:15AM B11.00001: First-principles calculations on dislocation-point defect interactions in Cu(In,Ga)Se$_2$ solar cell absorbers* [Invited] KARSTEN ALBE (Presenter), DANIEL A. BARRAGAN-YANI, FB Material- und Geowissenschaften, TU Darmstadt — In Cu(In,Ga)Se$_2$ based commercial solar cells, power-conversion efficiencies of more than 15% can be achieved, although significant dislocation densities are present. This implies that lattice dislocations in CIGSe-based absorbers are per se electrically inactive or possibly passivated by solute or impurity atoms.

While intrinsic point defects in this material class have been completely characterized by density functional theory calculations using hybrid functionals [1], studying dislocations remains a challenge for electronic structure calculations. In this talk, I will present a supercell approach using dislocation dipoles, that allows to study the influence of chemical reconstruction and solute segregation on the electrical activity of mixed dislocations in CISE and CGSe. I will discuss the interaction of various dislocation types with intrinsic [3] and extrinsic point defects [3] and address the importance of mechanical driving forces. Moreover, the computational results are directly compared with experimental data from high-resolution electron microscopy [4].


*Helmholtz Virtual Institute HV-I-520 “Microstructure Control for Thin-Film Solar Cells”
11:51AM B11.00002: Observation of Enormous Non-Linearity in the Output Electroluminescence Characteristics of Room-Temperature GaN-Based Microcavities*  
ANIRUDDHA BHATTACHARYA (Presenter), Department of Electrical Engineering and Computer Science, University of Michigan at Ann Arbor — Highly non-linear light ($\lambda \sim 380$ nm)-current characteristics are observed in a bulk GaN-based laterally-emitting microcavity diode at room temperature. The value of the non-linear slope, when plotted in a double logarithmic scale, increases from $\sim 2$ to $\sim 40$ at the threshold ($\sim 5$ kA/cm$^2$). The spectral characteristics remain essentially invariant with increasing excitation and no signatures of coherence are observed at any injection. Control measurements indirectly show that the electroluminescence originates from the p-type Mg:doped GaN contact layer. These phenomena are at least partially and qualitatively similar to previous observations of super-linear photoluminescence characteristics in Zn:doped GaN epilayers at $\sim 180$ K [1]. In our case, the super-linearity originates, most possibly, due to the redistribution of injected carriers between the radiative and non-radiative pathways over a particular excitation regime. Further analysis of these effects is in progress and will be presented.


*NSF (Grant No. DMR-1120923)

12:03PM B11.00003: The Near-Surface Electrostatic Environment of n-Doped Silicon Probed with a Moveable Dangling Bond Point Probe  
TALEANA HUFF (Presenter), THOMAS DIENEL, MOHAMMAD RASHIDI, ROSHAN ACHAL, WYATT VINE, ROBERT A WOLKOW, Physics, University of Alberta — With nanoelectronics reaching the limit of atom-sized devices, it has become critical to characterize how irregularities in the local environment can affect device functionality. This includes unwanted charge defects detuning binary logic atomic patterns [1], delicately coupled quantum computing states [2], and supra-layer molecular electronics [3]. In this work, we characterize charged subsurface defects on a hydrogen terminated silicon (100) sample, adding a possible explanation for a heretofore contentious negatively-charged defect. Through contact potential difference maps, taken with non-contact atomic force microscopy, variations in the electrostatic topography on a nanometer length scale are shown and correlated with alterations in the behavior of dangling bond charge state transitions. In addition, the spectroscopic signature of a single electron charge transition in a dangling bond is used as a charge sensor to directly probe the depth of charged defects, the local Debye screening length, and the effective dielectric constant close to the surface.


12:15PM B11.00004: Extinction of Random Telegraph Switching by “Cryogenic Annealing” in Small Area Si MOS Transistors*  
GANGYI HU, MARK LEE (Presenter), HISASHI SHICHIJO, University of Texas at Dallas, CLINT A NAQUIN, HAL EDWARDS, Texas Instruments, Inc. — Random telegraph switching (RTS) showing a slow decay in switching rate at cryogenic temperatures that leads to eventual extinction of the discrete fluctuations has been observed in the drain-source current ($I_{DS}$) of small area Si n-channel metal-oxide-semiconductor (NMOS) transistors. The RTS was characterized by $I_{DS}$ fluctuations between two discrete levels over a finite interval of gate bias. In all devices showing RTS, the average switching rate gradually diminished to zero over a time of 1 to 2 hours at 15 K while maintaining nearly constant fluctuation amplitude, so that the RTS eventually ceased. This decay in switching rate may be due to a metastable oxygen vacancy defect that gradually repairs itself after repeated capture and emission of charge. Once gone, RTS did not reappear in any subsequent measurements even after bias and temperature cycling, suggesting a mechanism to deactivate at least some forms of RTS through a “cryogenic anneal”.

*Work at UTD was supported by the National Science Foundation under Grant No. ECCS-1403421.
**12:27PM B11.00005: Hyperdoping silicon for intermediate band photoconductivity**  
YINING LIU (Presenter), Department of Electro-Optics and Photonics, University of Dayton, SHAO QI LIM, WENJIE YANG, Research School of Physics and Engineering, Australia National University, PHILLIPPE K CHOW, US Army ARDEC-Benet Labs, IMAD AGHA, Department of Physics, University of Dayton, JAMES S WILLIAMS, Research School of Physics and Engineering, Australia National University, JEFFREY M WARRENDER, US Army ARDEC-Benet Labs, JAY MATHEWS, Department of Physics, University of Dayton — Intermediate band formation in silicon could lead the way for photodetection well below the Si band gap. By incorporating transition metals into Si at levels well above the solid solubility limit, intermediate band absorption can lead to photoconductivity induced by photons with less than the energy of the band gap. These supersaturated solutions can be fabricated using the method of ion implantation followed by pulsed laser melting. This concept has been demonstrated with Si hyperdoped with Au or Ti, but the photoresponse of detectors based on this idea have low quantum efficiency. Here we report on enhancements in the photoresponse of Si:Au and Si:Ti based detectors from varying the implantation and laser melting conditions, as well as the formation of high-quality Ohmic contacts.

**12:39PM B11.00006: The evolution of atomic structure and chemical states of ultra-low energy high-dose Boron implanted Si via UV laser annealing**  
KUANG YAO LO (Presenter), FU-YING LEE, ZONG-ZHE WU, LI-CHI KAO, FENG-MING CHANG, Physics, National Cheng Kung University, Taiwan, YU-MING CHANG, Center for Condensed Matter Sciences, National Taiwan University, Taiwan — One of the most critical issues in the nano-device fabrication is to confirm the atomic structure evolution of the ultrathin shallow junction. In this report, UV Raman spectroscopy, X-ray absorption near edge structure (XANES), X-ray photoelectron spectroscopy (XPS) and reflective second harmonic generation (RSHG) are used to analyze the pulse laser induced atomic structure evolution of ultralow-energy high-dose Boron implanted Si(110) at the room and cold substrate temperature. The formation of Si-B bond after the laser irradiation was indicated by a peak feature around 480 cm\(^{-1}\) resolved in UV Raman spectra. Meanwhile, the evolution of absorption peak (\(-197\) eV) in XANES and the red shift of binding energy of Si element (\(-99\) eV) in XPS reveal that the changes in the chemical states of ultra shallow junction strongly correlate to the activation process of Boron implantation. These results were confirmed by RSHG measurement, which exhibits the form symmetrical Si-B bonds. The observation of HRTEM agreed with the substrate temperature effect in the recrystallization of Boron implanted region.

*Thanks the Ministry of Science and Technology of the Republic of China, Taiwan for financially supporting, MOST 106-2112-M-006-007, MOST 105-2112-M-006-012 and 105-2119-M-002-046-MY3.

**12:51PM B11.00007: Defect studies in Ge and GeSn thin films grown on Si**  
CHRISTINA SCOTT (Presenter), IMAD AGHA, JAY MATHEWS, Department of Physics, University of Dayton — Silicon (Si) is often used in electronics because of its beneficial conductive properties and cost efficiency. However, it has poor optical properties in the infrared. Si infrared photonic devices could be used for a number of military and civilian applications. One approach to solving this problem is to use epitaxy to grow materials with more favorable optical properties on top of Si, such as germanium (Ge) and germanium tin (GeSn). One challenge for epitaxy is minimizing threading dislocations in the epitaxial layers due to lattice mismatch. In this work, we investigate the quality of Ge and GeSn materials grown on Si using a new remote plasma enhanced chemical vapor deposition (CVD) process. The newly grown material was subjected to etch pit density tests in order to determine the density of threading dislocations. The results show that using this new method results in high quality achieved using traditional CVD methods while also increasing growth rates.

*Funding for this work was provided by an Air Force Office of Scientific Research Young Investigator Award, Grant No. FA95501710146.
1:03PM B11.00008: Crystal growth, electronic structure and optical properties of BaZrS$_3$ and its Ruddlesden-Popper phases*  

SHANYUAN NIU (Presenter), Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, KRISTOPHER WILLIAMS, Department of Chemical Engineering, Massachusetts Institute of Technology, WEI LI, Department of Materials Science and Engineering, University of Delaware, DEBARGHYA SARKAR, Ming Hsieh Department of Electrical Engineering, University of Southern California, FEI HOU, School of Materials Science and Engineering, University of New South Wales, BOYANG ZHAO, Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, KEVIN YE, Department of Materials Science and Engineering, Massachusetts Institute of Technology, ELISABETH BIANCO, MICHAEL E MCCONNEY, Materials and Manufacturing Directorate, Air Force Research Laboratory, RALF HAIGES, Loker Hydrocarbon Research Institute and Department of Chemistry, University of Southern California, DAVID SINGH, Department of Physics and Astronomy, University of Missouri, JAN SEIDEL, School of Materials Science and Engineering, University of New South Wales, RAFAEL JARAMILLO, Department of Materials Science and Engineering, Massachusetts Institute of Technology, REHAN KAPADIA, Ming Hsieh Department of Electrical Engineering, University of Southern California, WILLIAM A TISDALE, Department of Chemical Engineering, Massachusetts Institute of Technology, ANDERSON JANOTTI, Department of Materials Science and Engineering, University of Delaware, JAYAKANTH RAVICHANDRAN, Mork Family Department of Chemical Engineering and Materials Science, University of Southern California —

Transition metal perovskite chalcogenides (TMPCs) are a new class of semiconductors with $d^0$ configuration. The less electronegative chalcogen, compared to oxides, lead to reduced band gap, more covalent bonding, and other interesting physical properties. We report the crystal growth and physical property study of BaZrS$_3$, Ba$_3$Zr$_2$S$_7$ and Ba$_2$ZrS$_4$. Photoluminescence (PL) measurements were performed to study the optical properties. Scanning Kelvin probe microscopy and Hall measurements were carried out to study the electronic structure and transport phenomena. Optical band gap of 1.82, 1.28 and 1.33 eV for BaZrS$_3$, Ba$_3$Zr$_2$S$_7$, and Ba$_2$ZrS$_4$, respectively, were extracted from PL. Such band gap evolution trend is different from that observed in oxide and halide counterparts. Potential effect of octahedra tilting and Zr-S covalent bonding in determining the electronic structure were explored. External luminescence efficiency up to 0.2% and effective minority carrier lifetime longer than 65 ns in Ba$_3$Zr$_2$S$_7$ was also obtained by quantitative and time-resolved PL, respectively.

Reference:

*Link Energy Fellowship, APS FIP Distinguished Student program

1:15PM B11.00009: Source of $p$-type conductivity in ultrahigh thermal conducting cubic boron arsenide*  

JOHN LYONS (Presenter), United States Naval Research Laboratory, JOEL BASILE VARLEY, Lawrence Livermore National Laboratory, EVAN RICHARD GLASER, JAIME A. FREITAS, JR., JAMES CLIFFORD CULBERTSON, United States Naval Research Laboratory, FEI TIAN, GEETHAL AMILA GAMAGE, HAORAN SUN, HAMID REZA ZIYAE, ZHIFENG REN, University of Houston — Cubic boron arsenide (c-BAs) exhibits an ultrahigh thermal conductivity (κ) near 1300 W/m-K at room temperature. However, c-BAs is believed to incorporate high concentrations of crystal imperfections that can both quench κ and act as sources of unintentional $p$-type conductivity. This behavior has been attributed to native defects, but direct evidence of their presence in c-BAs crystals is lacking. Here we evaluate the properties of native defects in c-BAs using hybrid density functional theory. These calculations indicate that native defects cannot give rise to free holes; instead, we find that impurities such as Si and/or C readily incorporate on the As site and as shallow acceptors. These results are in excellent agreement with optical and magnetic resonance spectroscopy measurements, which reveal impurity-related processes including donor-acceptor pair recombination and evidence for effective-mass-like shallow acceptors.

*This work was supported by the ONR Basic Research Program and under ONR MURI Grant No. N00014-16-1-2436. Computations used the DoD Major Shared Resource Center at AFRL. This work was additionally performed under the auspices of the U.S. Department of Energy at Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344.
1:27PM B11.00010: Point defects and dopants of boron arsenide from first-principles calculations: donor compensation and doping asymmetry*  
SIEUN CHAE (Presenter), KELSEY MENGLE, JOHN HERON, EMMANOUIL KIOUPAKIS, University of Michigan — BAS has received attention due to its unusually high thermal conductivity, yet, its defect properties are relatively unknown. Particularly, point defects crucially affect its electronic, thermal, and optical properties as a semiconductor. Here, we apply hybrid density functional theory calculations to identify the formation energies and thermodynamic charge transition levels of native point defects, common impurities, and shallow dopants in BAS [1]. We find that AsB, VB, BAS, Bi-VB, AsB-BAS, are the dominant intrinsic defects, while CAs, CB, Hi are common impurities. BeB, SiAs and GeAs are predicted to be excellent shallow acceptors with low ionization energy (< 0.03 eV) and negligible compensation by other point defects. However, donors such as SeAs, TeAs, SiB, and GeB have a relatively large ionization energy (~0.15 eV) and are likely to be passivated by native defects such as BAS and VB, as well as CAs, Hi, and HB. The hole and electron doping asymmetry originates from the heavy effective mass of the conduction band due to its boron orbital character, as well as from boron-related intrinsic defects that compensate donors. 

*This work was supported by NSF DMREF program (1534221). Computational resources provided by DOE NERSC (DE-AC02-05CH11231).

1:39PM B11.00011: Effect of substitutional defects on the thermal conductivity of boron arsenide*  
NAKIB PROTIK (Presenter), Physics, Boston College, MAURO FAVA, NATALIO MINGO, LITEN, CEA-Grenoble, JESÚS CARRETE, GEORG MADSEN, Institute of Materials Chemistry, Technical University of Vienna, NAVANEETHA KRISHNAN RAVICHANDRAN, DAVID A BROIDO, Physics, Boston College — Cubic boron arsenide (BAs) has recently been confirmed as having unconventional ultrahigh thermal conductivity, $k$, [1-3], which is particularly sensitive to the presence of vacancy defects [4]. Here, using density functional theory based first principles methods, we calculate the effect of various defects on the lattice thermal conductivity of BAs. We treat the phonon-defect scattering using both the Born approximation and the infinite-order T-matrix method and assess the difference between the results from these two approaches. The phonon-defect scattering rates are combined with the three-phonon and four-phonon scattering rates to obtain a full solution of the phonon Boltzmann transport equation. The calculated thermal conductivities are compared with the most recent experimental measurements.


*N.H.P. and D. B. acknowledge support from ONR MURI Grant No. N00014-16-1-2436.

1:51PM B11.00012: Beyond diffusion limit defect imaging and independent determination of the spatial profiles of electron and hole density near a dislocation defect by combining Raman and photoluminescence (PL) imaging*  
CHANG-KUI HU, University of North Carolina at Charlotte and Wuhan University of Technology, QIONG CHEN, University of North Carolina at Charlotte, FENGXIANG CHEN, University of North Carolina at Charlotte and Wuhan University of Technology, TIMOTHY HURLEY GROERER, Davidson College, MARK W WANLASS, National Renewable Energy Laboratory, YONG ZHANG (Presenter), University of North Carolina at Charlotte — Although a large carrier diffusion length (DL) indicates high material quality, ironically it implies more carrier depletion by an individual extended defect. It also obscures the spatial resolution (SR) in PL imaging, where the SR is dictated by the carrier DL rather than by the optical diffraction limit. Raman imaging of the LO phonon-plasmon (LOPP) coupled mode can be used to recover the intrinsic SR of the optical system [1], as demonstrated by Raman imaging of dislocation defects in GaAs, achieving a 10-fold improvement in SR. Furthermore, by combining Raman and PL imaging near a dislocation defect, we can independently determine the electron and hole spatial profile, radiative and nonradiative recombination rate, which has not been possible using other techniques. We find that in GaAs the dislocation defect tends to behavior as a hope trap: the defect only depletes the electrons in a short range, whereas the impact range of the defect is much larger in PL imaging. The mismatch in the electron and hole distribution implies the formation of a polarization field near the defect. The imbalance between the two charge distributions suggests the diffusion is non-ambipolar. [1] Hu et al., Light: Sci. & Appl. 7, 23 (2018).

*ARO/Electronics

Monday, March 4, 2019 11:15 AM - 2:15 PM
11:15AM B12.00001: Reconfigurable Carbon Nanotube Network Devices

PRATHAMESH DHAKRAS (Presenter), SAMUEL LAGASSE, Colleges of Nanoscale Science and Engineering, State University of New York Polytechnic Institute, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, SHENG WANG, LIAN-MAO PENG, Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, JI UNG LEE, Colleges of Nanoscale Science and Engineering, State University of New York Polytechnic Institute — Semiconducting single-walled carbon nanotubes (SWNTs) are an attractive channel material for a wide range of applications, from flexible, low cost printed electronics to high performance field effect transistors. Though recent advances in developing high purity semiconducting SWNT solutions have yielded devices with excellent on/off ratios and improved ON currents, determining the true nature of conduction of a network with a mixture of metallic and semiconducting nanotubes remains a challenge. Here, we fabricated split-gate devices that can reconfigure as either a metal-oxide-semiconductor field effect transistor (MOSFET) or a p-n diode. The spacing between the split gates was varied from 10 μm down to 100 nm to allow a detailed comparison between properties of unipolar conduction (MOSFET) and that of ambipolar transport dominated by minority carriers (p-n Diode). In addition, we varied the metallic concentration of SWNTs in the network channel. We show that the conduction is determined not only by the metallic concentration, but also by the environment that acts as strong generation and recombination centers.


XUAN WANG, Beijing National Laboratory for Condensed Matter Physics, WEILU GAO, XINWEI LI, QI ZHANG, Electrical Engineering, Rice University, SÉBASTIAN NANOYT, Laboratoire Charles Coulomb, Université de Montpellier, ERIK H HAROZ, Explosive Sciences and Shock Physics Division, Los Alamos National Laboratory, JUNICHIRO KONO, Electrical Engineering, Rice University, WILLIAM RICE (Presenter), Physics and Astronomy, University of Wyoming — Single-wall carbon nanotubes (SWCNTs) exhibit a wide range of chirality-dependent physical phenomena. This dependency complicates in-depth understanding of ensemble behavior, since nanotube networks contain numerous chiralities. In particular, electronic-type mixing greatly hinders the development of a comprehensive picture of SWCNT ensemble electrical transport. Here, we systematically study temperature-dependent magnetoconductivity (MC) in semiconductor and metal SWCNTs. In the semiconductor-enriched network, we observe 2D variable-range hopping conduction from 5 to 290 K. Low-temperature MC reveals a large, negative MC from which we determine the wavefunction localization length and Fermi energy density of states. In contrast, the metal-enriched film shows positive MC that increases with decreasing temperature, a behavior we attribute to 2D weak localization. Using this model, we determine carrier phase coherence and describe the temperature-dependent conductivity. These extensive transport measurements on type-enriched SWCNTs provide insights, which pave the way for nanotube solid-state devices.

*WDR acknowledges support from the UW School of Energy Resources, and JK acknowledges support from DOE BES (DEFG02-06ER4630), NSF (ECCS-1708315), and the Welch Foundation (C-1509).


MITCHELL J. SENGTER (Presenter), DANIEL MCCULLEY, LEE ASPITARTE, Physics, Oregon State University, NEDA LOTFIZHAD, VIKRAM DESHPANDE, Department of Physics and Astronomy, University of Utah, ETHAN D. MINOT, Physics, Oregon State University — Metallic carbon nanotubes (m-CNTs) exhibit a remarkably large energy gap for electronic excitations. The gap often exceeds 100 meV when the m-CNT is suspended in free space, but the gap disappears when the m-CNT lies on a metal surface. The theoretical description of this gap remains controversial and more experiments are needed. We have built ultra-clean suspended CNT devices from CNTs of known diameter and chiral angle. The CNT chirality is identified with spectrally resolved scanning photocurrent microscopy and the energy gap is determined by measuring thermally-activated electron transport. Our results show that the gap scales exactly as 1/D, with no dependence on chiral angle. We also demonstrate that the gap can be tuned by submerging the suspended m-CNT in dielectric liquids. Our results put new constraints on competing theoretical descriptions of a Mott insulator state versus an excitonic insulator state.

*This work is supported by the National Science Foundation under Grant No. 1709800.
11:51 AM B12.00004: Field-Enhanced Exciton Dissociation in Carbon Nanotube Photodiodes* DANIEL MCCULLEY (Presenter), MITCHELL J. SENGERT, Oregon State University, ANDREA BERTONI, CNR Nano, ETHAN D. MINOT, Oregon State University — Low-dimensional materials may be useful for building solar cells that harness carrier multiplication and circumvent the Shockley-Queisser limit. For example, quantum dot solar cells with an internal quantum efficiency (IQE) > 100% have been reported. In this work, we search for carrier multiplication effects in CNTs. We use individually-contacted, ultra-clean, suspended, semiconducting carbon nanotubes of known chiral index. Previous work on this system showed an IQE ~ 30% when the built-in electric field was ~ 4 V/μm. Here we report an IQE ~ 80% when the electric field is increased to ~ 15 V/μm. At these high fields, photocurrent spectroscopy reveals extreme broadening of low-energy exciton peaks. We compare our results to theoretical predictions for field-induced exciton dissociation in CNTs, and develop a framework to describe the energy dissipation pathways.

*This work is funded by NSF grant 1709800.

12:03 PM B12.00005: Tip-enhanced Raman spectroscopy of CNTs in a picocavity KAI NAN (Presenter), SHARAD AMBARDAR, DMITRI VORONINE, Physics department, University of South Florida — Carbon nanotubes (CNTs) have optical and electronic properties which allow promising applications. Conventional atomic force microscopy (AFM) and tip-enhanced Raman scattering (TERS) provide topographic and chemically specific images that reveal nanoscale structure-functional relationships. By placing CNTs in a picocavity formed by a plasmonic scanning probe tip and a metallic surface we control the relative intensities of various CNT signals. We investigate the tip-sample distance dependence in the nanometer classical and sub-nanometer quantum plasmonic regimes. This quantum picophotonics approach provides a new platform for exploration of enhanced properties of low dimensional materials.

12:15 PM B12.00006: Exciton Relaxation in Carbon Nanotubes via Electronic-to-Vibrational Energy Transfer* KIRILL VELIZHANIN (Presenter), Los Alamos National Laboratory — Covalent functionalization of semiconducting single-wall carbon nanotubes (SWCNTs) can introduce new localized photoluminescent states that are strongly red-shifted from the emission commonly observed from the nanotube band-edge E_{11} exciton state. In addition to being the source of new photophysical behaviors, these states are drawing significant interest as the basis for emerging functionality. A particularly important feature of such exciton localization at defect sites is that, because the exciton is no longer free to diffusively sample photoluminescent quenching sites along the length of the SWCNT, its lifetime is significantly extended. We have recently demonstrated that an important recombination channel of such localized excitons is the electronic-to-vibrational energy transfer (EVET). This process is analogous to the Förster resonance energy transfer (FRET) except for the final state of this process is not electronically, but vibrationally excited molecules of the medium (e.g., solvent). In this talk we will discuss the basic physics of EVET and then proceed to estimating the EVET rate for a localized exciton in the SWCNT.

*This work was supported in part by Los Alamos National Laboratory (LANL) Directed Research and Development funds.

12:27 PM B12.00007: Binding Energy and Lifetime of Excitons in Metallic Nanotubes* LEI SHAN, MEGHA AGARWAL (Presenter), EUGENE MISHCHENKO, University of Utah — Due to the large screening of Coulomb interaction between electrons in higher dimensions in metallic materials, a bound state of electron-hole pair cannot be formed. However, in lower dimensional materials such as carbon nanotubes due to less effective screening of electrons allows the formation of bound state of electron-hole pair whose radius, R_{ex} ~ R. This is particularly unique to metallic nanotubes in a sense that the problem of describing excitons can now be considered 1D as compared to semiconducting nanotubes where exciton radius R_{ex} ~ R and excitons are neither 1D nor 2D. We are thus able to determine the binding energy of excitons in metallic nanotubes, is about 0.08 v/R. Additionally, because of the presence of the gapless subbands, there are processes where bound excitons are scattered into unbound electron-hole pairs belonging to the gapless subbands. Such processes lead to a finite exciton lifetime and the broadening of its spectral function. We calculate the corresponding decay rate of the excitons.

*This work was supported by DOE, Office of Basic Energy Sciences, Grant No. DE-FG02-06ER46313.
12:39PM B12.00008: Organic molecule adsorption effects on air-suspended carbon nanotubes* SHUNSUKE TANAKA (Presenter), AKIHIRO ISHII, YUICHIRO K. KATO, RIKEN — Environmental screening effects are large in carbon nanotubes due to their atomically thin nature, and therefore it is possible to control the optical properties with molecular adsorption [1,2]. Here, we investigate adsorption effects of copper phthalocyanine molecules on excitons and trions in air-suspended carbon nanotubes. By averaging the photoluminescence excitation spectra for tubes with the same chiralities, we observe that the exciton emission energy redshifts gradually with molecular deposition thickness. The trion emission is also observed at large deposition amounts, which could be due to charge transfer between the phthalocyanine molecules and carbon nanotubes. Analyzing the spectra for individual tubes, we find a good correlation between the exciton-trion energy separation and the exciton emission energy.


*Work supported in part by RIKEN (Incentive Research Projects), JSPS (KAKENHI JP16H05962), and MEXT (Nanotechnology Platform). We thank K. Kimura, H. Imada, and Y. Kim for the thermal evaporator. We acknowledge the Advanced Manufacturing Support Team at RIKEN for technical assistance.

12:51PM B12.00009: Interlayer interactions and radial breathing mode in double- and triple-walled carbon nanotube bundles JIA WERN HUE (Presenter), Department of Physics and Astronomy, The University of Alabama, Tuscaloosa, Alabama 35487, USA, THOMAS CH HIRSCHMANN, Attocube Systems AG, Königstraße 11a, 80539 Munich, Germany, STEPHEN K. DOORN, Center for Integrated Nanotechnologies, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, YOONG AHM KIM, School of Polymer Science and Engineering, Chonnam National University, 77 Yongbong-ro, Buk-gu, Gwangju, 61186, Republic of Korea, NEWTON M BARBOSA NETO, Instituto de Ciências Exatas e Naturais – Programa de Pós-graduação em Física, Universidade Federal do Pará, Belém PA 66075-110, Brazil, PAULO T ARAUJO, Department of Physics and Astronomy, The University of Alabama, Tuscaloosa, Alabama 35487, USA — A double-walled carbon nanotube (DWNT) can be considered a inner single-walled carbon nanotube (SWNT) protected by an outer SWNT. Likewise, a triple-walled carbon nanotube (TWNT) can considered an inner DWNT encapsulated by an outer SWNT. The signature in resonant Raman spectroscopy for carbon nanotubes is the radial breathing mode (RBM). For radial breathing modes (RBM), double- and triple-walled carbon nanotubes can be considered as coupled oscillators. The RBM frequency, $\omega_{\text{RBM}}$, is sensitive to environmental factors and interlayer interactions. For interlayer interactions, it is necessary to take into account curvature effects, particularly for smaller tubes, whether the constituent tubes are commensurate, and whether the inner tubes are really isolated from the environment from the outer tubes. Another matter of interest is how do the magnitudes of the interlayer interactions compare. Resonant Raman spectra of a DWNT bundle and TWNT bundle were taken. From those spectra, chiral indices were assigned and tube diameters calculated. Then, a comparison to the SWNT $\omega_{\text{RBM}}$ was made and the questions presented above answered.

1:03PM B12.00010: Energy barrier for carbon nanotube collapse RODRIGO CAPAZ (Presenter), RAFAEL RODRIGUES DEL GRANDE, Federal University of Rio de Janeiro, Brazil, ALEXANDRE FONSECA, Unicamp, Brazil — Small-diameter carbon nanotubes have circular cross section shapes, but the ground state of large diameter tubes correspond to a collapsed structure, stabilized by the van der Waals attraction of opposite sides of the nanotube wall. For those tubes, the circular cross section shape is metastable and it is interesting to investigate the energy barrier for jumping from one configuration to another. Previous theoretical works calculate the energy barrier by considering a transition pathway in which the nanotube collapses uniformly along its length, normally using periodic boundary conditions along the nanotube axis. This assumption is unphysical since it would give an infinite barrier for a nanotube of infinite length. In this work, we calculate the true energy barrier for carbon nanotube collapse by considering a transition pathway that consists of a local deformation that propagates itself along the carbon nanotube axis. This leads to finite and physically meaningful energy barriers in the limit of infinite nanotubes. For typical nanotube diameters, the energy barriers are so large that effectively prevent the collapse induced by temperature of an infinite nanotube. We also perform classical molecular dynamics that confirm these results.
Snap-Through Buckling Bi-Stability in Suspended Carbon Nanotube Resonators

Mechanical bi-stability based on snap-through (ST) buckling is a well-known phenomenon in micro-electromechanical systems (MEMS) which serves as the underlying mechanism for many practical applications such as switches, actuators, sensors, filters, and memory elements, to name a few.

Here, we report the first realization of a suspended carbon nanotube (CNT) based bi-stable resonators exhibiting ST buckling phenomena. Both the static and dynamic responses of the system were obtained through conductance and resonance frequency measurements, respectively. In both measurements, non-linear effects such as jumps, hysteresis, softening and hardening, and super and sub-harmonic excitations were observed.

Apart from these resonators being the smallest bi-stable electromechanical system based on ST buckling to date, our devices could also serve as excellent sensors with ultrahigh sensitivities, reaching electrostatic tunability values beyond 100MHz/V, which are also attractive for realization of mechanical quantum-bits.

Finally, we developed a comprehensive theoretical model based on the Euler-Bernoulli beam equation to support our findings.

Solution Sorting of 10 µm Long Single-Walled Carbon Nanotubes

Single-walled carbon nanotubes (SWCNTs) that are ultralong (>10 µm) and electronically pure may enable stretchable thin film transistors, ballistic conductors, and ultra-strong fibers. However, nanotubes are cut to short pieces (typically less than 1 µm) by sonication during solution processing. In this presentation, I will discuss an invention from our lab called “superacid-surfactant exchange (S2E)” which allows for non-destructive dispersion and scalable sorting of ultralong SWCNTs in aqueous solutions. The length of the isolated SWCNTs readily reaches 10 µm, with a narrow distribution. We further show that these ultralong nanotubes can be further sorted by electronic type to attain an electron mobility exceeding 90 cm² V⁻¹ s⁻¹ in fabricated thin film transistors.

Synthesis and Characterization of Single Walled Carbon Nanotubes (SWNT) Through Direct Decomposition Ferrocene

Carbon-based nanostructures, specifically carbon nanotubes due to their unique surface adsorption properties can become the choice materials for several applications. Here we present our results on synthesis and characterization of single walled carbon nanotubes (SWNT) through direct decomposition of metallocene. Specifically, ferrocene was utilized in this study. The effect of growth conditions on physical properties of these SWNT materials were studied in detail through volumetric gas adsorption measurements, Raman spectroscopic characterization as well as UV-Vis spectroscopy measurements. The correlation of some of the physical properties as it related to the growth conditions will be discussed in light of these characterization results.

Measuring the Electron Beam Induced Plasmon Response in Single-Walled Carbon Nanotube Devices

In this work, we examine the transport properties of individual single-walled carbon nanotubes, configured with split gates, as it is excited by a finely focused electron beam. We conduct the experiment in a scanning electron microscope (SEM) equipped with multiple nanopores. We measure the current from both ends of the nanotube as the electron beam is rastered to determine the mechanism of transport. Our analysis shows that the energetic beam launches plasmon excitations along the nanotube, which we measure as a sharp change in the current. The sign of the current on both ends of the nanotube is the same, which rules out other competing mechanisms, including electron-hole generation and thermal effects. We examine the transport properties as a function of beam energy and position, and nanotube doping.
Intrinsically Ultrastrong Plasmon-Exciton Interactions in Crystallized Films of Carbon Nanotubes

ABRAM FALK (Presenter), PO-HSUN HO, DAMON FARMER, PHAEDON AVOURIS, IBM Thomas J. Watson Research Center — We show that carbon nanotubes can be crystallized into chip-scale, two-dimensionally ordered films and that this new material enables intrinsically ultrastrong emitter-cavity interactions: rather than interacting with external cavities, nanotube excitons couple to the near-infrared plasmon resonances of the nanotubes themselves [1]. Our polycrystalline nanotube films have a hexagonal crystal structure, ~25 nm domains, and a 1.74 nm lattice constant. With this extremely high nanotube density and nearly ideal plasmon-exciton spatial overlap, plasmon-exciton coupling strengths reach 0.5 eV, which is 75% of the bare exciton energy and a near record for room-temperature ultrastrong coupling. Crystallized nanotube films provide a compelling foundation for high-ampacity conductors, low-power optical switches, and tunable optical antennas.


*This work was funded by IBM and the Postdoctoral Research Abroad Program of the Ministry of Science and Technology Taiwan (NSC 106-2917-I-564-012).

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B13 DMP: Materials (General) -- Modeling and Characterization

Model of the piezoelectric coefficient of hexagonal two-dimensional materials

LOK LEW YAN VOON (Presenter), University of West Georgia, MORTEN WILLATZEN, ZHONG-LIN WANG, Beijing Institute of Nanoenergy and Nanosystems — A quantum-mechanical microscopic model of the piezoelectric effect in two-dimensional materials is developed. The piezoelectric coefficient requires the calculation of an internal atomic displacement and an effective piezoelectric charge. The internal displacement is obtained from minimizing the strain energy given by a Keating-like model, while the effective charge takes into account the atomic displacements and also a redistribution of the electronic charge; a bond-orbital model is used to compute the latter. The final theory only requires atomic energies and the elasticity constants of the materials as input parameters. The piezoelectric coefficients of a number of II-V, III-V and IV-IV materials that could stably form in the planar hexagonal structure are computed; results for the IV-IV materials are obtained for the first time.

Nucleation Kinetics of Structural Phase Changes in Two-Dimensional Transition Metal Dichalcogenides

ADITI KRISHNAPRIYAN (Presenter), QIAN YANG, YAO ZHOU, Stanford University, EKIN D CUBUK, Google Brain, EVAN REED, Stanford University — Predictive capabilities for kinetic processes in materials are in their infancy, but kinetics are critical for a spectrum of energy applications ranging from phase change materials, catalysis, materials synthesis, and combustion. The structural phase transition between the metallic 1T or 1T' and semiconducting 2H structures in two-dimensional transition metal dichalcogenide materials is important to understand for synthesis and may provide exciting new opportunities for energy-efficient electronic and optical devices. However, very little is known about the mechanisms and kinetics of these phase changes or how to engineer the kinetics. We propose a novel electronic structure based method to determine the nucleation kinetics and timescales of this phase change. Furthermore, we discuss the curious fact that the interface energies between phases for this challenging problem are mathematically ill-defined. We also point to strategies on the engineering of kinetics in these phase change materials that take into account nucleation barriers and nucleation time.

*Department of Energy Computational Science Graduate Fellowship, NSF, Army Research Office, Office of Naval Research, and the Department of Energy National Nuclear Security Administration
11:39 AM B13.00003: Effective k.p models for phosphorene including the interband spin-orbit coupling* PAULO DE FARIA JR. (Presenter), University of Regensburg, MARCIN KURPAS, University of Silesia, MARTIN GMITRA, P. J. Safarik Univ. in Kosice, JAROSLAV FABIAN, University of Regensburg — Phosphorene is a two-dimensional semiconductor with direct band gap and promising spin-dependent properties[1,2]. In this study, we investigate effective k.p models for phosphorene including the interband spin-orbit coupling[3], a term previously overlooked in the literature. The inclusion of such interband spin-orbit coupling provides a reliable description of the anisotropic dipole transition and of the effective g-factors. We also investigate excitonic effects and found very good agreement with reported results in the literature. To obtain reliable k.p parameters we use a robust fitting approach that takes into account not only the band structure but also the k-dependence of the effective mass. With the increasing interest in two-dimensional systems, our effective k.p Hamiltonians can be combined with other already available models to investigate novel physical phenomena in van der Waals heterostructures. [1] M. Kurpas, M. Gmitra and J. Fabian, PRB 94, 155423 (2016). [2] A. Avsar et al., Nat. Phys. 13, 888 (2017). [3] P. E. Faria Junior et al., PRB 93, 235204 (2016).

*Supported by: Alexander von Humboldt Foundation, Capes, DFG SFB 689, DPG SFB 1277, MSWaaS SR 90/CVTISR/2018.

11:51 AM B13.00004: Spin-orbit-torque magnetic manipulation with 2D materials* [Invited] DANIEL RALPH (Presenter), Cornell University — Current-induced spin-orbit torques provide a promising strategy for efficient manipulation of nonvolatile magnetic memory and logic technologies. For best performance, both the layer of material that provides the spin-orbit torque and the magnetic layer being manipulated should be as thin as possible. Here we discuss experiments which probe the ultimate limits in which 2D materials are used for either the spin-orbit layer or the magnetic layer. We will also discuss initial experiments in which recently-discovered 2D magnetic materials are integrated with spin-orbit materials. Using mechanically exfoliated thin flakes of the insulating 2D ferromagnet Cr₂Ge₂Te₆ combined into a bilayer structure with tantalum, we have observed current-induced deflections of the out-of-plane magnetic moment of Cr₂Ge₂Te₆ and characterized the strength of the spin-orbit torque.

*This work was performed with G. M. Stiehl, V. Gupta, M. H. D. Guimaraes, D. MacNeill, N. D. Reynolds, R. Li, S. Karimeddiny, J. Mittelstaedt, N. Sivadas, I. El Baggari, L. F. Kourkoutis, C. Fennie, J. Park, and R. A. Buhrman, with support from DOE and SRC/DARPA.

12:27 PM B13.00005: Strain-induced structural phase transformation in two-dimensional molydenum tungsten diselenide alloy* AMEY ANANT APTE (Presenter), VIDYA KOCHAT, Materials Science & NanoEngineering, Rice University, PANKAJ RAJAK, ARAVIND KRISHNAMOORTHY, Physics & Astronomy, University of Southern California, PRAVEENA MANIMUNDA, Bruker Nano Surfaces, JORDAN HACHTEL, JUAN IDROBO, Center for Nanophase Materials Science, Oak Ridge National Laboratory, SYED ASIF AMANULLA, Bruker Nano Surfaces, PRIYA VASHISHTA, AIICHIRO NAKANO, RAJIV KALIA, Physics & Astronomy, University of Southern California, CHANDRA SEKHAR TIWARY, PULICKEL M AJAYAN, Materials Science & NanoEngineering, Rice University — Two-dimensional transition metal dichalcogenides (TMDs) show intriguing mechanical properties compared to their bulk counterparts. This behavior can be modified in alloyed TMDCs due to doping and defects. In this work we develop CVD synthesis of large-area monolayer MoWSe₂ alloy film on sapphire substrate. With Raman spectroscopy and mapping, we investigate the microscopic behavior of this alloy film transferred onto a flexible substrate as function of increasing bending strain. We observe the nature of crack propagation through the Mo and W-dominated regions in this 2D alloy film with differing stress concentration near the W-rich precipitates. Our molecular dynamics simulations illustrate how stress buildup at propagating crack tip in the film result in a 2H-1T phase transformation which is verified at micro- and nanoscale using Raman mapping and HAADF-STEM imaging. The MD simulations also predict increased crack resistance and healing in alloys compared to unalloyed pristine samples.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy (DoE), Office of Science, Basic Energy Sciences, under award number DE-SC00014607 and authored by UT-Battelle, LLC under contract no. DE-AC05-00OR22725 with the U.S. DoE.
12:39PM B13.00006: Quantum plasmonic imaging of 2D transition metal dichalcogenides  ALINA ZHUKOVA  
(Presenter), DMITRI VORONINE, University of South Florida —
Two-dimensional (2D) transition metal dichalcogenides (TMDs) are of particular interest due to their unique optoelectronic properties. Nano-optical imaging techniques such as tip-enhanced Raman spectroscopy (TERS) and tip-enhanced photoluminescence (TEPL) are useful tools for investigating the nanoscale properties of materials below the diffraction limit. We investigated the topography and optical properties of monolayer TMDs using atomic force microscopy (AFM), TERS, and TEPL. Near-field TEPL and TERS signals have been found to be successful in identifying distinct crystalline boundaries with higher spatial resolution compared to far-field imaging. Subwavelength optical characterization techniques are necessary to study nanoscale phenomena such as the lateral heterojunctions of 2D materials. We also performed tip-sample distance dependence experiments and observed quantum plasmonic effects. Specifically, manipulating the plasmonic tip location results in nano-optical imaging capabilities and plasmon-induced hot-electron injection. As a result, there is significant potential for applying quantum plasmonic effects to nanodevices with tunable photoresponse.

12:51PM B13.00007: Missing links towards understanding equilibrium shapes of hexagonal boron nitride: algorithm, hydrogen passivation, and temperature effects*  JINGZHAO ZHANG, WENJING ZHAO (Presenter), JUNYI ZHU, Physics, The Chinese University of HongKong — There is a large discrepancy between the experimental observations and the theoretical predictions in the morphology of hexagonal boron nitride (h-BN) nanosheets. Theoretically-predicted hexagons terminated by armchair edges are not observed in experiments; and experimentally-observed triangles terminated by zigzag edges are found theoretically unstable. There are two key issues in theoretical investigations, namely, an efficient and accurate algorithm of absolute formation energy of h-BN edges, and a good understanding of the role of hydrogen passivation during h-BN growth. Here, we first proposed an efficient algorithm to calculate asymmetric edges with a self-consistent accuracy of about 0.0014 eV/Å. This method can also potentially serve as a standard approach for other two-dimensional (2D) compound materials. Based on this algorithm, we constructed Wulff plot and discovered that only when edges are passivated by hydrogen atoms and temperature effects are taken into account can experimental morphology be explained.  
*This work was supported by the start-up funding, HKRGC funding with the Project Code of 14319416, and direct grants with the Project Codes of 4053233, 4053134, and 3132748, at CUHK.

1:03PM B13.00008: Plasmon excitations in trilayer AAB-stacked graphene  GODFREY GUMBS (Presenter), Physics Department, Hunter College/CUNY, CHIUN-YAN LIN, BOR-LUEN HUANG, MING-FA LIN, Physics Department, National Cheng Kung University — We report on the fascinating electronic properties and distinct plasma excitations for low-symmetry trilayer AAB-stacked graphene. For the undoped structure, there are three pairs of unusual valence and conduction subbands which give rise to nine allowed interband excitations, for which the imaginary (real) part of the polarizability exhibits 1D square root asymmetric peaks and 2D shoulder structures (pairs of antisymmetric peaks and logarithm type symmetric peaks). The low frequency acoustic plasmon, appearing as a prominent peak in the energy loss spectrum, can survive in a narrow gap system with large density-of-states from the valence band. This type of plasmon mode is similar to that in a narrow gap carbon nanotube. The mechanism responsible for this plasmon is the intraband conduction state excitations. Its frequency, intensity and critical momentum exhibit a non-monotonic dependence on the Fermi energy.

1:15PM B13.00009: Correlated SPM–TERS Imaging: Revealing Unexpected Nanoscale Heterogeneities in 2D Semiconductors.  ANDREY KRAYEV (Presenter), HORIBA Scientific — Here I report on the application of scanning probe microscopy (SPM) cross-correlated with tip enhanced Raman scattering (TERS) and photoluminescence (TEPL) imaging for detection of unexpected heterogeneities in TMDs. I'll demonstrate that few-layer flakes of WSe₂ exfoliated to gold or silver may possess doping heterogeneity with domains within 30-300nm range. These domains identified by Kelvin probe imaging showed different TERS response and generated photocurrent of opposite polarity. I'll further discuss how scanning capacitance microscopy can identify the grain boundaries (GB) in CVD-grown MoSe₂ crystals, while TERS characterization of such crystals transferred to gold reveals possible etching of MoSe₂ along GB during the transfer, an effect beneficial for photocatalytic activity. 3-rd example of the use of cross-correlated SPM and TERS/TEPL imaging of 2D semiconductors is a discovery of the nature of strong PL of WS₂ and WSe₂ transferred to gold via heat-assisted exfoliation. Through TERS/TEPL it was identified that PL is coming from nanoscale bubbles formed in TMD layers. Exciton funnelling towards the bubbles was also discovered, which resulted in strong enhancement of Raman/PL response from the bubbles, and in significant suppression of TERS/TEPL signal in adjacent area.
1:27PM B13.00010: Real-Space Mapping of Polaritons in 2D Materials  
TOBIAS GOKUS (Presenter), STEFAN MASTEL, ALEXANDER GOVYADINOV, Applications, neaspec GmbH — The performance of the next-generation electronic devices based on graphene and other 2D materials is strongly influenced by the structure-function relationship. Scattering-type scanning near-field optical microscopy (s-SNOM) is the ideal technology to investigate such material systems at the nanoscale. s-SNOM combines the best of two worlds: (i) the high spatial resolution of Atomic Force Microscopy (AFM) and (ii) the analytical power of optical microscopy and spectroscopy. Achieving an unmatched spatial resolution below 10 nanometer this technology opens a new era for modern nano-analytical applications such as chemical identification, free-carrier profiling and plasmonic near-field mapping. Recent research highlights on graphene and other 2D materials include contact-free access to the local conductivity, the electron mobility, and the intrinsic electron doping by resolving propagating phonon-, plasmon-, and exciton-polariton directly in space and time. In this presentation we will introduce the basic principles of near-field microscopy for imaging and spectroscopy with 10 nanometer spatial resolution and address their impact and key applications in the field of 2D materials.

1:39PM B13.00011: Real time optical observation and control of transition metal dichalcogenide synthesis*  
TALIP KASIRGA (Presenter), HAMID REZA RASOULI, NAVEED MEHMOOD, ONUR ÇAKIROĞLU, Materials Science and Nanotechnology, Bilkent University — Synthesis of atomically thin transition metal dichalcogenide (TMC) crystals have attracted tremendous amount of attention in the past few years. The common technique for the synthesis is to use a tubular split furnace with gas and exhaust connections. The precursors and the target substrate are placed in the hot zone of the furnace. The major shortcoming of the setup is the inaccessibility of the growth for real time characterizations. Thus, the growth has to be shut down blindly and the intermediate products that may lead to the growth has to be analysed later. Here, we developed a compact CVD chamber that allows real time optical observation of the crystal synthesis. Among our findings, for the first time we observed the formation of the atomically thin TMCs in real time, and characterized the various synthesis routes for several TMCs. By using the unique abilities we have with our chamber, we also observed the formation of the heterostructures. Furthermore, we demonstrated a directed synthesis of TMCs with prepatterned structures on a substrate.

*This work is supported by TUBITAK under Grant no:116M224

1:51PM B13.00012: Oxidation effect on WTe2 using optical second harmonic generation*  
YUJIN CHO (Presenter), University of Texas at Austin, NA HYUN JO, PAUL CANFIELD, Iowa State University, MICHAEL C DOWNER, University of Texas at Austin — A transition metal dichalcogenide WTe2 has recently drawn many researchers' attention because this material is Type-II Weyl semimetal in bulk and it is a topological insulator in a monolayer at low temperature. This material is known to be particularly sensitive to oxidation, which could alter its electronic and mechanical properties. Optical Second Harmonic Generation (SHG) microscopy is a good way to probe the small change at the surface due to its hypersensitivity to the structural changes. We used Ti:Sapphire laser, with 76 MHz repetition rate and 150 fs pulse, to see the oxidation effect on the rotational anisotropic SHG at a discrete oxidation level. We found out that the oxidation greatly affects SHG intensities in s-in/s-out polarization configuration. In this talk, I will be presenting a systematic study of oxidation effect on the bulk WTe2 as well as its spectroscopic response.

2 Z. Fei et al., Nat. Phys. 13, 677 (2017)

*This work is supported by Robert Welch Foundation, F-1038. N.H.Jo and P.C.Canfield was supported by the U.S. DOE/BES, Division of Materials Sciences and Engineering under Contract No. DE-AC02-07CH11358. Na Hyun Jo is supported by the Gordon and Betty Moore Foundation EPiQS Initiative (Grant No. GBMF4411)
Visualization of Photo-carrier Diffusion in Monolayer Transition Metal Dichalcogenides

ZHAODONG CHU (Presenter), JIAMIN QUAN, CHUN YUAN WANG, DAVID WANNLUND, Department of Physics, The University of Texas at Austin, ALI HAN, Physical Sciences and Engineering Division, King Abdullah University of Science and Technology, KEVIN HERRERA, DI WU, Department of Physics, The University of Texas at Austin, LAIN-JONG LI, Physical Sciences and Engineering Division, King Abdullah University of Science and Technology, CHIH-KANG SHIH, XIAOQIN (ELAINE) LI, KEJI LAI, Department of Physics, The University of Texas at Austin — Understanding of the spatial and temporal evolution of photo-generated charge carriers in atomically thin transition metal dichalcogenides (TMDs) is of critical importance for their application in optoelectronic devices. Using a light-assisted microwave impedance microscope (MIM), we demonstrate the first quantitative mapping of photo-carrier diffusion on monolayer TMDs. When the sample is illuminated by above-gap laser, the circular profile of local photoconductivity measured by the MIM is clearly broader than that of the laser spot. Numerical simulation shows that the free-carrier diffusion length of is on the order of micrometers, corresponding to a carrier lifetime of tens to hundreds of nanoseconds. Our work provides important insights to the remarkable electrical and optical properties of TMDs.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B14 DCMP: 2D Materials (Metals, Superconductors, and Correlated Materials) -- Magnetism BCEC 153C - Andrew May, Oak Ridge National Laboratory - Tag(s): Focus

11:15AM B14.00001: Magnetism in two dimensions [Invited] XIAODONG XU (Presenter), University of Washington — Selected by the organization chairs Kin Fai Mak and Cory Dean.

11:51AM B14.00002: Gate-tunable Room-temperature Ferromagnetism in Two-dimensional Fe₃GeTe₂ YUJUN DENG (Presenter), YIJUN YU, YICHEN SONG, Fudan University, JINGZHAO ZHANG, The Chinese University of Hong Kong, NAI ZHOU WANG, University of Science and Technology of China, ZEYUAN SUN, YANGFAN YI, YI ZHENG WU, Fudan University, JUNYI ZHU, The Chinese University of Hong Kong, JING WANG, Fudan University, XIANHUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Fudan University — The advent of two-dimensional van der Waals crystals creates new possibilities in developing novel spintronic devices. Recent experiments have demonstrated that it is possible to obtain two-dimensional ferromagnetic order in insulating Cr₂Ge₂Te₆ and CrI₃ at low temperatures. Here, we developed a new device fabrication technique, and successfully isolated monolayers from layered metallic magnet Fe₃GeTe₂. We found that the itinerant ferromagnetism persists in Fe₃GeTe₂ down to monolayer. The ferromagnetic transition temperature, T_c, is suppressed in pristine Fe₃GeTe₂ thin flakes. An ionic gate, however, dramatically raises the T_c up to room temperature. The gate-tunable room-temperature ferromagnetism in two-dimensional Fe₃GeTe₂ opens up opportunities for potential voltage-controlled magnetoelectronics.

12:03PM B14.00003: Magnetic properties of vanadium selenide epitaxial thin films* MASAKI NAKANO (Presenter), SATOSHI YOSHIDA, SAEED BAHRAMY, YUE WANG, HIDEKI MATSUOKA, YUKI MAJIMA, Department of Applied Physics, The University of Tokyo, YOSHIMITSU KOHAMA, The Institute for Solid State Physics, The University of Tokyo, YUTA OHIGASHI, YUTA KASHIWABARA, MASATO SAKANO, KIYOKO IISHIZAKA, YOSHIHIRO IWASA, Department of Applied Physics, The University of Tokyo — The discoveries of ferromagnetism in atomically-thin Cr₂Ge₂Te₆ and CrI₃ have opened up an opportunity for integration of magnetic 2D materials into van der Waals heterostructures. Moreover, the recent discovery of emergent room-temperature ferromagnetism in monolayer VSe₂ [1], which has been known as a paramagnetic metal in its bulk form, should provide an important step toward spintronics applications based on 2D materials, although the existence of ferromagnetism in monolayer VSe₂ is still controversial [2]. We have recently found that vanadium selenide epitaxial thin films fabricated by molecular-beam epitaxy (MBE) with our growth recipe [3] exhibit peculiar magnetic properties with clear anomalous Hall effect down to 2D limit. In this presentation, we will show transport properties of our MBE-grown vanadium selenide epitaxial thin films, and discuss possible origins of this emergent ferromagnetism in our samples. [1] M. Bonilla, et. al., Nat. Nanotechnol. 13, 289 (2018). [2] J. Feng, et. al., Nano Lett. 18, 4493 (2018). [3] M. Nakano, et. al., Nano Lett. 17, 5595 (2017).

*This work was supported by Grant-in-Aid for Scientific Research (No. 25000003) from the Japan Society for the Promotion of Science.
12:15PM B14.00004: Gate-controlled charge-doping of a Mott insulator in Graphene/α-RuCl₃ Heterostructures*

BOYI ZHOU (Presenter), JESSE BALGLEY, Washington University, St. Louis, PAULA J KELLEY, DAVID GEORGE MANDRUS, Oak Ridge National Laboratory, ERIK HENRIKSEN, Washington University, St. Louis — The layered antiferromagnetic Mott insulator α-RuCl₃ exhibits many phenomena consistent with the existence of a Kitaev quantum spin liquid. While most works on α-RuCl₃ so far have focused on pristine bulk samples, this material can be readily exfoliated down to monolayer thicknesses. Here we study the electronic transport of van der Waals heterostructure devices containing thin α-RuCl₃ flakes in contact with monolayer graphene Hall bars. We find an anomalously large conductivity implying the RuCl₃ has become charge-doped and is now conducting. The Hall coefficient data show a sharp increase in the density of the second conducting band (in the α-RuCl₃) as graphene is gated from hole- to electron-doped. Additionally, the resistivity at low temperature shows clear signals associated with magnetic phase transitions at temperatures 2-3 times higher than the native antiferromagnetic transition in α-RuCl₃.

*We acknowledge support from the Institute of Materials Science and Engineering at Washington University in St. Louis. A portion of this work was supported under NSF DMR-1810305.

12:27PM B14.00005: Ab initio mismatched interface theory of graphene on α-RuCl₃: doping and magnetism* ELI GERBER (Presenter), YUAN YAO, TOMAS ARIAS, EUN-AH KIM, Cornell University — The possibilities for creating van der Waals heterostructures are limitless with the rich palette including Mott insulating α-RuCl₃ and semi-metallic graphene. However, the study of such “mismatched interfaces” calls for an innovative way of capturing the underlying physics of these complex systems, that goes beyond standard ab initio methods. We propose a general strategy for studying such interfaces, “mismatched interface theory,” and apply it to a α-RuCl₃-graphene heterostructure in which there is significant lattice mismatch between the two crystals. Our results indicate charge transfer from graphene to the Ru layer in α-RuCl₃ directly proportional to the number of carbon atoms present in the system, corresponding to uniform doping of 4.7% in the α-RuCl₃-graphene heterostructure. We further demonstrate that this doping may be tuned by applying uniaxial pressure to the heterostructure, and investigate the effects of the doping on the zigzag- and ferromagnetic-ordered low-energy stable states of α-RuCl₃ which lie close to the antiferromagnetic Kitaev spin liquid.

*The authors acknowledge support through the NSF MRSEC program (DMR-1719875) and the Materials Innovation Platform grant DMR-1539918.

12:39PM B14.00006: Crystal Structure Reconstruction on Surface of Quantum Spin Liquid Candidate: α-RuCl₃ * ZHONGWEI DAI (Presenter), Center for Functional Nanomaterials, Brookhaven National Lab, JIE-XIANG YU, Department of Physics, University of New Hampshire, BOYI ZHOU, Department of Physics, Washington University in St. Louis, SAMUEL TENNEY, Center for Functional Nanomaterials, Brookhaven National Lab, PAIGE LAMPEN-KELLEY, Materials Science and Technology Division, Oak Ridge National Laboratory, DAVID GEORGE MANDRUS, Department of Material Science and Engineering, University of Tennessee, ERIK HENRIKSEN, Department of Physics, Washington University in St. Louis, JERZY T. SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Lab, KARSTEN POHL, JIADONG ZANG, Department of Physics, University of New Hampshire — α-RuCl₃ has emerged as a novel 2D material that potentially hosts quantum spin liquid state (QSL). Recent experimental reports of neutron scattering and thermal quantum Hall effect have provided indirect but promising evidence for the existence of QSL in α-RuCl₃. However, numerous controversies still remain in the current literatures about α-RuCl₃, such as its crystal structure and electronic structure. We used a unique surface sensitive technique, low energy electron microscopy (LEEM), combined with dynamical selected-area low energy electron diffraction (μLEED-IV) to study the 2D crystal structure of α-RuCl₃. We found an unexpected diffraction pattern on the surface of α-RuCl₃, which indicates intrinsic surface reconstruction that forms a superlattice. The superlattice most likely originates from the slight shift of atomic positions which results in unit cell distortion. The existence of a surface superlattice may significantly impacts the electronic and magnetic properties which in turn would potentially influence the existence of QSL in α-RuCl₃.

*This research used resources of the Center for Functional Nanomaterials and National Synchrotron Light Source II, which are U.S. DOE Office of Science Facilities, at Brookhaven National Laboratory under Contract No. DE-SC0012704.
DAVID MACNEILL (Presenter), Massachusetts Institute of Technology — Layered magnetic insulators that can be exfoliated are highly desirable, as we can potentially create topological states (e.g., quantum anomalous Hall effect) by incorporating them in van der Waals heterostructures. Such materials were finally realized in 2017 with the isolation of monolayer CrI3 and bilayer CrGeTe3. However, this field is in its infancy and few layer films seem to have complex properties different from bulk, such as the ferromagnetic to antiferromagnetic transition in CrI3. In this talk, I will discuss the use of electron tunneling through ultrathin magnetic insulators as a probe of their magnetic ground state and excitations [1]. We report giant magnetoresistance effects when tunneling through CrI3 and CrCl3 barriers with graphite electrodes, resulting from polarization of their antiferromagnetic ground states under an applied magnetic field. In CrI3 we also find inelastic electron tunneling suggesting the observation of Dirac magnon excitations. Finally, we note a large enhancement of the interlayer exchange in thin CrCl3 compared to bulk, and discuss its origins.


DAHLIA KLEIN (Presenter), DAVID MACNEILL, QIAN SONG, Massachusetts Institute of Technology, MINGYU XU, RAQUEL RIBEIRO, PAUL CANFIELD, Iowa State University, RICCARDO COMIN, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — The family of layered chromium trihalides has been studied for decades due to its rich magnetic phases coupled with insulating properties. The recent isolation of monolayer CrI3 has renewed interest in these materials to incorporate magnetism into 2D van der Waals heterostructures. Transition metal halide magnets have revealed intriguing ground states differing from the bulk when cleaved to thin films but this phenomenon is not yet understood. Here, we use electron tunneling through few-layer crystals of the layered antiferromagnet CrCl3 to probe its magnetic order in the ultrathin limit. By measuring the magnetoresistance in spin filter magnetic tunnel junctions, we measure the interlayer exchange in CrCl3 barriers two to four layers in thickness and find that it is greatly increased in thin films compared to bulk.

*NSF Graduate Research Fellowship: NSF Grant No. 1122374; Center for Integrated Quantum Materials: NSF Grant No. DMR-1231319; EPiQS Initiative: Gordon and Betty Moore Foundation Grant No. GBMF4541 & GBMF4411; Ames Laboratory Contract No. DE-AC02-07CH11358

SEUNG WOO JANG (Presenter), MIN YONG JEONG, HONGKEE YOON, SIHEON RYEE, MYUNG JOON HAN, Department of Physics, Korea Advanced Institute of Science and Technology (KAIST) — We performed a detailed microscopic analysis of the inter-layer magnetic couplings for bilayer CrI3. As the first step toward understanding the recent experimental observations and utilizing them for device applications, we estimated magnetic force response as well as total energy. Various van der Waals functionals unequivocally point to the ferromagnetic ground state for the low-temperature structured bilayer CrI3 which is further confirmed independently by magnetic force response calculations. The calculated orbital-dependent magnetic forces clearly show that eg-t2g interaction is the key to stabilize this ferromagnetic order. By suppressing this ferromagnetic interaction and enhancing antiferromagnetic orbital channels of eg-eg and t2g-t2g, one can realize the desirable antiferromagnetic order. We showed that high-temperature monoclinic stacking can be the case. Our results provide unique information and insight to understand the magnetism of multi-layer CrI3 paving the way to utilize it for applications.
FAZLE SUBHAN, JISANG HONG (Presenter), Pukyong National University — Two dimensional CrI3 system has attracted extensive research interest because it is an intrinsic 2D ferromagnetic material with a band gap. It has been found that the monolayer of CrI3 possesses an intrinsic ferromagnetic ordering with a finite band gap of 1.1 eV and it has also a strong perpendicular magnetocrystalline anisotropy. Besides, it has been experimentally reported that the anti-ferromagnetic interlayer coupling in bilayer CrI3 structure could be change by external charge doping. Nonetheless, despite a few experimental works on CrI3 system, it is rare to find the theoretical studies on bilayer CrI3. We investigated the magnetic properties of bilayer CrI3 using density functional approach. We found that the pristine bilayer CrI3 had an anti-ferromagnetic ground state. Interestingly, we obtained that the external pressure could induce a transition from anti-ferromagnetic to ferromagnetic state in bilayer CrI3 and the perpendicular magnetic anisotropy was still preserved even under the external pressure.

*Supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF:2016R1A2B4006406)

HIDEKI MATSUOKA (Presenter), MASAKI NAKANO, YOSHIHIRO IWASA, University of Tokyo — Emerging properties of van der Waals (vdW) materials at two-dimensional (2D) limit have been broadening their varieties, ranging from spin-orbit coupled transport properties, valley-polarized luminescence, spin-valley-locked superconductivities, to topological quantum transport. As one of big advantages of 2D materials, 2D physical phenomena could be more and more enriched by integrating different 2D materials into a heterostructure, so-called vdW heterostructures, providing a new high-quality platform for 2D physics. One recent breakthrough in 2D physics is observation of magnetism in vdW materials, which turned out to survive down to 2D limit. This type of magnet, so-called 2D magnet, has been integrated into various types of vdW heterostructures, while tuning magnetism itself at vdW heterostructures has been less investigated so far. Here we created magnetic vdW heterostructures by molecular-beam epitaxy, where a new type of 2D magnet, vanadium selenide epitaxial thin film, was incorporated. In the presentation, we will show transport properties of those heterostructures, and discuss the interface effect on 2D magnetism.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B15 DMP: 2D Materials (Semiconductors) -- Multilayers & Heterostructures I

11:15AM B15.00001: Twist-angle dependent Optical Second-Harmonic Generation from Transition Metal Dichalcogenides (TMD) Heterostructures WONTAEK KIM (Presenter), SUNMIN RYU, Pohang University of Science and Technology — Optical second-harmonic generation (SHG) by single and few-layer transition metal dichalcogenides (TMD) is highly efficient and sensitive to their structural symmetry. The SHG signal from artificially-stacked MoS2 bilayers can be understood as a superposition of SHG fields from the individual layers. However, this model has not been verified for TMD heterostructures. Here, we studied the SHG behavior of TMD hetero-bilayers of varying twist angle in comparison with homo-bilayers. When homo-bilayers were rotated over 2pi-azimuth with a fundamental beam normally incident on their basal planes, the polarization-resolved SHG signal exhibited a six-petal pattern with six azimuthal nodes, which agreed with the superposition model. The heterostructures, however, lacked the angular nodes because of an azimuth-independent signal in addition to the six-petal pattern. The fractional contribution of the constant signal was larger for more staggered hetero-bilayers. To explain these results, we propose that the anomaly originates from a non-zero phase difference between SHG fields generated in the individual monolayers. In addition, we show that the degree of the anomaly is sensitive to the fundamental's wavelength, as the phase depends on photon energy.
11:27AM B15.00002: Observation of negative photoconductance in van der Waals heterostructures* YU WANG (Presenter), Nanjing University, ERFU LIU, University of California, Riverside, WEIDA HU, Shanghai Institute of Technical Physics, SHIJUN LIANG, FENG MIAO, Nanjing University, — Van der Waals (vdW) heterostructures made of different two-dimensional (2D) materials exhibit interesting optoelectronic properties. For example, photodetection and photo-controllable memory devices are two of intriguing applications based on vdW heterostructures. However, the operating principle for most of these devices rely on the positive photoconductance (PPC) effect. Negative photoconductance (NPC) has not yet been observed in vdW heterostructures, which holds promise in constructing optoelectronic devices with low power consumption and high-speed frequency response. In this work [1], we for the first time observed the NPC phenomenon in ReS$_2$/h-BN/MoS$_2$ vdW heterostructures-based floating gate phototransistor. The devices show excellent memory properties. More importantly, we realized the transition between the PPC and the NPC in the floating gate phototransistor. With these findings, the vdW heterostructures may open up a novel avenue for the fabrication of photoelectronic nonvolatile memory devices and multifunctional photoconductive devices.


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11:39AM B15.00003: Interlayer translations in commensurately stacked transition metal dichalcogenide bilayers* MADELEINE PHILLIPS (Presenter), C STEPHEN HELLBERG, U.S. Naval Research Laboratory — Transition metal dichalcogenide (TMD) bilayers are promising candidates for optoelectronic device components. In addition to being semiconductors that are optically active in the visible light range, they can exist in a vast array of stacking orientations due to the weak van der Waals bonding between layers. To take advantage of this geometric flexibility, it is essential to understand how changes in stacking orientation affect the properties of TMD bilayers. In this work, we use density functional theory (DFT) to study the stacking variations brought about by interlayer translations in 0 and 180-degree stacked WSe$_2$/MoSe$_2$ and WS$_2$/MoS$_2$ bilayers. We show that the 180-degree stacked bilayers have a single ground state geometry, while the 0-degree stacked bilayers have two degenerate ground state stackings. We also describe how stacking orientation correlates with interlayer distance and electronic structure, and we suggest ways to probe stacking geometry in photoluminescence experiments.

*M.P. holds a National Research Council fellowship at NRL.

11:51AM B15.00004: Interlayer excitons in bilayer MoS2 with strong oscillator strength up to room temperature* BERNHARD URBASZEK (Presenter), IANN GERBER, EMMANUEL COURTADE, SHIVANGI SHREE, CEDRIC ROBERT, XAVIER MARIE, CNRS/INSA, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS Tsukuba — Coulomb bound electron-hole pairs, excitons, govern the optical properties of transition metal dichalcogenides (TMDs) like MoS$_2$ and WSe$_2$. TMD bilayers allow studying several exciton species: intralayer excitons with electrons and holes in the same layer and also interlayer excitons with the electron and the hole residing in different layers.

In this combined experimental and theoretical work we report on the observation of interlayer excitons in a high quality homobilayer MoS$_2$ sample encapsulated in hexagonal boron nitride (hBN). The interlayer exciton transition is located between the intralayer A and B excitons and is observable in reflectivity between 4 and 300 K, whereas no such transition is observed for the monolayer in the same structure in this energy range. Our peak attribution is supported by DFT calculations solving the Bethe-Salpeter equation after GW bandstructure calculations. We find in the calculated absorption spectrum a strong, spin allowed transition situated in energy between A and B intralayer excitons stemming from an electron residing on one and the hole residing in the other layer, both at the K-point of the Brillouin zone. We discuss the possibility of hybridization of exciton species and compare with our results on homotrilayer MoS$_2$.

*ANR 2D-vdW-spin
Saturation and photon-energy dependence of ultrafast charge transfer in vdW heterostructures

ERIC YUE MA (Presenter), BURAK GUZELTURK, Stanford University, GUOQING LI, LINYOU CAO, North Carolina State University, ZHI-XUN SHEN, AARON M LINDENBERG, TONY F HEINZ, Stanford University — We have directly monitored the interlayer charge transfer after photoexcitation in type-II van der Waals heterostructures of monolayer transition metal dichalcogenides. Charge transfer is found to occur on the fs time scale by recording the electromagnetic transient emitted at THz frequencies using THz time-domain spectroscopy. This approach, insensitive to spectral changes of the materials and competing charge-neutral processes, is ideal for studying the dynamics at high excitation fluences and as a function of excitation photon energy. At low excitation fluence, we observe a linear increase in the interlayer current with fluence. However, as the fluence is increased, we see a clear saturation. We analyze this effect in terms of band re-alignment induced by the electric field from charge transfer itself. Such unavoidable saturation puts a limit on the power handling capability of these heterostructures and needs to be carefully characterized for practical applications. With further calibration, such measurements also offer a new route to determine band offsets. We further report the insensitivity of charge transfer dynamics to excitation photon energy within the instrument response. We discuss its implication on the mechanism of interlayer charge transfer.

MoS2/Si and WS2/Si 2D/3D heterojunction photodiodes fabricated by low-temperature plasma enhanced CVD

SOYEONG KWON (Presenter), Physics, Ewha Womans University, YONGHUN KIM, Korea Institute of Materials Science (KIMS), JUNGEUN SONG, DONGRYE CHOI, EUNAH KIM, Physics, Ewha Womans University, JUNG-DAE KWON, Korea Institute of Materials Science (KIMS), BYUNGJIN CHO, Advanced Materials Engineering, Chungbuk National University, DONGWOOK KIM, Physics, Ewha Womans University — We prepared MoS2 and WS2 tri-layers directly on Si substrates using atmospheric-pressure plasma enhanced chemical vapor deposition (AP-PECVD). High pressure (over 100 Torr) plasma formation and low-temperature (under 200°C) growth of AP-PECVD enabled high-quality 2D/3D semiconductor (SC) heterojunctions on a large area (over 4 inch) at a high deposition rate (10 minutes for 2 inch). The fabricated devices showed clear rectifying behaviors and large shunt resistance, indicating formation of uniform heterojunction diodes. Relatively large dark current of the heterojunctions under reverse bias could be attributed to band-to-band tunneling and avalanche multiplication process. Temperature dependence of ideality factor was studied to understand the major recombination processes, based on the conventional 3D SC model. Both of the MoS2/Si and WS2/Si heterojunctions exhibited large and fast photocurrent responses to the laser illumination (wavelength: 532 nm). The measured photocurrent was linear to the laser power, indicating interfacial defect states could not suppress photo-generated carrier collection. All the results demonstrated high quality 2D/3D SC heterojunction photodiodes with clean interfaces were prepared by AP-PECVD.

High Degree Valley-Polarization from Interlayer Exciton in van der Waals Heterostructure

LONG ZHANG (Presenter), RAHUL GOGNA, University of Michigan, WILL W BURG, JASON HORNG, University of Texas at Austin, EUNICE PAIK, YU-HSUN CHOU, University of Michigan, KYOUNGHWAN KIM, EMANUEL TUTUC, University of Texas at Austin, HUI DENG, University of Michigan — Two-dimensional semiconductors promise valleytronics applications, where the valleys of the electronic bands, in addition to spin and charge, become a new degree of freedom for quantum engineering and information processing. Yet electron-hole exchange interactions lead to rapid valley depolarization and low valley polarizations (VPs) in monolayer materials. Here, by precisely aligning the momentum valleys of a WSe2 monolayer to a MoSe2 monolayer, we form a hetero-bilayer with bright interlayer excitons that inherit and preserve the VP from the intralayer ones while at the same time with greatly suppressed electron-hole exchange interactions. Using these heterobilayers, We demonstrate brightened spin triplet inter-layer excitons localized at the potential minimum of the moiré lattice with a VP up to 80% and a valley lifetime of 33 ns. Spin singlet transition localized at the same registry is also measured, with an as high but opposite VP. Our work leads the way of using van der Waals semiconductor heterostructures to control the charge transfer, VP, optical selection rules and other novel optoelectronic properties.

*All authors acknowledge the support by the Army Research Office under Awards W911NF-17-1-0312.
12:39PM B15.00008: Van der Waals TMDC Heterostructures: electronic structure dependence on number of layers*
MUHAMMAD SUFYAN RAMZAN (Presenter), AGNIESZKA BEETA KUC, Jacobs University Bremen — Two-dimensional (2D) transition metal dichalcogenides (TMDCs) of type MX\textsubscript{2} (M = Mo, W; X = S, Se) have attracted considerable attention in electronics and optoelectronics due to their extraordinary properties, which differ strongly between single layers and bulk materials. Moreover, weak van der Waals interactions between layers make it possible to exfoliate them and stack with different TMDC layers to form heterostructures, which offer remarkable electronic properties. In this work, we have studied interlayer coupling between various TMDC layers, which differ either in chalcogen or transition-metal atoms. Furthermore, we have investigated stacking on 3, 4, and 5 layers. The property we were interested in was the electronic structure, in particular, which stacking yields direct band gap materials. For instance, stacking a monolayer of WSe\textsubscript{2} on top of MoS\textsubscript{2} multi-layer (2 or more layers) can yield direct (type-II) band gap for up to 6-layers system (i.e., 1L WSe\textsubscript{2} and 5L MoS\textsubscript{2}) whereas vice versa yields in-direct gap for even 5-layers system (i.e., 1L MoS\textsubscript{2} and 4L WSe\textsubscript{2}). We believe that our findings could greatly contribute to the potential applications of heterostructure TMDCs in photovoltaics, energy harvesting, and solar cells.

*RTG-QM3 for financial support and ZIH for computing time.

12:51PM B15.00009: Characterization of the contact resistance in transition metal dichalcogenide heterojunctions
ADAM PFEIFLE, MARCELO KURODA (Presenter), Auburn University — Semiconducting (2H) transition metal dichalcogenides (TMDs) are known to form high resistance contacts with most metals. Recently, lateral heterojunctions formed by 2H and metallic (1T') phases of TMDs have been proposed to reduce the contact resistance in these systems. Here we combine first principles and quantum transport calculations to rationalize the contact resistance of heterojunctions accounting for their phases (2H and 1T'), composition (WTe\textsubscript{2}, MoTe\textsubscript{2}, WSe\textsubscript{2}, and MoSe\textsubscript{2}), and channel length. We find that telluride 1T' phases in metal/metal junctions are nearly ideal close to the Fermi level as Bloch states remain delocalized through the metal electrode and channel. Mixtures of 1T' selenides and tellurides depart from this ideal scenario due to the momentum mismatch of Bloch states that limit carrier injection. The coupling between metallic (1T') and semiconducting (2H) channels also shows large barriers (> 0.3 eV). The crossover between transport regimes governed by thermionic emission and tunneling is analyzed for the different compositions. We also discuss the presence of edge states in these heterostructures. This work may prove valuable to attaining low contact resistance suitable for optoelectronic applications based on two-dimensional materials.

1:03PM B15.00010: Quantum Transport in Transition Metal Dichalcogenide Monolayers and Twisted Bilayers*
[Invited] JAMES HONE (Presenter), Columbia University — This presentation will review our recent progress in studies of the magneto-transport properties of transition metal dichalcogenides. This work utilizes materials exfoliated from ultrahigh-purity single crystals grown by a flux synthesis technique, and encapsulation by h-BN to minimize external disorder. Ohmic contacts are achieved by work function control and dual-gating. These samples are studied in high magnetic fields by a combination of electrical transport measurements and probing the density of states using capacitance. I will describe a number of systems studied in this way, including WSe\textsubscript{2} monolayers, bilayers, and bilayers with small interlayer twist angles. In addition, recent studies of semiconducting and metallic forms MoTe\textsubscript{2} will be described.

*Sample synthesis and studies of MoTe2 are supported under NSF DMR-1420634
Studies of monolayer WSe2 are supported under DOE SC-0016703
Studies of twisted bilayer materials are supported under DOE DE-SC0019443

1:39PM B15.00011: Photon-Induced Suppression of Interlayer Tunneling in Van Der Waals Heterostructures*
WANG KONG TSE (Presenter), WOO-RAM LEE, University of Alabama — We present a theory for interlayer tunneling in van der Waals heterostructures driven under a strong electromagnetic field, using graphene/hBN/graphene as a paradigmatic example. Our theory predicts that strong anti-resonances appear at bias voltage values equal to an integer multiple of the light frequency. These features are found to originate from photon-assisted resonant tunneling transitions between Floquet sidebands of different graphene layers, and are unique to two-band systems due to the interplay of both intraband and interband tunneling transitions. Our results point to the possibility of tunneling localization in van der Waals heterostructures using strong electromagnetic fields.

*This work was supported by startup funds from the University of Alabama and by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Early Career Award #DE-SC0019326.
**1:51PM B15.00012: Ab initio Study and Search of Chalcogenide-oxide Interfaces**

YUXIN YIN (Presenter), JENNIFER COULTER, PRINEHA NARANG, Harvard University — The discovery of interface enhanced superconductivity has sparked interest in studying interfacial properties of quantum materials. Experimental and theoretical efforts highlight the relevance of spin fluctuation, orbital order and electron-phonon coupling to the onset enhanced superconducting behavior. However, the exact mechanism responsible for increased Tc is still not well-understood. Inspired by recent observations of interface enhanced superconductivity in FeSe/SrTiO3 system and ultrathin film CuS2, we use ab initio theoretical tools to investigate interfacial properties. We investigate interfacial effects on electronic structure, electron-electron and electron-phonon interactions, as well as study the effect of interlayer coupling in chalcogenide-oxide structures. Additionally, we aim to use our methods to identify superconducting interfaces in other chalcogenide material and substrate combinations. These theoretical investigations provide avenues to design and search for superconducting chalcogenide-oxide interfaces.

*We acknowledge support from ONR: N00014-18-1-2691 grant on High-Tc Superconductivity at Oxide-Chalcogenide Interfaces.

**2:03PM B15.00013: Effect of stacking orientation on the electronic and optical properties of 2D nitride heterostructures**

NOCONA SANDERS (Presenter), EMMANOUIL KIOUPAKIS, University of Michigan — Given the successful synthesis of 2D GaN and investigations into the properties of freestanding 2D nitrides, heterostructures of these materials are now of particular interest. Extreme quantum confinement is a viable method to shift light emission to shorter wavelengths, but in 2D nitrides this is counteracted by the quantum-confined Stark shift due to the strong inherent polarization perpendicular to the 2D plane. We report the electronic and optical properties of 2D BN, GaN, AlN, and InN in various stacking orientations, such that the electric fields are either aligned or anti-parallel in two possible configurations. We employ density functional theory and quasiparticle corrections with the GW method, as well as the Bethe-Salpeter Equation, to derive accurate band structures, exciton binding energies, and luminescence energies. Through understanding how the stacking arrangement influences the underlying electronic and optical properties, critical insight will be gained in how to improve 2D III-nitride-based optoelectronics through accessing the additional degree of freedom provided by polarization.

*This work was supported by the NSF ECCS-CDS&E program (1607796). Computational resources were provided by the DOE NERSC facility under Contract No. DE-AC02-05CH11231.

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**Monday, March 4, 2019 11:15 AM - 2:15 PM**

**Session B16 DMP: Transport in Nanostructures -- Single Molecules and Molecular Devices**

BCEC 155 - Han Htoon, Los Alamos National Laboratory - Tag(s): Focus


E-DEAN FUNG (Presenter), YAPING ZANG, LATHA VENKATARAMAN, Columbia University — The basic mechanism for light emission in Scanning Tunneling Microscopes (STM) is described by inelastic tunneling electrons which couple to localized surface plasmons. There is also growing interest in charge transfer plasmons which appear when electrically coupling metallic nanoparticles. Here, we use single molecules to form conductive bridges between an STM tip and substrate and study the complex relationship between tunneling electrons, charge transfer plasmons, and luminescence in molecular junctions. We employ the STM break junction technique to form thousands of Au point contacts and molecular junctions at ambient conditions and room temperature and measure the light emitted from these junctions using a Si photomultiplier. Since the current, junction bias, and emission signals are collected simultaneously, fluctuations in light emission can be correlated with changes in current and junction bias. Because the break junction procedure continuously modifies the local geometry, limits on the emission efficiency are experimentally determined. Finally, we explore the effect of different molecules on light emission.

*This work was supported primarily by the Center for Precision Assembly of Superstratic and Superatomic Solids at Columbia University NSF MRSEC (award no. DMR-1420634)*
NATHAN BAMBERGER (Presenter), JEFFREY IVIE, Department of Chemistry and Biochemistry, University of Arizona, ROLAND HIMMELHUBER, College of Optical Sciences, University of Arizona, OLIVER MONTI, Department of Chemistry and Biochemistry, University of Arizona — Designing circuits based on individual molecules has the potential to produce smaller and more powerful electronic devices. However, a continued challenge to studying the properties of such single molecule circuits is understanding the behavior of the linker group used to connect the molecule to electrodes. This linker plays a critical role because it controls both the electronic coupling and the available binding configurations for the molecule-electrode connections. We have studied a series of single molecule circuits using a mechanically controlled break junction set-up with custom high-speed amplification electronics. By changing both the identity and chemical environment of the molecular linker groups we can gain insight into how and why these linkers affect the value of and variation in molecular conductance. We also develop and use novel data analysis tools including advanced clustering methods to help disentangle the different types of junction behavior in an unbiased manner.

*National Science Foundation #DMR-1708443

11:39AM B16.00003: Two-stage Kondo effect in single Manganese phthalocyanine molecule transistor*  
XIAO GUO (Presenter), QIUHAO ZHU, WENJIE LIANG, Institute of Physics, Chinese Academy of Sciences — Charge and spin manipulation over single molecule is important for understanding various fundamental physical processes down to molecular level. In single molecule device, when the coupling between molecule and electrodes is enhanced, localize electron spin strongly interacts with electrons in the electrodes, forming Kondo effect. In this talk, I will discuss our efforts on manipulation of Kondo effect in single Manganese Phthalocyanine (MnPc) device. We use electromigration method fabricating single MnPc molecule field effect transistor successfully. Two stage Kondo and S=1/2 Kondo resonance were observed in different charge states. Two-stage Kondo effect was examined against temperature and electric field. Evolution of Kondo temperatures of the two stages in the field will be discussed. We also observed magnet field induced quantum phase transition between spin singlet and spin triplet in this system. These results illustrate spin control in multi electrons system at single molecule scale.

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Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. XDB30000000)
Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. XDB07030100)

11:51AM B16.00004: Many-body states description for transport and optical properties of molecular junctions with intra-molecule Coulomb interaction*  
KUNIYUKI MIWA (Presenter), MICHAEL GALPERIN, Department of Chemistry and Biochemistry, University of California San Diego — Recent progress of nano-fabrication and laser techniques at nanometer scale makes it possible to perform optical measurements in current-carrying molecular junctions. These advances give rise to the new branch of research coined molecular optoelectronics. With electrons involved in both quantum transport and optical scattering, theoretical challenge is description of these processes on the same footing. Here, we present theoretical analysis of quantum transport and optical response in molecular junctions with strong intra-molecule Coulomb interaction. The study employs molecular many-body states as a basis of consideration, which allows to take intra-molecular interactions exactly. To account for molecule-contacts coupling we use diagrammatic technique for the Hubbard nonequilibrium Green's functions (NEGF). We verify the methodology by comparing with other available techniques at the model level, and apply it to analyze experimental measurements of electroluminescence and photocurrent generation in molecular junctions.

*This work was supported in part by CHE - 1565939, US DOE (BES) DE-SC0018201. Part of computational work were performed using HOKUSAI system in RIKEN.
12:03PM B16.00005: Polaronic transport on conductive metal-organic frameworks from first principles  SEBASTIAN E REYES-LILLO (Presenter), Ciencias Fisicas, Universidad Andres Bello, JEFFREY B NEATON, Molecular Foundry, LBNL; UC Berkeley; Kavli ENSI — Hybrid organic-inorganic materials are an emerging class of functional materials with important technological applications in solar energy conversion, catalysis and carbon capture. Among these, metal-organic frameworks (MOFs) correspond to three-dimensional porous materials with potential applications in batteries and fuel cells. Recent studies have shown that polarons, localized quasi-particles formed by excess electronic charge and its self-induced local lattice distortion, play an important role in the transport and optoelectronic properties of electrically conductive MOFs; and therefore, in their overall performance in real devices. In this work, we revisit recent experimental results [1,2] and use theoretical and computational first principles methods to investigate the structural stability and electronic properties of electron polarons, as well as their transport properties. We describe our theoretical results for two specific hybrid organic-inorganic materials: the metallic doped system KxFe2(BDP)3 (0 < x < 2; BDP2− = 1,4-benzenedipyrrozolate) [1], and the two-dimensional ferrimagnetic and conductive system CrCl2(py2)2 (py = pyrazine) [2]. References: [1] Aubrey et al., Nature Materials 17, 625 (2018); [2] Pedersen et al., Nature Chemistry 10, 1056 (2018).

12:15PM B16.00006: Extracting Quantitative Information of electronic structures from Tunneling Molecular Junction I-V Characteristics using a Compact Analytical Model  ZUOTI XIE (Presenter), C. DANIEL FRISBIE, Chemical Engineering and Materials Science, University of Minnesota — One of the central challenges of molecular electronics is to establish clear connections between molecular structure, the ensuing electronic structure, and the current-voltage (I-V) characteristics of molecular junctions. In particular, the offset εh of the Fermi level relative to the appropriate frontier molecular orbital (HOMO in this case) and the electrode-molecule coupling strength Γ are recognized as two main factors that determine the electrical properties of a typical molecular junction. We show that a compact analytical model derived from the Landauer formalism provides a quantitative fit to the I-V data and yields values of εh and Γ that vary systematically with molecular structure and choice of electrode materials. We will present transport data and theoretical analysis of tunnel junctions based on oligophenylene monoand dithiols – with systematically varying lengths – and electrodes fabricated from Ag, Au and Pt metals. Furthermore, Ultraviolet photoelectron spectroscopy (UPS) was employed to determine the εh to be compared with the values predicted by the model from transport data. We will emphasize that the compact analytical analysis facilitates structure-property correlations and a powerful physical organic chemistry approach to molecular electronics.

12:27PM B16.00007: Angstrom-distance rulers using single molecule conductance measurements  NICHOLAS MILLER (Presenter), Boston University, MARIA KAMENETSKA, Physics and Chemistry, Boston University — Electron transport through single metal-molecule-metal junctions are exquisitely sensitive to the atomic scale geometry of the junction. Here, we use conductance signatures of single molecules on metal electrodes measured using the Scanning Tunneling Microscope-based Break Junction (STM-BJ) technique to map the Angstrom-scale arrangement of the atoms in the junctions. Using our “pull-push” technique, where we repeatedly pull apart, hold and then push the electrodes together in the presence of diamine molecules, we determine the conductance and geometry signatures of a series of these molecules. We find that the molecular conductance can be used to determine the distance between electrodes with Angstrom-scale precision. We discover that the odd or even number of carbon atoms in an alkanediamine molecule affects the mean elongation that the single molecule junction can sustain. Furthermore, by analyzing the statistical probability of forming the junctions with molecules of different lengths, we can infer the average shape of our electrodes.

12:39PM B16.00008: Single Molecule Conductance of Ferrocene at Cryogenic and Room Temperature  BRENT LAWSON (Presenter), MARIO KAMENETSKA, Physics, Boston University — Ferrocene and other metallocenes are organometallic species with a metal atom sandwiched between two aromatic rings whose overall spin, spectrum and other properties can be tuned synthetically by choice of metal atom. There is interest in these molecules as candidates for applications in single molecule electronics and spintronics. However, few electron transport measurements of single metallocene molecules on metal have been performed to date. Previous conductance measurements of ferrocene using single molecule break junctions employed anchoring groups to attach the ferrocene to the electrodes, thereby changing the molecular orbitals energy levels and attenuating electron transport. Here, we use Scanning Tunneling Microscope-based break junction technique to measure conductance of ferrocene on gold at room temperature and at 4 K in UHV. We are able to effectively trap the molecule between the tip and substrate while pushing the junction together and find that the molecule binds to gold directly through carbon atoms in the cyclopentadiene organic ligands sandwiching the iron, and has an average conductance of 0.012 G0. Using this technique, we investigate the effect of the metal atom on transport properties by measuring conductance through other metallocene molecules.
12:51PM B16.00009: Signatures of Conformational Dynamics and Electrode-Molecule Interactions in the Conductance Profile During Pulling of Single-Molecule Junctions  LEOPOLDO MEJIA RESTREPO (Presenter), IGNACIO FRANCO, Chemistry, University of Rochester — We demonstrate that conductance can act as a sensitive probe of conformational dynamics and electrode-molecule interactions during the equilibrium and non-equilibrium pulling of molecular junctions. To do so, we use a combination of classical molecular dynamics simulations and Landauer electron transport computations to investigate the conductance of a family of Au-alkanedithiol-Au junctions as they are mechanically elongated. The simulations show an overall decay of the conductance during pulling that is due to a decrease in the through-space electrode-molecule interactions, and that sensitivity depends on the electrode geometry. In addition, characteristic kinks induced by level alignment shifts (and to a lesser extent by quantum destructive interference) were also observed superimposed to the overall decay during pulling simulations. The latter effect depends on the variation of the molecular dihedral angles during pulling and therefore offers an efficient solution to experimentally monitor conformational dynamics at the single-molecule limit.

1:03PM B16.00010: charge transport in molecular transistor incorporating a pair of Mn-phthalocynine molecule*  WENJIE LIANG (Presenter), XIAO GUO, Institute of Physics — charge transport phenomena of single molecule transistor are of great interests not only to understand quantum transport in confined structure, but also to study molecular properties at individual molecule level. Single molecule transistors have been realized successfully in the past years and findings including Kondo resonance, quantum phase transition among others were discovered. In this talk, we will discuss our new experimental findings when two molecules were incorporated in a molecular devices. When two Mn phthalocynine molecules are close to each other, they will coupled to each other though electric static field and in some case exchange electrons in between, leading to unique and different physics picture depending on coupling strength. molecular gating and exchange coupling will be adressed.

*This research is supported by National Basic Research Program of China (2014CB920904), Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. XDB30000000 No. XDB07030100)

1:15PM B16.00011: Origin of high thermal conductivity in complex molecular crystals: an ab initio study of polythiophene  PEISHI CHENG (Presenter), AUSTIN MINNICH, NINA SHULUMBA, Caltech — Thermally conductive molecular crystals are of fundamental and practical interest in part because they are unlike typical complex crystals, which conduct heat poorly owing to their large phonon scattering phase space. While molecular crystals with high thermal conductivity in the range of tens of Wm⁻¹K⁻¹ have been known experimentally for decades, the microscopic origin of this property has remained unclear. Ab-initio methods that have been successfully applied to simple crystals have proved difficult to adapt to molecular crystals due to quantum nuclear motion and their complex primitive cells. Here, we report the thermal transport properties of crystalline polythiophene with 28 atoms per primitive cell using an ab-initio approach that rigorously includes finite temperature anharmonicity and quantum nuclear effects. The calculated room temperature thermal conductivity is 176 Wm⁻¹K⁻¹, a high value that arises from exceptional phonon focusing along the chain for certain branches and despite short lifetimes in the picosecond range. Our finding suggests that many complex molecular crystals with stiff intra-chain bonds are intrinsically good thermal conductors as phonon focusing occurs in any crystal with anisotropic bonds.

1:27PM B16.00012: Modeling structure and conductivity of atomic-scale break junctions  MO LI, EVAN MORAVANSKY, MANUEL SMEU (Presenter), Physics, Binghamton University - SUNY — A large number of single-molecule conductance measurements rely on the break junction approach in which a metal wire (typically Au) is stretched to the breaking point in the presence of the molecule of interest. As the wire breaks, a single molecule can bridge the gap between the electrodes and its conductance can be measured. This is a complex process during which many atomic rearrangements occur, resulting in complicated current versus distance traces that are difficult to interpret. We employ density functional theory (DFT) structure relaxations to investigate the possible geometries during a break junction experiment with and without the presence of molecules. Our focus is on Au electrodes, but we also consider other elements such as Ag and Pt. Next, we the relaxed structures and study their conductance properties with the non-equilibrium Green's function technique coupled with DFT (NEGF-DFT). Our results reveal an intriguing relationship about the evolution of conductance as the junction is stretched, which can be attributed to atomic rearrangements and orbital alignment. These computational analyses can provide guidance in interpreting experimental data.
ZHI LI (Presenter), University of Rochester, ALEXANDRE TKATCHENKO, University of Luxembourg, IGNACIO FRANCO, University of Rochester — We propose a computationally efficient strategy to accurately model nonreactive molecule−surface interactions that adapts density functional theory calculations with the Tkatchenko–Scheffler scheme for van der Waals interactions into a simple classical force field. The resulting force field requires just two adjustable parameters per atom type that are needed to capture short-range and polarization interactions. The developed strategy allows for classical molecular dynamics simulation of molecules on surfaces with the accuracy of high-level electronic structure methods but for system sizes (10^3 to 10^7 atoms) and timescales (picoseconds to microseconds) that go well beyond what can be achieved with first-principles methods. Parameters for H, sp^2 C, and O on Au(111) are developed and employed to atomistically model experiments that measure the conductance of a single polyfluorene on Au(111) as a continuous function of its length. The simulations qualitatively capture both the gross and fine features of the observed conductance decay during initial junction elongation and lead to a revised atomistic understanding of the experiment.


1:51PM B16.00014: Ab initio study of the single molecule conductance of TCNQ and F_4TCNQ using NEGF-DFT  
STUART SHEPARD (Presenter), MANUEL SMEU, Binghamton University — By investigating the conductance of single molecules we gain insight into the fundamental physics of electron transport. Such an understanding can lead to molecular-based electronic components and sensors. We study the transport properties of tetracyanoquinodimethane (TCNQ) and tetrafluoro-TCNQ (F_4TCNQ) at the level of density functional theory within the non-equilibrium Green's function formalism (NEGF-DFT). Experiments show at least three distinct conductance values for a single molecule of TCNQ and F_4TCNQ. We construct a model system which consists of two gold electrodes connected via a single molecule arranged in different orientations. Four orientations are defined: bidentate-bidentate (bi-bi), mono-bi, mono-mono, and flat. We find that conductance depends on the molecule's orientation between the electrodes which ranges over an order of magnitude. In both molecules, the bi-bi and mono-bi produce lower conductance (0.02 - 0.1 G_0) while the flat orientation gives a slightly higher conductance of 0.2 G_0. Surprisingly, the mono-mono shows the largest conductance at 0.4 and 0.6 G_0 for F_4TCNQ and TCNQ respectively. The results are in qualitative agreement with scanning tunneling microscopy break junction (STM-Bj) experiments, which find two low and one high conductance value.

2:03PM B16.00015: Auxiliary quantum master equation for nonequilibrium dual-fermion approach*  
FENG CHEN (Presenter), University of California, San Diego, GUY COHEN, School of Chemistry, Tel Aviv University, MICHAEL GALPERIN, University of California, San Diego — We introduce auxiliary quantum master equation - dual fermion approach (AQME-DF) and argue that it presents a convenient way to describe steady states of non-equilibrium correlated impurity systems. The combined scheme yields an expansion around a reference system much closer to the true system than in the previous considerations. This scheme also avoids long time propagation and hence is numerically cheaper. Results for Anderson impurity model (AIM) are presented as a benchmark.

*This material is based upon work supported by the National Science Foundation under CHE-1565939 and by the Department of Energy under DE-SC0018201

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B17 DCOMP: Matter in Extreme Environments: Hydrides  BCEC 156A - Yanming Ma, Jilin Univ -

Tag(s): Focus
11:15AM B17.00001: Near room temperature superconductivity in superhydrides at megabar pressures* [Invited]
RUSSELL HEMLEY (Presenter), School of Engineering and Applied Science, The George Washington University — Recent predictions and experimental observations of high $T_c$ superconductivity in hydrogen-rich materials at very high pressures are driving the search for superconductivity in the vicinity of room temperature. We confirmed the existence of a new class of such materials – superhydrides ($MH_x$, with $x > 6$) – and developed preparation techniques for their syntheses and characterization, including measurements of structural and transport properties, at megabar pressures. Four-probe electrical transport measurements of lanthanum superhydride samples display signatures of superconductivity at temperatures ranging from 150 K to above 280 K near 200 GPa. The experiments are supported by pseudo-four probe conductivity measurements, critical current determinations, low-temperature x-ray diffraction, and magnetic susceptibility measurements. These measurements of near-room temperature superconductivity are in good agreement with density functional and BCS theory-based calculations.

*This work was made possible by M. Somayazulu, M. Ahart, V. V. Struzhkin, Z. M. Geballe, A. K. Mishra, M. Baldini, Y. Meng, Hanyu Liu, and Ivan I. Naumov. This research was supported by EFRe, an Energy Frontier Research Center funded by DOE, Office of Science (DE-SC0001057). Instrumentation and facilities were supported by DOE/BES (DE-FG02-99ER45775; DE-AC02-06CH11357, ANL), DOE/NNSA (DE-NA-0002006, CDAC; DE-NA0001974, HPCAT), and NSF (DMR-1809783).

11:51AM B17.00002: High-Tc Conventional Superconductivity in Clathrate Hydrides: What can we learn from Electronic Structure?* LILIA BOERI (Presenter), Sapienza University of Rome, CHRISTOPH HEIL, SIMONE DI CATALDO, Institute for Theoretical and Computational Physics, Graz University of Technology, GIOVANNI BACHELET, Sapienza University of Rome — The current record-holder for superconductivity is a lanthanum superhydride ($LaH_{10}$), which crystallizes in a clathrate structure, in which hydrogen forms a dense lattice of interconnected cages. The highest $T_c$ reported is close to room temperature (265 K). $T_c$'s comparable, or even higher than this, have been predicted to occur in other clathrate hydrides with chemical formula $XH_6$ and $XH_{10}$, with $X$=Sc,Y,Mg,Ca.

In this contribution, using ab-initio Migdal-Eliashberg theory, we study the superconducting properties of this new broad class of superconductors, and trace them back to their unique electronic structure.

*We acknowledge funding from the Austrian Science Fund FWF projects No. J 3806-N36 and P 30269-N36 and Fondo Ateneo Sapienza 2017.

12:03PM B17.00003: Synthesis of cerium superhydride CeH$_9$ with 3-dimensional atomic hydrogen sublattice
NILESH SALKE (Presenter), Center for High Pressure Science & Technology Advanced Research (HPSTAR), Shanghai, 201203, China, M. MAHDI DAVARI ESFAHANI, Department of Geosciences, Center for Materials by Design, and Institute for Advanced Computational Science, State University of New York, Stony Brook, New York 11794-2100, U, YOUJUN ZHANG, Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China, IVAN KRUGLOV, Department of Problems of Physics and Energetics, Moscow Institute of Physics and Technology, 9 Institutskiy Lane, Dolgoprudny City, Moscow Region 141700, Russia, JIANSHI ZHOU, YAGUO WANG, Department of Mechanical Engineering, The University of Texas at Austin, Austin, Texas 78712, USA, ERAN GREENBERG, VITALI PRAKAPENKA, Center for Advanced Radiation Sources, University of Chicago, Illinois, 60637, USA, ARTEM OGANOV, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, 3 Nobel Street, Moscow 143026, Russia, JUNG-FU LIN, Department of Geological Sciences, The University of Texas at Austin, Austin, Texas 78712, USA — Hydrogen-rich super/polyhydrides were considered as an alternative to the monatomic metallic hydrogen to achieve superconductivity close to room temperature at relatively lower pressure. Concomitantly, superconductivity was reported in H$_3$S at record high $T_c$ of 203 K at 200 GPa. Synthesis of superhydrides is very challenging as most of these super/polyhydrides stabilize at very high pressure for e.g., FeH$_5$ and LaH$_{10}$ stabilized at 130 and 170 GPa respectively. However, it would be always useful if superhydrides are synthesized at lower possible pressure. With this motivation, we carried the experimental and theoretical studies on Ce-H system. We have successfully synthesized superhydride CeH$_9$ around 100 GPa in the laser-heated diamond anvil cell. Theoretical calculations were carried to understand the structure, stability and superconductivity of CeH$_9$. CeH$_9$ crystallized in a $P6_3/mmc$ clathrate structure with 3-dimensional atomic hydrogen sublattice. Synthesis of CeH$_9$ at feasible pressure range is very promising and hints towards the future possibility to achieve higher $T_c$ value with the lowest possible pressure in hydride superconductors. This study will also help to further investigate and understand hydride superconductivity at feasible pressure range.
Theoretical Investigation of Ternary Hydrogen-Rich Materials under Pressure

TIANGE BI (Presenter), EVA ZUREK, Chemistry, University at Buffalo — Investigations of chemical compounds under pressure has led to the discovery of novel materials with unique properties and chemical compositions that cannot form at ambient conditions. Hydrogen is believed to become metallic and even superconducting under pressure with a high transition temperature, but the metallization pressure has not been reached by current experiments. Our research mainly focuses on predicting the structures of novel superconducting hydrogen-rich materials using the open-source evolutionary algorithm XTALOPT coupled with density functional theory (DFT) calculations. Given only the chemical composition, this combination allows us to find the most stable structure of a solid under extreme conditions. Therefore, we present our predictions of ternary hydrides at high pressures including analysis of structural and electronic properties.

Strong Electron-Hole Symmetry Breaking in the High Temperature Superconductor H$_3$S.

SOHAM GHOSH (Presenter), WARREN E PICKETT, University of California, Davis — A favorable combination of strong electron-phonon coupling (EPC), high phonon frequency and substantial density of states (DOS) near the Fermi energy was predicted\(^1\) to produce a record superconducting critical temperature $T_c$ around 200K at high pressure, quickly followed by the experimental discovery by Drozdov et al.\(^2\) up to 203K at 160 GPa pressure. Several theoretical papers have confirmed and elaborated on the new phenomena that arise in H$_3$S. Here we employ first principles methods that reveal new aspects of H$_3$S. The electron and phonon self energies are calculated using the EPW code, and we analyze effects of the two nearby van Hove singularities (vHs) that create a sharp and narrow peak of the electron DOS in this material. Several features emerge: The interacting DOS (the spectral density) is severely affected by the strong electron-phonon coupling, and the electronic spectrum displays extreme examples of band renormalization and broadening that have been suggested to arise from strong EPC. Phonon self-energy features will also be presented.


High Field Magnetotransport in Superconducting Hydrides under Pressure

SHIRIN MOZAFFARI, LUIS BALICAS, National High Magnetic Field Lab, Florida State University, Tallahassee, USA, VASILY S. MINKOV, DMITRY KNYAZEV, MIKHAIL EREMETS, Max-Planck-Institut fur Chemie, Hahn-Meitner-Weg 1, 55128 Mainz, Germany, MARI EINAGA, KATSUYA SHIMIZU, Osaka University, Machikaneyamacho 1-3, Toyonaka, Osaka, 560-8531, Japan, DAN SUN, FEDOR BALAKIREV (Presenter), National High Magnetic Field Lab, Los Alamos National Laboratory, Los Alamos, USA — Hydrogen sulfide forms metallic phase under high pressure above one million atmospheres and becomes superconducting at temperatures as high as 203K at 160GPa. Despite record-breaking $T_c$ the basic properties of superconducting sulphur hydride/deuteride are found to be consistent with conventional Bardeen-Cooper-Schrieffer (BCS) theory. Early measurements of the superconducting phase diagram in magnetic fields up to 7T estimate upper critical fields of the order of 70T. We report magnetotransport studies of superconducting sulphur hydride in DC fields up to 35T and pulsed fields up to 65T. We find that upper critical field generally follow the Werthamer, Helfand and Hohenberg (WHH) formalism at low fields, while noticeable deviations from WHH appear at experimental limit of 65T.

*The work at NHMFL was supported by the National Science foundation under cooperative Grant Nos. DMR-1157490 and DMR-1644779, the U.S. DOE, and the State of Florida, and DoE-BES DE-SC0002613

High superconductivity in hydrides at high pressures

XUE LI (Presenter), State Key Laboratory of Superhard Materials, College of Physics, Jilin university, HANYU LIU, YANMING MA, Innovation Center for Computational Physics Methods and Software, College of Physics, Jilin university — The mechanisms for the strong electron-phonon coupling predicted for hydrogen-rich compounds with high superconducting critical temperature were examined within the Bardeen-Schrieffer-Cooper and Midgal-Eliashberg theory. In this study, we have explored some candidate structures for hydrides at high pressures. Electron-phonon coupling calculations predict the existence of new superconducting phases, some even exhibiting superconductivity in the range of room temperature. Further analysis shows that hydrogen-hydrogen vibrations played acritical role in enhancing electron-phonon coupling parameters. Moreover, the calculated stabilities indicate the materials are likely to be synthesized at pressures that are currently accessible in the laboratory. The results open the prospect for the design, synthesis, and recovery of new high-temperature superconductors with potential practical applications.
1:03PM B17.00008: Electronic Structure and Properties of Calcium and Iron Polyhydrides Under Pressure

EVA ZUREK (Presenter), Department of Chemistry, University at Buffalo — The recent synthesis of the calcium and iron polyhydride phases under pressure has inspired theoretical investigations of their structures and electronic structures. First principles calculations have helped to characterize a newly synthesized \( C2/m \) symmetry \( \text{Ca}_2\text{H}_5 \) phase at 25 GPa and an \( I4/mmm \) symmetry \( \text{CaH}_4 \) phase at 120 GPa. Both of these phases contain atomic and molecular hydrogen. The H-H distances in the molecular units are elongated as compared to those in elemental \( \text{H}_2 \) at the same pressure. Electronic structure calculations illustrate that the bond-lengthening mechanism under pressure in the solid state resembles the one responsible for lengthening the H-H bond in Kubas like molecular complexes. Crystal structure prediction techniques have also been employed to predict stable and metastable high hydrides of iron between 150-300 GPa that have not been discussed in other studies. Density functional theory calculations show that neither the \( I4/mmm \) nor the \( Cmca \) symmetry \( \text{FeH}_5 \) phases found to be stable are superconducting.

1:15PM B17.00009: Bipartite character of electronic structure in compressed \( \text{H}_3\text{S} \) and its relation to the high-Tc superconductivity*

RYOSUKE AKASHI (Presenter), University of Tokyo — The sulfur superhydride \( \text{H}_3\text{S} \) has attracted enormous interest since the discovery of the 200K superconductivity in this material under extreme pressure. According to the previous studies, its \( T_c \) is boosted by the peaked structure in the density of states (DOS) and its presence is robust against substitution of sulfur atoms to phosphorus etc.. Its persistence has been thought to emerge through some complicated interplay of the sulfur 3s, 3p and hydrogen 1s orbitals but clear explanation on it has yet been established. We disentangle the “complicated interplay” to clarify how the DOS peak emerges. In particular, we find that a sublattice model with decorated simple cubic structure well represents the electronic structure in this system near a two-dimensional manifold in the Brillouin zone, which is due to small inter-sublattice coupling dependent on the crystal wavenumber. We discuss this point and its possible relation to the robust DOS peak.

*MEXT Element Strategy Initiative to Form Core Research Center in Japan

1:27PM B17.00010: A New Analysis of Strong Electron-Phonon Coupling in Compressed Metal Hydrides*

YUNDI QUAN (Presenter), WARREN E PICKETT, University of California, Davis — The experimental discovery that \( \text{H}_3\text{S} \) becomes superconducting at 200 K under 160 GPa pressure has re-invigorated interest in metal hydrides under compression. Understanding the role of hydrogen relative to that of metal atom and the crystal structure is essential for designing materials with even higher \( T_c \). Importantly for \( \text{H}_3\text{S} \) and other hydrides, various physical quantities including the phonon spectra, the coupling strength \( \lambda \), and matrix elements can be clearly identified as contributions from either hydrogen or the metal atom. We systematically study a few classes of binary hydrides, viz. \( \text{H}_3\text{S} \), \( \text{CaH}_6 \), \( \text{MgH}_6 \) and recently reported lanthanum hydride to carry out this separation and gain a unique type of insight into the origin of strong electron-phonon coupling and high \( T_c \) in hydrides.

*We acknowledge funding from NSF DMR 1607139. This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562.
Probing Hydrogen in Metal Hydrides: Proton-NMR study of FeH up to 1.9 Mbar

THOMAS MEIER (Presenter), SAIANA KHANDEKHAeva, Bavarian Geoinstitute, Bayreuth University, SYLVAIN PETITGIRARD, Department of Earth Sciences, Institute of Geochemistry and Petrology, STELLA CHARITON, Bavarian Geoinstitute, Bayreuth University, TIMOFEY FEDOTENKO, NATALIA DUBROVINSKAIA, Material Physics and Technology at Extreme Conditions, Laboratory of Crystallography, University of Bayreuth, L. S. DUBROVINSKY, FLORIAN TRYBEL, GERD STEINLE-NEUMANN, Bavarian Geoinstitute, Bayreuth University — Investigation of electronic structures of metal hydrides remains an elusive challenge in high pressure laboratories. Using a novel high pressure NMR technique [1,2,3] we study face centred cubic iron hydride, FeHx with x = 1.0(1), synthesized in-situ in a diamond anvil cell at 30 GPa and temperatures above 1000 K by reaction of iron powder and paraffin. Signals stemming from metallic FeH were identified at protonic Knight shifts of about -1200 ppm. Measurement of the Korringa relation shows that FeH preserve Fermi-liquid like electronic behaviour between 30 and 63 GPa and from 154 GPa towards the highest pressures in this study. Between 63 GPa and 154 GPa the volume dependence of the Proton Knight shift shows an unexpected deviation of the free-electron V^2/3 Knight Shift curvature, indicating an electronic topological transition of the Fermi surface. This study demonstrates the possibility to investigate the electronic structures of hydrogen under chemical pre-compression in metal hydride systems at pressures not accessible by comparable methods.


*This study was financed by the Bavarian Geoinstitute and free state of Bavaria.

Spin-Lattice Model of Plutonium Hydride Nucleation

RYAN MULLEN (Presenter), NIR GOLDMAN, Materials Science Division, Lawrence Livermore National Laboratory — Plutonium hydride forms when plutonium is exposed to hydrogen gas or water vapor. The mechanism of plutonium hydride nucleation is a key material property in this process. Conducting experiments with plutonium is difficult and expensive due to its toxicity and radioactivity. Computer models allow us to probe the phase transition to plutonium hydride without physically handling plutonium.

We develop a spin-lattice model of plutonium hydride, PuH₂, wherein the presence of a hydrogen atom in an interstitial site is a binary variable. We parameterize the site energy of each interstitial as a function of the number of nearest-neighbor occupied sites from the DFT energies of a small system (N_{Pu} = 32). We then compute the phase equilibrium between Pu and PuH₂ from the spin-lattice model using a combination of Wang-Landau sampling and histogram reweighting. The size of the critical PuH₂ nucleus is then computed using a much larger system than would be accessible with DFT (N_{Pu} = 500,000).

*This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-ACS2-07NA27344. Document release number LLNL-ABS-760287.

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B18 DCOMP DCMP DAMOP: Machine Learning Material and Experimental Data II

BCEC 156B - Christof Weitenberg, University of Hamburg - Tag(s): Focus

Identifying quantum phase transitions using artificial neural networks on experimental data

CHRISTOF WEITENBERG (Presenter), University of Hamburg — Machine learning techniques such as artificial neural networks are currently revolutionizing many technological areas and have also proven successful in quantum physics applications. Here we employ an artificial neural network and deep learning techniques to identify quantum phase transitions from single-shot experimental momentum-space density images of ultracold quantum gases and obtain results, which were not feasible with conventional methods. We map out the complete two-dimensional topological phase diagram of the Haldane model and provide an accurate characterization of the superfluid-to-Mott-insulator transition in an inhomogeneous Bose-Hubbard system. Our work points the way to unravel complex phase diagrams of general experimental systems, where the Hamiltonian and the order parameters might not be known.

*We acknowledge financial support from the Deutsche Forschungsgemeinschaft via the Research Unit FOR 2414 and the Collaborative Research Center SFB 925.
11:51AM B18.00002: Classifying Snapshots of the Doped Hubbard Model with Machine Learning  
ANNABELLE BOHRDT (Presenter), Technical University of Munich, CHRISTIE S CHIU, GEOFFREY JJ, MUQING XU, DANIEL GREIF, MARKUS GREINER, EUGENE DEMLER, Physics Department, Harvard University, FABIAN GRUSDT, MICHAEL KNAP, Technical University of Munich — Quantum gas microscopes for ultracold atoms can provide high-resolution real-space snapshots of complex many-body systems. We implement machine learning to analyze and classify such snapshots of ultracold atoms, which realize the Fermi-Hubbard model on a square lattice. At half-filling, we find that machine learning successfully identifies a crossover in the character of magnetic correlations with increasing temperature, in concurrence with the peak of the uniform spin susceptibility. We then extend the approach to assess two theoretical descriptions of doped antiferromagnets: a doped quantum spin liquid and a geometric string theory describing hidden spin order. Up to intermediate doping values, our algorithm tends to classify experimental snapshots as geometric-string-like, as compared to the dosed spin liquid or to experimental images at high temperatures. Our results demonstrate the potential for machine learning in processing the wealth of data obtained through quantum gas microscopy for new physical insights.

*This work was supported in part by Materials research by Information Integration Initiative (MI2I) project of the Support Program for Starting Up Innovation Hub from Japan Science and Technology Agency (JST), by Japan Society for the Promotion of Science (JSPS) KAKENHI Grant Number JP 18K13474, and by Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan as a social and scientific priority issue (Creation of new functional devices and high-performance materials to support next-generation industries; CDMSI) to be tackled by using a post-K computer.

12:03PM B18.00003: Detecting nematic order in STM/STS data with artificial intelligence†  
JEREMY GOETZ (Presenter), Binghamton University, YI ZHANG, MICHAEL LAWLER, Department of Physics, Cornell University — Detecting the subtle yet phase defining features in Scanning Tunneling Microscopy and Spectroscopy (STM/STS) data remains an important challenge in quantum materials. We meet the challenge of detecting nematic order from local density of states data with supervised machine learning and artificial neural networks for the difficult scenario without sharp features such as visible lattice Bragg peaks or Friedel oscillation signatures in the Fourier transform spectrum. We train the artificial neural networks to classify simulated data of isotropic and anisotropic two-dimensional metals in the presence of disorder. The supervised machine learning succeeds only with at least one hidden layer in the ANN architecture, suggesting the classification scheme is non-linear. We apply the finalized ANN to experimental STM data on CaFe$_2$As$_2$ and it predicts nematic symmetry breaking with 99% confidence (probability 0.99), in agreement with previous analysis.

*MJL acknowledges supported in part by the National Science Foundation under Grant No. NSF PHY-1125915. MJL acknowledge the kind hospitality from KITP at the preliminary stages of the work. Y.Z. was supported by NSF DMR-1308089 and Bethe fellowship at Cornell University.

12:15PM B18.00004: Revealing Patterns in Scanning Probe Microscopy Data via Machine Learning Techniques*  
ERIC HUDSON (Presenter), RJJU BANERJEE, LAVISH PABBI, ANNA BINION, KEVIN CRUST, WILLIAM DUSCH, Pennsylvania State University — Machine Learning (ML) techniques have become prevalent in many diverse fields of research, with the goal of helping extract information from large, complex datasets. Its penetration into condensed matter physics is still however relatively shallow, even for application to results from techniques such as scanning tunneling microscopy (STM), where the image-based nature of the data would naturally seem to lend itself to now standard ML investigations. Here we present results of ML techniques applied to both topographic and spectroscopic STM data, demonstrating the power of these techniques to reveal previously hidden connections between the two and hence help improve our understanding of the relationship between structure and electronic properties at the atomic scale.

*This work was supported by the National Science Foundation Grant MRI-1229138.

12:27PM B18.00005: Crystal Structure Prediction by Bayesian Optimization and Evolutionary Algorithm†  
TOMOKI YAMASHITA (Presenter), National Institute for Materials Science, SHINICHI KANEHIRA, Osaka University, NOBUYA SATO, National Institute of Advanced Industrial Science and Technology, HIORI KINO, National Institute for Materials Science, KOJI TSUDA, The University of Tokyo, TAKASHI MIYAKE, National Institute of Advanced Industrial Science and Technology, TAMIO OGUCHI, Osaka University — Crystal structure prediction methods such as random search (RS) and evolutionary algorithm (EA) have attracted attention. Previously we have developed a searching algorithm accelerated by Bayesian optimization (BO). BO is a selection-type algorithm which can efficiently select potential candidates by machine learning. First, we compared searching efficiency among RS, EA, and BO in the small system of Si$_{16}$. In each algorithm, a hundred structures were searched. The importance of random generation is found compared with evolutionary operations even in EA. RS could be the most efficient for small systems. Furthermore, we develop a hybrid algorithm of BO and EA, and discuss the searching efficiency in large systems.

*This work was supported in part by Materials research by Information Integration Initiative (MI2I) project of the Support Program for Starting Up Innovation Hub from Japan Science and Technology Agency (JST), by Japan Society for the Promotion of Science (JSPS) KAKENHI Grant Number JP 18K13474, and by Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan as a social and scientific priority issue (Creation of new functional devices and high-performance materials to support next-generation industries; CDMSI) to be tackled by using a post-K computer.
12:39PM B18.00006: Phonon Calculations of Phase Change Materials Using Machine-Learning Methods  YOUNGJAE CHOI (Presenter), WOOIL YANG, SEUNG-HOON JHI, POSTECH, Korean Physical Society — Machine-learning (ML) methods for constructing the potential-energy-surface (PES) have been developed and being widely applied to the systems that may be inaccessible by conventional \textit{ab initio} calculations [1, 2, 3]. Dynamical properties of the systems can also be analyzed utilizing calculated PES from the ML methods [2, 4]. One issue that should be addressed for proper application of the ML methods is the transferability of the PES, in particular for calculation of the dynamical properties in various phases. In this study, we used the ML methods to calculate the PES and phonon modes of phase change materials and carried out the transferability analysis by controlling the training sets and force errors.


12:51PM B18.00007: Developing computationally efficient potential models by genetic programming  ALBERTO HERNANDEZ (Presenter), ADARSH BALASUBRAMANIAN, FENGLIN YUAN, TIM MUELLER, Johns Hopkins University — The length and time scales of atomistic simulations are limited by the computational cost of the methods used to predict material properties. We have developed a machine learning algorithm based on genetic programming to discover computationally efficient and parsimonious potential models. Genetic programming is an evolutionary algorithm that can search the space of functional forms, facilitating the optimization of the computational efficiency without the need of selecting an expression a priori. Our approach was validated by rediscovering the Lennard Jones potential and the Sutton Chen embedded atom model from training data generated using these models. By using training data generated from density functional theory calculations, we found simple and fast potential models for elemental systems. We present our approach, the forms of the discovered models, and assessments of their transferability, accuracy and speed.

1:03PM B18.00008: ICA method for identifying collective modes  YADONG WU (Presenter), HUI ZHAI, Tsinghua University — The independent component analysis method is applied to images of ultra-cold atoms. We present this model-independent method to identify the collective modes which are mixed together in a Bose-Einstein condensate from large sets of images. Machine learning method can extract features very well and ICA method can separate these mixed modes very well.

1:15PM B18.00009: "Perfect crime" of machine-learning potentials: 100-fold speed-up with no detectable trace of using machine learning in the final result*  KONSTANTIN GUBAEV, EVGENY PODRYABINKIN, Skolkovo Institute of Science and Technology, GUS HART, Physics and Astronomy, Brigham Young University, ALEXANDER SHAPEEV (Presenter), Skolkovo Institute of Science and Technology — Machine-learning interatomic potentials have been showing significant progress in accelerating atomistic modeling while preserving near DFT accuracy. To make use of such potentials, one must prepare a training dataset of atomistic configurations evaluated with DFT. This can be automated by active learning, allowing one to develop algorithms for automatically predicting materials properties with near-DFT accuracy with speedups of a few orders of magnitude. The only downside of such algorithms is a numerical error in the final answer arising from the deviation of a machine-learning potential from DFT. In my talk, I will show that, in some applications, one could develop algorithms that are free even from that numerical error. For the application of obtaining thermodynamically stable ternary alloy structures I will present an algorithm for screening out high-energy structures, thus accelerating a baseline DFT-based high-throughput algorithm by a factor of 100, leaving zero error in the final answer when compared to DFT. This alludes to the "perfect crime": machine-learning potentials offer very large speed-ups, but the final result is indistinguishable from the one obtained by pure DFT.

*This work was supported by the Russian Science Foundation (grant number 18-13-00479).
Deep Learning of Lennard-Jones Potential Parameterization

ALIREZA MORADZADEH (Presenter), N. R. ALURU, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, IL, USA — In this study, a deep neural network is developed to parameterize van der Waals interactions at various thermodynamic states based on the pair-correlation functions obtained through MD simulation of about 52 μs. After training, the network not only performs with high accuracy and fidelity for van der Waals particles but also performs well for correlations obtained from all-atom MD simulation of complex molecules. The network is capable of developing coarse-grained force fields within the theoretical limitation and accuracy imposed by van der Waals interactions. The accuracy and fidelity of the method are investigated by computing the total variation in the radial distribution function and the Kullback-Leibler divergence for the coarse-grained model development, while the mean-squared error is used to characterize the performance for the vdW particles. Our results show that deep learning is able to obtain the solution to inverse-problem of liquid-state theory under the assumption of a predetermined pair potential in both all-atom and coarse-grained models with a computational cost that is several orders of magnitude faster than other available methods in the literature.

A direct and local deep learning model for atomic forces in solids

NATALIA KURITZ, Physical Electronics, Tel-Aviv University, GOREN GORDON, Industrial Engineering, Tel-Aviv University, AMIR NATAN (Presenter), Physical Electronics, Tel-Aviv University — We demonstrate a direct and local Deep Learning (DL) model for atomic forces. We apply this model for bulk aluminum, silicon and sodium and show that the model errors are comparable to other state of the art algorithms. Our model allows the calculation of forces in large cells using a training data that we built from smaller cells that were calculated with Density Functional Theory (DFT). In addition, we examine the question of temperature transferability of the model and show that we can train the model with data that was produced at a high temperature and then test it on data that was produced at lower temperatures. We also explore the physical properties of the system (e.g. number of nearest neighbors) effect on the model convergence with respect to some of its parameters. Finally, we discuss why the performance of such local models is better in some materials in comparison to others.

Machine Learning Correlates CDW Properties with Local Gap in Cuprates

KAYLIE HAUSKNECHT (Presenter), TATIANA WEBB, Department of Physics, Harvard University, MICHAEL C BOYER, Department of Physics, Clark University, YI YIN, Department of Physics, Zhejiang University, TAKESHI KONDO, ISSP, University of Tokyo, TSUNEHIRO TAKEUCHI, Toyota Technological Institute, HIROSHI IKUTA, Department of Materials Physics, Nagoya University, ERIC HUDSON, Department of Physics, Pennsylvania State University, JENNIFER HOFFMAN, Department of Physics, Harvard University — With the advent of atomic resolution imaging techniques comes the challenge of disentangling the intrinsic electronic properties of materials from their stochastic atomic-scale disorder. In the past decade, machine learning (ML) image analysis techniques have rapidly evolved, and their applications in physics are just emerging. Here, we use ML to test correlation hypotheses between spatially resolved measurements of disordered materials to overcome the limitations of standard Fourier analysis techniques. We apply artificial neural networks to uncover the doping-dependence of the density wave (DW) structure in the cuprate superconductor (Pb,Bi)_{2}(Sr,La)_{2}CuO_{6+δ} (Bi-2201) imaged via scanning tunneling microscopy. In Bi-based cuprates, the electronic inhomogeneity, caused by local variations in doping, limits the precision of DW wavevector measurements. Our ML algorithm overcomes this limitation and allows clear differentiation between commensurate and incommensurate DW instabilities with physically distinct mechanisms. More broadly, our work lays the foundation for a ML approach to quantify intrinsic periodic order and correlations from datasets where these trends are masked by disorder.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B19 DCOMP DCMP: Precision Many Body Physics II

Session B19 DCOMP DCMP: Precision Many Body Physics II
BCEC 156C - Boris Svistunov, University of Massachusetts Amherst - Tag(s): Focus
11:15AM B19.00001: Spatial Charge and Spin Correlations in the 2D Fermi-Hubbard Model: Comparison between quantum Monte Carlo simulations and optical lattice emulators* [Invited] NANDINI TRIVEDI (Presenter), Ohio State University — I will report on the current status and challenges faced by quantum Monte Carlo simulations to obtain quantitative information about the spatially resolved charge and spin correlations in the two-dimensional Fermi-Hubbard model. The computational results will be compared with those obtained in site-resolved imaging experiments with fermionic atoms in optical lattices. I will also discuss results with and without a Zeeman field at a wide range of temperatures, including temperatures below currently reachable in experiments. Some of the open questions I will discuss are: (1) Are there signatures of fractionalization of the fermionic spectral function? (2) How close are we to observing d-wave superconductivity in the simulations and experiments? (3) What is the sign problem and in which regions of parameter space is it most problematic?


* (a) NSF Division of Materials Research grant 1309461; (b) partial support by a grant from the Simons Foundation (343227)

11:51AM B19.00002: Metal to insulator crossover and non-Fermi-liquid physics in the half-filled 2d Hubbard model AARAM JOO KIM, Department of Physics, King's College London, FEDOR SIMKOVIC, Collège de France, EVGENY KOZIK (Presenter), Department of Physics, King's College London — We present a controlled study of the finite-temperature crossover from the metallic to insulating regime in the half-filled 2D Hubbard model using Diagrammatic Monte Carlo techniques in the thermodynamic limit. Our results for one- and two-body properties confirm absence of the metal- to-insulator transition at any non-zero coupling and relate the insulating behavior to development of extended antiferromagnetic (AFM) correlations. The crossover is marked by the AFM correlation length extending beyond one lattice constant and involves an intermediate non-Fermi-liquid regime with a partially gapped Fermi surface. We observe the peculiar behavior of thermodynamic observables at the crossover indicative of the Slater-type insulator scenario.

12:03PM B19.00003: Pair Density Wave in the doped t-J model with ring exchange on triangular lattice XIAO YAN XU (Presenter), KAM TUEN LAW, Department of Physics, Hong Kong University of Science and Technology, PATRICK LEE, Department of Physics, Massachusetts Institute of Technology — In our former work (PRL 121 046401 (2018)), we found a quantum spin liquid with spinon Fermi surface in the two dimensional spin-1/2 Heisenberg model with four-spin ring exchange on triangular lattice. In this work we dope the spinon Fermi surface phase by studying the t-J model with four-spin ring exchange. We perform density matrix renormalization group calculations on four-leg cylinders of triangular lattice and find clear signatures of pair density wave. The pair correlation function is oscillatory, even though it decays rapidly with distance with a power law larger than 2. The doping dependence of the decay and the period are studied. This is the first example where the pairing density wave is the dominate pairing in a system without a spin gap.

12:15PM B19.00004: An Auxiliary Field Quantum Monte Carlo study of the Hubbard Kanamori model* HONGXIA HAO (Presenter), BRENDA RUBENSTEIN, Brown University, HAO SHI, Simons Foundation — In the eld of strongly-correlated many-electron systems, the Hubbard Kanamori model has been extensively studied as a prototype for transition-metal oxides, to accurately describe interesting problems like magnetic properties, phase transitions, and unconventional superconductivity. The model is multiorbital in nature and contains Hunds coupling terms. However, due to the sign problem, it is mainly studied in the framework of Dynamical Mean-Field Theory (DMFT). We study the model using the ground state Auxiliary Field Quantum Monte Carlo (AFQMC) method. Different decomposition strategies for the Hunds coupling and pair-exchange terms are proposed for Hubbard-Stratonovich transformation. The Constrained Path Approximation and Phaseless Approximation are used to control the sign and phase problem. Systematic tests are carried out and shown the high accuracy of this approach. The ground state properties of real material Ca2RuO4 will be discussed.

*Supported by Center for Computation and Visualization (CCV) at Brown University and Extreme Science and Engineering Discovery Environment (XSEDE). The Flatiron Institute is supported by the Simons Foundation.
12:27PM B19.00005: Study of competing phases in the half filled Hubbard-Holstein model by "sign-free" determinantal Langevin simulations
SEHER KARAKUZU (Presenter), SANDRO SORELLA, International School for Advanced Studies — Understanding the properties of strongly correlated models is a challenging problem since many analytical tools cannot be applied due to the complicated nature of the problems. Here, we apply numerical methods in order to investigate the ground state thermodynamic limit properties of the so-called Hubbard-Holstein model in two spatial dimensions. We show that it is possible to perform "sign-problem-free" path integration for the model at half-filling by an appropriate choice of Hubbard-Stratonovich transformation and exact integration of phononic degrees of freedom. We apply an efficient first-order accelerated Langevin dynamics algorithm to evaluate all relevant correlation functions of the model. Preliminary calculations at $U/t=4$ and $U/t=1$, $\omega_0/t=1$, indicate a strong competition of antiferromagnetic and charge-density-wave orders. We observe signatures of a quite extended region around $U\approx g^2/\omega_0$ without either antiferromagnetic or charge-density-wave orders, separating into two quantum critical points at zero temperature. Furthermore, the phase diagram of the model will be presented for moderate phonon frequencies $\omega_0$. The possible extension of the current technique to finite temperature is under study.

12:39PM B19.00006: Hubbard model analysis with dynamical mean-field theory and selective configuration interaction
CARLOS MEJUTO ZAERA (Presenter), NORM TUBMAN, BIRGITTA K WHALEY, University of California, Berkeley — The two-dimensional square lattice Hubbard model has been one of the most investigated Hamiltonian systems in condensed matter physics during the last few decades. Despite extensive efforts and numerous theoretical studies, there is still debate about its zero temperature phase diagram. Here, we present numerical results obtained using adaptive selected configuration interaction (ASCI) techniques for both finite size clusters and the thermodynamic limit, with the latter obtained by combining ASCI with dynamical mean-field theory (DMFT). We study basic spectral properties together with two-point correlation functions of spin and charge, for a variety of particle fillings and interaction strengths. Away from half-filling and for a wide range of interaction strengths, the finite size cluster results indicate that the ground state wave function presents a shell structure similar to that of atomic or molecular systems. In the bulk ASCI-DMFT calculations we study the effect of the bath discretization on the spectral properties.

*We thank the Fundacion Bancaria La Caixa for financial support.

12:51PM B19.00007: Crossovers caused by the Mott transition away from long-range ordered phases
CHARLES-DAVID HÉBERT (Presenter), Institut quantique, RQMP, Université de Sherbrooke, MAXIME CHARLEBOIS, Institut quantique, RQMP, Université de Sherbrooke — The dynamical mean-field description of the Mott transition explains high-temperature crossovers caused by local correlations. However, these crossovers can be wiped out by long-range order. Frustrated lattices are generally necessary to prevent long-range magnetic order. Yet many calculations are done on unfrustrated clusters. Using cluster extensions of dynamical mean-field theory for system sizes up to $4x4$, we compare the results obtained on the square and on the triangular lattices to identify possible modifications of the crossovers that could arise from antiferromagnetic correlations. In particular, we verify whether on the triangular lattice, the first order Mott transition extends above the antiferromagnetic order, as seen in some materials.

*Canada First Excellence Research Fund, NSERC Grant RGPIN-2014-04584, Research Chair in the Theory of Quantum Materials, Compute Canada, Calcul Québec, CIFAR

1:03PM B19.00008: Recent advances in Diagrammatic Monte Carlo
RICCARDO ROSSI (Presenter), Simons Foundation — In this talk, I will present some of the recent advances obtained in the automatic high-order computations of Feynman diagrams for fermionic systems. I will discuss in particular the Connected Determinant Monte Carlo algorithm (CDet) [1, 2] and its extensions, and I will present results for the Fermi-Hubbard model as the paradigmatic strongly-correlated fermionic system.

1:15PM B19.00009: Functional renormalization group study of the three-dimensional Hubbard model*  JANNIS EHR LICH (Presenter), Peter-Gruenberg-Institut, Forschungszentrum Juelich, CARSTEN HONERKAMP, Inst. for Theoretical Solid State Physics, RWTH Aachen University — We present the extension of the truncated unity functional renormalization group (TUfRG) approach to three-dimensional lattice models for interacting fermions. This provides a flexible method for detecting ordering tendencies which treats all fluctuation channels on equal footing.

As a first example, we study the Hubbard model on the simple cubic lattice. We determine the leading ordering tendencies for low temperatures and the corresponding energy scales for ordering. At half filling and for repulsive interaction, the transition scale to an antiferromagnetic (AFM) ground state shows good agreement with other numerical methods. In addition, we investigate the competition between AFM and d-wave superconducting ordering away from half filling.

*We acknowledge financial support by DFG RTG 1995

1:27PM B19.00010: Multiloop functional renormalization group for the two-dimensional Hubbard model: Loop convergence of the response functions  AGNESE TAGLIAVINI, CORNELIA HILLE, University of Tübingen, FABIAN B. KUGLER, LMU, SABINE ANDERGASSEN (Presenter), University of Tübingen, ALESSANDRO TOSCHI, TU Vienna, CARSTEN HONERKAMP, RWTH Aachen University — We present a functional renormalization group (fRG) study of the two dimensional Hubbard model, performed with an algorithmic implementation which lifts some of the common approximations made in fRG calculations. In particular, in our fRG flow; (i) we take explicitly into account the momentum and the frequency dependence of the vertex functions; (ii) we include the feedback effect of the self-energy; (iii) we implement the recently introduced multiloop extension which allows us to sum up all the diagrams of the parquet approximation with their exact weight. Due to its iterative structure based on successive one-loop computations, the loop convergence of the fRG results can be obtained with an affordable numerical effort. In particular, focusing on the analysis of the physical response functions, we show that the results become independent from the chosen cutoff scheme and from the way the fRG susceptibilities are computed, i.e., either through flowing couplings to external fields, or through a “post-processing” contraction of the interaction vertex at the end of the flow. The presented substantial refinement of fRG-based computation schemes paves a promising route towards future quantitative fRG analyses of more challenging systems and/or parameter regimes.

1:39PM B19.00011: Ground-State Superfluid Phase Diagram of the Two-Dimensional Fermionic Hubbard Model with Next-Nearest-Neighbour Hopping*  FEDOR SIMKOVIC (Presenter), Department of Physics, King's College London, YOUJIN DENG, Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, EVGENY KOZIK, Department of Physics, King's College London — In this work, we employ the Bold Diagrammatic Monte Carlo method to establish the superfluid phase diagram in terms of density and interaction strength and for several values of next-nearest-neighbour hopping. We find that although a multitude of superfluid states persists up to moderate interactions the picture changes severely compared to the weak-coupling interaction limit. We investigate into how relative proximity to the Van Hove filling affects superfluid order parameters and find that this effect diminishes with increasing interaction strength.

*Simons Collaboration on the Many-Electron Problem

1:51PM B19.00012: Superconducting paring induced by the Mott stripe in t-J ladders*  CHEN CHENG (Presenter), RUBEM MONDAINI, Beijing Computational Science Research Center, MARCOS RIGOL, Department of Physics, The Pennsylvania State University — Stripe formation is ubiquitous in the doped cuprates family and in corresponding numerical studies on 2D lattices. However, the complex competition of different orders makes it difficult to understand how they precisely affect the superconducting pairing in high-temperature superconductors. Alternatively, we study a simplified ladder system with doped outer-legs and a Mott stripe core, produced by the interplay of strong repulsion and the large negative on-site potential in the inner legs. By using the density matrix renormalization group method in 4-leg ladders, we show that, for anisotropic exchange couplings, a novel singlet-pair superconducting phase occurs with the fermions in the pairs residing on different sides of the Mott insulating stripe. In this phase, the binding energy is negative and the interleg singlet-pair correlation function decays algebraically with distance, in contrast to other correlations that are exponentially decaying. We expect our findings to shed light on the pairing mechanisms for the high-temperature superconductivity, and potentially highlight novel types of pairing mechanisms in AMO experiments. Part of this work is published as Phys. Rev. B 98, 121112(R) (2018).

*We acknowledge NSAF-U1530401, NSFC-11674021, and 11650110441, and NSF-PHY-1707482.
Superconductivity in the Hubbard model: a hidden-order diagnostics from the Luther-Emery phase on ladders  

LUCA FAUSTO TOCCHIO (Presenter), Institute for Condensed Matter Physics and Complex Systems, Politecnico di Torino, Italy, FEDERICO BECCA, Democritos National Simulation Center, Istituto Officina dei Materiali del CNR and International School for Advanced Studies (SISSA), Trieste, Italy, ARIANNA MONTORSI, Institute for Condensed Matter Physics and Complex Systems, Politecnico di Torino, Italy — Short-range antiferromagnetic correlations are known to open a spin gap in the repulsive Hubbard model on ladders with $M$ legs, when $M$ is even. We show that the spin gap originates from the formation of correlated pairs of electrons with opposite spin, captured by the hidden ordering of a spin-parity operator. Since both spin gap and parity vanish in the two-dimensional limit, we introduce the fractional generalization of spin parity and prove that it remains finite in the thermodynamic limit. Our results are based upon variational wave functions and Monte Carlo calculations: Performing a finite size-scaling analysis with growing $M$, we show that the doping region where the parity is finite coincides with the range in which superconductivity is observed in two spatial dimensions. Our observations support the idea that superconductivity emerges out of spin gapped phases on ladders, driven by a spin-pairing mechanism, in which the ordering is conveniently captured by the finiteness of the fractional spin-parity operator.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B20 DCOMP DMP: First-principles Modeling of Excited-state Phenomena in Materials II: Many-body Perturbation Theory (Techniques and Applications)

Correlated multi-particle excitations: Green's function formalism for trions and biexcitons*  

FELIPE DA JORNADA (Presenter), ANDREA CEPELLOTTI, STEVEN G. LOUIE, UC Berkeley and Lawrence Berkeley National Lab — With the experimental isolation of atomically thin one- and two-dimensional materials, it is now possible to measure a variety of charged and neutral multiparticle excitations (trions, biexcitons, etc.) in these systems, many of which display large binding energies. On the theory side, however, while quasiparticle and neutral optical excitations have been successfully treated in many materials with the first-principles GW and GW plus Bethe-Salpeter equation (GW-BSE) approaches, respectively, similar many-body and parameter-free approaches are not available to compute and understand correlated multi-particle excitations. Accordingly, past theoretical studies were often limited to treatments based on model Hamiltonians. In this talk, we present results from a new ab initio approach based on the interacting 3- and 4-particle Green's function formalism to compute multiparticle excitations [1]. Our new diagrammatic approach that makes use of appropriate screened Coulomb interactions, combined with a high-performance computing implementation, allows us to predict without adjustable parameters that trions and biexcitons in carbon nanotubes are stable at room temperature, and also to reveal in details electronic correlation in these multiparticle excitations. We will also comment on how this formalism can be employed to investigate other high-order excited-state phenomena in the bulk and at the nanoscale.


*This work was supported by the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) at LBNL, funded by the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources provided by NERSC and XSEDE.
FULVIO PALEARI (Presenter), University of Luxembourg, HENRIQUE MIRANDA, Université Catholique de Louvain, ALEJANDRO MOLINA-SANCHEZ, University of Valencia, LUDGER WIRTZ, University of Luxembourg — We present an ab initio method to calculate phonon-assisted absorption and emission spectra when strong excitonic effects are present. We apply the method to bulk hexagonal BN, a material with indirect band gap which exhibits strong luminescence in the UV range. We first calculate the excitons at the wave vector $q_i$ of the indirect gap with the Bethe-Salpeter equation. The coupling of these excitons with the various phonon modes at $q_i$ is investigated with group theory and then expressed in terms of a product of the mean square displacement of the atoms and the second derivative of the optical response function with respect to atomic displacement along the phonon eigenvectors. The derivatives are calculated numerically with a finite difference scheme in a supercell commensurate with $q_i$. We use detailed balance arguments to obtain the intensity ratio between emission and absorption processes. Our results[1] explain recent luminescence experiments[2] and reveal the exciton-phonon coupling channels responsible for the emission lines.


Juan de la Cierva program (MINECO, Spain): Grant IJCI-2015-25799.
F.R.S.-FNRS: PDR Grants HTBaSE T.1071.15.

XIAO ZHANG (Presenter), ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — The Bethe-Salpeter equation (BSE) is a theoretical spectroscopy technique that accurately describes optical absorption by considering the screened electron-hole Coulomb interaction. In practice, the frequency dependence of screening is oftentimes neglected to reduce computational cost. This static approximation is often valid due to small exciton-binding energies in bulk inorganic semiconductors, compared to plasmon frequencies. However, for materials with large exciton-binding energies, such as finite and low-dimensional systems, dynamical screening can become important. To explore this, we incorporated dynamical electronic screening into the BSE approach and quantify its impact from first-principles calculations. We study the optical absorption of linear oligoacene crystals and show that the exciton binding energy is on the order of 1 eV. Furthermore, we compute corrections due to dynamic screening, and show that these can be of comparable size, i.e. an order of magnitude larger than in inorganic semiconductors. We also show that including this effect significantly improves agreement of exciton binding energies with experimental results.

*This work is supported by the NSF (DMR-1555153) and Blue Waters (OCI-0725070, ACI-1238993, and the state of IL).

TIANLUN HUANG (Presenter), SAHAR SHARIFZADEH, Boston University — Perylene-3,4,9,10-tetracarboxylic diimide (PTCDI) are promising optoelectronic materials; they possess strong optical absorption and emission properties, along with a propensity for self-assembly and excellent stability. We utilize density functional theory and many-body perturbation theory within the GW/BSE approximation to investigate the optoelectronic properties of a periodic assembly of PTCDI DNA base surrogates. We predict a bandstructure with significant bandwidth (~0.8 eV) and several spatially delocalized low-energy optically excited-states. By incorporating electron-phonon interactions, we determine that at finite temperature, the bandwidth is reduced and exciton binding increased, leading to localization of excited-states.

*We are grateful for funding from NSF (DMR-1610031).

SIVAN REFAELY-ABRAMSON (Presenter), Materials and Interfaces, Weizmann Institute of Science, Israel, JONAH HABER, FELIPE DA JORNADA, STEVEN G. LOUIE, JEFFREY B NEATON, Physics, University of California, Berkeley — We study structural effects on single- and multi-exciton processes in organic molecular crystals. We use many-body perturbation theory within the GW approximation and the Bethe-Salpeter equation approach to calculate and compare the quasiparticle and excitonic band structures of different polymorphs of solid pentacene, and explore their implications for excited-state processes. We find that structural differences between known phases can lead to large effects on exciton-exciton interactions; and in particular, we predict very different singlet fission rates, revealing a strong sensitivity between singlet fission efficiency and crystal phase. We explore the effect of phonons on this picture, and discuss the implications of our findings on design principles and pathways to optimize photogeneration processes in organic crystals. This work supported by the Department of Energy; computational resources provided by NERSC.
12:39PM B20.00006: Computational discovery of new materials for intermolecular singlet fission in the solid state*  
[invited] NOA MAROM (Presenter), Carnegie Mellon University — Intermolecular singlet fission (SF) is the conversion of one photogenerated singlet exciton into two triplet excitons localized on different molecules. SF has the potential to significantly enhance the conversion efficiency of organic solar cells by harvesting two charge carriers from one photon. However, few materials are presently known to exhibit intermolecular SF in the solid state. Using many-body perturbation theory in the GW approximation and Bethe-Salpeter equation (BSE), we have elucidated the effect of crystal packing on the excitonic properties of molecular crystals. To assess the likelihood of new materials to exhibit SF, we have proposed a two-dimensional descriptor based on the thermodynamic driving force for SF and the degree of singlet exciton charge transfer character. To evaluate the latter we have developed the double-Bader analysis method for exciton wave-functions from BSE calculations. We have identified several promising candidates for intermolecular SF in the solid state including monoclinic rubrene, quaterrylene, and phenylated pentacene derivatives.

*Funded by the Charles E. Kaufman Foundation and AFOR grant FA9550-18-1-0248

1:15PM B20.00007: Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission  
XIAOPENG WANG (Presenter), XINGYU ALFRED LIU, RITHWIK TOM, Carnegie Mellon University, CAMERON COOK, BOHDAN SCHATSCHNEIDER, Cal Poly Pomona, NOA MAROM, Carnegie Mellon University — Singlet fission (SF), the conversion of one singlet exciton into two triplet excitons, may improve the efficiency of organic photovoltaics. Only a few materials have been experimentally observed to undergo intermolecular SF, most of which are acenes and their derivatives. Using many-body perturbation theory in the GW approximation and the Bethe-Salpeter equation (BSE), we systematically investigate the electronic and excitonic properties of tetracene, pentacene, and their phenylated derivatives in the gas phase and solid state. Their potential for SF is evaluated with respect to the thermodynamic driving force and the singlet exciton charge transfer character. In both gas phase and solid state, pentacene and its derivatives are more promising than tetracene and its derivatives. Within a group of phenylated derivatives with the same acene backbone, increasing the number of phenyl side groups is detrimental for SF in the gas phase. However, solid state properties are additionally affected by intermolecular interactions. We find that a higher number of phenyl side groups results in crystal structures with weak π-stacking and slip stacking, which exhibit higher SF driving force in the solid state.

1:27PM B20.00008: The Spin-Flip BSE approach and applications to simple molecular systems*  
BRADFORD BARKER (Presenter), DAVID STRUBBE, Physics, University of California, Merced — The spin-flip (SF) method allows for description of multi-reference states by considering excitations of a single high-spin reference state, and it has been successfully used in time-dependent density-functional theory (SF-TDDFT) and configuration interaction (SF-CI) approaches to describe molecules with unpaired spins. While SF-TDDFT is significantly less computationally expensive than SF-CI, it has difficulty describing double excitations, Rydberg states, and bond-breaking with conventional functionals. Just as the GW/Bethe-Salpeter (BSE) approach, with its ab initio long-ranged and non-local interaction kernel, allows for a systematic improvement of calculated optical absorption spectra over TDDFT, we consider a spin-flip BSE (SF-BSE) approach to improve SF-TDDFT. This method has a more moderate expense than SF-CI and can be used also for extended systems. We present the theory of SF-BSE and apply it to simple molecular examples of bond-breaking and unpaired spins.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, CTC and CPIMS Programs, under Award DE-SC0019053.

1:39PM B20.00009: Conjugation length dependence on the electronic and optical properties of oligothiophene-F4TCNQ complexes*  
ANA VALENCIA (Presenter), CATERINA COCCHI, Department of Physics, Humboldt-Universitaet zu Berlin, Germany — To understand how the donor conjugation length affects the doping mechanisms in organic semiconductors [1], we investigate a series of charge transfer (CT) complexes formed by oligothiophene molecules of increasing length doped by the acceptor F4TCNQ. Using hybrid DFT as a starting point, we assess the electronic and optical properties of these systems from many-body perturbation theory (GW and the Bethe-Salpeter equation). We find that the frontier orbitals (HOMO and LUMO) have CT character in all complexes, while deeper occupied and higher virtual states depend on the nT length. The first bright excitation is dominated by the HOMO-LUMO transition occurring approximately at the same energy in all systems. At increasing donor length, higher-energy peaks exhibit different character depending on the donor conjugation length. The rationale offered by our results contributes to clarify the excitation processes in organic donor/acceptor complexes.


*Work founded by the German Research Foundation, grant HE 5866/2-1.
1:51PM B20.00010: First-principles prediction of free-electron screening of the electron-hole interaction in hybrid perovskite MAPbI3* JOSHUA LEVEILLEE (Presenter), ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Hybrid organic-inorganic perovskite MAPbI3 has captivated the solar cell community as a high-efficiency photovoltaic material. Recent reports find high intrinsic charged defect concentrations in MAPbI3 which donate free electrons to the material. Due to these, the Coulomb potential between electrons and holes is further screened and the exciton binding energy decreases. We use first-principles methods based on many-body perturbation theory to determine the influence of free-electron screening on the predicted excitonic properties and the optical spectrum of MAPbI3. Electronic band structures and gaps are predicted using Hedin's GW approximation, including the spin-orbit interaction. Electron-hole excitation energies and optical spectra are calculated using the Bethe-Salpeter framework. Our calculations show that exciton binding energies span the experimentally observed range of 31 to 2.5 meV as the free-electron concentration varies between $10^{12}$ and $10^{19}$ cm$^{-3}$. The corresponding optical spectra are found in good agreement with experimental results, suggesting that free-carrier screening plays an important role in the optical response of MAPbI3.

*Support by the National Science Foundation, Grant Nos. CBET-1437230 and DMR-1555153

2:03PM B20.00011: First-principles Studies of Tl Activated Halide Scintillator Phosphor Materials: Towards an Understanding of the Scintillation Mechanism* ANDREW CANNING (Presenter), MAURO DEL BEN, EDITH BOURRET, Lawrence Berkeley National Laboratory — Tl doped halide scintillator phosphors are amongst the most commonly used gamma ray detector materials for medical imaging, high energy physics and nuclear materials detection applications (e.g. CsI:Tl, NaI:Tl). Even so the complete scintillation process in these materials is still poorly understood. In particular in recent years there has been great interest in co-doping these materials to try and improve their detection performance. We have performed first-principles studies based on GGA, hybrid functionals and the GW/BSE method in tandem with experiments to understand the scintillation mechanism in these materials and how it could be improved by co-doping. In particular we have looked at the Tl exciton optical emission states and energy transfer mechanisms from the gamma ray to the Tl. Recently there has also been interest in new Tl bulk scintillators such as TLYC (Tl$_2$LiYCl$_6$) which we have also studied.

*This work is supported by the Department of Energy, National Nuclear Security Administration, Office of Defense Nuclear Nonproliferation Research and Development and carried out at Lawrence Berkeley National Laboratory under contract #AC02-05CH11231. This work does not constitute an express or implied endorsement on the part of the government

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B21 DCOMP DBIO DMP GSOFT: Exploring Free Energy Landscapes in Biology and Materials Science I BCEC 157B - Pratyush Tiwary, University of Maryland, College Park - Tag(s): Focus

11:15AM B21.00001: Incorporating experimental data into long timescale simulations of macromolecules* [Invited] CECILIA CLEMENTI (Presenter), Department of Chemistry, Rice University — Recent breakthroughs in experimental technologies and in high-performance computing have enabled unprecedented measurements and simulations of complex biophysical systems such as macromolecules. However, experiments provide only a partial view of macromolecular processes and are limited in their temporal and spatial resolution. On the other hand, atomistic simulations are still not able to sample the conformation space of large complexes, thus leaving significant gaps in our ability to study molecular processes at a biophysically relevant scale. We present our efforts to bridge these gaps, by using experimental data as a starting point in a computational modeling approach. We use models at different resolutions and “anchor” them to experimental measurements, to provide quantitatively accurate representations of systems of interest, and address open biophysical questions.

*National Science Foundation CHE-1265929, CHE-1738990, and PHY-1427654
Welch Foundation C-1570
Helix Mediated Aggregation in Poly-Glutamine Tracts

In protein aggregation related neurodegenerative diseases, a disease specific host protein misfolds and adopts a metastable, aggregation prone conformation. For Huntington's disease, the htt exon I domain is the smallest physiological N-terminal fragment that forms disease related poly-glutamine rich fibrils. Exon I consists of a glutamine tract, flanked by a 17 amino acid long fragment (httNT) and a proline rich fragment. The presence of httNT fragment has been shown to significantly accelerate the formation of poly-glutamine rich fibrils. In this study, we test the helix mediated aggregation mechanism of glutamine tracts as proposed by the Wetzel group by using molecular dynamics simulations. Analysis of httNT fragment in bulk water suggests only a weak helix propensity. However, when several fragments come into contact they adopt the alpha-helix conformation and form bundles. When the httNT fragment is flanked to the poly-glutamine tract, these bundles lead to a dramatic increase in glutamine concentration. By using a coarse grained model, we study the beta-sheet formation and show that, in agreement with the Wetzel group's hypothesis, beta-sheet propensity significantly increases in these bundles compared to the isolated poly-glutamine tracts.

*TUBITAK (project no 116z512)
12:51PM B21.00007: Nonlinear and Hierarchical Discovery of Slow Molecular Modes using Sequential Learning with Natural Constraints  WEI CHEN (Presenter), Physics, University of Illinois at Urbana-Champaign, HYTHEM SIDKY, ANDREW L FERGUSON, Institute for Molecular Engineering, University of Chicago — Discovering the slow modes governing molecular dynamics can unveil new mechanistic understanding and provide collective variables along which to direct enhanced sampling. Time-lagged independent component analysis (tICA) is a well-developed method that discovers linear combination of molecular features as slow modes. The linearity of tICA, however, hampers its capacity to discover nonlinear modes. Nonlinear feature engineering can prove profitable but is typically reliant on human intuition or expensive preprocessing. Kernel tICA integrates tICA and kernel trick to effect nonlinear discovery, but is computationally expensive and selection and tuning of the kernel limits its generalizability. Time-lagged autoencoders and variational dynamics encoders are neural networks that can identify the slowest mode but are unable to resolve higher-order modes. In this work, we introduce a sequential learning method that we term hierarchical dynamics encoder (HDE) as a novel neural network that sequentially learns hierarchical nonlinear slow CVs. Each CV is orthogonal to all previously learned CVs, and orthogonality is imposed naturally without regularization. We demonstrate HDEs for several toy systems where the true slow modes are known, and in simulations of peptides and proteins.

1:03PM B21.00008: Learning reaction coordinate on-the-fly for sampling complex biomolecular systems with SGOOP and metadynamics  DEBABRATA PRAMANIK (Presenter), Chemistry and Biochemistry and Institute for Physical Science and Technology, University of Maryland, College Park, USA, ADAM KELLS, Department of Chemistry, King's College London, United Kingdom, ZACHARY SMITH, Biophysics Program and Institute for Physical Science and Technology, University of Maryland, College Park, USA, PRATYUSH TIWARY, Chemistry and Biochemistry and Institute for Physical Science and Technology, University of Maryland, College Park, USA — Understanding functioning and stabilizing/destabilizing forces of biomolecules such as protein-ligand and protein-DNA are highly desirable due to implication in basic biology as well as diseases. Experiments can be useful in measuring various thermodynamic quantities, but they cannot, at least directly, provide microscopic details and kinetics, pathways etc. Here, we complement experiments with all-atom molecular dynamics (MD) simulations. Unfortunately MD is limited by a huge time scale problem. We attempt to solve it through developing sampling methods based on statistical mechanics and demonstrate progress on model systems and in ambitious systems such as protein-ligand interactions and transcription factor-DNA interactions. One of the specific issues we will address is the need to know beforehand an accurate reaction coordinate (RC), which is a challenge for any biased simulation. Recently, we have shown how to construct a 1-dimensional RC by a method called “spectral gap optimization of order parameters (SGOOP)”. Here we will show how to extend its scope by introducing a simple but powerful extension based on the notion of conditional probability factorization for systems with inherent complexity and where a 1-d RC is not enough to accurately capture the energy landscape.

1:15PM B21.00009: Understanding Binding Dynamics in Host-Guest Systems with Advanced Sampling Simulations  ANNE LEONHARD (Presenter), JONATHAN WHITMER, University of Notre Dame — Host-guest complexes are useful for applications in biomaterials science and engineering, including drug delivery, separations, transport regulation, and novel hydrogels. Highly-specific binding interactions are a key feature of such systems, and as such knowledge of systems' binding affinity, free energy landscapes, and binding pathways is critical. Here, we propose that advanced sampling techniques, such as the Adaptive Biasing Force and Artificial Neural Network methods, are promising ways to explore free energy landscapes of host-guest systems due to their ability to quickly sample the full phase space. We apply these methods to calculation of binding affinities between an array of small molecules and curcurbit[n]uril hosts. These binding affinities calculated with advanced sampling methods are compared to previously-published experimentally- and computationally-obtained values and obtain exceptional agreement with each. We also discuss how such methods might be generalized to more complex systems of interest in the biomolecular and materials simulations communities.
Ζ-Glycine: Insight into the Mechanism of a Polymorphic Phase Transition

CRAIG L. BULL, GILES FLOWITT-HILL, ISIS Neutron and Muon Source, STEFANO DE GIRONCOLI (Presenter), EMINE KUCUKBENLI, International School for Advanced Studies, SIMON PARSONS, The University of Edinburgh, CONG-HUY PHAM, International School for Advanced Studies, HELEN PLAYFORD, ISIS Neutron and Muon Source, MATTHEW G. TUCKER, Oak Ridge National Laboratory — Glycine is the simplest amino acid and a great test-bed for studying polymorphism in molecular crystals. With five phases having been structurally characterized at atmospheric or high pressure, it is a well-studied system both experimentally and theoretically. Yet a sixth form, the ζ phase, was discovered over a decade ago as a short-lived intermediate upon decompression of a high-pressure phase. However, its structure has remained unsolved despite several theoretical investigations to glycine polymorphism. We have recently reported [1] the structure of the elusive ζ phase, which was resolved thanks to the collaboration between crystal structure prediction procedure based on fully ab initio total energy calculations combined with a genetic algorithm, and neutron powder diffraction data obtained on a sample trapped at 100 K. Here we will discuss the approach that led to the successful theoretical prediction of this phase, the lessons that can be learnt and applied to similar systems, and mention remaining challenges for a predictive ab initio crystal structure prediction process.


A Climbing Multi-String Method to Map Free-Energy Saddles and Minima*

GOURAV SHRIVASTAV (Presenter), CAMERON ABRAMS, Department of Chemical and Biological Engineering, Drexel University — Finding stationary points, minima or saddles, on hyperdimensional free energy surface is crucial to gain insights about the possible transition events and to compute the associated transition rates. Though minima can be easily found, the tasks of locating saddles and measuring their energies relative to their associated minima remain challenging, especially in high-dimensional spaces. We propose here a modified climbing string method to locate multiple saddles by initiating multiple strings in one go. For a given minimum, strings propagate by gradient flow in the path space, with one end fixed and other end climbing across the free energy profile to locate a saddle. The convergence of multiple strings to a common saddle is avoided by checking repulsive forces between the climbing ends. The presence of multiple images along the string helps to ensure the direct connectivity between the minimum and saddles and to compute the free energy along the path. Hence, the climbing multi-string method can be used to map the network of directly connected stationary points in the free energy hypersurface. We demonstrate this method to locate saddle points in two-dimensional and four-dimensional free energy surface of alanine dipeptide and alanine tripeptide, respectively.

*NIH GM 100472.

Conformational free energy surface of cyclooctane from metadynamics in the collective variable space of autoencoder neural network*

BUMJOON SEO (Presenter), SEULWOO KIM, MINHWAN LEE, YOUNWOO LEE, WON BO LEE, Seoul National University — For rare event problems in which the important free energy basins are separated by large barriers, enhanced sampling methods provide the means to perform simulations within tractable timescales. Metadynamics simulation, which is one of the widely used enhanced sampling methods, requires the definition of a set of collective variables for accumulating the bias potentials. An important aspect of the collective variables is their dimensionality because the efficiency of the method decreases exponentially with the dimensionality. We present here a methodology of incorporating the codes from an autoencoder neural network as the collective variables for metadynamics simulations. This dimensionality reduction of an eight-dimensional space of dihedral angles into a three-dimensional space of features enables the computation of the conformational free energy surface of cyclooctane.

*This research was supported by Creative Materials Discovery Program through the National Research Foundation of Korea (NRF) funded by Ministry of Science and ICT (2018M3D1A1058624).
Disordered peptide chains in a coarse-grained model*  

MAREK CIEPLAK (Presenter), LUKASZ MIODUSZEWSKI, Institute of Physics, Polish Academy of Sciences — We construct a one-bead-per-residue coarse-grained dynamical model to describe intrinsically disordered proteins at significantly longer timescales than in the all-atom models. It yields structural results that are consistent with many all-atom and experimental data on these systems. We demonstrate that the geometrical properties of various homopeptides differ substantially in this model. The (breakable) contacts between the beads are determined during the course of the time evolution.\n

*Funded by the EU Joint Programme in Neurodegenerative Diseas project (JPND CD FP-668-059) through the NCN grant 2014/15/Z/NZ1/0037 (Poland)

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B22 DCOMP DMP DCP DBIO: Building the Bridge to Exascale: Applications and Opportunities for Materials, Chemistry, and Biology II

11:15AM B22.00001: Towards catalysis modeling with QMC*  
VIRAAJ JAYARAM (Presenter), University of Chicago, RYAN PEDERSON, LIANG LI, ANOUAR BENALI, YE LUO, MARIA CHAN, Argonne National Lab — Predictive modeling of catalytic processes on surfaces is challenging because of large uncertainties in computed energetics using density functional theory (DFT), and exponential dependence of catalyst performance on energies. In particular, the use of various DFT functionals and approximations results in qualitatively different results. The problem is compounded when treating transition metal oxides where a host of DFT errors persist. In this work, made possible by leadership scale high performance computers, we use quantum Monte Carlo (QMC) to determine the adsorption energies of the CO molecule on CuO (110) surface for various geometries determined by different DFT approximations. The relationships between geometry and energies, and between DFT and QMC results, will be discussed.

*An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.

11:27AM B22.00002: Accelerating quantum Monte Carlo simulations on many-core processors via OpenMP nested threading*  
YE LUO (Presenter), Argonne National Laboratory —

The massively parallel nature of quantum Monte Carlo is ideally suited to petascale computers which have enabled a wide range of applications to relatively large molecular and extended systems. The current scheme to achieve the shortest time-to-solution is placing one walker per core on multi/many-core processors. However, this strategy meets a great challenge from upcoming Exascale computers where much larger problem will be solved. The time to advance a walker and the memory need of it scale cubically and quadratically as a function of the electron counts in the system. On current computers, large problems already force us to leave cores idle for fitting them in memory. In addition, adding more walkers reduces the production steps for a given amount of samples but do not reduce the equilibration steps, which causes even more waste. In order to reduce the time-to-solution and reduce the memory footprint, we introduce nested threading to distribute the computation of each walker over several cores. We explore threading algorithms with minimal overhead and demonstrate a good scaling.

*This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.
11:39AM B22.00003: Structure and magnetism in bulk and uniaxially strained LaCoO$_{3-x}$ through ab-initio diffusion quantum Monte Carlo*  
KAYAHAN SARITAS (Presenter), JARON KROGEL, HO NYUNG LEE, FERNANDO REBOREDO, Materials Science and Technology Division, Oak Ridge National Laboratory — Advances in high-performance computing (HPC) is allowing the use of ambitious methods in materials science with unprecedented accuracy. Density Functional Theory (DFT) accuracy is not sufficient for challenging problems, as it depends critically on the empirical corrections applied, such as Hubbard-U and exchange mixing. For example, DFT has not yet been able to discern the microscopic origin of the ferromagnetic (FM) state in uniaxially strained LaCoO$_3$ thin films. In contrast, Diffusion quantum Monte Carlo (DMC) method treats electrons explicitly, solving the many-body Schrodinger equation with minimum approximations. DMC has been applied to an increasingly larger set of materials with excellent agreement. In this presentation, we report ground state energies, magnetism, defect formation energies in uniaxially strained LaCoO$_{3-x}$ using DMC. DMC yields an antiferromagnetic ground state for bulk uniaxially strained LaCoO$_3$ which agrees with the recent experiments. A transition between high-spin AFM and FM structures is also identified in the uniaxially strained structures, which may help explain the spin transition in thin films.

*The work was supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

11:51AM B22.00004: Accelerating Large-Scale GW Calculations on Many-Core and Hybrid CPU+GPU HPC Systems*  
MAURO DEL BEN (Presenter), Lawrence Berkeley National Laboratory, FELIPE DA JORNADA, University of California at Berkeley and Lawrence Berkeley National Laboratory, ANDREW CANNING, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory, JACK DESLIPPE, National Energy Research Scientific Computing Center (NERSC), Lawrence Berkeley National Laboratory — The novel electronic and optical properties found in complex materials represent the basis for the development of many emerging technologies. The rational design of such technologies requires an accurate quantum mechanical predictive capability (e.g., the GW approximation within many-body perturbation theory and beyond) that can run in reasonable timescales on available high performance computing (HPC) facilities. In this talk we summarize the advances in method development and code optimization of the BerkeleyGW software package targeted for many-core and hybrid CPU+GPU architectures. In particular showing how we have combined methods to reduce the prefactor of the calculations with an optimal implementation suitable for many-core architectures which allowed us to achieve excellent parallel scalability (>500k cores), high fraction of peak performance and thus excellent time to solution for systems up to thousands of atoms. We show how these developments can be combined to take advantages of GPU accelerators.

*Work supported by the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) at LBL, as part of the Computational Materials Sciences Program, funded by the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources provided by NERSC.

12:03PM B22.00005: Large scale GW and BSE calculations using interoperable software building blocks*  
MARCO GOVONI (Presenter), Materials Science Division and Institute for Molecular Engineering, Argonne National laboratory, HE MA, NGOC LINH NGUYEN, University of Chicago, FRANCOIS GYGI, Computer Science, University of California Davis, GIULIA GALLI, University of Chicago — The modeling of light-matter interaction in complex heterogenous systems is key to several materials design problems. A microscopic modeling of two-particle correlation functions requires the solution of the Bethe-Salpeter equation (BSE) based on many body perturbation theory. However, the application of BSE-GW calculations to complex nanostructured, disordered or defective materials has been hindered by high computational costs. We present a method, implemented into interoperable software building blocks, to compute optical spectra and exciton binding energies based on the solution of the Liouville equation and the calculation of the screened Coulomb interaction in finite field. The method does not require the explicit evaluation of dielectric matrices nor of virtual electronic states, and can be easily applied to large systems, beyond the random phase approximation. Localized orbitals obtained from Bloch states using bisection techniques are used to reduce the complexity of the calculation and enable the efficient use of hybrid functionals. We will discuss the advantages of this paradigm, and provide results for the calculation of spectroscopic features of promising materials for spin qubits.

*This work was supported by MICCoM, as part of the CMS Program funded by the U.S. DOE.
12:15PM B22.00006: Pushing the Accuracy Limits of Scalable Fixed-Node Diffusion Monte Carlo for Noncovalent Interactions* MATUS DUBECKY (Presenter), Physics, University of Ostrava — Single-determinant (SD) fixed-node diffusion Monte Carlo (FNDMC) gains popularity as a benchmark tool scalable to large noncovalent systems although its accuracy limits are not yet fully mapped out. Some of the recent results suggest that accuracy of SD FNDMC is capable of achieving benchmark accuracy for a rich class of noncovalent systems, larger than expected before. The talk will summarize recent progress and current accuracy limits of bias-cancellation-based SD FNDMC for molecules and noncovalent crystals. The best available “recipe” suitable for a wide class of noncovalent systems will be sketched out.

*Financial support by Czech Science Foundation (18-24321Y) and University of Ostrava (UO, IRP201826) is gratefully acknowledged.

12:27PM B22.00007: Deep Machine Learning for Atomically-Resolved Imaging Experiments: Physics Extraction and Feedback* [Invited] MAXIM ZIATDINOV (Presenter), Oak Ridge National Laboratory — Development of the imaging tools such as electron, optical, and scanning probe microscopy in the last decade of 20th century has opened floodgates of imaging data, in the form of images, movies, and hyperspectral data sets. These contain information on the minute details of atomic structure and electronic, magnetic, and phonon functionalities, chemical transformation mechanisms, and quantum phenomena. However, the bottleneck in analysis and knowledge extraction from large volumes of raw imaging data is often human domain expert. Here I will show how utilization of deep artificial neural networks (aka deep learning) offers a path to overcome limitations of human analysis. I will specifically discuss applications of deep learning for rapid fully automated identification of individual atomic types and positions from scanning transmission electron microscopy images, using theoretical or labeled experimental images as a training set. We used this approach to construct reaction pathways for point defects in 2D materials, trace the structural evolution of atomic species during the electron beam manipulation, and create the library of defect configurations in silicon- and vacancy doped graphene. I will discuss specific examples where we showed that coupling of sulphur vacancy to molybdenum dopants in tungsten disulfide and reactions of silicon impurity on the edge and in the bulk of graphene can be explored quantitatively and mapped on the Markov model, giving rise to the transition probabilities on single atomic defect level. The work on genetic engineering optimization framework for automatic design of deep learning network architecture and hyperparameters optimal specifically for electron microscopy datasets will be addressed. Finally, I will discuss how a synergy of deep learning image analytics and real-time feedback allows harnessing beam-induced atomic and bond dynamics to enable direct atom-by-atom fabrication.

*U.S. Department of Energy, Basic Energy Sciences

1:03PM B22.00008: Decoding Inverse Imaging Problems in Materials with Distributed Deep Learning* NOUAMANE LAANAIT (Presenter), ALBINA Y BORISEVICH, Oak Ridge National Laboratory, ALEXANDER SERGEEV, Uber Technologies, Inc., SEAN TREICHLER, NVIDIA Corporation, MICHAEL A. MATHESON, Oak Ridge National Laboratory — Materials physics abounds with challenging inverse problems, from inverse materials design to reconstruction of material properties from imaging/scattering data. One of the oldest inverse problems in materials is the reconstruction of the local atomic scattering potential from convergent beam electron diffraction (CBED). In this talk, we will present results on a potential reconstruction approach based on deep neural networks (DNN). In particular, we used data parallelism to distribute the training of a DNN over 12,000 GPUs on the Summit supercomputer. By efficient utilization of Summit’s burst buffer and half-precision arithmetics, the data processing rates of the DNN reached upwards of 100 GB/s, allowing for the processing of local CBED patterns from 60,000+ crystal structures in the matter of minutes. We will present challenges encountered in distributed training at these scales, such as I/O bottlenecks and DNN convergence and how they can be mitigated. Finally, initial results on our DNN-based reconstruction of local atomic potentials of strontium irridate superlattices will be presented.

*This work used resources of the Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy.
ExaTN - A Scalable Exascale Math Library for Hierarchical Tensor Network Representations and Simulations

ExaTN is a math library of parallel numerical primitives for processing operations based on hierarchical tensor representations. Our library provides a scalable infrastructure for building a performance portable framework for simulating strongly correlated quantum systems on heterogeneous HPC platforms such as Titan and Summit. Our framework is the first to deliver a massively parallel implementation of the multiscale entanglement renormalization ansatz (MERA), a promising hierarchical tensor decomposition scheme capable of expressing local expectation values in strongly entangled quantum systems efficiently. In this talk, we will present our integrated framework for processing hierarchical tensor representations on exascale HPC systems via a multi-level asynchronous task-based programming model. This provides scientists with a capability for simulating strongly entangled systems in condensed matter physics.

*Laboratory Directed Research and Development Program ORNL
2:03PM B22.00013: UV/vis absorption spectra database auto-generated for optical applications via the Argonne data science program*  EDWARD J. BEARD, Cavendish Laboratory, Department of Physics, University of Cambridge, GANESH SIVARAMAN (Presenter), ALVARO VAZQUEZ-MAYAGOITIA, VENKATRAM VISHWANATH, Argonne Leadership Computing Facility, Argonne National Laboratory, JACQUELINE M COLE, Cavendish Laboratory, Department of Physics, University of Cambridge — A large corpus of material and experimental data exists in historic scientific literature. Natural language processing and data-mining approaches can be applied to curated scientific literature to extract chemical information for targeted functionality and applications. This talk focuses on development of a UV/vis absorption spectra database by means of a complex quantum chemistry workflow built on the top of the ChemDataExtractor tool [1] by leveraging DOE Argonne leadership computing facilities as a part of the data science project allocation. We show results of retrieving chemical information and experimental properties from a large sample of scientific literature (~ 400,000) with chemdataextractor. Some electronic structure properties of a large subset of compounds are modeled using quantum chemistry workflows for benchmarking and validation. Finally, the quality of the database is discussed based on validation metrics and its applicability to optical applications.

*This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B23 GIMS: Advances in Scanned Probe Microscopy I: Novel Approaches and Ultrasensitive Detection BCEC 158 - Tag(s): Focus

11:15AM B23.00001: Nanoscale magnetometry using scanning single spin quantum sensors [Invited]  RICHARD MALETINSKY (Presenter), University of Basel — tbd

11:51AM B23.00002: Three-dimensional AFM imaging of hydration and flexible surface structures at solid-liquid interfaces* [Invited]  TAKESHI FUKUMA (Presenter), Kanazawa University — At a solid-liquid interface, water interacts with a surface to present a non-uniform distribution referred to as hydration structure. In addition, if the surface consists of soft organic or biological molecules, the flexible surface structures often exhibit thermal fluctuations to present a three-dimensional (3D) distribution. These 3D hydration and flexible surface structures play critical roles in various interfacial phenomena such as protein folding, crystal growth, self-assembly, molecular recognition, metal corrosion, friction and anti-fouling. However, these 3D structures are hard to visualize by conventional imaging techniques. Here, we aim to solve this problem by 3D-AFM [1]. In 3D-AFM, a tip is scanned in vertical and lateral directions to cover the 3D interfacial space. During the scan, the tip interacts with the surrounding molecules so that the measured 3D force distribution shows molecular-scale contrasts reflecting the molecular distributions. So far, several groups have shown that the method can visualize 3D hydration structures on minerals (e.g. mica, calcite and fluorite) and biological molecules (e.g. bR, GroEL and DNA). In addition, it was shown that 3D-AFM can visualize 3D distribution of fluctuating molecules such as lipid headgroups at a membrane surface [2] and surfactants on an HOPG substrate. More recently, the possibility of visualizing 3D hydrations above heterogeneous structures such as point defects and complex minerals have been explored. Furthermore, there has been an attempt to visualize dynamic changes of the 3D hydration structures by improving the operation speed of 3D-AFM. In this study, we present an overview of these advanced 3D-AFM techniques and their applications.


*This work was supported by the World Premier International Research Center Initiative (WPI), MEXT, Japan.
12:27PM B23.00003: Single-atom nuclear magnetic resonance (NMR) using scanning tunneling microscopy*  

KAI YANG (Presenter), PHILIP WILLKE, YUJEONG BAE, IBM Almaden Research Center, ALEJANDRO FERRÓN, Universidad Nacional del Nordeste, JOSE LADO, ETH Zurich, ARZHANG ARDAVAN, University of Oxford, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory (INL), ANDREAS HEINRICH, Center for Quantum Nanoscience, Institute for Basic Science (IBS), CHRISTOPHER LUTZ, IBM Almaden Research Center — Nuclear spins are sensitive probes in chemistry and materials science as well as promising candidates for quantum information processing. Manipulating nuclear spins in condensed matter systems is difficult due to the small nuclear magnetic moment, leading to low polarizations, and addressing them individually is particularly challenging. Here, we demonstrate NMR of individual atoms on a surface in a scanning tunneling microscope (STM) [1]. To achieve NMR, we first polarize nuclear spins using spin-polarized tunneling current. By employing the flip-flop hyperfine interaction, the spin angular momentum of tunneling electrons is transferred to the nucleus. The nuclear polarization is controlled by the current, and read out by electron spin resonance [2, 3]. We further use NMR to sense the local magnetic environment of the electron spin of a single atom. The electrical polarization and driving of the nuclear spin states enable the local spin manipulation for nuclear spintronics and detection of the atomic-scale magnetic environment in nanomagnets.


*We acknowledge financial support from the Office of Naval Research.

12:39PM B23.00004: Downscaling of multiprobe STM experiments: towards atomic level understanding of transport phenomena*  

MAREK KOLMER (Presenter), WONHEE KO, AN-PING LI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Multiprobe scanning tunneling microscopy (STM) based techniques allow determination of electronic and spin transport in variety of systems supported on surfaces of solid materials. Classical 2- and 4-probe methods are currently considered as universal tools for in-situ transport measurements on mesoscopic scales (typically hundreds of nanometers). Alternatively, application of scanning tunneling potentiometry (STP) visualizes potential change during such mesoscopic charge current transport with a nominal nanometer resolution. Here, on chosen examples we would like to discuss our efforts towards changing of this mesoscopic experimental paradigm by downscaling of 2-probe STM and STP experiments towards the atomic level. In this case the charge and spin current supplying probes are positioned in atomically defined locations with respect to the characterized nanosystem. In such configuration multiprobe techniques could directly visualize quantum nature of coherent carriers.

*Part of this work was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a DOE Office of Science User Facility.

12:51PM B23.00005: Array atomic force microscopy for real-time multi-parametric analysis*  

QINGQING YANG (Presenter), Materials Science and Engineering, UC San Diego, QIAN MA, ZHAOWEI LIU, Electrical and Computer Engineering, UC San Diego, RATNESH LAL, Bioengineering, UC San Diego — Nanoscale multipoint structure-function analysis is essential for deciphering complexity of multiscale biological and physical system. Here, we describe a prototype of dispersive optics-based array AFM capable of simultaneously monitoring multiple probe-sample interactions in air and in liquid. A single supercontinuum laser beam is utilized to spatially and spectrally map multiple cantilevers, so that the beam deflection from individual cantilever can be isolated and recorded by distinct wavelength selection. This new design provides a remarkably simplified yet effective solution to overcome optical crosstalk, while maintaining high sensitivity and compatibility with probe-based sensors. We demonstrate the versatility and robustness of our system on parallel multi-parametric imaging, as well as monitoring live hearts cells intercellular activity. This approach provides new opportunities for studying emergent properties of atomic-scale mechanical and physicochemical interactions in a wide range of biological and physical networks.

*This work was supported by the National Institute on Aging of National Institutes of Health (Grant AG028709).
1:03PM B23.00006: Nanofabricated tips as a platform for double-tip and device based scanning tunneling microscopy
MAARTEN LEEUWENHOEK (Presenter), RICHARD NORTE, Delft University of Technology, KOEN BASTIAANS, DOOHEE CHO, IRENE BATTISTI, Leiden University, YAROSLAV BLANTER, Delft University of Technology, MILAN P ALLAN, Leiden University, SIMON GROEBLACHER, Delft University of Technology — We introduce a new kind of tip for scanning tunneling microscopy (STM) and report on its fabrication and performance [1]. By fully incorporating a metallic tip on a silicon chip using modern micromachining and nanofabrication techniques, we realize so-called smart tips and show the possibility of device-based STM tips. Contrary to traditional etched/grinded wire tips, these can be integrated in lithographically defined electrical circuits, photonic circuits and mechanical systems. We experimentally demonstrate the high performance of the smart tips, both in stability and resolution. In situ tip preparation methods are possible and we verify that they can resolve the herringbone reconstruction and Friedel oscillations on Au(111) surfaces. Smart tips can allow to considerably extend the range of STM, for example by enabling high-frequency tips to study noise on majorana zero modes and spin resonances, local gating using two tips or spin sensitive devices. As an example we present in detail two isolated tips with sub-50 nm apex-to-apex distance and calculations of how this can be used to measure electron correlations at the nanoscale.


1:15PM B23.00007: FEBID-grown iron and cobalt nanowires as magnetic force sensors*
HINRICH MATTIAT (Presenter), NICOLA ROSSI, BORIS GROSS, University of Basel, JAVIER PABLO-NAVARRO, CÉSAR MAGÉN, JOSE MARIA DE TERESA NOGUERAS, Physics, Universidad de Zaragoza, MARTINO POGGIO, University of Basel — Nanowires (NW) fabricated by focused electron beam induced deposition (FEBID) of magnetic materials such as iron and cobalt [1] are ideal candidates as magnetic force transducers [2]. The ability to produce nanometer-scale structures with extremely high aspect ratios should allow for magnetic probes with both high force sensitivity and fine spatial resolution. Here, we characterize the mechanical properties of magnetic FEBID-grown NWs using optical interferometry. Furthermore, we study their magnetic behavior through measurements of dynamic torque magnetometry [2]. Due to the large shape anisotropy, the equilibrium magnetization points along the NW, giving rise to a tiny magnetic monopole-like tip for magnetic force sensing. We confirm such behavior by scanning the NW over a micron-sized, current-carrying wire and recording its mechanical response driven by the Biot-Savart magnetic field. Our results, combined with ongoing progress in FEBID manufacturing of nanowires, hold great promise for new types of mechanical sensors for magnetic field imaging at the nanometer-scale.


*Swiss NSF (200020-178863); ERC Starting Grant NWScan (334767).

1:27PM B23.00008: Imaging and Controlling Pseudospin and Berry Phase of Dirac Fermions by Symmetry-Assisted Coherent Scattering
YI-TING CHEN (Presenter), MORGAN BRUBAKER, HARI MANOHARAN, Stanford University — In lattice materials, the solution of the Schrödinger equation is a set of Bloch waves. The dispersion of these components defines the band structure and is crucial to electronic transport and thermodynamic properties. Scanning tunneling microscopy (STM) is a powerful tool to study electronic properties with exceptional spatial resolution. Because coherent scattering induced by impurities strongly depends on the band structure of a material, by imaging the pattern of coherent scattering, the band structure can be probed in momentum space as well. Using atom manipulation with STM, we show that the coherent scattering term can be separated from the non-scattering term. As a result, the contrast of the coherent scattering pattern is amplified and the details of the band structure of Dirac fermions in graphene, including complete Dirac cones and their trigonal warping, are revealed. Furthermore, by tuning the symmetry of the scattering center using atom manipulation, we show that pseudospin can be resolved and that a signature of the underlying Berry phase can be observed. The results indicate that the interplay of the symmetry of wave functions and that of a single scattering center provides a new way to image and control the internal degrees of freedom of quantum matter.


*Swiss NSF (200020-178863); ERC Starting Grant NWScan (334767).
1:39PM B23.00009: Using real space pseudopotentials to simulate non-contact atomic force microscopy images of organic molecules*  
DINGXIN FAN (Presenter), JAMES CHELIKOWSKY, University of Texas at Austin — Non-contact atomic force microscopy (nc-AFM) is a popular instrument to visualize the nano world with unprecedented resolution. nc-AFM, with a CO functionalized probe tip, can be used to distinguish different organic molecules, and serves as a very powerful analytical tool in organic chemistry research to identify the molecular structures of reactants, intermediates and products. However, a one-to-one mapping between the functional groups and nc-AFM images is often lacking. We employ a real-space pseudopotential method to simulate nc-AFM images and to provide a “database” for various functional groups, such as -C≡C-, -C=C-, and -C=O. We will also assess new functionalized tips by performing calculations to simulate nc-AFM images.

*We acknowledge support from the U.S. Department of Energy under DE-FG02-06ER46286 and the Welch Foundation under Grant No. F-1837. The National Energy Research Scientific Computing (NERSC) and the Texas Advanced Computing Center (TACC) provided computational resources.

1:51PM B23.00010: Subtleties in the use of a quadrant cell photodiode in an optical lever*  
PAUL NAKROSHIS (Presenter), BENJAMIN MONTGOMERY, University of Southern Maine — Quadrant cell photodiodes are often used in an optical lever to deliver a digital “zero-crossing” signal (either for determining the period or for a static position signal). However, one can also continuously monitor the analog output of a quad-cell photodiode to determine time dependent positioning information (albeit over a narrow range). Unfortunately, the response of a quadrant cell photodiode to the passage of a gaussian laser beam is a non-trivial function of the beam radius. We have created a detailed (python based) computational model of a quadrant cell photodiode, and compared the model to experimental measurements. We remark the accuracy of the model as well as some important frequency spectrum implications of the detector response which are very relevant when analyzing the power spectrum of a quadrant cell signal.

*Funding for this work came from the University of Southern Maine.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B24 DAMOP: Open Quantum Systems BCEC 159 - Barry Sanders - Tag(s): Focus

11:15AM B24.00001: Dissipative quantum error correction and application to quantum sensing with trapped ions  
[Invited] FLORENTIN REITER, Harvard University, ANDERS SORENSEN, Niels Bohr Institute, PETER ZOLLER, University of Innsbruck, CHRISTINE MUSCHIK (Presenter), Institute for Quantum Computing — Quantum-enhanced measurements hold the promise to improve high-precision sensing ranging from the definition of time standards to the determination of fundamental constants of nature. However, quantum sensors lose their sensitivity in the presence of noise. To protect them, the use of quantum error correcting codes has been proposed. Trapped ions are an excellent technological platform for both quantum sensing and quantum error correction. Here we present a quantum error correction scheme that harnesses dissipation to stabilize a trapped-ion qubit. In our approach, always-on couplings to an engineered environment protect the qubit against spin- or phase flips. Our dissipative error correction scheme operates in a fully autonomous manner without the need to perform measurements or feedback operations. We show that the resulting enhanced coherence time translates into a significantly enhanced precision for quantum measurements. Our work constitutes a stepping stone towards the paradigm of self-correcting quantum information processing.
**11:51AM B24.00002: Analysis of matter-wave emission into a structured vacuum**  
MICHAEL STEWART (Presenter), JOONHYUK KWON, DOMINIK SCHNEBLE, Stony Brook University — Ultracold atoms in optical lattices realize a tunable open quantum system in the context of matter-wave emission into vacuum. Recent studies [1, 2] have demonstrated drastic departures from Markovian spontaneous emission into a vacuum near an energetic boundary, as well as the existence of a bound matter-wave and emitter state below it. In this talk we theoretically analyze the effects of introducing an emission vacuum with a band structure mirroring that of a photonic crystal. We find exotic decay dynamics arising from the analytic structure of the self-energy, including a beating between bound states at opposite edges of a band. The dynamic depends on the interplay between coupling strength and bandwidth, which can be easily tuned in the optical lattice platform.


*This work is supported by the National Science Foundation, Grand No. PHY-1607633

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**12:03PM B24.00003: Novel Entanglement-preserving approach for universal dissipation mechanisms in quantum nanophotonics**  
ZIHAO CHEN (Presenter), YAO ZHOU, JUNG-TSUNG SHEN, Electrical and System Engineering, Washington University in St. Louis — Ubiquitously in quantum nanophotonics, photons may be scattered off system impurities to the reservoir, or absorbed by reservoir degrees of freedom, which manifest as different dissipation mechanisms of scattering loss or material loss. Conventionally, fruitful density matrix approach (DMA) is adopted to study such effects, which averages out reservoir degrees of freedom in the reduced density matrix dynamics. While such an approach can incorporate the information that shuttles back and forth between system and reservoir, it does not preserve photon-photon entanglement in the system or the system-reservoir entanglement.

Here we present a novel wave-function-based approach that preserves the entanglement information, to study both dissipation mechanisms for an arbitrary photonic Fock state process. For the scattering loss scenario, when the dissipated photon does not return to the system, we show that the effects can be incorporated by using a reduced Hamiltonian description. For the material loss scenario, nonetheless, returning nature of dissipated photons fundamentally modifies multi-photon entanglement to invalidate the reduced Hamiltonian description. Moreover, our approach reveals how scattering matrix and transport properties are modified, which is beyond the scope of DMA.

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**12:15PM B24.00004: Coherent frequency transfer of optical nonlinearities by feedback control of a non-degenerate optical parametric oscillator**  
EDWIN NG (Presenter), TATSUHIRO ONODERA, RYOTATSU YANAGIMOTO, HIDEO MABUCHI, Stanford University — Strong, coherent optical nonlinearities, such as those found in atom-cavity QED systems, are key resources for ultra-low-power optical information processing. However, such nonlinearities often arise from resonant effects occurring in a narrow band of frequencies, limiting their utility within heterogeneous networks of optical devices. At the same time, optical parametric oscillators (OPOs) are a robust platform for tunable light generation, converting pump light into signal and idler light at potentially vastly different frequencies. Here, we consider a coherent feedback scheme in which a narrowband nonlinear device, modelled as a Kerr cavity, is connected by an optical feedback loop to the signal port of an non-degenerate OPO below threshold. We use the SLH formalism to derive a rigorous input-output quantum model for this composite device, and we show by numerical simulation that the nonlinear input-output behavior of the Kerr cavity can be transferred to the idler port of the OPO, thus implementing a coherent transfer of the optical nonlinearity from one frequency to another.

*This work has been supported by the NSF under award number PHY-1648807.*

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RENZO VILLAZON (Presenter), ANATOLI S POLKOVNIKOV, ANUSHYA CHANDRAN, Boston University — Fast forward protocols can be used to engineer rapid adiabatic processes by dynamically tuning available control parameters. For open systems, constructing local transitionless protocols can be a challenging task since one cannot access the bath degrees of freedom needed to prevent non-adiabatic excitations. We present a local fast forward protocol for a particle in a tunable harmonic potential coupled to a bath of optical phonons, which we treat microscopically without making the standard Markovian or Lindbladian approximations. This protocol can be experimentally realized by dynamically tuning the system’s frequency and driving its coupling to the environment with a high-frequency Floquet drive. We show that this protocol effectively implements a rapid isothermal process and apply it to realize a fast heat engine operating near the Carnot efficiency.

*NSF: DMR-1752759  
Sloan Fellowship  
NSF DMR-1813499  
AFOSR FA9550-16-1-0334

12:39PM B24.00006: Non-Gaussian quantum phenomena in synchronously-pumped optical parametric oscillator*  
TATSUHIRO ONODERA (Presenter), EDWIN NG, PETER MCMAHON, ALIREZA MARANDI, HIDEO MABUCHI, Stanford University — The synchronously-pumped optical parametric oscillator (SPOPO) below threshold has been engineered to generate multimode squeezing and entanglement among the various frequency components of the broadband pulses. A natural question to ask is whether new phenomena exist in the above-threshold regime of the SPOPO. To this end, we have developed a quantum input-output model of the SPOPO that is rigorously valid above threshold. In this model, we have found theoretical evidence of rich multimode non-Gaussian quantum phenomena such as the generation of multimode cat states, which can be engineered by designing the pump spectrum and dispersion of the SPOPO appropriately. We also showed that, consistent with classical intuition, field enhancement due to the localization of the pulse envelope in time enhances the effective nonlinearity by the (large) number of interacting modes. Because of this enhancement, we speculate that non-Gaussian states may be experimentally accessible in the future with near-term, on-chip photonic platforms, such as thin-film lithium niobate.

**This work has been supported by the NSF under award number PHY-1648807.

12:51PM B24.00007: Non-Markovian dynamics revealed at the bound state in continuum*  
SAVANNAH GARMON (Presenter), KENICHI NOBA, Osaka Prefecture University, GONZALO ORDONEZ, Butler University, DVIRA SEGAL, University of Toronto — We propose a methodical approach to controlling and enhancing deviations from exponential decay in quantum and optical systems by exploiting recent progress surrounding another subtle effect: the bound states in continuum, which have been observed in optical waveguide array experiments within this past decade. Specifically, we show that by populating an initial state orthogonal to that of the bound state in continuum, it is possible to engineer system parameters for which the usual exponential decay process is suppressed in favor of inverse power law dynamics and coherent effects that typically would be extremely difficult to detect in experiment. We demonstrate our method using a model based on an optical waveguide array experiment, and further show that the method is robust even in the face of significant detuning from the precise location of the bound state in continuum.


*This work was supported by JSPS KAKENHI Grants No. JP18K03466 and JP16K05481 as well as the Research Foundation for Opto-Science and Technology (S.G.) and the Canada Research Chair Program (D.S.).
1:03PM B24.00008: Two-Photon Scattering in USC regime  VANESSA PAULISCH, Max-Planck-Institute of Quantum Optics, TAO SHI, Institute of Theoretical Physics, Chinese Academy of Sciences, JUAN JOSE GARCIA-RIPELL (Presenter), Institute of Fundamental Physics, CSIC — In this work we study the scattering of pairs of photons by a two-level system ultrastrongly coupled to a one-dimensional waveguide [1]. We describe this problem using a spin-boson model with an Ohmic environment \( J(\omega) = \pi \alpha \omega \). We show that when coupling strength lays is about \( \alpha \leq 1 \), the dynamics is well approximated by a polaron Hamiltonian, under the approximation of a conserved number of excitations. In this regime, we develop analytical predictions for the single- and two-photon scattering matrix computed with a Green's function method. These predictions are verified against time-evolved matrix-product-state simulations of propagating wavepackets interacting with a two-level system, showing the accuracy of the approximation. Our predictions for two-photon scattering can be verified using the scattering tomography techniques from Ref. [2].


1:15PM B24.00009: Bloch state scattering in the Brillouin zone*  LINDA E REICHL, MAX PORTER (Presenter), AARON BARR, ARIEL BARR, University of Texas at Austin — Systems with space-periodic Hamiltonians have unique scattering properties, just as time-periodic ones do. We use Wigner-Eisenbud (reaction matrix) scattering theory to consider a two-dimensional scattering system in which one dimension is a periodic lattice and the other is localized in space. The scattering and decay properties can then be described by sets of channels, where sets are indexed by Bloch momenta and channels within sets are indexed by incident waves' quantized kinetic energy parallel to the lattice. In the case where the lattice unit cell has reflection symmetry we find that the lattice can sustain formation of antisymmetric bound states in the continuum. Breaking the unit cell symmetry then causes those bound states to become quasibound and slowly decay. We also find in the lowest energy channel that reflection probability increases when varying Bloch momentum.

*The authors thank the Robert A. Welch Foundation (Grant No. F-1051) for support of this work.

1:27PM B24.00010: Emergent Finite Frequency Criticality of Driven-Dissipative Correlated Lattice Bosons  ORAZIO SCARLATELLA (Presenter), Institute de Physique Théorique-CEA/Saclay, Université Paris Saclay, France, Gif-sur-Yvette, ROSARIO FAZIO, ICTP, Italy, Trieste. NEST, Scuola Normale Superiore & Istituto Nanoscienze-CNR. Italy, Pisa., MARCO SCHIRO, Institute de Physique Théorique-CEA/Saclay, Université Paris Saclay, CNRS, France, Gif-sur-Yvette — Critical points and phase transitions are characterized by diverging susceptibilities, reflecting the tendency of the system toward spontaneous symmetry breaking. Equilibrium statistical mechanics bounds these instabilities to occur at zero frequency, giving rise to static order parameters. In this work we argue that a prototype model of correlated driven-dissipative lattice bosons, of direct relevance for upcoming generation of circuit QED arrays experiments, exhibits a susceptibility sharply diverging at a finite non-zero frequency, which is an emerging scale set by interactions and non-equilibrium effects. In the broken-symmetry phase the corresponding macroscopic order parameter becomes non-stationary and oscillates in time without damping, thus breaking continuous time-translational symmetry. Our work, connecting breaking of time translational invariance to divergent finite frequency susceptibilities, which are of direct physical relevance, could potentially be extended to study other time-domain instabilities in non-equilibrium quantum systems, including Floquet time crystals and quantum synchronization.

1:39PM B24.00011: Spectral Decomposition of Green's Functions of Open Quantum Systems  MARCO SCHIRO (Presenter), ORAZIO SCARLATELLA, Institute for Theoretical Physics, CEA Saclay, CNRS, AASHISH CLERK, Institute for Molecular Engineering, University of Chicago — We derive a Lehmann-style representation of spectral functions of Markovian driven-dissipative systems, and discuss how this can be employed to obtain physical intuition. Focusing on a specific model of a non-linear driven Kerr cavity, we discuss the connections between spectral functions changing sign and population inversion in the steady state. Surprisingly, we find that dissipation can change the sign of spectral functions, with direct physical implications, even in absence of steady state population inversion.
1:51PM B24.00012: Coarse-grained master equation is valid for a fast bath and any drive* EVGENY MOZGUNOV
(Presenter), USC — We compare three master equations: Davies-Lindblad, Redfield, and the recent Coarse-grained completely positive equation[1]. We note that the Redfield equation is valid for a fast bath regardless of the relative strength of the coupling to the system Hamiltonian. The main obstruction to using it is its non-positivity. We show how an attempt to make Redfield positive results in the Coarse-grained master equation. Our new derivation allows to estimate the error of the resulting completely positive equation. Much like Redfield, this equation is applicable for fast bath even if the system Hamiltonian is driven. We thus present a completely positive open system master equation that is a controlled approximation to true evolution for any time-dependence of the system Hamiltonian. The fast bath assumption includes any bath with time correlation function decaying faster than $1/t^2$ which is the case for the Ohmic bath. For Ohmic bath, equation is still applicable up to a large timescale.


*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.

2:03PM B24.00013: A solution ansatz for Lindblad master equation with a dynamical system theory approach* GEHAD SADIEK (Presenter), Department of Applied Physics and Astronomy, University of Sharjah, Sharjah 27272, UAE, ELSAYED I. LASHIN, Department of Physics, Ain Shams University, Cairo 11566, Egypt —

We study interacting quantum systems coupled to a dissipative Markovian environment. We use an ansatz for the solution of Lindblad master equation of the composite system, which splits the time evolution of the system into two parts, unitary evolution of the wave function of the free system and time evolution of the density matrix coefficients of the composite system mainly controlled by the Lindblad operators. We show that the obtained system of first order linear differential equations, autonomous or otherwise, governing the density matrix coefficients can be treated using the machinery of dynamical system theory to reveal all the information about the system dynamics and its asymptotic behavior, fixed points (steady states) and limiting oscillatory behavior (limit cycle), with minimal amount of work. For the sake of illustration, we apply this technique to an interacting spin-1/2 XXZ system coupled to a dissipative environment, which demonstrates the main aspects of the approach.

*This work has been supported by The office of V.C. of research and graduate studies, University of Sharjah under Grant No. 16021-43030-P.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B25 DPOLY: Biopolymers and Sustainable Polymers BCEC 160A - Alexander Klotz, Massachusetts Institute of Technology

11:15AM B25.00001: Fabrication of Nano/micro-fiber Materials from Rigid Rod Peptide Chains via Electrospinning and Their Mechanical Properties* KYUNGHEE KIM (Presenter), CHRISTOPHER KLOXIN, University of Delaware, JEFFERY G SAVEN, University of Pennsylvania, DARRIN POCHAN, University of Delaware — Peptides are ideal candidates for the design and controlled assembly of nanoscale materials due to their potential to assemble with almost atomistic precision as in biological systems. The ability to create rigid rod chains composed of individual peptide bundles and to develop nano/microfibers containing the stiff chains offers the opportunity to develop unique structural features and a remarkable combination of high stiffness, high strength, large elasticity and elongation. This study is to facilitate nano/microfiber electrospinning, focusing on the use of synthetic peptides and to measure initial physical properties of peptide-based fibers. Computationally-designed peptides formed designed coiled coil bundles that serve as supramolecular monomers in chain formation. The bundle chains, or “bundlemers” display rigid-rod character due to intrabundle and interbundle physical and covalent interactions. The resultant rigid chains are employed to fabricate nano/micro-fibers via electrospinning. The mechanical properties of electrospun rod fibers are investigated as a function of bundlemer rod length, intra- or inter-chain interactions (both before and/or after electrospinning), and bundle type included in the bundlemer chains.

*DOE award #18A01039
**11:27AM B25.00002: Self-Assembly of poly(D-glucose carbonate) Amphiphilic Block copolymers in Solution**

YOUNG LEE (Presenter), University of Delaware, KAREN L. WOOLEY, Chemistry, Texas A&M University, ARTHI JAYARAMAN, DARRIN POCHAN, University of Delaware — With a rising interest in developing and implementing more environmentally-friendly materials, the study of self-assembly behavior of a next generation natural-source based polymers is crucial. Sugar-derived poly(D-glucose carbonate) (PGC) amphiphilic block copolymers with targeted block compositions, chain lengths and side chain chemistries were synthesized. The bulk solution assembly behavior of PGCs was explored using a range of solvent environments (e.g. water-miscible organic solvent compositions or pH-induced structural transitions). The assembled nanostructure shows a morphological transition from a micellar to a fibrillar nanostructure that is dependent on parameters affecting the degree of side chain ionization. These findings allow us to discover a variety of robust nanostructures that can be achieved by non-traditional polymers and their potential to be used in many applications. Additionally, conformations of homopolymer PGC with different side chains were measured via small-angle neutron scattering (SANS) in an effort to better understand the assembly formation behavior of the PGCs when used as blocks in amphiphile creation. Finally, new efforts to correlate scattering, electron microscopy, and simulation data will be presented.

*NSF DMREF-1629156


JOHN ATKINSON (Presenter), University of Guelph, JONATHAN NICKELS, University of Cincinnati, MICHELLE MICHALSKI, ADRIAN SCHWAN, University of Guelph, JOHN KATSARAS, Oak Ridge National Lab, JOHN DUTCHER, University of Guelph — Phytoglycogen is a polysaccharide produced in the form of compact nanoparticles by sweet corn. The nanoparticles have exceptional properties that emerge from their highly-branched, dendrimeric structure and their unique interaction with water, which makes them desirable as additives for applications in personal care, food and biomedicine. Our initial small angle neutron scattering (SANS) study on phytoglycogen nanoparticles [1] revealed unique insights into their structure and hydration. By hydrophobically modifying the hydrophilic nanoparticles, we can change the nature of their interactions in a tunable manner. Specifically, we modified phytoglycogen nanoparticles by covalently attaching octenyl succinate anhydride (OSA), for which the octenyl groups convey a hydrophobic character. We used small angle neutron scattering at the Oak Ridge National Laboratory to perform a comprehensive study of OSA-modified phytoglycogen with different degrees of substitution. We synthesized deuterated OSA (dOSA) and used dOSA-phytoglycogen and OSA-phytoglycogen in contrast series SANS experiments to create a comprehensive picture of the radial distribution of the OSA molecules on the phytoglycogen nanoparticles.


**11:51AM B25.00004: Binding of Proteins to Phytoglycogen Nanoparticles, a Novel, Sustainable, Soft Colloid**

KATHLEEN CHARLESWORTH (Presenter), AIDAN MAXWELL, JOHN DUTCHER, University of Guelph — Phytoglycogen is a glucose polymer that occurs naturally in the form of highly branched, compact nanoparticles. Because of their tree-like or dendrimeric structure, phytoglycogen nanoparticles have unique properties, such as a strong interaction with water and uniformity in size, which makes them attractive for use in applications ranging from cosmetics to drug delivery. Many of these applications rely on the binding of small molecules onto phytoglycogen nanoparticles. Surface Plasmon Resonance (SPR) is a sensitive experimental technique, based on the resonant absorption of light within an ultrathin gold film, that can be used to measure the binding kinetics and affinities of small molecules. I will discuss our success in creating a stable phytoglycogen-functionalized gold surface, which has allowed us to use SPR to quantify the binding of various proteins to the phytoglycogen nanoparticles.

**12:03PM B25.00005: Influence of poly(N-isopropylacrylamide) grafting density on the temperature dependent fibril formation of methylcellulose**

MCKENZIE COUGHLIN (Presenter), SVETLANA MOROZOVA, PETER SCHMIDT, S. PIRIL ERTEM, THERESA M. REINEKE, FRANK BATES, TIMOTHY LODGE, University of Minnesota — Methylcellulose (MC) is a water-soluble cellulose ether that is used in a variety of commercial products due to its thermoreversible gelation at ca. 60 °C, near the lower critical solution temperature (LCST) of MC. It is known that this gelation is caused by the formation of a fibrillar network upon heating. Recently, we demonstrated that the MC fibril structure can be modified and that the fibril formation can be suppressed by grafting short poly(ethylene glycol) (PEG) chains onto the MC backbone. With this new understanding, we have grafted poly(N-isopropylacrylamide) (PNIPAm) chains onto the MC backbone at various grafting densities; PNIPAm displays LCST behavior in water at ca. 32 °C. Utilizing static and dynamic light scattering, we characterize the chain conformation and variation in the overall radius of the chains as a function of grafting density and temperature. Small-amplitude oscillatory shear reveals changes in the gelation behavior and modulus of the two polymers. Fibril formation and fibril structure are studied using small-angle X-ray scattering and cryogenic transmission electron microscopy. The influence of PNIPAm grafts on the temperature dependence of MC fibril formation is compared with the results from PEG-grafted MC.
Correlation of Mechanical and Hydration Properties of Soft Phytoglycogen Nanoparticles

MICHAEL GROSSUTTI (Presenter), JOHN DUTCHER, University of Guelph — Phytoglycogen nanoparticles are highly-branched polymers of glucose that are produced as soft, compact nanoparticles by sweet corn. By combining the results of dialysis, ellipsometry and gravimetric analysis experiments, we have constructed a master plot of the osmotic pressure-concentration curve for phytoglycogen nanoparticles with values ranging over seven orders of magnitude. The distinctive shape of the osmotic pressure-concentration curve for phytoglycogen differs significantly from that of dextran, a lightly-branched polysaccharide that is chemically identical but does not occur in the form of particles. Specifically, there is a well-defined plateau in the logarithm of the osmotic pressure at phytoglycogen nanoparticle concentrations corresponding to contact between the particles. By recasting the dependence of the osmotic pressure on concentration in terms of its dependence on the effective separation of the particles, we identify three distinct regimes of interactions between the particles: a weak repulsion before contact; a stronger repulsion upon initial contact and compression (intermediate regime); and an even stronger repulsion for large particle compressions (concentrated regime). This analysis has allowed us to relate the mechanical stiffness to particle hydration.

Tensile properties for solid films of deoxyribonucleic acid containing hydrated ionic liquids

HISAO MATSUNO (Presenter), YUMA MORIMITSU, Kyushu University, NOBORU OHTA, HIROSHI SEKIGUCHI, Japan Synchrotron Radiation Research Institute, ATSUSHI TAKAHARA, KEIJI TANAKA, Kyushu University — Mechanical properties of deoxyribonucleic acid (DNA) solid films strongly depend on the water content; from glassy-like to rubbery-like via semi-crystalline-like. Also, the incorporation of intermolecular cross-linking between DNA strands impacts on them. These imply a possibility of DNA solids as an eco-friendly structural material. However, to accelerate such a trend, there exists a challenging problem that water evaporates from the film in a short time, causing a change of the mechanical properties. In this study, aggregation states and tensile properties of the DNA films containing a hydrated ionic liquid, choline dihydrogen phosphate (CDP), were studied. The stress-strain (S-S) curve was strongly dependent on the amount of CDP in the films. A 8-wt% CDP film behaved like a glassy polymer. As the CDP content increased, the shape of S-S curves changed to ductility-like or rubbery-like polymers. In the case of a 23-wt% CDP film, the yield stress decreased more strikingly and the clear strain hardening, like elastomers, was observed. Overall, the breaking point and energy increased, and the Young's modulus and yield stress decreased with increasing CDP amount. And also, these properties were maintained for more than several days because hydrated CDP could be hardly evaporated.
Early results showed more penetration of acetophenone into the LDPE when the positive electrode was on the acetophenone side. This suggests that acetophenone ionization and electrophoretic transport of the ions enhance acetophenone penetration. Ionization of the crosslinking byproducts and subsequent electrophoretic migration of the charges may be one reason for high local electric fields and ultimate dielectric failure.
1:51PM B25.00014: 1/f Noise in Solid-state Nanopore: Generation Mechanism and Prevention Methods  KAZUMA MATSUI (Presenter), YUSUKE GOTO, RENA AKAHORI, Hitachi, MICHIRU FUJIOKA, Hitachi High-Technologies, TAKESHI ISHIDA, TAKAHIDE YOKOI, ITARU YANAGI, KEN-ICHI TAKEDA, Hitachi — To realize DNA sequencing with solid-state nanopore, reduction of an ionic current noise is an important issue. Especially, low-frequency (1/f) noise causes a serious problem reducing read accuracy of DNA sequencing. Its origin has been heavily debated, but not yet clarified.

In this research, we found that 1/f noise is generated from the surface charge fluctuations due to an exchange reaction of alkali metal ions (M+) and protons (H+) on a nanopore wall. We hypothesized the charge fluctuations are dependent on the equilibrium constants of the reaction, and measured baseline current with various cations. Surprisingly, the order of 1/f noise intensity follows the theoretical one estimated from their equilibrium constants.

We also developed a new 1/f noise reduction method by suppressing the exchange reaction. The nanopore wall was coated with divalent cations, which lead to prevent the adsorption of other ions because those adsorption affinity is higher than other ions. As a result, we successfully and effectively reduced 1/f noise with this method.

2:03PM B25.00015: Elucidating the microstructural basis for the lasting radial strength of poly (L-lactide) bioresorbable vascular scaffolds during hydrolysis*  KARTHIK RAMACHANDRAN (Presenter), TIZIANA DI LUCCIO, ARTEMIS AILIANOU, Chemistry and Chemical Engineering, California Institute of Technology, MARY BETH KOSSUTH, JAMES PAUL OBERHAUSER, Global Product Development, Abbott Vascular, JULIE A KORNFIELD, Chemistry and Chemical Engineering, California Institute of Technology — Drug-eluting metal stents (DES) are the current standard-of-care for restoring blood flow through an occluded artery. However, DES are made from metal alloys that are non-biodegradable and consequently, inhibit arterial vasomotion and pose a risk of thrombosis, a dreaded complication. Bioresorbable vascular scaffolds (BVS) made from poly L-lactide (PLLA) are emerging as a promising alternative to permanent metal stents. The clinically-approved BVS (FDA-approval in 2016) supports the occluded artery for the requisite 3-6 months but is completely resorbed in 2-3 years. As a result, the BVS restores arterial vasomotion and can eliminate the late onset of thrombosis. The clinically-approved BVS presents a paradox as it hydrolyzes in the body – it suffers a ~40% decrease in molecular weight ($M_n$) but shows no decrease in radial strength. Using X-ray microdiffraction, we discovered that the BVS develops a unique microstructure in localized regions that make up <3% of the scaffold. These regions resist hydrolysis and reinforce struts in the BVS that are the most vulnerable to fracture. Thus, the global measure of degradation does not capture the presence of chains with $M_n$ higher than average in regions that have a disproportional impact on strength.

*NIH, Caltech, Abbott Vascular

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B26 DQI: Superconducting Circuits: Remote Entanglement and Waveguide QED

BCEC 160B - Mollie Schwartz, MIT Lincoln Laboratory

11:15AM B26.00001: Particle production in ultrastrong-coupling waveguide QED* NIGUEL GHEERAERT (Presenter), Néel Institute, CNRS and Université Grenoble-Alpes, XIN ZHANG, Department of Physics, Duke University, THÉO SÉPULCRE, Néel Institute, CNRS and Université Grenoble-Alpes, SOUMYA BERA, Department of Physics, Indian Institute of Technology Bombay, NICOLAS ROCHE, Néel Institute, CNRS and Université Grenoble-Alpes, HAROLD U BARANGER, Department of Physics, Duke University, SERGE FLORENS, Néel Institute, CNRS and Université Grenoble-Alpes — In recent years, the field of light-matter interaction has made a further stride forward with the advent of superconducting qubits ultra-strongly coupled to open waveguides. In this setting, the qubit becomes simultaneously coupled to many different modes of the waveguide, leading to a wealth of non-linear dynamical phenomena.

First, I will show how one can tackle the time-evolution of such a non-trivial system using a novel numerical technique based on an expansion of the full state vector in terms of multi-mode coherent states. Inspired by earlier semi-classical approaches, this numerically exact method provides an important advance compared to the state-of-the-art techniques that have been used so far to study the many-mode ultra-strong coupling regime.

I will then move on to present the central prediction of my work concerning the scattering of low-power coherent signals on a qubit. Most remarkably, I will show that the qubit non-linearity, transferred to the waveguide through the ultra-strong light-matter interaction, is able to split photons from the incoming beam into several lower-energy photons. This splitting leads to the emergence of a low-frequency continuum in the scattered power spectrum that dominates the inelastic signal.

*The Nanoscience Foundation
Waveguide-mediated interaction of artificial atoms in the strong coupling regime, part 1

XUEYUE ZHANG (Presenter), EUN JONG KIM, MOHAMMAD MIRHOSSEINI, ALP SIPAHIGIL, Caltech, PAUL DIETERLE, Harvard University, ANDREW J KELLER, ANA ASENJO-GARCIA, Caltech, DARRICK CHANG, ICF, OSKAR PAINTER, Caltech — Embedding of multiple quantum emitters to a common one-dimensional radiation channel gives rise to emergent collective effects: collective emission and long-range exchange interaction. Collective emission leads to super- and sub-radiant states while the signature of exchange interaction, coherent cooperative dynamics, has been obscured by the radiative decay into the one-dimensional channel. In this work, we utilize the sub-radiant state to trap the radiation, acting as an atomic cavity, and strongly couple a probe quantum emitter to the sub-radiant state, effectively creating an atom-cavity system [New J. Phys. 15, 063003 (2012)]. We implement the scheme with transmon qubits coupled to a microwave coplanar waveguide. We discuss the building blocks and design of the qubit-waveguide system, and the characterization of individual waveguide-coupled qubits which highlights the requirements for observing coherent cooperative dynamics. arXiv:1809.09752

This work was supported by the AFOSR MURI Quantum Photonic Matter (grant FA9550-16-1-0323), the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center (grant PHY-1125565).

Waveguide-mediated interaction of artificial atoms in the strong coupling regime, part 2

EUN JONG KIM (Presenter), XUEYUE ZHANG, MOHAMMAD MIRHOSSEINI, ALP SIPAHIGIL, Caltech, PAUL DIETERLE, Harvard University, ANDREW J KELLER, ANA ASENJO-GARCIA, Caltech, DARRICK CHANG, ICF, OSKAR PAINTER, Caltech — Photon-mediated interactions of quantum emitters in a one-dimensional radiation channel leads to collective emission and long-range exchange interaction. Observation of coherent cooperative dynamics via such interactions, however, has been obscured by radiative decay into the one-dimensional channel. Here, we employ transmon qubits and a microwave coplanar waveguide as artificial atoms coupled to a one-dimensional channel. We circumvent the radiative decay problem by utilizing the entangled dark state of a qubit array arising from collective waveguide emission. The entangled dark state, with a suppressed decay rate, effectively traps radiation as an atomic cavity while exhibiting a large exchange interaction rate with a designated probe qubit. We report the observation of coherent cooperative dynamics in the strong coupling regime and characterize the coherence properties of the collective states involved in the dynamics. In addition, we discuss potential applications of this platform and practical challenges in such systems. arXiv:1809.09752

This work was supported by the AFOSR MURI Quantum Photonic Matter (grant FA9550-16-1-0323), the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center (grant PHY-1125565).

Waveguide QED with a giant transmon

A.M. VADIRAJ (Presenter), C.W.S CHANG, IBRAHIM NSANZINEZA, CHRISTOPHER WILSON, Electrical and Computer Engineering, Institute for Quantum Computing, University of Waterloo — In a typical waveguide QED system, a quantum emitter, such as a superconducting transmon qubit, is coupled to a superconducting waveguide in order to study its interaction with the electromagnetic field. In these systems, the emitter is approximated as a point-like object when compared to the wavelength of light. However, recent experiments [1] demonstrated the ability to couple a transmon to surface acoustic waves (SAW) that have a wavelength much smaller than the transmon, thereby creating a “giant” artificial atom. Inspired by these results, there is a recent proposal [2] to couple a transmon at multiple points of a microwave waveguide, with wavelength-scale distances between each coupling point, also making a giant transmon. The proposal predicts the ability to custom design the relaxation rates of different transmon levels and proposes several interesting applications such as single-atom lasing and tunable coupling. We will present preliminary characterization of such a device.

Studying collective effects in 3D waveguide QED with frequency and time-domain resolved spectroscopy

ALEKSEI SHARAFIEV (Presenter), MATHIEU JUAN, Inst Quantum Optics & Quantum Info, MAXIMILIAN ZANNER, University of Innsbruck, JUAN JOSE GARCIA-RIPOLL, Institute of Polymer Science and Technology, Madrid, GERHARD KIRCHMAIR, University of Innsbruck — Collective behavior of coupled quantum emitters has been studied extensively theoretically starting from seminal Dicke's paper. Experimentally however many of the theoretical predictions have never been checked since it requires sophisticated experimental techniques. The recently appeared platform of 3D cQED offers unique opportunities in controlling independent qubits and their respective couplings control as well as long coherence times. We experimentally realized a system, which allows to investigate frequency chirping in a Dicke physics model, as well as to study cooperative behavior against collective noise and parameters spread. We study the system dynamics in frequency, as well as time-domain and compare it to theoretical predictions.
12:15PM B26.00006: Real-time detection of an itinerant microwave photon using dressed-state engineering* 
ZHIRONG LIN (Presenter), RIKEN and Shanghai Institute of Microsystem and Information Technology, SHUMPEI MASUDA, Tokyo Medical and Dental University, KUNIHIRO INOMATA, National Institute of Advanced Industrial Science and Technology, KAZUKI KOSHINO, Tokyo Medical and Dental University, TSUYOSHI YAMAMOTO, NEC Corporation, YASUNOBU NAKAMURA, The University of Tokyo — Several schemes for single microwave photon detection have been proposed and demonstrated lately in circuit quantum electrodynamics. However, all experimental demonstration to date are performed in the time-gated mode. In this presentation, we demonstrate a real-time detection of itinerant microwave photons. In our setup, a superconducting flux qubit is coupled to two resonators, which have substantial difference in the dispersive shifts. Under an adequate choice of the frequency and the power of the qubit drive, one resonator is used to form an impedance-matched Λ system that deterministically captures incoming photons, and the other is used for continuous monitoring of the event. We observe quantum jump produced by an itinerant microwave photon and attain a single-photon-detection efficiency of ~0.35. The detection efficiency of this detector is limited by the relatively short qubit relaxation time.

*This work was supported in part by JST ERATO (Grant No. JPMJER1601), JSPS KAKENHI (No. 16K05497, No. 26220601 and No. 18K03486), and ALS, The University of Tokyo.

12:27PM B26.00007: Quantum non demolition parity measurements of itinerant microwave fields 
JEAN-CLAUDE BESSE (Presenter), SIMONE GASPARINETTI, MICHELE COLLODO, ANTS REMM, CHRISTOPHER EICHLER, ANDREAS WALLRAFF, ETH Zurich — Capitalizing on recent demonstrations of quantum non demolition (QND) detection of individual itinerant microwave photons [1,2] we demonstrate parity measurements applied to input fields with photon number up to ten.

Defining a mode to be characterized by the temporal shape of a displacement field added onto it, we recover its Wigner function without making use of reconstruction or maximum likelihood methods. We present results of this phase space tomography method for propagating fields for various classical and quantum input fields.

The non demolition character of the measurement also allows for heralding highly non-classical states of light, such as multi-photon cat states, which are relevant for quantum information processing.


12:39PM B26.00008: Violating Bell’s Inequality with Remotely-Connected Superconducting Qubits* 
YOUPENG ZHONG (Presenter), HUNG-SHEN CHANG, University of Chicago, KEVIN SATZINGER, UC Santa Barbara; University of Chicago, MING-HAN CHOU, AUDREY BIENFAIT, CHRISTOPHER CONNER, ETIENNE DUMUR, JOEL GREBEL, University of Chicago, GREGORY A PEAIERS, UC Santa Barbara; University of Chicago, RHYS G POVEY, DAVID SCHUSTER, ANDREW N CLELAND, University of Chicago — Quantum communication relies on the efficient generation of entanglement between remote quantum nodes, due to entanglement's key role in achieving and verifying secure communications. Remote entanglement has been realized using a number of different probabilistic schemes, but deterministic remote entanglement has only recently been demonstrated, using a variety of superconducting circuit approaches. However, the deterministic violation of a Bell inequality, a strong measure of quantum correlation, has not to date been demonstrated in a superconducting quantum communication architecture, in part because achieving sufficiently strong correlation requires fast and accurate control of the emission and capture of the entangling photons. Here we present a simple and robust architecture for achieving this benchmark result in a superconducting system.

*This effort is supported by the Army Research Office under contract W911NF-15-2-0058, the Air Force Office of Scientific Research, and the Department of Energy. This work was partially supported by the UChicago MRSEC (NSF DMR-1420709) and made use of the Pritzker Nanofabrication Facility, which receives support from ShyNE, a node of the National Science Foundation’s National Nanotechnology Coordinated Infrastructure (NSF NNCI-1542205).
12:51PM B26.00009: Microwave remote state preparation vs. quantum cryptography

FRANK DEPPE (Presenter), KIRILL FEDOROV, STEFAN POGORZALEK, MINGXING XU, QU-MING CHEN, MICHAEL FISCHER, MICHAEL RENGER, EDWAR XIE, Walther-Meißner-Institut & Physik-Department, Bayerische Akademie der Wissenschaften & Technische Universität München, ACHIM MARX, Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, RUDOLF O GROSS, Walther-Meißner-Institut & Physik-Department, Bayerische Akademie der Wissenschaften & Technische Universität München — Quantum communication protocols employ nonclassical correlations as a resource for an efficient transfer of quantum states [R. Di Candia et al., EPJ Quantum Technol. 2, 25 (2015)]. As a fundamental protocol, remote state preparation (RSP) aims at the preparation of a known quantum state at a remote location using classical communication and quantum entanglement. In our experiment, we use flux-driven Josephson parametric amplifiers and linear circuit elements to generate propagating two-mode squeezed (TMS) microwave states acting as quantum resource [K. G. Fedorov et al., Phys. Rev. Lett. 117, 020502 (2016); K. G. Fedorov et al., Sci. Rep. 8, 6416 (2018)]. Combined with a classical feedforward, we use these TMS states to remotely prepare single-mode squeezed states. Furthermore, we analyze the consumption of quantum discord in our experiment and interpret our results in the framework of a quantum cryptographic protocol analogous to the Vernam cipher.

*The authors acknowledge support from the EU Quantum Flagship project QMiCS, the German Research Foundation (DFG) through FE 1564/1-1 and the excellence cluster 'Nanosystems Initiative Munich (NIM)', the IMPRS 'Quantum Science and Technology', and the doctorate program ExQM of the Elite Network of Bavaria.

1:03PM B26.00010: Generating Non-Classical and Spatially-Correlated Photons in a Waveguide QED Architecture

BHARATH KANNAN (Presenter), DANIEL CAMPBELL, RONI WINIK, Research Laboratory of Electronics, Massachusetts Institute of Technology, DAVID K KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, JONILYN L YODER, MIT Lincoln Laboratory, Massachusetts Institute of Technology, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, WILLIAM D OLIVER, Department of Physics, Research Laboratory of Electronics, MIT Lincoln Laboratory, Massachusetts Institute of Technology — In waveguide quantum electrodynamics (wQED), atoms interact with a guided continuum of photonic modes. These systems can serve as a platform to study exotic radiation phenomena. The electrical distance between atoms along the waveguide is controllable by tuning the frequency, and thus the wavelength, of light emitted from the atoms. This enables the exploration of a wide variety of radiation phenomena. In this work, we experimentally study devices with multiple superconducting transmon qubits that are strongly coupled to a one-dimensional co-planar waveguide. We present experimental results demonstrating the generation of non-classical and spatially correlated photons in a wQED setting.

*This research was funded in part by an IC Postdoctoral Fellowship; a National Defense Science and Engineering Graduate Fellowship, and by the Department of Defense via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.

1:15PM B26.00011: Quantum Communication with Microwave Photons

ANDREAS WALLRAFF (Presenter), ETH Zurich — Sharing information coherently between physically separated chips in a network of quantum computers could be an essential element for realizing a viable quantum information processing system. A direct, deterministic quantum channel may be advantageous both for larger scale fault-tolerant or non-error-corrected quantum processors realizing universal quantum computation or solving noisy intermediate-scale quantum (NISQ) problems. We implement a deterministic state transfer and entanglement protocol between individually packaged chips connected by coaxial lines [1]. Individual chips may serve as universal nodes capable of sending, receiving, storing, and processing quantum information. Our protocol is based on an all-microwave process, which entangles or transfers the state of a superconducting qubit with a time-symmetric itinerant single photon. We transfer qubit states at rates of 50 kHz, absorb photons at the receiving node with a probability of 98 %, achieve a transfer process fidelity of 80 %, prepare on demand remote entanglement with a fidelity of 79 % and show that time bin encoding can be used to further improve these metrics.

**1:27PM B26.00012: Raman Transitions between two Superconducting Cavity Modules via Parametric Conversion:**

**Part I** JAMES TEOH (Presenter), LUKE BURKHART, CHRISTOPHER J AXLINE, YAXING ZHANG, LUIGI FRUNZIO, MICHEL H. DEVORET, STEVEN GIRVIN, LIANG JIANG, ROBERT J SCHOELKOPF, Yale Univ — We investigate a simple quantum network capable of state transfer and entanglement between superconducting 3D cavities in two spatially separated modules. Bidirectional communication between the cavity modes is established by coupling each cavity to the same standing-wave mode of a superconducting coaxial cable via parametric conversion. The system can be made robust to loss in the cable by using off-resonant conversion to engineer a virtual Raman transition between the three modes (cavity-cable-cavity), which suppresses the population of the lossy cable mode. Preliminary experimental results regarding state transfer will be discussed.

*This work is supported by US Army Research Office grant W911NF-18-1-0212

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**1:39PM B26.00013: Raman Transitions between two Superconducting Cavity Modules via Parametric Conversion:**

**Part II** LUKE BURKHART (Presenter), JAMES TEOH, CHRISTOPHER J AXLINE, YAXING ZHANG, LUIGI FRUNZIO, MICHEL H. DEVORET, STEVEN GIRVIN, LIANG JIANG, ROBERT J SCHOELKOPF, Yale Univ — Entanglement generation between modules in a quantum network allows for gates between qubits in separate modules. A partial swap of population between two modes can be used to generate entanglement. We engineer such an entangling operation with a virtual Raman transition via a standing-wave mode of a coaxial cable. Preliminary results towards generating on-demand entanglement between two modules will be shown. Schemes for improving the entanglement by making use of multiphoton quantum states will be discussed.

*This work is supported by US Army Research Office grant W911NF-18-1-0212.

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**1:51PM B26.00014: Generation of a microwave time-bin qubit with a superconducting qubit** JESPER ILVES (Presenter), SHOTA YAMAZAKI, SHINGO KONO, YOSHIKI SUNADA, MINKYU KIM, The University of Tokyo, KAZUKI KOSHINO, Tokyo Medical and Dental University, YASUNOBU NAKAMURA, The University of Tokyo — Quantum information can be encoded in a propagating photonic qubit by constructing a set of computational basis states with one or more modes of light. This encoding scheme defines the characteristic properties of the qubit such as its decoherence properties and how it retains phase information. By encoding the qubit in a basis constructed from two orthogonal temporal modes, as a time-bin qubit, it is possible to detect and correct photon decay during information transfer with a parity measurement. We experimentally demonstrate a protocol for deterministic on-demand generation of a time-bin qubit in the microwave regime through microwave-driven coherent control of a transmon qubit placed in a three-dimensional cavity. To perform quantum state tomography on a prepared time-bin qubit state, we apply iterative maximum likelihood estimation on time-bin encoded single-photon signal squeezed in different quadratures. We also discuss different factors affecting the time-bin qubit state preparation fidelity. Our protocol can be used as a means of realizing robust information transfer in quantum networks.

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**2:03PM B26.00015: Time-Bin Entanglement Between Remote Superconducting Cavities** EVAN ZALYS-GELLER (Presenter), PHILLIPE CAMPAGNE-IBARCQ, ANIRUDH NARLA, SHYAM SHANKAR, Yale Univ, CHRISTOPHER J AXLINE, ETH Zurich, LUKE BURKHART, Yale Univ, WOLFGANG PFAFF, Microsoft, LUIGI FRUNZIO, ROBERT J SCHOELKOPF, MICHEL H. DEVORET, Yale Univ — Generation of entanglement between qubits connected by a lossy channel is an important primitive for large scale quantum information processing. Time-bin entanglement allows one to counter this imperfection through detection of photon loss errors in the channel. We present an experiment for time-bin entanglement between remote superconducting cavities. Stimulating a particular three-body Raman transition performs an entangling gate between a flying photon, target system, and an ancillary mode used as an entanglement witness. This ancillary mode, equivalent to a photon detector, is used to herald success of the protocol. The success rate of this protocol is expected to reach the transmission of the channel. Through local measurement of the ancillary modes, we can detect photon loss errors in the channel and herald the creation of an entangled Fock state between the remote cavities. We discuss experimental progress towards the implementation of this protocol.

*Work supported by ARO, AFOSR, ONR, NSF and YINQE.

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**Monday, March 4, 2019 11:15 AM - 2:15 PM**

**Session B27 DQI: Superconducting Circuits: Quantum Simulations and Many-Body Physics** BCEC 160C
Predicting the dynamics of quantum systems is a primary example of an intensive computational task that could be efficiently solved with a near term quantum computer. To pursue this goal, we have fabricated a 9-qubit linear chain device made of superconducting circuits with nearest neighbor couplings. Our device is unique because it features frequency tunable qubits and an adjustable inter-qubit coupling strength, making it well suited to the simulation of quantum systems. We use the device to generate high-fidelity, multi-qubit, analog dynamics evolving under a Bose-Hubbard Hamiltonian. In this talk, we discuss the calibration of this device for quantum simulation. Once calibrated we use this device to probe the basic physics of thermalization. Specifically, we use transport measurements to distinguish localized and diffusive behavior. To complement this, we use echo techniques to characterize the propagation of entanglement in these regimes. This shows qualitative differences between how energy and entropy flow in the system.

The rich physics of strongly-correlated quantum materials can be explored in synthetic systems built with microwave photons in superconducting circuits in the circuit QED paradigm. However, the intrinsic loss in photonic platforms makes many-body quantum state preparation a challenge. We build a 1D Bose-Hubbard lattice for photons where capacitively coupled transmon qubits serve as lattice sites, and the transmon anharmonicity corresponds to strong photon-photon interaction. We employ an engineered reservoir to realize a dissipatively stabilized site and couple it to the lattice to stabilize a n=1 Mott insulator. Site-resolved microscopy allow detailed studies of the thermalization process through the dynamics of defect propagation and removal in the Mott phase. By probing two-site correlations, we could investigate the emergence of correlations and entanglement in these driven-dissipative systems.

This work was supported by Army Research Office grant W911NF-15-1-0397
Support was provided by the Chicago MRSEC, which is funded by NSF through grant DMR-1420709.
This work was supported by MURI ARO Grant No. W911NF-15-1-0397
This work was also supported by NSF Grant No. ECCS - 1542205

Encoding quantum information in the higher energy levels of the transmon circuit provides a hardware efficient way to harness a larger Hilbert space in existing quantum processors while also increasing their connectivity. Furthermore, a network of qutrits (three-level systems) is naturally suited to experimentally demonstrate recently identified connections between high energy physics and quantum information, such as holographic quantum error correction codes and the physics of scrambling. Here we report on the control of a five-qutrit processor and our progress toward characterizing the scrambling of quantum information. We implement a circuit to measure the decay of out-of-time ordered correlators, a hallmark of scrambling, in a method that distinguishes between decoherence and scrambling. The same circuit can be viewed as a teleportation protocol where quantum information is scrambled by a black hole and then decoded through measurement of emitted Hawking photons.

This work was supported by the Army Research Office and the Department of Energy.

The field of circuit QED has emerged as a rich platform for both quantum computation and quantum simulation. Lattices of coplanar waveguide (CPW) resonators realize artificial photonic materials in the tight-binding limit. In combination with qubit-mediated photon-photon interactions, these systems can be used to study dynamical phase transitions and many-body phenomena in driven-dissipative systems. In this talk, we will show how graph-theory and graph-level operations can be used to tailor the single-particle band structures of such systems. In particular, we will show that the process of taking a line graph produces controllably gapped flat bands at −2 and that subdividing all graph edges produces Dirac cones from formerly quadratic band edges and chiral flat bands at zero energy.

This research was supported by the Princeton Materials Science Postdoctoral Fellowship and Army Research Office Grant W911NF-15-1-0397.
12:03PM B27.00005: Tunable-profile qubit-photon bound state interactions with superconducting circuits*  
BASIL SMITHHAM (Presenter), Princeton University, NEEREJA SUNDARESAN, IBM T.J. Watson Research Center, PRZEMYSLAW BIENIAS, REX LUNGDREN, QI/QuICS NIST/University of Maryland, College Park, ALEXEY V GORSHKOV, QI/QuICS NIST/University of Maryland, College Park, ANDREW HOUCK, Princeton University — Strongly coupling qubits to the band edge of a photonic crystal results in the formation of qubit-photon dressed bound states. The photonic components of these bound states are exponentially localized around the qubit positions and represent the inter-bound state interaction profiles. Tunability of the exponential localization length of bound state interactions has been experimentally demonstrated in superconducting circuits of two transmons coupled to a microwave photonic crystal [1]. To expand the range of 1D quantum models that can be probed with qubits coupled to photonic crystals, proposals have been put forth to engineer non-exponential interaction profiles by further dressing the systems with external driving fields [2]. We present experimental progress towards characterizing the effective bound states of transmons coupled to photonic crystals driven by auxiliary microwave tones. By driving the photonic crystal with multiple tones we aim to engineer non-exponential effective interactions, with the goal of accessing a broader class of tunable spin models.


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12:15PM B27.00006: Emulating Majorana Fermions Using Transmon Qubits with Application to Topological Quantum Computing  
ALIREZA NAJAFI-YAZDI (Presenter), Anyon Systems Inc — Majorana Fermions are fermionic modes with non-abelian dynamics and are of significant interest to realize topologically protected quantum processors. There have been significant efforts by the community to realize the Majorana modes in solid-state devices. Despite significant progress, fabricating and operating a Majorana qubit has proven to be extremely challenging.

In this talk, we propose a different approach: instead of trying to realize Majorana modes in solid-state systems such as Superconducting/Semiconducting nanowires, we propose to engineer an array of transmon qubits to realize a meta material with Majorana modes. We will present an example design of such system, the chip layout, as well as discuss braiding, fusion, and readout schemes. We will also discuss intricacies and constraints associated with practical device fabrication procedures.

12:27PM B27.00007: High coherence quantum simulation of coherent backscattering in an effective two-level system composed of two superconducting qubits*  
ANA GRAMAJO (Presenter), Research Laboratory of Electronics, Massachusetts Institute of Technology, Bariloche Atomic Center, DAN CAMPBELL, BHRAT KANNAN, Research Laboratory of Electronics, Massachusetts Institute of Technology, DAVID K KIM, ALEXANDER MELVILLE, MIT Lincoln Laboratory, BETHANY M NIEDZIELSKI, Department of Physics, Massachusetts Institute of Technology, JONILYN L YODER, MIT Lincoln Laboratory, DANIEL DOMÍNGUEZ, MARÍA JOSÉ SÁNCHEZ, Balseiro Institute, Bariloche Atomic Centre, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, WILLIAM D OLIVER, Research Laboratory of Electronics, MIT Lincoln Laboratory, Department of Physics, Massachusetts Institute of Technology — In a recent experiment by Gustavsson et al. [1], a superconducting flux qubit was used to model scattering events using multiple Landau-Zener transitions by driving the qubit periodically back and forth through an avoided crossing. In highly coherent systems, time-reversal symmetry in the driving field should give rise to a dip in the average transition rate (averaged over many quantum trajectories), by analogy with weak localization in condensed matter systems. We experimentally emulate the scattering events with multiple Landau-Zener transitions in an effective two-level system, seeking to demonstrate the theoretically predicted weak localization phenomenon in this system, Ferrón et al. [2]. The effects of system-bath coupling are accurately simulated by a Floquet-Markov master equation.


*This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.
12:39PM B27.00008: Demonstration of a non-stoquastic Hamiltonian in coupled superconducting flux qubits

ISIL OZFIDAN (Presenter), CHUNQING DENG, MOHAMMAD AMIN, ANATOLY SMIRNOV, TREVOR LANTING, D-Wave Systems —
Currently available quantum annealers (QA) provide solutions to the transverse field Ising model with thousands of magnetically coupled qubits. To achieve a non-stoquastic Hamiltonian with QA, coupling via two canonically conjugate (orthogonal) degrees of freedom is necessary. Furthermore this orthogonal coupling can potentially enhance the performance of QA processors and enable an extended range of quantum simulations. Here we present one- and two-qubit microwave spectroscopy as well as time evolution measurements on two superconducting flux qubits coupled via two orthogonal degrees of freedom, charge and flux. We show that the electrostatic interaction, realized through a coupling capacitor, produces $\sigma_y\sigma_y$ coupling in the computational basis and leads to broken gauge invariance. We also observe emergence of $\sigma_x\sigma_x$ coupling through higher energy states of each rf-SQUID. Finally, we show that the reduced two qubit Hamiltonian is nonstoquastic across a wide range of parameters.

12:51PM B27.00009: Metamaterial Slow-Light Waveguide for Finite Range Interactions and Non-Markovian Dynamics with Superconducting Qubits*

VINICIUS FERREIRA (Presenter), JASH BANKER, MOHAMMAD MIRHOSSEINI, ALP SIPAHIGIL, OSKAR PAINTER, Applied Physics and Material Science, Caltech — The ability to engineer the dispersion of light through subwavelength patterning of bulk materials has been a powerful tool for studying the influence of novel electromagnetic environments on light-matter interactions. Here, we present the experimental realization of an on-chip superconducting metamaterial waveguide composed of an array of coupled resonators of subwavelength size and negligible frequency disorder. By matching the array boundaries to 50Ω coplanar waveguides, our design achieves an 80MHz bandwidth photonic channel with nearly constant group index of ~650, as well as extinction of more than 70dB outside of the passband. Coupling transmon qubits to this metamaterial allows us to study non-Markovian dynamics of a single qubit's interaction with the photonic bath, as well as collective non-Markovian dynamics of multiple qubits. Moreover, far from the passband, we can dynamically measure finite-range qubit-qubit interactions that extend beyond nearest neighbor and depend on detuning from the bandedge. We thus establish our metamaterial design as an attractive platform for studying photon-mediated non-Markovian dynamics and quantum many-body physics.

*AFOSR MURI Quantum Photonic Matter
Institute for Quantum Information and Matter (IQIM)

1:03PM B27.00010: Roadmap to a superconducting quantum many body simulator

YARIV YANAY (Presenter), Laboritory for Physical Sciences, DANIEL CAMPBELL, JOCHEN BRAUMÜLLER, Massachusetts Institute of Technology, WILLIAM D OLIVER, Massachusetts Institute of Technology and MIT Lincoln Laboratory, CHARLES TAHAN, Laboratory for Physical Sciences — A superconducting circuit constructed from a repeating pattern of identical unit cells comprising qubits or resonators can be used to simulate a quantum many body system of spins or bosons. While single or few qubit systems have been repeatedly demonstrated in the last few years, the majority of those require tuning each individual qubit frequency through individual control lines. Here, we propose how a larger two-dimensional system can be realized with far fewer control lines by focusing on qubit designs that can be uniformly fabricated, with deviation from the design frequency acting as disorder. We examine the operating regimes for such a system and the required fabrication accuracy, as well as readout and control schemes. We discuss how a such a superconducting system could be prepared in non-thermal states in different parts of the many-body spectrum, and consider what observables could be accessed and whether they could be used to test assumptions on entanglement entropy and eigenstate thermalization in 2D systems.

1:15PM B27.00011: Synthetic quantum materials in superconducting circuits*

RUICHAO MA (Presenter), BRENDA SAXBERG, CLAI OWENS, JONATHAN SIMON, DAVID SCHUSTER, University of Chicago — Superconducting circuits have emerged as a competitive platform for quantum computation, satisfying the challenges of controllability, long coherence and strong interactions. Here we apply this toolbox to the exploration of strongly correlated quantum matter, building a Bose-Hubbard lattice for photons in the strongly interacting regime. We develop a versatile recipe for the dissipative preparation of incompressible many-body phases through reservoir engineering and apply it in our system to realize the first Mott insulator of photons. Site- and time-resolved readout of the lattice allows microscopic observation of the lattice dynamics. The low entropy Mott state can serve as a starting point for studying other strongly correlated phases, e.g. a Tonks-Girardeau gas of interacting defects. The dissipative preparation demonstrated in this work also enable future exploration of elusive interacting topological phases.

*This work was supported by the Chicago MRSEC, which is funded by NSF through grant DMR-1420709; and by ARO Grant No. W911NF-15-1-0397.
1:27PM B27.00012: Time-Resolved Measurements of Energy Transport in a System of Coupled Superconducting Qubits Inspired by Simulations of Photosynthetic Processes  GRAHAM J. NORRIS (Presenter), ANTON POTOČNIK, MICHELE COLLODO, ABDULKADIR AKIN, SIMONE GASPARINETTI, CHRISTOPHER EICHLER, ANDREAS WALLRAFF, Department of Physics, ETH Zurich — Engineered quantum systems have recently found application as a test-bed for answering open questions about energy transport in complex open quantum systems such as photosynthetic systems. Using a circuit incorporating three superconducting transmon qubits, we simulate energy transport with electron-phonon interactions, where we emulate longitudinal coupling to different types of phononic baths by applying engineered flux noise to the qubits. Previously, we considered the effects of noise on energy transport efficiency in steady-state measurements under continuous driving [1]. To study the transport of single photons, we now switch to pulsed excitations and time-resolved measurements. We verify the quantum nature of the excitations transported through the system in anti-bunching measurements, showing second-order correlation functions with \( g^{(2)}(0) < 0.05 \), observe coherent oscillations of the emitted power indicative of static coherence, and study the efficiency of transport as a function of noise type.


1:39PM B27.00013: Quantum impurity in a 1D photonic crystal* ANDREI VRAJITOAREA (Presenter), Princeton University, REX LUNDGREN, YIDAN WANG, PRZEMYSŁAW BIENIAS, ALEXEY GORSHKOV, JQI-NIST, ANDREW HOUCK, Princeton University — Quantum impurity problems are described in terms of a single quantum-mechanical degree of freedom interacting with a dissipative reservoir. Superconducting circuits offer an ideal platform for studying the quantum dynamics of artificial atoms embedded in the electromagnetic continuum of a one-dimensional waveguide, reaching non-perturbative coupling regimes in the spin-boson model for an ohmic bath. Parallel experiments have explored transmon qubits strongly coupled to a photonic crystal, where the impurity hybridizes with the band structure resulting in a photonic bound state inside the gap. In this talk we present recent efforts in further pushing the coupling strength with the stepped impedance microwave crystal, using an artificial atom with a large magnetic moment, the fluxonium circuit. The goal of this experiment is to explore how photon scattering inside the waveguide is influenced by the significance of counter-rotating coupling terms and by the nonlinear photon dispersion in the crystal.

*This work is supported by the National Science Foundation under Grant no. PHY-1607160.

1:51PM B27.00014: Quantum impurity physics simulation with superconducting circuits I: perturbative regime NITISH JITENDRAKUMAR MEHTA (Presenter), ROMAN KUZMIN, NICHOLAS GRABON, RAY MENCIA, VLADIMIR MANUCHARYAN, University of Maryland, College Park — We report our progress in the field of quantum impurity simulations with superconducting circuits. Our simulator consists of a split Josephson junction terminating a high-impedance transmission line, which is made of a linear chain of up to 40,000 junctions [1,2]. In part I, we start with a relatively large area split-junction, such that its quartic anharmonicity can be treated as a perturbation. In this regime, the system is well-described by a Caldeira-Leggett model of a quantum degree of freedom interacting with an Ohmic bath. The interaction effects are revealed through the measurement of the frequency shifts of over 100 discrete modes of the bath. In part II, we explore small-area impurity junction where the non-linearity is non-perturbative. Now the system can be described by a boundary sine-Gordon quantum impurity model. It is expected that inelastic scattering of single photons becomes the dominant photon loss mechanism, with the loss frequency dependence containing information on the many-body correlation functions. We will present the measurements at various line impedances and impurity parameters.


2:03PM B27.00015: Quantum impurity physics simulation with superconducting circuits II: many-body regime ROMAN KUZMIN (Presenter), NITISH JITENDRAKUMAR MEHTA, NICHOLAS GRABON, RAY MENCIA, VLADIMIR MANUCHARYAN, University of Maryland, College Park — We report our progress in the field of quantum impurity simulations with superconducting circuits. Our simulator consists of a split Josephson junction terminating a high-impedance transmission line, which is made of a linear chain of up to 40,000 junctions [1,2]. In part I, we start with a relatively large area split-junction, such that its quartic anharmonicity can be treated as a perturbation. In this regime, the system is well-described by a Caldeira-Leggett model of a quantum degree of freedom interacting with an Ohmic bath. The interaction effects are revealed through the measurement of the frequency shifts of over 100 discrete modes of the bath. In part II, we explore small-area impurity junction where the non-linearity is non-perturbative. Now the system can be described by a boundary sine-Gordon quantum impurity model. It is expected that inelastic scattering of single photons becomes the dominant photon loss mechanism, with the loss frequency dependence containing information on the many-body correlation functions. We will present the measurements at various line impedances and impurity parameters.

11:15AM B28.00001: Spurious topological entanglement entropy and subsystem symmetries in compactified cubic code
DOMINIC WILLIAMSON (Presenter), ARPIT DUA, MENG CHENG, Yale Univ — Compactifying one direction of the cubic code results in a family of two dimensional topological orders, equivalent to stacks of toric code enriched by translation symmetry. Surprisingly, some of these models have unbroken rigid 1D subsystem symmetries that lead to spurious contributions to the topological entanglement entropy. These spurious contributions can appear in a bulk computation of the topological entanglement entropy from a linear combination of subregion entropies with cancelling boundary terms. We introduce an entropic quantity that measures the presence of such spurious contributions.

11:27AM B28.00002: Low overhead Clifford gates from joint measurements in surface, color, and hyperbolic codes*
SEYED ALI HOSSEINI LAVASANI (Presenter), MAISSAM BARKESHLI, Department of Physics, University of Maryland College Park — One of the most promising routes towards fault-tolerant quantum computation utilizes topological quantum error correcting codes, such as the $\mathbb{Z}_2$ surface code. Logical qubits can be encoded in a variety of ways in the surface code. However proposed fault-tolerant implementations of the Clifford group in these schemes are limited and often require unnecessary overhead. In this work, we show that within any encoding scheme for the logical qubits, we can fault-tolerantly implement the full Clifford group by using joint measurements involving a single appropriately encoded logical ancilla. This allows us to provide new low overhead implementations of the full Clifford group in surface codes as well as color codes. It also provides the first proposed implementations of the full Clifford group in hyperbolic codes. We further use our methods to propose state-of-the-art encoding schemes for small numbers of logical qubits. To our knowledge, this is the optimal proposal to date, and thus may be useful for demonstration of fault-tolerant logical gates in small near-term quantum computers.

*This work is supported by NSF CAREER (DMR-1753240) and JQI-PFC-UMD.

11:39AM B28.00003: Universal logical gate sets on encoded qubits using constant depth unitary circuits* [Invited]
MAISSAM BARKESHLI (Presenter), Physics, University of Maryland, College Park — A basic question in the theory of fault-tolerant quantum computation is to understand the fundamental space-time overhead required for performing a universal logical set of gates on encoded qubits to arbitrary accuracy. In this talk, I will demonstrate how braiding and Dehn twists in arbitrary (Abelian and non-Abelian) topological codes can be implemented through constant depth unitary circuits, where the depth is independent of the code distance. These circuits consist of a local constant depth unitary circuit followed by a permutation on physical qubits. When applied to the Fibonacci Turaev-Viro codes, they provide the first example of a universal logical gate set through constant depth unitary circuits. Other methods require either measurements, with follow-up gate operations that depend on the results of those measurements, or require local unitary circuits whose depth increases linearly with code distance. Our results can be extended to the context of hyperbolic Turaev-Viro codes as well, which have constant space overhead (constant rate encoding). I will discuss the fault-tolerance properties of these circuits, and how they provide some of the most optimal schemes to date in terms of space-time overhead for universal fault-tolerant quantum computation.

*NSF CAREER (DMR-1753240), Alfred P. Sloan Foundation, JQI-UMD-PFC

12:15PM B28.00004: Exotic quantum wires from symmetry-enriched topological order interfaces*
WEIYI DING (Presenter), SHENGHAN JIANG, JASON ALICEA, Physics, California Institute of Technology — When two identical chiral topological orders merge, the gapless modes at their interface can annihilate—thereby forming a single, uninterrupted topological phase. We study such interfaces when one of the two phases is promoted to a symmetry-enriched topological order exhibiting an anyon-permuting symmetry. In this case symmetry provides an obstruction to gapping the interface; moreover, we show that the gapless, symmetry-preserving interface can realize nontrivial critical points with no fine-tuning required. Such exotic “quantum wires” can provide efficient building blocks for assembling two-dimensional topological orders hosting anyons with universal braid statistics.

*Caltech Summer Undergraduate Research Fellowships (SURF)
National Science Foundation through grant DMR-1723367
CHUN-XIAO LIU (Presenter), Delft University of Technology, CHING-KAI CHIU, Kavli Institute of Theoretical Sciences — Braiding Majorana zero modes is an important approach to understand the physics of the non-Abelian statistics. To experimentally achieve this approach, accurately reading the change of the quantum state through the braiding process is an essential step. In this talk, we propose an experimental protocol to read the braiding change of the Majorana zero modes. The scheme includes four spatially-separated Majorana zero modes on top of a Coulomb blockaded topological superconductor. The reading of the braiding change is implemented by measuring the tunnel conductance in the strong Coulomb blockade regime for two overlapped Majorana zero modes.

*Supported by the Strategic Priority Research Program of the Chinese Academy of Sciences, Grant No. XDB28000000

SAGAR VIJAY (Presenter), Physics, Harvard University — Recently, there has been a growing effort to store quantum information in fermion states, so that a qubit is encoded in the fermion occupation number or the fermion number parity. Using fermions as the carriers of quantum information necessitates a new computational model and new error-correcting codes, as Fermi statistics forbids a mapping of local quantum gates acting on fermions to local gates acting on bosons. Motivated by on-going experiments, we introduce a variety of fermionic quantum codes that are able to correct for fermion parity-preserving and parity-violating (“quasiparticle poisoning”) errors. First, we discuss a surface code of Majorana fermions, along with its implementation, and demonstrate that the threshold error-rates for this code are superior to that of bosonic surface codes. We then introduce a generic construction of fermion codes from weakly self-dual classical, binary error-correcting codes, and use this method to find the shortest fermion code to correct for quasiparticle poisoning errors and other codes that correct higher-weight errors. We conclude by discussing physical implementations of codes with shorter code distance.

Supported by the Harvard Society of Fellows

ZHI LI (Presenter), ROGER MONG, University of Pittsburgh — We consider the finite-temperature topological entanglement entropy (TEE) for topological-ordered systems. We found, quite generally, that the finite-temperature TEE is a piece-wise constant function for CSS codes, which include the toric code and some fracton models like Haah's code and the X-cube model. We also discuss the phase transition structure of CSS codes and possible connections with self-correctness.

OSCAR VIYUELA (Presenter), SAGAR VIJAY, LIANG FU, Department of Physics, Massachusetts Institute of Technology — The Majorana Surface Code (MSC) is a topological quantum code constructed out of interacting Majorana fermions, which can be used to store quantum information and perform topological quantum computation. In this talk, we show how purely fermionic errors (quasiparticle poisoning events) can be corrected provided the error rate is below a certain threshold. In addition, we show how bosonic and measurement errors poses higher error thresholds than spin-based topological memories like the Surface Code and the Color Code. These results together with the inherent protection against thermal fluctuations given by the superconducting gap make the MSC a strong candidate for a robust topological quantum memory.

ARPIT DUA (Presenter), DOMINIC WILLIAMSON, MENG CHENG, Yale Univ — We employ quantities generalizing the two-dimensional S-matrix invariant to categorize 3D stabilizers models into type-I fracton models, type-II fracton models, TQFTs and stacks of 2D Toric codes. These quantities count the numbers of anticommuting string-string, string-membrane and membrane-membrane operators. The scaling behavior of these quantities with the size of the strings and membranes gives a signature of the class of topological order. We also investigate two-dimensional compactifications of three-dimensional fracton models. We find the two-dimensional topological phases produced as a function of compactification radius and uncover translation symmetry-enrichment that leads to twisted boundary conditions. This allows us to interpret the complicated ground space degeneracy of type-II 3D fracton models in terms of the symmetry enriched anyons in the compactified model.
Classifying Subsystem Symmetry Protected Topological Phases

TRITHEP DEVAKUL (Presenter), Princeton University, DOMINIC WILLIAMSON, Yale University, YIZHI YOU, Princeton University, FIONA BURNELL, University of Minnesota, SHIVAJI SONDHI, Princeton University — We discuss symmetry protected topological (SPT) phases in 2D systems with subsystem symmetries: symmetries which act on rigid subsystems, such as along straight lines or fractals. The total symmetry group of such systems grows with system size and is infinitely large in the thermodynamic limit. Systems with linear subsystem symmetries exhibit a phenomenon wherein two states from different phases may differ only along a subsystem — leading to an infinitude of possible phases.

To address this issue we identify and classify the "intrinsic" information of phase which can be measured locally. This may be likened to equivalence classes of phases which differ by only transformations along subsystems.

We show that for linear subsystem SPTs, despite there being infinitely many phases, the classification of this intrinsic information is finite and depends only on the on-site symmetry group.

For fractal subsystem symmetries, this is not necessary: locality is enough to enforce a certain translation symmetry which leads to a number of possible phases.

We give an upper bound for the number of phases in such models where Hamiltonian terms are supported within L-by-L boxes.

These phases showcase how subsystem symmetries can lead to intriguing new physics even in simple cases.

A braiding quantum circuit based on the 4π Josephson effect

JOHN STENGER (Presenter), MICHAEL HATRIDGE, SERGEY M FROLOV, DAVID PEKKER, University of Pittsburgh — We propose a topological qubit in which braiding and readout are mediated by the 4π Majorana-Josephson effect. The braidonium device consists of three Majorana nanowires that come together to make a tri-junction; in order to control the superconducting phase differences at the tri-junction the nanowires are enclosed in a ring made of a conventional superconductor; and in order to perform initialization/readout one of the nanowires is coupled to a fluxonium qubit through a topological Josephson junction. We analyze how flux-based control and readout protocols can be used to demonstrate braiding and qubit operation for realistic materials and circuit parameters.

*Work is supported by NSF PIRE-1743717. S.M.F. is supported by NSF DMR-1743972, ONR, and ARO.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B29 DQI: Superconducting Qubits: Hamiltonian Engineering and Design Tools

11:15AM B29.00001: Quantization of Large Superconducting Circuits with Tensor Networks

KRISTINA COLLADAY (Presenter), MATTHEW WEIPPERT, DAVID FERGUSON, RYAN J EPSTEIN, Northrop Grumman — We introduce a novel method for efficient quantum simulation of large superconducting circuits using matrix product states (MPS) and the density matrix renormalization group (DMRG) technique. We analyze an LC oscillator containing a chain of Josephson junctions, forming a superinductor. We obtain the lowest-lying eigenstates and energies, and calculate physical observables of interest for chain lengths in the range of 5-65 Josephson junctions. We quantify simulation convergence through comparison with exact diagonalization (when possible) and quantum state variance. Our approach reaches far beyond the resource limitations of brute-force exact diagonalization.

*This work is supported by IARPA and ARO.

11:27AM B29.00002: Towards Total Quantum System Characterization

GERARDO PAZ SILVA (Presenter), YA CAO, IVONNE GUEVARA PRIETO, Griffith University, CHRISTOPHER FERRIE, University of Technology Sydney — Quantum enabled technologies promise to deliver the next technological revolution. However, their realization requires a degree of control over quantum systems that is still elusive. The problem stems from our imperfect knowledge of the physical quantities ruling their evolution. To overcome this, system characterization tools such as Hamiltonian learning, noise spectroscopy, and state tomography have been devised. However, the success of each of these schemes often requires the knowledge provided by the other. For example, Hamiltonian learning protocols estimate the parameters of a Hamiltonian ruling the evolution of a set of qubits but require knowledge of any noise affecting them to be successful, while noise spectroscopy protocols can characterize the noise affecting the system of interest but require knowledge of the deterministic part of the Hamiltonian.

In this talk, we will present a limited-access total quantum system characterization tool. We show that it is possible to simultaneously extract the information that Hamiltonian learning, noise spectroscopy, and state tomography of a composite quantum system provide, when only limited-access is available, i.e., when fast and reliable control and measurements are possible in only a subsystem.
**11:39 AM B29.00003: Exact quantization of superconducting circuits**

MOHAMMAD H. ANSARI (Presenter), Forschungszentrum Julich — Circuits consisting of weak anharmonic qubits coupled to cavity multimodes are theoretically quantized beyond dispersive regime. In order to do this, we obtain a unitary transformation that diagonalizes harmonic sector of the circuit. Weak anharmonicity does not alter normal mode basis, however, it modifies energy levels. Using our formalism, we quantify two circuits of: 1) a transmon coupled to a resonator, and 2) two transmons coupled to a bus resonator. In both circuits, we determine dressed frequencies and Kerr nonlinearities in closed form formulas. Our results are valid for arbitrary frequency detuning and coupling within and beyond dispersive regime.


*Support from Intelligence Advanced Research Projects Activity (IARPA) under contract W911NF-16-0114 is gratefully acknowledged.

**11:51 AM B29.00004: Numerical Methods for Current Mirror Qubit Simulations**

DANIEL WEISS (Presenter), Department of Physics and Astronomy, Northwestern University, DAVID FERGUSON, MOE S KHALIL, Northrop Grumman Corporation, ANDY C. Y. LI, Scientific Computing Division, Fermi National Accelerator Laboratory, JENS KOCH, Department of Physics and Astronomy, Northwestern University — Current Mirror Qubits (CMQs) are an example of “noise insensitive” superconducting qubits predicted to exhibit longer coherence times than conventional superconducting qubits even when exposed to the same noise environment. CMQs also have the advantage of not requiring detailed tune-up or fabrication precision to achieve noise insensitivity. However, given the large number of circuit components that comprise such qubits, direct numerical diagonalization of the qubit’s Hamiltonian using a product basis is numerically intractable. This presents a challenge for verifying projected noise immunity for realistic circuits that include fabrication imperfections or control offsets. This talk discusses various numerical models for CMQs that address this challenge, and presents initial comparisons between these models and experimental realizations of these qubits.


*This research was supported by the Army Research Office under contract W911NF-17-C-0024.

**12:03 PM B29.00005: Quantum Engineering Design of Superconducting Qubits**

DAVID FERGUSON (Presenter), DAVID CLARKE, Northrop Grumman, DANIEL WEISS, JENS KOCH, Northwestern University — Many novel superconducting qubits have circuits with a large number of quantum components. Such circuits can require quantum engineering design, i.e., the numerical simulation of a large Hilbert space to determine optimal device performance. For this purpose, we introduce the Villain periodically Continued Harmonic Oscillator Basis (VCHOB). This general method allows for automated and efficient numerical diagonalization of superconducting circuits, increasing the types of circuits for which quantum engineering design is possible.

*This research was supported by the Army Research Office under contract W911NF-17-C-0024

**12:15 PM B29.00006: Energy-participation approach to the design of quantum Josephson circuits**

ZLATKO MINEV (Presenter), Department of Applied Physics, Yale University, New Haven, Connecticut 06511, USA, ZAKI LEGHTAS, Centre Automatique et Systèmes, Mines-ParisTech and Laboratoire Pierre Aigrain, École Normale Supérieure, Paris, France, SHANTANU O. MUNDHADA, Department of Applied Physics, Yale University, New Haven, Connecticut 06511, USA, IOAN-MIHAI POP, Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany, LYSANDER CHRISTAKIS, MICHEL H. DEVORET, Department of Applied Physics, Yale University, New Haven, Connecticut 06511, USA — Superconducting circuits incorporating non-linear devices, such as Josephson tunnel junctions and nanowires, are among the leading platforms for emerging quantum technologies. Promising applications require designing and optimizing circuits with ever-increasing complexity and controlling their dissipative and Hamiltonian parameters to several significant digits. Therefore, there is a growing need for a systematic, simple, and robust approach for precise circuit design, extensible to increased complexity. In this talk, we present such an approach to unify the design of dissipation and Hamiltonians around a single concept — the energy participation, a number between zero and one — in a single-step electromagnetic simulation. This markedly reduces the required number of simulations and allows for robust extension to complex systems. The approach is general purpose, valid for arbitrary non-linear devices and circuit architectures. We present experimental results on a variety of circuit quantum electrodynamics (cQED) devices and architectures, 3D and flip-chip (2.5D), which exhibit percent-level agreement for Hamiltonian parameters over five-orders of magnitude and across a dozen devices.

*Work supported by: ARO, ONR, NSF, AFOSR, and YINQE
Circuit quantization serves as a link between physical circuits and quantum Hamiltonians. The standard procedure [1] established decades ago implicitly assumes the external magnetic flux threading a circuit loop to be static. However, time-dependence arises inevitably when flux modulation or noise are considered. Naïve application of the existing circuit-quantization procedure can then lead to inconsistencies in predictions of qubit relaxation times. In this talk, we present a generalized approach to circuit quantization valid in the presence of time-dependent external sources. Our results uncover the reason for the inconsistency and resolve it, and are applicable to a wide range of circuits utilizing time-varying external fields.


*This research was supported by the Center for Applied Physics and Superconducting Technologies, Northwestern University and Fermi National Accelerator Laboratory.

Bayesian inference uses Bayes' theorem to update the probability of a hypothesis and as a result can be used to great effect when trying to learn the Hamiltonian of a quantum system. In comparison to traditional techniques for characterisation it has the benefit of providing statistically relevant information about the learning procedure, enabling more efficient data taking and revealing limits of the model provided to produce the data. It can be used to compare how well different models fit measured data and hence diagnose noise sources. We demonstrate this by applying it to a superconductor semiconductor 'gatemon' qubit and use it to learn the parameters of the Hamiltonian.

*We would like to acknowledge Microsoft Project Q, the U.S. Army Research Office, the Swiss National Science Foundation, the Danish National Research Foundation and NCCR QSIT.

The dynamics in a system of coupled qubits is proven to be computationally hard. Harnessing the computation power associated with these complex dynamics requires controlling the evolution with high fidelity, which in turn requires knowing the physical parameters of the system with high accuracy. Using a few coupled superconducting qubits, we discuss a method for extracting the values of the physical parameters of the system. In addition to the direct spectroscopy of the eigen-modes of the system, we generate controlled dynamics and measure the evolution of certain observables to refine the knowledge of the parameters obtained from spectroscopy. We discuss the accuracy of this calibration technique in terms of the requirements for performing a classically challenging computation.

We show that number non-conserving terms in the Josephson anharmonicity lead to a renormalization of the lifetime of microwave-driven superconducting qubits. Using a method of unitary transformations, we account for the frequently neglected number non-conserving terms in the Josephson potential, and show that they generate drive- and anharmonicity-dependent corrections of the qubit and readout resonator relaxation rates. Simultaneously, the number-conserving terms yield the known Kerr corrections to the eigenfrequencies of the system. We present our results in the form of effective master equations with renormalized Hamiltonian and collapse operators. Effective master equations provide an efficient tool to extract drive-, state- and anharmonicity-dependent relaxation rates.
1:15PM B29.00011: Drive-induced lifetime renormalization of superconducting qubits II: The Readout Problem
ALEXANDRU PETRESCU (Presenter), Université de Sherbrooke, MOHAMMAD MOEIN MALEKAKHLAGH, HAKAN TURECI, Princeton University —
Recent experiments found a strong dependence of qubit relaxation rates on the readout drive power. The observed dynamics cannot be fully explained by previous theoretical approaches based on the Jaynes-Cummings, Rabi or Kerr based models. We show that an effective master equation that accounts for renormalization of dissipative parameters due to number non-conserving terms inherent in the Josephson nonlinearity captures with good qualitative agreement this strong dependence. We account for a realistic experimental setting with a finite bath temperature and an additional pure dephasing channel, both of which are shown to significantly enhance the qubit relaxation renormalization with drive. Effective master equations for driven Josephson circuits appear to provide an accurate and computationally resource-efficient approach to experimentally relevant settings.

1:27PM B29.00012: Computational modeling of decay and hybridization in superconducting circuits
MICHAEL SCHEER (Presenter), MAXWELL B BLOCK, Rigetti Computing — We present a circuit theoretic technique for computing the complex frequencies and eigenmodes of superconducting circuits with radiative loss. We show that the transmon loss rates obtained by our method agree with the established approximation C/Re[Y] away from resonance and do not diverge near resonance. Additionally, we demonstrate that in systems with significant radiative loss, couplings between modes cannot be accurately computed if the loss is neglected. Our simulation technique is useful for designing complex superconducting quantum processors.

1:39PM B29.00013: Enablement of near-term quantum processors by architectural yield engineering*
SAMI ROSENBLATT (Presenter), JARED B HERTZBERG, JOSÉ CHAVEZ-GARCIA, NICHOLAS T BRONN, HANHEE PAIK, MARTIN SANDBERG, EASWAR M MAGESAN, JOHN A SMOLIN, JENG-BANG YAU, VIVEKANANDA ADIGA, MARKUS BRINK, JERRY M. CHOW, IBM Thomas J. Watson Research Center — Scaling of near-term quantum processors depends on complex architectures where maintaining low gate error rates relies on utilizing the highest coherence times available. In the case of fixed-frequency transmon qubits coupled via cross-resonance gates, multi-qubit operation is feasible as long as the excitation energies of neighboring qubits are similar but non-degenerate. Meeting this condition consistently in a large lattice of qubits requires precise Josephson junction fabrication and accurate frequency forecasting. In this talk, we will compare measured qubit frequencies to resistance measurements of Josephson junctions, and use a statistical model to suggest strategies for useful device yields at the 50 qubit and larger scale.

*We acknowledge support from IARPA under Contract No. W911NF-16-0114.

1:51PM B29.00014: Frequency trimming of superconducting fixed-frequency qubits
MUSTAFA BAL (Presenter), JUNLING LONG, RUSSELL LAKE, XIAN WU, COREY RAE MCRAE, HSIAANG-SHENG KU, National Institute of Standards and Technology Boulder, JARED B HERTZBERG, NICHOLAS T BRONN, JERRY M. CHOW, IBM T. J. Watson Research Center, DAVID PAPPAS, National Institute of Standards and Technology Boulder — There has been significant progress to increase the number of superconducting fixed-frequency qubits for multi-qubit gates. The variations in fabrication limits the precision in qubit frequency to within ~ 200 MHz of the design value [1], which could lead to undesired frequency crowding. We developed a frequency trimming process to correct the frequencies of the measured qubits. The frequency trimming involves first a chemical process to remove all on-chip wirebonds, followed by lithography and dry etch to trench the dielectric substrate near the qubit to tune the frequency to the target design value. We present fabrication process details, simulations, and qubit measurements.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B30 GSOFT: Liquid Crystals I  BCEC 162B - Cristina Martin Linares, Johns Hopkins University

11:15AM B30.00001: Liquid-Liquid Interfaces and Grain Boundaries Engineering of Soft Crystals  XIAO LI (Presenter), University of Chicago, JOSÉ A. MARTÍNEZ-GONZÁLEZ, Universidad Autónoma de San Luis Potosí, XUEDAN MA, Argonne National Laboratory, ORLANDO GUZMÁN, Universidad Autónoma Metropolitana, KANGHO PARK, JUAN DE PABLO, PAUL F NEALEY, University of Chicago — In solid state science, a considerable challenge remains in the development of techniques toward grain-boundary engineering, which is fundamental for designing materials with specific mechanical properties. Meanwhile, in soft matter a significant number of natural phenomena take place at liquid-liquid interfaces. Similar to grain boundaries of solid crystals, liquid-liquid interfaces lack of shape control, placing limits to applications in biosensing, photonics, directed self-assembly and adsorption phenomena. In this work, we build on soft-matter heteroepitaxy to grow, not solids, but single crystals of cubic liquid-crystalline BPs. Specifically, we rely on accurately designed binary-anchoring patterned substrates that facilitate spontaneous BP nucleation over the whole patterned region. This leads to a distortion-free BP-crystal, with a uniform lattice orientation that depends on the symmetry of the pattern used. Based on such liquid-liquid interfacial behavior, we produce large, stable and single-crystal BP-domains can serve as an alternative for engineering materials with accurately localized regions that respond sensitively to contaminants, incident light, electric or magnetic fields and other external stimuli.

11:27AM B30.00002: Cylindrical fiber cored by a double twisted chiral nematic  ADRIAN REYES (Presenter), GERARDO J. VÁZQUEZ, Instituto de Física, Universidad Nacional Autónoma de México — Abstract
We consider an electromagnetic field propagating within a waveguide consisting of a material having double helix, as those found in some chiral nematic materials such as blue phases, which lies along the axis of the fiber. We establish the electromagnetic equation governing the dynamics of the propagating modes and solve them numerically. We found the band structure of the mentioned modes, the profiles field amplitudes and the Poynting vector distributions versus the radius of the fiber. We discuss the composition and conditions for this modes to propagate.

11:39AM B30.00003: First-order smectic-hexatic phase transition in thick liquid crystal films*  IVAN ZALUZHNYY (Presenter), Department of Physics, University of California San Diego, RUSLAN KURTA, European XFEL, NASTASIA MUKHARAMOVA, YOUNG YONG KIM, RUSLAN KHUBBUTDINOV, DMITRY DZHIGAEV, Photon Science, Deutsches Elektronen-Synchrotron DESY, VLADIMIR LEBEDEV, ELENA PIKINA, EFIM KATS, Landau Institute for Theoretical Physics, NOEL ANTHONY CLARK, Department of Physics, University of Colorado Boulder, MICHAEL SPRUNG, Photon Science, Deutsches Elektronen-Synchrotron DESY, BORIS OSTROVSKIĬ, FSRC "Crystallography and photonics", IVAN VARTANYANTS, Photon Science, Deutsches Elektronen-Synchrotron DESY — Synchrotron studies with a focused x-ray beam of the first-order smectic-A – hexatic-B (Sm-A – Hex-B) phase transition in 2-10 μm thick free standing films of 54COOBC compound are presented. The Hex-B phase is distinguished from Sm-A phase by long-range bond-orientational (BO) order, which can be conveniently studied by the angular X-ray cross-correlation analysis (XCCA). Discontinuity in temperature dependence of positional correlation length and the BO order parameter as well as direct observation of phase coexistence clearly indicate the first-order character of the phase transition. Experimental data unambiguously show that the width of temperature region of two phases coexistence increases with film thickness. This effect is explained on the basis of Landau mean-field theory in the vicinity of a tricritical point by anomalous penetration of the Hex-B order parameter into the film interior.

*The project was supported by Helmholtz Association’s Initiative and Networking Fund and the Russian Science Foundation (18-41-06001, 18-12-00108), and the Ministry of Science and Higher Education of Russia (0033-2018-0003).
**11:51AM B30.00004: Liquid Crystal Flat Optical Elements**

ZIYUAN ZHOU (Presenter), MIAO JIANG, HAO YU, YUBING GUO, TARAS TURIV, O D LAVRENTOVICH, QI-HUO WEI, Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, Ohio, 44242, USA — Thin liquid crystal films (LCs) with well-defined molecular orientations are an exceptional platform for making flat optical devices based on the Pancharatnam-Berry phase. Here we present a new approach to designing and fabricating liquid crystal flat optical elements such as micro-lenses and beam-shapers. We show the molecular orientation patterns for shaping a light beam into desired intensity profiles can be designed using a generalized Snell's law, and that such liquid crystal flat optical elements can be made with high throughput and high resolution by using a plasmonic-metamask-based photopatterning approach.

*NSF CMMI-1663394

**12:03PM B30.00005: Cellulose Nanocrystals confined to polymer microgels**

SUJIN LEE (Presenter), ELSA REICHMANIS, MOHAN SRINIVASARAO, JUNG OK PARK, Georgia Institute of Technology — Liquid crystals that are confined within curved boundaries are of interest to many scientists due to their important role in optoelectronic technologies. As such, intensive research has been conducted with various types of liquid crystals constrained to droplets or cylindrical environments. Such studies are significant because the curvature of liquid crystals costs elastic energy, and hence, we observe rich physical phenomena such as change in the director field that otherwise would have been hidden. Most of the fundamental studies of liquid crystalline phase of the cellulose nanocrystals were conducted as a film type or in the cells with flat boundaries, limited to certain concentrations. Here, we report cellulose nanocrystals confined to pNIPAM microspheres using inverse emulsion polymerization technique with microfluidics device. The chiral nematic phase of cellulose nanocrystals are preserved within the polymer matrix, as characterized by optical microscopy. The droplet radius, R of the microgels can be adjusted by changing the volumetric flow rate of oil phase in a microfluidics device. Notably, the fabricated CNCs-PNIPAM microgels are able to exhibit swelling-deswelling behavior upon temperature change with well-organized structure.

**12:15PM B30.00006: Anisotropic diffusion of islands and topological defects in dipolar chains of islands in freely-suspended SmC liquid crystal films**

CHEOL PARK (Presenter), ERIC MINOR, JOSEPH E MACLENNAN, MATTHEW GLASER, NOEL ANTHONY CLARK, University of Colorado, Boulder — Islands, disk-like inclusions of extra layers in few-layer thick, freely-suspended tilted smectic liquid crystal films, stabilize +2π chiral vortices in the two-dimensional \(XY\) field giving the azimuthal orientation of the local molecular tilt. We have studied the Brownian motion of islands and their companion -1 defects on the background film in a dipolar chain of islands. The mean square fluctuations of the position are strongly anisotropic, the island mobility parallel to the chain direction being up to four times smaller than their mobility perpendicular to the chain. Measurements of thermal fluctuations of islands and topological defects in dipole chains will be compared with theoretical predictions.

*This work was supported by NASA Grants No. NNX-13AQ81G and No. NNX17AC74G and by the Soft Materials Research Center under NSF MRSEC Grants No. DMR-0820579 and DMR-1420736.

**12:27PM B30.00007: Two-Dimensional Hexagonal Boron Nitride Nanosheet as an Ion-Capturing Planar-Alignment Agent in a Liquid Crystal-Based Electro-Optic Device**

RAJRATAN BASU, LUKAS ATWOOD (Presenter), United States Naval Academy — The two-dimensional (2D) hexagonal boron nitride (h-BN) nanosheet is employed as a planar-alignment agent on one side of a liquid crystal (LC) cell, where the other side of the cell has a standard planar-alining polyimide (PI) layer. The LC exhibits uniform planar-alignment in this h-BN/PI hybrid cell. The free-ion impurities in the LC are found to be suppressed dramatically in this h-BN/PI hybrid cell compared to that in a standard PI/PI LC cell. The free-ion concentration is reduced in the hybrid cell due to the 2D h-BN nanosheet's ion-capturing process. The reduction of ionic impurities results in an accelerated electro-optic response of the LC in the hybrid cell. The dielectric anisotropy of the LC is enhanced in the h-BN/PI hybrid cell, indicating an improved orientational order parameter of the LC due to the reduction of ionic impurities.

*This work was supported by the Office of Naval Research (N0001418WX01842; N0001418WX01543) and the Naval Academy Research Council (NARC) 2018.
**12:39PM B30.00008: Study of phase behavior and (meta)stability of model surfactant solutions by microfluidic thermal fluctuation platform**  
HAOYU WANG (Presenter), SEPIDEH KHODAPARAST, JOAO CABRAL, Imperial College London  
— Metastability poses considerable challenges for the practical utilization of surfactant solutions subjected to ubiquitous temperature fluctuations. We first investigate aqueous solutions of a model biodegradable surfactant system (Linear Alkylate Sulfonate, LAS) at low concentrations, examining the mechanism and kinetics of the transition from micellar to multilamellar vesicle (MLV) phase, in the absence of salt and external flow. We then employ a novel microfluidic platform designed to rapidly modulate temperature fields and detect phase changes, coupled with optical microscopy and small angle neutron scattering (SANS). We resolve the MLV structure and decouple the nucleation and growth kinetics across the metastable zone width by imposing the square-wave temperature profiles. Finally, we demonstrate the imposition of complex temperature profiles, mirroring diurnal and seasonal variations, and their consequences to LAS micellar solution stability.

*This work is funded by the Centre for Process Innovation, Procter & Gamble, and BP.

**12:51PM B30.00009: Chiral symmetry-breaking dynamics in the phase transformation of nematic droplets**  
NASSER ABUKHDEIR (Presenter), FRED FU, Chemical Engineering, University of Waterloo  
— Chiral symmetry-breaking equilibrium textures in deformable and nondeformable droplets of achiral nematic liquid crystals (LCs) have long been observed for a broad range of LC compounds and conditions. Most of the observed chiral symmetry-breaking phenomena in achiral nematic LCs have involved spherical nematic droplets, which serve as ideal geometries for studying the interaction between surface and bulk elastic effects on nematic texture.

In this work, continuum simulations are performed of the formation of an initially isotropic phase nematic LC confined within a nanoscale nondeformable droplet with weak homeotropic surface anchoring conditions. Simulation conditions are chosen for the case where the equilibrium nematic texture is uniform. Beginning with an initial quench of the isotropic phase droplet, nematic formation occurs, initially forming an unstable radial-like texture. Subsequently, a spontaneous symmetry-breaking twist-mediated defect escape mechanism is observed for material parameters corresponding to pentyl-cyanobiphenyl (SCB) prior to the droplet evolving to stable uniform texture. Notably, this dynamic mechanism does not occur in simulations using the single-constant elastic constant approximation.

**1:03PM B30.00010: Brownian Dynamics of Particles “Dressed” by Chiral Director Configurations in Lyotropic Chromonic Liquid Crystals**  
ANGEL MARTINEZ (Presenter), University of Pennsylvania, PETER COLLINGS, Swarthmore College, A. G. YODH, University of Pennsylvania  
— We employ video microscopy to study the Brownian dynamics of colloidal particles suspended in the uniaxially aligned nematic phase of a lyotropic chromonic liquid crystal (LCLC), Disodium Cromoglycate (DSCG). DSCG is water soluble, and its nematic phase is characterized by an unusually large elastic anisotropy. Our measurements of the mean-square displacement for polystyrene-based colloidal microspheres show sub-diffusive behaviors along directions parallel and perpendicular to the nematic director. The dynamics parallel to the far-field director is sub-diffusive for lag times as long as several seconds and then diffusive beyond that, while the dynamics perpendicular to the far-field director continues to display complicated and unexpected sub-diffusive behavior for hundreds of seconds of lag time. Also, spherical colloids suspended in LCLCs can induce two symmetrically and energetically distinct director field configurations and we consider the effects of these differences on the diffusion dynamics of LCLC colloids. The origin of these deviations from conventional diffusion theory are discussed and our results are compared to previous diffusion experiments in conventional nematic liquid crystals.

*NSF Grant No. DMR16-07378  
PENN MRSEC Grant No. DMR17-20530  
NASA Grant No. NNX13AL27G

**1:15PM B30.00011: Interaction of liquid crystal skyrmions with curved boundaries**  
AVADH SAXENA (Presenter), AYHAN DUZGUN, Los Alamos National Laboratory  
— A liquid crystal cell is made by confining the liquid crystal material between two plates usually made of glass. In recent years, long-lived skyrmions, which are topological defect structures of the director field, have been realized in chiral nematic liquid crystal cells by means of establishing equilibrium between a background electric field and surface anchoring. These skyrmions interact with each other as well as with field gradients. In this work, we present numerical studies where an additional electric field, surface anchoring or light is used to generate “walls” to guide the motion of skyrmions. Specifically, we explore the motion of skyrmions near curved boundaries and how it is affected by the curvature.
1:27PM B30.00012: Magnetic Effects in Confined Nematic Liquid Crystal Droplets*  
SOPHIE ETTINGER (Presenter), ANGEL MARTINEZ, ALEXIS DE LA COTTE, Physics and Astronomy, University of Pennsylvania, PETER COLLINGS, Physics and Astronomy, Swarthmore College, ARJUN G YODH, Physics and Astronomy, University of Pennsylvania  
We study the structural transition of nematic liquid crystal (NLC) droplets with homeotropic anchoring in a uniform magnetic field. Confining NLC in droplets creates competition between surface anchoring energy and bulk elasticity, giving rise to distortions and defects. The effects of an electric field on the equilibrium director conformation of NLC droplets are well known, but studies using a magnetic field are scarcer due to the low magnetic susceptibility of most NLCs. We have developed a variable magnet mounted on a polarized microscope that can deliver up to 0.5T of uniform field. With this mechanism, we study the stability of hedgehog defects and the resulting Fréedericksz transition in NLC droplets. We confirm, as predicted theoretically, the formation of a ring defect whose radius increases with field strength as the director approaches a uniformly aligned state. We establish stability diagrams for NLC droplets of various radii and conduct comparative analysis of experimental and calculated threshold fields. Overall, this project aims to elucidate the director configurations of NLCs in confined geometries and to explore their bulk response to external magnetic fields.

*This work is supported by NSF DMR16-07378, PENN MRSEC Grant DMR-1720530, and NASA Grant NNX08AO0G.

1:39PM B30.00013: Liquid Crystals and the Optical Theorem  
XI CHEN (Presenter), NOEL ANTHONY CLARK, Soft Material Research Center, Department of Physics, University of Colorado, Boulder CO,80309  
The “optical theorem” is the calculation of plane electromagnetic wave propagation through a transparent dielectric slab, that views the slab as a uniformly distributed collection of point scatterers in a vacuum. The theorem shows that the apparent index of refraction of the slab is the result of the interference of the net forward scattered light with the incident beam. We are exploring this effect for the case where the slab is a nematic liquid crystal, probing in particular the effect of the strong scattering by director fluctuations on refractive index, and thus on phase fluctuations in the outgoing radiation.

*This work was supported by the Soft Materials Research Center under NSF MRSEC Grant DMR-1420736.

1:51PM B30.00014: Bent-Core Liquid Crystal with Polar Electro-optic Switching in the SmE phase  
Authors: Rayshan Visvanathan,1,2 Xi Chen,2, 3 Renfan Shao,2, 3 Min Shuai,2 Alexandra E. Duncan,2, 3 Eva D. Korblova,2, 4 Edward Guzman,2, 4 David M*  
RAYSHAN VISVANATHAN (Presenter), XI CHEN, RENFAN SHAO, MIN SHUAI, ALEXANDRA E DUNCAN, EVA D KORBLOVA, EDWARD GUZMAN, DAVID M WALBA, MATTHEW GLASER, JOSEPH E MACLENNAN, NOEL ANTHONY CLARK, University of Colorado, Boulder  
Polarizing optical microscopy and x-ray scattering measurements show that a new achiral, bent-core liquid crystal compound, W898, with a rigid core and a flexible tail exhibits a biaxial smectic phase with orthorhombic symmetry. Upon cooling from a higher temperature SmAPA phase, a SmE-like phase with long-ranged bond-orientational order and short-ranged, centered rectangular, in-plane positional order with local herringbone correlations forms. In this phase, the layers are macroscopically polar, and an applied electric field couples to the polarization to reorient the molecules, inducing a dramatic and rapid birefringence change in liquid crystal cells with planar alignment.

*This work was supported by the Soft Materials Research Center under NSF MRSEC Grant No. DMR-1420736 and NSF MRSEC Grant No. DMR-0820579.

2:03PM B30.00015: Interpretation of saddle-splay and the Oseen-Frank free energy*  
JONATHAN SELINGER (Presenter), Kent State University  
In this talk, we re-examine the oldest question in liquid-crystal physics: What are the elastic modes of a nematic liquid crystal? For this analysis, we use a recent mathematical construction [1], which breaks the director gradient tensor into four distinct types of mathematical objects. Based on this construction, we suggest an interpretation of saddle-splay as bulk rather than surface elasticity. This interpretation leads to an alternative way to think about several previous results in liquid-crystal physics, including: (1) free energy balance between cholesteric and blue phases, (2) director deformations in hybrid-aligned-nematic cells, (3) spontaneous twist of achiral liquid crystals confined in a torus or a cylinder, and (4) curvature of smectic layers.


*This work is supported by NSF Grant No. DMR-1409658.

Monday, March 4, 2019 11:15 AM - 2:15 PM
11:15AM B31.00001: Structure and reactivity of two-dimensional silica and zeolites* [Invited] JOACHIM SAUER (Presenter), Humboldt University of Berlin — Density functional theory is applied to solve the structures of ultrathin silica and zeolite films on metal substrates based on experimental information including LEED, IR-RAS, and STM. Specifically we discuss crystalline films consisting of one or two layers of corner-sharing TO₄-tetrahedra (T=Si, Al) on Mo(112) and Ru(0001) surfaces. We also discuss the formation of amorphous phases that can be directly imaged in real space by STM, and the substitution of Si with Ti and Fe which is not isomorphous but leads to new structure types. Joined computational – surface science studies on thin film zeolite models provide information for the limiting case of a flat surface corresponding to an infinitely large pore diameter. Whereas the non-specific adsorption energy is smaller on flat surfaces than inside zeolite pores, the acidity is significantly higher as OH frequency shifts on adsorption of molecules indicate. The consequences for understanding the acidity of layered powder materials (ZSM-5 layers) is discussed.

*This work has been funded by German Research Foundation (DFG)

11:51AM B31.00002: Hierarchical Zeolites: Synthesis and Applications [Invited] MICHELE OSTRAAT (Presenter), Advanced Materials, Aramco Services Company — Zeolites have been used extensively as industrial solid-acid catalysts in the oil refining and petrochemical industries due to their unique pore structures, acidity, and stability. Over the past two decades, innovations in synthesizing hierarchical zeolites have received continuous attention in both academia and industry for the potential to optimize catalytic performance of zeolite materials for in a wide range of refining and petrochemical applications that involve conversion of bulky molecules. The manipulation of hierarchy in zeolites can be achieved by different synthetic strategies that result in distinctive zeolites with various morphological, structural, and compositional characteristics. In this talk, we will discuss our recent progress on developing and optimizing hierarchical zeolites using top-down routes as well as bottom-up approaches with hard and soft templates and will summarize many of the unique underlying features for these different synthesis routes and their implications for large-scale industrial production of zeolites. We will also provide highlights on the utilization of these materials for important industrial applications related to oil refining and chemical productions.

12:27PM B31.00003: 2D Materials and Membranes for Biorefining and Hydrocarbon Separations [Invited] SANKAR NAIR (Presenter), Georgia Institute of Technology — The advent of 2D nanoporous materials has created exciting new possibilities in the scalable and economically viable fabrication of membranes for chemical separations. This talk will focus on our recent work in two areas of 2D membrane science and technology. Firstly, we will discuss new advances in the fabrication, modification, and scale-up of graphene oxide (GO) membranes, as well as their use in challenging applications in biorefining such as the fractionation of kraft black liquor and other related processes. Secondly, we will discuss our latest work on fabrication of 2D zeolite membranes on scalable hollow fiber platforms, and their applications in the separation of organic mixtures such as hydrocarbons from petrochemical processes or oxygenated molecules obtained from biomass conversion.

1:03PM B31.00004: Polymer-Grafted Nanoparticle Membranes with Unprecedented Gas-Separation Performance [Invited] SANAT KUMAR (Presenter), Chemical Engineering, Columbia University — Recent work has shown that nanoparticles grafted with polymer chains (GNPs) possess unusual collective properties. Their gas permeability shows non-monotonic behavior with increasing polymer length, with peak permeability increases of 8-20 times relative to the neat polymer. Similarly, their mechanical properties change from brittle to tough around the chain length with peak gas permeability. We show by combining small angle x-ray scattering, x-ray photon correlation spectroscopy and linear rheology that this behavior reflects the transition of the GNP materials from a jammed, soft glass-like state to liquid-like behavior with increasing chain length. For chain lengths below this transition, polymers on adjacent nanoparticles do not interpenetrate. Polymer melt incompressibility then results in a system where the coronas distort so that they tile space yielding a jammed (disordered) colloidal state. At longer chain lengths, this colloidal behavior disappears because chains on adjacent coronas interpenetrate. Since the dynamic properties of these systems, spanning time scale from the ps to the macroscopic, are affected by this transition we postulate that all of their transport properties should show anomalous behavior.
Regioselective Epoxide Ring Opening with Alcohols Using Heterogeneous Lewis Acidic Nano-Zeolites* [Invited] NICHOLAS BRUNELLI (Presenter), AAMENA PARULKAR, NITISH DESHPANDE, ALEXANDER SPANOS, RUTUJA JOSHI, BRIAN DIEP, Ohio State University, AMBARISH KULKARNI, UC Davis — Epoxides are versatile intermediates that can be ring opened using different nucleophiles to produce a wide variety of valuable chemicals. The key challenge for this reaction is selectivity. The regioselectivity of epoxide ring opening reactions for alcohols is examined using Lewis acidic catalysts. Through comparing catalytic activities, it is found that Sn-Beta is more active than other similar Lewis acidic catalytic materials such as Sn-MFI and Sn-SBA-15. For all materials, high regioselectivity of >99% is obtained when using epichlorohydrin with methanol. With large substrates such as epoxy hexane, diffusion limitations are encountered that can be overcome through creating zeolites with particle sizes less than 100 nm such as nano-Sn-MFI. These materials can be readily recycled while retaining high catalytic activity and selectivity. Hot filtration tests demonstrate that these catalysts are heterogeneous in nature and stable. Larger substrates such as epoxy octane result in diffusion limitations. We demonstrate the use of a new SDA to produce nano-Sn-Beta. This material can catalyze even larger structures. Overall, this demonstrates the importance of tuning material design to create highly active catalytic materials.

*This work was supported by NSF CBET Career (1653587), Ohio State University Institute of Materials Research (IMR-FG0211), and ACS-PRF (55946-DNIS).

Monday, March 4, 2019 11:15 AM - 1:15 PM

Session B32 DCP: Gas Phase Clusters - Experiment and Theory in Concert (B): Metal Clusters BCEC 204A - Marie-Pierre Gaigeot - Tag(s): Focus

11:15AM B32.00001: Mass Spectrometry and Theoretical Chemistry in Service of Catalysis Research: A Ménage-à-Trois at Its Best [Invited] HELMUT SCHWARZ (Presenter), Chemistry, Technische Universität Berlin — The ultimate goal in heterogeneous catalysis is to make use of each and every atom of supported (metal) catalysts, i.e. in the extreme to perform single-atom catalysis (SAC). While this arduous task constitutes a non-trivial, if not daunting challenge in 'real-life' chemistry, in the gas phase SAC can be achieved in a rather straightforward manner by conducting experiments with mass-selected species under (near) single-collision conditions. These mass spectrometry-based studies on isolated reactants, when complemented by state-of-the-art computational and spectroscopic work, provide an ideal arena for probing the energetics and kinetics of a chemical process in an unperturbed environment at a strictly molecular level without being obscured by ill-defined side effects. Thus, the concept of SAC can be explored or, more generally, the mechanisms of reactions and the active parts of single-site catalysts, the so-called 'aristocratic' atoms, can be identified.

Examples discussed include:
(i) The room-temperature, cluster-oxide mediated redox reactions of the CO/N₂O couple which, arguably constitute one of the most prominent oxidation processes, and
(ii) novel metal-mediated C-H bond activation and C-C coupling of methane, which are regarded as one of the holy grails in chemistry.

References:
(2) H. Schwarz, S. Shaik, J. Li, J. Am. Chem. Soc. 2017, 139, 17201
(3) H. Schwarz, Angew. Chem. Int. Ed. 2011, 51, 1009

11:51AM B32.00002: From Clusters To Cluster Complexes* [Invited] MASAHIKO ICHIHASHI (Presenter), Cluster Research Laboratory, Toyota Technological Institute, HIDEHO ODAKA, East Tokyo Laboratory, Genesis Research Institute, Inc. — Adsorption and reactions of molecules on metal clusters have been considered as a fundamental model of catalysis, and attracted much attention both in basic science and industrial areas. Then, the elucidation of their geometric and electronic structures provides a helpful insight into the reaction mechanisms to improve the catalytic properties. Infrared spectra of the nanocatalyst in a helium cluster give much information on the structures related to the reactivity. Recently we have developed a technique to form cluster complexes, Coₘ⁺Heₙ and Coₘ⁺NOHeₙ, by use of low-energy collision between helium clusters and metal cluster ions. This technique can provide significant amount of the cluster complexes, and we demonstrate the formation and the spectroscopy of the cluster complexes.

*This work was supported by the Special Cluster Research Project of Genesis Research Institute, Inc. and by JSPS KAKENHI Grant Number 17K04975.
GEREON NIEDNER-SCHATTEBURG (Presenter), Chemistry and Research Center OPTIMAS, Technische Universität Kaiserslautern (TUK) — We are investigating the surface morphology and adsorbate bonding properties of naked transition metal clusters under cryo conditions, and we have conducted a series of spectroscopic, kinetic and computational studies of the N$_2$ adsorption onto size selected Cobalt and Nickel clusters [1-4], as well as a case study of N$_2$ and H$_2$ co-adsorption onto a selected Ruthenium cluster [5]. In the course of these studies we chose to investigate Iron clusters and Iron-Rhodium nanoalloys as well. We found some Iron clusters reluctant to attach neither Nitrogen N$_2$ nor Hydrogen H$_2$. This presentation puts the current level of understanding to the stage.


*This work is supported by the Deutsche Forschungsgemeinschaft (DFG) in the framework of the Transregional Collaborative Research Center 3MET.de on Homogeneous and Heterogeneous Transition Metal Complexes.

LIAM HOWARD-FABRETTO (Presenter), GUNTER G ANDERSSON, Institute for Nanoscale Science & Technology, Flinders University, SCOTT ANDERSON, TIMOTHY GOREY, Department of Chemistry, University of Utah, GREGORY METHA, Chemistry, The University of Adelaide, VLADIMIR GOLOVKO, The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury — Metal clusters are groups of metal atoms with sizes ranging between 2 and 100 atoms, possessing unique electronic and catalytic properties. This work aims to measure the valence electron density of states for titania-supported Ru$_3$ clusters using the complimentary techniques UPS and metastable induced electron spectroscopy (MIES), and XPS will be used to determine the elemental composition. Ru clusters have been shown to be among the most active catalysts for industry-relevant reactions such as CO hydrogenation.

Two approaches to cluster deposition will be compared. The first is vaporisation of ligand-protected Ru$_3$(CO)$_{12}$ clusters onto a titania substrate under ultra-high vacuum, and subsequent heat-removal of the CO ligands to leave the bare Ru$_3$. The second is using a size-selected, laser ablation cluster source to deposit bare Ru$_3$ directly onto the substrates. It is known that the properties of supported clusters can differ depending on the deposition method, however these two common methods have never been directly compared for these clusters.

*Supported by the US army project FA5209-16-R-0017.
We acknowledge the expertise, equipment, and support provided by the Australian Microscopy and Microanalysis Research Facility (AMMRF) and the Australian National Fabrication Facility (ANFF).

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B33 FiAP: Advanced Materials for Applications: Fabrication, Lithography and Instrumentation BCEC 204B - Ronald Warzoha - Tag(s): Focus
Strained polymer films are commonly used as dielectric materials in high energy density capacitors, and processed such that they have significant anisotropy in a variety of materials parameters. In order to interrogate the influence of this anisotropy in thermal transport characteristics, we use the Transient Electro Thermal Technique (TET). TET enables characterization of novel materials with micrometer dimensions, without necessitating bulk production, reducing the time and cost of materials research. Using TET, we are able to obtain resolution of anisotropy in strained polymer films simply by modifying the orientation of the measurement. We compare the results of this thermal diffusivity obtained via TET analysis to the expected enhancement in thermal diffusivity results, from molecular dynamics modeling, of mechanically strained polymers. These findings demonstrate the utility of this for use in novel, laboratory-scale, polymer-based dielectric film fabrication.

Origin of long-lived photostriction in molecular ferroelectrics

Croconic Acid (CA) exhibits ferroelectricity due to proton displacement between molecules. Utilizing Time resolved x-ray spectroscopy under UV irradiation, we were able to observe lattice dilation effect with time scale over few seconds indicative of a long-lived metastable structure. The origin of the lattice dilation cannot be attributed to thermal effects due to its anisotropic characteristics. To elucidate the photon-induced electron structure change, current measurements were performed under different irradiation wavelengths of which only UV light exposure gives second-long excitation and relaxation time. Since the energy of the UV radiation is comparable to the bandgap in CA, the origin of photostriction could be solely attributed to the localized proton transfer between adjacent CA molecules.

This work is primarily supported by the National Science Foundation (Grant No. DMR-1420645) and the NSF-DMR #1708790. Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

Theory and simulation of charge injection at metal-polymer interfaces

In this work, we construct in silico atomic and molecular models of metal-polymer interfaces for two polymers commonly used in HVDC applications, namely polyethylene (PE) and polypropylene (PP). Using first-principles electronic structure calculations, we compute charge injection barriers for our interface systems. The effect of chemical and structural features, such as extrinsic chemical defects in the polymer (e.g., C=O and C-Cl groups) and physical morphology (e.g., amorphous vs crystalline regions in the polymer) are also considered.

Our results indicate potential avenues for the rational design of polymeric insulators that are more resistant to charge leakage.

Unravelling The Behaviour in a TCNQ Based Molecular Solid

Molecular solids present many advantages over their inorganic counterparts, however their more work is needed to bring our understanding up to that of other types of materials. One interesting problem is using organic based compounds to create functional materials, pairing the existence of magnetism and electrical behaviour. Within this talk, I will focus on triethylammonium 7,7,8,8-tetracyanoquinodimethane (TEA(TCNQ)₂), a quasi-1D system where an electron is shared between two TCNQ molecules creating a delocalised radical anion. Dielectric measurements have shown anomalies at two temperatures and these match with both a structural and magnetic phase transition. Our recent study has shown that the system enters a 3D Ising ground state and not simply undergoing a spin-transition as was previously thought. This is helping to further our knowledge of the system and highlight it's potential as a functional material.

We would like to acknowledge RIKEN and the ISIS Neutron and Muon Source, STFC, for access to the RIKEN-RAL muon facility.
Ultrafast photoexcited carrier dynamics in violanthrone-79 thin films

Kateryna Kushnir (Presenter), Taylor Trottier, Patrick Devlin Fitzgerald, Andrew Mendizabal, Physics Department, Worcester Polytechnic Institute, Christopher R Lambert, Biomedical Engineering, Chemistry & Biochemistry, Worcester Polytechnic Institute, Lyubov Titova, Physics Department, Worcester Polytechnic Institute — Violanthrone-79 (VO-79) is a promising organic semiconductor, molecules of which consist of large aromatic cores and aliphatic side chains. Strong π - π interactions promote stacking of individual molecules and forming nanoaggregates in solutions when dissolved in polar solvents like toluene and chloroform. Introduction of small amounts of poor solvents such as hexane enhances aggregation and results in highly crystalline morphology. We have studied optical and electronic properties of VO-79 thin films prepared from VO-79/chloroform solution at a concentration above the aggregation threshold, as well as those prepared from VO-79 solutions in chloroform/hexane mix. Using optical pump – THz probe spectroscopy, we have demonstrated that delocalization of π electrons in the film results in band-like carriers that remain free within individual aggregates for tens of picoseconds after photoexcitation. We correlate carrier dynamics in films containing VO-79 nanoaggregates with their morphology and optical properties as revealed by the photoluminescence spectroscopy. Observation of long-lived, mobile photocarriers suggests possible applications of VO-79 in organic optoelectronic and solar energy conversion devices.

*We acknowledge financial support from ACS PRF 56734-DNI6

Ferroelectric switching kinetics of large area Croconic acid thin films

Shashi Poddar (Presenter), Xuanyuan Jiang, Physics, University of Nebraska Lincoln, Yifan Yuan, Mechanical & Materials Engineering, University of Nebraska Lincoln, Xiaoshan Xu, Physics, University of Nebraska Lincoln — In the present work, large area ferroelectric thin films of Croconic acid with thickness ranging from 10-50 nm have been fabricated by physical vapor deposition on ITO substrates at ~ 30 C. The films, on being annealed up to room temperature, show excellent wetting forming polycrystalline films. The AFM morphology exhibits stable grains with lateral dimensions of 50-200 nm often exhibiting a monodomain polar states which can be reversibly switched as evidenced by piezoresponse force microscopy. Since the switching mechanism here solely relies on the proton tautomerism localized in the -OH- hydrogen bonds, studying local switching kinetics of the individual polar grains may unveil a novel mechanism of domain nucleation and switching in these molecular ferroelectric systems.

*This work is supported by the grant DE-SC0019173 funded by the U.S. Department of Energy, Office of Science.

Metal-semiconductor contact effects and temperature-dependence of carrier transport in large-grain organic semiconductor thin film transistors

Jing Wan (Presenter), Yang Li, Department of Physics and Materials Science Program, University of Vermont, Jonathan Hollin, Adam Whalley, Department of Chemistry, University of Vermont, Randall Headrick, Department of Physics and Materials Science Program, University of Vermont — The pen-writer solution deposition method is used to deposit 2,7-dioclyl[1]benzothieno[3,2-b][1]benzothiophene (C8-BTBT) organic semiconductor thin films and also polymer dielectric layers. Organic transistors with source/drain contact layers either below or on top of the semiconductor layer and with or without surface treatment are investigated. Contact resistance produces a pronounced non-linearity in the output characteristics at low drain voltage, which is found to be consistent with a Schottky Barrier model. By treating the Au electrode with pentafluorobenzenethiol (PFBT) in a bottom contact geometry, the contact resistance is greatly reduced. An optimized geometry is obtained by using pen-written Cytop™ dielectric in a top-gate/bottom-contact structure, which exhibits a near-intrinsic average mobility, up to 9.0 cm²/V-s for C8-BTBT thin films deposited at high writing speed (25mm/s) and deposition on a heated substrate (60°C). We will report temperature-dependent carrier transport results for individual devices with both a top gate (with cytop dielectric) and bottom gate (with silicon dioxide dielectric) to compare results at both interfaces of the same C8-BTBT thin film.

*This work is supported by the National Science Foundation under award DMR-1701774.
Entropic elasticity and negative thermal expansion in ScF₃

IGOR ZALIZNYAK, DAVID WENDT, EMIL BOZIN, Brookhaven National Laboratory, KATHARINE L. PAGE, JOERG NEUEFEIND, Oak Ridge National Laboratory, BRENT T FULTZ, California Institute of Technology, ALEXEY TKACHENKO (Presenter), Brookhaven National Laboratory — Negative thermal expansion (NTE) is common in polymers and biomolecules, where its origin can be traced to entropic elasticity, but is rare in solids where it is desirable for applications. We report pair distribution function (PDF) analysis of neutron total scattering tracking the local structure and relative atomic positions in ScF₃ as it shrinks with increasing temperature. In agreement with previous X-ray studies¹,², we find that Sc-F bond slightly expands on warming, while the lattice spacing decreases. The correlation in positions of the neighbor F atoms rapidly fades on warming, consistent with simple model of F transverse thermal motion constrained only by the rigid Sc-F bond. This indicates that entropic stiffness rendered by strong Sc-F bond is at the origin of NTE in ScF₃. We thus observe universality of the NTE phenomenon across hard and soft matter, which opens new avenues for predictive modelling of this effect in solids.


*Work at BNL supported by Division of Materials Sciences and Engineering under contract DE-SC0012704, at ORNL's Spallation Neutron Source by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

Atomic Calligraphy: A MEMS Based Nanomanufacturing Technique

LAWRENCE BARRETT (Presenter), RICHARD LALLY, THOMAS STARK, JEREMY REEVES, DAVID JOHN BISHOP, Boston University — Atomic Calligraphy is a nanomanufacturing technique with the potential to combine resolutions below 10 nm with high throughputs. It works by combining two technologies, stencil lithography which is essentially shadow masking a flux atoms and microelectromechanical systems (MEMS). Stencil lithography is useable over large areas, inexpensive to implement, useable with fragile materials and on fragile surfaces. However, it has several challenges including: clogging of the stencil, limited resolution due to the dimensions of the evaporation source and the distance to the target, and imprecise alignment between stencil and target. Here, we present on overcoming these challenges using a variety of MEMS technologies including joule heating, precision springs, capacitive sensing and capacitive actuation.

*This work is funded by the DARPA Atoms to Product Program.

Focused Electrohydrodynamic Printing Technology by Incorporating an Einzel Lens

MATTHEW STROHMAYER (Presenter), ATUL DHALL, PUJHITHA RAMESH, NATALYA TOKRANOVA, JAMES CASTRACANE, CARL VENTRICE, SUNY Polytechnic Institute — Additive manufacturing (AM) shows great promise for both research and industrial applications. The main advantages of AM include limited waste and the ability to build complicated structures. The most common techniques for AM are fused deposition manufacturing, digital light printing, and ink jetting. All of these techniques suffer from resolution and material limitations. Recently, a cost-effective, versatile method of high-resolution printing called electrohydrodynamic (EHD) printing has been introduced. This method allows for spatial resolution in the hundreds of nanometers. This method works similarly to a typical ink jetting system, except instead of the ink/polymer being pushed out of a tip, it is pulled out by an applied electric field. This allows for the resultant droplet to be smaller than the needle diameter. Coulomb's law limits the ultimate resolution of this technique. To overcome this resolution limitation, we have incorporated an Einzel lens into the system to focus the droplets. This helps the droplets overcome the repulsive force from Coulomb's law and leads to better spatial resolution.

Superalloy Radiative Heat Transfer in Additive Manufacturing

ERIN CURRY (Presenter), RAINER HEBERT, PAMIR ALPAY, SANJUBALA SAHOO, JASON HANCOCK, University of Connecticut — Direct Laser Metal Sintering (DLMS) is a layer-by-layer additive manufacturing process using a high power focused source such a laser or electron beam. As the metal powder melts, the melt pool experiences non-equilibrium thermalization processes involving convection, evaporation, plasma creation and radiative cooling, expected to be most important at high temperature. Developing a fundamental understanding of the melt pool cooling rate through the radiative cooling is invaluable to controlling microstructure of the final product. In DLMS a high energy melting source is focused to a small spot size on the build plate and travels across the powder layer at a high velocity, all of which parameters make in-situ measurements of melt pool temperature from radiative cooling difficult. We discuss approaches to spatially resolved temperature analysis of the DLMS melt pool as well as a combined experimental and theoretical optical property investigation of superalloys typically used in DLMS.

*University of Connecticut
1:27PM B33.00012: Cathodoluminescence-based nanoscopic thermometry in a lanthanide-doped phosphor
CLARICE D AIELLO (Presenter), Bioengineering Dept., Stanford University, ANDREA D PICKEL, Mechanical Engineering Dept., UC Berkeley, EDWARD BARNARD, Molecular Foundry, Lawrence Berkeley National Laboratory, REBECCA WAI, Chemistry Dept., UC Berkeley, CHRISTIAN MONACHON, Attolight AG, EDWARD WONG, SHAUL ALONI, FRANK OGLETREE, Molecular Foundry, Lawrence Berkeley National Laboratory, CHRIS DAMES, Mechanical Engineering Dept., UC Berkeley, NAOMI GINSBERG, Chemistry Dept., UC Berkeley — Crucial to analyze phenomena as varied as plasmonic hot spots and the spread of cancer in living tissue, nanoscale thermometry is challenging: probes are usually larger than the sample under study, and contact techniques may alter the sample temperature itself. Many photostable nanomaterials whose luminescence is temperature-dependent, such as lanthanide-doped phosphors, have been shown to be good non-contact thermometric sensors when optically excited. Using such nanomaterials, in this work we accomplished the key milestone of enabling far-field thermometry with a spatial resolution that is not diffraction-limited at readout. We explore thermal effects on the cathodoluminescence of lanthanide-doped NaYF₄ nanoparticles. Whereas cathodoluminescence from such lanthanide-doped nanomaterials has been previously observed, here we use quantitative features of such emission for the first time towards an application beyond localization. We demonstrate a thermometry scheme that is based on cathodoluminescence lifetime changes as a function of temperature that achieves ~ 30 mK sensitivity in sub-μm nanoparticle patches. The scheme is robust against spurious effects related to electron beam radiation damage and optical alignment fluctuations.

1:39PM B33.00013: Modeling Performance of Ultra-Sensitive In-Orbit Infrared Telescopes
WILLIAM ATKINSON (Presenter), Boeing — This paper evaluates considerations in minimizing disruptions of scientific data in ultra-sensitive Infrared (IR) spaced-based telescopes by charged particles in space radiation. The particles modeled are protons, alphas, and heavier ions with an atomic number as high as that of iron. Performance results of proposed designs are based on a model developed at Boeing. The components modeled are the spectra of the ion species in cosmic rays and solar flares, the transport of the primary ions and secondary particles produced including neutrons, the generation electron hole pairs (EHPs) by the particles penetrating the focal point array (FPA), and a component modeling transfer of EHPs from generation to recombination. Results indicate noise levels above 100 EHPs by secondary particles alone per pixel in intense space weather events, these observations agree with empirical data sources. Space based IR astronomical observatories now have a noise level of 100 electrons/pixel indicating the need of detailed radiation transport models; in near future designs where the pixel pitch reduces from 25 to 5 microns, the radiation model component becomes even more significant. Measures reducing the number of electrons per pixel below the threshold are discussed.

1:51PM B33.00014: Revisiting the Non-linear transport behaviors in conducting polymer
JIAWEI WANG (Presenter), LING LI, MING LIU, Institute of Microelectronics, Chinese Academy of Sciences — The non-linear transport in conducting polymers usually refers to the non-ohmic current-voltage (IV) relationship at low temperature, and are widely reported in both molecular doped and field effect doped polymers, power-law dependence of conductance on temperature, at low voltage (eV<<k_BT) and current on voltage, at high voltage (eV>>k_BT) are universally observed in the non-linear regime. We investigated the charge transport in polymer materials PBTTT doped with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ), very revealing information was obtained via a simple contrast investigation between PBTTT films of different crystalline degrees. We found that only the transport behavior of highly crystalline PBTTT film at low-T could satisfy what Luttinger Liquid theory predicts, while those of poor ordered film showed non-power-law relationship. Simultaneously, fit of other non-linear transport models with our data was investigated. We finally proposed our model based on the microstructure of the PBTTT film with considering the interplay between Fermi liquids and Luttinger liquids.

Monday, March 4, 2019 11:15 AM - 1:39 PM

Session B34 DCMP: Fundamentals of Solid/Aqueous-Electrolyte interfaces BCEC 205A - Jorg Zegenhagen, Diamond Light Source - Tag(s): Invited
11:15AM B34.00001: Probing the charge distribution at the electrochemical interface [Invited] YVONNE GRUNDER
(Presenter), CHRISTOPHER LUCAS, University of Liverpool, YVES JOLY, CNRS, Grenoble INP, Institut Neel — In-situ surface x-ray diffraction has enabled an atomic/molecular-level understanding of the interface under reactive conditions, including its potential and time dependence, to be developed. While information about the atomic structure of the electrode surface in electrochemical in-situ cells has been widely investigated, insight into the charge distribution and the structure of the electrolyte at the interface is still lacking. A fundamental understanding of the nature of the charge transfer, especially the influence of the applied potential and the screening by the electrolyte, is a major goal in electrochemistry to better understand electrochemical processes and charge transfer during adsorption and deposition. [1]

In-situ studies of the chemical bonding are rather difficult due to the presence of the electrolyte, as standard characterisation techniques which are mostly UHV based cannot be applied. Thus combining x-ray spectroscopy and x-ray diffraction to gain site specific information about the charge distribution at buried interfaces is a promising tool. [2,3] Examples of how the use of surface x-ray scattering techniques can help to characterise electrochemical interfaces in-situ in order to link, structure, reactivity and stability will be presented. Advances in these directions offer possibilities in elucidating atomic scale models of the electrochemical interface and thus will help to establish structure-stability-reactivity relationships.

References:

11:51AM B34.00002: Monitoring electrochemical and electrocatalytic interface processes on the atomic and nanometer scale by operando surface X-ray scattering [Invited] OLAF MAGNUSSSEN (Presenter), Experimental and Applied Physics, Kiel University — The need for sustainable energy, reduction of pollutants, and the environmental benign processing of chemicals has spurred worldwide scientific activities in electrochemical energy science and electrocatalysis. These processes occur at the interfaces of solid electrodes in contact with complex liquid environments under conditions, which are difficult to access by most surface analytic techniques. For a better understanding of structure-property relationships and reaction-induced morphological changes, experimental approaches are required that provide direct insight into the atomic and nanoscale interface structure.

Modern synchrotron-based X-ray scattering methods provide unique opportunities for such operando studies. They allow monitoring structural changes at electrode surfaces with high structure sensitivity on (sub-) second time scales. The talk will give an overview of the current state of this field. It will specifically highlight the advantages of using very high photon energies (70 keV) in combination with 2D X-ray detectors. This new approach enables e.g. detailed determination of complex, dynamically changing interface structures and microdiffraction studies of spatially heterogeneous materials. The application of these methods will be demonstrated by studies of Pt oxidation and transition metal oxide catalysts for water splitting. In the first case, a strong dependence of the oxidation mechanism on the Pt surface structure was observed, resulting in pronouncedly different Pt dissolution and nanoscale restructuring. The second example will focus on epitaxial Co oxide thin films, which were monitored in the oxygen evolution regime up to current densities as high as 150 mA cm⁻². Whereas CoOOH(001) films were perfectly stable under these conditions, oxygen evolution on Co₃O₄(111) films occurs on a disordered nm-thick skin layer, which forms highly reversibly at potentials 300 mV negative of the onset of this electrocatalytic reaction.
12:27PM B34.00003: Transition-metal-oxide/liquid interfaces [Invited] ULRIKE DIEBOLD (Presenter), Institute of Applied Physics, TU Wien — Transition metal oxides are promising systems for photo- and electrocatalysis. For a molecular-scale understanding of the underlying mechanisms and processes, experiments on well-characterized samples are necessary, i.e., specific facets of single crystals with a known composition, geometry, and defect structure.

In the talk we will address the question whether the atomic structure of selected oxide surfaces survives the exposure to liquid water. We use a novel apparatus that allows to expose samples to liquids without them leaving the ultrahigh vacuum (UHV) environment [1]. We find that the TiO$_2$(110) surface maintains its (1x1) termination [2] and that the (2x1) overlayer observed after water exposure in air results in an ordered layer of carboxylates. In contrast, exposure to liquid water lifts the TiO$_2$(011)-(2x1) reconstruction and results in full hydroxylation [3]. We have also tested the several iron oxide surfaces [4, 5], and find hints that the pairs of dissociated and intact water molecules that form on these [4] and several other metal oxides are present in the liquid phase as well. Magnetite Fe$_3$O$_4$ was tested for OER in alkaline conditions, and was found to be stable at the nanoscopic scale, with a facet-dependent reactivity [5].


1:03PM B34.00004: Molecular Self-Assemblies as Templates for Electrochemically Deposited Nanostructures [Invited] MANFRED BUCK (Presenter), School of Chemistry, University of St Andrews — Ranging from porous networks to dense layers, the structural and functional versatility of aromatic molecules provides a diversity of options for controlling processes at the liquid/solid interface. This includes the electrochemical interface where the level of control intrinsic to electrochemical processes combines favourably with the control of charge transfer, interfacial energies and chemical functionality by highly organized molecular assemblies.

This combination can be taken advantage of for the generation of nanostructures by templated electrodeposition using molecular patterns produced by either bottom-up self-assembly or top down lithography. While structures down to the 20 nm range are relatively straightforward to achieve, progress in the move towards the bottom end of the nanoscale will be critically dependent not only on the precision of template structures but also on the level of control over the dynamics of processes such as diffusion and nucleation which, ultimately, become the limiting factors. To address these issues requires to go beyond the usual application of organized molecular layers to render electrodes electrochemically passive. As illustrated by the electrodeposition of metals, utilising a more varied design than non-functionalized single component layers offers interesting prospects for the generation of ultrasmall structures such as a reduction in the percolation threshold or self-limiting layer formation enabled by coordination controlled deposition.

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B35 DQI: Silicon Spin Qubits BCEC 205B - Emily Pritchett, HRL Laboratories - Tag(s): Focus

11:15AM B35.00001: Spin Qubits at Intel [Invited] JIM CLARKE (Presenter), Intel Corporation — Intel is developing a 300mm process line for spin qubit devices using state-of-the-art immersion lithography and isotopically pure epitaxial silicon layers. Both Si-MOS and Si/SiGe devices are being evaluated in this multi-layer integration scheme. In this talk, we will be sharing our current progress towards spin qubits starting with substrate characterization. Transistors and quantum dot devices are then co-fabricated on the same wafer and allow calibration to Intel’s internal transistor processes. Electrical characterization and feedback is accomplished through wafer scale testing at both room temperature and 1.6K prior to milli-kelvin testing. Accelerated testing across a 300mm wafer provides a vast amount of data that can be used for continuous improvement in both performance and variability. This removes one of the bottlenecks towards a large scale system: trying to deliver an exponentially fast compute technology with a slow and linear characterization scheme using only dilution refrigerators.
11:51AM B35.00002: A novel Si/SiGe heterostructure for quantum dot spin qubits  THOMAS MCJUNKIN (Presenter), EVAN R MACQUARRIE, SAMUEL NEYENS, BRANDUR THORGRIMSSON, JOELLE CORRIGAN, JOHN DODSON, Department of Physics, University of Wisconsin-Madison, DONALD E SAVAGE, MAX G LAGALLY, Department of Materials Science and Engineering, University of Wisconsin-Madison, MARK G FRIESEN, SUSAN COPPERSMITH, MARK ALAN ERIKSSON, Department of Physics, University of Wisconsin-Madison — Motivated by a desire to increase the energy splitting between the two low-lying valley states in a silicon quantum well, a Si/SiGe heterostructure is grown via UHV-CVD with a ~1 nm layer of SiGe buried ~2 nm beneath the upper interface of a silicon quantum well. High resolution STEM measurements confirm that this thin epitaxial layer is abrupt on the side facing the substrate and gradual on the side facing the surface. We report Shubnikov-de Haas and quantum Hall measurements, finding a transport mobility in excess of 100,000 cm²/(V s) at 6 x 10¹¹ cm⁻² carrier density and a series of stable oscillations in measurements of the longitudinal voltage as a function of magnetic field and carrier density (a fan diagram). We report both activation energy measurements in the quantum Hall regime and measurements of the excited state spectrum in gate-defined quantum dots fabricated in this material.

12:03PM B35.00003: Coherent control of a semiconductor quantum dot qubit, encoded by valley-states in Si⁺ NICHOLAS PENTHORN, JOSHUA S SCHOENFIELD (Presenter), HONGWEN JIANG, UCLA — Traditionally, spin and charge of individual electrons are used to encode a qubit in gated-defined semiconductor quantum dots. Valley states of electrons in silicon represents another degree of freedom in addition to spin and charge degree of freedoms. In this talk, we demonstrate the coherent control of a semiconductor quantum dot qubit, encoded by valley-states in Si. A double quantum dot device, fabricated on a SiGe hetero-structure, is used for the experiment. We found that either one of the quantum dots can be used to encode a qubit. The left dot has a valley splitting of 5.3 GHz (or 22 ueV), while the right dot has a different splitting of 8.2 GHz (or 34 ueV). The x-axis control of the qubit is done by either timed x-rotation near the anti-crossing point of the two valley eigenstates, or by the Landau-Zener effect using a slowly rising/falling pulse. The z-axis control is done at the region when the energy separation of the two valley levels is nearly detuning independent, which offers a protection against charge noise. Fast qubit operations, in the range of a few GHz, for both x and z rotations, are realized.

*This work is supported by ARO under grant # W911NF-17-1-0242.

12:15PM B35.00004: Spin-Blockade Spectroscopy of Si/SiGe Quantum Dots  EDWARD CHEN (Presenter), HRL Laboratories — We introduce a technique for measuring the singlet-triplet energy splitting in undoped, accumulation-mode Si/SiGe quantum dots [1]. We find that the measured splitting varies smoothly as a function of confinement gate biases and are also consistent to those obtained using photon-assisted tunneling (PAT) spectroscopy at the (2,0)-(1,1) charge transition. Because our technique operates in the limits of both large and small singlet-triplet energy splittings, we are able to show that the splitting can be limited by the lateral orbital excitation energy rather than solely by the valley splitting in the silicon well.


12:27PM B35.00005: Valley and orbital state spectroscopy of a Si/SiGe triple quantum dot  JOHN DODSON (Presenter), JOELLE BAER, JOSE CARLOS ABADILLO-URIEL, NATHAN HOLMAN, TREVOR KNAPP, BRANDUR THORGRIMSSON, EVAN R MACQUARRIE, SAMUEL NEYENS, THOMAS MCJUNKIN, RYAN FOOTE, University of Wisconsin - Madison, LISA EDGE, HRL Laboratories, LLC, MARK G FRIESEN, SUSAN COPPERSMITH, MARK ALAN ERIKSSON, University of Wisconsin - Madison — Valley and orbital states have important consequences for silicon based qubits, and a thorough understanding of their interaction in the few electron regime is crucial in forming robust qubits. While many spin-based qubits operate best with large valley and orbital splittings, valley qubits such as the quantum dot hybrid qubit [1] utilize the valley degree of freedom for its logical states. Here we present measurements of valley and orbital energies using excited state spectroscopy in a triple quantum dot fabricated using an Al-AlₓO₁₋ₓ-Al overlapping gate design. Valley splitting is shown to vary as a function of electron occupancy in the N=1 to N=4 regime between 35 and 70 µeV. We observe that higher lying orbital levels have a larger valley splitting, and we present tight binding simulations consistent with this observation. The spatial dependence of the valley splitting in a linear array of quantum dots is also investigated. Finally, we observe anomalously low orbital splittings of 200-400 µeV that could have potential applications to new readout mechanisms for certain silicon based qubits.

Here, we study the spin relaxation and dephasing in an MBE-grown $^{28}\text{Si}/\text{SiGe}$ device with a residual $^{29}\text{Si}$ concentration of less than 60 ppm. In our devices, instead of using a micromagnet, one of the electrostatic gates is replaced by a cobalt nanomagnet to generate the magnetic field gradient required for electrical dipole spin resonance. We find a maximum $T_1 = 480$ ms and present a detailed study of the spin relaxation time $T_1$ as a function of magnetic field. We observe a spin relaxation hotspot due to enhanced spin-valley mixing at a Zeeman energy of 207 µeV and find this large valley splitting to be tunable with the gate voltages. Finally, we discuss the long spin dephasing times $T_2^*$ and $T_2^{\text{echo}}$ obtained in this device.


*This project is sponsored by the German Research Foundation (DFG).
Charge noise induced spin decoherence in a double quantum dot: Effects of a micromagnet

XINYU ZHAO (Presenter), XUEDONG HU, University at Buffalo, The State University of New York — Charge noise is one of the largest error sources preventing the high-fidelity quantum computing in semiconductor systems. We study the decoherence of an electron spin in a double quantum dot in the presence of an inhomogeneous magnetic field and induced by a non-Markovian charge noise. We derive a master equation based on the stochastic Schrodinger equation. By analyzing the physical process represented by each term in the master equation, we show how the properties of the charge noise affect spin decoherence and how an orbital charge noise affects the spin dynamics through the inhomogeneous magnetic field. We find that a longer correlation time can slow down spin decoherence, particularly during the early stage of an evolution. A relation between the spin relaxation rate and the gradient of the magnetic field is given. The stochastic approach used to derive master equation can be also extended to other semiconductor systems in the presence of charge noise. Our results present a systematic approach to study decoherence processes caused by charge noise, particularly for quantum dots in an inhomogeneous magnetic field.

Spin decoherence in a quantum dot due to micro-magnets

PEIHAO HUANG (Presenter), Shenzhen Institute for Quantum Science and Engineering, and Department of Physics, Southern University of Science and Technology, XUEDONG HU, Department of Physics, University at Buffalo — A spin qubit in a semiconductor quantum dot is a promising candidate for quantum information processing for scalability and miniaturization. Micro-magnets have been proven to be effective to mediate the coupling of a spin qubit to photon and electrical control field. In this work, we study spin decoherence in a quantum dot mediated by the magnetic field gradient created by micro-magnets. The spin relaxation mediated by magnetic field gradient shows different magnetic field dependence compare with spin relaxation mediated by spin-orbit coupling. Furthermore, to the first order of the magnetic field gradient, there is finite spin dephasing due to 1/f charge noise. We discuss the consequence of the new spin decoherence mechanisms on the number of qubit operations.

Targeted enrichment of $^{28}\text{Si}$ for quantum computing

KE TANG (Presenter), HYUN-SOO KIM, ARUNA RAMANAYAKA, DAVID S SIMONS, JOSHUA POMEROY, National Institute of Standards and Technology — We report on the growth of isotopically enriched $^{28}\text{Si}$ epitaxial films with precisely controlled enrichment levels, ranging from natural abundance ratio of 92.2% all the way to 99.99987% (0.832ppm $^{29}\text{Si}$). Isotopically enriched $^{28}\text{Si}$ is regarded as an ideal host material for semiconducting quantum computing due to the lack of $^{29}\text{Si}$ nuclear spins. However, the detailed mechanisms for quantum decoherence and the exact level of enrichment needed remain unknown. Here we use hyperthermal energy ion beam deposition with silane gas to deposit epitaxial $^{28}\text{Si}$. In the meantime, we switch the mass selective magnetic field periodically to control the $^{29}\text{Si}$ concentration. A model predicting the residual $^{29}\text{Si}$ isotope fraction and the corresponding secondary ion mass spectrometry (SIMS) analysis are presented. Cross-sectional SEM/TEM will also been shown for the deposited $^{28}\text{Si}$ film throughout the range of enrichments.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B36 GMAG: Exotic Dynamics of Pyrochlore Magnets

Excitation Continuum in a Pyrochlore S=1 Heisenberg Magnet* [Invited] KEMP PLUMB (Presenter), Brown University — The existence of a spin-liquid for Heisenberg spins on the pyrochlore lattice was first speculated by Jacques Villain nearly 40 years ago and it is now recognized that the ground state of this model is a Coulomb spin liquid. However, experimental realizations are scarce. In this talk, I will discuss a new pyrochlore lattice magnet, NaCaNi$_2$F$_7$, which realizes the isotropic Coulomb spin liquid with $S=1$ spins and the complication of random Na$^+$ - Ca$^{2+}$ charge disorder in the crystal structure. I will present neutron scattering and calorimetric measurements that were used to uncover the magnetic correlations in this material and determine the magnetic Hamiltonian. The ionic disorder creates a rugged energy landscape that acts to freeze a small fraction of the magnetic degrees of freedom. However, the energy scale set by this disorder is small, and the Heisenberg interactions prevail. Only a small fraction of the available moment is frozen, and the magnetism in NaCaNi$_2$F$_7$ is dominated by a persistently fluctuating component that appears as a broad continuum of magnetic signal in inelastic neutron scattering measurements. These measurements demonstrate a beautiful realization of the Coulomb spin liquid and provide new insight into the interplay between disorder and magnetic exchange interactions in highly frustrated magnets.

*Work at the Institute for Quantum Matter was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering under grant DE-FG02-08ER46544.
11:51AM B36.00002: Novel Photogalvanic Effects in Weyl Semimetals [Invited] NAOTO NAGAOSA (Presenter), Department of Applied Physics, University of Tokyo — Photovoltaic effect is attracting growing interest from the viewpoint of the geometrical quantal phase of Bloch wavefunctions, i.e., Berry phase. The interband transitions between bands cause the shift of the electrons due to the difference in the intra-cell coordinates encoded as the Berry phase connection, resulting in the shift current without the external bias voltage. On the other hand, it has been known that the Weyl fermion is the source or sink of the Berry curvature, i.e., monopole or anti-monopole in momentum space, and leads to the enhanced Berry phase phenomena. Therefore, it is natural to expect the novel photovoltaic effect there. In this talk, I will describe the physical mechanism of shift current, and its features such as I-V characteristics, dependence on the mean free time, and noise, and discuss its realizations in Weyl semimetals such as the surface state of topological insulator, and TaAs. This talk is based on the works with collaborators T. Morimoto, K.W. Kim, H.Ishizuka, Y.Zhang, J.v. d.Brink, C. Felser, B. Yan, N. Ogawa, T. Hayata, M. Ueda, M. Sotome, M. Nakamura, J. Fujioka, M. Ogino, Y. Kaneko, M. Kawasaki, and Y. Tokura.

12:27PM B36.00003: Metamagnetism, Criticality and Dynamics in the Quantum Spin Ice Pr2Zr2O7 [Invited] NAN TANG (Presenter), AKITO SAKAI, ISSP, University of Tokyo, KENTA KIMURA, GSFS, University of Tokyo, SHOTA NAKAMURA, Department of Physical Science and Engineering, Nagoya Institute of Technology, YOUSKE MATSUMOTO, Max-Planck Institute, TOSHIRO SAKAKIBARA, SATORU NAKATSUJI, ISSP, University of Tokyo — Geometrical frustration may prevent the formation of long-range magnetic order, giving rise to a diverse range of novel ground states. One of such an unusual state is called quantum spin liquid (QSL) possibly realized in quantum spin ice systems. Its excitations behave like charged particles interacting with linearly dispersive “photon”, protected by hidden topological order parameter. Yet, the properties of quantum phase transition between such topological phases remain unknown and are waiting to be established. Pr-based pyrochlore compounds such as Pr2Ir2O7 and Pr2Zr2O7 are known to be quantum spin ice systems. Pr2Ir2O7 is a fascinating material exhibiting various exotic phenomena such as the spontaneous anomalous Hall effect [1]. In contrast to Pr2Ir2O7, the insulating Pr2Zr2O7 renders a simplified platform to explore the physics of quantum spin ice. K. Kimura et al. [2] reported the absence of “pinch points” in the inelastic neutron scattering spectrum of Pr2Zr2O7, suggesting the breakdown of the ice rule owing to quantum fluctuations — a promising hint of a U(1) QSL state. In a recent study [3], it was found that structural disorder acts as a transverse field on the non-Kramers Pr3+ ion in Pr2Zr2O7, stabilizing the QSL state. Under a magnetic field along the [111] axis, classical spin ice materials undergo a 1st-order metamagnetic transition [4]. Although theoretical studies [5] predict the existence of metamagnetic transition in quantum spin ice, a comprehensive investigation is still lacking. Here, we report magnetization, thermal expansion, and magnetostriction measurements on Pr2Zr2O7. These measurements aim to clarify the nature of the metamagnetic transition and to probe possible topological quantum criticality.

Reference

1:03PM B36.00004: Magnetic moment fragmentation and dynamical spin ice features in Neodymium pyrochlores [Invited] ALEXANDROS SAMARTZIS, JIANHUI XU, VIVEK K. ANAND, NAZMUL ISLAM, Helmholtz-Zentrum Berlin, JACQUES OLLIVIER, Institut Laue Langevin, TATIANA GUIDI, Rutherford Appleton Laboratory, GEORG EHLERS, Oak Ridge National Laboratory, YiXi SU, Heinz Maier-Leibnitz Zentrum, BELLA LAKE (Presenter), Helmholtz-Zentrum Berlin — Neodymium pyrochlores show rich, complex and exotic physical phenomena. The Nd3+ ions have a well-isolated ground state doublet with octupolar-dipolar symmetry and they interact with each other via highly anisotropic exchange interactions. We have studied two members of this family Nd2Zr2O7 and Nd2Hf2O7. Both show long-range all-in-all-out antiferromagnetic order revealing broken gauge symmetry in the ground state. The lowest energy excitations form a flat, gapped mode with a pinch-point structure factor suggesting a proximate gauge symmetry leading to dynamical spin ice. At higher energies there are dispersive spin-wave modes which touch the flat mode, at the pinch points. They have a pinch point pattern of their own which is rotated with respect to that of the flat mode and which give rise to half-moon features in constant energy slices. The coexistence of long-range magnetic order, the pinch-point mode and half-moon features originate from fragmentation of the Nd3+ magnetic moment into divergence-free and divergence-full parts. Finally at temperatures just above the Neel temperature, the pinch point mode becomes gapless and the spin-waves broaden suggesting a spinon continuum.
Neutron scattering signatures of pyrochlore spin liquids and nematic phases* [Invited] LUDOVIC JAUBERT (Presenter), CNRS / LOMA, University of Bordeaux, OWEN BENTON, RIKEN, HAN YAN, Okinawa Institute of Science and Technology, MATHIEU TAILLEFUMIER, ETH Zurich, NICHOLAS SHANNON, Okinawa Institute of Science and Technology, JAAN OITMAA, University of New South Wales, RAJIV SINGH, University of California, Davis, TOMONARI MIZOGUCHI, University of Tsukuba, RODERICH MOESSNER, MPI-PKS Dresden, MASAFUMI UDAGAWA, University of Gakushuin — Research on spin liquids has gradually evolved from the search of systems that do not order, to the quest of exotic quasi-particles and emergent gauge fields. But how to measure a gauge field in experiments? Neutron scattering certainly offers a helpful microscopic probe, e.g. with Coulomb gauge fields famously identified by pinch points in spin ice materials. But there is no spin-liquid analog of a Bragg peak; the very diversity of spin liquids makes them both fascinating and evasive.

In this talk, we will explore a broad range of pyrochlore physics with anisotropic exchange and further neighbour couplings, in order to explain the connection between several characteristic patterns of neutron scattering, their underlying Hamiltonian models and the strongly correlated magnetic phases they support. For example, "half-moon" patterns are a dispersive complement to the pinch points [1,2] that have been observed in Tb2Ti2O7 [3] and NaCaNi2F7 [4], while in tensor spin liquids, the pinch points may evolve into lines [5] or 4-fold singularities characteristic of higher-rank U(1) gauge fields [6,9]. To conclude, we will discuss the nematic "hidden" order stabilised when the symmetry of the Heisenberg antiferromagnet is lowered by frustrating anisotropic exchange [7,8,9].


Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B37 GMAG DCMP: Spin Liquids: Theory and Experiment

Critical Spin Liquid versus Valence Bond Glass in Triangular Lattice Organic κ-(ET)2Cu2(CN)3*

KIRA M. RIEDL, ROSER VALENTI, STEPHEN WINTER (Presenter), Institute for Theoretical Physics, Goethe University Frankfurt — The organic triangular-lattice antiferromagnet κ-(ET)2Cu2(CN)3 has been extensively discussed as a quantum spin liquid (QSL) candidate. Recently, an intriguing quantum critical behaviour was suggested from low-temperature B/T scaling of the magnetic torque experiments [1]. Through microscopic analysis of all anisotropic contributions, including Dzyaloshinskii-Moriya and multi-spin scalar chiral interactions, we highlight significant deviations of the experimental observations from a quantum critical scenario. Instead, we show that disorder-induced spin defects provide a comprehensive explanation of the low-temperature properties[2]. These spins are attributed to valence bond defects that emerge spontaneously as the QSL enters a valence bond glass phase at low temperature. This theoretical treatment is applicable to a general class of frustrated magnetic systems; similar scaling is also observed in the Kagome lattice antiferromagnet Herbertsmithite[3].


*The work was supported by the Deutsche Forschungsgemeinschaft (DFG) through project SFB/TRR49.
11:27 AM B37.00002: Charge Order without Spin Order in the Layered Frustrated Magnet κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl$^*$

TERESA LE (Presenter), ANDREJ PUSTOGOW, HSIN-HUA WANG, YONGKANG LUO, University of California, Los Angeles, ELENA GATI, MICHAEL LANG, Institute of Physics, Goethe-University Frankfurt, STUART E BROWN, University of California, Los Angeles —

There are several quasi two-dimensional materials which do not order magnetically, including a number of geometrically frustrated organic charge transfer salts. To investigate the interplay between charge order (which may affect the frustration) and magnetic order, we use $^1$H NMR spectroscopy to examine the magnetic properties of κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl, which exhibits a first-order metal-insulator transition to a charge ordered state at $T_{CO} = 30K$. The high-temperature metallic phase exhibits Fermi-liquid behavior with constant $(T_1T)^{-1}$, while the spin-lattice relaxation rate is subject to an abrupt enhancement at $T_{CO}$ and shows a standard paramagnetic response down to 2 K, below which the relaxation rates decrease as $1/T_1 \sim T^2$. The smooth temperature dependence of $T_1$ and the absence of changes in the NMR spectra rule out magnetic order down to 25 mK suggesting decoupling of the spin and charge degrees of freedom, while the CO is expected to reduce the frustration. These observations are discussed in the context of the ground state without magnetic order. Ongoing field-dependent measurements may elucidate whether the magnetic interactions are subject to 1D physics.

*This work was supported by the National Science Foundation (DMR-1709304).

11:39 AM B37.00003: Quantum valence bond ice and its relation to κ-H$_3$(Cat-EDT-TTF)$_2$

MASAHIKO YAMADA (Presenter), YASUHIRO TADA, Univ of Tokyo-Kashiwanoha — Motivated by the discovery of the coexistence of unfrozen spin and dipole fluctuations in an organic quantum spin liquid called κ-H$_3$(Cat-EDT-TTF)$_2$ [1], we propose a new asymptotically solvable model, where a quantum spin liquid (resonating valence bond) state is accompanied by quantum proton motion, which we name quantum valence bond ice. We can regard this state as a quantum spin-dipole liquid in the sense that quantum spin fluctuations are triggered by the coupling to the quantum proton motion. In the classical version of this model, there are macroscopically degenerate ground states, and quantum fluctuations of the proton motion will lift the degeneracy. The resulting quantum ground state should be regarded as the U(1) spin liquid phase in 3 dimensions, connected to Anderson’s resonating valence bond state [2] in the perturbative level.


11:51 AM B37.00004: Effect of randomness on spin excitations in quantum spin liquid state of 1T-TaS$_2$

HINAKO MURAYAMA (Presenter), YUKI SATO, TOMOYA TANIGUCHI, RYO KURIHARA, XIANGZHUO XING, SHIGERU KASAHARA, YUICHI KASAHARA, Department of Physics, Kyoto University, MASARO YOSHIDA, CEMS, RIKEN, YOSHIHIRO IWASA, Quantum-Phase Electronics Center and Department of Applied Physics, University of Tokyo, MARCIN KONCZYKOWSKI, Laboratoire des Solides Irradies, Ecole Polytechnique, YUJI MATSUDA, Department of Physics, Kyoto University —

Quantum spin liquid (QSL) is a novel state of matter where the ground states are quantum mechanically entangled and have several characteristic features, including fractional excitations. However, the nature of QSLs remains elusive. To tackle this problem, studying the effect of quenched disorder is of vital importance.

Recently, 1T-TaS$_2$ has aroused great interest as a candidate material that hosts a QSL ground state on two-dimensional perfect triangular lattice as suggested both theoretically and experimentally[1, 2]. To study the effect of randomness on the QSL state, we performed thermal conductivity and specific heat measurements on pure, Se-doped and electron irradiated 1T-TaS$_2$. The results indicate the coexistence of itinerant and localized gapless spin excitations, suggesting a novel spin liquid state where itinerant quasiparticles coexist with randomly distributed orphan spins forming localized random singlets. In addition, thermal conductivity reveals the suppression of gapless spin excitations by Se-doping, indicating that the itinerant gapless spin excitations are sensitive to randomness. We will also discuss the effect of randomness on the specific heat.

12:03PM B37.00005: Spin-Liquid-Like State in the Triangular Lattice Antiferromagnet TbInO3*  
MIN GYU KIM  
(Presenter), Rutgers University, New Brunswick, BARRY L. WINN, SONGXUE CHI, ANDREI T SAVICI, Oak Ridge National Lab, JOSE A RODRIGUEZ, NIST, YANBIN LI, XIANGHAN XU, JAE WOOK KIM, SANG-WOOK CHEONG, VALERY KIRYUKHIN, Rutgers University, New Brunswick — Unpolarized and polarized inelastic neutron scattering studies in single crystals of the triangular-lattice (TL) antiferromagnets TbInO3 and TbIn0.95 Mn0.05 O3 are reported. Broad gapless magnetic excitations are located at the TL Brillouin zone boundary. They show a weak enhancement near the M points at the lowest energies, and shift to the K points with increasing energy. At higher energies, a broad dispersing excitation branch, also centered at the zone boundary, is observed after a gap. No signs of magnetic order are found down to the temperatures 100 times smaller than the effective interaction energy given by the excitation bandwidth, indicating a very strong frustration. The fluctuating magnetic moment exceeds one half of the Tb3+ free-ion value and is confined to the TL plane. These observations strongly suggest a triangular-lattice-based spin liquid state in TbInO3.

*This work at Rutgers University was supported by U.S. Department of Energy Grant No. DE-FG02-07ER46382.

12:15PM B37.00006: Spin Dynamics of the Elemental Quantum Spin Liquid β-Mn*  
JOSEPH PADDISON (Presenter),  
Department of Physics, University of Cambridge, ROSS STEWART, ISIS Neutron and Muon Source, Rutherford Appleton Laboratory — Pure β-Mn is the only elemental metal that shows quantum spin-liquid-like behavior [1]. Its magnetic Mn atoms occupy a frustrated three-dimensional network of corner-sharing triangles. Unlike all other transition metals, β-Mn does not show long-range magnetic order to the lowest measured temperatures (~0.3 K). Instead, its magnetic response is dominated by strong antiferromagnetic spin fluctuations that persist up to room temperature and exhibit non-Fermi-liquid scaling [2].

We present neutron-scattering measurements of the spin dynamics of β-Mn over a wide range of momentum transfer, energy transfer, and temperature. Our measurements allow us to parameterize an effective Hamiltonian [3] that reveals the temperature dependence of the on-site magnetic moment and the magnetic interactions. Our results shed new light on the unusual magnetic behaviour of this remarkable element and demonstrate an experiment-driven approach to parameterizing magnetic interactions in metals.


*Churchill College, Cambridge (UK) to J.A.M.P. and STFC (UK) to J.R.S.

12:27PM B37.00007: Dynamical spin structure factor from a variational Monte Carlo perspective*  
[Invited] FEDERICO BECCA (Presenter), National Research Council — The spin dynamical structure factor is computed within a variational framework to study frustrated Heisenberg models in one and two dimensions. Starting from Gutzwiller-projected fermionic wave functions, the low-energy spectrum is constructed by considering two-spinon excitations. Benchmarks on the one-dimensional J1-J2 model are considered. Here, an excellent description of both the gapless and gapped (dimerized) phases is obtained [1]. In the square lattice, we obtain the distinctive spectral signatures of the transition between the Neel and the spin-liquid phases that takes place for J2/J1 ~0.45. By increasing the frustration, the magnon excitation at q=(π,0) and (0,π) broadens, suggesting the tendency towards a spin fractionalization. In addition, its energy softens, indicating the presence of gapless states at the transition and within the spin-liquid phase [2]. On the triangular lattice, we assess the possibility to have the magnon decay, as suggested by using spin-wave approaches for non-collinear magnetic orders [3]. The evolution of the spin dynamical structure factor when approaching the magnetically disordered phase in presence of a next-nearest-neighbor coupling J2 is also included [4]. Preliminary calculations on the kagome lattice are also discussed.


*Support from the National Research Council (CNR) is acknowledged.
We investigate signatures of spin liquids with spinon Fermi surfaces in electron spin resonance experiments. We focus on the magnetic field (h) and temperature (T) dependence of the linewidth $\eta$ of the resonance peak in the ESR absorption spectrum. We show that in the presence of DM interaction, the linewidth is determined by the low-energy U(1) gauge fluctuations resulting in a characteristic $\eta \sim h^{2/3}$ scaling at $T=0$ and a more complicated behavior $T/h + T^{2/3} f(h/T)$, with an explicit form of the scaling function $f(x)$, at finite $T$. We find that exchange anisotropy results in a weaker $h$ and $T$ dependence of $\eta$. We discuss relevance of our findings to experiments on the spin liquid candidate $\kappa$-ET and related materials.

*Supported by NSF DMR-1507054 and DOE DE-FG02-08ER46524.

Coulombic quantum spin liquids (C-QSLs) whose low energy excitations are U(1) gauge fluctuations realize massive quantum entanglement in quantum magnets. They have been suggested to be hosted in several three-dimensional materials including a pyrochlore structure, $\text{A}_2\text{B}_2\text{O}_7$. In this study, we present a phenomenological theory of C-QSLs and their phase transitions in the extended Landau paradigm. Within extended Landau paradigm which can be achieved by enlarging symmetry group, we obtain richer phase diagrams than the conventional order only diagrams. As a specific example, we construct the effective theory of conventional order parameters of a lattice symmetry($G$) and emergent excitations of C-QSLs($\sim G$) in the extended Landau paradigm. Namely, we write down all terms respecting a lattice symmetry and gauge invariance and investigate possible phase structures. For example, we apply our theory to systems with an all-in-all-out (AIAO) order parameter and U(1) gauge fluctuation dubbed Coulombic AIAO (AIAO*). Phenomenologically we obtain characteristic heat capacities and magnetic responses characterizing phases. Our theory may be directly applied to an insulating pyrochlore system where both A and B sites are magnetically active and one of them forms a U(1) quantum spin liquids.

We present the global phase diagram of the Heisenberg model on the body-centered cubic (BCC) lattice with nearest-neighbor $J_1$, second nearest-neighbor $J_2$ and third nearest-neighbor $J_3$ exchange couplings, for both antiferromagnetic and ferromagnetic $J_1$, $J_2$, and $J_3$. The classical phase diagram is shown to host four commensurate magnetic orders [ferromagnet $q=(0,0,0)$, Néel antiferromagnet $q=(2\pi,0,0)$, $q=(\pi,\pi,0)$, and $q=(\pi,\pi,\pi)$], and three incommensurate helimagnetic orders, namely, a one-, two- and three-dimensional spiral. The corresponding quantum spin-1/2 model is investigated employing the pseudofermion functional renormalization group (PFFRG) method. It is shown that quantum fluctuations (i) stabilize a quantum spin liquid phase over an appreciable region in parameter space centered around tri-critical points, (ii) strongly renormalize the phase boundaries (compared to those of the classical model), (iii) shift the pitch vector of the helimagnetic orders. We obtain the critical ordering temperatures for the $S=1/2$ model from Quantum Monte Carlo in the unfrustrated parameter regime, and compare it with the estimates obtained from one- and two-loop PFFRG. In the frustrated regime of the model, we compare our estimates with results available from other methods.
1:39PM B37.00011: Control of Magnetic and Topological Orders with a DC Electric Field*  
KAZUAKI TAKASAN (Presenter), Department of Physics, Kyoto University, MASAHIRO SATO, Department of Physics, Ibaraki University — In this talk, we present our theoretical proposal which provides a new route to control magnetic and topological orders in a broad class of insulating magnets with a DC electric field [1]. We show from the strong-coupling expansion that magnetic exchange interactions along the electric-field direction are generally enhanced in Mott insulators. It indicates that we can control the spatial structure of the interactions in magnets with a DC electric field. To illustrate this idea, we particularly focus on two kinds of magnets, frustrated magnets and quasi-one-dimensional magnets, and obtain phase diagrams including several magnetic or topological ordered phases such as quantum spin liquids and Haldane-gap states. Our proposal is effective especially for magnets in the vicinity of quantum critical points, and would also be applicable for magnets under low-frequency AC electric fields such as terahertz laser pulses. Our result would pave a promising way to control the exotic states of matter in magnets.


*This work is supported by JSPS KAKENHI (Grant No. JP16J05078, JP17K05513 and JP15H02117) and Grant-in-Aid for Scientific Research on Innovative Area, Nano Spin Conversion Science (Grant No. 17H05174).

1:51PM B37.00012: Construction of matrix product state for the Gutwiller projected variational wavefunctions  
AMIR MOHAMMADAGHAEI (Presenter), University of California, Riverside, BELA BAUER, Station Q, Microsoft Research, KIRILL SHTENGEL, University of California, Riverside, RYAN MISHMASH, University of California, Berkeley — An accurate description of various quantum spin liquid states using tensor network methods remains notoriously challenging. For large quasi-1D systems, the density matrix renormalization group and related methods usually require significant computational resources and sometimes fail to converge to a satisfactory state. On the other hand, variational wavefunctions acquired from the Gutwiller projection of gaussian fermionic theories has long served as both a theoretical starting point for construction of such spin liquid states and as an inspiration for numerical variational Monte Carlo (VMC) to calculate observables of interest. In this work, we examine a different method by exploring the possibility of constructing a matrix product state (MPS) representation for a Gutwiller-projected state from two given MPS representations of gaussian fermionic theories. We investigate the complexity of different approaches to achieve this goal and test the methods on two copies of a single half-filled band of spin-1/2 fermionic spinons. We then apply this method to two MPS of multi-band fermionic spinon theories in an attempt to describe spin liquid states on a quasi-1D strips of triangular and kagome-like lattices and compare to the complexity of the traditional VMC approach.

2:03PM B37.00013: Bridging partons and coupled-wire approaches to quantum spin liquids.*  
EYAL LEVIATAN (Presenter), DAVID MROSS, Weizmann Institute of Science — Quantum spin systems which avoid symmetry-breaking order, e.g., due to geometric frustration, can instead form so-called quantum spin liquids. These phases, characterized by fractional excitations and emergent gauge fields, are thought to be realized in an increasing number of quasi-two-dimensional materials. In my talk, I will show how a wide range of gapped as well as gapless spin liquids can be accessed by a generalization of the ‘coupled-wire’ technique. In particular, I will construct explicit Hamiltonians that realize these phases and show how this method allows transparent access to subtle questions regarding the emergent gauge field, such as confinement. I will compare and contrast this approach to the popular parton-construction, and highlight the respective advantages.

*This work was supported by the Minerva foundation with funding from the Federal German Ministry for Education and Research.

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B38 GMAG DMP: 2D Magnetism I  
BCEC 206B - Mark Meisel, University of Florida - Tag(s): Focus
11:15AM B38.00001: Criticality in Two-Dimensional Quantum Antiferromagnets (2D QAF) [Invited] CHRISTOPHER LANDEE (Presenter), Clark University — Low Dimensional (LoD) physics has long provided opportunities (both analytical and experimental) for exploring criticality in model systems that are more tractable than the more formidable 3D analogs. In particular, magnetic LoD compounds have provided multiple physical realizations with which theoretical predictions can be tested. The quantum (S = ½) two-dimensional model clearly reveals the influence of exchange anisotropy (Ising, XY, Heisenberg) and quantum fluctuations upon criticality: the Ising model spontaneously orders, the XY system undergoes a topological transition, and the Heisenberg analog (2D QHAF) remains disordered at any finite temperature. There are many crystalline compounds accurately described as 2D quantum Ising antiferromagnets but the equivalent XY and Heisenberg materials remain in development.

In practice, all known crystalline realizations of 2D QHAF magnetically order at low temperatures due to a combination of interlayer exchange (J_{3d}) and/or exchange anisotropy (Δ). Simulations of the ideal (J_{3d}=0) 2D QHAF [1] revealed that a ratio Δ/J < 0.01 will induce either XY or -l-order at low temperatures and also revealed that the ideal 2D QHAF becomes a perfect 2D QXYAF in an applied field [2]. This talk will describe the approaches followed in the Clark University group in pursuit of the ideal 2D QHAF, as illustrated in the compound [Cu(pz)_{2}(2-HO-py)_{2}](PF_{6})_{2}.


11:51AM B38.00002: Single crystal EPR analysis of pyrazine bridged layered complexes‡ JEFFREY MONROE (Presenter), Chemistry, Clark University, CHRISTOPHER LANDEE, Physics, Clark University, FREDRICK T GREENAWAY, Chemistry, Clark University, JAN L WIKAIRA, Chemistry, University of Canterbury, MARK M TURNBULL, Chemistry, Clark University — Over the last three decades our group has endeavored to model the antiferromagnetic interactions of the copper-oxide high-temperature superconductors via crystal engineering of low dimensional copper(II) systems. Our efforts have led us to systems of the type [Cu(pz)_{2}(L)_{2}](A)_{2} which contain well isolated pyrazine-bridged square-lattices with Heisenberg antiferromagnetic superexchange. We report primarily on [Cu(pz)_{2}(2-hydroxypyridine)_{2}](PF_{6})_{2}. The single crystal EPR linewidth as a function of temperature and angle at X-Band are investigated in three orientations where XYZ=abc. The linewidth is investigated in terms of g-anisotropy, dipolar spin-diffusion, antisymmetric and anisotropic exchange. The linewidth in the ac and bc planes follow a cos^{2}(θ) dependence indicating the dominant contributions to the linewidth are the anisotropic and antisymmetric exchange. These results are compared to those from other techniques including NMR and SQUID magnetometry. The effects of these interactions on the 3D ordering temperature are considered.

References:

*Acknowledgements
Alan A. Jones Endowed Graduate Fellowship Fund in Chemistry

12:03PM B38.00003: Low-dimensional quantum magnets supported by non-covalent interactions‡ JAMIE MANSON (Presenter), JACQUELINE VILLA, DANIELLE VILLA, Chemistry, Eastern Washington University, WILLIAM BLACKMORE, ROBERT WILLIAMS, JAMIE BRAMBLEBY, PAUL GODDARD, Physics, University of Warwick, JOHN SINGLETON, NHML, Los Alamos Natl Lab, ROGER JOHNSON, Physics, University of Oxford, SAUL H. LAPIKUS, Advanced Photon Source, Argonne Natl Lab, BENJAMIN HUDDART, THOMAS HICKEN, TOM LANCASTER, Physics, Durham University, STEVE BLUNDELL, Physics, University of Oxford, FAN XIAO, Muon-spec Lab, Paul Scherrer Institut, JOHN SCHLUETER, DMR, NSF — At ambient pressure, [Ni(HF_{2})(pyz)_{2}]SbF_{6} contains S = 1 Ni(II) ions arranged in a tetragonal network consisting of 1D Ni-FHF-Ni chains (J) cross-linked by pyrazine (pyz) ligands (J'). Previous work determined D = 13.3 K, J = 10.4 K and J' = 1.4 K [1]. Below T_{N} = 12.2 K, long-range magnetic order sets in and, as revealed by neutron diffraction, is of the XY-type with Ni(II) moments occupying any collinear orientation in the crystallographic ab-plane. Pressure-dependent X-ray powder diffraction data reveal a first-order structural phase transition at 3 GPa which leads to a distorted monoclinic network and kinked magnetic exchange pathways. In this high-pressure regime, the magnetic ground state switches to Ising-like with concomitant reduction in T_{N}. The related quasi-1D chain, NiI_{2}(3,5-lutidine)_{4}, also forms a tetragonal lattice but consis of discrete molecular units. A chain-like motif affords close Ni-I...I-Ni contacts and strong magnetic coupling. Evidence suggests that this material is a rare isotropic Haldane chain with J = 17.5 K and D = 6.3 K [2]. Time permitting, structural and magnetic properties of each material will be presented.


*NSF DMR-1703003 (EWU), DMR-1157490 (MagLab), DoE, FL, ERC, EPSRC
Honeycomb lattice antiferromagnets have been of tremendous research interests due to their complex magnetic structures ranging from Neél, zigzag, stripy, and spin liquid depending on details of competing exchange interactions. To study these interesting magnetic states, we have synthesized single crystals of a novel spin-3 honeycomb lattice antiferromagnet, Tb$_2$Ir$_3$Ga$_9$, which is a member of a large family of compounds with chemical formula R$_2$T$_3$X$_9$ (R = rare-earth element, T = d-element, and X = p-block element). Structural analysis showed the crystals have formed in orthorhombic symmetry with space group 63 ($\text{Cmcm}$). From the magnetization measurements, we find characteristics of low-dimensional magnetism followed by a long range ordering at 12 K. As determined both by magnetometry and powder neutron diffraction, the Tb spins lie strictly along the a-axis, parallel to the Tb-Tb contact. Two spin-flop transitions are observed when the field is applied parallel to this axis, separated by a plateau corresponding to $M=\frac{M_s}{2}$. Magnetoresistance data reflect the anisotropy and contains features that correlate with the spin flop transitions. We propose a model for the magnetic ground state and a phenomenological theory for the magnetic interactions.

Hydroxy halides M$_2$(OH)$_3$X (M = transition metal, X = Cl, Br, I) represent a family to investigate novel quantum phenomena arising from the magnetic frustration. For instance, via doing Zn into Cu sites in the parent cinoactacamite Cu$_2$(OH)$_3$Cl, herbertsmithite ZnCu$_3$(OH)$_6$Cl$_2$ hosts a perfect two-dimensional kagome magnetic lattice and exhibits quantum spin liquid state without long range magnetic ordering. In this paper, we report a comprehensive study of botallackite Cu$_2$(OH)$_3$Br, a compound with distorted quasi-two dimensional triangular magnetic lattice, via magnetic susceptibility, heat capacity, neutron diffraction, and inelastic neutron scattering measurements. Density functional theory calculations to understand the exchange interactions of this system will be briefly discussed as well.

The copper compound Cu$_2$(OH)$_3$Br has relatively few experimental studies, and, to the best of our knowledge, this material has not been approached from first principles before. Previous experimental work on the isostructural compound Cu$_2$(OH)$_3$Cl has demonstrated an interesting frustrated magnetic phase below the Neel temperature. Furthermore, upon substitution of the halogen ion, the Neel temperature was shown to grow with increasing halogen ion size for Cu$_2$(OH)$_3$Cl, Cu$_2$(OH)$_3$Br, and Cu$_2$(OH)$_3$I, possibly providing insight into the superexchange mechanism in this material. In this talk, we present the results of our first principles calculations on the compound Cu$_2$(OH)$_3$Br. We discuss the magnetic phase; in particular, we find the exchange constants and elucidate the interplay between magnetism and orbital configuration.

Finding skyrmions in different kinds of structures has attracted a lot of attention but also remains a challenge. Here we study the adsorption of transition metal atoms (Cr, Mn, Fe, and Co) deposited on top of a monolayer MoS$_2$ where the transition metal atoms form a triangular lattice. First-principles DFT calculations suggest that the magnetic ordering of this triangular lattice corresponds to a 120-degree antiferromagnetic structure. Heisenberg exchange parameters, single-ion anisotropy constants, and Dzyaloshinskii-Moriya vectors are extracted by choosing different spin configurations and calculating the total energy differences. For the considered transition metal atoms, the ground states are found to be spin spirals formed from 120-degree antiferromagnetic states. Our study shows the potential to find skyrmions in such triangular lattices.
Orbital and Charge Participation in the Magnetic Phases of Intercalated Fe$_{1/3}$TaS$_2$, Fe$_{1/3}$NbS$_2$ and Their Alloys

Conrad Stansbury (Presenter), Claudia Fatuzzo, Eran Maniv, Spencer Doyle, Caolan John, James G. Analytis, Alessandra Lanzara, University of California, Berkeley — The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction has been used to understand the origin of (anti)ferromagnetic behavior in some magnetic transition metal intercalated dichalcogenides (TMDs). Despite the clean picture that RKKY presents, little has been said about the interplay of intercalate magnetism with the low temperature phases in disulfide TMDs. By using angle resolved photoemission spectroscopy (ARPES) and optical spectroscopies we are able to provide a new picture for the onset of magnetic phases over a family of transition metal intercalates on the basis of charge transfer. The interaction between magnetism and other forms of order in 2H-NbS$_2$ and 2H-TaS$_2$ will also be explored.

Controlling and Tuning the Magnetic Ground State in an Intercalated Transition Metal Dichalcogenide

Spencer Doyle (Presenter), Caolan John, Eran Maniv, James G. Analytis, University of California, Berkeley — It is possible to engineer magnetism in layered TMDs X$_2$ (X=transition metal) via intercalation of magnetic transition metals. In particular, iron intercalation (1/3 Fe per X site) introduces a two-dimensional magnetic sublattice between X$_2$ layers. Despite adopting identical crystal structures with near-identical lattice parameters, the magnetic ground states of Fe$_{1/3}$NbS$_2$ and Fe$_{1/3}$TaS$_2$ are antiferromagnetic and ferromagnetic, respectively. Due to their chemical similarity, these two materials can form end members of an alloying series Fe$_{1/3}$Nb$_{1-x}$Ta$_x$S$_2$. Due to the different magnetic orderings of its end members, this alloying series permits the substitutional control of the magnetic ground state of the material system. I will present our thermodynamic measurements and findings.

*The Analytis Lab is supported by the Gordon and Betty Moore Foundation's EPiQS initiative through Grant GBMF4374. The Analytis Lab is supported by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-05CH11231. Spencer Doyle is supported by the Summer Undergraduate Research Fellowship L&S McKinley Fund.

Anomalous Hall Effect Mechanisms in Quasi-2D van der Waals Ferromagnet Fe$_{0.29}$TaS$_2$

Ranran Cai (Presenter), Wenyu Xing, HuiBing Zhou, YangYang Chen, Yunyan Yao, Yang Ma, Xincheng Xie, Shuang Jia, Wei Han, International Center for Quantum Materials, Peking University — The recent emergence of two-dimensional (2D) van der Waals ferromagnets has provided a new platform for exploring magnetism in the flatland and for designing 2D ferromagnet-based spintronics devices. Despite intensive studies, the anomalous Hall effect (AHE) mechanisms in 2D van der Waals ferromagnets have not been investigated yet. In this talk, I will present the AHE mechanisms in quasi-2D van der Waals ferromagnet Fe$_{0.29}$TaS$_2$ via systematically measuring Fe$_{0.29}$TaS$_2$ devices with thickness from 14 nm to bulk single crystal. The dominant AHE mechanism is found to be skew scattering in bulk single crystal, and the contribution from intrinsic mechanism emerges and become more relevant as the Fe$_{0.29}$TaS$_2$ thickness decrease. Besides, the coercive field in Fe$_{0.29}$TaS$_2$ thin flake decrease as the Fe$_{0.29}$TaS$_2$ thickness decrease.

*National Basic Research Programs of China, National Natural Science Foundation of China and the Key Research Program of the Chinese Academy of Sciences

Ab-initio study of the magnetic interaction between vanadium impurities in ultra-narrow graphene nanoribbons

Romeo de Coss (Presenter), Department Applied Physics, Cinvestav, Juan Hernández-Aacute;NdeZ-Tecoralco, Instituto de Fisica, BUAP, Miguel Eduardo Cifuentes Quintal, Department Applied Physics, Cinvestav, Lilía Méza-Montés, Instituto de Fisica, BUAP — The exchange interaction between two substitutional vanadium atoms in graphene nanoribbons is studied using ab-initio calculations. The exchange coupling was obtained as the energy difference between the ferro- and antiferro-magnetic configurations. In order to evaluate the effects of quantum confinement and edge magnetism on the exchange interaction, we have studied nanoribbons with zigzag and armchair edges. For comparison we also calculated the 2V-impurities in the bulk (graphene) system. In all the studied cases the exchange coupling shows an oscillatory behavior with the distance between the vanadium impurities, but the values depends on the type of edge structure (AC or ZZ). The present results show the relevance of including the quantum confinement effect and the edge structure in modeling the interaction between magnetic impurities in ultra-narrow graphene nanoribbons. The understanding of the exchange interaction between magnetic impurities in graphene nanoribbons plays an important role in the design of possible novel spintronic devices and quantum gates for quantum computing.

*Computer resources, technical expertise and support was provided by Laboratorio Nacional de Supercómputo del Sureste de México, This work was supported by CONACyT-México under grant No. 288344.
1:51PM B38.00012: Local broken symmetry and spin transport in frustrated Heisenberg model in low dimension*  
LEONARDO DOS SANTOS LIMA (Presenter), Física, Centro Federal de Educação Tecnológica de Minas Gerais — The local spontaneous symmetry breaking is a general phenomena in condensed matter physics. It is characterized by the fact that the action has a local symmetry but the quantum theory, instead of having a unique vacuum state which respects this symmetry, has a family of degenerate vacua that transform into each other under the action of the symmetry group. A simple example is given by a ferromagnetic model in which the action governing its microscopic dynamics is invariant under spatial rotations. A kind of local gauge invariance or spontaneous breaking of U(1) gauge symmetry is realized in nature in the phenomenon of superconductivity.

We have proposed a Meissner mechanism for the spin transport in quantum spin systems. Besides, we study the behavior of the AC spin conductivity in the neighborhood of a quantum phase transition in a frustrated spin model such as the antiferromagnet in the compass lattice with single ion anisotropy at $T = 0$. 

*Conselho Nacional de Desenvolvimento Científico e Tecnológico CNPq

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B39 GMAG DMP: Spin transport and Hall effect  
BCEC 207 - Xiaojin (Elaine) Li, Univ of Texas, Austin -  
Tag(s): Focus

11:15AM B39.00001: Spin-to-Charge Conversion in Bi Films and Bi/Ag Bilayers*  
[Invited] DI YUE (Presenter), Department of Physics, Fudan University, WEIWEI LIN, Department of Physics and Astronomy, Johns Hopkins University, JIAJIA LI, XIAOFENG JIN, Department of Physics, Fudan University, C. L. CHIEN, Department of Physics and Astronomy, Johns Hopkins University — Recently, there have been reports on the superior prowess of bismuth (Bi) in spin-to-charge conversion, including large spin Hall angle and long spin diffusion length, qualities that are highly favorable for exploring pure spin current phenomena and devices [1]. Bi/Ag bilayers have also been featured prominently in the inverse Rashba-Edelstein effect (IREE), a related effect offering strong spin-to-charge conversion at interfaces [2,3]. One notes that in most cases the spin injection has been accomplished by spin pumping from Py, a process well known to harbor a variety of parasitic effects due to metallic Py that complicate the voltage measurements of the inverse spin Hall effect (ISHE).

In this work [4], we use thermal injection from a ferromagnetic insulator YIG into Bi films and Bi/Ag bilayers, demonstrated to be without the parasitic effects. The Bi layers of various thicknesses have been made by both MBE and sputtering at 77 K with similar results. The contribution of the pure spin current can be unequivocally determined by the insertion of a MgO(3 nm) layer, which blocks the spin current and eliminates the ISHE voltage. In sharp contrast to previous results, we have observed much shorter spin diffusion length in Bi of about 1 nm and negligibly small spin Hall angle. We have also observed no evidence of the IREE in the Bi/Ag bilayers. We note that Bi is a well-known thermoelectric material with low carrier concentration and very large Nernst voltage.


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11:51AM B39.00002: Spin Hall Effect in Ni_{x}Cu_{1-x} Alloys  MARK KELLER (Presenter), KATY GERACE, MONIKA ARORA, JUSTIN
SHAW, THOMAS SILVIA, National Institute of Standards and Technology Boulder — We report a large spin Hall conductivity, $\sigma_{SH}$
in, high resistivity, paramagnetic Ni_{60}Cu_{40}. The value is comparable to what we reported for Pt [1]. Broadband FMR
measurements of ferromagnet/nonmagnet bilayers provide an accurate measure of $\sigma_{SH}$, and simultaneously the damping
due to spin pumping, when the various contributions to the inductively detected signal are analyzed as described in [2].
These measurements do not require patterning of the bilayer, nor perpendicular anisotropy of the ferromagnet. In a
series of samples with the layer structure substrate/Ta(3)/Py(3.5)/Ni_{x}Cu_{1-x}(d)/Ta(3) (thickness in nm), we varied Ni fraction $x$
for $d = 10$ nm and varied thickness $d$ for $x = 0.6$, a composition with a magnetic ordering critical temperature $T_C = 140$ K.
Room temperature FMR measurements with a saturating out-of-plane field showed a substantial $\sigma_{SH}$ for all compositions
we deposited, $0.3 \leq x \leq 0.75$, with a maximum at $x = 0.7$ where $T_C = 270$ K. For the thickness series at $x = 0.6$, we use the
approach detailed in [1] to extract a spin diffusion length of $(7.8 \pm 0.5)$ nm and a spin Hall ratio of $0.81 \pm 0.14$. Both values
are about twice as large as we reported for Pt [1].

12:03PM B39.00003: Anomalous and spin Hall effect in tunnel junctions with spin orbit interaction  CHRISTIAN
ORTIZ PAUYAC (Presenter), RIKEN — Considering a tight binding model in Keldysh formalism we describe the anomalous
and spin Hall effect in tunnel junctions with Rashba spin orbit coupling. Two types of structures are
considered, conventional magnetic tunnel junctions (normal metal - insulator - ferromagnet) and spin filter tunnel
junctions (normal metal - magnetic insulator - ferromagnet). We show that the magnitudes of the anomalous and spin Hall
effects are enhanced in the presence of magnetic insulators. In both types of structures the angular dependence exhibit a
cosine and sine behavior.

12:15PM B39.00004: Observation of the nonlinear anomalous Hall effect in 2D WTe2/Pt heterostructures*  MOHAMMED ALGHAMDI
(Presenter), MARK LOHMANN, JUNXUE LI, Department of Physics and Astronomy, University of California, Riverside, TANG SU,
International Center for Quantum Materials, School of Physics, Peking University, KENJI WATANABE, TAKASHI TANIGUCHI, National
Institute for Materials Science, PALANI RAJA JOTHI, BONIFACE FOWKA, Department of Chemistry, University of California, Riverside,
JING SHI, Department of Physics and Astronomy, University of California, Riverside — Van der Waals (vdW) layered ferromagnets
have become a hot topic of research lately within the two-dimensional materials community due to the ability to study
magnetic properties from a single atomic layer. Fe$_3$GeTe$_2$ (FGT) is one of very few known metallic members of the vdW
ferromagnetic materials family. It has strong perpendicular magnetic anisotropy (PMA) and Curie temperature, $T_C \sim 220$ K,
which makes FGT a good candidate material to study the effect of spin-orbit torque (SOT) on the magnetization of 2D
ferromagnet in FGT/heavy metal heterostructures. For this study we fabricated heterostructures of FGT/Pt with 5 nm of Pt
sputtered onto the surface of ~ 15 nm – 50 nm flakes of FGT. We measured the first and second harmonic Hall responses
to an applied magnetic field in the in-plane parallel and perpendicular to current directions. We also measured the angular
dependence of the 2 $\omega$ signal with fixed in-plane fields larger than the field required to saturate the magnetization in the
hard axis direction. Our analysis of the 2 $\omega$ signals show that damping-like SOT is at least an order of magnitude greater
than the negligible field-like SOT and thus it is the dominant mechanism acting on the magnetization of FGT.

*This work was supported by DOE (USA) BES Award No. DE-FG02-07ER46351.

12:27PM B39.00005: Observation of the nonlinear anomalous Hall effect in 2D WTe$_2$  KAIFEI KANG (Presenter),
TINGXIN LI, Applied and engineering physics, Cornell University, EGON SOHN, Physics, Cornell University, JIE SHAN, Applied and
engineering physics, Cornell University, KIN FAI MAK, Physics, Cornell University — The Hall effect has been observed in systems
with broken time reversal symmetry, such as the ordinary Hall effect in solids under a magnetic field and the anomalous
Hall effect (AHE) in magnetic materials. Theories have indicated that in nonmagnetic materials with certain low crystal
symmetries, a nonlinear Hall effect can be observed under zero magnetic field, in which the Hall voltage scales
quadratically to the longitudinal current. Here we report an observation of such effect in atomically thin Td WTe$_2$ flakes, a
semimetal with only one mirror plane along the crystal b axis. In our angle-resolved electrical measurements, we observed
a sinusoidal angular dependence of the nonlinear Hall effect, in which the effect maximizes when the driven current is
perpendicular to the mirror plane and minimizes when it aligns to the mirror plane. This effect can be described as an
anomalous Hall effect with a current induced magnetization. We further studied the temperature and doping dependence
of the nonlinear hall conductivity. The result suggests that both intrinsic Berry curvature dipole and extrinsic spin-
dependent scatterings contribute to the observed nonlinear AHE.
12:39PM B39.00006: Anomalous Hall effect in Pt/\text{Cr}_2\text{Ge}_2\text{Te}_6 heterostructures*  MARK LOHMANN (Presenter), University of California, Riverside, TANG SU, International Center for Quantum Materials, School of Physics, Peking University, MOHAMMED ALGHAMDI, BEN NIU, University of California, Riverside, YUSHENG HOU, University of California, Irvine, MOHAMMED ALDOSARY, University of California, Riverside, WENYU XING, JIANGNAN ZHONG, SHUANG JIA, WEI HAN, International Center for Quantum Materials, School of Physics, Peking University, RUQIAN WU, University of California, Irvine, YONGTAO CUI, JING SHI, University of California, Riverside — Understanding the physical properties of 2D ferromagnets such as \text{Cr}_2\text{Ge}_2\text{Te}_6 (CGT), amongst a plethora of others, has accelerated due to their properties in one to few layers as well as their ability to easily form heterostructures with other 2D materials. This feature is extremely attractive due to the possibility of manipulating interfacial interactions via proximity coupling. Here we demonstrate the anomalous Hall effect (AHE) in Pt thin films sputtered onto the surface of thin exfoliated flakes of CGT which must originate in Pt since CGT is essentially an insulator at low temperatures. The AHE loops persist up to T_c ~ 60 K which matches well to the bulk value. Low-temperature magnetic force microscopy of Pt/CGT reveals magnetic field dependent domain structures consistent with the AHE behavior. The origin of the AHE in Pt/CGT heterostructures is explored through density functional theory calculations. The method used in this study is a powerful tool to understand magnetism in 2D ferromagnetic insulators and provides a new platform for the study of magnetic proximity exchange and spin-dependent transport phenomena.

*This work is support by DOE (USA) BES Award No. DE-FG02-07ER46351

DFT calculations at UC Irvine was supported by DOE-BES Grant No. DE-FG02-05ER46237 and NERSC

12:51PM B39.00007: Semiclassical theory of the spin transport of Bloch electrons LIANG DONG (Presenter), QIAN NIU, Physics, University of Texas at Austin — The semiclassical wave-packet theory is a powerful method in studying transport properties. Usually, the charge center of the wave-packet is used to denote the position of a semiclassical electron. In fact, wave-packets with finite size can have other centers which gives an additional degree of freedom. We develop a semiclassical theory where different centers (e.g spin center) can be chosen depending on which physical property (e.g spin) we are interested in. We give an example by applying this theory to calculate the spin transport.

1:03PM B39.00008: Two-band magnetoresistance in spin-filter \text{CrVTiAl} GREGORY STEPHEN (Presenter), CHRISTOPHER LANE, IOANA G BUDA, Northeastern University, DAVID E GRAF, National High Magnetic Field Lab, STANISLAW KAPRZYK, AGH University of Science and Technology, BERNARDO BARBIELLINI, Lappeenranta University of Technology, ARUN BANSIL, DONALD E HEIMAN, Northeastern University — Thin films of spin-filter material \text{CrVTiAl} were grown via sputtering, and their magnetotransport properties have been studied up to B=35 T. The resistivity vs T shows 2-channel semiconducting behavior with a disordered gapless channel and an activated gapped channel. Magnetoresistance measurements provide values for the mobilities of the two conducting channels, 900 and 50 cm^2/Vs. This leads to a ratio of 18:1 for the effective masses, which corresponds to that predicted by density functional theory. Hall and magnetization measurements reveal a small moment saturating near 15 T that is assigned to partial non-compensation of the sublattices. These results combined with previous studies [1,2] show \text{CrVTiAl} to be a compensated ferrimagnet with a spin-polarized electronic structure.


1:15PM B39.00009: Intrinsic spin currents in ferromagnets* VIVEK AMIN (Presenter), Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, JUNWEN LI, Joint Institute for Computational Sciences, University of Tennessee, Knoxville, MARK STILES, PAUL HANEY, Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg — We present first principles calculations showing that an applied electric field generates intrinsic spin currents in ferromagnets that flow perpendicularly to the electric field. Reduced symmetry in ferromagnets with spin-orbit coupling enable a wide variety of such spin currents. However, we find the total spin current is approximately given by the sum of a magnetization-independent spin current with the symmetry of the spin Hall effect and a spin-polarized anomalous Hall current. We also present a simple tight-binding model that captures the relevant physics. Intrinsic spin currents are not subject to dephasing, enabling their spin polarizations to be misaligned with the magnetization, which is crucial to explain the magnetization-independent spin Hall effect. The spin Hall conductivity and spin anomalous Hall conductivities of transition metal ferromagnets can be comparable to Pt, opening new avenues for efficient spin current generation in spintronic devices.

*Vivek Amin acknowledges support under the Cooperative Research Agreement between the University of Maryland and the National Institute of Standards and Technology Center for Nanoscale Science and Technology, Award 70NANB14H209, through the University of Maryland.

1:27PM B39.00010: ABSTRACT WITHDRAWN
1:39PM B39.00011: Symmetric and anti-symmetric contributions in mixed spin-current effects in a NiO/Pt nanostructure*  
F. L. A. MACHADO (Presenter), P. R. T. RIBEIRO, M. GAMINO, A. AZEVEDO, SERGIO M REZENDE,  
Departamento de Física, Universidade Federal de Pernambuco, Recife, Pernambuco, Brazil. — Spin-currents generated by thermal gradients are efficiently converted into charge-currents by the inverse spin-Hall effect in films of metals presenting strong spin-orbit coupling. The nature of the thermal induced effects depends on the relative orientation among the directions of the spin-current, the applied magnetic field ($H$), the thermal gradient and the electrical contacts in the metallic film. Mixings in the currents generated by different effects are expected to occur. In this work, the $H$-dependent anti-symmetric spin-Seebeck effect (SSE) was generated altogether with the symmetric planar Nernst effect in a NiO(100 nm)/Pt(6 nm) nanostructure grown on a 0.5 mm thick Si substrate. A sample holder adapted to a PPMS was used for measuring the voltage in the Pt-film for $H$ in the range ±85 kOe and for temperatures ($T$) varying from 100 to 300 K. A simple procedure developed for separating the SSE from the planar Nernst effect yielded magnitudes for the SSE in the range ±30 pAcm/K for a temperature different of 10 K across the sample at 300 K. The magnitude of the SSE signal was found to vary with $H$ and $T$ in good agreement with a drift-diffusion magnonic theory.

*Work supported by CNPq, FACEPE, CAPES and FINEP (Brazilian Agencies).

1:51PM B39.00012: Effects of oxidation on the spin-orbit torques and domain textures in ultrathin Pt/Co/AlOx heterostructures  
JUNXIAO FENG (Presenter), MARVIN MÜLLER, EVA GRIMALDI, PIETRO GAMBARDELLA, Department of Materials, ETH Zurich — We investigated the correlation between structure, oxidation, and magnetic properties of Pt/Co/AlOx, Pt/CoOx/Co/AlOx and PtOx/Co/AlOx heterostructures. We find that the anomalous Hall resistance, magnetoresistance, magnetic anisotropy, and domain texture are affected in a systematic way by the degree of oxidation of the Co/AlOx, CoO/Co and PtOx/Co interfaces. Moreover, we find that oxidation also influences the spin-orbit torques as well as the current-induced domain-wall motion and switching.

2:03PM B39.00013: Modeling electrical detection of current generated spin in topological insulator surface states*  
CONNIE LI (Presenter), OLAF M VAN T ERVE, United States Naval Research Laboratory, CHENHUI YAN, LIAN LI, Physics and Astronomy, West Virginia University, BEREND JONKER, United States Naval Research Laboratory — Current generated spin in topological insulator (TI) surface states due to spin-momentum locking has been detected recently using FM/tunnel barrier contacts, where the projection of the TI spin onto the magnetization of the FM is measured as a voltage. However, opposing signs of the spin voltage have been reported, attributed to the coexistence of trivial 2DEG states on the TI surface that may exhibit opposite current-induced polarization. Models based on electrochemical potential have been presented to determine the sign of the spin voltage expected for the TI surface states, however neglecting critical experimental parameters. Here we present a Mott two-spin current resistor model which takes into account parameters such as spin-dependent interface resistances, and show that such inclusion can lead to a crossing of the voltage profiles for the spin-up and spin-down electrons within the channel, which can lead to measured spin voltages of either sign. These findings offer a resolution of the ongoing controversy regarding opposite signs of spin signal reported in the literature, and highlight the importance of including realistic experimental parameters in the model.

*Supported by core programs at Naval Research Laboratory, and from DOE (DE-SC0017632) at West Virginia University.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B40 GMAG DMP DCOMP: Complex Oxide Films and Heterostructures I BCEC 208 - George Sterbinsky, Argonne National Laboratory - Tag(s): Focus
Evidence of antiferromagnetism as the driver of the metal-insulator transition in vanadium sesquioxide (V$_2$O$_3$)°

[Invited] JUAN TRASTOY (Presenter), Department of Physics and Center for Advanced Nanoscience, University of California, San Diego — Metal-insulator transitions (MITs) in strongly-correlated materials result from the interplay of many degrees of freedom, such as electronic, magnetic or structural. Untangling these contributions has remained a longstanding problem in condensed matter physics. In this work, we have investigated V$_2$O$_3$, an archetypal strongly-correlated material with a MIT where electronic, structural and magnetic phase transitions occur simultaneously. By performing magneto-resistance (MR) measurements across the MIT we acted on the magnetic degree of freedom and revealed an anomalous behavior: the MR crosses over to negative values and seemingly diverges as the MIT takes place. To gain physical insight, we study the antiferromagnetic MIT in a Hubbard model in the presence of a magnetic field by high precision dynamical mean-field theory calculations. We find the model results accurately reproduce the unusual experimental behavior. Furthermore, they reveal a simple mechanism where the magnetic field impedes the antiferromagnetic ordering of one sublattice, thus preventing the opening of the gap. Our study provides strong evidence that the origin of the MIT in V$_2$O$_3$ is the opening of an antiferromagnetic gap.

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This work was performed in collaboration with A. Camjayi from Universidad de Buenos Aires; J. del Valle, Y. Kalcheim and I.K. Schuller from UC San Diego; and J.-P. Crocombette, J.E. Villegas, M. Rozenberg and D. Ravelosona from Université Paris-Saclay. Magnetic measurements were supported by the Office of Basic Energy Science, U.S. Department of Energy, under grant DEFG02 87ER-45332, and fabrication and characterization by the Vannevar Bush Faculty Fellowship funded by the Office of Naval Research through grant N00014-15-1-2848. The work was also supported by ERC grant Nr. 647100 “Suspintronics”. The author would like to thank Fundación Ramón Areces (Spain) for a postdoctoral fellowship.

Large linear magnetoresistance in ultraclean SrVO$_3$°

MATTHEW BRAHLEK (Presenter), JONG MOK OK, ELIZABETH SKOROPATA, HO NYUNG LEE, Materials Science and Technology Division, Oak Ridge National Laboratory, JASON LAPANO, ROMAN ENGEL-HERBERT, Pennsylvania State University, PATRICK IRVIN, JEREMY LEVY, physics, University of Pittsburgh — Observations of linear magnetoresistance have a near 100-year history with origins ranging from effects of open Fermi surface in polycrystalline metals, pushing materials like bismuth to the quantum limit, to large scale inhomogeneity/defect clusters in silver chalcogenides—such diversity has long given rise to controversy. This talk will focus on the surprising observation of a non-saturating linear magnetoresistance that appears in ultraclean, molecular beam epitaxy-grown thin films of the correlated metal SrVO$_3$. The unusual nature of this observation is that the linear magnetoresistance appears only when the samples are in the ultraclean limit and sets in far below the quantum limit; this strongly implies that this is an intrinsic feature of the electronic structure. As such both intrinsic effects, coming from the Fermi surface geometry and electron-electron correlations, and extrinsic effects, particularly defect structures common to perovskites, will be discussed.

°Work supported by the Office of Basic Energy Science, U.S. Department of Energy, Divisions of Materials Sciences and Scientific User Facilities

Spin colossal magnetoresistance in an antiferromagnetic insulator°

DAZHI HOU (Presenter), Tohoku University, ZHIYONG QIU, School of Materials Science and Engineering, Dalian University of Technology, JOSEPH BARKER, Tohoku University, KEI YAMAMOTO, Advanced Science Research Center, Japan Atomic Energy Agency, OLENA GOMONAY, Institut für Physik, Johannes Gutenberg Universität Mainz, EIJJI SAITOH, Department of applied physics, University of Tokyo — Colossal magnetoresistance (CMR) refers to a large change in electrical conductivity induced by a magnetic field in the vicinity of a metal–insulator transition and has inspired extensive studies for decades. Here we demonstrate an analogous spin effect near the Néel temperature, $T_N = 296$ K, of the antiferromagnetic insulator Cr$_2$O$_3$. Using a yttrium iron garnet YIG/Cr$_2$O$_3$/Pt trilayer, we injected a spin current from the YIG into the Cr$_2$O$_3$ layer and collected, via the inverse spin Hall effect, the spin signal transmitted into the heavy metal Pt. We observed a two orders of magnitude difference in the transmitted spin current within 14 K of the Néel temperature. This transition between spin conducting and non-conducting states was also modulated by a magnetic field in isothermal conditions. This effect, which we term spin colossal magnetoresistance (SCMR), has the potential to simplify the design of fundamental spintronics components, for instance, by enabling the realization of spin-current switches or spin-current-based memories.

Reference:

°Grant-in-Aid for young scientists (B) (JP17K14331)
**12:15PM B40.00004: Observation of non-Fermi liquid behaviors on high-mobility LaNiO$_3^*$**

CHANGJIANG LIU (Presenter), TERENCE BRETTZ-SULLIVAN, FRIEDERIKE WROBEL, GENSHENG WANG, DESHUN HONG, JOHN E. PEARSON, J SAMUEL JIANG, JIANJIE ZHANG, CLARENCE CHANG, Argonne National Laboratory, ALEXEY SUSLOV, National High Magnetic Field Lab, MICHAEL NORMAN, ANAND BHATTACHARYA, Argonne National Laboratory — LaNiO$_3$ (LNO) is a special member of the rare-earth perovskite nickelate family, as it does not show metal-insulator or magnetic transitions at low temperatures. Whether or not LNO behaves like a Fermi liquid in the low temperature regime with quadratic temperature dependence of resistivity remains an open question. Recent measurements of the electronic structure and theoretical calculations support the presence of structural and magnetic instabilities in LNO. However, the impact of these instabilities has yet to be clarified in transport measurements, partly because preparing high-quality LNO samples had been challenging due to a propensity towards oxygen vacancy formation. Here, we report on the observation of non-Fermi liquid transport behaviors at sub-Kelvin temperatures in high-mobility LNO thin films grown by ozone-assisted molecular beam epitaxy. The resistivity of these samples can be lower than 4 $\mu\Omega$ cm at $T = 2$ K, with residual resistivity ratios (RRR) [$\rho (300 \text{ K}) / \rho (2 \text{ K})$] > 24.

*Supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. The use of facilities at the Center for Nanoscale Materials was supported by the US Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

**12:27PM B40.00005: Direct Imaging Revealing Halved Ferromagnetism in Tensile-Strained LaCoO$_3$ Thin Films**

XIAOFANG ZHAI (Presenter), QIYUAN FENG, DECHAO MENG, QINGYOU LU, YALIN LU, University of Science and Technology of China — The enigma of the emergent ferromagnetic state in tensile-strained LaCoO$_3$ thin films remains to be explored since there is a longstanding controversy between the theory and experiments. It is that all experiments can only find at most half of the magnetic moment predicted by the theory. Here we show the experimental evidence of the rare halved occupation of the ferromagnetic state in tensile-strained LaCoO$_3$ thin films by the direct magnetic imaging technique using a low-temperature magnetic force microscope. The film was grown by the atomic layer-by-layer laser molecular beam epitaxy and exhibits the coherently strained lattice structure and the stoichiometric composition. The direct magnetic imaging revealed that percolated ferromagnetic regions with typical sizes between 100 nm and 200 nm occupy about 50% of the entire film, down to the lowest achievable temperature of 4.5 K and up to the largest magnetic field of 13.4 T. Our study demonstrated the halved occupation of the ferromagnetic phase in the LaCoO$_3$ ultrathin films as the real microscopic state of the emergent ferromagnetism.

**12:39PM B40.00006: Interplay between Strain-Stabilized Ferromagnetism and Charge Transport in Epitaxial LaCoO$_{3-\delta}$ Thin Films**

VIPUL CHATURVEDI (Presenter), JEFFERY J WALTER, ARPITA PAUL, JONG S JEONG, University of Minnesota, ALEXANDER GRUTTER, BRIAN KIRBY, JULIE BORCHERS, National Institute of Standards and Technology, K. ANDRE MKHOYAN, TURAN BIROL, CHRIS LEIGHTON, University of Minnesota — The presence of ferromagnetic (FM) order in epitaxial LaCoO$_3$ (LCO) thin films, in stark contrast to bulk, has gathered substantial recent attention. Due to the insulating nature of this strain-stabilized FM, however, little attention has been paid to electronic transport. Here, we present a systematic study of epitaxial LCO films (8-22 nm thick) grown under both tensile (on SrTiO$_3$ and LSAT) and compressive strain (on LaAlO$_3$ and SrLaAlO$_4$), emphasizing not only magnetism but also transport. Tensile films exhibit ferromagnetism with saturation magnetization 1-1.5 $\mu_B$/Co and Curie temperature ~80 K, consistent with prior work. Polarized neutron reflectometry has also been performed, revealing a uniform magnetization depth profile with thickness. Most notably, transport, which is semiconducting in all cases, reveals an unanticipated correlation between strain-state and majority carrier type, supported by density functional theory calculations suggesting significant changes in conduction band structure under strain. This provides important clues to the origin of FM in this material.

*Supported by DOE Center for Quantum Materials under DOE-SC0016371.
Most multiferroic materials with coexisting ferroelectric and magnetic order exhibit cycloidal antiferromagnetism with wavelength much larger than lattice spacing. The prototypical example is bismuth ferrite (BiFeO3 or BFO), a room-temperature multiferroic considered for a number of technological applications, including magnetic memories with electric-write capability. While most applications require small sizes such as nanoparticles, little is known about the state of these materials when their sizes are comparable to the cycloid wavelength. This work describes a theory of cycloid magnetism in nanoparticles. It is argued that magnetic anisotropy close to the surface has a huge impact on the ground state cycloidal wavevector, leading to several observable consequences. For certain sizes the cycloidal wavevector is bistable, an effect that may be exploited in the design of novel memory devices.

*We acknowledge support from NSERC (Canada), RGPIN/03938-2015.

NiO is a Mott insulator that orders antiferromagnetically below 520 K. The transition temperature drops with Li-doping and becomes first ferrimagnetic and later antiferromagnetic with a Néel temperature of 9 K. Despite intense study of NiO and other Mott insulators, the evolution of correlations with charge doping, which give rise to spectacular phenomena (including superconductivity in cuprates), is poorly understood to date. Here, we combine atomic layer-by-layer molecular beam epitaxy growth of charge doped NiO with density functional theory (DFT) and Quantum Monte Carlo (QMC) simulations. We analyze the band gap with spectroscopic ellipsometry as a function of hole (K) and electron (In) doping, and compare the results with DFT and QMC. Moreover, we measure the distortion of the lattice caused by the large K with extended x-ray absorption fine structure and find a distortion much larger than predicted by DFT.

1 D. Alders et al., EPL 32(3), 259 (1995)

*Supported by the U.S. DOE, Office of Science, BES, Materials Sciences and Engineering Division, as part of the Comp. Materials Sciences Program and Center for Predictive Simulation of Functional Materials

Magnon spin transport through antiferromagnetic NiO GEERT HOOGBOOM (Presenter), BART VAN WEES, Physics of Nanodevices, Zernike Institute for Advanced Materials — Thus far, antiferromagnets (AFMs) played a passive role of pinning in giant magnetoresistance. AFMs hold promise of ultrafast and lossless AFM transport devices when one is able to simultaneously generate and detect spin currents, while having control over the magnetic moment directions. AFMs have no stray fields so we made use of either the magnetic easy-plane character or an attached ferromagnet to manipulate its magnetic moments. Electrical and thermal injection of magnon spins occurs by a charge current through Pt, creating an interface spin accumulation via the Spin Hall Effect (SHE) and a thermally based magnon gradient. Resulting spin currents are detected by the inverse SHE, showing a 90° and 180° shift in the electrical and thermal signal respectively. Moreover, magnons that are detected non-locally revealed that both injection and detection is dependent on the magnetic texture of the NiO layer.

[1] Jungwirth et al., NNANO 11, 231
[2] Hoogeboom et al., APL 111, 052409
The cation distribution in piezoelectric ferromagnetic GaFeO$_3$(010) thin films*  JAEYOUNG KIM (Presenter), Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science, DONG-HWAN KIM, Department of Physics, POSTECH — GaFeO$_3$ is well known piezoelectric ferrimagnet where electron and spin degree of freedoms are coupled. There are four different cationic sites and the disorder in the occupation of them makes it ferrimagnet. Therefore, it is very important to study the site disorder in a specific specimen so as to understand a wide variety of ferromagnetic properties found in different GaFeO$_3$’s. Usually the site occupation of cations can be studied with neutron diffraction and Mösbauer spectroscopy. But, mostly they are not available for thin films. In this work, we have developed a new procedure to identify the site occupation of the cations by measuring X-ray absorption spectroscopy and X-ray magnetic circular dichroism and comparing them with cluster calculations. We apply it to undoped and Co-doped (2%) Ga$_{0.6}$Fe$_{1.4}$O$_3$ thin films and successfully explain the role of doped Co ions and why they have far different ferromagnetic properties.

*This work was supported by IBS - R014 -A2

Spin Transport across Antiferromagnetic Cr$_2$O$_3$ Films Grown on Y$_3$Fe$_5$O$_{12}$*  YAWEN LIU (Presenter), WEI YUAN, Department of Physics and Astronomy, University of California, Riverside, QIMING SHAO, KANG WANG, Department of Electrical Engineering, University of California, Los Angeles, JING SHI, Department of Physics and Astronomy, University of California, Riverside — Spin transport in heterostructures containing antiferromagnetic materials has attracted a lot of attention due to the enhanced transmission of the pure spin current and the interesting orientation dependence. Compared with NiO, Cr$_2$O$_3$ is a better-defined antiferromagnet for its uniaxial anisotropy. Here we report a spin transport study of YIG/Cr$_2$O$_3$/Pt heterostructures, in which both YIG and Cr$_2$O$_3$ are grown by PLD. RHEED patterns indicate that Cr$_2$O$_3$ is textured polycrystalline on single crystal YIG with preferred c-axis along the easy axis of the YIG. We perform both magnetoresistance(MR) and spin Seebeck effect (SSE) measurements. When the in-plane magnetic field is applied along or perpendicular to the c-axis of textured Cr$_2$O$_3$, the high-field MR responses in both directions resemble those of the YIG/Pt. When the field is along the c-axis of textured Cr$_2$O$_3$, MR shows an additional peak feature ~1T at 5 K, and the peak position moves to higher fields at higher temperatures, indicative of the spin-flop transition of Cr$_2$O$_3$. The SSE signal shows a sign reversal at low temperature, which does not exist in YIG/Pt and therefore is also attributed to the Cr$_2$O$_3$.

*This work was supported by SHINES, which is funded by the U.S.DOE, Office of Science, Basic Energy Sciences under Award SC0012670.

Hexagonal YbFeO$_3$ thin-film heterostructures grown by pulsed laser deposition*  YU YUN (Presenter), YUEWEI YIN, XUANYUAN JIANG, XIAOSHAN XU, University of Nebraska - Lincoln — Multiferroic materials have drawn significant attention because of its potential application in information processing and storage. Hexagonal ferrites (h-RFeO$_3$, R=Y, Dy-Lu), as identified multiferroic materials, have recently been predicted to have a magnetoelectric effect. To verify theoretical predictions, exploring the suitable substrates and bottom electrodes for the growth of hexagonal ferrites is a big challenge. In our study, we have successfully fabricated high-quality YbFeO$_3$ thin films on the STO (111) substrate with La$_{0.3}$Sr$_{0.7}$MnO$_3$ bottom electrode grown by pulsed laser deposition system. The crystal structure is characterized by X-ray diffraction, and the electron transport properties are investigated from 20 K to 300 K. Our experiments in YbFeO$_3$ multiferroic thin films pave the way for the further investigation of magnetoelectric effects in the hexagonal ferrites.

*This work was supported by the NSF DMR-1454618.
2:03PM B40.00013: The role of disorder and defects in the ferromagnetic resonance of spinel ferrite thin films
JACOB WISSER (Presenter), Applied Physics, Stanford University, SATORU EMORI, Physics, Virginia Tech, LAUREN RIDDIFORD, Applied Physics, Stanford University, PENG LI, Geballe Laboratory for Advanced Materials, Stanford University, KRISHNAMURTHY MAHALINGHAM, BRITTANY T. URWIN, BRANDON HOWE, Air Force Research Laboratory, ALEXANDER GRUTTER, BRIAN KIRBY, NIST Center for Neutron Research, YURI SUZUKI, Applied Physics, Stanford University — Spin current generation in heterostructures requires low magnetic damping spin-current sources. To this end, we seek to minimize disorder and defects in spin-current source materials and improve interface quality. In this work, we find that epitaxial spinel ferrite MgAl0.5Fe1.5O4 (MAFO) films exhibit low damping and coercivity in the 10-15nm thickness range with a Gilbert damping parameter $\alpha \approx 0.001$ and coercive field $H_c < 5$ Oe. Transmission electron microscopy results indicate these films grow coherently strained on MgAl2O4 substrates with minimal defects. Gilbert damping rapidly increases outside of this thickness range, with $\alpha \approx 0.004$ for 5nm films and $\alpha \approx 0.03$ for 40nm films. Dislocations form at the film/substrate interface in 40nm films, indicating that the film relaxes, causing increased damping and coercivity ($H_c > 50$ Oe). A thickness-dependent magnetization study of MAFO films from 1-45nm thick indicates the presence of a 1.6nm magnetically-dead layer, less than half that found in yttrium iron garnet films. This layer is confirmed to exist at the film/substrate interface by depth profiling via polarized beam neutron reflectivity. The nature of this dead layer is crucial to device integration, and we will discuss interfacing this oxide with platinum and copper/platinum overlayers.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B41 GMAG DMP: Novel Magnetic Structures and Excitations I
BCEC 209 - Adam Ahmed, Ohio State University - Tag(s): Focus

11:15AM B41.00001: Anatomy of Dzyaloshinskii–Moriya interaction at interfaces: from Fert-Levy type DMI at Co/Pt to Rashba effect induced DMI at Co/graphene* [invited] HONGXIN YANG (Presenter), Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences — The antisymmetric exchange interaction, Dzyaloshinskii-Moriya Interaction (DMI), has gained an intense research effort due to its crucial role in the creation, annihilation and the influence on the dynamics of magnetic Skyrmions and chiral domain wall. Here, we will present a general DMI calculation approach based on DFT total energy calculations and show the calculated DMI at Co/Pt interfaces and the comparison with experiments. We will address the main features and microscopic mechanism of typical Fert-Levy type DMI at Co/Pt interface from first-principles by clearing up several fundamental questions: how does the DMI extend away from the interface? Where is the corresponding electronic energy source located? [1] How to design enhanced DMI systems? [2,3] Moreover, we will go beyond Fert-Levy type DMI systems to avoid using heavy metals but with simple ferromagnet/graphene interfaces. [4] At the end, we will give a perspective on the topic with new systems which may also give large DMI but are different to FM/HM and FM/graphene.


*We acknowledge the French ANR SOSPIN, ESPERADO and ULTRASKY projects, HPC resources from CEA/Grenoble, GENCI-CINES (Grants No. 2012, No. 2013-096971 and C2016097605), the European Union’s Horizon 2020 Research and Innovation Programme under grant agreement No. 696656 (GRAPHENE FLAGSHIP), and the National Natural Science Foundation of China (11874059).
12:03PM B41.00003: Laser-induced ultrafast magneto-optic dynamics on low-dimensional carbon nanostructures*  
CHUN LI (Presenter), RUI HUANG, YIMING ZHANG, Northwestern Polytechnical University, GEORGIOS AL LEFKIDIS, WOLFGANG HUEBNER, University of Kaiserslautern — Carbon nanostructures constitute a family of novel molecular materials, with great potential applications for future nanoscale spintronics devices. Here, the ultrafast magneto-optic dynamics behavior of carbon nanostructures (including graphene and endohedral fullerenes) are investigated by taking advantage of suitable Λ processes[1-3]. For graphene nanoflakes, different attaching locations of the magnetic elements at the graphene boundary are considered. It is shown that the spin density is typically localized on a single magnetic atom, which leads to localized spin switching within subpicosecond time regime. For the endohedral fullerenes, it is found that both spin switching and spin transfer can be achieved on the experimentally synthesized system Sc3N@C80. The spin density, which for the fully relaxed system is equally distributed among the three Sc atoms, becomes strongly localized by the applied strain, leading to fast, clear-cut, spin-transfer processes. In particular, the fastest spin-transfer process can be accomplished within 100 fs.

References

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12:15PM B41.00004: Time-dependent ab initio insight to the ultrafast demagnetization mechanism  
ZHANGHUI CHEN (Presenter), LIN-WANG WANG, Lawrence Berkeley National Laboratory — Laser induced ultrafast demagnetization process has a great potential in future spintronic devices. Ever since its discovery, this subject has been studied intensively. However, the fundamental physics is still not well understood. There are several long-standing problems regarding the demagnetization mechanism. One major issue is the remarkable underestimation in ab initio simulation. At the same intensity of laser, the theoretical demagnetization rate can be ten times smaller than the experimental observation. Here, we present an ultrafast real-time time-dependent density functional theory method, together with atomic Landau-Lifshitz-Gilbert model, to investigate this problem. Our results show that one important reason for the underestimation is the missing of initial spin disorder, which can significantly enhance the demagnetization to the experimentally observed rate. This spin disorder connects the electronic structure theory with the phenomenological three-temperature model. We have also systematically studied the roles of various interactions which are heavily debated. In particular, we found that electron-electron interaction and spin-orbit interaction play extremely important roles, while electron-phonon and light-spin interactions are not essential.

12:27PM B41.00005: Photocontrol of magnetic structure in a metallic ferromagnet*  
ATSUSHI ONO (Presenter), SUMIO ISHIHARA, Department of Physics, Tohoku University — We study theoretically photoinduced phenomena in a metallic ferromagnet described by the double-exchange (DE) model, where conduction electrons mediate the ferromagnetic (FM) DE interaction between localized magnetic moments in equilibrium. We found that the DE interaction acts as the antiferromagnetic (AFM) interaction in highly photoexcited states, which is in sharp contrast to the conventional DE mechanism. Numerical computations of real-time dynamics described by the Schrödinger equation combined with the Landau-Lifshitz-Gilbert equation reveal that the FM metallic initial state is transformed into the AFM steady state through a transient state with emergent topological magnetic defects. We also calculated magnetic excitation spectra in the photoirradiated FM metallic state by using the Floquet Green function method and found that magnon is softened by photoirradiation, which indicates that the AFM instability is induced by the Stoner excitation in the Floquet state.

*This work was supported by JSPS KAKENHI Grant JSPS KAKENHI Grant Numbers JP15H02100, JP17H02916, JP18H05208, and JP18J10246.

12:39PM B41.00006: All-Optical Deterministic Switching of Synthetic CoCrPt Ferrimagnets*  
BRADLEE K. BEAUCHAMP (Presenter), School of Materials Engineering, Purdue University, AVEEK DUTTA, ALEXANDRA BOLTASSEVA, VLADIMIR M SHALAEV, School of Electrical and Computer Engineering, Purdue University, ERNESTO MARINERO, School of Materials Engineering, Purdue University — Ultrafast magnetic switching via femtosecond laser pulses is vital for increasing the speed of spintronic devices and has been demonstrated in various ferrimagnetic materials. However, this switching has not yet been demonstrated in synthetic ferrimagnetic hcp CoPtCr alloys. The synthetic ferrimagnetic trilayers consist of two CoCrPt layers antiferromagnetically coupled via a thin Ru spacer. Synthetic ferrimagnetic thin film trilayers have the potential to be switched in the sub-picosecond time regime. CoCrPt is a highly anisotropic magnetic material with low saturation magnetization, making it optimal for magnetic recording. Here we demonstrate all-optical helicity-dependent switching of CoCrPt/Ru/CoCrPt thin film trilayers using circularly polarized, 65 femtosecond, 800 nm KrF laser pulses.

*This work was conducted under the auspice of the Office of Naval Research, Award N00014-18-1-2481.
12:51PM B41.00007: Optical Control of Magnetic Orientation in Epitaxial CoFe$_2$O$_4$ Films  YI-CHUN CHEN (Presenter), YI-DE LIOU, I-TSE TSAI, JAN-CHI YANG, Department of Physics, National Cheng Kung University — Complex oxides have caught significant attention for the development of the next-generation electronic devices due to their versatile functionalities and the tunability via the external stimuli, such as electrical and magnetic fields. To broaden the application of complex oxides, the new pathway to control the physical properties is on demand. Cobalt ferrite (CoFe$_2$O$_4$, CFO), a ferrimagnetic inverse spinel, which has advantages of high magnetization and coercivity for magnetic data storage, is investigated in this study. We introduce the high density laser to illuminate the epitaxial CFO film and control the magnetic orientation of the film at ambient temperature. Effects of various illumination conditions of CW and pulsed lasers are systematically investigated. Magnetic force microscopy (MFM) and X-ray magnetic circular dichroism coupled to photoemission electron microscopy (XMCD-PEEM) are used to investigate the magnetic orientation of the optical-modulated area. The possible mechanism for modulating magnetic structures is thus determined as the thermal effect combined with magnetostatic couplings.

1:03PM B41.00008: Ultrafast transfer of magnetization on magnetic sublattices in half-metallic Co$_2$MnGe heusler alloys  PHOEBE TENGDIN (Presenter), CHRISTIAN GENTRY, DMITRIY ZUSIN, ADAM Z BLONSKY, JILA, University of Colorado, Boulder, JUSTIN SHAW, HANS T. NEMBACH, MONIKA ARORA, THOMAS SILVA, National Institute of Standards and Technology, Boulder CO, YAROSLAV KVASHNIN, ERNA DELCZEZ, OLLE ERIKSSON, Uppsala University, HENRY C KAPTEYN, MARGARET MARY MURNANE, JILA, University of Colorado, Boulder — Heusler alloys are exciting materials for future applications because they display a wide range of tunable electronic and magnetic interactions such as metallicity, ferromagnetism, superconductivity, and giant magneto-resistance. However, laser-induced spin dynamics in heuslers were expected to be slower than in conventional metallic ferromagnets, due to the presence of a blocked spin channel. Here we directly observe ultrafast spin transfer from one magnetic sublattice to another in half-metallic heusler alloy Co$_2$MnGe, that occurs on the timescale of the femtosecond laser excitation. Ultrafast high harmonic pulses make it possible to simultaneously record the element-specific magnetic dynamics of Co and Mn as the material undergoes demagnetization. The magnetization of Co is transiently enhanced by 10% within 60 fs, while that of Mn rapidly quenches. By comparing our data to density functional theory, we show that optical excitation can directly transfer spin from one magnetic sublattice to another, due to spin-polarized optical excitation pathways. The observed transient enhancement of ferromagnetic ordering demonstrates fast manipulation of spin by light, thus providing a path towards spintronics logic devices that can operate on femtosecond or even attosecond timescales.

1:15PM B41.00009: Revisiting half-metallicity of Co-based full Heusler alloys from non-empirical DFT+U method*  KENJI NAWA (Presenter), YOSHIIO MIURA, National Institute for Materials Science — The half-metallic (HM) ferromagnet, which has 100% spin polarization at the Fermi level ($E_F$), is great advantage to enhance efficiency of spin-dependent tunneling property. In particular, Co-based full Heusler alloys have been paid much attention because of the HM and high Curie temperature. The density functional theory (DFT) calculations are expected to play a key role for searching the HM materials and understanding an origin of HM. However, the DFT methods within the local density approximation often fail to predict the HM due to localized $d$ electrons around $E_F$. In this work, we revisit electronic structure of Co$_2$MnSi by the DFT+U method, where +U parameters representing correlation effect are derived from linear response theory. We revealed important atomic orbital hybridizations, which mainly dominate energy gap at $E_F$. Although the Co$_2$MnSi is not HM, our energy diagram provides a new guideline to tune the HM gap. We extended our calculations to quaternary systems Co$_2$(Y,Mn)Si, where Y is $3d$ transition metals. We found the systems with Y of Ti, V, Cr, and Fe show the HM when composition of Y is selected appropriately.

*This work was supported by JSPS KAKENHI Grant Numbers JP16H06332 and JP17H06152, and by ImPACT Program of Council for Science, Technology and Innovation, Japan.

1:27PM B41.00010: Half-metallic surfaces in thin-film Ti$_2$MnAl$_{0.5}$Sn$_{0.5}$  PAVEL LUKASHEV (Presenter), SAM PROPHET, RISHABH DALAL, University of Northern Iowa, PARASHU KHAREL, South Dakota State University — Materials exhibiting a high degree of spin polarization are in demand in spintronics. Room-temperature half-metals are considered ideal candidates, as they behave as an insulator for one spin channel and as a conductor for the other spin channel. In addition, for nano-size devices, one has to take into account possible modification of electronic structure in thin-film geometry, due to the potential presence of surface/interface states. Typically, these states have a detrimental impact on half-metallicity. Here, we employ density functional calculations to explore an inverse Heusler compound, Ti$_2$MnAl$_{0.5}$Sn$_{0.5}$, which exhibits half-metallic electronic structure in bulk geometry. We show that in thin-film geometry, the type of termination surface has a decisive effect on half-metallicity of this material. In particular, we analyze six possible termination configurations, and show that for four of them, energy states emerge in the minority-spin band gap, significantly reducing the spin polarization. At the same time, two termination surfaces preserve half-metallic properties of this material. Thus, our results show that a judicious choice of the termination surface may be a crucial factor in nano-device applications, where highly spin-polarized current is needed.
1:39PM B41.00011: Why is the Curie temperature of Co2FeSi so high?* GUANHUA QIN (Presenter), University of Missouri, WEI REN, Shanghai University, DAVID SINGH, University of Missouri — We have investigated the Curie temperature of Co2FeSi and Co2TiSi by using first principle calculations. The full heusler alloy Co2FeSi has large magnetic moment per f.u. 6μB and very high Curie temperature ~1100K. And the value for Tc is 380K for half-metallic ferromagnetism Co2TiSi. We Compare these two systems using models and calculations of magnon dispersions.

*Work at the University of Missouri is supported by the Department of Energy, Basic Energy Sciences, Award DE-SC0019114.

1:51PM B41.00012: Electronic structure and magnetic properties in T2AlB2 (T = Fe, Mn, Cr, Co, and Ni) and their alloys* BRUCE HARMON, MATTHEW J. KRAMER, LIQIN KE (Presenter), Ames Laboratory, U.S. DOE, Ames, Iowa 50011, USA — Fe2AlB2 is one of the promising candidates for magnetic refrigeration technology and has attracted great attention since the recent discovery of its substantial magnetocaloric effect around room temperature. The electronic structure and intrinsic magnetic properties of Fe2AlB2-related compounds and their alloys have been investigated using density functional theory. For Fe2AlB2, the crystallographic a axis is the easy axis, in agreement with experiment. The magnetic ground state of Mn2AlB2 is found to be ferromagnetic in the basal ab plane, but antiferromagnetic along the c axis. All 3d dopants considered decrease the magnetization and Curie temperature in Fe2AlB2. Electron doping with Co or Ni has a stronger effect on the decreasing of Curie temperature in Fe2AlB2 than hole doping with Mn or Cr. However, a larger amount of Mn doping in Fe2AlB2 promotes a ferromagnetic to antiferromagnetic transition. A very anisotropic magnetoelastic effect is found in Fe2AlB2: the magnetization has a much stronger dependence on the lattice parameter c than on a or b, which is explained by electronic-structure features near the Fermi level. (Ref: PRB 95, 104427)

*This work was supported by the U.S. Department of Energy, Advanced Research Projects Agency-Energy (ARPA-E) under Grant No. 1002-2147.

2:03PM B41.00013: Magnetic and magnetocaloric properties of Co doped Ni-Mn-Sn Heusler alloys at high magnetic field and pressure* SUDIP PANDEY (Presenter), Department of Physics, Southern Illinois University Carbondale, IL 62901, USA, YURY KOSHKID'KO, Institute of Low Temperature and Structural Research PAS, Wroclaw, 53-421 Poland, IGOR DUBENKO, ANIL ARYAL, Department of Physics, Southern Illinois University Carbondale, IL 62901, USA, ALEXANDER B. GRANOFSKY, Faculty of Physics, Lomonosov Moscow State University, Moscow, 119991 Russia, SHANE STADLER, Department of Physics & Astronomy, Louisiana State University, LA 70803 USA, NAUSHAD ALI, Department of Physics, Southern Illinois University Carbondale, IL 62901, USA — The magnetic and magnetocaloric properties of Ni45Mn43CoSn11 have been investigated using direct method for magnetic field changes up to 14 T, heat capacity measurements, and magnetization with hydrostatic pressure applications. A large reversible magnetocaloric effect resulted in a ΔT_{ad} of about ~−11 K and 5 K for a magnetic field change of 14 T in the vicinity of magnetostructural (T_A~260 K) and magnetic (T_C~320K) transition, respectively. The impact of thermomagnetic history on ΔT_{ad} at high magnetic fields has been revealed. Significant changes in the relaxation time of ΔT_{ad} depending on the type of phase transitions, magnetization, and demagnetization cycle are discussed. The density of states and Debye temperature have been estimated from heat capacity measurements. The mixed effects of pressure and magnetic field on the transition temperature is discussed.

*This work was supported by the Office of Basic Energy Sciences, Material Science Division of the U.S. Department of Energy, DOE Grant No. DE-FG02-06ER46291 (SIU) and DE-FG02-13ER46946 (LSU). YK acknowledges support from a grant from the National Science Center Poland (NCN) under the SONATA program (2016/21/D/ST3/03435).

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B42 DQI: Gates in Superconducting Qubits BCEC 210A - Antonio Corcoles, IBM Thomas J. Watson Research Center - Tag(s): Focus
11:15AM B42.00001: Characterization of Single- and Two-qubit Gates between Transmons and Capacitively Shunted Flux Qubits  JASEUNG KU (Presenter), YEBIN LIU, BRITTON L PLOURDE, Syracuse University, XUEXIN XU, MOHAMMAD H. ANSARI, Peter Grünberg Institute, JARED B HERTZBERG, MARKUS BRINK, JERRY M. CHOW, IBM T.J. Watson Research Center — Capacitively shunted flux qubits (CSFQs) with high coherence hold promise for improved single- and two-qubit gate operations due to their relatively large and positive anharmonicity. When paired with transmon qubits, CSFQs may lead to a novel regime for two-qubit gates based on the cross resonance interaction. We fabricated a two-qubit system consisting of a CSFQ and a fixed-frequency transmon coupled via a bus cavity and we characterized the fidelity of single- and two-qubit gate operations. In this talk, we will present experimental results from these measurements.

11:27AM B42.00002: Characterization of Single- and Two-qubit Gates between Transmons and Capacitively Shunted Flux Qubits: Part 2, Theory  XUEXIN XU (Presenter), MOHAMMAD H. ANSARI, Peter Grünberg Institute, Forschungszentrum Jülich, JASEUNG KU, YEBIN LIU, BRITTON L PLOURDE, Syracuse University, JARED B HERTZBERG, MARKUS BRINK, JERRY M. CHOW, IBM T J Watson Res Ctr — We theoretically model an experiment on a superconducting circuit made of a capacitively shunted flux qubit (CSFQ) and a Transmon qubit both capacitively coupled to a bus resonator in dispersive regime. To model this circuit we take into account the contribution of higher excited states in qubits and block-diagonalize the Hamiltonian perturbatively in the regime of small interaction couplings compared to frequency detuning. We apply external driving microwave pulses over all energy levels and consider the transitions they impose effectively within the computational subspace. More specifically we study single qubit gates and cross-resonance gate, and analyze the fidelity of their operations. Our theoretical results are in agreement with experiment, showing a promising approach to controllably improve single- and two-qubit gate operations in such circuits due to the relatively large and positive anharmonicity of CSFQ.

11:39AM B42.00003: Demonstration of a high fidelity entangling gate in a superconducting architecture  SABRINA HONG (Presenter), PRASAHNT SIVARAJAH, ANTHONY POLLORENO, NICOLAS DIDIER, EYOB SETE, JOSHUA COMBES, KYLE GULSHEN, MARCUS DA SILVA, ALEXANDER PAPAGEORGE, Rigetti Computing — We demonstrate a high fidelity entangling gate in an architecture of alternating fixed and tunable qubits by directly modulating the flux of the tunable qubit. We achieve this by parking the DC flux of the tunable gate where the qubit is first-order insensitive to $1/f$ DC flux noise in addition to performing the flux modulated gate at an “AC sweet spot” where the qubit is first-order insensitive to noise under flux modulation, allowing us to leverage a higher ratio of gate time to coherence time. In addition to characterizing the gate using standard protocols, we qualify its performance over long periods of time, self-consistently assessing the gate fidelity and drift therein.

11:51AM B42.00004: Quantum Gates between Multi-modal Quantum Circuits*  SUMERU HAZRA (Presenter), KISHOR SALUNKHE, GAURAV BOTHARA, ANIRBAN BHATTACHARJEE, SUMAN KUNDU, MEGHAN P. PATANKAR, Tata Institute of Fundamental Research, TANAY ROY, Department of Physics, University of Chicago, IL, USA, RAJAMANI VIJAYARAGHAVAN, Tata Institute of Fundamental Research — Maximum interqubit connectivity and ability to do fast multiqubit operation are key ingredients towards building an efficient quantum processor. We have recently demonstrated trimon, a multimodal device[1,2] with all-to-all longitudinal coupling as a three-qubit quantum processor[3]. Always on strong longitudinal coupling and maximum interqubit interactions in such devices lead to simple implementation of fast high fidelity multiqubit gates. In order to scale up, we propose to use the trimon as a building block for a larger quantum processor using cross resonance drive[4] to turn on interaction between two such units. We will first discuss the coupling of a transmon and a longitudinally coupled two-qubit device named dimon, and explain how to construct a two-qubit CNOT gate. We will present preliminary experimental data and discuss extensions to gates between multiple dimon/trimon blocks. Finally, we will discuss the possibility of using dimon to improve connectivity and directionality of gates in transversely coupled multiqubit systems.


*Department of Atomic Energy, Government of India
12:03PM B42.00005: Fast single qubit gates in a capacitively shunted fluxonium* HELIN ZHANG (Presenter), University of Chicago — A capacitively shunted fluxonium circuit has among the longest lifetimes seen in cQED due to the exponential suppression of the charge transition matrix element from the extra capacitance. The suppressed matrix elements however make it challenging to perform fast fluxon gates via charge coupling, requiring the use of excited fluxonium levels and Raman transitions [1]. Here, we present and characterize new protocols for performing fast single-qubit gates near half flux quantum, using fast flux modulation. The low transition frequencies near half flux quantum allow for adiabatic gates, and direct synthesis of flux pulses. These approaches increase the ease of control of fluxonium circuit at its highest coherence point, and thereby its feasibility as a building block for future quantum information processors.


*This work was supported by ARO Grant No. W911NF-15-1-0421; SUB0000079

12:15PM B42.00006: Sub-100ns entangling gates between two strongly coupled transmon qubits* JUNLING LONG (Presenter), HSIANG-SHENG KU, RUSSELL LAKE, XIAN WU, MUSTAFA BAL, COREY RAE MCRAE, DAVID PAPPAS, National Institute of Standards and Technology, Boulder — Superconducting qubits are very promising candidates for realizing a fault-tolerant quantum computer. However, implementing two-qubit entangling gates with short gate operation time and high fidelity is still a challenge with superconducting qubits. In this talk, we demonstrate a new type of two-qubit entangling gate, the SWIPHT gate [1], on a coupled-transmon device. The two-transmon system, strongly coupled through a bus resonator, is tuned into the secondary resonance regime, where the effective $\sigma_1^z\sigma_2^z$ interaction is enhanced due to the coupling to higher levels of the transmons. Unconditional single qubit gates two-transmon systems with strong $\sigma_1^z\sigma_2^z$ interaction were developed. This allows a SWIPHT CNOT gate with roughly 90 ns gate time. The gate fidelity is extracted by quantum process tomography.


*All the authors acknowledge support of the NIST Quantum Based Metrology Initiative

12:27PM B42.00007: Black-box optimization of quantum gates for two coupled transmons* ZHAOQI LENG (Presenter), PRANAV MUNDADA, ANDREW HOUCK, Princeton University — As qubit coherence time sets a limit on the total time available for performing quantum gates, realizing high-fidelity, fast quantum gates is critical for enabling long-depth quantum circuits in the non-fault-tolerant regime and represents a path way towards fault tolerant quantum computation. Here, we present simulated and experimental results on using black-box optimization to tune up quantum gates for two transmon qubits coupled via a bus cavity. This optimization procedure does not require any knowledge of gradients derived from the system Hamiltonian, and thus it is ideal for automatic gate optimization on large quantum systems.

*This work is supported by IARPA under contract W911NF-16-1-0114

12:39PM B42.00008: High fidelity fermionic simulation gates with superconducting gmon qubits BROOKS FOXEN (Presenter), BEN CHIARO, MATTHEW MCEWEN, University of California, Santa Barbara, JOHN M MARTINIS, Google Inc. — We present an experimental realization of a high-fidelity 2-qubit continuous fermionic simulation (fSim) gateset using superconducting gmon qubits. Each fSim gate is parameterized by two angles: the $|01\rangle$ to $|10\rangle$ swap angle $\theta$, and the conditional phase angle $\varphi$. The full fSim($\theta$, $\varphi$) gateset covering $\theta$: $[0^\circ, 90^\circ]$ and $\varphi$: $[-180^\circ, 180^\circ]$ includes both the iSwap (fSim$(90^\circ, 0^\circ)$) and controlled-Z (fSim$(0^\circ, 180^\circ)$) gates making it applicable to error correction, quantum supremacy, and pre-error correction applications including quantum chemistry and quantum approximate optimization algorithms.
12:51PM B42.00009: Experimental Realization of non-Adiabatic Shortcut to non-Abelian Geometric Gates

TONGXING YAN (Presenter), BAOJIE LIU, School of Physics, Southern University of Science and Technology of China, KAI XU, CHAO SONG, Department of Physics, Zhejiang University, SONG LIU, ZHENSHENG ZHANG, School of Physics, Southern University of Science and Technology of China, HUI DENG, ZHIQIUAN YAN, HAO RONG, CAS Center for Excellence and Synergetic Innovation Center in Quantum Information and Quantum Physics, University of Science and Technology of China, KEQIANG HUANG, Institute of Physics, Chinese Academy of Sciences, MAN-HONG YUNG, YUANZHEN CHEN, DAPENG YU, School of Physics, Southern University of Science and Technology of China — When a quantum system is driven slowly through a parametric cycle in a degenerate Hilbert space, the state would acquire a non-Abelian geometric phase, which is stable and forms the foundation for holonomic quantum computation (HQC). However, in the adiabatic limit, the environmental decoherence becomes a significant source of errors. Recently, various non-adiabatic holonomic quantum computation (NHQC) schemes have been proposed, but all at the price of increased sensitivity to control errors. Here we propose and experimentally demonstrate that HQC via shortcut to adiabaticity (STA) can be constructed with only three energy levels, using a superconducting qubit. With this scheme, all holonomic single-qubit operations can be realized non-adiabatically through a single cycle evolution. As a result, we are able to experimentally benchmark the stability of STA+HQC against NHQC. The flexibility and simplicity of our scheme makes it also implementable on other quantum systems.

*Natural Science Foundation of Guangdong Province (2017B030308003), the Guangdong Innovative and Entrepreneurial Research Team Program (No.2016ZT06D348), and the Science Technology and Innovation Commission of Shenzhen Municipality (ZDSYS20170303165926217, JCYJ20170412152620376).

1:03PM B42.00010: High-fidelity parametric entangling gates at AC flux sweet spots [Invited] NICOLAS DIDIER (Presenter), EYOB A SETE, JOSHUA COMBES, MARCUS DA SILVA, Rigetti Computing — Realizing high-fidelity two-qubit gates is one of the main challenges in building quantum processors. A major limitation is often decoherence, in particular dephasing due to the ubiquitous presence of flux noise in tunable qubits. Under static magnetic flux biases, the dephasing time is greatly enhanced when the tunable qubit is parked at flux insensitive operating points, commonly referred to as "sweet spots". We show that under flux bias modulation around such DC flux sweet spots, even though the qubit continuously explores regions sensitive to flux noise, there exists a modulation amplitude where the qubit is insensitive to low-frequency flux fluctuations like 1/f noise - the AC flux sweet spot. We show how this sweet spot is preserved in presence of instrumental white noise by lowpass filtering the flux line. We present how the AC flux sweet spot allows to reach state-of-the-art fidelities in parametrically-activated entangling gates. arXiv:1807.01310.

1:39PM B42.00011: Coherent, Landau-Zener control of a superconducting composite qubit* DANIEL CAMPBELL (Presenter), BHARATH KANNAN, Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, MA 02139, YUN-PIL SHIM, Laboratory for Physical Sciences, Department of Physics, University of Maryland, College Park, MD 20740, RONI WINIK, Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, MA 02139, ALEXANDER MELVILLE, BETHANY M. NIEDZIELSKI, JONILYN L YODER, MIT Lincoln Laboratory, 244 Wood Street, Lexington, MA 02421, CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD 20740, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, MA 02139, WILLIAM D OLIVER, Research Laboratory of Electronics, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, MIT Lincoln Laboratory, 244 Wood Street, Lexington, MA — We consider a computational subspace defined by two transmons coupled with a fixed capacitance. Following Ref. 1, we identify the resonantly coupled, hybridized states as a composite qubit (CQB). The CQB architecture has the desirable property that universal single-CQB gates may be implemented using solely coherent, Landau-Zener control methods based on fast, broadband pulses, without need for microwave control signals. The fidelity of these single-CQB gates is comparable to current state-of-the-art implementations.2 We present these experimental demonstrations and discuss the susceptibility of the CQB to various noise channels.

1Shim, Y.-P. and Tahan, C. Nat. Commun. 7 11059 (2016).

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1:51PM B42.00012: Fault-tolerant and Continuous Holonomic Gates for Topologically Protected Qubits.  

ANDREY KLOTS (Presenter), LARA FAORO, ROBERT F MCDERMOTT, LEV B IOFFE, University of Wisconsin-Madison — We present the design of the topologically protected qubit that allows fault tolerant discrete operations together with the continuous holonomic \( \exp(i\theta \sigma_z) \)-gates. Topological protection of qubits is meaningless without ability to perform fault tolerant operations. These transformations should involve at least the generators of the discrete fault tolerant Clifford group and a rotation at an arbitrary angle such as \( \pi/3 \). We propose a superconducting circuit that satisfies these criteria. The proposed qubit allows protected \( \pi/2 \)-rotations in charge (Q)- and flux (\( \Phi \))-channels. Furthermore, by moving the state of the qubit along the closed loop in the \( \{Q, \Phi\} \)-space we can controllably and continuously gain a finite Berry phase difference between 0 and 1 states that is weakly sensitive to the errors in charge and flux biases.

The qubit is based on superconducting 0-\( \pi \) elements which effectively act as \( \pi \)-periodic Josephson junctions. The discrete gate operations are characterized by the exponential suppression of the flux and charge noise. The continuous holonomic operation maintains exponential suppression of the flux noise and has the quadratic suppression of the charge noise.

*We thank ARO HiPS W911NF-18-1-0106

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B43 DCMP: Nonlinear Optics in Topological Semimetals

11:15AM B43.00001: Origins of strong and/or quantized nonlinear optical responses in Weyl semimetals  

JOEL MOORE (Presenter), University of California, Berkeley, and Lawrence Berkeley National Laboratory — Weyl semimetals and other topological materials can support unique electromagnetic responses different from ordinary matter. This talk starts with a brief review of the theory of linear and nonlinear optics in crystals, including recent work on how geometric properties of Bloch states such as the Berry curvature can lead to simplified expressions and sum rules. Previous results show that in Weyl semimetals, nonlinear optics is likely to be a more fruitful ground for novel behavior than linear response. In addition to the Weyl semimetal TaAs whose nonlinear optical properties are the subject of intense study, we explain how other Weyl materials lacking mirror symmetry (and certain related compounds) should have an approximately quantized circular photogalvanic effect (CPGE) and discuss the status of experimental searches for this effect in various materials.

The main results described were obtained in collaborative works with F. de Juan, B. M. Fregoso, A. G. Grushin, T. Morimoto, J. W. Orenstein, and D. Parker.

11:51AM B43.00002: Colossal Bulk Photovoltaic Effect in a Weyl Semimetal*  

GAVIN B OSTERHOUDT (Presenter), LAURA KATHARINA DIEBEL, MASON GRAY, XU YANG, JOHN STANCO, Boston College, XIANGWEI HUANG, Max Planck Institute for Chemical Physics of Solid, BING SHEN, NI NI, Univ of California Los Angeles, PHILIP MOLL, Ecole Polytechnique Federale de Lausanne, YING RAN, KENNETH BURCH, Boston College — The bulk photovoltaic effect (BPVE) is a second-order non-linear optical effect which directly converts light into an electrical current. This effect is intimately related to the topological nature of the material, and is in fact directly proportional to the Berry connection. We present photocurrent measurements on the Weyl semimetal TaAs, where the diverging Berry connection leads to the largest observed BPVE, as well as the first observation of BPVE utilizing mid-infrared radiation.

*U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Award No. DE-SC0018675
National Science Foundation, Award No. DMR-1709987
DAAD RISE Fellowship
National Science Foundation, Award No. DMR-1151440
U.S. Departramnt of Energy, Office of Science, Office of Basic Energy Research, Award No. DE-SC0011978
European Research Council, European Union Horizon 2020 Research and Innovation Programme, No. 715730
12:27PM B43.00003: Berry Curvature Enhanced Nonlinear Photogalvanic Response of Type-II Weyl Cone* [Invited]
DONG SUN (Presenter), Peking University — In this talk, signatures of the singular topology in a type-II Weyl semimetal TaIrTe$_4$ is revealed in the photo responses, which are shown to be directly related to the divergence of Berry curvature. As a result of the divergence of Berry curvature at the Weyl nodes, TaIrTe$_4$ exhibits unusually large photo responsivity of 130.2 mA/W with 4-mm excitation in an unbiased field effect transistor at room temperature arising from the third-order nonlinear optical response. Furthermore, the circularly polarized galvanic response is also enhanced at 4-mm, possibly due to the same Berry curvature singularity enhancement with the shift current. Considering the optical selection rule of Weyl cones with opposite chirality, it may open new experimental possibilities for studying and controlling the chiral polarization of Weyl Fermions through an in-plane DC electric field in addition to the optical helicities.

*This project has been supported by the National Natural Science Foundation of China (NSFC Grant Nos. 11674013, 91750109).

1:03PM B43.00004: Nonlinear transport and optical responses in atomically thin WTe$_2$ [Invited] QIONG MA (Presenter), Massachusetts Institute of Technology — Many exotic quantum phenomena of today's forefront materials arise from the interplay among symmetry, topology, quantum geometry and correlations. Therefore, their detection and characterization require one to probe multiple aspects of the materials. We demonstrate nonlinear electrical transport and infrared optoelectronic measurements as symmetry sensitive probes of the low energy electron states in novel metals/semimetals. Using monolayer and bilayer WTe$_2$ as examples, I will show how nonlinear electrical transport and infrared photocurrent can reveal the Berry curvature properties in a highly symmetry sensitive way. In particular, the nonlinear electrical transport in bilayer WTe$_2$ uncovers a new type of Hall effect, the nonlinear Hall effect. Interestingly, this is an electrical Hall effect in a nonmagnetic material and in the absence of external magnetic field. Coupled with the gate tunability of 2D materials, we demonstrate that such nonlinear Hall effect provides a powerful tool to detect the Berry curvature of nonmagnetic quantum materials in an energy-resolved way.

1:39PM B43.00005: Fragile Topological Bands With Stable Index at Half-Filling in Twisted Bilayer Graphene [Invited] B ANDREI BERNEVIG (Presenter), Princeton University — Using an approximate but crucial particle-hole symmetry, we prove that half-filled graphene has bands that exhibit Wannier (Wilson loop) flow, and hence have to be topological. While this Wannier flow can be interrupted by the addition of certain bands, a topological index remains stable, and characterizes the set of bands. We then show that electron-phonon interaction in this set of bands can cause large superconducting temperatures and predict a certain set of angles where superconductivity should be observed.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B44 DCMP: Hole Spins in Semiconductor Quantum Dots BCEC 210C - Alex Hamilton, University of New South Wales - Tag(s): Invited

11:15AM B44.00001: High-fidelity single and two-qubit gates in germanium* [Invited] MENNO VELDHORST (Presenter), QuTech, Delft University of Technology — The promise of quantum computation with quantum dots inspired over two decades of intensive research on creating and manipulating single spins in semiconductor structures. The main focus was initially on GaAs, because of device maturity, and later on silicon, that can be isotopically purified to support extremely long quantum coherence times. Here, I will present germanium as a material that can combine these assets to form an excellent quantum material [1]. I will present the first planar germanium quantum dots, hosting single holes. I will show excellent quantum dot behavior with great control [2]. Single qubits can be defined on these holes with fidelities over 99% and can be coupled to execute two-qubit logic gates. Interestingly, these systems can also make contact to superconductors. I will present our latest effort on hybrid structures, including micro meter long supercurrents and supercurrent discretization [2,3]. Germanium bears therefore great promise for fast and coherent quantum hardware.


*Support though a FOM Projectruimte of the Foundation for Fundamental Research on Matter (FOM), associated with the Netherlands Organisation for Scientific Research (NWO) is acknowledged.
11:51AM B44.00002: Hole spins in quantum wires and quantum dots*  [Invited]  ALEX R HAMILTON (Presenter), Univ of New South Wales — The spin states of heavy holes in semiconductor nanostructures are attracting significant attention for quantum information applications, with rapid progress being made by a number of groups over the past few years. In this talk I will discuss our recent progress studying spin properties of holes in silicon and gallium arsenide quantum wires and dots. In GaAs hole quantum wires we observe highly anisotropic spin properties, which can be used to directly probe the spin-orbit interaction in holes [1,2], as well as evidence for an emergeny spin gap. In silicon single quantum dots we are able to study the spin shell filling sequence for the first 8 holes, which is consistent with the Fock-Darwin states of a circular 2D quantum dot. However while the spin filling obeys Hund's first rule, the hole-hole interaction energy is 90% of the orbital energy [3]. In few hole GaAs and Si double quantum dots we observe Pauli spin blockade, and find that the lifting of the spin blockade by an external magnetic field is highly anisotropic. These results highlight the promise, and challenges, of using holes for spin qubits.


*This work was supported by the Australian Research Council.

12:27PM B44.00003: A Ge heavy hole spin qubit  [Invited]  GEORGIOS KATSAROS (Presenter), Institute of Science and Technology Austria — The interest in hole spins as potential qubits has strongly increased in the past few years. Due to the intrinsically large spin orbit coupling, hole spins should be electrically tunable and show high Rabi frequencies. Indeed in 2016, the first electrically tunable hole spin qubit with Rabi frequencies as high as 70MHz was demonstrated [1]. In our group we work with Ge. Results on the first Ge hole spin qubit will be presented. The qubit is formed in a Ge hut wire [2] double quantum dot. Rabi-frequencies of 140 MHz were reached [3] and Ramsey experiments revealed dephasing times T2* exceeding 130 ns. Furthermore, by measuring the spin relaxation time of holes in Ge hut wires an upper bound for the coherence time could be extracted [4]. While these experiments underline the potential of hole spins in Ge, randomly grown nanowires are not very appealing for the creation of more complex qubit devices. Latest results on positioned hut wires which emphasize the potential of this material platform for scalable quantum devices will be presented.


1:03PM B44.00004: Quantum electronics with holes in Si/Ge*  [Invited]  SILVANO DE FRANCESCHI (Presenter), Univ. Grenoble Alpes & CEA — Silicon and germanium form the core materials of the well-established microelectronics industry. Lately, they have enabled remarkable progress also in the rising field of quantum technologies, generating at the same time new fundamental questions and technological challenges. In fact, there is still a lot to know about these well-known semiconducting materials and their potential for quantum electronics. In this talk, I will focus on hole-based systems made from silicon and silicon-germanium nanostructures. I will present recent experiments dealing with spin-related effects in silicon quantum dot devices, and discuss their implications for hole-spin qubits. I will also report the realization of prototypical hybrid superconductor-semiconductor devices exploiting the superconducting proximity effect in a high-mobility two-dimensional hole gas confined to a germanium quantum well.

*This work has received financial support from the EU H2020 research and innovation program, through the “MOS-QUITO” project (grant n. 688539) and through the ERC Synergy project “QuCube” (grant n. 810504), and from the Agence Nationale de la Recherche, through the OH RISQUE "TOPONANO" project.
Hole quantum dots in planar silicon and in GeSi nanowires* [Invited] FLORIS ZWANENBURG (Presenter), University of Twente — Ge/Si core/shell nanowires are suitable candidates for electrically driven spin qubits, and for the creation of Majorana fermions [1]. In highly tuneable hole quantum dots [2, 3], we observe shell filling of new orbitals and corresponding Pauli spin blockade [4]. In nanowires with superconducting Al leads we create a Josephson junction via proximity-induced superconductivity. A gate-tuneable supercurrent is observed with a maximum of ~60 nA [5]. We identify two different regimes: Cooper pair tunnelling via multiple subbands in the open regime the device [6], while near depletion the supercurrent is carried by single-particle levels of a quantum dot operating in the few-hole regime [5].

Secondly, we create ambipolar quantum dots in silicon nanoMOSFETs. We investigate the conformity of Al, Ti and Pd nanoscale gates by means of transmission electron microscopy [7]. We define low-disorder electron quantum dots with Pd gates [8], and depletion-mode hole quantum dots in undoped silicon [9]. For the latter we use fixed charge in a SiO2/Al2O3 dielectric stack to induce a 2DHG at the Si/SiO2 interface. The depletion-mode design avoids complex multilayer architectures requiring precision alignment and allows directly adopting best practices already developed for depletion dots in other material systems.


*This work is supported by the Netherlands Organisation for Scientific Research (NWO).

Monday, March 4, 2019 11:15 AM - 1:51 PM

Session B45 DCMP: Semiconductor Surfaces, Films, and Nanostructures BCEC 211 - Elena Cimpoiasu, United States Naval Academy

Uranium Surface Nitridation and Its Application in Uranium Passivation* KEZHAO LIU (Presenter), QIFA PAN, RUILONG YANG, KANGWEI ZHU, XIAOFANG WANG, JING LIU, YIN HU, Institute of Materials, China Academy of Engineering Physics — Uranium plays a significant role in the nuclear industry. However, it is chemically active and very easy to be oxidized and corroded in the environment. Therefore, it is very important to study the corrosion and oxidation behavior of uranium metal and to find the appropriate anti-corrosion treatment technology. This report briefly introduces our recent progress in surface nitridation of uranium and its application in anti-corrosion. The relationship between the preparation technologies and the composition as well as structure of the surface layer was studied. By using TEM, AES and XPS, it is found that surface nitriding can effectively improve the corrosion resistance of the metal uranium. The nitride with high nitrogen content exhibits better oxidation resistance than the one with low nitrogen content. This may due to the formation of uranium oxynitride in the nitride with high content. It can prevent the occurrence of further oxidation corrosion. These findings will contribute to the development of metal uranium surface corrosion protection technology.

*This work is supported by the National Natural Science Foundation of China (Grant No. U1630250).
11:27 AM B45.00002: The Experimental Research on Oxidation Kinetics of Uranium Surface Treated by Laser Nitriding* YIN HU (Presenter), HAIBO LI, JIANWEI QIN, XIAOFANG WANG, YONGBIN ZHANG, YANZHI ZHANG, KEZHAO LIU, Institute of Materials, China Academy of Engineering Physics — The oxidation kinetics of uranium surface treated by pulsed laser nitriding, which has been proved to be protective during storing at room temperature in the atmosphere, were studied using reflectance spectroscopy and X-ray diffraction (XRD) technique.

The growth of the oxide thickness firstly follows a parabolic growth model for the nitriding uranium with O2, which is coincided with the diffusion barrier model. And the initial regime of slow oxide-film growth is followed by a much faster growth stage of a linear curve, resulting from the cracking of the initial oxide layer. It has been shown that the critical thickness reached at the onset of the transition is about 300 nm in this work.

The activation energy equaling to 98 kJ/mol was obtained by monitoring the oxide growth in the first stage, and 85.9 kJ/mol in the second stage. In comparison, the growth of oxide thickness of untreated uranium was also monitored, indicating that corrosion resistance could be obviously improved after nitriding treatment. It may result from the formation of U-N-O compound after oxidation, which would resist the diffusion of oxygen ions in the oxide layer.

*This work is supported by the National Natural Science Foundation of China (Grant No. U1630250).

11:39 AM B45.00003: Metallic surface states induced perturbation in electron affinity of epitaxial AlN films* MONU MISHRA (Presenter), GOVIND GUPTA, Advanced Materials and Devices, CSIR-National Physical Laboratory — We report the influence of metallic surface states induced alteration in the electron affinity of epitaxial AlN films. A systematic and in-depth photoemission analysis of epitaxial AlN films grown under different conditions by plasma-assisted molecular beam epitaxy system was performed. The presence of remnant metallic aluminium and native oxide (with different contribution) on the surface (and sub-surface) perturbed the surface chemistry and electronic structure of the grown films. However, no significant change in the morphology of the films was witnessed. It was observed that these metallic states pin the Fermi Level (FL) near valence band edge and lead to the reduction of electron affinity (EA). The metallic states initiate charge transfer from surface to bulk which induces change in the surface and interface dipoles strength. Therefore, the EA of the films varied between 0.6 - 1.0 eV due to the variation in contribution of metallic states and native oxide. However, the surface barrier height (SBH) increased (4.2 - 3.5 eV) adversely due to the availability of donor-like surface states in metallic aluminium rich films.

*Monu Mishra acknowledges CSIR for Senior Research Fellowship

11:51 AM B45.00004: Plasma Nitriding and Carbon Assisted Plasma Nitriding of Tantalum* RUILONG YANG (Presenter), KANGWEI ZHU, Institute of Materials, China Academy of Engineering Physics — Plasma nitriding and carbon assisted plasma nitriding of tantalum were carried out. The nitride layer prepared with pure N2 is composed of TaN and Ta2N with hexagonal structure and a nitriding depth of 500 nm. The carbon assisted plasma nitriding process was carried out with the addition of methane into N2 gas (5% and 10% in volume ratio) as carbon source. The carbonitride films were found to be composed of a larger number of micro-crystals nearly 1 um in size, with a uniform and compact surface, as revealed by scanning electron microscopy (SEM). TaC1-xNx with a face-centered-cubic (FCC) and Ta2C1-xNx with hexagonal structure were identified by X-ray diffraction(XRD). The auger electron spectroscopy (AES) depth profiles reveal that the diffusion depth of nitrogen increased from 500 nm in nitride film to 1.5-3 μm in carbonitride films. The high solubility of nitrogen in tantalum carbide might be the main cause that promoted the diffusion of nitrogen during the plasma carbonitriding process.

*This work was supported by Foundation of President of China Academy of Engineering Physics (YZJLX2016006), and partially supported by Key Project of Natural Science Foundation of China (U1630250), National Fund Project (CXTQ 20171631302), Material Fund (TP201402-3).
12:03PM B45.00005: Atomic layer epitaxy of aluminum nitride: Unraveling the connection between hydrogen plasma and carbon contamination  STEVEN ERWIN (Presenter), JOHN LYONS, United States Naval Research Laboratory — Atomistic control over the growth of semiconductor thin films, such as aluminum nitride, is a long-sought goal in materials physics. One promising approach is plasma-assisted atomic layer epitaxy, in which separate reactant precursors are employed to grow the cation and anion layers in alternating deposition steps. The use of a plasma during the growth — most often a hydrogen plasma — is now routine and generally considered critical, but the precise role of the plasma is not well understood. We propose a theoretical atomistic model and elucidate its consequences using analytical rate equations, density-functional theory, and kinetic Monte Carlo statistical simulations. We show that using a plasma has two important consequences, one beneficial and one detrimental. The plasma produces atomic hydrogen in the gas phase, which is important for removing methyl radicals left over from the aluminum precursor molecules. But atomic hydrogen also leads to atomic carbon on the surface and, moreover, opens a channel for trapping these carbon atoms as impurities in the subsurface region, where they remain as unwanted contaminants. Understanding this dual role leads us to propose a solution for the carbon contamination problem which leaves the main benefit of the plasma largely unaffected.

12:15PM B45.00006: The Effect of Embedded Ag versus Au Nanoparticles on the Photovoltaic Conversion Efficiency in CdTe/CdS Thin Films*  OLIVIA RODGERS (Presenter), YUNIS YILMAZ, SELAM WOLDEGERIMA, MEHMET ALPER SAHINER, Seton Hall University — The addition of metal nanoparticles to photovoltaic cells creates the possibility of improving cell efficiency and reducing production costs. Impressive improvements in photovoltaic conversion efficiencies were found in CdTe/CdS/ITO (indium tin oxide) based solar cells with the addition of embedded Ag nanoparticles. Ag nanoparticles were deposited between the CdS and CdTe layers through pulse laser deposition method. Structural and electrical characterizing was achieved using x-ray diffraction ellipsometry, scanning electron microscopy, energy dispersive x-ray diffraction, atomic force microscopy and Keithley source meter photovoltaic measurement set. Previous research revealed that the photovoltaic conversion efficiency exhibits sensitive dependence on the size and the particle density of the embedded Ag nanoparticles. This work focuses on identifying at what amount of Ag deposition time will yield maximum efficiency. A similar study was conducted using Au nanoparticles deposited with the same parameters. An assessment of the differences between Ag and Au nanoparticles size and density was done. More importantly, a comparison on the photovoltaic conversion efficiency in thin films with Au versus Ag nanoparticles will be discussed.

*NSF Award #:DMI-0420952 and TUBITAK-2221 Award

12:27PM B45.00007: Non-classical effects of extrinsic doping on Au quantum wires  ZAMIN MAMIYEV (Presenter), CHRISTOPH TEGENKAMP, HERBERT PFNÜR, Institute for Solid State Physics, Leibniz University of Hannover — Self-assembled atomic wires on vicinal Si(hhk) surfaces are very versatile quasi-1D objects to study their interaction with the embedding environment [1,2]. Here we employ plasmon spectroscopy to study the response of Au-induced quantum wires to extrinsic doping by hydrogen adsorption. Si(553) and Si(557) surfaces are used as templates, which form double and single atomic strands per terrace upon evaporation of 0.48ML and 0.19ML of Au, respectively. The present study shows that the plasmonic excitation on both surfaces is strongly modified upon hydrogenation of the Si environment. These modifications are specific to the structural Au motif on the surface. Although hydrogen adsorption never happens on the Au chains directly, it clearly modifies the band structure of the whole system including the Au chains. The effects range from simple charge donation and changes of band filling, as for Si(553)-Au, to opening of band gaps partly even close to the Fermi energy as for Si(557)-Au, that will be discussed in detail.

12:39PM B45.00008: Kinetics of a Solid-Solid Charge Transfer Reaction*  
YING PAN, Harvard University, DIMOS POULIKAKOS, Mechanical and Process Engineering, ETH, NATE J. CIRA, YE TAO (Presenter), Harvard University — We present an analysis of the kinetics of charge transfer at a solid-solid interface. The study was enabled by measuring the conductance of ultra-thin, fully suspended single-crystalline silicon nanowires across 7 orders of magnitude with a detection sensitivity of order single event over a 10^3 μm^2 reaction area. We find that a classic, first-order process is unable to capture the reaction progress and propose a new kinetic model based on a continuum of reactant geometries inherently present at typical solid-solid interfaces. The new model captures the kinetic manifestation of heterogeneity in a single, global rate constant. Quantitative agreement with data and an analysis of the parameters suggest that this model may be generally applicable to charge transfer at solid-solid interfaces.

*Rowland Postdoctoral Fellowship and Rowland Fellowships

12:51PM B45.00009: Growth of CuMnAs by molecular beam epitaxy: Control over structure and properties*  
FILIP KRIZEK (Presenter), ZDENĚK KASPAR, MARTIN BRAJER, JAN ZUBÁČ, Department of Spintronics and Nanoelectronics, Institute of Physics of the Czech Academy of Sciences, ALIKSEI VETUSHKA, Department of Thin Films and Nanostructure, Institute of Physics of the Czech Academy of Sciences, JOÃO GODINHO, DOMINIK KRIEGNER, ZBYNĚK ŠOBÁN, Department of Spintronics and Nanoelectronics, Institute of Physics of the Czech Academy of Sciences, RICHARD CHAMPION, PETER WADLEY, School of Physics and Astronomy, University of Nottingham, KAMIL OLEJNÍK, TOMAS JUNGWIRTH, VÍT NOVÁK, Department of Spintronics and Nanoelectronics, Institute of Physics of the Czech Academy of Sciences — Antiferromagnetic materials have recently attracted significant attention in connection with the discovery of a way to electrically manipulate their magnetic ordering [1]. Especially magnetic reorientation of tetragonal CuMnAs layers by electrical current has potential for future industrial applications of antiferromagnetic materials [2]. We will present a detailed strategy for growth of CuMnAs by molecular beam epitaxy, while focusing on crystallinity of the grown thin films. These typically contain different densities of specific structural defects, which likely influence their electrical and magnetic properties. This, together with ageing in ambient conditions and significant surface roughness complicates practical implementations of CuMnAs thin films. We will show how careful tuning of the growth conditions improves the structural properties of the material and how growth parameters are reflected in conductivity, Hall coefficient and effectivity of Néel vector manipulation.


*This work is supported by the Czech Ministry of Education LNSM-LNSpin, the EU FET Open RIA Grant no. 766566 and Grant GA UK no. 886137.

1:03PM B45.00010: Preparation of epitaxial ScF3 thin films – a negative thermal expansion material  
AMANI JAYAKODY (Presenter), ZHIWEI ZHANG, University of Connecticut, ZHIHAI ZHU, Massachusetts Institute of Technology, HOPE R WHITELOCK, University of Colorado, JOSEPH I BUDNICK, JASON HANCOCK, BARRETT OTIS WELLS, University of Connecticut — Scandium trifluoride (ScF3) is known for a pronounced negative thermal expansion over a wide range of temperature, from 10 K to 1100 K. The structure of ScF3 can be described as an ABX3 perovskite with an empty A-site. Growing films of ScF3 allows for tuning the lattice constant, the thermal expansion, and the construction of devices based upon differential thermal expansion. We have investigated the growth of ScF3 films on oxide and fluoride substrates using pulsed laser deposition (PLD). There are several unique features to this material that pose challenges for PLD growth: poor adhesion of ScF3 pressed powder targets, a narrow stability range, and complex interfaces between fluorides and oxides. Nonetheless, we have found growth routes for producing films with very good epitaxy and narrow mosaic. This report describes the growth and initial characterization of high quality ScF3 films.
Atom-Scale Dynamics in Surface-Catalyzed Nitrogen Incorporation in Epitaxial Growth of Gallium Nitride

KIEU MY BUI (Presenter), IMASS, Nagoya University, MAURO BOERO, IPCMS, University of Strasbourg, KENJI SHIRAISHI, ATSUSHI OSHIYAMA, IMASS, Nagoya University — GaN is a principal material in optoelectronics and now emerging as a key material in power electronics [1]. One of the challenges to the device fabrication is the formation of higher quality thin films of GaN, that is not yet achieved to date. We here report density-functional total-energy electronic-structure calculations [2] and Car-Parrinello Molecular Dynamics simulations [3] that clarify atom-scale mechanisms of N incorporation in GaN bonding network during Metal Organic Vapor Phase Epitaxy (MOVPE). The results obtained for the first time in this work include (i) that Ga atoms on the growing surface are extremely mobile at the growth temperature, forming a liquid-like phase, and (ii) that ammonia NH3 and its related species NHx intervene into the weak Ga-Ga bond on the growing surface spontaneously or with surprisingly small energy barriers. This finding leads to a conclusion that the epitaxial growth is a reaction enhanced by the existence of weak surface Ga-Ga bonds. Computations have been performed with our own real-space code highly tuned and scalable on for massively parallel HPC architectures.


A SCAN+rVV10 study of Thiophene adsorption on Ir, Rh, and Ag (100)*

ABDELKADER KARA (Presenter), WALTER MALONE, University of Central Florida — Using density functional theory we study the adsorption of thiophene on Ir, Rh, and Ag(100) surfaces. Specifically, we employ the meta-GGA SCAN+rVV10 functional. To assess the performance of SCAN+rVV10 we compared our SCAN+rVV10 results to results calculated using the popular van der Waals (vdW) inclusive GGA functional, optB88-vdW. To find the equilibrium adsorption geometry, we explore a variety of adsorption sites with the plane of the molecule both parallel and perpendicular to the surface. Along with the equilibrium adsorption geometry we present various geometric and electronic properties of the adsorbate/substrate systems such as adsorption energy, adsorption height, buckling of the first layer of the substrate, charge transfer to the molecule, change in the width and center of the substrate's d-band, and change in the surface's work function. We find over all surfaces both functionals predict thiophene to adsorb parallel to the surface. Besides the consensus on a flat adsorption site, generally we find SCAN+rVV10 and optB88-vdW to agree very well concerning thiophene adsorption over Ag(100) and moderately well concerning thiophene adsorption over Rh(100) and Ir(100).

*This work was supported by the DOE-BES DE-FG02-11ER16243. This research used resources of NERSC.

A Density Functional Theory Study of the Adsorption of Thiophene on Transition Metal Surfaces

WALTER MALONE (Presenter), ABDELKADER KARA, WILLIAM KADEN, University of Central Florida — Using density functional theory we study the adsorption of thiophene (C4H4S) over a wide variety of transition metal surfaces including V, Cr, Ta, W, Mo, Nb, Co, and Al(100). To account for long range dispersion we utilize the van der Waals (vdW) inclusive optB88-vdW functional. We explore several adsorption sites with the plane of the molecule either parallel or perpendicular to the surface. We find that on all of the surfaces thiophene prefers to bond in a flat configuration. Along with the equilibrium adsorption sites, we present a variety of other properties of the substrate/adsorbate system including adsorption energy, adsorption height, C-S bond lengths, and charge transfer to the molecule. Using the previously mentioned geometric and electronic data we find the thiophene/substrate interaction increases moving from right to left on the periodic table. Focusing specifically on charge transfer to the thiophene molecule, we find a strong correlation between the charge transfer to thiophene's S atom and the thiophene/substrate interaction, which we build into a descriptor for the surfaces' reactivity.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B46 DMP GMAG: 4d/5d Transition Metal Systems -- Ruthenates and RuCl3
ANDY CHRISTIANSON (Presenter), Materials Science and Technology Division, Oak Ridge National Laboratory — The double perovskite structure type is extremely flexible and accommodates a large fraction of the elements in the periodic table. Of particular interest are double perovskites containing magnetic 4d or 5d transition metal elements. Such materials exhibit novel phenomena including high ferrimagnetic transition temperatures in conjunction with half metallic or insulating behavior. One of the key remaining challenges is to accurately determine effective spin Hamiltonians to achieve a deeper understanding of this class of materials. This talk will focus on our efforts to determine the effective spin Hamiltonians with inelastic neutron scattering in materials including Sr$_2$ScOsO$_6$, Sr$_2$FeOsO$_6$, Sr$_2$MgOsO$_6$, Ca$_3$LiOsO$_6$, Ca$_3$LiRuO$_6$, and Ba$_2$LaRuO$_6$. Interestingly, all of the Osmates in the above list exhibit significant gaps in the magnetic excitation spectrum, despite being nominally in the 5d$^3$ electronic configuration. This provides an indication of strong spin-orbit effects that would not normally be expected for a 5d$^3$ half-filled t$_2g$ multiplet. We will also discuss what can be learned about the nature of the exchange interactions from inelastic neutron scattering on polycrystalline samples and how such experimental studies can be used to constrain models for effective spin Hamiltonians in double perovskites and related transition metal oxides.

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

QIANG HAN (Presenter), Physics, Columbia University, RAFAEL M FERNANDES, Physics, University of Minnesota, ANDREW MILLIS, Center for Computational Quantum Physics, Flatiron Institute, Physics Department, Columbia University — A general Ginzburg-Landau free energy is proposed for the metal-insulator transition (MIT) in correlated oxides, which incorporates magnetism, octahedral distortions, strain as well as the electronic transition. The theory is used to elucidate important experimental features observed across thermal-induced and current induced MIT in 2-1-4 and Ti-doped 3-2-7 calcium ruthenate compounds, including the coexistence of metallic and insulating domains, occurrence, orientation and lengths of stripes at the domain boundaries, as well as the impact of uniaxial and biaxial strain on the transition temperatures and elasto-resistance. Generalization to MIT in other systems is presented.

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CHRISTOPHER DIETL (Presenter), Institute for Basic Science, JOEL BERTINSHAW, SHYAM KANTA SINHA, GEORG CRISTIANI, GENNADY LOGVENOV, YURY KHAYDUKOV, THOMAS KELLER, KATRIN FURSICH, GIDEOK KIM, DANIEL PUTZKY, Max Planck Institute for Solid State Research, LAURENCE BOUCHENOIRE, XMas, European Synchrotron Radiation Facility, JOERG STREMPFER, Advanced Photon Source, Argonne National Laboratory, SONIA FRANCOUAL, Deutsches Elektronen-Synchrotron, YONGSEONG CHOI, Advanced Photon Source, Argonne National Laboratory, PETER WOCHNER, SHYJUMON IBRAHIMKUTTY, PETER VAN AKEN, Max Planck Institute for Solid State Research, BUMJOON KIM, Institute for Basic Science, BERNHARD KEIMER, Max Planck Institute for Solid State Research — We report a comprehensive study of epitaxial Ca$_2$RuO$_4$ thin films using resonant X-ray scattering at the Ru-L$_2$ and L$_3$ absorption edges, which directly probe the Ru 4d valence states. The strong modification of the electronic properties by biaxial strain is readily seen in transport measurements, which reveal a tuning from an insulator (on NdCaAlO$_4$(110) substrates) to a metal (on LaSrAlO$_3$(001)). Using magnetometry and resonant X-ray scattering, we can identify ferromagnetic phases in films on LaSrAlO$_3$(001), LaSrAlO$_3$(110) and LaAlO$_3$(100) substrates and antiferromagnetic phases in films on NdCaAlO$_4$(110), LaSrAlO$_3$(110) and LaAlO$_3$(100). The antiferromagnetic phases are most compatible with the B-Type magnetic structure found in the pressurized bulk system exhibiting a $T_N$=$150$ K. While the magnetic moment direction is typically along (010) in bulk Ca$_2$RuO$_4$, a polarization analysis of magnetic reflections of the film on NCAO(110) shows an unusual magnetic moment direction towards (-102).

*We acknowledge financial support by the European Research Council under Advanced Grant No. 669550 (Com4Com).
**12:15PM B46.00004: Investigation on the Itinerant/Local Magnetic Nature in SrRuO$_3$ by ARPES**

JI SEOP OH (Presenter), SE YOUNG PARK, Institute for Basic Science, WONSHIK KYUNG, Lawrence Berkeley National Laboratory, NAOKI KIKUGAWA, National Institute for Material Science, YOSHIYUKI YOSHIDA, National Institute of Advanced Industrial Science and Technology, JUNYOUNG KWON, Institute for Basic Science, SIMON K MOSER, ROLAND KOCH, CHRIS JOZWIAK, AARON BOSTWICK, ELI ROTENBERG, Lawrence Berkeley National Laboratory, CHANGYOUNG KIM, TAE WON NOH, Institute for Basic Science — SrRuO$_3$ (SRO), one of the most famous perovskite metallic ferromagnets, has been the center of various research perspectives. One of the key issue with a long-time standing debate is the origin of ferromagnetism with metallicity. We studied the three-dimensional electronic structure of SRO single crystals by angle-resolved photoemission spectroscopy. We determined the inner potential of SRO single crystals for the first time. We also measured band dispersions on high symmetry planes and opened a way to cross-check theoretical electronic structures of SRO, which has not been accomplished during last 20 years. We also obtained temperature dependence of the ferromagnetic exchange splitting. These results implied the existence of short-range magnetic order above the Curie temperature and supported the dual nature of itinerant/local magnetism in SRO. Detailed experimental results and analyses will be presented and discussed.

**12:27PM B46.00005: Magnetic susceptibility in the Hund’s metal Sr$_2$RuO$_4$ from the dynamical two-particle vertex**

HUGO STRAND (Presenter), MANUEL ZINGL, NILS WENTZELL, OLIVIER PARCOLLET, ANTOINE GEORGES, Center for Computational Quantum Physics, Flatiron Institute — Strontium Ruthenate (Sr$_2$RuO$_4$) is a strongly correlated complex oxide for which crystals with exquisite purity can be prepared, allowing for a wealth of experimental studies. It displays unconventional superconductivity, Hund’s metal physics, and an incommensurate anti-ferromagnetic spin response.

To understand the interplay of collective spin excitations and the Fermi liquid quasi particles we have performed density functional theory and dynamical mean field theory calculations of the dynamic magnetic susceptibility using the Bethe-Salpeter equation, comparing to recent inelastic neutron scattering results.

The crucial importance of local quantum fluctuations in the vertex is established by comparison with the static random phase approximation. We also study the spin-orbit driven anisotropy and disentangle the orbital contributions. Our findings confirm that this material is close to a magnetic instability, as revealed by its sensitivity to impurity substitutions. Finally, by comparing the local and momentum dependent response, we pinpoint signatures of Hund’s metal physics in the inelastic neutron spectra.

*The Flatiron Institute is a division of the Simons Foundation.

**12:39PM B46.00006: Hall number sign changes in Sr$_2$RuO$_4$ reveal coherent-to-incoherent and elastic-to-inelastic crossovers**

MANUEL ZINGL (Presenter), CCQ, Flatiron Institute, JERNEJ MRAVLJE, Department of Theoretical Physics, Institute Jozef Stefan, MARKUS AICHHORN, Institute of Theoretical and Computational Physics, Graz University of Technology, OLIVIER PARCOLLET, ANTOINE GEORGES, CCQ, Flatiron Institute — The 4d transition metal oxide Sr$_2$RuO$_4$ exhibits an unusual temperature dependence of its Hall number with two sign reversals: it is negative at low temperature below 30K (Fermi liquid temperature), turns positive, reaches a maximum and turns negative again at ~120K. We show that this non-monotonic behavior is due to the strong temperature-dependence of the ratio of inelastic scattering rates between the xy and xz/yz orbitals. This ratio becomes remarkably large upon cooling into the Fermi liquid regime, but is overshadowed at lower temperatures by impurity scattering. Another pivotal factor to account for the full temperature dependence is the spin-orbit coupling, as it impacts the topography of the Fermi surface sheets and strongly mixes their orbital character. By considering all these effects, we are able to reveal the significance of both sign changes: the one at 30K is a direct consequence of the crossover from elastic to inelastic scattering, while the higher-T one is associated with the coherence-to-incoherence crossover due to electronic correlations. These qualitative conclusions are supported by quantitative calculations using a Boltzmann transport theory in combination with dynamical mean-field theory, taking into account the electronic structure of the material.
Electric field driven octahedral rotation in Sr$_2$RuO$_4$ and its underlying mechanism

WONSHIK KYUNG (Presenter), Lawrence Berkeley National Laboratory, CHOONG HYUN KIM, CCES-IBS, YEONG KWAN KIM, KAIIST, BEOMYOUNG KIM, Lawrence Berkeley National Laboratory, CHUL KIM, Yonsei University, WOOBIN JUNG, JUNYOUNG KWON, MINSOO KIM, CCES-IBS, AARON BOSTWICK, JONATHAN DENLINGER, Lawrence Berkeley National Laboratory, YOSHIYUKI YOSHIDA, AIST, CHANGYOUNG KIM, CCES-IBS — One of the key goals in the research of perovskite transition metal oxides (TMOs) is to design and control their physical properties, for which MO$_6$ (M=transition metal) octahedron rotation (OR) is considered to be one of the key control parameters. We show, through a combined study of angle resolved photoemission, low energy electron diffraction and first-principles calculations, that OR can be induced and thus be tuned with electric field in Sr$_2$RuO$_4$. Originally rotated octahedra in the surface layer of Sr$_2$RuO$_4$ are restored to the bulk structure upon K dosing on the surface. Our theoretical investigation shows that OR in Sr$_2$RuO$_4$ originates from surface electric field which can be controlled via the screening effect of the overlaid K layer and that the variation of Sr-Sr vertical distance is responsible for the coupling between OR and electric field. Our finding raises a possibility for electric field control of physical properties through the variation of the OR angle even for non-piezoelectric materials.

Quantum continuum fluctuations in glassy perovskite Ca(Co$_{0.15}$Ru$_{0.85}$)O$_3$

DEEPAK K SINGH (Presenter), YIYAO CHEN, ASHUTOSH DAHAL, Department of Physics and Astronomy, University of Missouri, JOSE A RODRIGUEZ, GUANGYONG XU, NIST Center for Neutron Research, THOMAS HEITMANN, University of Missouri Research Reactor, University of Missouri, VITALII DUGAEV, Department of Physics and Medical Engineering, Rzeszow University of Technology, ARTHUR ERNST, Max Planck Institute of Microstructure Physics — The quantum spin continuum and classical spin freezing, associated with a glassy state, represent two opposite extremes of a correlated electronic material. Here, we report the coexistence of a quantum spin continuum with a weak spin glass order in Co-doped CaRuO$_3$ perovskite near the chemical doping dependent metal-insulator transition boundary. Inelastic neutron measurements on Ca(Co$_{0.15}$Ru$_{0.85}$)O$_3$ at low temperature, $T = 1.5$ K, reveal a continuum spectrum in the Q-E space due to uncorrelated spin fluctuations. This persists across the glass transition at $T_G \approx 23$ K. Furthermore, scaling of the dynamic susceptibility yields a very small scaling coefficient $\alpha \approx 0.1$, suggesting extreme locality of the dynamic properties. The experimental results indicate the realization of a narrow regime where the distinction between continuum dynamic behavior and glass-like regimes is reduced.

Direct evidence of orbital-selective confinement effect of Ru 4$d$ orbitals in SrRuO$_3$ ultrathin film

SOONMIN KANG (Presenter), Seoul National University, YI TSENG, Swiss Light Source, Paul Scherrer Institut, BEOM HYUN KIM, Korea Institute for Advanced Study, SEOKHWAN YUN, BYUNGMIN SOHN, BONGJU KIM, Seoul National University, DANIEL MCNALLY, EUGENIO PARIS, Swiss Light Source, Paul Scherrer Institut, CHUL KIM, CHANGYOUNG KIM, TAE WON NOH, Seoul National University, SUMIO IŞIHARA, Department of Physics, Tohoku University, SCHMITT THORSTEN, Swiss Light Source, Paul Scherrer Institut, JE-GUEN PARK, Seoul National University — The electronic structure of SrRuO$_3$ thin film with the thickness from 50 to 1 unit cell (u.c.) is investigated via the resonant inelastic x-ray scattering (RIXS) technique at the O K-edge to unravel the intriguing interplay of orbital and charge degrees of freedom. We found that orbital-selective quantum confinement effect (QCE) induces the splitting of peaks in RIXS spectra of thin films, which corresponds to the charge transfer from O 2$p$ to Ru 4$d$ orbitals. At the same time, we observed a spectral weight transfer from electron-hole continuum to intersite $d$-$d$ excitation across the metal-to-insulator transition (MIT) occurring between 5 and 4 u.c. samples. From these two clear observations, we conclude that QCE gives rise to a Mott insulating phase in ultrathin SrRuO$_3$ films. Our interpretation of the RIXS spectra is supported by configuration interaction calculations of RuO$_6$ cluster models.

*The research at MU is supported by DOE, Office of Basic Energy Sciences under grant no. DE-SC0014461.

*The work at IBS CCES is supported by Institute of Basic Science in Korea. The work at PSI is supported by the Swiss National Science Foundation through the NCCR MARVEL and the Sinergia network Mott Physics Beyond the Heisenberg Model (MPBH). We also thank Korea Institute for Advanced Study for providing computing resources (KIAS Center for Advanced Computation Linux Cluster System) for this work.
Substitution of 4d magnetic ions of a Kitaev-Heisenberg magnet by 3d magnetic ions: the case of Ru$_{1-x}$Cr$_x$Cl$_3$* 

GÄEL BASTIEN (Presenter), Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, 01171 Dresden, Germany, MARIA ROSLOVA, Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, 01062 Dresden, Germany, MOHAMMAD HOSSEIN HAGHIGHI, KAVITA MEHLAWAT, KONSTANTIN NENKOV, Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, 01171 Dresden, Germany, JENS HUNGER, ANNA ISAEVA, Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, 01062 Dresden, Germany, MATTHIAS VOJTA, Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany, THOMAS DOERT, Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, 01062 Dresden, Germany, ANJA WOLTER, BERND BÜCHNER, Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, 01171 Dresden, Germany — The Jeff$=1/2$ Mott insulator alpha-RuCl$_3$ is a promising candidate for the realization of the Kitaev-Heisenberg model. It harbors an antiferromagnetic ground state below $T_N=7$K, however, this ordered state can be suppressed by a magnetic field through a quantum critical point toward a possible quantum spin liquid [1]. In this study, the Ru$^{3+}$ ions with Jeff$=1/2$ moments were partially substituted by Cr$^{3+}$ ions with S=3/2. The effect of this substitution on the magnetic interactions, the magnetic ground state and the field-induced quantum spin liquid were studied by means of magnetization, ac susceptibility and specific heat measurements. The ground state of Ru$_{1-x}$Cr$_x$Cl$_3$ was found to be a spin glass on a broad Cr concentration range with a maximum of the freezing temperature around $x=0.5$. Moreover, the evolution of the magnetic anisotropy with the substitution reveals a rather complex nature of the magnetic interaction between the Ru and Cr magnetic moments.


*This research has been supported by the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement No 796048.
1:51PM B46.00012: An effective spin Hamiltonian for α-RuCl₃ and finite temperature properties* PONTUS LAURELL (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CASEY EICHSTAEDT, Department of Physics and Astronomy, University of Tennessee, Knoxville, YI ZHANG, Department of Physics and Astronomy, Louisiana State University, TOM BERLJIN, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, ADOLFO GERMAN EGUILUZ, Department of Physics and Astronomy, University of Tennessee, Knoxville, YOUHEI YAMAJI, Department of Applied Physics, University of Tokyo, SATOSHI OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory — We study the magnetic interactions in the Kitaev spin-liquid candidate α-RuCl₃ using ab initio, exact diagonalization, and thermal pure quantum state methods. First we derive a new effective Hamiltonian, using an ab initio downfolding scheme based on a density functional theory calculation for the monoclinic crystal structure (space group C2/m). The calculation includes local crystal field splitting, and local and non-local spin-orbit coupling. Both local and nonlocal Coulomb interactions are computed using the constrained RPA method, and the interaction parameters for the effective spin Hamiltonian are determined using second order perturbation theory. We report both zero and finite temperature properties for this and previously proposed models, including dynamical spin structure factors and the specific heat. Our results highlight the importance of further range anisotropic spin-spin interactions, both for producing the zigzag magnetic order and for predictions beyond static properties at zero temperature.

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

2:03PM B46.00013: Electronic transport in thin crystals of transition metal oxides with Heisenberg-Kitaev physics* JOSUE RODRIGUEZ (Presenter), AMIRARI DIEGO, California State University, Long Beach, NICHOLAS BREZNAY, Harvey Mudd College, ROBERT KEALHOFER, GILBERT LOPEZ, University of California Berkeley, DAVID ROSSER, FRANCISCO RAMIREZ, NAOMY MARRUFO, SAMANTHA CROUCH, California State University, Long Beach, JAMES G. ANALYTIS, University of California Berkeley, CLAUDIA OJEDA-ARISTIZABAL, California State University, Long Beach — Josue Rodriguez, Amirari Diego, Gilbert Lopez, Nicholas P. Breznay, Robert Kealhofer, David Rosser, Francisco Ramirez, Naomy Marrufo, Samantha Crouch, James G. Analytis and Claudia Ojeda-Aristizabal

Sodium Iridate (Na₂IrO₃) and Ruthenium Chloride (RuCl₃) present exciting phenomena thanks to the honeycomb arrangement of their ions and the interplay of electronic correlations and spin-orbit coupling. They constitute a close experimental realization of the the Kitaev-Heisenberg model. Magnetic susceptibility and heat capacity measurements in bulk crystals have shown signature of magnetic ordered states [1]. We have integrated exfoliated thin crystals of Na₂IrO₃ and RuCl₃ into an electronic device and performed electronic transport measurements, finding through temperature dependent resistance measurements anomalies that correspond to the magnetic ordered transition for Na₂IrO₃.


*This project was funded by the Department of Energy award number DE-SC0018154

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B47 GERA: Catalytic Energy Generation BCEC 213 - Filip Podjaski
11:15AM B47.00001: Mechanism of water oxidation catalyzed by cobalt-intercalated layered MnO2: confinement and intercalant local ordering* JINLIANG NING (Presenter), JAMES FURNESS, YUBO ZHANG, Department of Physics and Engineering Physics, Tulane University, AKILA C. THENUWARA, RICHARD C REMSING, MICHAEL L KLEIN, DANIEL R. STRONGIN, Department of Chemistry, Temple University, JIANWEI SUN, Department of Physics and Engineering Physics, Tulane University — To lower the overpotential is a persistent goal for (photo)electrochemistry reactions, which can be facilitated by selectively stabilizing one reaction intermediate over another. In this mechanistic SCAN+rVV101,2 study of the oxygen evolution reaction (OER) catalysed by cobalt-intercalated layered MnO2, we show that confinement effects and local cobalt atomic ordering in the interlayer space can be used to tune the adsorption energies of O, OH, and OOH reaction intermediates and the scaling relationship between them. Interlayer confinement destabilizes the OER intermediates, but clustering Co atoms can selectively stabilize OOH. With considering both effects, our model predicts an overpotential of 0.30 V, in excellent agreement with the experimental result of 0.36 V. In addition to giving mechanistic explanation for experimental findings, these insights illuminate a route for engineering non-toxic precious-metal-free catalysts through designed layered materials.

*Supported by the DOE Energy Frontier Research Centers (DE-SC0012575).

11:27AM B47.00002: Photocatalytic oxygen evolution reactivity at surface edges and corners of anatase TiO2 nanoparticles revealed by coupled quantum mechanical and molecular mechanical simulations* LIXIN SUN (Presenter), BILGE YILDIZ, Nuclear Science and Engineering, Massachusetts Institute of Technology — Coupled quantum mechanical and molecular mechanical (QM/MM) method is applied to investigate the oxygen evolution reactions (OER) on a realistic 9.5-nm long anatase TiO2 nanoparticle. The nanoparticle surface has easier electron and hole localization behavior on some of the corners and edges, compared to flat surfaces. As a result, OER reaction energy can be reduced by 0.1 - 0.5 eV at the corners and edges. However, since some of the structures with low reaction energies are also prone to form electron polarons, its high OER activity can be compromised due to electron-hole recombination. By considering both factors, the (101) facet and the edge between (101) and (011) facets are found to be the most active for OER, while the remaining corners and edges can be active for reduction reactions. Unlike early works where four-fold coordinated Ti4c was attributed to the only reason for active corners and edges, this work shows that Madelung potential, surface relaxation can also be the cause of active surface.

*The authors are grateful for the support of this research by DOE-Basic Energy Sciences, grant number DE-SC0002633, and the for the computational support by the National Science Foundation through the XSEDE Science Gateways programme, grant number TGDMR120025.

11:39AM B47.00003: Operando studies of carbon removal and contaminants in solid oxide fuel cells* JEFFREY OWRUTSKY (Presenter), WILLIAM A. MAZA, United States Naval Research Laboratory, DANIEL STEINHURST, Nova Research, Inc., STANISLOV TSOI, United States Naval Research Laboratory, BRYAN EIGENBRODT, Chemistry, Villanova University, ROBERT WALKER, Chemistry and Biochemistry, Montana State University — Solid oxide fuel cells (SOFCs) are attractive devices for power generation due to their fuel flexibility. These devices present challenges for real time, direct observations because they operate at high temperatures (> 700 °C). We have developed and used several methods for real-time, operando studies, including infrared emission, near infrared thermal imaging and Raman spectroscopy which are combined with ex situ infrared spectroscopy and mass spectrometry of the products and concurrent electrochemical measurements for comprehensive investigations of the effects of contaminants and remediation approaches. We characterized the products, primarily CO and CO2, as well as anode temperature changes to explore the effects of various mixtures of H2 and O2 on carbon removal from Ni-YSZ anodes as well as during partial methane oxidation for SOFC operation. The prevalent processes effectively reduce to steam reforming with hydroxyl as a primary reaction intermediate. We also report initial studies of sulfur effects based on SOFC operation with methane and compare the results to similar studies for chlorine degradation to identify whether there are common themes.

*This work supported by the Office of Naval Research.
11:51AM B47.00004: Characterization of Platinum Nanoparticles Utilized in Photocatalytic Hydrogen Synthesis*

DANIEL BOYCE (Presenter), JOHN COLTON, MATTHEW RICHARDS, Brigham Young University — Hydrogen (H₂) gas is a possible alternate fuel to help meet increasing worldwide energy needs, but a major obstacle in the use of H₂ for green, environmentally-friendly fuel is the energetic and chemical requirements to synthesize the gas. We are studying the use of photocatalytic reactions to produce H₂, where a light-absorbing substance acts as a catalyst in shuttling electrons from a donor to protons that are reduced into H₂. Previous research conducted at BYU showed that platinum nanoparticles bound to ferritin catalyzed the photoreaction of methyl viologen to reduce protons in an organic acid offered an increase in hydrogen production efficiency by up to 100 times over platinum black (a commonly available platinum-based catalyst). We are reporting on our efforts to optimize the synthesis of the platinum nanoparticles bound to ferritin that are used in this photocatalytic system and how we characterize these nanoparticles, as well as how these characteristics affect H₂ production.

*We'd like to thank the Brigham Young University Physics Department and the National Science Foundation (grant no. 1757998) for their generous funding.

12:03PM B47.00005: First-principles Studies on the Structural and Electronic Modifications of Nitrogen Electrochemical Reduction on Anatase TiO₂(101) Surface*

YANNING ZHANG (Presenter), TONGWEI WU, University of Electronic Science and Technology of China — The conversion of dinitrogen (N₂) to ammonia (NH₃) through an electrochemical reduction process is attracting increasing attentions due to its great importance in both the biosphere and the fertilizer industry. In this work, we performed systematic density functional theory (DFT) studies on the nitrogen reduction reaction (NRR) mechanisms on both clean and O-decorated TiO₂(101) surfaces at an atomic scale. Our calculation results showed that the Ti₄C₂VO₂c site most likely serves as the active site for NRR process, and the V₂O₂c-decorated TiO₂(101) surface exhibits outstanding NRR catalytic activity through a mixed mechanism compared with the clean anatase TiO₂(101) surface. We further studied the effect of structural and electronic features on N₂ fixation and activation on TiO₂(101) surface. The introduction of surface oxygen vacancy should enhance the nitrogen adsorption obviously with an adsorption energy of -0.46 eV, and the tuning of Ti³⁺ concentration further changes the adsorption energy, such as to -0.65 eV if the concentrations of Ti³⁺ can be decreased to 4%. Our calculation results may provide some guidelines in the design of new catalysts for NRR.

*Work was supported by the National Nature Science Foundation of China (No. 11874005).

12:15PM B47.00006: Optimizing proton conductivity in alkaline-earth zirconates through defect engineering*

ANDREW ROWBERG (Presenter), Materials Department, University of California, Santa Barbara, LEIGH WESTON, Energy Technologies Area, Lawrence Berkeley National Laboratory, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — The alkaline-earth zirconates (AeZrO₃; Ae = Sr, Ca, Ba) are among the best solid-state proton conductors and as such have energy applications in solid-state hydrogen fuel cells. They crystallize as perovskite oxides of the form ABO₃. Oxygen vacancies form readily in these systems, and upon exposure to water, these vacancies are filled and the materials are populated with protons. To incorporate oxygen vacancies, acceptor dopants such as Sc and Y substituting on the Zr-site are used; however, these dopants can simultaneously incorporate as A-site donors and self-compensate. We study the properties of these dopants using first-principles calculations with a hybrid functional. We characterize the bulk properties and study the formation of native and extrinsic point defects. We examine the propensity for self-compensation of Sc and Y, as well as possible A-site and O-site acceptors. We find that certain alkali metal A-site dopants (Na in CaZrO₃, K in SrZrO₃, and Rb in BaZrO₃) incorporate oxygen vacancies in higher concentrations than Sc and Y, while also circumventing the problem of self-compensation. Furthermore, these acceptors have low proton binding energies, making them good choices to improve proton conductivity in the zirconates.

*This project was supported by DOE and NSF.
calculate the charge-voltage response of various reconstructions of a solvated SrTiO3 surface, revealing that interfacial long-range polarization of the semiconductor electrode under electrical bias. Using this comprehensive model, we predict the relation between electrochemical stability, band alignment, and photocatalytic activity taking into account the develop an embedded quantum-mechanical approach using the self-consistent continuum solvation (SCCS) model to to-hydrogen efficiency for these materials is critically dependent on the electrochemical state of their surface. Here, we investigate the role of a different physical property, namely, the diffusivity, in hydrogen evolution reaction. On typical catalytic metal surfaces, the diffusivity of hydrogen is high, and the binding strength is the dominant controlling factor. In contrast, the diffusion barrier on the surfaces or edges of two-dimensional catalytic materials such as MoS2 is found to be inversely proportional to the binding strength. This relatively large diffusion barrier may serve as another important factor on such surfaces. Moreover, the charge density wave of a catalytic surface can also significantly modulate the diffusion barrier. These findings provide important insights into how to design efficient catalysts for enhanced hydrogen evolution reaction.

12:39PM B47.00008: Role of diffusivity in hydrogen evolution reaction  JIANG ZENG (Presenter), LEIQIANG LI, PING CUI, University of Science and Technology of China, JOHN P PERDEW, Temple University, ZHENYU ZHANG, University of Science and Technology of China — The hydrogen binding strength on a catalyst is known to be an important factor in electrochemical hydrogen evolution. Although much effort has been exerted to improve the binding strength to exploit precious-metal-free catalysts, their performance is still inferior to that of platinum. Based on first-principles calculations, here we investigate the role of a different physical property, namely, the diffusivity, in hydrogen evolution reaction. On typical catalytic metal surfaces, the diffusivity of hydrogen is high, and the binding strength is the dominant controlling factor. In contrast, the diffusion barrier on the surfaces or edges of two-dimensional catalytic materials such as MoS2 is found to be inversely proportional to the binding strength. This relatively large diffusion barrier may serve as another important factor on such surfaces. Moreover, the charge density wave of a catalytic surface can also significantly modulate the diffusion barrier. These findings provide important insights into how to design efficient catalysts for enhanced hydrogen evolution reaction.

12:51PM B47.00009: Configuration entropy of protons in doped-BaHfO3 at finite temperature, an ab-initio based cluster expansion study*  LEI ZHANG (Presenter), MEILIN LIU, Georgia Institute of Technology — Doped-BaHfO3 is a promising solid state protonic conducting electrolyte for solid oxide fuel cells. A widely-recognized feature in aliovalent-doped solid state ionic is that the conductivity of charge carriers, is governed by two competing factors, i.e. concentration and mobility. At finite temperature, e.g. 500 Celsius, point defects has non-negligible configurational and vibrational entropies. The interplay between entropic and electronic energetic creates a non-trivial thermodynamic phase diagram, describing defect ordering, segregation and randomization. This also inevitably modulates kinetic properties of protons. By using ab-initio density functional theory calculations as input, a cluster-expansion model was constructed and utilized in this multi-sublattice cubic perovskite system. A comprehensive thermodynamic and kinetic understanding was generated hereafter, with suggestions about optimal doping concentration and heat treatment protocol.

*This work is supported by Phillips 66.

1:03PM B47.00010: Influence of Sr leaching on the catalytic activity of reconstructed SrTiO3 photoelectrodes*  YIHUANG XIONG (Presenter), ISMAILA DABO, Pennsylvania State University — Perovskite photoelectrodes are being extensively studied in the search for photocatalytic materials for hydrogen production through water splitting. The solar-to-hydrogen efficiency for these materials is critically dependent on the electrochemical state of their surface. Here, we develop an embedded quantum-mechanical approach using the self-consistent continuum solvation (SCCS) model to predict the relation between electrochemical stability, band alignment, and photocatalytic activity taking into account the long-range polarization of the semiconductor electrode under electrical bias. Using this comprehensive model, we calculate the charge-voltage response of various reconstructions of a solvated SrTiO3 surface, revealing that interfacial charge trapping exerts primary control on the electrical response, electronic structure, and surface stability of the photoelectrode. Our results provide a detailed molecular-level interpretation of the enhanced photocatalytic activity of SrTiO3 upon the voltage-induced restructuring of the semiconductor-solution interface.

*The authors acknowledge financial support from the National Science Foundation under grant number DMR-1729338.
1:15PM B47.0001: Adsorption characteristics of small aromatic molecules on silica/Ru(0001)  MUHAMMAD SAJID (Presenter), WILLIAM KADEN, ABDELKADER KARA, University of Central Florida — Organic molecules are part of future materials for electronic devices. The performance of these devices depends strongly on the atomic and electronic characteristics at the organic-substrate interface, which is necessary to provide support and/or conduction for the device. To develop a catalogue of anchor-group-dependent trends in these characteristics, we have undertaken a joint computational/experimental study of aromatic molecules (benzene, pyridine and thiophene) bound to Ru(0001), both with and without silica sheets inserted between the two. The silica sheets have been chosen to provide an experimentally accomplishable means of varying the separation between the adsorbate molecules and metal by growing them as monolayer or bilayer. Using DFT with vdW corrections, the models of above-mentioned systems will be presented along with their electronic properties (workfunction, charge transfer etc.). Accompanying, XPS measurements will provide complementary experimental data to compare electronic predictions. These will include changes in workfunction, valence-band measurements, and core-level XPS analysis with Auger Parameter analysis for improved deconvolutions of initial and final-state contributions to binding energy shifts.

1:27PM B47.00012: Understanding the role of vacancy-vacancy interaction and hydrogen-hydrogen coupling in hydrogen bonding on MoS2 surfaces*  LIPING YU (Presenter), Department of Physics and Astronomy, University of Maine, ADRIENN RUZSINSZKY, QIMIN YAN, Department of Physics, Temple University — MoS2 is a promising nonprecious electrochemical catalyst for catalyzing hydrogen production from water. It has been found that (i) the catalytic reaction activity depends on the concentration of sulfur vacancies, and (ii) the free energy of hydrogen adsorption varies with the coverage of hydrogen adsorbates. However, microscopically, the physical factors responsible for such finding remain unclear. In this talk, we will present a microscopic model to understand the effects of vacancy-vacancy interaction and hydrogen-hydrogen coupling. We find that the effect of vacancy-vacancy interaction on hydrogen-surface bonding becomes considerable only when they are separated by less than 1.1 nm. When one hydrogen atom is adsorbed at a sulfur vacancy, the interaction between this sulfur vacancy and others nearby will be largely disabled. Such disabling decreases the adsorption energy and hence strengthens the binding. Similarly, the hydrogen-hydrogen interaction also becomes important only when they are close enough. However, instead of being disabled, such interaction is introduced upon hydrogen adsorption, which increases the adsorption energy and weakens the binding. The generation of those results will also be briefly discussed.

*Supported by DOE BES Energy Frontier Research Center.

1:39PM B47.00013: Defect-mediated charge and mass transport in energy materials  KHANG HOANG (Presenter), North Dakota State University — Conventional solid-oxide fuel cells (SOFCs) based on yttria-stabilized zirconia (YSZ) electrolytes and Ni-YSZ cermet anodes suffer performance degradation due to problems associated with the Ni-based anodes such as redox cycling instability, nickel agglomeration, carbon deposition, and sulfur poisoning. It is thus necessary to search for new, Ni-free materials that may hold potential for overcoming these problems. Recently, Ba3Ti3O6(BO3)2 has been identified as a possible candidate for SOFC anodes or anode composites [1]. The oxyborate material undergoes a change from ionic under oxidizing and soft reducing conditions to mainly electronic transport under an extreme reducing atmosphere typical of anode environment, leading to a drastic enhancement in the electrical conductivity. In this talk, we introduce a theoretical framework, based on defect physics, to understand changes in the electrical transport mechanism caused by changes in the environment and to explore and design new materials for SOFC applications. [1] Doux et al., ACS Appl. Energy Mater. 1, 510 (2018).
In this work, La$_{0.6}$Sr$_{0.4}$FeO$_{3-δ}$ (LSF64) thin films are employed as model systems and the biaxial strain is introduced by growing LSF64 thin films epitaxially on substrates with different lattice constants. Coupling surface chemical information from in-situ ambient pressure X-ray spectroscopy with morphological and structural information from electron microscopy, we found that in-plane biaxial strain can be a powerful tool in optimizing the particle dispersion of the exsolution products. The observed strain dependence of exsolution advances our abilities to control them and enhance the performance of catalysts for clean energy technologies.

Monday, March 4, 2019 11:15 AM - 1:15 PM

Session B48 DFD GSNP: Fluid-Structure Interactions (FSI)

11:15AM B48.00001: Wave interaction with flexible vegetation: connecting individual blade dynamics to meadow scale wave decay* [Invited] JIARUI LEI, HEIDI NEPF (Presenter), Massachusetts Institute of Technology — Flexible plants move in response to wave orbital velocity, which diminishes wave decay relative to rigid plants. The impact of reconfiguration and blade motion on wave decay has been characterized using an effective blade length, $l_e$, which represents the length of a rigid blade that generates the same drag as the flexible blade of length $l$. The effective blade length depends on the Cauchy number, which represents the ratio of hydrodynamic drag to blade stiffness, and on the ratio of blade length to wave orbital excursion. This laboratory study considered how scaling laws determined for individual blades could be used to predict the wave decay over a meadow of multiple plants. First, the drag force on and motion of individual model blades was studied for a range of wave conditions to provide empirical coefficients for the theoretically determined scaling laws for effective blade length, $l_e$. Second, the effective blade length predicted for individual blades was incorporated into a meadow-scale model to predict wave decay over a meadow. Third, wave decay was measured over meadows of different plant density (shoots per bed area), and the measured decay was used to validate the wave-decay model.

*This work was supported by the National Science Foundation grant EAR 1659923.

11:51AM B48.00002: An Eulerian method for mixed soft and rigid body interactions in incompressible fluids XIAOLIN WANG (Presenter), Harvard University, KEN KAMRIN, MIT, CHRISTOPHER RYCROFT, Harvard University — Fluid-solid interaction problems are encountered in many engineering and biological applications, but are challenging to simulate due to the coupling between the two material phases. Here, we propose a fully Eulerian approach for solving fluid-solid interactions that is simple to implement and capable of simulating complex multi-body interactions. When the solid is rigid, a projection step is formulated as a composite linear system that simultaneously enforces the rigidity and incompressibility constraints. When the solid is soft, a reference map technique is applied to characterize the body deformation in an Eulerian framework. Several examples including a single body, multiple bodies, and soft-rigid combinations will be presented, with potential applications to biological systems.

12:03PM B48.00003: A Method for Deriving Fluid-Structure Interaction Reduced-Order Models for Cerebral Aneurysms SUYUE HAN (Presenter), YAHYA MODARRES-SADEGHI, University of Massachusetts Amherst — A Reduced Order Modeling (ROM) method is discussed for Fluid-Structure Interaction problems in cerebral aneurysm. In this method, we first conduct training CFD simulations with pre-defined structural motion using the fixed mesh method, and then use the snapshot POD method to generate POD modes for both the flow field and the structure. Instead of using traditional topology-changing method, the CFD simulation is enhanced by a fixed mesh method to handle large-amplitude displacements or structural deformation without changing the mesh connectivity, thus consuming much less time. The POD ROM method is also enhanced by the same fixed mesh method, so that the training CFD simulation could be combined with the ROM smoothly. Besides, by implementing a fixed mesh method into the ROM, there is no need for iteratively calculating the forces acting on the structure for every time step. After generating POD modes for both the fluid and the structure using a fixed mesh, we couple these fluid and structure POD modes to create the FSI ROMs.
Flow-induced vibration of an inclined flexible cylinder in tandem arrangement

BANAFSHEH SEYED-AGHAZADEH (Presenter), Miami University — Flow-induced vibration (FIV) of a flexible inclined circular cylinder placed in the wake of a stationary cylinder is studied, experimentally. A highly flexible circular cylinder with an aspect ratio of 47 and a mass ratio of 120 was held fixed at both ends and placed inclined at 45° to the incoming flow in the test-section of a subsonic wind tunnel. The inclined flexible cylinder lied in the wake of an upstream stationary cylinder of equal diameter and inclination. The dynamic response of the downstream cylinder is studied for center-to-center spacing range from 3 to 7 times the cylinder diameter, in the reduced velocity range of $U^*=3.6-48.5$ and the Reynolds number range of $Re = 260-3750$.

The validity of the independence principle, which states that the behavior of an inclined cylinder is essentially driven by the normal component of the incoming flow velocity, has been previously investigated for a single flexible cylinder. The objective of this study is to examine the effects of inclination on FIV response of cylinders in tandem arrangements. Dynamic response of the inclined flexible cylinder in terms of the excited structural modes, frequencies of oscillations, and modal weight contributions is compared to those of a normal incidence flexible cylinder in tandem arrangement.

Numerical study on the flow-induced vibrations of a flexibly-mounted cavity at the rear of a bluff body

José I Jiménez-González (Presenter), Carlos García-Baena, Javier F. Aceituno, Department of Mechanical and Mining Engineering, Universidad de Jaén (Spain) — We carry out a computational study on the flow-induced vibrations (FIV) of a rigid cavity, flexibly mounted at the rear of a D-shaped body of height $H$, subject to a cross-stream of velocity $u_\infty$.

Simulations are performed for laminar Reynolds numbers to characterize the interaction between wake and parallel rotary plates, connected to the rear edges of the body using torsional hinges. The FIV amplitude response and the effect on force coefficients are investigated for several values of hinge's torsional stiffness $k$, which provide with different natural oscillation frequencies $f_n$ and reduced velocities $U^*=u_\infty/f_nH$. A large FIV response is found for $U^*>2$, where plates oscillate in phase at the shedding frequency. Such response increases the mean drag and fluctuating lift, although reductions are found $U^*<2$, where a weaker FIV response is characterized by oscillation of plates in counter-phase. Finally, to validate the results, we develop a multibody model that allows to retrieve the local aerodynamic forces and torque acting on the plates, using the motion obtained from simulations as input. A final analysis is performed in terms of torque's components and phase between wake forcing and plates' response.

This work was supported by the Spanish MINECO under Project DPI2017-89746-R

Flutter control using nonlinear tuned magnetic vibration absorbers

Xavier Amadolese (Presenter), Arnaud Malher, Laboratoire d'Hydrodynamique — We will talk about the effects of nonlinear tuned magnetic vibration absorbers on the instability threshold and post-critical flutter of two-degrees-of-freedom « pitch-plunge » wing section. Two post-critical scenarios will be examined: a coupled-mode flutter scenario exhibiting limit cycle oscillations characterized by moderate amplitude in plunge and low amplitude in pitch, and a more complex flutter scenario exhibiting a second post-critical bifurcation from coupled-mode flutter to high amplitude symmetric stall flutter. Magnetic vibration absorbers have been used in plunge, in pitch or in both, and tuned as nonlinear vibration absorbers with cubic stiffness. Their efficiency will be examined in the light of wind tunnel tests and simulations. The latter have been obtained using an analytical aeroelastic model, including a nonlinear unsteady aerodynamic formulation, coupled with the vibration absorbers.

*This work was supported by the grants DYSACCI from Direction Générale de l'Armement (DGA).
Flutter instability of a reconfiguring beam*  MOHAMMAD TARI (Presenter), FREDERICK GOSSELIN, ERIK LAURENDEAU, Mechanical Engineering, Polytechnique Montreal — Reconfiguration refers to static and dynamic aeroelastic deflections of structures to flow that provide benefits, such as reduced aerodynamic drag. Assuming small structural deformations, the linear theory is used predominantly in engineering applications. However, large deformations of the trees and aquatic plants can only be explained through large deformation theory. The aim of this research is to study experimentally and numerically the flutter instability in slender structures which deform with great amplitude. In particular, we extend the reduced order model of Leclercq & de Langre1 to a RANS coupled with a nonlinear beam model handling large displacements. Since the flutter in such flexible structures arises from the strong interaction of the physics of the fluid and the structure domains, we use a partitioned strongly coupled approach with our in-house structural and fluid solvers. This approach enables us to study flutter and provides insights into the drag reduction mechanisms of flexible structures.


*The work benefited from the financial support of the Natural Sciences and Engineering Research Council of Canada. Computations were made on Calcul Quebec clusters.

To leak or not to leak: deformation of perforated elastic strips driven through a viscous fluid
PEDRO REIS (Presenter), MATTEO PEZZULLA, LORENZO SICONOLFI, FRANCOIS GALLAIRE, Institute of Mechanical Engineering, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland — From dandelions and insect wings to wire fences and parachutes, there are numerous natural and technological instances of porous flexible structures that deform due to fluid loading. Whereas fluid flow through bulk porous media has been studied extensively, the interaction between a perforated, deformable object and a surrounding viscous fluid has received much less attention. Here, we microfabricate flexible, porous, and slender strips containing a precisely designed array of voids that target set permeabilities. We then drive these perforated strips through a fluid, at low Reynolds number conditions, and quantify the extent of deformation due to viscous loading. We use a reduced theoretical model based on Kirchhoff-Euler beam theory coupled with a description of the fluid loading to deduce the drag force from the deflected shape of the strip. In parallel, we perform ad-hoc numerical simulations to capture the details of the fluid-structure interaction, thereby uncovering a nontrivial effect of permeability on the drag experienced by the porous structure. We hope that the gained insight may guide the design of flexible structures that optimize their porosity and permeability to enhance drag, towards light-weight high-drag slender objects.

Monday, March 4, 2019 11:15 AM - 2:03 PM
Session B49 DPOLY GSOFT: Advanced Deposition Methods for Polymers and Soft Materials

Initiated Chemical Vapor Deposition onto Moving Liquid Surfaces*  PRATHAMESH KARANDIKAR (Presenter), MARK M DE LUNA, MALANCHA GUPTA, University of Southern California — In this talk, we will demonstrate that initiated chemical vapor deposition (iCVD) can be used to deposit thin functional films onto low vapor pressure liquids such as silicone oils and ionic liquids. The substrate viscosity, surface tension, monomer solubility and process parameters such as deposition time and deposition rate determine the polymer structure on the liquid. The spreading coefficient of the polymer on the liquid surface can be used to predict the thermodynamically preferred polymer morphology. Films, nanoparticles, and gels can be formed. We demonstrate that modifications to the deposition chamber can enable in situ modulation of the liquids in a vacuum allowing polymer deposition on moving liquids. We demonstrate liquid motion in silicone oils of viscosities ranging from 5 cSt to 50 cSt. We study the deposition of fluorinated polymers on the moving liquids and demonstrate that the mechanical response of the polymer films can be tuned by the use of a crosslinker ethylene glycol diacrylate. Our experimental findings allow for further understanding of nucleation and growth mechanisms of polymer films on liquid surfaces by inducing liquid motion and allows us to probe the mechanical strength of thin films.

*Department of Energy, Office of Basic Sciences.
11:27 AM B49.00002: Initiated Chemical Vapor Deposition of Copolymer Based Electrolytes for 3D Microbatteries

WENHAO LI (Presenter), LAURA BRADLEY, JAMES J WATKINS, Polymer Science and Engineering, University of Massachusetts at Amherst — Reliable fabrication of nanoscale, solid-state polymer electrolytes (SPEs) with conformal 3D coating capability and good ionic conductivity is one major challenge toward fully assembled 3D microbatteries. Here we utilize initiated chemical vapor deposition (iCVD) to produce sub-micron copolymer thin films comprised of hydroxyethyl methacrylate (HEMA) and ethylene glycol diacrylate (EGDA). These copolymer films are subsequently converted into SPEs via solution-based lithium salt doping and demonstrate ionic conductivity of \((6.1 \pm 2.7) \times 10^{-6} \text{ S cm}^{-1}\) at room temperature, the highest value reported to date for nanoscale SPEs. An investigation of copolymer composition, crosslinking density, polarity, structural relaxation is presented to explain the ion conduction.

11:39 AM B49.00003: Vapor Deposited Polymers: from Fundamentals to Commercialization [Invited]

KAREN GLEASON (Presenter), Department of Chemical Engineering, Massachusetts Institute of Technology — Chemical vapor deposition (CVD), as practiced by the semiconductor industry, typically utilizes high powers and high temperatures to drive non-selective chemistry. However, employing selective chemistry allows deposition rates of CVD organic films to be high, even when energy input is low. The CVD method is ideally suited for insoluble and infusible materials such as fluoropolymers, crosslinked organic networks, and conjugated semiconducting and conducting polymers. To date, a portfolio of >70 CVD homopolymers and copolymers have been demonstrated. The conformal nature of CVD polymerization enables the facile integration of organic thin films into device prototypes onto thermally sensitive and mechanical flexible substrates. Scale up of the process has facilitated the commercialization of CVD polymer technology.

12:15 PM B49.00004: iCVD Solid Nanoadhesives for Precision Assembly at Near Room Temperature*

XAVIER LEPRO (Presenter), Materials Science Division, Lawrence Livermore National Laboratory, JOHN SIMON MILLER, Materials Engineering Division, Lawrence Livermore National Laboratory, GAVIN WINTER, SALMAAN BAXAMUSA, Materials Science Division, Lawrence Livermore National Laboratory — Adhesives are widely used in manufacturing processes to bond components. Due to their ubiquity in consumer goods, adhesives and sealants form a mature $50B industry with decades of investment in formulation chemistry for various applications. However, nearly all adhesives are based on the application of viscous resins which cure based on chemical reaction, solvent evaporation, or cooling of a hot melt. Capillary forces from liquid-like resins both prevent the formation of thin (<1 μm) bondlines and can wick or damage porous materials such as foams, aerogels and other delicate structures at the nano and microscale.

Here we synthesized adhesive solid polymers directly from vapor-phase reagents by initiated chemical vapor deposition (iCVD) avoiding any liquid intermediates while achieving thickness control within tens of nanometers. We formulated thermoplastics that bond physically rather than chemically by inducing polymer chain interdiffusion when the polymer is heated above its glass transition temperature, \(T_g\). Whereas chemical cure near room temperature requires liquid-phase metal catalysts or UV light, this approach allows to engineer \(T_g\) via polymer composition.

*Supported by the 18-FS-032 LDRD program. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-760356

12:27 PM B49.00005: Using volatile liquid oxidant in PEDOT synthesis by oxidative Chemical Vapor Deposition (oCVD)*

MEYSAM HEYDARI GHARAHCHESHMEH (Presenter), KAREN GLEASON, Chemical Engineering, Massachusetts Institute of Technology (MIT) — Conducting Polymers (CPs) are desired for next generation flexible, stretchable, wearable, and large-area electronic devices. The oxidative Chemical Vapor Deposition (oCVD) is a versatile deposition technique with the potential for commercial production of CPs in large-scale applications. Here, we report the oCVD poly(3,4-polyethylene dioxythiophene) (PEDOT) synthesis using a volatile liquid oxidant. The flow rate of volatile liquid oxidant to the oCVD reactor is more controllable than its solid oxidants counterparts, which resulted in better control of the oxidant surface concentration. In addition, the main advantage of using volatile liquid oxidant is that the final CPs thin films exploit directly in device fabrication without the need for any post-deposition rinsing step to remove unreacted oxidants and oxidation by-products. The texture and structural properties of deposited oCVD PEDOT films with volatile oxidant as a function of deposition temperature and a fraction of oxidant saturation pressure (P/P_{sat}) were investigated. It was noted that the orientation of oCVD PEDOT films is highly influenced by the process parameters and has a significant impact on electrical conductivity.

*This work was supported by Eni S.p.A. under the Eni-MIT Alliance Solar Frontiers Program
Selective spin-on deposition of polymers on heterogeneous surfaces*  
YUANYI ZHANG (Presenter), COLTON D'AMBRA, CRAIG HAWKER, RACHEL SEGALMAN, CHRISTOPHER M BATES, University of California, Santa Barbara — Traditional photolithography relies on the manipulation of spun cast polymer films using a complex sequence of processing steps to generate patterns for device fabrication. Selective deposition holds promise to reduce this economic burden and enable self-aligned fabrication by directly coating material only on desired regions of a heterogeneous surface. Our work introduces a strategy to achieve selective polymer deposition via spin coating without necessitating superfluous processing steps (e.g., thermal annealing, etching). This talk will focus on understanding the interplay between polymer design, spin coating conditions, and consequent thin film characteristics.


*This work was supported in part by Semiconductor Research Corporation (SRC).

Morphology and Thermal Properties of Semi-Crystalline Polymer Films by Slow Deposition

RODNEY PRIESTLEY (Presenter), Princeton University — Thin-film growth via physical vapor deposition (PVD) has been successfully exploited for the delicate control of film structure for molecular and atomic systems. The application of such a high-energetic process for polymeric film growth has been an enduring challenge. However, the recent development of Matrix Assisted Pulsed Laser Evaporation (MAPLE) has provided a new means to deposit a variety of macromolecules in a manner similar to PVD. Here, employing MAPLE for the growth of semi-crystalline polymer thin films, we show the ability to tune film morphology by manipulation of substrate temperature. This is accomplished by exploiting the effects of temperature on polymer crystal nucleation and dynamics. During slow film growth, crystal nucleation can either be permitted or suppressed, and crystal thickness can be tuned by temperature modulation. Finally, by combining MAPLE deposition with flash DSC, we demonstrate the ability to measure the extent of crystallinity and melting temperature of thin films grown over a wide temperature range.

Thin films of ultramonodisperse polystyrene polymers

ADAM RAEGEN (Presenter), JAMES FORREST, Physics and Astronomy, University of Waterloo — We present a study of the aging of thin films composed of ultramonodisperse polymeric/oligomeric samples. Purified polymeric samples of known molecular weight and polydispersity are deposited via thermal evaporation onto actively cooled silicon substrates, forming uniform films. Ellipsometry allows us to investigate the thickness and refractive index of these vapour deposited films. We compare calorimetric glass transitions of these films with different production parameters.

Confined Polymer Crystallization in Vapor-Deposited PE/PMMA Blend Films*

YUCHENG WANG (Presenter), RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — Polymer blends are widely applied in technologies because they can join features from individual components to optimize performance. However, for thin films comprising immiscible polymers, it is challenging to precisely control the film structure because of the spontaneous phase separation, which can influence the resulting properties in an undesirable way. In this work, we utilize a vapor deposition technique termed matrix-assisted pulsed laser evaporation (MAPLE) to process thin films of PE/PMMA and illustrate that the technique can effectively control the size of phase separation. During MAPLE, thin films are formed atop a temperature-controlled substrate by the addition of separate nanoscale polymer droplets at an ultra-slow rate, thereby confining the phase separation within a much smaller scale relative to films processed via other means. Employing a fast scanning calorimeter, we demonstrate the ability to shift the crystallization temperatures of PE by ~20°C as a result of confinement and temperature during deposition. We also show the preservation of film structures beyond melting.

*I acknowledge the support of the National Science Foundation (NSF) Materials Research Science and Engineering Center program through the Princeton Center for Complex Materials (DMR-1420541).
Emulsion Target Process-Structure-Property Relationships in Resonant Infrared Matrix-Assisted Pulsed Laser Evaporation (RIR-MAPLE) for Selective Deposition of Crystalline Phases in Polymer Thin Films

ADRIENNE STIFF-ROBERTS (Presenter), SPENCER FERGUSON, CASSANDRA WILLIAMS, Electrical and Computer Engineering, Duke University, BUANG ZHANG, University Program in Materials Science and Engineering, Duke University — The semi-crystalline phase of polyfluorene (β-PFO) is desirable for blue polymer LEDs because it yields higher carrier mobilities that lower operating voltage and increase device lifetime. However, the use of poor solvents in solution-based deposition to obtain high β-PFO content also degrades surface quality. Previous research on emulsion-based RIR-MAPLE deposition has shown that emulsion characteristics impact β-PFO content in thin films. In contrast to solution-based deposition, RIR-MAPLE increases β-PFO content to 6% without degrading surface morphology.

The goal of the current work is to establish the process-structure-property relationships of RIR-MAPLE emulsion targets to achieve 42% β-PFO content (for phase stability) by controlling emulsion chemistry and deposition rate. The emulsified polymer particle size will be measured by dynamic light scattering, the structure of PFO films will be characterized by atomic force microscopy, and the β-PFO concentration will be measured using photoluminescence and/or UV-absorbance spectroscopy. In addition, basic device performance of PFO-based LEDs will be measured to determine the impact on device performance.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B50 DPOLY: UKPPG/DPOLY Polymer Lecture Exchange: Advances in Film Formation and Chain Dynamics

IGNACIO MARTIN-FABIANI (Presenter), Loughborough University — Colloidal self-assembly methods, using particles suspended in a solvent as the building blocks, have been recently proposed as a single-step alternative for obtaining surfaces “on demand”.¹ We recently proved experimentally how in blends of polymer colloids of two different sizes, small particles can segregate during drying into a layer on top of the larger particles.² The moving interface causes a density, and hence a pressure, gradient in the drying film, which pushes larger particles away from the moving interface faster than it pushes smaller particles. By using stimuli-responsive particles, which swell with increasing pH, it is possible to switch stratification on and off by just changing the pH of the initial dispersion.³ For a certain size, stratification is suppressed because of the increased solids content, which reduces particle mobility and reduces the osmotic pressure gradient. This type of self-assembly allows the independent control of the properties of the top and the bottom of the final film, dictated by the functionality of the large and small particles. Modelling shows it is a really strong and reliable effect, taking place for a wide range of particle size ratios and evaporation rates. However, agreement with experiments is limited, because of coffee-ring effects and Marangoni flows that are not usually present in models. In this talk, I will discuss the progress we made in this field and how we can harness the Physics of polymer colloid systems to control the final film structure towards a certain application.

References

Programming surface energy driven Marangoni convection to pattern polymer films

CHRISTOPHER ELLISON (Presenter), University of Minnesota — The Marangoni effect describes how fluid flows in response to gradients in surface energy. We recently developed a method for photochemically preprogramming spatial surface energy patterns in glassy polystyrene (PS) thin films. UV irradiation through a mask selectively dehydrogenates the PS, thus increasing surface energy in the UV exposed regions compared to the unexposed regions. After heating the film to the liquid state, transport of polymer occurs from regions of low surface energy to regions of high surface energy. This method can be harnessed to rapidly manufacture polymer films possessing prescribed three-dimensional topographies reflective of the original light exposure pattern without solvent washes or etching procedures. To better understand this phenomenon, a theoretical model will be presented that reveals the physics of this process, its limits and ways to apply it efficiently for various target metrics.
12:03PM B50.00003: Influence of Hydrodynamic Interactions on Stratification in Drying Mixtures

ANTONIA STAT (Presenter), Princeton University, MICHAEL HOWARD, McKetta Department of Chemical Engineering, University of Texas, Austin, ATHANASSIOS PANAGIOTOPoulos, Princeton University — It is desirable to control the structure of dried multicomponent films for many technologies, but there is an incomplete theoretical understanding of how evaporation affects film structure. Recent experiments[^1] showed that mixtures of small and large colloids unexpectedly stratify with the small colloids counterintuitively on top of the large colloids. Stratification can be modeled without hydrodynamic interactions (HIs) using dynamic density functional theory, but it was recently suggested[^2] that HIs cannot be reasonably neglected. We investigated the influence of HIs on stratification using nonequilibrium simulations of polymer films with explicit and implicit solvent models.[^3] The short chains stratified on top of the long chains in the implicit solvent (no HIs) in agreement with previous theoretical models and simulations. However, the explicit solvent model did not stratify at the same drying conditions due to HIs. Our work shows that it is critical to include HIs into models for drying films.


*Financial support was provided by the Princeton Center for Complex Materials, a NSF MRSEC (award DMR-1420541).

12:15PM B50.00004: Strategies to improve the unconfined melt electrospinning process via incorporation of ionically conductive particles

ELNAZ SHABANI (Presenter), CHENGXI LI, REBECCA J KOMER, LAURA CLARKE, JASON R BOCHINSKI, RUSSELL E GORGA, BRENTON BOLAND, NEELAM SHEORAN, North Carolina State University — By utilizing a sharp-edged flat plate, multiple parallel jets can be electrospun spontaneously from unconfined polymer melts. In this work polyethylene was electrospun from a thin film of the polymer melt heated on an electrically-grounded flat plate. This technique can produce fibers with a throughput rate of about 50 mg/min without the possibility of clogging which frequently happens in traditional single needle electrospinning due to high viscosity of polymer melts. The effect of increased melt conductivity through salt additives on fiber diameter was studied to present a method for fabrication of smaller diameter fibers from highly-insulating polymer thermoplastics. Also, The environmental temperature, specifically in the spin-line shows to have a significant impact on the fiber diameter and the spinning process.

*Support from The National Science Foundation Grant #1635113

12:27PM B50.00005: Creating thin film compositional polymer libraries using electrospray deposition

KRISTOF TOTH (Presenter), Yale University, GREGORY DOERK, KEVIN G. YAGER, Brookhaven National Lab, CHINEDUM OSUJI, University of Pennsylvania — Electrospray deposition (ESD) enables the growth of polymer thin films in a precise and continuous manner by the delivery of sub-micron droplets of dilute polymer solutions to a heated substrate. By combining ESD with programmable motor control and gradient solution pumping in a first-of-its-kind user tool at the Center for Functional Nanomaterials at Brookhaven National Laboratory, we show the ability to create one or two-dimensional compositional gradient nanoscale films via ESD. These capabilities make it possible to construct thin film multicomponent “libraries” on a single substrate to rapidly and significantly characterize composition-dependent properties, in particular, thin films involving homopolymer and block copolymer (BCP) blends. We report the design, construction, and validation of a gradient ESD tool which allows users to carefully control the jet stability, flow composition, spray position, and substrate temperature. Paired with synchrotron small angle X-ray scattering (SAXS), this tool forms an integral part of a new platform for high-throughput, autonomous characterization and design of self-assembling polymer blends as well as functional soft materials more generally.

*NSF DMR-1410568
NSF GRFP DGE-1122492
12:39PM B50.00006: Understanding the Deformation of Polymer Thin Films Under Hydration  PETER DUDENAS (Presenter), University of California, Berkeley, ADAM Z WEBER, AHMET KUSOGLU, Lawrence Berkeley National Lab — Understanding the impact of interfaces and surfaces on hydrophilic/amphiphilic polymers including ionomers is of increasing interest as functional polymer coatings and thin-film devices become more ubiquitous. In these thin-film systems, confinement and interfacial energy impact a variety of properties including Tg, modulus, and morphology; the degree of hydration will also significantly impact these properties. Because of this, the characterization of mechanical properties for polymer thin films and networks under hydration remains a challenge. Here, we report the swelling-induced deformation of model hydrogel and block copolymer films as a function of thickness, cross-linking, and surface functionalization to understand the effect of confinement and surface interactions on polymer swelling and swelling-induced stresses. A cantilever bending method is used to characterize the mechanical response which is correlated to morphology using in-situ grazing incidence x-ray scattering. The results and techniques are applicable to understand the structure-functionality of a wide variety of polymers, including hydrogels, ion-conducting polymers for energy conversion, and block copolymers.

12:51PM B50.00007: AFM Observation of the Movements of Single Linear Chains in a Precursor Film of a Spreading Polymer Blend Melt  YASUHIRO WATANABE, JIRO KUMAKI (Presenter), Yamagata University — We have successfully visualized the movements of single chains in a precursor film of a spreading polymer melt on a substrate at the molecular level by atomic force microscopy (AFM). A polymer melt spreading on a substrate forms a precursor film with a thickness comparable to a monolayer at the flow front. Previously, Sheiko and coworkers successfully observed the movements of polymer brush molecules in the precursor film of a spreading melt (Phys. Rev. Lett. 2004, 93, 206103), however, those of conventional linear polymers have not yet been observed due to the limited resolution of the present AFM instruments. We observed a mixture of a poly(methyl methacrylate) (PMMA) oligomer with a small amount of a high-molecular-weight isotactic (it) PMMA polymer, and successfully observed the movements of the it-PMMA polymer chains flowing in the precursor film of the spreading melt at the molecular level. The movements of the individual PMMA chains will be discussed in detail.

1:03PM B50.00008: Lattice Self-Consistent Field Calculations of Ring Polymer Brushes*  QIANG WANG (Presenter), Colorado State Univ, WENJUAN QIU, BAOHUI LI, Nankai University, China — We report the first systematic study using lattice self-consistent field (LSCF) calculations of ring homopolymer brushes grafted onto a flat and homogeneous surface and immersed in an explicit and athermal solvent, which are either uncompressed, compressed by a flat and impenetrable surface, or compressed by an identical brush.[1] Our results clearly show that ring brushes are slightly less stretched than, thus nearly but not completely identical to, the “equivalent” linear brushes having half the chain length and double the grafting density. Our LSCF results are consistent with the molecular simulation results reported in the literature[2,3], except the previous finding that the normal pressure of two opposing ring brushes is only half of the “equivalent” linear brushes at melt density.[3]


*This work was supported by the National Natural Science Foundation of China (21574071, 21528401, 20925414), by the PCSIRT (IRT1257), and by the 111 Project (B16027).

1:15PM B50.00009: Comprehensive scaling theory for entanglement in melts and solutions of flexible and stiff polymer chains*  SCOTT MILNER (Presenter), Pennsylvania State University — The entanglement length Ne is a key parameter for all entangled polymer fluids, for which no comprehensive scaling theory yet exists. We have pieces of a theory; the Lin-Noolandi (LN) argument predicts Ne scaling for flexible chains that agrees with data on melts. There are arguments for how Ne should depend on polymer volume fraction, but which are not obviously consistent with LN. Morse scaling describes entanglement for stiff chains, consistent with data. Everaers proposed an ansatz that Ne depends only on “arc-length concentration”, as if chains were uncrossable threads. This ansatz is consistent with simulation of bead-spring chains but not with LN, it has no role for packing length, the central parameter in LN scaling. We propose a comprehensive scaling theory which includes LN in one limit, thread ansatz in another, and reduces to Morse scaling for stiff chains. Our new ingredient is the observation that the typical distance of closest approach between two chains is governed by packing length or chain diameter, whichever is larger. If a chain is sufficiently flexible and bulky, the packing length is relevant; but for stiffened bead-spring chains without sidegroups, the packing length is likely smaller than the chain diameter, so thread scaling applies.

*DMR-1507980
**1:27PM B50.00010: Effect of Polymer Architectures on the Entanglement of Combs and Bottlebrushes**

HEYI LIANG, Department of Polymer Science, University of Akron, BENJAMIN J. MORGAN, Department of Chemistry, University of North Carolina at Chapel Hill, GUOJUN XIE, MICHAEL MARTINEZ, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, SERGEI SHEIKO, Department of Chemistry, University of North Carolina at Chapel Hill, ANDREY DOBRYNIN (Presenter),Department of Polymer Science, University of Akron — We study correlations between the entanglement plateau modulus and architecture of graft polymers in a melt. To distinguish between two types of graft polymers – combs and bottlebrushes – we introduce the crowding parameter Φ, which describes mutual interpenetration of the neighboring macromolecules. In comb systems, both the backbones and sparsely grafted side chains are coiled and allow side chains of neighboring macromolecules to overlap (Φ<1). In bottlebrush systems, however, the steric repulsion between densely grafted side chains results in chain extension and inhibits side chain interpenetration (Φ≥1). The ratio $G_{e,gr}/G_{e,lin} \approx \phi^3(1+(\Phi/0.7)^3)$ of the plateau modulus of a graft polymer melt, $G_{e,gr}$, to that of a linear polymer melt, $G_{e,lin}$, is a universal function of the crowding parameter $\Phi=\phi^{-1}n_{sc}^{-1/2}$ and graft polymer composition $\phi=n_g/(n_g+n_{sc})$, where $n_{sc}$ and $n_g$ are the degrees of polymerization of side chains and a spacer separating consecutive side chains along the backbone, respectively. Such universal behavior is verified by poly(n-butyl acrylate) combs and other graft polymers reported in literatures. For graft polymers with entangled side chains, the $G_{e,gr}/G_{e,lin}$ ratio is proportional to $\phi^2$.

*NSF DMR 1407645, 1436201, 1436219, 1624569

**1:39PM B50.00011: Entanglement in semiflexible polymer melts and solutions from simulations**

SAI VINEETH BOBBILI (Presenter), SCOTT MILNER, Department of Chemical Engineering, Pennsylvania State University — The Lin-Noolandi scaling argument predicts the entanglement molecular weight from chain geometry, and is well supported by experimental results for real polymers. The argument assumes that polymers are flexible within their tubes, which fails at some point as chains become stiffer. Everaers has made a different scaling proposal, which crosses over from semiflexible chains to stiff chains as described by Morse. Everaers’ ansatz is consistent with simulation data for a range of bead-spring melts, but is not consistent with LN. In this work, we use MD simulations to explore a wide range of entangled bead-spring ring chains, to find out how entanglement properties vary with chain stiffness and concentration. To topologically equilibrate ring chains, we soften the short-range repulsive potential to allow chains to cross. We calculate entanglement properties using three techniques: chain shrinking to find the primitive path, measuring the tube diameter by the width of the “cloud” of monomer positions about the primitive path, and directly measuring the plateau modulus. As chain stiffness varies, we observe three distinct scaling regimes, suggestive of LN scaling, semiflexible chains, and stiff chains.

*We acknowledge funding from National Science Foundation under Grant No. DMR-1507980.

**1:51PM B50.00012: Polymer Structures and Their Glass Transition Temperatures: An Intriguing Relationship**

TIANYU LI, CNMS, Oak Ridge National Laboratory, HUIQUN WANG, JIMMY W MAYS, Department of Chemistry, The University of Tennessee, KUNLUN HONG (Presenter), CNMS, Oak Ridge National Laboratory — Abstract: Polymer structure play an essential role in dictating chain stiffness and glass transition temperature (Tg). The characteristic ratio ($C_w$) is an important parameter to describe chain stiffness. In general, polymers with stiffer chains have higher glass transition temperature and correspondingly higher $C_w$. However, for poly(n-alkyl methacrylates), this is not always true. For example, poly(ethyl methacrylate) has Tg of 65 °C and $C_w$ of 8.2, but poly(n-hexyl methacrylate) has Tg of -5 °C and $C_w$ of 11.1. Furthermore, poly(n-alkyl acrylates) generally have lower Tgs than the corresponding poly(n-alkyl methacrylate) but actually have higher $C_w$ values. We believe other structural characteristics, such as stereoisomerism, might play a role in these discrepancies. In this contribution we discuss the intriguing relationships of polymer structure (chain stiffness) and glass transition temperatures with relation to structural parameters and solution properties of well-characterized poly(meth)acrylates.

*Funding Acknowledgement: This research was conducted at the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Lab (ORNL), which is a DOE Office of Science User Facility.
Phase-separating fluid and polymer mixtures provide a flexible platform for the design of functional materials containing multiple segregated domains. External electric fields provide a modality for biasing this behavior and tuning the miscibility of such mixtures; however, fundamental understanding of electric field effects on phase behavior has been limited by disagreement between theoretical predictions and experimental results.

In this talk, we report progress for a study of binary phase separation in dielectric fluids, performed using a recently developed field theory representation for polarizable molecular species. Polarizability contrast in such systems leads to van der Waals (VDW) interactions that favor immiscibility, inducing aggregation of the more strongly polarizable molecular species, and subsequent demixing. In addition to VDW interactions, which arise from local fluctuations in the polarization of the fluid, the mixture also admits a mean-field dielectric response to the applied field, which favors miscibility of the fluid. The effect of molecular architecture is also considered.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B51 DPOLY: Advanced Scattering Techniques to Inform the Design of Polymeric Systems  BCEC 253A - Gila Stein, Univ of Tennessee, Knoxville - Tag(s): Invited

11:15AM B51.00001: Exploiting the process of thin film printing for structure manipulation tracked by grazing incidence scattering* [Invited]  EVA M. HERZIG (Presenter), Dynamics and Structure Formation - Herzig Group, Universität Bayreuth, STEPHEPN PRÖLLER, OLIVER FILONIK, Munich School of Engineering - Herzig Group, TU München, CHRISTOPHER GREVE, MICHAEL BUCHHORN, Dynamics and Structure Formation - Herzig Group, Universität Bayreuth, MIHAEL CORIC, JENNY LEBERT, Munich School of Engineering - Herzig Group, TU München — Thin films can have intriguing properties that are exploitable for consumer good applications. Such properties are strongly linked to the morphology on the nanoscale within such thin films. X-ray scattering can be a very powerful tool to resolve such structures, and also, to carry out time-resolved measurements to track the actual formation of the final nanostructures.

We have developed a dedicated set-up that allows us to print, manipulate and examine functional thin films [1]. Using X-rays we have previously demonstrated that structure formation is then trackable and can be used to gain insights into the effect of processing parameters on the structure formation process [2]. While continuously improving the processing and characterization capabilities, we are currently starting to systematically investigate different processing parameters like temperature and solvent atmosphere to understand structure formation mechanisms and their control in various thin film solar cell material systems.


*Funding from Bayerisches Staatsministerium für Bildung und Kultus, Wissenschaft und Kunst as well as BaCaTec and IGSSE is gratefully acknowledged.

11:51AM B51.00002: Packaging Plastics - Structure-Property Relationships [Invited]  DAVID G BUCKNALL (Presenter), Hariot-Watt University — The use of various experimental methods have been widely employed to study polymer deformation. Despite these previous studies, there still remains a disconnect between the molecular architecture, i.e. branch content, molecular weight between branches, etc, and the macroscopic mechanical properties. The nature of the uniaxial deformation behavior of polymers can be explained using continuum models, a surprisingly simple yet effective example of which is the spring and dashpot model of Haward and Thackray. Such models try and interpret the observed behavior in terms of viscous and elastic components associated with the crystalline and amorphous phases within the semi-crystalline polymer regions. However, these continuum models only provide a very indirect correlation between the observed mechanical behavior and the molecular structure. In this talk, the use of in-situ X-ray scattering experiments will be discussed which have enabled development of a more complete molecular interpretation of the deformation processes in polyolefins and polyesters. These results have allowed us to make direct correlations between the molecular architecture and the mechanical properties.
12:27PM B51.00003: Correlating Thermodynamic Assembly to Functional and Structural Performance of Polymeric Systems by Comprehensive Analysis of Neutron Scattering* [Invited]  
MARK DADMUN (Presenter), University of Tennessee — Small angle scattering is often used to determine the size and shape of polymeric materials, but more thorough analysis of the scattering from multi-component polymer systems provides interfacial surface area, average domain size, and importantly, phase composition. For instance, polyimide aerogels (PIA) saturated with ionic liquids are promising materials as robust electrolytes for next generation batteries. Careful analysis of SANS data from PIA/ionic liquid constructs show that the ionic liquid penetrates the polyimide skeleton. This unexpected structure clearly impacts charge transport and therefore performance of the aerogel as a battery component. This mixing behavior must be more fully understood to rationally utilize these promising materials in devices. We will also present examples of how similar analyses of scattering data provide crucial insight into the correlation of thermodynamic structure and performance in energy harvesting nanocomposites, the relationship between structure and dynamics in all-polymer nanocomposites, and the impact of deposition conditions on the lateral and vertical phase separation in polymer blend thin films.

*Portions of this research were supported by the Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division as well as the National Science Foundation (DMR-1409034 and DMR-1808946).

1:03PM B51.00004: Interfacial structure and dynamics in nanoparticle-polymer composites [Invited]  
RANA ASHKAR (Presenter), Virginia Tech — Nanoparticle-polymer hybrids and composites are central to a wide range of advanced multifunctional materials and technological applications. The premise of such systems lies in the myriad of possibilities that they offer in synergistically integrating particle and polymer properties to obtain significantly improved material performance. The past few decades of research on nanoparticle-based materials have remarkably enhanced our understanding of their macroscopic behavior and have resulted in an array of novel technologies. Yet, the demand for increasingly sophisticated applications of nanoparticle-polymer composites requires design rules that allow control of nanoscale interactions between the nanoparticles and their host environment. Such interactions manifest in unique interfacial structural and dynamical properties which ultimately determine the emergent material behavior. In this talk, I highlight the role of neutron scattering in directly observing and resolving interfacial properties that are critical to the design and performance of nanoparticle-polymer hybrids and composites.

1:39PM B51.00005: Polymer electrolytes for battery technology [Invited]  
JANNA MARANAS (Presenter), Pennsylvania State University — Polymer electrolytes have potential for use in next generation lithium and sodium batteries. Replacing the liquid electrolyte currently used has several advantages: it allows use of high energy density solid lithium as the anode, removes toxic solvents, improves safety, and eliminates the need for heavy casings. Despite their advantages, the conductivity of polymer electrolytes is not sufficient for use in batteries. As a result, considerable effort towards improving conductivity and understanding mechanisms of lithium transport has taken place over the last 30 years. This talk considers the interplay of conductivity, crystallinity, local coordination and polymer dynamics in solid polymer electrolytes. Using a combination of experimental and computational technique, we propose the possibility of high charge mobility using ion aggregates and percolated nanofiller networks.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B52 DPOLY DBIO: Polyelectrolyte Complexation I: Coacervates and More BCEC 253B -
Debra Audus, National Institute of Standards and Technology - Tag(s): Focus

11:15AM B52.00001: Complexation of homologous polymers with variable polarity  
JIAN QIN (Presenter), SEAN FRIEDOWITZ, JUNZHE LOU, YAN XIA, Stanford University — Polyelectrolyte complexation is sensitive to both long-ranged electrostatic interaction and short-ranged effects including solvation and ion association. We synthesized polyanions and polycations with identical backbone, variable length, and controlled solvation environment around charges. Systematic dependences on molecular weight and local environment are revealed by accurate polymer compositions determined using spectroscopic measurements, for nine sets of polymer pairs. Using two fitting parameters, the backbone solubility parameter and the ion-binding strength, the results are quantitatively described by a solution free energy model that incorporates properly charge connectivity and ion-binding equilibrium.
11:27AM B52.00002: Non-stoichiometric Coacervation between Hyaluronic Acid and Chitosan* BASAK KAYITMAZER (Presenter), ALAADDIN FARUK KOKSAL, ELIF KILIC IYILIK, Department of Chemistry, Bogazici University, OZGE KARABIYIK ACAR, GAMZE KOSE, Department of Genetics and Bioengineering, Yeditepe University — Hyaluronic acid and chitosan present a unique non-cognate pair where both polyelectrolytes are semi-flexible and have pH-dependent charges. These oppositely charged polysaccharides go into liquid-liquid phase separation far away from zero-zeta potential, which usually takes place at 1:1 charge ratios for other oppositely charged macroion-pairs. In this presentation, we explore the reasons behind non-stoichiometric coacervation for the HA/CHI pair. We also briefly studied effect of counterions on the coacervation window; i.e. extend of charge ratios where coacervation prevailed. If the counterion was present as a small ion of the solvent solution (Na⁺ or Ca²⁺), then its chaotropic nature had an effect of keeping the polymer hydrated despite the tendency to release the water molecules upon association of the polymers. This effect was enhanced when the polyelectrolyte had glutamate instead of chloride as its counterion. Since glutamate was a large zwitterion where the charge was distributed around different atoms, it served to extend the coacervation window.

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11:39AM B52.00003: Lower critical solution temperature in polyelectrolyte complex coacervates VIVEK PRABHU (Presenter), SAMIM ALI, Materials Science and Engineering Division, National Institute of Standards and Technology, MARKUS BLEUEL, Center for Neutron Research, National Institute of Standards and Technology — Measurements on a common linear oppositely-charged polyelectrolyte complex system, potassium-poly(styrene sulfonate) and poly(diallyl dimethyl ammonium bromide), shows liquid-liquid phase separation upon heating, or lower critical solution temperature behavior. The experimental accessibility of the critical temperature occurs for a narrow range of monovalent salt concentration (Cs) with coexistence curves narrowing with increasing Cs that reduces the polymer concentration (Cp) in the polymer-rich phase. We will describe a qualitative comparison of this phase behavior to available mean field models.

11:51AM B52.00004: Coacervate-driven self-assembly with Transfer Matrix Theory and Self-Consistent Field Theory GARY MIN CHIANG ONG (Presenter), CHARLES SING, University of Illinois at Urbana-Champaign — Complex coacervation occurs when two oppositely charged polyelectrolytes phase separate in an aqueous salt solution, resulting in a polymer dense coacervate phase and a polymer-dilute supernatant phase. Block copolyelectrolytes, which consists of both charged and neutral blocks, use this driving force to self-assemble into geometries which include micelles, vesicles and hexagonal rods. Coacervate-based materials provide advantages in (for example) the delivery of biologic materials, as encapsulation can be performed in the absence of organic solvent while maintaining stability of proteins. Recent advances in coacervation theory and simulations are used to understand the thermodynamics of coacervation-driven self-assembly. Transfer matrix theory is incorporated into self-consistent field theory (SCFT) to study how parameters like salt concentration, total polymer concentration and charge fraction of block copolyelectrolyes can affect the phase behavior of assembled structures, which is crucial in assisting in the design of materials. We show assembly that is analogous to uncharged block copolymer assembly in solution, and limits to standard coacervate phase behavior in the limit of long charged blocks.

12:03PM B52.00005: Structure and rheology of polyelectrolytes in length-mismatched coacervates AMANDA MARCIEL (Presenter), Chemical and Biomolecular Engineering, Rice University, MATTHEW TIRRELL, IME, The University of Chicago — Polyelectrolyte complexes are highly tunable materials that span from low-viscosity liquids (coacervates) to high-modulus solids with high water content, making them attractive as surface coating, membrane purification and bioadhesive materials. However, most of their properties and their effects with salt, pH, polymer ratio and temperature have only been qualitatively described. Here, we present an investigation of the structure and chain conformations, and rheological properties of polyelectrolyte complex (PEC) coacervates comprising biomimetic model polyelectrolytes with mismatched lengths. This model system allows the chain length (6 – 800-mer), side-chain functionality and chirality (L, D) to be tuned while keeping the backbone chemistry constant, thus enabling a systematic investigation of polyelectrolyte chain conformation in the liquid coacervate phase.
KEVIN SHEN (Presenter), Chemical Engineering, University of California Santa Barbara, ZHEN-GANG WANG, Chemistry and Chemical Engineering, Caltech — We study electrostatic correlations by quantifying the relative contributions of linear-response ionic atmospheres (as first described by Debye and Huckel) and counterion condensation (CC). Even for aqueous solutions of highly charged polyelectrolytes, CC may contribute less than half of the (electrostatic) osmotic coefficient drop. We further show that after CC sets in, its relative contribution to the osmotic coefficient actually decreases with increasing concentration. We quantify the strength of CC in terms of an electrostatic binding constant that captures both direct interactions between condensing charges as well as non-local effects of screening and chain connectivity. Critically, we retain the discrete nature of the polyelectrolyte backbone and counterions – this preserves "residual" electrostatic fluctuations of condensed charge pairs. Depending on the strength of residual charge fluctuations, CC can either stabilize or destabilize polyelectrolyte solutions against phase separation.

*KS thanks support by the NSF-GRFP fellowship and Jacobs Institute for Molecular Engineering for Medicine (JIMEM).

MICHAEL RUBINSTEIN (Presenter), Mechanical Engineering and Materials Science, Biomedical Engineering, Physics, and Chemistry, Duke University, SERGEY PANYUKOV, P. N. Lebedev Physics Institute, Russian Academy of Sciences, QI LIAO, Institute of Chemistry, Chinese Academy of Sciences, CHRISTIAN APONTE-RIVERA, Mechanical Engineering and Materials Science, Duke University — We develop a scaling theory and perform molecular dynamic simulations of weakly interacting coacervates with electrostatic interaction energy per charge less than thermal energy $kT$. Such liquid coacervates formed by oppositely charged polyelectrolytes can be asymmetric in charge density and number of charges per chain. We predict that these coacervates form interpenetrating solutions with two correlation lengths and two qualitatively different types of conformations of polyelectrolytes with lower and higher charge densities, which are analogous to chain conformations in quasi-neutral and in polyelectrolyte solutions, respectively. Weaker charged chains are attracted to and adsorbed on stronger charged chains forming a screening "coat" around the stronger charged polyelectrolytes. We present scaling prediction for polymeric diffusion coefficient, viscosity and stress relaxation function of these coacervates. Salt added at lower concentrations screens the repulsion between stronger charged chains, thereby reducing the thickness of the screening coat and resulting in the non-zero net polymer charge in the coacervate. At higher salt concentrations salt screens the attraction between oppositely charged chains, decreasing the coacervate concentration and its polymeric charge density. Thus, we predict a non-monotonic salt concentration dependence of polymeric charge density for asymmetric coacervates. Phase diagram for a mixture of oppositely charged polyelectrolytes at various compositions is proposed for different salt concentrations.

*This work was supported by NSF, NIH and CFF.

JEFFREY TING (Presenter), SIQI MENG, LU LI, HAO WU, University of Chicago, AMANDA MARCEL, Chemical and Biomolecular Engineering, Rice University, MATTHEW TIRRELL, University of Chicago — Polyelectrolyte complexes that form solid-like precipitates in water strongly resemble kinetically trapped solid mixtures and present formidable challenges in reproducing reliable properties and functionality. However, salt can be employed to break intermolecular ion pairs and process these nonequilibrium assemblies from a rubbery to a viscous liquid-like state. Here, we explore this transition with a pairing of RAFT-derived poly(styrene sulfonate sodium) (PSS) and poly(vinyl benzyl trimethylammonium chloride) (PVBTMA), using a combination of rheology, small angle X-ray scattering (SAXS), optical imaging, and thermal characterization. PSS and PVBTMA homopolyelectrolytes were synthesized at different molar masses with low dispersity; sodium bromide was chosen to probe individual chain and complex features. With no added salt, solid-like aggregates precipitated from solution. At 2.5 M salt, viscoelastic behavior was observed – shifting of the storage/loss moduli exhibited excellent time-salt superposition. Systematic SAXS studies were in good agreement with morphologies at various combinations of molar mass and salt. Finally, thermogravimetric analysis of the separate complex and supernatant phases enabled us to quantify the partitioning of salt and water.

*NIST CHiMaD (70NANB14H012)
1:15PM B52.00009: Guanidinium can Break and Form Strongly Associating Ion-Complexes  
KAZI SADMAN (Presenter), QIFENG WANG, KENNETH R SHULL, Northwestern University — Guanidinium is one of nature's strongest denaturants and is also a motif that appears in several interfacial contexts such as the RGD sequence involved in cell adhesion, cell penetrating peptides, and anti-microbial molecules. It is important to quantify the origin of guanidinium's ion-specific interactions, so that its unique behavior may be exploited in synthetic applications. Here we show that guanidinium ions can both break and form strongly associating ion-complexes in a context-dependent way. These insights into guanidinium's behavior are elucidated using polyelectrolyte complexes (PECs), where inter-polymer ion-pairs between oppositely charged polymers play an important role in determining material stability. We demonstrate that guanidinium salts are very effective in dissolving the poly(styrenesulfonate)/poly(allylamine) (PSS:PAH) complex, which has one of the highest measured polycation-polyanion association affinities. We also demonstrate that incorporating guanidinium charges directly into the polyelectrolyte results in a complex that remains stable under highly denaturing conditions. The model system of PSS:PAH is used to glean insights into guanidinium's denaturing activity, and to broadly comment on the nature of ion-specific interactions in charged macromolecules.

1:27PM B52.00010: Thermodynamic Characterization of Complex Coacervates of Oppositely Charged Biopolymers*
FATMA AKCAY OGUR (Presenter), FATMA AHU AKIN, NAYRA KAVAFYAN, BUSRA GUN, BASAK KAYITMAZER, Department of Chemistry, Bogazici University — Complex coacervation occurs between two oppositely charged macromolecules which go into macroscopic phase separation and form two liquid phases: polyelectrolyte-rich (coacervate) and polyelectrolyte-poor (dilute) phase. There are several areas of application for coacervates in food, cosmetics, pharmaceuticals, and medical adhesives industries. Hyaluronic acid (HA) and chitosan (CH), which are semi-flexible biopolymers, are weak polyacids and polybases, respectively. In this study, isothermal titration calorimetry (ITC) and turbidity experiments were employed to understand the thermodynamics of complex formation and phase separation for this non-cognate biopolymer system. Parameters that affect coacervation (charge ratio of polyelectrolytes, pH, ionic strength, molecular weight of polyelectrolytes) were varied to determine binding constants, change in enthalpy, change in entropy, molar heat capacity, and stoichiometry of soluble complex formation and coacervation. By systematically changing these variables, we determined that HA/CH interaction was predominantly entropic as a result of counterion release.

*This work was supported by the Scientific and Technological Research Council of Turkey (TUBITAK), Grant No:116Z096

1:39PM B52.00011: The free energy profile of complexation of two oppositely charged polyelectrolyte chains*
SOU MIK MITRA (Presenter), ARINDAM KUNDAGRAMI, Department of Physical Sciences & Centre for Advanced Functional Materials, Indian Institute of Science Education and Research Kolkata — We report a study of the complexation process of two oppositely charged polyelectrolyte (PE) chains in dilute solution interacting through an attractive screened Coulomb potential. The system is modeled using the PE chain free energy within the uniform spherical expansion approximation where the two PE chains as well as the neutral complex are considered to be hypothetical spheres whose radii quantitatively denote the sizes of the respective chains. The two chains start overlapping due to attraction between the monomers, as well as the entropy gain of free counterions. The complexation process ends up in the formation of a neutral coacervate through mutual adsorption of oppositely charged monomers, with associated release of all counterions of both types. The free energy profile that follows this pathway is studied by obtaining the variations of the total free energy, as well as the various individual energy and entropy contributions, as functions of the extent of overlap of the two chains. Also the behavior of the chain size and charge as functions of overlap is presented. These results elucidate the competition of the various driving forces, both enthalpic and entropic in nature, which lead to complexation.

*Ministry of Human Resource Development (MHRD), Government of India
1:51PM B52.00012: Confined Impingement Jet Mixing of Charged Polymers for Functional Structured Colloids and Encapsulation  DOUGLAS SCOTT (Presenter), ROBERT K PRUD’HOMME, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — Confined impingement jet (CIJ) mixing has been demonstrated as a scalable continuous process, thus enabling the mass production of structured nanocolloids consisting of distinct polymer domains as well as the encapsulation of sensitive active ingredients (SAIs) via the technique of flash nanoprecipitation (FNP). Due to the fast mixing in a CIJ mixer, competing timescales of mixing and aggregation dictate final particle size and morphology. Yet, incorporating charged polymers (e.g., ionomers and polyelectrolytes) and their additional timescales of electrostatic interactions has yet to be characterized in detail as a pathway for fabricating functional colloids. Here, we explore the impact of hydrophobic ionomers on traditional FNP for forming complex nanocolloids for use as amphiphilic colloidal surfactants in emulsification studies. The use of ionomers for stabilization of SAIs in a non-traditional medium is also presented. Additionally, the nascent technique of flash nanocomplexation (FNC) is developed as a scalable route for generating polyelectrolyte complexes where process parameters of charge ratio, charge density, and molecular weight disparity are explored in the context of fast mixing times. The application of FNC to the sustainable encapsulation of SAIs is demonstrated.

2:03PM B52.00013: Gradient Nanoporous Poly(ionic liquid) Complex Membrane as Soft Actuators*  JIAYIN YUAN (Presenter), Department of Materials and Environmental Chemistry, Stockholm university — This talk deals with nanoporous polyelectrolyte complex membranes by using poly(ionic liquid)s (PILs).1 PILs are the polymerization products of ionic liquids (ILs) and combine some properties and functions of ILs with polymers. We exploited PILs in the fabrication of nanoporous membranes via electrostatic complexation of PILs with polyacids.2 The porous structure results from phase separation of a hydrophobic PIL in water accompanied by ionic crosslinking between PIL and polyacids. The nanoporous membrane carries a gradient profile in the cross-linking density along the cross-section, triggered by the diffusive penetration of ammonia into the PIL-polyacid blend film. The membrane pore size is tunable from nano- to micrometer scale. The membrane features high actuation speed in response to acetone vapor and serves as environmental sensors to detect solvent quality.3,4

References

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Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B53 GSNP GSOFT: Disordered Networks: From Mechanical Properties to Failure
BCEC 253C - J. M. Schwarz - Tag(s): Invited

11:15AM B53.00001: Experimental study of failure in a granular material [Invited]  DAVID HOUDOUX, THAI BINH NGUYEN, JEROME CRASSOUS, AXELLE AMON (Presenter), University of Rennes 1 — Solid amorphous materials, when submitted to large enough stresses, display localization of the deformation. This localization can take several forms from local plastic events to shear-bands formation. I will present recent experimental results showing how those processes occur in a granular material submitted to a biaxial test.

Our observations show that failure in a sheared granular material is a multi-scale process both on a spatial point of view and on strain increments point of view. When a small strain increment is used to define the deformation field, plasticity occurs in the form of local rearrangements. Those local events can be interpreted as elementary contributions building up in a macroscopic plastic flow on larger strain increments. Correlation between the rearrangements can be evidenced and a transient self-organization of the flow at intermediate strain increments is observed with the formation of intermittent micro-bands. The coupling between the rearrangements is due to the elastic redistribution of the stress when a plastic event takes place. This structuration of the plastic flow corresponds to the fluctuating part of the plastic field and is clearly of a different nature from the final, permanent, shear-band which is a feature of the mean plastic field, defined on large strain increments. We have shown that the shear band emerges through a bifurcation of the mean plastic field. This bifurcation is linked to the emergence of an angle linked to the internal friction of the material which is clearly distinct from the orientation of the anisotropic elastic coupling. I will discuss the interpretation of our observations in the framework of current theoretical models of the plasticity of granular materials.
11:51AM B53.00002: Mechanics of cells in disordered environments [Invited] CHASE BROEDERSZ (Presenter), Physics, LMU Munich — Living cells typically grow and move in a 3D fibrous matrix such as collagen. Macroscopically, these biopolymer matrices exhibit striking nonlinear mechanical responses. At the scale of the cell, the network is highly disordered. The implications of the extreme mechanical response and structural disorder of the matrix for cells embedded in the meshwork remain largely elusive. In fact, it is unknown what the network mechanics looks like from the perspective of such a cell, and it is unclear how the cell interacts with this network at the microscopic scale to sense stiffness and regulate the mechanics of its surrounding matrix. In this talk, I will present our recent theoretical and experimental progress to understand how cells mechanically interface with their environment. Finally, I will discuss how such structured confining environments, which we mimick by using micropatterns, affect cell migration.

12:27PM B53.00003: Towards a virtual bone lab: multiscale interplay between architecture, complexity, and dynamics* [Invited] JEAN CARLSON (Presenter), CHANTAL NGUYEN, AVIK MONDAL, University of California, Santa Barbara, XIAO MA, AHMED ELBANNA, Civil and Environmental Engineering, University of Illinois at Urbana Champaign — Trabecular bone is a flexible, lightweight tissue that exhibits hierarchical mechanisms of fracture resistance across scales. At the mesoscale, it resembles a web of interconnected struts (trabeculae) that erode with age and diseases such as osteoporosis, resulting in increased fracture propensity. Recent ex vivo experiments have indicated that the traditional macroscale diagnostic marker of osteoporosis, bone mineral density (BMD), correlates poorly with bone strength when used as a sole predictor, but that it can explain much of the variation in bone strength when considered in conjunction with architectural features. We introduce a novel approach to modeling trabecular bone that combines network analysis with simulations of mechanical loading and failure, enabling a unique characterization of how bone architecture contributes to robustness and resilience. We generate network models from tomographic images of real human vertebral bone. Weighted edges represent trabeculae and nodes represent branch points where trabeculae meet. We simulate loading and deformation on finite element models in which edges are replaced by beams, resulting in a considerable reduction in computation time in comparison with fine-grained models used for in silico validation. The beam-element analysis facilitates direct comparison of mechanics and topology at multiple scales ranging from that of individual edges (beams) to the network as a whole. In addition, we discuss implications of our work in the context of clinical application, facilitated by advances in data acquisition methods for assessing fine tissue structure, and we highlight future directions for integrating our results into a comprehensive characterization of bone that links its molecular constituents at the nanoscale to its architecture at large.

*NSF IIP-1548339; ARO (ICB) W911NF-09-D-0001.

1:03PM B53.00004: A quasi-continuum approach for modeling fracture in disordered networked materials: Can small world architectures save the day? [Invited] AHMED ELBANNA (Presenter), AHMED N GHAREEB, University of Illinois at Urbana-Champaign — The skeleton of many natural and artificial structures may be abstracted as networks of nonlinearly interacting elements. Examples include rubber, gels, soft tissues, and lattice materials. Understanding the multiscale nature of deformation and failure of networked structures hold key for uncovering origins of fragility in many complex systems including biological tissues and enables designing novel materials. However, these processes are intrinsically multiscale and for large scale structures it is computationally prohibitive to adopt a full discrete approach. Here, we introduce a new adaptive numerical algorithm for solving polymer networks, the building blocks in many biological and engineering systems, using an extended version of the Quasi-Continuum (QC) method. In regions of high interest, for example near defects or cracks, each polymer chain is idealized using the worm like chain model. Away from these imperfections, the network structure is computationally homogenized, using Hill-Mandell's principle, to yield an anisotropic material tensor consistent with the underlying network structure. Dynamic adaptivity provides a seamless transition across the two models. Overall, the proposed method provides a multi-resolution capability by retaining explicit representation of small scale heterogeneities and topological features, where they matter near the crack tips, while still accurately accounting for bulk elasticity and loading. We illustrate the efficiency of the method by applying it to study the fracture of large scale polymer network problems as realized in experiments on hydrogels. We further apply the method to test the influence of network topology on its fracture resistance and demonstrate that networks with small-world architectures, balancing clustering and average path length, may lead to an optimum fracture toughness. We discuss the implications of our findings for the analysis and design of tough networks.
Disordered networks are used widely to study heterogeneous material failure. These structures are inherent to many systems, such as rigid foams or granular materials. In particular, the latter exhibit highly heterogeneous force chain networks that appear to control the response of such media to external perturbations. To characterize these networks, we focus on their mechanical stability. We study the uniaxial response of networks with geometry derived from the force chains observed in granular experiments. We perform experiments on samples created by laser-cutting these networks from acrylic sheets. We find that the mean degree of the network is a control parameter of the failure behavior, which ranges from ductile to brittle. We explain this ductile-brittle transition with rigidity analysis using a frictional (3,3)-pebble game algorithm. We find that the brittle behavior corresponds to the emergence of a percolating rigid cluster occurring at a mean degree close to the isostatic value of a high friction coefficient packing. Moreover, we find that for networks close to the transition point, failure events predominantly occur within the floppy regions between the rigid clusters. To perform an analysis that is not restricted to the networks close to the transition point, we develop a test to study the failure locations. We use a measure taken from network-science tools and capable of identifying likely failure locations in the samples. It consists in comparing the relative importance of the beams of the lattice by studying their geodesic edge betweenness centrality.

*James S. McDonnell Foundation

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B54 DPOLY GSOFT DFD DBIO: Extreme Deformation I: Cavitation and Yielding

11:15AM B54.00001: Laser-induced Cavitation Dynamics of Polydimethylsiloxane with Varying Cross-Linking Density and Molecular Weight* SACCHITA TIWARI (Presenter), Mechanical and Industrial Engineering, University of Massachusetts, Amherst, YUE ZHENG, Mechanical and Aerospace Engineering, University of California San Diego, California, AMIR KAZEMI-MORIDANI, Mechanical and Industrial Engineering, University of Massachusetts, Amherst, KELLY MCLEOD, IPEK SACLIGIL, CHRISTOPHER BARNEY, ALFRED CROSBY, GREGORY TEW, Polymer Science and Engineering, University of Massachusetts, Amherst, SHENGQIANG CAI, Mechanical and Aerospace Engineering, University of California San Diego, California, JAE-HWANG LEE, Mechanical and Industrial Engineering, University of Massachusetts, Amherst — High-strain-rate mechanical properties of a cross-linked polymeric model system are relevant to understanding the dynamics and damage mechanisms of various biological tissues under HSR mechanical stimuli. We present the characterization of two material systems: 1) a commercially available polydimethylsiloxane (Sylgard 184) prepared with varying crosslinking times at fixed temperature; 2) a UV-curable polydimethylsiloxane having different controlled molecular weights. For high-strain-rate characterization, we performed laser-induced cavitation with ablation seeds. The ablation seed in a specimen was vaporized without dielectric breakdown, and produced a rapidly expanding cavity. The expansion dynamics of the laser-induced cavity was observed using ultrafast imaging. The dataset obtained from time-dependent radii of cavities was numerically analyzed, and the material's HSR mechanical parameters were identified. This study can lead us to establish a high-strain-rate mechanical characterization method for soft materials including various tissues.

*This research was supported by the Office of Naval Research under contract N00014-17-1-2056.
11:27AM B54.00002: Modeling high-strain-rate microcavitation in soft materials: the role of material response*

ANASTASIA TZOUMAKA (Presenter), DAVID HENANN, Brown University — High-strain-rate inertial microcavitation has been shown to be an effective method for mechanical characterization of soft materials. To model inertial microcavitation Rayleigh-Plesset-based approaches are commonly used to capture the cavitation dynamics; however, these approaches are limited to simple viscoelastic constitutive models for the soft material, such as the Kelvin-Voigt model, since the implementation of more complex viscoelastic models requires the integration of complex mathematical expressions. To circumvent this limitation, we have developed a finite-element-based numerical simulation capability for inertial microcavitation that enables the incorporation of more complex constitutive laws. In this talk, we consider nonlinear elastic and power-law viscous constitutive laws and present a deeper investigation of the role of the elasticity and rheology of the soft material on the consequent cavitation dynamics. We apply our simulation capability by comparing computational results with experimental data from high-strain-rate inertial microcavitation of polyacrylamide and collagen gels in order to mechanically characterize these materials at high strain rates.

*This work was supported by funds from ONR through Grant N00014-18-1-2625.

11:39AM B54.00003: Crack Geometry Dependence on Kinetic Energy and Loading Rate in High-Speed Cavitation

MATTHEW MILNER (Presenter), SHELBY HUTCHENS, University of Illinois at Urbana-Champaign — Temporary cavitation occurs when a projectile impacts a soft material causing a large radial expansion of the wound tract immediately after the projectile passes. Though cavity size is known to scale with the kinetic energy of the projectile, the fracture-governed damage accompanying this large deformation remains poorly understood. Using a custom designed table-top ballistic cavitation device, we replicate the temporary cavity phenomenon in soft tissue simulants on a small scale by applying a fast, high-pressure pulse of air through a needle. Temporary cavities produced via air pulse (characterized by energy density, loading rate, and needle size) isolate the damage accompanying large and dynamic stretches from that associated with more complicated impact dynamics such as projectile tumble. We find that increasing kinetic energy density and loading rate both result in greater crack area, while transforming the fracture geometry from a single planar crack to multiple radial cracks. As a result, the dependence of accumulated damage, quantified with crack surface area, increases super-linearly with kinetic energy while the temporary cavitation volume is verified to remain approximately linear over the range of energies tested.

11:51AM B54.00004: Inertial Microcavitation in Soft Matter*

JIN YANG, Mechanical Engineering, University of Wisconsin-Madison, JONATHAN ESTRADA, ERIC JOHNSEN, Mechanical Engineering, University of Michigan, DAVID HENANN, Brown University, CHRISTIAN FRANCK (Presenter), Mechanical Engineering, University of Wisconsin-Madison — The last two decades have seen significant advances in the manufacturing and design of soft matter materials with tunable control across orders of magnitude in length scale and elastic modulus. Characterization of the mechanical behavior of this new class of emerging complex soft materials has been challenging, especially in the inertial regime at strain rates beyond 100/s. In this talk I will present an overview of how inertial microcavitation can be exploited to mechanically characterize soft matter at high and ultra-high strain rates (i.e., $10^2 - 10^8$ 1/s) using inertial microcavitation rheometry (IMR). Specifically, I will show how such an approach that features both rigorous experimental and theoretical advances, can be leveraged to inform about the time and length-scale dependent material behavior of complex soft matter.

*We gratefully acknowledge support from the Office of Naval Research (Dr. Timothy Bentley) under grants N000141612872 and N000141712058.

12:27PM B54.00005: The Sound of Light: Using optical breakdown to drive extreme mechanical excitations*

ATHANASIOS ATHANASSIADIS (Presenter), Massachusetts Institute of Technology — When a high-power laser is focused to a small spot in a fluid, nonlinear interactions at the focus can excite a plasma that expands explosively and emits a strong mechanical shock wave into the ambient medium. This phenomenon — called optical breakdown — can generate peak pressures exceeding 1 MPa a centimeter from the source, with pressure pulses typically lasting less than 1 microsecond. In liquids, optical breakdown is accompanied by the growth of a vapor bubble that rapidly expands from micron to millimeter scales. Together, the ultrafast shock and subsequent bubble expansion can be used to probe the dynamic mechanical response of materials at short time scales and large stress scales. In this talk, I will demonstrate how I have leveraged optical breakdown to remotely measure the mechanical properties of submerged solids. I will show how the mechanical excitation can be tuned optically, and discuss how this technique can be adapted to measure the mechanical response of soft media.

*This work was supported by the Office of Naval Research.
12:39PM B54.00006: Molecular Dynamics Simulation of Polymeric Systems Under Shock Deformation∗

JOHN P MIKHAIL (Presenter), GREGORY C RUTLEDGE, Department of Chemical Engineering, Massachusetts Institute of Technology —

Currently, mechanisms by which polymeric systems respond to extreme deformation conditions, in particular deformation due to shock waves, are not fully understood. This work uses molecular dynamics (MD) simulations of atomistically detailed models of both homogeneous and heterogeneous polymeric materials (with structural variations on the nanometer scale) to study the underlying physics of system response to shock waves. Simulations are performed using both equilibrium ("Hugoniostatted") and nonequilibrium MD. Semicrystalline polymers with different configurations and degrees of crystallinity are examined, with shocks applied either isotropically or directionally with respect to the crystalline-amorphous interface. The Hugoniot curves are calculated, along with shock velocity and particle velocity. Analysis of the vibrational state of the systems identifies normal modes, along with changes in the vibrational signature pre- to post-shock. This analysis enables validation against experimental results obtainable via Raman or IR spectroscopy and provides insight into deformation mechanisms.

∗This material is based upon work supported in part by the U. S. Army Research Office through the Institute for Soldier Nanotechnologies at MIT, under Cooperative Agreement Number W911NF-18-2-0048.

12:51PM B54.00007: Rheological properties of small-molecule liquids in elastohydrodynamic lubrication∗

MARK OWEN ROBBINS (Presenter), Department of Physics and Astronomy, Johns Hopkins University, VIKRAM JADHAO, Intelligent Systems Engineering, Indiana University Bloomington — There is an ongoing debate concerning the rheological model that accurately captures the flow of small-molecule liquids in elastohydrodynamic lubrication (EHL). In EHL, liquids experience extreme pressures (>0.5 GPa) and strain rates (>100,000 s^-1). Rheological properties of squalane, a representative EHL fluid, are investigated using nonequilibrium molecular dynamics simulations for pressures up to 1.2 GPa, strain rates between 10^5 – 10^10 s^-1, and temperatures up to 100 C. Simulation results are consistent with experimental data for a broad range of equilibrium and nonequilibrium conditions. At high temperatures and low pressures, where Newtonian viscosity of squalane is low, shear-thinning associated with molecular alignment is observed, which can be described by power-law fluid models. As Newtonian viscosity rises above ~1 Pa-s, shear-thinning is increasingly dominated by thermally-activated flow processes. In these conditions, the stress-strain-rate behavior from simulations and available experimental data is consistent with the Eyring equation for over 10 decades in strain rate. The macroscopic rheological properties are correlated with underlying molecular orientation and dynamics.

∗This work is supported by the Army Research Laboratory through Grant W911NF-12-2-0022.

1:03PM B54.00008: A Molecular View: the Mechanical Behavior of Polymer Networks∗

ZIYU YE (Presenter), ROBERT RIGGLEMAN, University of Pennsylvania — Crosslinked polymer networks swollen in solvent, such as hydrogels, have gained much attention for their unique structural and mechanical properties that mimic natural materials and biological tissues. Since the network structure is linked to material properties, it is important to understand the dynamic behavior of the network during mechanical deformation. As many synthetic and natural soft materials are highly inhomogeneous, an important step is to elucidate how structural heterogeneities, such as network defects and phase boundaries, affect the response of the network to deformation. We use coarse-grained molecular dynamics to investigate the response of swollen polymer networks to deformation and the influence of network heterogeneities on the response. We examine the influence of network structures on soft materials’ bulk mechanical properties using tensile deformation to study both reversible and irreversible responses in gels as a function of polymer concentration, strand length, and network defects. We find that the network formation process will dictate local network structure, which is highly correlated to the dynamic material response under deformation.

∗ONR-40004251
Expansion Instabilities of Tube-Like Defects in Polymer Gels Subjected to Hydrostatic Pressure

CHRISTOPHER BARNEY (Presenter), University of Massachusetts Amherst, YUE ZHENG, SHENGQIANG CAI, Mechanical Engineering, University of California San Diego, ALFRED CROSBY, University of Massachusetts Amherst — Cavitation in soft solids is defined as the unstable expansion of a void within a body subjected to a negative hydrostatic pressure. Classically this expansion has been modeled assuming an initially spherical cavity, but the advent of needle-induced cavitation makes an initially cylindrical geometry experimentally relevant. Tube-like defects of varying aspect ratio are first created at the tip of a needle by incorporating a retraction step to the needle insertion process after puncturing soft polymer gels. Instability-like expansion of the cylindrical defects is then experimentally observed at pressures comparable to those expected of a spherical geometry. Complementary modeling shows that the change in initial geometry has little effect on the critical cavitation pressure. Together these measurements demonstrate that the onset pressure of instability-like expansion of cylindrical voids in soft gels does not deviate considerably from the classical spherical model which enables the confident measurement of local elastic properties in soft gels and biological tissues.

Cavitation to Study Brain Mechanics and Tissue Interface Strength

CAREY DOUGAN (Presenter), Chemical Engineering, University of Massachusetts, YUE ZHENG, Department of Mechanical and Aerospace Engineering, University of California, San Diego, CHRISTOPHER BARNEY, Polymer Science and Engineering, University of Massachusetts, SUALYNETH GALARZA, Chemical Engineering, University of Massachusetts, SHENGQIANG CAI, Department of Mechanical and Aerospace Engineering, University of California, San Diego, ALFRED CROSBY, Polymer Science and Engineering, University of Massachusetts, SHELLY PEYTON, Chemical Engineering, University of Massachusetts — Cavitation is the rapid expansion of an instability within a material. There is a considerable need to study cavitation in biological tissue, as cavitation-related damage has been implicated in explosive blast injuries on military personnel. Post-mortem analysis of human brains exposed to blasts revealed scarring at boundaries between white and gray matter, at the outermost layer, and at blood vessel/tissue interfaces. Our technique introduces a single bubble at the tip of a needle at a specific location and depth to determine localized brain properties and the impact of tissue boundaries on cavitation damage path. Finite element modeling concludes that if a tissue-tissue interface is weaker than the needle injection path, the cavitation damage propagates along the interface. Our data suggests that interfaces synergistically facilitate fracture propagation at critical pressures 5 kPa less than required to cavitate bulk thalamus. When cavitation occurs near the corpus callosum, we observe a fracture propagation along the corpus callosum and cerebral cortex interface. In deeper regions, fracture separates the amygdala from the thalamus region of brain. This approach allows us to study cavitation damage paths to better understand the mechanism for brain injury.

Volume-controlled Cavity Expansion for Probing of Local Elastic Properties in Soft Materials

SHABNAM RAAYAI (Presenter), ZHANTAO CHEN, TAL COHEN, Massachusetts Institute of Technology — Ability to measure the mechanical properties of soft biological materials in vivo can enable physicians in offering more accurate diagnosis of diseases such as cancer. Needle-based cavity expansion techniques are thus capturing the attention of researchers for measurement of the local nonlinear elastic properties in soft materials. Here we introduce a volume-controlled cavity expansion procedure that builds on the Cavitation Rheology technique [1] without relying on the maximum recorded pressure. We show that by employing an effective cavity radius based on our volume measurements we can consistently collapse the experimental results onto the theoretical predictions, regardless of the specific damage or instability mechanism exhibited by the material. We confirm the applicability of this technique by using PDMS samples, presenting good agreement with results obtained via conventional techniques with less than 5% of scatter. Moreover, since this method does not require visual tracking of the cavity, it can be applied to measure the nonlinear elastic response in opaque samples.

The yielding transition of soft colloids

STEFANO AIME (Presenter), John A. Paulson School of Engineering and Applied Science, Harvard University, DOMENICO TRUZZOLILLO, LAURENCE RAMOS, LUCA CIPPELLETTI, Laboratoire Charles Coulomb, Université de Montpellier — We investigate the yielding transition of dense suspensions of colloids interacting via a soft repulsive potential by simultaneously measuring their mechanical response and microscopic dynamics under an oscillating shear deformation.

At low strain amplitude, all systems exhibit ultraslow, ballistic dynamics characterized by a compressed exponential relaxation of correlators, similar to those reported for many jammed soft materials at rest. Upon increasing the strain amplitude, in correspondence to the onset of the non-linear rheological response, we observe a dynamic transition towards a steady state characterized by fast stretched exponential, diffusive-like relaxations, reminiscent of those measured in supercooled liquids at rest.

Although the sharpness of the transition depends on the potential details, this scenario seems to be generic to soft colloids. We show that its main features are captured by an Ising-like model, with dynamic facilitation coupling the relaxation of neighboring sites, and we discuss intriguing analogies with thermodynamic phase transitions.

Plasticity effects in thin film wrinkling: Wrinkling behavior of plastic films bonded to elastomers with large strain mismatch

RAHUL GOPALAN RAMACHANDRAN (Presenter), JUNYU YANG, SAMEER DAMLE, SPANDAN MAITI, SACHIN VELANKAR, University of Pittsburgh — We examine the mechanics of composite films comprising a SEPS elastomer layer sandwiched between two thinner surface layers of plastic (polyethylene). Upon stretching such composite films to over twice their length and then releasing, the plastic surface films develop a highly wrinkled surface texture. The mechanism for this texturing is that during stretching, the plastic layers yield and stretch irreversibly whereas the elastomer stretches reversibly. Thus upon releasing, the plastic layers buckle due to compressive stress imposed by the elastomer. Although the wrinkling process appears somewhat similar to the wrinkling of a stiff elastic film bonded to a soft elastic substrate, our experiments and simulations show that plasticity plays a major role at all stages: (1) during stretching, the plastic layer yields in tension; (2) during recovery, the plastic layer first yields in-plane in compression and then buckles; (3) post-buckling, plastic hinges are formed at high-curvature regions. Homogeneous wrinkles are predicted only within a finite window of material properties: if the yield stress is too low, the plastic layers yield in-plane without wrinkling, whereas if the yield stress is too high, non-homogeneous wrinkles are predicted.

Machine Learning for Modelling Microstructure Evolution in Polymer Mixtures

NIGEL CLARKE (Presenter), University of Sheffield — Our aim is to enhance our modelling capabilities for microstructure evolution with machine learning. In particular, we focus on Gaussian processes (GPs), a popular non-parametric class of models used extensively in ML and uncertainty quantification, which have well documented predictive abilities. In our preliminary studies, we apply existing GP methodology to microstructure evolution to determine the feasibility of generating an emulator to supplement more traditional, computationally intense, approaches. As an exemplar, we focus on the non-linear Cahn-Hilliard equation for describing phase separation in blends. Spatio-temporal problems are particularly challenging for ML due to their high dimensionality, hence we use a method recently proposed for using machine learning to predict video images, based on the idea of light cones, in which the present is only dependent on the past in the immediate spatial neighbourhood, analogous to real-space time-stepping numerical schemes for PDEs. We will present results which highlight the both the strengths and challenges of using ML for modelling microstructure.

*We thank the UK Engineering and Physical Sciences Research Council (EP/S014985/1) for financial support.
11:39AM B55.00003: Impact of Dataset Uncertainties on Machine Learning Model predictions: The Example of Polymer Glass Transition Temperatures*  
ANURAG JHA (Presenter), ANAND CHANDRASEKARAN, CHIHO KIM, RAMAMURTHY RAMPRASAD, Georgia Institute of Technology — Data-driven methods are seeing a revival and are deeply influencing multiple aspects of materials research. Materials property data from computations or experiments, are being utilized to create surrogate models using machine learning (ML) techniques. These models can be utilized to provide rapid predictions of the properties of new materials at a fraction of the cost compared to actual experimentation or computation. Moreover, a variety of techniques are being explored to “invert” the property prediction pipeline to allow for designing materials with desired target set of property values. The quality of the developed surrogate model, depends on the quality (and quantity) of the dataset used in the model training. Often, different experimental studies may report different values for the same property of the same material. This may be due to variations in measurement techniques, conditions, and sample quality among others. How should one treat these variances and what is their impact? This question needs to be answered specifically, since it is paramount to the development of a good prediction model and helps understand its limitations.

*The authors acknowledge support of this work by the Toyota Research Institute through the Accelerated Materials Design and Discovery program.

11:51AM B55.00004: Molecular dynamics and machine learning assisted design of conjugated polymers for improved ionic conductivity*  
CHRISTIAN NOWAK (Presenter), MAYANK MISRA, FERNANDO A ESCOBEDO, Chemical and Biomolecular Engineering, Cornell University — Ionic transport in conjugated polymers is an area of increasing interest for applications involving such devices as sensors, batteries, and electronic ion pumps. In a previous work we used computational models to investigate the effect on ionic conductivity of specific chemistries of side chains attached to a polythiophene (PT) backbone, and made predictions that have been confirmed by experiments. Here we extend our materials design approach such that a chemical group “library” is considered from which polymers can be constructed. We employ two differing machine learning approaches to converge on a general set of high performing chemistries: a genetic algorithm and a neural network. We only consider PT-like molecules and take advantage of the fact that the crystalline arrangements simplify the task of microstructure modeling/prediction. We find some general trends for designing materials with improved ionic conductivity; namely, biasing the ion solvating groups towards the chain ends while still retaining good percolation of the solvation sites. Our ongoing efforts are focused on extending this scheme for optimization ionic conductivity to molecules with more complex morphologies such as Bolaamphiphiles.

*This work was supported by National Science Foundation (DMREF-1629369)

12:03PM B55.00005: A charge density prediction model for organic molecules using Deep Neural Networks*  
DEEPAK KAMAL (Presenter), ANAND CHANDRASHEKARAN, RAMAMURTHY RAMPRASAD, Georgia Institute of Technology — In an attempt to accelerate the pace of materials discovery, the community is increasingly using machine learning (ML) based techniques to rapidly map structure property relationships in materials. The Machine Learning methods has the advantage that their computational costs are negligible compared to those of the customary methods like density functional theory (DFT). The simulation properties of polymers is one such example where this limitation is most apparent. Here we propose a method to accurately predict charge densities of large organic systems by learning from pre-calculated examples of smaller systems. We present a novel fingerprint scheme which can numerically represent the local atomic environment. We then use a Neural Networks based models to learn the functional map between the local environments and the charge densities. Further, we introduce a recursive approach to improve these models by selectively incorporating poorly predicted examples. These charge densities are then used to calculate properties which depend on the charge density distribution like the dipole moments, dielectric properties for a host of unseen molecules thus eliminating the need to explicitly solve the laborious Kohn-Sham equations.

*Office of Naval Research : N0014-17-1-2656, a MURI grant.
Bayesian Optimization for Designing Polymer Electrolytes with a Higher Lithium-ion Conductivity

TIAN XIE (Presenter), YANMING WANG, ARTHUR FRANCE-LANORD, YANG SHAO-HORN, JEFFREY C GROSSMAN, Massachusetts Institute of Technology — Solid polymer electrolytes (SPEs) are candidates for the next generation battery technology due to their safety, stability, and low manufacturing cost. However, the lithium-ion (Li-ion) conductivities of SPEs are still 2-3 orders of magnitudes lower than what is needed for practical applications. In this work, we combine a Bayesian optimization (BO) scheme and coarse-grained molecular dynamics (CGMD) to explore the materials space of SPEs to improve their Li-ion conductivity. The SPEs in the CGMD models are a mixture of polymers and lithium salts in which the salt concentration, polymer/salt interaction strengths, and polymer compositions can be changed continuously and independently. We demonstrate that BO can significantly improve the efficiency of space exploration, which enables us to find the optimum SPE with the highest Li-ion conductivity despite the high computation cost of CGMD simulations. In addition, the Li-ion conductivity predictions from the BO provides a guideline for improving the performance of existing SPEs by changing their components accordingly. Finally, we validate our method by comparing the predictions with fully atomistic molecular dynamics and experimental measurements.


BING CAO, University of Alberta, LAWRENCE A ADUTWUM, Pharmaceutical Chemistry, University of Ghana, ANTON O OLIYNYK, ERIK LUBER (Presenter), BRIAN C OLSEN, ARTHUR MAR, JILLIAN M BURIAK, University of Alberta — Organic solar cells (OSCs) are a potential cost-effective way to transform solar energy into electricity due to their potential for low-cost and high-throughput roll-to-roll production.[1] Improving the power conversion efficiency (PCE) and stability of OSCs are two of the most important tasks on the way toward commercialization. While much effort has been focused on developing new materials, optimization of processing conditions is equally important, where optimization is typically done in a haphazard manner using the experimenter’s “intuition” or through one-variable-at-a-time (Edisonian) manipulation. However, such methods can fail to find the maximum PCE due to the high dimensionality parameter space of processing conditions and correlations between parameters. Moreover, laboratory-scale OSC fabrication is often low-throughput, time-consuming and expensive. Herein, we report an approach that uses Design of Experiments (DOE) along with machine learning (ML) to optimize solar cell efficiency. DoE is used to systematically explore the parameter space of processing conditions and ML is then utilized to estimate the PCE landscape as a function of the processing parameters. This process is then applied recursively to successively smaller regions of parameters space in regions of interest. Utilizing this process allows experimentalists to explore a larger parameter space with fewer experimental trials while obtaining valid and objective conclusions. Specific examples of concrete improvement of the power conversion efficiency of OSCs will be described.

Using Particle Swarm Optimization and SCFT to agnostically identify the stable and low-lying metastable competitive morphologies of block copolymers

CAROL TSAI (Presenter), KRIS T DELANEY, GLENN FREDRICKSON, University of California, Santa Barbara — The unguided search for the stable phase of a block copolymer of a given composition and architecture is a problem of global optimization with important ramifications from a materials discovery perspective. We discuss the development of a reciprocal-space Particle Swarm Optimization (PSO)-SCFT method in which Fourier components of SCFT fields near the principal shell are manipulated. Effectively, PSO-SCFT facilitates the search through a space of reciprocal-space SCFT seeds which yield a variety of morphologies. Using intensive free energy as a fitness metric by which to compare these morphologies, the PSO-SCFT methodology allows us to agnostically identify low-lying competitive and stable morphologies. In this talk, we present results for applying PSO-SCFT to conformationally symmetric diblock copolymers and miktoarm star polymers, and discuss the successes and challenges of the method.

*This project is supported by Toyota Research Institute.

*This work was supported by Future Energy Systems of the University of Alberta (https://futureenergysystems.ca; Grant Nos. T12-P04 and T12-P01), the Natural Sciences and Engineering Research Council (NSERC, Grant Nos. RGPIN-2014-05195 and RGPIN-2018-04294), Alberta Innovates Technology Futures (Grant No. ATIF iCORE IC50-T1 G2013000198), and the Canada Research Chairs program (CRC 207142).

1:03PM B55.00008: Using Particle Swarm Optimization and SCFT to agnostically identify the stable and low-lying metastable competitive morphologies of block copolymers

CAROL TSAI (Presenter), KRIS T DELANEY, GLENN FREDRICKSON, University of California, Santa Barbara — The unguided search for the stable phase of a block copolymer of a given composition and architecture is a problem of global optimization with important ramifications from a materials discovery perspective. We discuss the development of a reciprocal-space Particle Swarm Optimization (PSO)-SCFT method in which Fourier components of SCFT fields near the principal shell are manipulated. Effectively, PSO-SCFT facilitates the search through a space of reciprocal-space SCFT seeds which yield a variety of morphologies. Using intensive free energy as a fitness metric by which to compare these morphologies, the PSO-SCFT methodology allows us to agnostically identify low-lying competitive and stable morphologies. In this talk, we present results for applying PSO-SCFT to conformationally symmetric diblock copolymers and miktoarm star polymers, and discuss the successes and challenges of the method.

*NSF-GRFP
NSF-DMR 1506008
Prediction of suitable solvents and non-solvents for polymers using machine learning techniques

SHRUTI VENKATRAM (Presenter), CHIHO KIM, ANAND CHANDRASEKARAN, RAMAMURTHY RAMPRASAD, Georgia Institute of Technology — Solvent selection is essential for formulations in industrial and research processes like paints, cosmetics and pharmaceuticals. Identifying appropriate solvents for a polymer formulation is usually done by trial-and-error, and therefore, is time-consuming. To mitigate this problem, quantitative measures of solvent-polymer miscibility known as solubility parameters have been developed in the past. In the present study, we first assessed the performance of the Hildebrand solubility parameter to predict solvents for a set of benchmark polymers. Machine learning techniques, trained on a dataset of known polymer Hildebrand solubility parameters, were then used to predict the solubility parameter of a queried polymer. Matching the predicted value with known solvent solubility parameters was then utilized to identify suitable solvents and non-solvents for the queried polymer. This capability has been implemented at www.polymergenome.org.

Applying Machine Learning to Structural Analysis using Pythia

MATTHEW SPELLINGS (Presenter), JULIA DSHEMUCHADSE, SHARON GLOTZER, University of Michigan — The recent explosion of interest and progress in machine learning (ML) methods has driven a proliferation of their application to soft matter systems. ML promises to deliver novel, automatic characterization techniques to solve previously insurmountable problems and it has already been successfully applied in several key areas for both disordered and ordered materials. However, researchers attempting to utilize ML methods often encounter challenges in finding the most appropriate representation of their data. To help alleviate this problem and foster reproducibility in these applications, we present Pythia, an open-source Python library for generating numerical descriptions of particle configurations. Pythia provides a palette of descriptors for users to select from, ranging from the simple to sophisticated. We demonstrate how Pythia can be combined with standard ML methods to quickly identify structures, analyze crystal grains, and study nucleation and growth of complex colloidal crystalline phases—all in a high-throughput manner.

End-to-End Characterization of Colloidal Particles through Holographic Microscopy and Deep Convolutional Neural Networks

LAUREN ALTMAN (Presenter), DAVID GRIER, MARK D HANNEL II, Center for Soft Matter Research, New York University — Analyzing holograms of colloidal particles with Lorenz-Mie theory yields the particles’ sizes, refractive indexes and three-dimensional positions, all with exquisite precision and accuracy. No other technique provides such a wealth of particle-resolved and time-resolved characterization data. The underlying fits to Lorenz-Mie theory, however, require estimates for the particles’ positions and properties that are good enough to ensure convergence to the optimal solution. Here, we demonstrate that this estimation problem can be solved with a single, specially structured deep convolutional neural network. The machine-learning approach to holographic particle characterization is orders of magnitude faster than conventional image-analysis techniques, substantially more robust against image defects, and yields answers that already are sufficiently precise for many applications. We demonstrate the method’s efficacy through experimental measurements of the properties and dynamics of model colloidal systems.

An Anisotropic Langevin Equation for Protein Dynamics

ERIC BEYERLE (Presenter), MARINA GIUSEPPINA GUENZA, University of Oregon — The analysis and description of protein motions is greatly facilitated by reducing the effective dimensionality of the system through coarse-graining and transforming to decoupled normal-mode coordinates. We have developed a coarse-grained, diffusive, Langevin equation to model protein dynamics, the Langevin Equation for Protein Dynamics (LE4PD), which accounts for hydrodynamic effects and mode-dependent free-energy barriers. Here, we extend the LE4PD to describe anisotropic, directional fluctuations of a protein’s residues, projected along the alpha-carbons. We compare the dynamics predicted by the LE4PD to a conventional method to model protein dynamics, principal component analysis (PCA), which does not account for free-energy barriers or possess an associated equation of motion. Testing the formalism on a molecular dynamics simulation of ubiquitin, coarse-grained at the alpha-carbon level, when both free-energy barriers and hydrodynamic effects are neglected, the normal modes predicted by both methods are identical. However, we find that including the barriers and hydrodynamic effects in the mode-dependent description can alter significantly the predicted kinetic and dynamic properties of the protein.

*This work is supported by the Office of Naval Research through grants N00014-17-1-2656 and N00014-16-1-2580.

*NSF Grant No. CHE-1665466, NSF Grant No. ACI-1548562.
2:03PM B55.00013: Machine-learning solver for modified diffusion equations* QIANSHI WEI (Presenter), University of Waterloo, YING JIANG, Chemistry, Beihang University, JEFF Z. Y. CHEN, University of Waterloo — A feedforward neural network has a remarkable property which allows the network itself to be a universal approximator for any function. Here we present a universal machine-learning based solver for multivariable partial differential equations. The algorithm approximates the target functions by neural networks and adjusts the network parameters to approach the desirable solutions. The idea can be easily adopted for dealing with multivariable coupled integrodifferential equations, such as those in the self-consistent field theory for predicting polymer microphase-separated structures.

*Natural Science and Engineering Council of Canada (NSERC), Beihang University, and the National Science Foundation of China (NSFC, Grants No. 21574006 and No.21622401).

Monday, March 4, 2019 11:15 AM - 1:51 PM

Session B56 GSNP DBIO: Network Theory II BCEC 255 - Albert-Laszlo Barabasi

11:15AM B56.00001: Distribution efficiency and structure of complex networks. GEORGIOS GOUNARIS (Presenter), MIGUEL RUIZ GARCIA, ELENI KATIFORI, University of Pennsylvania — Optimized transport networks play a key role in the function of various artificial and natural systems, such as plant or animal vasculature. Part of the function of these flow networks is to efficiently distribute nutrients to the organism. In the case of the animal circulatory system, the oxygen distributed to the tissues is carried by the red blood cells flowing through the capillaries in the blood plasma. The architecture of the network, as defined by its structure and topology controls both the energy dissipated in transferring the viscous fluid (e.g. the blood through the capillaries) and the efficiency of the nutrient transport (e.g. how the oxygen is distributed in the tissue). In this work, we investigate the optimal structure of networks when both energy optimization and transport efficiency are considered. We discuss how the network structure is affected by the trade-offs of different optimization functionals that compete to impose hierarchy and uniformity to the same network.

11:27AM B56.00002: Optimal noise-canceling networks* HENRIK RONELLENFITSCH (Presenter), JORN DUNKEL, Massachusetts Institute of Technology, MICHAEL WILCZEK, Theory of turbulent flows, Max Planck Institute for Dynamics and Self-Organization — From the cerebral cortex to large-scale power grids, natural and engineered networks face the challenge of converting noisy inputs into robust signals. The input fluctuations often exhibit complex yet statistically reproducible correlations that reflect underlying internal or environmental processes such as synaptic noise or atmospheric turbulence. This raises the practically and biophysically relevant question of whether and how noise-filtering can be hard-wired directly into a network's architecture. By considering generic phase oscillator arrays under cost constraints, we explore the design, efficiency and topology of noise-canceling networks. We find that when the input fluctuations become more correlated in space or time, optimal network architectures become sparser and more hierarchically organized, resembling the vasculature in plants or animals. Our results provide concrete guiding principles for designing more robust and efficient power grids and sensor networks.

*This work was supported by an Edmund F. Kelly Research Award (J.D.) and a James S. McDonnell Foundation Complex Systems Scholar Award (J.D.).

11:39AM B56.00003: The fundamental advantages of temporal networks AMING LI, Department of Zoology and Oxford Centre for Integrative Systems Biology, University of Oxford, SEAN CORNELIUS (Presenter), Center for Complex Network Research, Northeastern University, YANG-YU LIU, Channing Division of Network Medicine, Harvard Medical School, LONG WANG, Center for Systems and Control, Peking University, ALBERT BARABASI, Center for Complex Network Research, Northeastern University — Most networked systems of scientific interest are characterized by temporal links, meaning the network's structure changes over time. It has been shown that link temporality, by disrupting network paths, can slow down or otherwise hinder many dynamical processes, from information spreading to accessibility. Considering the ubiquity of temporal networks in nature, we ask: Are there any advantages of the networks' temporality? Here we develop an analytical framework to study the critical process of control in temporal networks. We show that temporal networks can, compared to their static counterparts, reach controllability faster, demand orders of magnitude less control energy, and allow control trajectories that are considerably more compact than those characterizing static networks. Thus, temporality ensures a degree of flexibility that would be unattainable in static networks, enhancing our ability to control them.
11:51AM B56.00004: Persistence in Random and Disordered Networks.* OMAR MALIK (Presenter), ALAA M MOUSSAWI, DAVID HUNT, Rensselaer Polytechnic Institute, MELINDA VARGA, ZOLTAN TOROCZKAI, University of Notre Dame, BOLESŁAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — To better understand the lifetime and temporal dynamics of activities and trends in social networks, we initiated investigations of diffusive persistence in various graphs. Persistence is defined as the probability that the diffusive field at a given node has not changed sign up to a certain time (or in general, that node remained inactive/active). We investigated disordered networks (characterized by the fraction of removed edges) and found that the behavior of the persistence probability depended on the topology of the network. In 2D networks we have found that above the percolation threshold diffusive persistence scale scales similarly to that of the original two-dimensional regular lattice, i.e., a power law with an exponent of 0.18. At the percolation threshold, the scaling changes to one with 0.12. This new exponent is the result of the interplay of diffusive persistence and the underlying structural transition in the disordered lattice at the percolation threshold. In contrast, we found that in random networks without a regular structure, such as Erdős-Rényi networks, no simple power-law scaling behavior exists above the percolation threshold.

*Supported in part by DARPA, ARL NS-CTA, and ONR.

12:03PM B56.00005: Global suppression effect on the infinite-order percolation transitions in growing networks BYUNGNAM KAHNG (Presenter), S. M. OH, Department of Physics and Astronomy, Seoul National University, S.-W. SON, Department of Applied Physics, Hanyang University — The percolation transition in growing networks can be of infinite order, following the Berezinskii-Kosteritz-Thouless (BKT) transition. Examples can be found in diverse systems ranging from socio- to bio-networks such as the coauthorship networks and the protein interaction networks. Here we are interested in how such an infinite-order percolation transition is changed by global suppression (GS) effect. In fact, about a half century ago, Thouless showed that $1/r^2$-type long-range interactions in the one-dimensional Ising model change the phase transition type from second order to first order. One may think that the GS dynamics plays a similar role of changing percolation transitions in complex systems. We show that the BKT transition breaks down, but the features of infinite-order, second-order, and first-order transitions all emerge in a single framework. The critical region below the BKT transition point is extended and the power-law behavior of the cluster size distribution reaches the state with the exponent two, suggesting that the system has the maximum diversity of cluster sizes. We also elucidate the underlying mechanisms and show that those features are universal. Forming such extreme diversity by the GS dynamics may be helpful for establishing stabilized complex systems.

12:15PM B56.00006: Walks in rough energy landscapes: a network model RICCARDO GIUSEPPE MARGIOTTA (Presenter), REIMER KUEHN, PETER SOLLICH, King's College London — A simple way to describe the slow relaxation and ageing of a glass is to consider the system as a point in configuration-space hopping between local energy minima. The associated Markov process is specified by the distribution of these minima and the transition rates between them. Previous studies have explored the analytically tractable mean-field case [Bouchaud et al, 96] where the network of allowed transitions is fully connected. We consider a more elaborate version of the model by introducing the concept of distance among minima: the evolution takes place on sparse networks. This brings the problem into the realm of sparse random matrices. We therefore base our analysis on the spectral properties of the infinitesimal generator of the process - the master operator. We use the cavity method to evaluate the average eigenvalue spectrum and degree of localisation of eigenstates in the thermodynamic limit. These quantities are key in determining the dynamics of the system and can be used to compute time-dependent observables such as the return probability. Our findings show that eigenstates have attributes arising from a non-trivial combination of the corresponding mean field and infinite temperature limits of the model, indicating the existence of three different regimes in time.
12:27PM B56.00007: Disintegration of Different Types of Networks by Overload under Massive Attack† GABRIEL CWILICH (Presenter), Yeshiva University, YOSEF KORNBLUTH, Mechanical Engineering, Massachusetts Institute of Technology, SERGEY BULDYREV, Yeshiva University — We discuss a network which has a fraction of its nodes fail initially, and the redistribution of the betweenness centrality of the remaining nodes leads to subsequent failures, as in the Motter and Lai model; the subsequent change of the betweenness can lead to a cascade of failures that might disintegrate the network. There is a threshold in the size of the initial attack that leads to disintegration. The transition switches from first order to second when the tolerance of the nodes increases for networks with a narrow distribution of the degrees of their nodes (Erdős-Rényi, random regular, small-world). In the case of broader distributions, like a power law with exponent smaller than 3, the destruction of the initial nodes tends to stabilize the network, the value of the threshold goes to zero and the transition remains second order for all tolerances. We present an analytic calculation of the behavior of the betweenness of the different nodes during the disintegration and extensive numerical simulations. We consider the influence of the localized nature of the initial attacks on the disintegration. We show that these type of networks are, surprisingly, much more resilient vis-à-vis localized attacks.

†This research was supported by HDTRA1-14-1-0017.

12:39PM B56.00008: Transfractal Stochastic Nets CHRISTOPHER DIGGANS (Presenter), Information Systems Division, Air Force Research Laboratory, DANIEL BEN-AVRAHAM, Physics, Clarkson University, ERIK BOLLT, Mathematics, Clarkson University — A stochastic extension of the (u,v)-flower graph recursion is given for the case where u=1, which produces small-world, transfinite dimensional hierarchical graphs. Inspired by the two equivalent (for the non-stochastic case) means of propagation, two approaches are provided. Both rely on using a list of possible v values and a probability distribution, e.g. v=[v_1, v_2] and p=[p,1-p], and both converge to the same statistics for large graph order. The first, less restrictive case entails choosing a random v value for each edge at each generation; the second, producing a more symmetric result, involves choosing a random value for v at each generation to be consistent across that step. The main contribution of these constructions is the ability to tune desirable network parameters such as assortativity and the exponent of the power law degree distribution. An additional area of interest for the second method is exact eigenvalue propagation, which has been determined for the case of v∈[2,3]. As part of this work, a general result was found for propagating the eigenvalues of recursive quadrangularizations of any simple graph.

12:51PM B56.00009: From the betweenness centrality in street networks to structural invariants in random planar graphs* ALEC KIRKLEY, Physics, University of Michigan, HUGO BARBOSA, Physics & Astronomy, University of Rochester, MARC BARTHELEMY, Institut de Physique Theorique, CEA Saclay, GOURAB GHOSHAL (Presenter), Physics & Astronomy, University of Rochester — The betweenness centrality, a path-based global measure of flow, is a static predictor of congestion and load on networks. Here we demonstrate that its statistical distribution is invariant for planar networks, that are used to model many infrastructural and biological systems. Empirical analysis of street networks from 97 cities worldwide, along with simulations of random planar graph models, indicates the observed invariance to be a consequence of a bimodal regime consisting of an underlying tree structure for high betweenness nodes, and a low betweenness regime corresponding to loops providing local path alternatives. Furthermore, the high betweenness nodes display a non-trivial spatial clustering with increasing spatial correlation as a function of the edge-density. Our results suggest that the spatial distribution of betweenness is a more accurate discriminator than its statistics for comparing static congestion patterns and its evolution across cities as demonstrated by analyzing 200 years of street data for Paris.

*This work was partially supported by the US Army Research Office under Agreement Number W911NF-17-1-0127. M.B. thanks the city of Paris (Paris 2030) for funding and the geohistoricaldata group for discussions and data.

1:03PM B56.00010: Topology of tangledness of network embeddings YANCHEN LIU (Presenter), NIMA DEHMAMY, ALBERT-LASZLO BARABASI, Northeastern University — The force directed layout (FDL; mass and spring model) is a class of layouts in which the position of the nodes are highly correlated with the network structure. In three dimensional space, one can embed any network without link crossings. However, as in glassy systems, the number of low energy configurations in FDL is extremely large, and distinguishing between them is very difficult. Here we introduce a topological measure, which we call the graph linking number, that allows us to classify some of these energy states. We study the relation between graph linking number and the energy of the FDL. We find that the graph linking number for FDL is much lower than random layouts. Also, the distribution of graph linking number in FDL for networks with different topologies can be very different. For some network topologies, e.g. lattices, there is a strong correlation between the graph linking number and energy, while for other network topologies, e.g. Erdős-Renyi and Barabasi-Albert networks we observe less correlation between graph linking number and energy. This shows that the graph linking number is capturing a new interesting aspect of the topology of embeddings not captured by the energy and is therefore useful for classification of graph embeddings.
1:15PM B56.00011: The hidden role of coupled wave network topology on the dynamics of nonlinear lattices

SOPHIA SKLAN (Presenter), Physics and Applied Physics, Nanyang Technological University, BAOWEN LI, Mechanical Engineering, University of Colorado, Boulder — In most systems, its division into interacting constituent elements gives rise to a natural network structure. Analyzing the dynamics of these elements and the topology of these natural graphs gave rise to the fields of (nonlinear) dynamics and network science, respectively. However, just as an object in a potential well can be described as both a particle (real space representation) and a wave (reciprocal or Fourier space representation), the "natural" network structure of these interacting constituent elements is not unique. In particular, in this work we develop a formalism for Fourier Transforming these networks to create a new class of interacting constituent elements - the coupled wave network - and discuss the nontrivial experimental realizations of these structures. This perspective unifies many previously distinct structures, most prominently the set of local nonlinear lattice models, and reveals new forms of order in nonlinear media. Notably, by analyzing the topological characteristics of nonlinear scattering processes, we can control the system's dynamics and isolate the different dynamical regimes that arise from this reciprocal network structure, including the bounding scattering topologies.

1:27PM B56.00012: Structure and Dynamics of Cultured Neuronal Networks*

EMILY S.C. CHING (Presenter), The Chinese University of Hong Kong — We have developed a method that can reconstruct the connectivity structure of a weighted directed network using only time-series measurements of the dynamics of the nodes. Our method is guided by noise-induced mathematical relations. We apply this method to reconstruct cultured neuronal networks using the electrical signals recorded in cultures of cortices of rat embryos by multi-electrode arrays. The reconstructed neuronal networks have 4095 nodes; their connection probability and proportion of the giant strongly connected component are comparable to those of the chemical synapse network of C. Elegans, and both are small-world networks. Our method can further reconstruct the average incoming and outgoing coupling strength of each node and whether the nodes are excitatory or inhibitory. We obtain various interesting results about the distributions of the in-degree and out-degree, and the average incoming and outgoing coupling strength of the nodes. Moreover, we find that the spike rate of the nodes is related to their network properties. Using this relation, we can predict whether a node has high or low spike rate with high accuracy.

*We acknowledge the Hong Kong Research Grants Council (Grant No. CUHK 14304017) for support.

1:39PM B56.00013: Directed aging and memory: Teaching an old foam new tricks

NIDHI PASHINE (Presenter), DANIEL HEXNER, University of Chicago, ANDREA LIU, University of Pennsylvania, SIDNEY ROBERT NAGEL, University of Chicago — As a material ages, its physical properties change. Under an applied stress, it plastically deforms in order to relieve the internal stress in incremental steps. At each instant, it lowers the stress in the most effective way. Thus, over long times, the final state of the material depends on the external stresses it was exposed to during the aging process. A material thus has a memory of the stresses to which it was exposed during the aging process. We exploit this property and direct the aging process with specific protocols in such a way that our material reaches a distinct, final state with a prescribed and desired functionality. In order to demonstrate this behavior, we use sheets of foam that we cut with a laser cutter and place under stress in such a way that the material develops unusual elastic properties. To accelerate the aging process, we apply heat to the sample. We have been able to modify the Poisson's ratio of our system considerably; we can make a sample that was initially nearly incompressible and make it auxetic (negative Poisson's ratio). We can likewise take an auxetic sample and make it incompressible. We have also been able to train local behavior so that a sample responds with a prescribed local deformation in response to a global perturbation.

Monday, March 4, 2019 11:15 AM - 2:03 PM

Session B57 GSNP GSOFT: Physics of Liquids II BCEC 256 - Yang Zhang, University of Illinois at Urbana-Champaign -
Tag(s): Focus
11:15AM B57.00001: Colloidal physics with DNA particles [Invited] FRANCESCO SCIORTINO (Presenter), Sapienza University of Rome — DNA oligomers can nowadays be assembled to produce a large variety of nanometric constructs, via a cascade of self-assembly processes, each one guided by the length of complementary sequences of distinct DNA strands. In the talk I will show that it is possible to build bulk quantities of DNA-made nanoparticles that closely match idealized colloids, transferring modern in-paper and in-silico intuitions into experimental realizations[1-4]. I will show how unconventional collective behaviors, recently explored theoretically, can indeed be reproduced in the lab. Among others I will discuss how the selectivity of the DNA interactions can be exploited to create gels that form both on cooling and on heating [5-6], how to create networks with swappable bonds[7], how to create systems residing on the verge of a percolation transition.


11:51AM B57.00002: Contrasting Dielectric Properties of Electrolyte Solutions with Polar and Polarizable Solvents DOUGLAS GRZETIC (Presenter), KRIS T DELANEY, GLENN FREDRICKSON, University of California, Santa Barbara — We examine the dielectric constant of electrolyte solutions with a polar and/or polarizable small-molecule solvent using a classical field-theoretic approach. We compute corrections to the dielectric constant and screening length due to intra- and inter-molecular correlations via a self-consistent one-loop approximation, accounting for the excluded volume of both solvent and electrolyte. The theory predicts either a non-linear dielectric decrement or increment with increasing salt, depending on whether the fluid correlations are dominated by the dipolar or polarizable nature of the solvent. These contrasting regimes of non-linear dielectric behavior are consistent with those seen experimentally in high- and low-dielectric-constant electrolyte solutions.

12:03PM B57.00003: Ion Solvation at Thermodynamic Extremes from First Principles* VIKTOR ROZSA (Presenter), Institute for Molecular Engineering, Univ. of Chicago, GIULIA GALLI, Institute for Molecular Engineering, Univ. of Chicago; Department of Chemistry, Univ. of Chicago; Materials Science Division, Argonne National Laboratory — The properties of aqueous salt solutions at high pressure and temperature are crucial to understanding geochemically relevant fluids. We report on the properties of aqueous monovalent ions at high pressure and temperature (1 GPa/1000 K, 11 GPa/1000 K), as obtained from first-principles molecular dynamics simulations [1]. In particular, we discuss the effect of ions on the structure and diffusion of water and the effect of water dissociation occurring under pressure, on ion solvation. We further analyze vibrational signatures of solvated ions, by comparing computed infrared and Raman spectra of salty and pure water [2] at the same conditions. Finally we present results for ionic conductivity and dielectric constants.

[1] We acknowledge support from the DOE NNSA Stewardship Science Graduate Fellowship under grant number DE-NA0003864 and MICCoM as part of the Computational Materials Sciences Program funded by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

12:15PM B57.00004: A Universal Equation of State for Hard Polyhedra THI VO (Presenter), SHARON GLOTZER, Chemical Engineering, University of Michigan - Ann Arbor — The empirical formulation of the ideal gas law marked a major turning point in the development of theoretical models aimed at describing fluid behaviors. Its extension to real systems, however, often result in deviations upon comparison with experimental observations due to the presence of both excluded volume and attractive interactions in non-ideal particles. Consideration of particle shape further complicates the development of a universal theoretical framework, although there have been several attempts with varying degrees of accuracy for convex shapes. Here, we introduce a new equation of state for hard polyhedra. The derived expression not only shows excellent agreement with simulations, but also suggests a “corresponding state”-like behavior, allowing for a reduction across shape space onto a single master curve as well as prediction of the order-disorder transition density for polyhedra.
**12:27PM B57.00005: Dynamical Criticality in Higher-Dimensional Equilibrium Glasses Obtained by Swap Monte Carlo**

PATRICK CHARBONNEAU (Presenter), Duke University, LUDOVIC BERTHIER, Université de Montpellier, SILVIO FRANZ, Université Paris-Sud, JOYJIT KUNDU, Duke University — Recent implementation of the swap Monte Carlo algorithm to suitably optimized continuously polydisperse mixtures has been remarkably successful in bypassing the sluggishness associated with glass formation in dimensions, \( d=2 \) to \( 8 \). This advance has renewed the interest in exploring the finite-dimensional echo of the dynamical transition, which leads to a power-law diverging relaxation time in mean-field treatments and in the mode-coupling theory of glasses. Despite competing activated processes, such as hopping and glass nucleation, traces of the dynamics criticality can be observed, especially on the glass-side of the transition. The mean-field-like features of caging and of the dynamical susceptibility are here specifically examined.

*This research was supported by a grant from the Simons Foundation

**12:39PM B57.00006: All-atom Metadynamics Simulations of the Hierarchical Folding Dynamics of Proteins on the Timescale of Seconds**

NATHAN WALTER (Presenter), YANG ZHANG, University of Illinois at Urbana-Champaign — Molecular dynamics simulations have proven instrumental to the understanding of molecular biophysics. However, the temporal constraints of molecular dynamics simulations have limited attempts to capture the protein folding process at the atomic scale. Herein, we circumvent this limitation by using all-atom metadynamics algorithm to directly sample the potential-energy landscape of numerous proteins. Previous applications of the original metadynamics method to proteins penalized select collective variables of the protein assumed to be principle to the folding process. Rather, our method penalizes the full coordinate space of the protein resulting in a 3N-dimensional sampled energy-landscape, unbiased by \textit{a priori} assumptions. With all-atom sampling, over collective variable sampling, a single simulation captures the folding and unfolding process multiple times, enabling the simulation of protein dynamics on scales of seconds, orders of magnitude longer than recorded molecular dynamics simulations. Further, we predict the folded state of the protein, and the activation barrier and the timescale associated with the folding process of the proteins. We will present these findings for several well-studied proteins, to validate our results, and several new proteins, as a novel extension.


ZHIXIA LI (Presenter), LILY ROBERTSON, University of Illinois at Urbana-Champaign, ILYA A SHKROB, Chemical Sciences and Engineering Division, Argonne National Laboratory, JOERG NEUEFEIND, Chemical and Engineering Materials Division, Oak Ridge National Laboratory, KYLE SMITH, University of Illinois at Urbana-Champaign, LU ZHANG, Chemical Sciences and Engineering Division, Argonne National Laboratory, JEFFREY S MOORE, YANG ZHANG, University of Illinois at Urbana-Champaign — Molecular dynamics are promising methods to compute numerous properties of nonaqueous electrolytes, but quantitative predictions depend critically on the prescribed force fields. Here, we show that several quantum-mechanically refined force fields for the lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) - acetonitrile electrolyte yield structures that are in good agreement with the experimental neutron pair distribution function (PDF), while dynamics is dramatically different and inconsistent with NMR measurements. Such glaring discrepancies indicate that inadequate representation of long-range interactions leads to excessive frustration in the free energy landscape. Better agreement is achieved by proportionally scaling down the atomic charges of the ions. This simplification enabled the simulation of concentration dependences of ionic diffusion for 0.2-2 M LiTFSI solutions without sacrificing fit quality of the PDFs. We argue that not only structures but also dynamics constitute important checkpoints on the road to computationally design functional electrolytes.

*The research was financially supported by the Joint Center for Energy Storage Research (JCESR), an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.
1:03PM B57.00008: Stabilization of Trp-cage within Confinement by Optimizing the Interface Hydrophobicity*  
YANQIN ZHAI (Presenter), ZHIKUN CAI, YANG ZHANG, Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign — Understanding the interaction between proteins and confining interfaces is a critical step towards revealing the folding behaviors of protein in cellular context. In particular, the hydrophobicity of the confinement is an important factor that may affect the hydrophobic collapsing of the proteins. Hence, to study the hydrophobic effects of the confinement on the protein behaviors, we performed molecular dynamics simulations of Trp-cage miniprotein sandwiched between two graphene sheets with varying hydrophobicity by tuning the interaction potential. The structural variations of the protein was characterized by the average root-mean-square-displacement, the radius of gyration of the backbone, and the mean contact area between individual residues and the confining interfaces. The results revealed that the confinement tends to stabilize the native state of Trp-cage by reducing its configurational entropy. Specifically, two stabilization mechanisms were identified. The protein may be stabilized by moderately hydrophobic confinement through gentle adsorption and yet without destroying the hydrophobic core of the Trp-cage, or, by highly hydrophilic confinement via volume exclusion caused by dense water layers.

*Award number DE-SC-0014804 supported by DOE is acknowledged.

1:15PM B57.00009: Two-step crystallization pathways of hard particle systems via a metastable fluid-fluid phase transition  
SANGMIN LEE (Presenter), Chemical Engineering, University of Michigan, ERIN TEICH, Applied Physics Program, University of Michigan, MICHAEL ENGEL, Institute for Multiscale Simulation, University Erlangen-Nürnberg, SHARON GLOTZER, Chemical Engineering, University of Michigan — Multi-step crystallization pathways are often found in biomineralization, protein crystallization and tetrahedrally coordinated systems, where a single or multiple intermediate state appear during the crystallization process. Despite the importance of those materials, universal characteristics shared by the multi-step crystallization process are not well understood. Here, we report three hard particle systems (truncated tetrahedra, pentagonal bipyramids and triangular bipyramids) exhibiting two-step crystallization via a metastable fluid-fluid phase transition. Monte Carlo simulations reveal that these systems first form a high-density fluid with prenucleation motifs in the form of clusters, fibers, and networks from a low-density fluid. Subsequently, complex crystal structures (cF432, oF244 and cP92) nucleate from the high-density fluid. Our observations demonstrate the existence of diverse crystallization pathways in entropic systems and reveal various dimensionalities of prenucleation motifs.

1:27PM B57.00010: Weak Secondary Relaxation in Molecular Glass Formers*  
SUDIPTA GUPTA (Presenter), Department of Chemistry, Louisiana State University — The physics of glass formers and the glassy dynamics is one of the great mysteries in science. For example, the structural α relaxation, which characterizes the freezing of molecular motions on approaching the glass transition, is well known. However, in recent years in addition to the α relaxation additional secondary dynamic processes were found. Like the so-called excess wing relaxation so far mostly been investigated by dielectric spectroscopy, a method that mainly couples to only one aspect of molecular mobility, namely reorientational motions of molecules carrying a dipolar moment. We present neutron-scattering results, sensitive to density-density fluctuations, on glycerols, in presence of salts and nanoparticles, to identify the nature of this secondary relaxation. New aspects in neutron scattering have been revealed: (i) The first is the unprecedented detection of the excess wing using neutron-scattering experiments, (ii) the systematic comparison between neutron scattering and dielectric measurements, (iii) the characteristic length scale of the secondary relaxation, and (iv) The importance of dynamic heterogeneities in these relaxations.


*U.S. DOE
German DFG
1:39PM B57.00011: Cluster connectivity and medium-range order in metallic glass*  
XIAOYA WEI, SI LAN, XUN-LI WANG (Presenter), City University of Hong Kong — Bulk metallic glasses were discovered more than 30 years ago. It has been established that, for multicomponent metallic glass alloys, the short-range order or the fundamental building block is characterized by solute-centered clusters. Over longer length scales, the clusters are packed on a fractal network forming the medium-range order. Still, there remain many questions on the structure of metallic glasses, particularly with regard to the development of short- and medium-range orders during structure evolution induced by temperature or mechanical deformation. The experimental results seem to show that during crystallization, mechanical deformation, and liquid-to-liquid phase transformation, the short-range order is enhanced but there are no substantial changes in the structure order. Rather, it is the connectivity between clusters at medium-range scale, that drives the dynamic response. In this paper, we explore the meaning of cluster connectivity and apply the concept to explain our experimental observations.

*This work is supported by the Research Grants Council of Hong Kong Special Administrative Region (CityU Project No. 11216215).

1:51PM B57.00012: Revisiting the Fragile-to-Strong Crossover in Metallic Glass-Forming Liquids: The Case of the \( \text{Cu}_x\text{Zr}_y\text{Al}_{100-2x} \) Alloy*  
RENÉ ALBERTO ALVAREZ-DONADO, SAMUEL CAJAHUARINGA, ALEX ANTONELLI (Presenter), Universidade Estadual de Campinas — A reliable description of the dynamic properties of metallic glass-forming liquids is highly important for the understanding of the glass forming ability of these materials. To this end, we investigate the behavior of the diffusion coefficient, vibrational spectra, and shear viscosity of the \( \text{Cu}_x\text{Zr}_y\text{Al}_{100-2x} \) alloy (for \( x = 50, 49, 46 \)) through molecular dynamics simulations. The glass transition temperatures (T_g) we obtained for different compositions are in good agreement with both experimental and computational findings, indicating an increase of T_g with the amount of aluminum in the alloy. The inverse of the diffusion coefficient as a function of temperature shows a fragile-to-strong crossover at temperatures (T_fs) in the vicinity of T_g (730 K ≤ T_fs ≤ 797 K), which are significantly lower than previous estimates. These results are corroborated by the development of an excess of vibrational modes at temperatures just below T_fs. Shear viscosity as a function of T_g/T also displays the expected Arrhenius behavior below T_fs. Moreover, our results indicate another dynamic crossover related to the onset of dynamical heterogeneities at a temperature about 1200 K, which much higher than T_fs.

*The authors acknowledge the Brazilian funding agencies FAPESP, CNPq, and CAPES
11:27AM B58.00002: Self-assembly of Nematic Liquid Crystals in Drying Drops of Lysozyme Protein Solution
ANUSUYA PAL (Presenter), GERMANO IANNACCHIONE, DEPARTMENT OF PHYSICS, Worcester Polytechnic Institute — In the recent years, an active area of research involves liquid crystals (LCs), e.g. 5CB (4-Cyano-4'-pentylbiphenyl) for sensing biological and chemical analytes. Another active area studies drying protein drops resulting in emergent patterns at the final dried state. In this presentation, these two areas are bridged by adding 5CB, with initial protein solution of lysozyme and de-ionized water. The investigation is done using bright-field and cross-polarizing microscopy, analyzed using ImageJ and Fiji and quantified using statistical tests. It is observed that the crack patterns in the final dried state of the protein is influenced by the presence of small amounts of 5CB. Since the protein lysozyme is not birefringent, cross-polarizing microscopy closely monitors the distribution of the LC, while the bright-field microscopy probes the crack patterns that emerge. The time evolution of the drying dynamics of the drops with and without 5CB are monitored. It is concluded that partial phase separation of LC makes some LC remains mixed and some dispersed into the domains formed by protein cracks. This work demonstrates the utility of using a bulk thermotropic LC as a probe material in a protein solution, revealing new information on the protein self-assembly during the drying process.

11:39AM B58.00003: Towards a Bayesian Interpretation of DNA Self-assembly in Hydrogels
IRIA PANTAZI (Presenter), ERIKA EISER, Physics, University of Cambridge — While widely known as the molecule of life, DNA is also an amazing building block at the nanoscale, since it allows the design and programming of the structure and dynamics of functional nanomaterials. A class of such materials are DNA hydrogels, which exploit elastic or viscous behaviour that is finely regulated by temperature. These functional materials are promising candidates for medical applications, and specifically controlled drug delivery, tissue engineering and biosensing.

In my research I am using computational tools to study the self-assembly of branched-shaped DNA building blocks that form a hydrogel. By using molecular dynamics I am simulating the assembling process, and calculate the equilibrium elastic and viscous moduli of DNA hydrogels. Moreover, I am working towards the design of a model that will employ Bayesian inference in order to associate the hydrogel properties with the different configurations of the DNA building blocks. In my talk I will outline the significance of a model that will describe DNA hydrogels, and how it can lead to the design of novel DNA-based materials.

11:51AM B58.00004: Self-Assembly of DNA origami capsids
STEFAN PAQUAY (Presenter), Brandeis University, CHRISTIAN SIGL, HENDRIK DIETZ, Physics, Technische Universität München, SETH FRADEN, MICHAEL F HAGAN, Brandeis University — DNA origami is an fruitful method to create a wide range of simple and complex objects on the nanometer scale. By folding DNA into truncated tetrahedra (“triangles”) with protrusions and recessions on their outer edges, one can add attractive interaction between these triangles.

With the right design these triangles self-assemble into icosahedra similarly to virus coat proteins but on larger length- and timescales, with potential applications in functional materials.

To guide the design of these building blocks we perform molecular dynamics and kinetic Monte Carlo simulations of coarse-grained, rigid triangles with reactive patches. Specifically, we aim to identify regimes at which the triangles optimally self-assemble into icosahedra of 20 and 60 subunits. Finally, we qualitatively compare the predicted self-assembly kinetics and structures to experiments.

*This project is funded by the Brandeis MRSEC, NIH and the William Keck Foundation
12:03PM B58.00005: The self-assembly of icosahedral shells depends on kinetics and thermodynamics*  
BOTOND TYUKODI (Presenter), FARZANEH MOHAJERANI, Brandeis University, GREGORY GRASON, UMass Amherst, MICHAEL F HAGAN, Brandeis University — We study the out-of-equilibrium self-assembly of subunits whose equilibrium ground state corresponds to an icosahedral shell, in the absence of template. We adapt a method introduced by Rostkoff and Geissler [1], which allows computationally efficient simulation of self-assembly via microscopically reversible dynamics. This allows sampling the non-equilibrium distribution of shell morphologies that arises at long, but finite times, over a wide range of shell sizes. We find that the size and morphology distribution is determined by a competition between kinetic and thermodynamic factors, and can vary significantly from the ground state equilibrium distribution as also seen in dynamical simulations [2]. Our results are general and should be applicable to diverse systems, including the self-assembly of viral capsids, bacterial microcompartments, nano tubules, or DNA origami subunits.

*This work was supported by Award Number R01GM108021 from the National Institute Of General Medical Sciences and the Brandeis Center for Bioinspired Soft Materials, an NSF MRSEC, DMR-1420382.

12:15PM B58.00006: Solvent Effects in Nanocrystal Self-Assembly*  
THOMAS WALTMANN (Presenter), ALEX TRAVESSET, Iowa State University — Materials which are composed of long-range, ordered nanocrystals exhibit many potentially revolutionary properties as compared with traditional materials. There is much to be learned about the dynamics associated with the assembly of these materials. We have previously characterized the equilibrium configuration of arrangements of highly symmetric nanocrystal clusters, and we seek now to determine solvent effects during the process of assembly via computer simulation. We have simulated the process of solvent evaporation using HOOMD and HOODLT and have found that the preferred orientation of the nanocrystals is on the boundary of the liquid solvent. As solvent is evaporated, the nanocrystals are forced to move closer together until the solvent is evaporated out completely, leaving behind nanocrystals in ordered structures.

*NSF, DMR-CMMT 1606336 ¦ ¦ CDS\&E: Design Principles for Ordering Nanoparticles into Super-crystals"

12:27PM B58.00007: Folding dynamics of colloidal clusters  
SOLOMON BARKLEY (Presenter), ELLEN D KLEIN, VINOTHAN N MANOHARAN, Harvard University — We follow the evolution of colloidal clusters from a well-defined initial configuration towards various stable structures in order to understand how a system traverses a free-energy landscape. We use optical tweezers to assemble individual colloidal particles into an initial extended structure held together by a short-range attraction between particles. Particles diffuse across their neighbours' surfaces, lowering the cluster's free energy when particles come into contact. We precisely track the coordinates of all particles in the rearranging cluster throughout this assembly process with a three-dimensional imaging technique, digital holographic microscopy, and we quantify the various pathways from the initial state to the ground states.

12:39PM B58.00008: Band Gap Optimization of Colloidal MgCu2 Photonic Crystals  
JOHNATHON GALES (Presenter), ETIENNE DUCROT, DAVID J PINE, CSMR, New York University — It was recently shown that a colloidal MgCu2 lattice can be self-assembled using a combination of DNA coated spheres and compressed tetrahedral clusters of spheres. The spheres and compressed clusters form two interpenetrating sublattices, diamond and pyrochlore, respectively. Both sublattices have a photonic band gap. We calculate the photonic band structures of the compressed cluster crystals, which differ from those of the standard pyrochlore lattice that has been considered previously. We find that the compression of the clusters can make the band gap significantly wider than for the typical pyrochlore lattices. We can precisely tune the compression of our synthesized tetrahedral clusters, giving us the opportunity to explore the full range of MgCu2 assembly and optimize their photonic properties.
optically active materials. This work paves the way to exploiting LC interfaces as a means to direct spontaneously formed, reconfigurable, and standing smectic-A films, in which the elasticity arising from the director field distortion and capillary interactions arising from interface deformation compete to direct the assembly of particles. New colloidal assemblies and patterns, ranging from 1D chains to 2D aggregates, sensitive to the initial wetting conditions of particles at the smectic film, are reported. Furthermore, colloidal particles at complex fluid interfaces and within films assemble to form ordered structures via interactions that include capillarity, elasticity, and other fields. Here we study microparticle interactions within free-standing smectic-A films, in which the elasticity arising from the director field distortion and capillary interactions arising from interface deformation compete to direct the assembly of particles. New colloidal assemblies and patterns, ranging from 1D chains to 2D aggregates, sensitive to the initial wetting conditions of particles at the smectic film, are reported. This work paves the way to exploiting LC interfaces as a means to direct spontaneously formed, reconfigurable, and optically active materials.

*National Science Foundation (NSF) through Materials Research Science and Engineering Centers Grant DMR-1120901 and NSF Grant DMR-1262047.

1:03PM B58.00010: Polymeric Janus Nanoparticles at Water/Oil Interfaces YUFENG JIANG (Presenter), University of California, Berkeley, RAMZI CHAKROUN, ANDRÉ GRÖSCHEL, Physical Chemistry, University of Duisburg-Essen, THOMAS RUSSELL, Polymer Science and Engineering, University of Massachusetts Amherst — We present a study on the assembly of polymeric Janus nanoparticles (pJNPs) at the toluene/water interface. The soft spherical polymeric Janus nanoparticles pJNPs, made by cross-linking polystyrene-block-polybutadiene-block-poly(methyl methacrylate) (PS-PB-PMMA), show a high interfacial activity, even though neither component is soluble in water. The preferential affinity of the PMMA to the aqueous phase causes a spreading of the PMMA block at the interface. Unlike hard NPs where, after the interfacial tension has decreased and stabilized, only a small volume reduction of the pendant droplet is required to induce wrinkling, for soft pJNPs, there must be a significant reduction in the pendant drop volume to induce wrinkling. A series of pJNPs where the molecular weight at constant weight fraction or where the weight fraction at constant molecular weight of the brushes and cores were varied to probe the influence of molecular weight, brush lengths and volume fractions of the component arms on the areal density of the assemblies and the response of the assemblies to a compression. We also investigated the influence of metal ions in the aqueous phase that can complex with the PMMA on the assembly, packing, stability and responsiveness of pJNP assemblies.

1:15PM B58.00011: Rational Design of Anisotropic Colloids to Self-assemble Open Lattices with Omnidirectional Band Gaps YUTAO MA (Presenter), ANDREW L FERGUSON, The Institute for Molecular Engineering, University of Chicago — Patchy colloids possessing anisotropic interactions are versatile building blocks for the self-assembly of complex functional materials. The main challenge in assembling these materials is the rational and efficient discovery of colloidal architectures and chemistries that make the desired aggregate both thermodynamically stable and kinetically accessible. We have previously devised an inverse design strategy termed "landscape engineering" wherein we combine molecular simulations, nonlinear dimensionality reduction, and genetic algorithms to recover and sculpt the low-dimensional free energy landscape governing assembly by rational modulation of building block design. We apply this data-driven design strategy to perform de novo design of patchy colloids that spontaneously assemble into an open pyrochlore lattice with an omnidirectional photonic bandgap. Our particle design assembles the crystal in a two-stage hierarchy where tetrahedral clusters representing the fundamental motif of the crystal are formed at high temperature with >90% yield, and then a gentle ramp to low temperature induces the aggregation of the tetrahedra into the pyrochlore lattice. Our design approach can be extended to other finite-sized and periodic assemblies including Platonic solids and diamond lattices.

1:27PM B58.00012: Interactions and Energy Scales in Self Assembly and Directed Assembly of Nanocrystal Superlattices ALEX TRAVESSET (Presenter), Iowa State University — Long range ordered structures of nanocrystals or nanoparticles are known as superlattices. We, and others, have shown that the cohesive energy of nanocrystals in superlattices is very large, of the order of hundreds of $k_B T$. In this talk we will show theoretical and computational results on nanocrystals capped with hydrocarbons showing how these systems overcome these scales and successfully self-assemble into ordered structures with long range order. Irrespective of the interactions, these systems show a tendency towards local icosahedral order. Time permitting, issues related to polydispersity will be discussed.

*The work is funded by NSF, DMR-CMMT 1606336 `CDS&E: Design Principles for Ordering Nanoparticles into Super-crystals"
Three-dimensional particle-based simulations of fluctuation-stabilized copolymer mesophases

CODY BEZIK (Presenter), Institute for Molecular Engineering, University of Chicago, ABELARDO RAMIREZ-HERNANDEZ, Department of Chemical Engineering, The University of Texas at San Antonio, JUAN DE PABLO, Institute for Molecular Engineering, University of Chicago — Binary blends of $A-(B-b-(B-b-A'))_n$ miktoarm star block copolymers and A homopolymers have been experimentally shown to self-assemble into an aperiodic “bricks-and-mortar” mesophase, which combines a continuous “mortar” phase of the B-type polymer with a discrete “bricks” phase of the A-type polymer. Such materials have been proposed for use as thermoplastic elastomers, combining high mechanical strength and high elastic recovery. It has been demonstrated theoretically that the mesophase is not predicted to exist in the absence of thermal fluctuations, suggesting it is a unique fluctuation-stabilized morphology. A critical feature of this mesophase is that the A-type domains possess a wide range of sizes, from tens to hundreds of nanometers, representing a challenge to simulation-based approaches. Consequently, prior theoretical work has been limited to simulation in two-dimensions. In this work, we use three-dimensional particle-based simulations, which include fluctuations, to extend understanding of the phase diagram of these blends. Our simulations verify that the bricks-and-mortar mesophase emerges in the presence of three-dimensional thermal fluctuations and more accurately capture experimental systems’ phase behavior.

Characterization of Martensitic Phase Transformations in Blue Phase Liquid Crystals Using Resonant Soft X-ray Scattering*

HYEONGMIN JIN, Northwestern Argonne Institute of Science and Engineering, Northwestern University, XIAO LI (Presenter), JAMES DOLAN, Institute for Molecular Engineering, University of Chicago, R. JOSEPH KLINE, National Institute of Standards and Technology, PAUL F NEALEY, Institute for Molecular Engineering, University of Chicago — In this work, we introduce resonant soft X-ray scattering (RSoXS)[1] to study the martensitic transformation of blue phase (BP) liquid crystals (LCs).[2] The combination of RSoXS and single crystal BP LCs—directed and stabilized by the chemically-nanopatterned surfaces—enable to provide a clear picture of how the BP lattice symmetry and molecular orientations change during this transformation. In particular, twin lamellae formation is observed during martensitic transformation to release the residual strain caused by the rapid martensitic transformation. We anticipate that these experiments will provide one of the most comprehensive studies yet of BP and, therefore, soft matter martensitic phase transformations.


*This work was supported by the U.S. Department of Commerce, National Institute of Standards and Technology under the award 70NHNBI4H012 as part of the Center for Hierarchical Materials Design. This research used the cleanroom resources at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science user facility operated by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

The Effects of Ligand Concentration on the Mechanical Properties of Nanoparticle Films*

SOPHIE MACFARLAND (Presenter), MORGAN REIK, MELANIE S CALABRO, BINHUA LIN, STUART A RICE, University of Chicago — When dodecanethiol-ligated gold nanoparticles are deposited on an air-water interface, they self-assemble into Langmuir films. Experiments in which the films are compressed uniaxially have demonstrated that as the ligand concentration decreases, the ligand-ligand and ligand-core interactions change and the 2-dimensional compressive and shear moduli of the films increases. However, these experiments were largely done upon films while on an air-water interface – this study focuses on films which are dried and removed from the air-water interface. It is important, since many potential applications of these films are in electronic devices, which require the films to operate in a dry environment. This study examines how variations in the concentrations of ligands in a gold nanoparticle solution and by extension the fractional surface coverage, impact a dried film's mechanical properties. Specifically, the Young's Moduli of the films are measured through contact-mode Atomic Force Microscopy (AFM), which demonstrates that low thiol concentrations are conducive to higher young's moduli.

*This work was supported by the NSF through the University of Chicago MRSEC program (DMR-1420709) and by ChemMatCARS funded by the NSF (CHE-1346572)
11:15AM B59.00001: Fragility in shear jamming of dense frictional suspensions* RYOHEI SETO (Presenter), Chemical Engineering, Kyoto University, ABHINENDRA SINGH, James Franck Institute and Institute for Molecular Engineering, University of Chicago, OMER SEDES, MORTON M DENN, Levich Institute, City College of New York, BULBUL CHAKRABORTY, Physics, Brandeis University, JEFFREY MORRIS, Levich Institute, City College of New York — Particulate systems often undergo fluid-solid transition. The packing fraction that corresponds to this particular transition is often found to be protocol dependent. In case of frictional particulate systems, starting from a force-free random configuration at $\phi > \phi_{sj}^{\mu}$ and subjected to shear by constant stress, some rearrangements (i.e., flowing) may occur before getting jammed. Such shear jammed states may flow again by changing the direction of the applied stress; such states are termed "fragile." We quantify this fragility with a stress reversal simulation and identify the point where the fragility vanishes as the isotropic jamming point $\phi_{j}^{\mu}$. We also present a shear-jamming phase diagram of stress-dependent suspension model with a critical-load friction model.

*This study was supported by JSPS KAKENHI Grants No. JP17K05618.

11:27AM B59.00002: Uncovering Instabilities in the Spatiotemporal Dynamics of a Shear-Thickening Cornstarch Suspension* BRICE SAINT-MICHEL, THOMAS GIBAUD, SEBASTIEN MANNEVILLE (Presenter), Physics, Ecole Normale Supérieure de Lyon — We explore unsteady dynamics in a dense cornstarch suspension by coupling long rheological measurements under constant shear stresses to ultrasound imaging. We demonstrate that unsteadiness in DST results from localized bands that travel along the vorticity direction with a specific signature on the global shear rate response. These propagating events coexist with quiescent phases for stresses slightly above DST onset, resulting in intermittent, turbulentlike dynamics. Deeper into DST, events proliferate, leading to simpler, Gaussian dynamics. We interpret our results in terms of unstable vorticity bands as inferred from recent model and numerical simulations.

*This research was supported in part by the National Science Foundation under Grant No. NSF PHY-1748958 through the KITP program on the Physics of Dense Suspensions.

11:39AM B59.00003: Shear jamming, DST and fragile of frictional granular materials under oscillatory shear* MICHIO OTSU, Graduate School of Engineering Science, Osaka University, HISAO HAYAKAWA (Presenter), Yukawa Institute for Theoretical Physics, Kyoto University — The mechanical response of two-dimensional frictional granular materials under an oscillatory shear in a constant volume are numerically investigated. It is confirmed that the shear storage modulus $G'$ depends on the initial amplitude of the oscillation to prepare the system before the measurement. For sufficiently large initial strain amplitude, the shear jammed state satisfying $G' > 0$ is observed even if the packing fraction is below the jamming point. The fragile state is also identified as a long lived metastable state where $G'$ depends on the phase of the oscillatory shear. The dynamic viscosity evaluated from the shear loss modulus $G''$ exhibits a sudden jump similar to the discontinuous shear thickening in the fragile state.[1]

In this talk we also show some preliminary results of hydrodynamic simulation for colloidal suspensions to discuss shear jamming and DST as well as the behavior of dry granular particles under the pressure control protocol.


*This work is partially supported by the Grantin-Aid of MEXT for Scientific Research (Grant No. 16H04025 and No. 17H05420).
11:51AM B59.00004: Using orthogonal shear and acoustic excitation to tune thickening and jamming in suspensions

ITAI COHEN (Presenter), NEIL YC LIN, MEERA RAMASWAMY, RAN NIU, PRATEEK SEHGAL, BRIAN J. KIRBY, Cornell University — Running fast enough over a tub of thickening cornstarch suspension and not sinking is one of the most entertaining science demonstrations garnering millions of viewers every year. As stress is applied to the suspension, the cornstarch particles come close enough to form force chains that are capable of supporting the weight of a person. This thickening, while fun for demonstrations, causes problems for efficient processing of industrial suspensions and garners a high cost. Previously we showed that by applying fast orthogonal perturbations, the viscosity of suspensions under shear can be tuned and decreased by over an order of magnitude. Here, we show that impact driven jamming can be eliminated using a similar technique. Specifically, we conducted a series of impact and extensional flow experiments while cyclically oscillating the bottom plate of our rheometer about the vertical axis. We observe a drastic reduction in the normal forces when the oscillations are turned on. These experiments have the potential to alter suspension processing methods used in numerous industries.

*This work was supported by NSF CBET-PMP Award No. 1232666, NSF CBET-PMP Award No. 1509308 and NSF PHY17-48958.

12:27PM B59.00005: Dynamics of Localized Stresses in Shear-thickening Cornstarch Suspensions

VIKRAM RATHEE (Presenter), DANIEL BLAIR, JEFFREY S URBACH, Georgetown University — Dense colloidal and cornstarch suspensions are common examples of shear thickening suspensions. Spatially resolved surface stresses in a model colloidal suspension using boundary stress microscopy (BSM) revealed dynamic regions of substantially increased local stresses that appear intermittently and move in shear direction. We report BSM of cornstarch suspensions and also find large stress heterogeneities, but with very different dynamics. Above critical stress, the heterogeneous regions propagate along the vorticity direction, perpendicular to shear direction, while at higher applied stresses we do observe propagation in the shear direction similar to the behavior observed in colloidal suspensions.

*NSF Award DMR-1809890

12:39PM B59.00006: Connecting shear jamming and discontinuous shear thickening

IAN MADDEN (Presenter), ERIK LUIJTEN, Northwestern University — Shear stress can induce jamming at packing fractions below the static jamming packing fraction. Here we investigate shear-jamming transitions in a model of two-dimensional shear-jammed discs, observing a transient shear-jamming behavior corresponding to fragile states before the shear-jamming transition. The existence of these states below the onset of shear-jamming was first discovered by Bi et al. (Nature 480, 355–358 (2011)), and further investigation uncovered the related phenomenon of discontinuous shear thickening (Nature 532, 214-217 (2016)). We use molecular dynamics simulations to connect theory to experiment, revealing discontinuous shear thickening and transient shear-jamming to be intimately related. Using this knowledge, we obtain guidance for the design of an experimental system that can reproduce our result.

12:51PM B59.00007: Microscopic signatures of yielding in concentrated nanoemulsions under large-amplitude oscillatory shear

ROBERT LEHENY (Presenter), Johns Hopkins University, MICHAEL C. ROGERS, University of Ottawa, KUI CHEN, Johns Hopkins University, MATTHEW J PAGENKOPP, THOMAS G MASON, UCLA, SURESH NARAYANAN, Argonne National Laboratory, JAMES HARDEN, University of Ottawa — Yielding occurs when a solid is stressed beyond its elastic limit. Signatures of yielding at the nano-to-microscale are irreversible changes to the material's structure. In amorphous solids, the intrinsic disorder makes identifying these microstructural changes difficult. We describe x-ray photon correlation spectroscopy experiments on a series of concentrated oil-in-water nanoemulsions subjected to in situ large-amplitude oscillatory shear in which we characterize the shear-induced droplet dynamics associated with yielding [1]. The dynamics include irreversible rearrangements among the droplets that occur in some regions of the nanoemulsions during a given shear cycle and residual strain-like displacements in those regions that do not re-arrange. We observe a power-law distribution in the size of regions undergoing rearrangement. The values of the onset strains for re-arrangement correlate with the concentration-dependent macroscopic yielding behavior. Specifically, they occur below the strains at which the nanoemulsions become effectively fluidized and, except for the lowest concentration sample in the study, significantly above the threshold strain for nonlinear rheological response.

1:03PM B59.00008: Traction force rheology of colloidal polycrystals and glasses* ZSOLT TERDIK (Presenter), DAVID A WEITZ, FRANS A SPAEPEN, Harvard University — Micron sized colloidal particles in a solution can be assembled and ordered into densely packed polycrystals or disordered glasses. Due to the large size and slow dynamics of colloidal particles, confocal microscopy can be used to directly measure the 3D structure of dynamics of colloidal solids. Measuring the stress response, in addition to visualization, is a challenge because large colloids (which are essential for confocal microscopy) and thermal interaction energies necessarily give rise to solid phases with exceptionally small elastic constants on the order of 10-100 mPa. We introduce a new technique, traction force rheology, to directly measure the mechanical response of colloidal polycrystals and glasses while simultaneously visualizing the microstructure. The method consists of a bilayer of colloidal solid sitting atop a well calibrated soft polymer gel of comparable shear modulus. The composite bilayer is sheared and the shear stresses are inferred from the displacement of embedded tracer particles in the gel. To complement the direct stress measurements, we visualize, in 3D, the time evolution of the complex microstructure including dislocation and grain boundaries in colloidal polycrystals and flow defects in the colloidal glass.

*NSF DMR-1611089

1:15PM B59.00009: Using oscillatory shear to tune the viscosity of shear thickening suspensions* MEERA RAMASWAMY (Presenter), Cornell University, ABHISHEK SHETTY, Anton Paar, ITAI COHEN, Cornell University — When concentrated colloidal suspensions are under stress, their viscosity can increase by over an order of magnitude. These shear thickening suspensions have many interesting technological applications but are also extremely difficult to process in an industrial setting due to the strong dependence of the flow properties on the shear rate. Previous work has shown that the viscosity of these suspensions can be tuned by applying fast orthogonal perturbations to the system. This behavior, however, was only demonstrated for a few values of applied stress and one suspension volume fraction. We are using a custom built attachment to a standard Anton Paar rheometer, to extend these previous measurements to various volume fractions, applied stresses, and system sizes. In this talk, I will describe our results which show that dethickening due to orthogonal shear is volume dependent, and a non-monotonic dependence on the primary applied strain rate. Understanding these trends has consequences for applications involving shear thickening fluids ranging from 3D printing to the processing of cement.

*This research was supported by NSF PHY17-48958, NSF CBET-PMP Award No. 1232666 and NSF CBET-PMP Award No. 1509308.

1:27PM B59.00010: Multiparticle finite element model of highly deformed hydrogel assemblies CRAIG MALONEY, AHMED ELGAILANI (Presenter), Mechanical and Industrial Engineering, Northeastern University — Abstract: Packings of hydrogel particles, like any granular material, become rigid when volumetrically confined. At low confinement near the onset of rigidity, linear elastic contact mechanics should provide a good description of the interparticle forces. At higher confinement, the particles become strongly deformed and linear elastic contact mechanics no longer provides a reasonable description of the interparticle forces. Here, we report on simulations using a multiparticle finite element technique, employing the Flory-Rehner constitutive law, to model the full non-linear elastic deformation of all particles in the packing. We show that the shear modulus (μ) of the packing depends strongly on confining pressure (p) with a crossover from a low-pressure regime where μ ~ p^{1/2} to a high-pressure strongly-faceted regime where μ ~ p^{1/4} where interstitial space has essentially vanished and the facet geometry no longer evolves with pressure.

1:39PM B59.00011: Yielding Versus Jamming: Critical Scaling of Sheared Soft-Core Disks JACOB THOMPSON (Presenter), ABE CLARK, Physics, Naval Postgraduate School — Using discrete element simulations, we study critical behavior for yielding of assemblies of soft-core repulsive disks over a range of dimensionless pressures P. We isotropically compress the disks in a shear-periodic (Lees-Edwards) geometry and then perform quasi-static simple shear. After each shear strain step, we relax the potential energy and dilate or compress the grains to maintain fixed pressure P and then evaluate the shear stress τ. We find that the number density of mechanically stable (MS) states and the strain between MS states obey finite-size scaling consistent with a diverging length scale ξ ~ |Σ-Σc|^{-ν}, where Σ=τ/P. We observe two distinct values of ν: one during the initial stress buildup, ν ≈ 1.7, and another characterizing the slips during steady state shear, ν ≈ 1.1. The critical stress Σc increases as P is decreased and approaches a constant in the low-P limit, Σc ≈ 0.1. However, the critical behavior (including the values of scaling exponents) is otherwise independent of P over several orders of magnitude, including well above the jamming transition. Our results show that critical scaling behavior associated with yielding is distinct from jamming, which may explain similarities among nonlocal flows of granular materials, emulsions, and other soft materials.
1:51PM B59.00012: Structural evolution of amorphous systems during large scale deformation* ETHAN STANIFER (Presenter), M. LISA MANNING, Syracuse University — Granular and amorphous materials deform plastically via localized structural rearrangements, although it remains unclear how microscopic structure and material preparation control such events. To address this question, many tools have been developed that use features of the linear response or dynamical matrix to predict the locations of localized rearrangements using structural information alone. However, these methods become less predictive across an avalanche, where stress fluctuations generated by one localized rearrangement can trigger other rearrangements resulting in a large-scale structural change that is not captured by the linear response at the beginning of the avalanche. Therefore, we develop a method to study the linear response of a system during an avalanche. Specifically, we use dimensionality reduction to project the Hessian and forces into the space orthogonal to the minimization direction, and other unstable directions. We extend existing tools for identifying structural defects using this reduced Hessian and study how the population of structural defects evolves during an avalanche with a goal of developing a statistical description of structural evolution during large-scale mechanical instabilities.

*This work was funded by the Simons Foundation Grant No. 454947

2:03PM B59.00013: Colloidal drops under extreme stress SRI SHTI ARORA (Presenter), MICHELLE R DRISCO LL, Northwestern University — We investigate the non-Newtonian behavior of dense colloidal suspensions by impacting a millimetric size droplet onto a solid surface. This method provides a unique platform to gain insight into suspension flow at high stresses and velocity gradients, a regime that is non-trivial to access using conventional rheometric techniques. Here, we present a comprehensive study of colloidal drop impact. We measure the maximal spread of the impacting colloidal drop while varying impact velocity and particle volume fraction. We find that the extent of spreading decreases with increasing volume fraction or decreasing impact velocity. Moreover, there exists a critical volume fraction below which the colloidal drop spreads radially into a flattened disc as commonly observed for Newtonian fluids. Above this critical volume fraction, no inertial spreading is observed, suggesting the onset of a jamming transition inside the colloidal drop. Furthermore, we observe a variety of elastic behaviors which manifest above the critical volume fraction and are controlled by impact velocity.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B60 DMP GMAG: DMP Prize Session BCEC 258A - Nitin Samarth, Pennsylvania State University - Tag(s): Invited

11:15AM B60.00001: James C. McGroddy Prize for New Materials Talk: FA Catalogue of Topological Materials Using Topological Quantum Chemistry [Invited] ANDREI B BERNEVIG (Presenter), Princeton University — We will show how, using a new theory called Topological Quantum Chemistry, thousands of new topological materials can be predicted, classified and discovered. The result is that more than 30 percent of all materials in nature are topological.
CLAUDIA FELSER (Presenter), Max Planck Institute for Chemical Physics of Solids — Topology, a mathematical concept, recently became a hot and truly transdisciplinary topic in condensed matter physics, solid state chemistry and materials science. Since there is a direct connection between real space: atoms, valence electrons, bonds and orbitals, and reciprocal space: bands, Fermi surfaces and Berry curvature, a simple classification of topological materials in a single particle picture should be possible [1]. One important criterion for the identification of the topological material is, in the language of chemistry, the inert pair effect of the s-electrons in heavy elements, and the symmetry of the crystal structure. Binary phosphides are an ideal material class for a systematic study of Dirac, Weyl and new Fermion physics, since these compounds can be grown as high-quality single crystals. A new class of topological phases that have Weyl points was also predicted in the family that includes NbP, NbAs, TaP, MoP and WP2 [2-5]. In magnetic materials the Berry curvature and the classical anomalous Hall and spin Hall effect helps to identify potentially interesting candidates. As a consequence, the magnetic Heusler compounds have already been identified as Weyl semimetals: for example, Co2YZ, Mn3Sn and Co5Sn2S2 [6]. The Anomalous Hall angle also helps to identify materials in which a quantum anomalous Hall effect should be possible in thin films. Even beyond this reciprocal Berry curvature, Heusler compounds with non-collinear magnetic structures also possess real-space topological states in the form of magnetic antiskyrmions, which have not yet been observed in other materials [7].


*This work was financially supported by the ERC Advanced Grant No. (742068) “TOPMAT”.

XI DAI (Presenter), Physics, Hong Kong University of Science & Technology — Quasi-particles and collective modes are two fundamental aspects that characterize a quantum mater in additional to its ground state features. For example, the low energy physics for Fermi liquid phase in He-III was featured not only by Fermionic quasi-particles near the chemical potential, but also by fruitful collective modes in the long wave length limit, including several different sound waves that can propagate through it under different circumstances. On the other hand, it is very difficult for sound waves to be carried by the electron liquid in the ordinary metals, due to the fact that long range Coulomb interaction among electrons will generate plasmon gap for ordinary electron density waves and thus prohibits the propagation of sound waves through the electron liquid. In the present paper, we propose an unique type of acoustic collective modes formed by Weyl fermions under the magnetic field, which is called chiral zero sound (CZS). The CZS only exists and propagates along an external magnetic field for Weyl semi-metal systems containing multiple-pairs of Weyl points. The sound velocity of CZS is proportional to the field strength in the weak field limit, whereas oscillates dramatically in the strong field limit generating completely new mechanism for quantum oscillations through the dynamics of neutral Bosonic excitation, which may manifests itself in the thermal conductivity measurements under magnetic field.

JULIA MUNDY (Presenter), Harvard University — Materials systems with many strongly interacting degrees of freedom can host some of the most exotic physical states known. In thin films, the interface between two distinct quantum materials forms a further playground to engineer emergent ground states. Here we demonstrate how we can combine atomically-precise thin film synthesis with picoscale imaging of the resulting structure, to design, construct and probe novel quantum materials at the sub-Angstrom length scales. We will consider a series of complex oxide superlattices where tuning the local distortions of the lattice can lead to dramatic changes in the electronic and magnetic properties of the system. We will demonstrate how this technical approach allows us to stabilize previously metastable “hidden” ground states to construct the first room-temperature strong multiferroic material and a high energy density antiferroelectric system.
11:15AM B61.00001: Excitations in an active smarticle gas*  AKASH VARDHAN (Presenter), ZACHARY JACKSON, WILLIAM C SAVOIE, KURT A WIESENFEILD, DANIEL GOLDMAN, Georgia Institute of Technology — <p style="margin: 0px 0px 10.66px;">Spontaneous stable excitations can arise unexpectedly from homogenous many body systems, e.g. oscillons observed in vibrating granular media, and rotons in superfluid helium. We have observed several such long lived excitations in a gas of active matter particles called “smarticles”. Smarticles are small 3 link planar robots. Each smarticle measures 14X2.5X3 cm<sup>3</sup>, where only the center link is on the ground. In the experiments they are placed on a frictional surface, and change their shape periodically, while interacting with each other via collisions. Although fairly limited in their locomotive capabilities on their own in the considered experimental configuration, interesting behavior is revealed when we allow these smart, active granular materials to mingle. We study the simplest case where two smarticles interact with each other. These two particle excitons demonstrate bouts of coordinated motion synchronized both in their gaits, and spatial orientations. We also witness a unique case of locomotion emerging from their mechanics, wherein the collective executes general planar motion.</p>

*College of Physics, Georgia Tech.

11:27AM B61.00002: Attractor symmetry and stability in symmetric self-driven oscillator networks*  IAN HUNTER (Presenter), MICHAEL NORTON, JAMES SHEEHY, Physics, Brandeis University, BOLUN CHEN, Neuroscience, Brandeis University, YOUSSEF FAHMY, Physics, Brandeis University, LANIJAH FLAGG, Physics, Hampton University, CHRIS SIMONETTI, SETH FRADEN, Physics, Brandeis University — The dynamics governing networks of identical oscillators are unchanged by node interchange symmetries, or automorphisms, of the network. Equivariant dynamical system theory predicts such networks consequently must possess steady states, and flow invariant manifolds where particular nodes, exchanged by subgroups of network symmetries, are synchronized. Homogeneous microreactors containing the oscillatory Belousov Zhabotinsky (BZ) reaction, coupled by diffusion, allow the experimental study of symmetric self-driven oscillator networks. A ring of 4 inhibitory-coupled BZ reactors was studied as a model system. This system exhibits symmetric gaits found in quadrupedal animals as its attractors. Experimental invariant manifolds, steady states, and stabilities are compared to those theoretically predicted using methods generalizable to other networks.

* We acknowledge financial support from the NSF DMREF-1534890 and the microfluidics facility of the NSF MRSEC DMR-1420382.

11:39AM B61.00003: Domain wall creep and depinning: a scalar field model approach  NIRVANA CABALLERO (Presenter), University of Geneva - Bariloche Atomic Center - CONICET, EZEQUIEL FERRERO, Bariloche Atomic Center - CONICET, ALEJANDRO B. KOLTON, Bariloche Atomic Center - Balseiro Institute - CONICET, JAVIER CURIALE, VINCENT JEUDY, Laboratoire de Physique des Solides, Universite Paris-Sud, SEBASTIAN BUSTINGORRY, Bariloche Atomic Center - CONICET, THIERRY GIAMARCHI, University of Geneva — Domain wall motion is at the heart of new magneto-electronic technologies and hence the need for a deeper understanding of domain wall (DW) dynamics in magnetic systems. In this context, numerical simulations using simple models can capture the main ingredients responsible for the complex observed DW behavior. We present a scalar-field model for the magnetization dynamics of quasi-two-dimensional systems with a perpendicular easy axis of magnetization which allows a direct comparison with typical experimental protocols, used in polar magneto-optical Kerr effect microscopy experiments. We show that the thermally activated creep and depinning regimes of DW motion can be reached, and the effect of different quenched disorder implementations can be assessed with the model. Moreover, our model has material-dependent tunable parameters and allows to reproduce experimental velocity-field curves. In particular, we show how the structural disorder should be modeled to reproduce Pt/Co/Pt velocity-field curves in a broad range of temperatures (ranging from 4K to room temperature). We also use this model to make a connection with DW with defects such as bubbles and overhangs. We examine in particular observables such as the two-dimensional structure factor both numerically and analytically.
11:51AM B61.00004: Modeling the relative dynamics of DNA-coated colloids*  MIRANDA HOLMES-CERFON (Presenter), JAMES LEE-THORP, Courant Institute of Mathematical Sciences — A versatile way to make colloids with programmable interactions is to coat them with strands of sticky DNA. However, the DNA changes the dynamics of the colloids, in ways that can push the system out of equilibrium on experimental timescales. We construct a coarse-grained theoretical model for the relative dynamics of DNA-coated colloids (which is similar to models of molecular motors), and use it to argue that (a) DNA induces friction between the points of contact that can be about 100 times larger than hydrodynamic friction, for relevant experimental parameters, and (b) the friction for particles rolling could be several orders of magnitude smaller than the friction for sliding, when the DNA is very short and stiff. Therefore, we speculate that in certain experimental systems such colloids could act like gears, and assemble into metastable states that would not be observed in their true equilibrium.

*MRSEC Program of the National Science Foundation (DMR-1420073)
Department of Energy (DE-SC0012296)
Alfred P. Sloan foundation (FG-2018-10656)

12:03PM B61.00005: Driving Frustrated Lattices of Active Droplets*  ANTON MOLINA (Presenter), Stanford University, STEFAN KARPITSCHKA, Dynamics and Self-Organization, Max Planck Institute, MANU PRAKASH, Stanford University — Self-organization is the process by which interacting building blocks arrange themselves into an ordered structure. While there are many examples of self organization, there are no examples which explore the use of external fields to drive self-organizing particles in a geometrically frustrated environment. Here, we explore frustrated self-organization in a novel system comprised of self-propelled droplets. Ensembles of these droplets interact with one another, via a vapor-mediated and long-ranged potential, displaying dynamic behavior that resembles chemotaxis. We present an experiment that confines droplets to hexagonal lattice sites, using gravity to drive the system away from equilibrium. Hence, we study the relationship between single particle dynamics and the statistics of ensemble organization. In this geometrically frustrated environment we observe a phase transition of droplet self-assembly as a function of the driving from equilibrium. Comparison to simulation allows us to connect our experimental results to statistically relevant distributions, thereby connecting observations of single particle dynamics and local accommodation of frustration to statistical physics.

*AM is supported by the National Science Foundation Graduate Fellowship Research Fellowship Program.

12:15PM B61.00006: Self-assembly of nanoscale braided structures  EDVIN MEMET (Presenter), MOHAMMAD SHAHJAMALI, CHENG ZENG, ISAAC BRUSS, VINOTHAN N MANOHARAN, LAKSHMINARAYANAN MAHADEVAN, Harvard University — Capillarity, along with bending and cohesive forces, can induce assembly of nanopillar/micropillar arrays into a wide variety of structures. Experiments we performed involving seven hexagonally arranged pillars reveal a surprising transition from straight to twisted conformations. Separately, we also found that large arrays (e.g. 30x30, 10x40) of high-aspect ratio pillars can assemble into various structures, including chiral, globally twisted morphologies. Here we use numerical and scaling methods to understand how the rate of drying, capillarity, bending, and cohesion control the physics of elastocapillary-driven self-assembly.

12:27PM B61.00007: Simulations on encapsulation of multiple cargoes in bacterial microcompartments*  LEV TSIDILKOVSKI (Presenter), FARZANEH MOHAJERANI, MICHAEL F HAGAN, Brandeis University — Bacterial microcompartments are self-assembling protein shells that encapsulate enzymes or other proteins, similar to eukaryotic organelles. Bacteria use them to sequester toxic intermediates from the cytoplasm, or to accelerate the rates of chemical reactions through co-localization of reagents. In this talk I will describe coarse-grained computational models that allow Brownian dynamics simulations of self-assembly of microcompartments around multiple cargo species (e.g. enzymes). Based on these simulations, we have identified multiple factors that control encapsulation. In particular, the simulations show that the relative interaction strengths among the different cargo species play a key role in determining the amount and spatial organization of each species, as well as the nature of assembly pathways. I will also describe the effects of other control parameters (e.g. interactions between cargo and shell), thus providing a basis for utilizing bacterial microcompartments as customizable nanoreactors.

*This work was supported by Award Number R01GM108021 from the National Institute Of General Medical Sciences and the Brandeis Center for Bioinspired Soft Materials, an NSF MRSEC, DMR-1420382.
12:39PM B61.00008: Driven Widom-Rowlinson lattice gas

RONALD DICKMAN (Presenter), Physics, UFMG, ROYCE ZIA, Physics, Virginia Tech. — In the Widom-Rowlinson lattice gas, two particle species (A, B) diffuse freely via particle-hole exchange, subject to both on-site exclusion and prohibition of A-B nearest-neighbor pairs. As an athermal system, the overall densities are the only control parameters. As the density increases, a phase transition occurs, leading to ordered states with A- and B-rich domains separated by hole-rich interfaces. Using Monte Carlo simulations, we analyze the effect of imposing a drive on this system, biasing particle moves along one direction. Novel features emerge, including structure factors with kink singularities (best fitted to $|q|$), maxima at non-vanishing wavevector values, oscillating correlation functions, and ordering into multiple striped domains perpendicular to the drive, with a preferred wavelength depending on density and drive intensity. Interfaces between the domains are statistically rough, in sharp contrast with those in the Katz-Lebowitz-Spohn model, in which the drive suppresses interfacial roughness. Defining an order parameter (to account for the emergence of multistripe states), we map out the phase diagram in the density-drive plane.

*This work was supported by CNPq and CAPES, Brazil.

12:51PM B61.00009: Self-assembly, aggregation, and phase behavior of driven and active colloids

ERIK LUIJTEN (Presenter), Northwestern University — Colloidal suspensions are a prototypical example of systems that can be either passive or active. I will demonstrate how various forms of dynamics and different types of interactions result in unexpected and until now largely unexplored aggregation and phase behavior. These observations, obtained through a combination of experiments and computer simulations, reveal striking connections between colloidal self-assembly and collective dynamics, and between dynamic behavior and equilibrium thermodynamics. Moreover, a remarkable variety of collective dynamics can be realized through simple variation of external electric fields. These observations provoke new thoughts on the nature of "soft" materials and our ability to manipulate them.

*This research was supported by the U.S. National Science Foundation under Grant No. DMR-1610796.

1:27PM B61.00010: Feasibility of prediction in driven-dissipative system displaying effective ergodicity breaking

CHONKIT PUN (Presenter), W. KLEIN, Department of Physics, Boston University, HARVEY GOULD, Department of Physics, Clark University — Using machine learning techniques we forecast the size of avalanches in the Olami-Feder-Christensen model using spatial information at different values of noise. We use the convolutional neural network and find that prediction is possible at low noise effective non-ergodic phase and not possible at the high noise effective ergodic phase. By looking at the higher level structures learned from the convolutional neural network, we can identify precursors of large events. Our goal is to understand the theoretical limitations of forecasting extreme events in complex systems.


DEBASHISH CHOWDHURY (Presenter), BHAVYA MISHRA, Indian Institute of Technology Kanpur — The totally asymmetric simple exclusion process (TASEP) was originally introduced fifty years ago as a model for the synthesis of biopolymers, called protein, by macromolecular machines called ribosome. In that formulation, the mRNA template for protein synthesis, that also serves as the track for the motor-like movement of the ribosomes, is represented by a lattice. We introduce a 3-species exclusion model that captures some of the hitherto neglected, but crucially important, details of the initiation of protein synthesis. We study the interference of the synthesis of two different proteins, the templates for which are encoded on two different, but overlapping, segments of the same lattice. We formulate the process of search for the start sites for protein synthesis as first-passage problems and calculate the mean initiation times for the synthesis of the two species of proteins. We show how the mean initiation times get affected by "leaky scanning" and the interference of the three exclusion processes.

*This work is supported by J.C. Bose National Fellowship from SERB (DC) and SRF from UGC (BM).

1:51PM B61.00012: Pressure exerted by confined active particles

MICHA KORNREICH (Presenter), PAUL M CHAIKIN, New York University — Mechanical pressure, defined as the force applied perpendicular to the surface of an object per unit area, takes dramatically different forms in and out of equilibrium [1]. To experimentally measure the pressure exerted by an out of equilibrium system, we confine self-propelled particles in a negative dielectrophoretic trap. Knowing the potential profile, the density profile reveals the pressure. In equilibrium, pressure is exclusively governed by bulk properties such as density and temperature. In contrast, when the particles are activated, using either an in-plane rotating magnetic field or light-activated self-phoretic particles, we find that the force exerted on the confining trap boundaries depends on the shape of the boundary dielectrophoretic force fields.

2:03PM B61.00013: Surfing on protein waves: proteophoresis as a mechanism for bacterial genome partitioning*
JEAN-CHARLES WALTER (Presenter), CNRS, JÉRÔME DORIGNAC, VLADIMIR LORMAN, Université de Montpellier, JÉRÔME RECH, JEAN-YVES BOJET, MARCELO NOLLMANN, JOHN PALMERI, CNRS, ANDREA PARMEGGIANI, FRÉDÉRIC GENIET, Université de Montpellier — Efficient bacterial chromosome segregation typically requires the coordinated action of a three-component, fueled by adenosine triphosphate machinery called the partition complex. We present a phenomenological model accounting for the dynamic activity of this system that is also relevant for the physics of catalytic particles in active environments. The model is obtained by coupling simple linear reaction-diffusion equations with a proteophoresis, or “volumetric” chemophoresis, force field that arises from protein-protein interactions and provides a physically viable mechanism for complex translocation. This minimal description captures most known experimental observations: dynamic oscillations of complex components, complex separation and subsequent symmetrical positioning. The predictions of our model are in phenomenological agreement with and provide substantial insight into recent experiments. From a non-linear physics view point, this system explores the active separation of matter at micrometric scales with a dynamical instability between static positioning and travelling wave regimes triggered by the dynamical spontaneous breaking of rotational symmetry.


Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B62 GPC: Detecting Signals in a Noisy Climate System

11:15AM B62.00001: Insights Regarding Observational Requirements For Climate Change Signal Detection [Invited]
BRUCE WIELICKI (Presenter), Science Directorate, NASA Langley Research Center — Climate change signals must be detected against both the noise of internal natural variability as well as a wide range of uncertainties in the observing system. Observing system uncertainties include SI traceable accuracy, instrument stability over a decade or longer, calibration across data gaps, changing instrument designs, changing sampling of the earth, and changing data analysis methods. Most current observations used for climate change signals were not designed with climate change uncertainties in mind (National Academy of Sciences Continuity Report for NASA, Nov. 2015). Examples are given of how to set requirements for climate change observations relative to anticipated climate change signals and climate system natural variability. Given that we currently lack an observing system designed specifically for climate change, what would such a system look like? Design principles are provided, and examples are given of how more accurate observations can narrow key scientific uncertainties in climate change. Examples will also be presented of observations that can meet these much more challenging climate change requirements. The lack of a designed climate observing system naturally raises the question of the societal return on investment of providing such a system. Recent published estimates using state of the art economic integrated assessment models (IAMS) suggest a return of ~ 50 per1 invested. Society will be managing the Earth's Climate System actively or passively, wisely or unwisely, for the indefinite future. The world has had an internationally designed, committed, and shared weather observing system for many decades. It is time to begin an equivalent international climate change observing system. The motivation for such systems are the same: a better future for society.
ENS0 Change in Climate Projections: Forced Response or Internal Variability?* [Invited]  NICOLA MAHER (Presenter), DANIELA MATEI, SEBASTIAN MILINSKI, JOCHEM MAROTZKE, Ocean in the Earth System, Max Planck Institute for Meteorology — The El Niño-Southern Oscillation (ENSO) is the dominant driver of interannual variability globally and has effects which are felt in many remote regions of the world. As such it is vital to assess the potential future changes of ENSO. However, there is little consensus on how ENSO sea surface temperature (SST) may change in a future with increasing greenhouse gas emissions and underlying warming (Bellenger et al., 2014; Collins et al., 2010; Guilyardi et al., 2012; Ham & Kug, 2016), with large differences found between different Coupled Model Intercomparison Project 5 (CMIP5) model projections (Collins et al., 2010; Guilyardi et al., 2012). The range of projections of ENSO in the future could be due to differences in model physics, resulting in different projections from different models. However, the role of internal variability must also be considered. Such internal variations can result in different projections from single ensemble members of the same climate model. A large ensemble of a single model can be used to estimate this internal variability, and together with other model ensembles can be used to address uncertainties in model physics.

Two large ensembles are used to quantify the extent to which internal variability can contribute to long-term changes in ENSO characteristics. The range of simulated ENSO amplitude changes in the large ensemble historical simulations encompasses 90% of the Coupled Model Intercomparison Project 5 historical simulations and 80% of moderate (RCP4.5) and strong (RCP8.5) warming scenarios. When considering projected ENSO pattern changes, model differences are also important. We find that ENSO has high internal variability and that single realizations of a model can produce very different results to the ensemble mean response. Due to this variability, 30-40 ensemble members of a single model are needed to robustly compute absolute ENSO variance to a 10% error when 30-year analysis periods are used.

*Alexander von Humboldt Foundation

12:27PM B62.00003: From months to Milankovitch: how timescale-dependent interactions in the coupled Earth system determine the spectrum of climate variability and response.* [Invited]  CRISTIAN PROISTOESCU (Presenter), JISAO, University of Washington — Acting as both signal and noise, stochastic internal variability dominates the observational record of Earth's energy budget. While variability confounds estimates of anthropogenic climate change, it can also be leveraged for insight into the underlying physics, provided one understands both the governing stochastic processes, and the ways in which they are encoded in the statistics of observable quantities.

I will show how the frequency spectrum of Earth's temperature variability is determined by - and informs on - the climate system's radiative damping efficiency. This damping efficiency determines how much radiation the system sheds to space for a given change in surface temperature, and it is set by how the different components of the climate system - atmosphere, ocean, cryosphere, and the carbon cycle, interact across a range of timescales. The theoretical model for a timescale-dependent radiative damping efficiency is constrained by a combination of observations of broad-band variability drawn from both instrumental records as well as proxies of past climate change.

*C.P. is supported by a postdoctoral fellowship from the Joint Institute for the Study of the Atmosphere and Ocean

1:03PM B62.00004: The climate change signal in hurricanes [Invited]  CHIA-YING LEE (Presenter), ADAM SOBEL, MICHAEL TIPPETT, SUZANA CAMARGO, Columbia University — In this presentation, I will discuss results from our ongoing research on detecting climate change signal in hurricane activity in the recent history. A question that is frequently asked during or after an extreme hurricane season like 2017 is whether such extreme season becomes more frequent or is simply one of the statistical flukes. Such question is hard to answer by using observational data alone as the length of high-quality hurricane record is too short. Therefore, we study this question by a combination of observations, statistical-dynamical downscaling modeling and high-resolution global dynamical modeling approaches. Simulations driven by reanalysis data will be used to estimate historical trends. Simulations driven by outputs from global climate models as well as those directly output from high-resolution global models are used to estimate the roles of radiative forcing, natural variability, and their combination. I will show the comparison of various climatological measures of TC activity from observations and model-based estimates for the current, pre-industrial, and near future periods. In addition to our work, I will also discuss other recent studies on detecting climate change signal on hurricanes.
Detecting changes in marine ecosystems and ocean colour* [Invited] STEPHANIE DUTKIEWICZ (Presenter), OLIVER JAHN, EAPS, Massachusetts Institute of Technology, ANNA HICKMAN, University of Southampton, STEPHANIE HENSON, National Oceanography Centre Southampton, CLAUDIE BEAULIEU, University of California, Santa Cruz, ERWAN MONIER, University of California, Davis — Monitoring changes in marine phytoplankton is important as they form the foundation of the marine food web and are crucial in the carbon cycle. Climate change is affecting marine phytoplankton by altering their nutrient, temperature, light and chemical environments. Often Chlorophyll-a (Chl-a) is used to track changes in phytoplankton, since there are global, regular satellite-derived estimates, and such studies suggesting complex, but as yet limited, patterns of long-term change over the last two decades. However, satellite sensors do not measure Chl-a directly. Instead, Chl-a is estimated from remote sensing reflectance (RRS): the ratio of upwelling radiance to the downwelling irradiance at the ocean's surface. We use a unique ocean physics, biogeochemistry and ecosystem model that explicitly includes a representation of the ocean's optical properties to explore how climate change signals are manifested in Chl-a, phytoplankton communities, and ocean colour over the course of the 21st century. We show that RRS in the blue-green spectrum is likely to have a stronger and earlier climate change-driven signal than Chl-a. This is because RRS integrates not only changes to Chl-a, but also alterations in other optically important constituents. Phytoplankton community structure, which strongly affects ocean optics, is likely to show one of the clearest and most rapid signatures of changes to the base of the marine ecosystem.

*NASA (grant NNX16AR47G)

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B63 DBIO GSNP: Evolutionary and Ecological Dynamics II: Eco-evolutionary Feedback

Infect, replicate, and diffuse on: how bacteriophage grows and evolves during a spatial range expansion* [Invited] DIANA FUSCO (Presenter), University of Cambridge — Spatially growing populations are ubiquitous across scales, ranging from the human migration out of Africa to the spreading of diseases. In contrast to well-mixed populations where an individual's chance of survival is only determined by its fitness, in spatially growing populations the physical location of an individual plays a crucial role: the individuals at the edge of the expanding front benefit from having access to virgin territory and giving their offspring the same advantage. The emerging population dynamic results in an evolutionary dynamic dominated by noise, with extreme consequences such as the accumulation of deleterious mutations at the population's front.

To investigate how spatial range expansion affects the evolutionary dynamic of a population, we employ the bacteriophage T7-E. coli system. In an evolutionary experiment lasting only 7 days, we were able to evolve a T7 strain that more than doubled its spreading speed on a bacterial lawn compared to its ancestor. The seeming lack of accumulation of deleterious mutations at the front raised questions regarding the physical nature of the traveling wave describing the expansion front of T7, which was traditionally assumed to behave like a pulled wave at long time scales. In contrast to the assumptions used in the FKPP reaction-diffusion equation generating pulled waves, diffusion rate measurements show that phage dispersal is non-uniform along the range expansion since it depends on the local bacterial density. Using stochastic simulations, we find that this effect can have dramatic consequences on the phage genetic diversity at the front and on the adaptation potential of the population. The underlying physical origin of the effect broadens the relevance of our findings to a wide range of host-pathogen systems that share this feature.

*EPSRC Doctoral Training Partnership Postgraduate Funding
Mitochondria are organelles found in almost all eukaryotic cells. They are highly dynamic and once formed, they can undergo changes in size and content via the processes of fusion, fission, and mitophagy. Mitochondria are famously known as the powerhouse of the cell for their role in cellular energy production. They are also essential for cell signaling and apoptosis, and have their own DNA, called mtDNA, which is maternally inherited. The same cell can have multiple variants of mtDNA, and harmful alterations in mtDNA can accumulate over time resulting in pathological changes in mitochondrial function and disease states. We develop and study a mathematical model to understand and predict the population dynamics of mtDNA and how it is correlated to changes in mitochondrial bioenergetics. We examine the spatiotemporal evolution of populations of healthy and dysfunctional mitochondria subject to mitochondrial biogenesis, fission, fusion, mitophagy, and changes in the mitochondrial membrane potential, and determine their relative impact on mtDNA population dynamics. Our results may provide insights into how different mtDNA populations survive and evolve under different selection pressures and the origins of mtDNA disorders.

*This work was supported by a grant from the Moore Foundation.

11:51AM B63.00002: Dynamics of mtDNA populations in mammalian cells: role of mitochondrial dynamics and its interplay with mitochondrial membrane potential†  BRANDON BOGNER (Presenter), KELLIANNE E KORNICK, LEO SUTTER, School of Physics and Astronomy, Rochester Institute of Technology, REBECCA ZATHANG, School of Chemical Sciences, Rochester Institute of Technology, MOUMITA DAS, School of Physics and Astronomy, Rochester Institute of Technology — Mitochondria are organelles found in almost all eukaryotic cells. They are highly dynamic and once formed, they can undergo changes in size and content via the processes of fusion, fission, and mitophagy. Mitochondria are famously known as the powerhouse of the cell for their role in cellular energy production. They are also essential for cell signaling and apoptosis, and have their own DNA, called mtDNA, which is maternally inherited. The same cell can have multiple variants of mtDNA, and harmful alterations in mtDNA can accumulate over time resulting in pathological changes in mitochondrial function and disease states. We develop and study a mathematical model to understand and predict the population dynamics of mtDNA and how it is correlated to changes in mitochondrial bioenergetics. We examine the spatiotemporal evolution of populations of healthy and dysfunctional mitochondria subject to mitochondrial biogenesis, fission, fusion, mitophagy, and changes in the mitochondrial membrane potential, and determine their relative impact on mtDNA population dynamics. Our results may provide insights into how different mtDNA populations survive and evolve under different selection pressures and the origins of mtDNA disorders.

12:03PM B63.00003: Frequency- and Amplitude-Dependent Microbial Population Dynamics during Cycles of Feast and Famine† JASON RYAN MERRITT, SEPPE KUEHN (Presenter), University of Illinois at Urbana-Champaign — In nature microbial populations are subject to fluctuating nutrient levels. Nutrient fluctuations are important for evolutionary and ecological dynamics in microbial communities since they impact growth rates, population sizes, and biofilm formation. Here we show that when populations of *Escherichia coli* are subjected to cycles of nutrient excess (feasts) and scarcity (famine) their abundance dynamics during famines depend on the frequency and amplitude of feasts. We show that frequency and amplitude dependent dynamics in planktonic populations arise from nutrient and history dependent rates of aggregation and dispersal. These conclusions are enabled by precision measurements performed with automated continuous culture devices coupled to custom fluorescence microscopes. The instruments automatically sample, image and count single-cells drawn from continuously-cultured populations on a timescale of minutes for periods of weeks. The quality of the data enable us to construct a concise phenomenological model that recapitulates our experimental observations. Our results show that the statistical properties of environmental fluctuations have substantial impacts on spatial structure in bacterial populations driving large changes in abundance dynamics.

*NSF (PHY 0822613 and PHY 1430124)

12:15PM B63.00004: Evolutionarily stable coexistence in a single nutrient: optimization and cross-feeding ZHIYUAN LI (Presenter), Princeton University, BO LIU, Peking University, NED WINGREEN, Princeton University — Two questions on coexistence have perplexed community ecologists for nearly a century: first, the “paradox of the plankton”, that nature world possess tremendous diversity while theoretical models suggested the number of species can hardly exceeds the number of nutrients. Second, evolution has been shown to exacerbate this paradox. As species are constantly evolving towards optimality, which may produce a supreme winner that takes over the habitat. To investigate these questions, we utilized and extended the graphical tools of resource-competition theory to relate and unify multiple models for microbial diversity, and quantified the optimal metabolic strategies in resource competition models in general. This framework was then applied to metabolic models that allows species to increase dimension in nutrient space by secreting metabolites. With this simple model, we explored the possibilities of coexistence though cross-feeding on a single supply nutrient, and investigated general criteria for such co-existence to be evolutionarily stable.

12:27PM B63.00005: Diversification of investment strategies in an ecological public goods game driven by the spatial structure of the population JOSEPH RAUCH (Presenter), JANE KONDEV, Brandeis University, ALVARO SANCHEZ, Yale University — Ecology and evolution work in tandem to create biodiversity, especially when they act on similar timescales, as can happen in microbial populations. Frequency and density dependent ecological models, like the public goods game, are known to be capable of supporting diverse populations. Recent experiments have shown diversification of gene expression in a bacterial population for a gene expressing a public good. Motivated by these observations we study an ecological public goods model and compare the extent to which mutations can fix in a population and generate diversity in a well-mixed situation and one with spatial structure. We show that rapid diversification within an ecological public goods game can drastically vary depending on the time scale of evolution and the time scale of ecological dynamics. While populations in a well-mixed model quickly come to equilibrium, limiting the amount of diversity typically to two dominant investment strategies; models with spatial structure prolong the time to equilibrium and allow multiple mutants to fix themselves in the population. Our theoretical studies agree with the experimental observations and point to a general principle how ecological public good games in spatially extended microbial population can lead to rapid diversification.
The evolution of multicellular life from single-celled ancestors is one of the most radical shifts in the history of life on earth, and sets the stage for evolution of more complex life forms. Despite the significance of this transition, we know little about the process by which cells first assemble groups and form multicellular organisms. We study this problem experimentally; a single mutation in the ACE2 gene of Baker’s yeast S. cerevisiae prevents mother and daughter cells from separating after cellular division. These yeast clusters, called ‘snowflake’ yeast, comprise a few hundred cells and grow to a maximum diameter of 200 microns. To evolve larger multicellular size, snowflake yeast clusters must mitigate forces strong enough to fracture cell-cell bonds. After a year of artificial selection for larger multicellular size, five populations of snowflake yeast surprisingly evolved to grow to a maximum diameter of 1 mm. In this work we investigate how nascent multicellular clusters evolve to overcome substantial mechanical constraints and dramatically increase their size.

Avalanche critical fluctuations are an important dynamic feature of many systems including earthquakes and magnet polarization. They are caused by sudden release of potential built up by frustration in energy dissipation. Here, we introduce the concept of resource frustration in ecological systems to describe transient buildup of resources within a community which are then dissipated via avalanche-like events of individual species growth. We developed a general model to predict the conditions under which this type of fluctuations emerge in ecological systems and identified scaling laws and critical exponents of these avalanche events. We also demonstrated that these scaling laws are universal across multiple model microbial communities, (e.g., siderophore dependence and auxotrophic mutualism) using consumer-resource models. Our results reveal a novel class of transient phenomena in ecology and provide mechanisms by which stochastic fluctuations in individual components amplify and propagate throughout the ecological system.

This work was supported by the NSF GRFP (Grant No. DGE-1656466) & NIH award T32 HG003284.

1:15PM B63.00009: What do metabolic constraints inform us about the emergence of early stable bacterial communities? GA CHING LUI (Presenter), SIDHARTHA GOYAL, Physics, University of Toronto — Stability of an ecosystem is determined by its composition. As a system gains stability, one of the major trends observed during ecological succession, which refers to the development of a community, is an increase in compositional diversity [1]. It has been shown that multispecies systems can support a larger community with more surviving species at steady state when the variability across pairwise coupling strengths between species is smaller [2]. But how a small system with one species and no foreign invaders develops into a large diverse system remains an open question. Here, we consider the stability of a system under constant nutrient flux [3] when a species is competing with its closely related mutants to understand how early diversity is established. Using adiabatic approximation and discarding higher order terms, we recover the reduced dynamics for chemostats similar to Lotka-Volterra systems. By introducing small perturbations to the growth rates of the otherwise identical species constrained by rates of metabolic regulations, the rules for obtaining stable multispecies communities are obtained.

1:27PM B63.00010: Eco-evolutionary hysteresis in bacterial genomes driven by horizontal gene transfer  
AKSHIT GOYAL (Presenter), Simons Centre for the Study of Living Machines, National Centre for Biological Sciences (NCBS-TIFR) — Many naturally-occurring bacteria lead a lifestyle of metabolic dependency, i.e. they depend on others for crucial resources. We do not understand what factors drive bacteria towards this lifestyle, and how. Here, we systematically explain the role of horizontal gene transfer (HGT) in metabolic dependency evolution. Across 835 bacterial species, we mapped gene dynamics on a deep evolutionary tree, and assessed the impact of HGT and gene loss on bacterial metabolic networks. Our analyses suggest that genes acquired by HGT can affect which genes are later lost. Dependency evolution by gene loss is contingent on earlier HGT via two steps. First, we find that HGT and gene loss act on contrasting regions of metabolic networks—losses remove existing anabolic routes; HGT adds new catabolic routes. This increases the chance of new metabolic interactions between bacteria, which is a prerequisite for dependency evolution. Second, we show how gaining new routes can promote the loss of specific ancestral routes (termed "eco-evolutionary hysteresis", EEH). Phylogenetic patterns indicate that both types of dependencies—those mediated by EEH and pure gene loss—are equally likely. Our results highlight HGT as an important driver of metabolic dependency evolution in bacteria.

1:39PM B63.00011: Species Packing with Generalized Resource Dynamics*  
WENPING CUI (Presenter), Department of Physics, Boston College, Boston University, ROBERT MARSLAND, PANKAJ MEHTA, Department of Physics, Boston University — An important question in ecology is to understand how species assemble under different resource dynamics. Here we explored generalized MacArthur’s resource models with two different resource dynamics: self-renewing(original MacArthur’s) and external-supplied resource dynamics. A statistical physics inspired cavity method is used to solve two resource dynamics analytically. Surprisingly, we find that two resource dynamics have different upper bounds of species packing. We show that external-supplied resource dynamics can introduce higher order competition between species and affect coexistence patterns dramatically.

*NIH NIGMS grant 1R35GM119461, Simons Investigator in the Mathematical Modeling of Living Systems (MMLS), the Scialog Program sponsored jointly by Research Corporation for Science Advancement

1:51PM B63.00012: Resource utilization determines growth rates and evolution in simple multi-species evolutionary model.  
JOSHUA DIJKSMAN (Presenter), Wageningen University & Research — Species proliferate in an ecosystem if resources are abundant. Populous species at the same time deplete resources, which undermines their expansion. This suggests that resource utilization, appropriately quantified, should set their growth rate. By defining a species by the amount of different resources it consumes, and using the alignment of this vector with the vector of available resources as species growth rate, we can implement growth but also drift in species composition, and hence entire ecosystem evolution through speciation and adaptation. Our approach displays all the salient features of ecosystem evolution. We can evolve ecosystems even by initiating dynamics out of a single primordial ancestor. Despite the nonlinear and stochastic nature of this MacArthur-style approach, the modeling approach yields a robust, universal solution for the mean ecosystem fitness dynamics that is resilient against resource shocks. More generally, ecosystem fitness depends in an intuitive way on model parameters such as resource influx, reproduction rate and evolutionary noise. Our resource utilization approach to growth modeling so provides a general but simple starting point to evolutionary ecosystem dynamics.

2:03PM B63.00013: MEST-SPACETIME STRUCTURE, MASSENERGY STRUCTURE, AND ORIGIN of LIFE  
DAYONG CAO (Presenter), Avoid Earth Extinction Association — MEST is a balance systemic model of mass, energy, space, and time.

According to Einstein field equation and negative Einstein equation, there are massenergy center with massenergy structure and spacetime center with spacetime structure which has gravity of the spacetime (as negative gravity).

The spacetime center structure can explain of dark matter and dark energy. A balance structure between massenergy and spacetime can explain of the homogeneous, isotropic, and flat structure of the universe. It can suppose a balance system between the sun and a dark sun as a spacetime center of Oort cloud which is dark matter-dark energy.

Beginning of the solar system, there have dark matter around baby sun. The dark matter with ring structure (of spacetime center structure) impacted on the stellar matter with open structure, and create organic macromolecule of the life's system with open system and closed system together. The impactions also could cause mass extinction, and could make natural gas, oil, and coals.

The period of the mass extinction has relationship with orbit of revolution of solar system, Galactic Spiral Arm, and balance system between sun and dark sun.
http://meetings.aps.org/Meeting/APR16/Session/M13.8
11:15AM B64.00001: Inferring the helix-helix electrostatic interaction strength from the structure of dense DNA toroids*  Luca Barberi (Presenter), LPTMS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, Amélie Leforestier, Françoise Livolant, LPS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, Martin Lenz, LPTMS, CNRS, Univ. Paris-Sud, Université Paris-Saclay — DNA is often condensed to remarkably dense phases, where one or more chains are curved at scales comparable to their persistence length. This can happen in the presence of highly valent cations, like in the capsids of some bacteriophage viruses, where a long DNA chain is rolled up to nearly crystalline densities with spermidine(3+) and putrescine(2+). Despite their biological relevance, cation-mediated helix-helix electrostatic interactions remain poorly understood and their experimental measurement limited to arrays of locally parallel DNA helices. These forces relying on strong spatial correlations between charges on neighbouring helices, straight DNA chains may interact differently than curved ones. We are able to infer the strength of helix-helix electrostatic forces in a spermine(4+)-condensed DNA toroid, predicting with a minimal model the inter-helical spacing spatial inhomogeneities observed in our recent cryo-electron microscopy experiments. Our results suggest that electrostatic cohesion may be one order of magnitude weaker in toroids than in other DNA condensates with less local curvature. Curvature-reduced electrostatic interactions may facilitate DNA ejection dynamics in bacteriophages.

*ANR-11-IDEX-0003-02; ANR-12-BSV5-0023-01; ANR-10-LABX-0039-PALM

11:27AM B64.00002: The Nanomechanics of Cellulose Synthesis*  Lori Goldner (Presenter), Nina Zehfroosh, Tobias I. Baskin, University of Massachusetts Amherst — Despite its ubiquity and technological importance, cellulose is synthesized in plants by a process that is poorly understood. Cellulose is a crystalline fiber made up of glucan chains synthesized by a large enzymatic complex that resides in the plant cell membrane. Decisive progress was made more than a decade ago when fluorescently-tagged complexes were first observed moving in the cell membranes of living plants. Complexes move with a speed between 100 and 400 nm/min and this motion is presumed to be related to the rate of cellulose synthesis. We present the results of a careful study of CESA motion in two different plant species over a wide range of timescales. We show several surprising aspects of this motion and discuss models to explain it. After accounting for localization error, the mean squared displacement (MSD) of the moving cellulose synthase complexes shows subdiffusive timescales below 10 seconds suggesting short-range trapping. Over longer timescales, an extant model and particle MSDs support a Brownian ratchet mechanism. However, initial indications are that step-size distributions are non-Gaussian, indicating that a Brownian ratchet alone may not be sufficient to explain CESA mechanics.

*Support for this work was from DOE DE-FG-03ER15421 and NSF PHY-1205989.

11:39AM B64.00003: On the behavior of random RNA secondary structures near the glass transition*  William Baez, Department of Physics, Ohio State University, Kay J. Wiese, CNRS-Laboratoire de Physique Théorique, Ecole Normale Supérieure, Ralf Bundschuh (Presenter), Department of Physics, Ohio State University — RNA forms elaborate secondary structures through intramolecular base pairing. These structures perform critical biological functions within each cell. Due to the availability of a polynomial algorithm to calculate the partition function over these structures, they are also a suitable system for the statistical physics of disordered systems. In this model, below the denaturation temperature, random RNA secondary structures exist in one of two phases: a strongly disordered, low-temperature glass phase, and a weakly disordered, high-temperature molten phase. The probability of two bases to pair decays with their distance with an exponent 3/2 in the molten phase, and about 4/3 in the glass phase. Inspired by previous results from a renormalized field theory of the glass transition separating the two phases, we numerically study this transition. We introduce distinct order parameters for each phase, that both vanish at the critical point. We finally explore the driving mechanism behind this transition.

*This material is based upon work supported by the National Science Foundation under Grants No. DMR-1410172 and DMR-1719316.
11:51AM B64.00004: Salivary mucin glycopolymers reduce virulence traits of cavity-causing *Streptococcus mutans*

CAROLINE WERLANG (Presenter), WESLEY CHEN, KATHARINA RIBBECK, Massachusetts Institute of Technology — Dry mouth is a condition characterized by an underproduction of saliva that affects one in five American adults. This reduction in salivary mucus is associated with higher incidences of cavities, oral ulcers, and microbial infections in the mouth. Saliva's protective effects are derived from mucins, gel-forming proteins. These natural brush polymers display over two-hundred unique glycan motifs. Reconstituted salivary mucin gels have been shown to prevent biofilm formation of *Streptococcus mutans*, bacteria whose adherence to teeth causes cavities. Here, we show that mucin affects other virulence behaviors of these bacteria, reducing population-level signaling and gene transfer, which can spread antibiotic resistance. This evidence points to mucin gels' unique ability to regulate the phenotypes of potentially pathogenic microbes. We also present our continuing efforts to design synthetic mucin-mimetic glycopolymers and test their efficacy at reducing microbial virulence. We hope that these principles can be used to develop mucin-inspired therapeutic polymers that could potentially alleviate the severity of dry mouth related symptoms based off of saliva's natural protection mechanisms.

*This work was supported by the NSF MRSEC Program award DMR1419807 and the NSF GRFP award 1122374.

12:03PM B64.00005: Molecular characterization of mucus binding

JACOB WITTEN (Presenter), TAHOURA SAMAD, KATHARINA RIBBECK, Biological Engineering, Massachusetts Institute of Technology — Mucus coats all wet epithelial surfaces of the body. Binding of small molecules to mucus has an important role in human health, as it may affect the diffusivity and activity of drugs and toxins that act in a mucosal environment. Despite the importance of mucus-small molecule binding, there is a lack of data revealing the precise physicochemical features of small molecules that lead to mucus binding. We developed a novel equilibrium dialysis assay to measure the binding of small molecules to mucin and other mucus components at unprecedented throughput, and combined this assay with a small molecule microarray to identify a novel mucin binding motif. Furthermore, we showed that for molecules with this motif, binding to mucins and the mucus-associated biopolymers DNA and alginate is modulated by differences in hydrophobicity and charge. Finally, we showed that molecules without the motif exhibited different trends from molecules with the motif, suggesting a complex dependence of mucin binding on molecular physicochemical properties.


12:15PM B64.00006: Microfluidic delivery of cutting enzymes for fragmentation of surface-adsorbed DNA molecules

JULIA BUDASSI (Presenter), Stony Brook University, ALAN GAN, East Brunswick High School, East Brunswick, NJ 08816, ALBERT TIAN, Ward Melville High School, E. Setauket, NY 11733, JONATHAN SOKOLOV, Stony Brook University — We describe a method for fragmenting DNA molecules surface-adsorbed and immobilized onto a polymethyl methacrylate (PMMA) coated silicon substrate by ‘molecular combing’ [1]. Microfluidic channels were formed into polydimethylsiloxane (PDMS) stamps using the soft lithography technique. The channel widths varied from 3.5 to 7 microns. The channels were pre-filled with a buffer solution by the channel outgas method [2]. Bovine serum albumin was diffused into the channels to coat the PDMS surfaces (which would otherwise strongly adsorb the DNase I cutting enzyme). DNase I was allowed to diffuse into the channel for 1 hour, resulting in efficient and precise fragmentation of the DNAs over the full channel length of 10mm. Applications to DNA sequencing will be discussed.


*Funding from NSF-AGEP (1344267) is gratefully acknowledged.
12:27PM B64.00007: Anomalous, non-Gaussian, viscoelastic and age-dependent dynamics of histone-like nucleoid structuring proteins in live Escherichia coli*  
YONG WANG (Presenter), ASMAA SADOON, Department of Physics, University of Arkansas — We report our measurements of the dynamics of H-NS proteins, which interact with both proteins and DNA simultaneously, in live E. coli bacteria. The dynamics turn out to differ significantly from other molecules reported previously. A new power-law distribution was observed for the diffusion coefficients of individual H-NS proteins. In addition, we observed a new distribution of displacements, which does not follow the Gaussian, Cauchy, or Laplace distributions, but the Pearson Type VII distribution. Furthermore, we experimentally measured, for the first time, the time/frequency dependence of the complex modulus of the bacterial cytoplasm, which deviates from the viscoelasticity of homogeneous protein solutions and shows a glass-liquid transition. Lastly, we observed that the dynamics of H-NS protein is cell-length/cell-age dependent. The findings are expected to fundamentally change the current views on bacterial cytoplasm and diffusional dynamics of molecules in bacteria.

*Arkansas Biosciences Institute (Grants No. ABI-0189, No. ABI-0226, and No. ABI-0277)  
National Science Foundation (Grant No. 1826642)

12:39PM B64.00008: Spatially-defined active matter using DNA strands  
ANIS SENOUSSI (Presenter), JEAN-CHRISTOPHE GALAS, ANDRÉ ESTEVEZ-TORRES, Sorbonne Universite and CNRS, Laboratoire Jean Perrin, Paris, France — Living systems have the incredible ability to organize themselves from molecules to the macroscopic scale. To understand the complex processes involved, we are reproducing some features of morphogenesis by rationally designing spatiotemporal patterns in artificial active materials. Taking advantages of the predictable interactions between their sequences, we use nucleic acids as elementary bricks to build complex active systems.

We designed a minimal system composed of protein filaments and modified molecular motors that can convert chemical energy into large-scale mechanical work upon the addition of a specific DNA strand. We expressed and purified each molecular components and rationally-assembled them to create a DNA-responsive material. This material undergoes macroscopic changes resulting in global or local contractions. This approach can be used to create original out-of-equilibrium systems that link a DNA-based chemical reaction network capable of generating a concentration landscape, as previously demonstrated [1], with a force-generating system.


12:51PM B64.00009: Selective response of DNA sequences at THz frequencies from numerical simulation*  
ALEXANDER SHVONSKI (Presenter), VICTORIA GABRIELE, KRZYSZTOF KEMPA, Boston College — We numerically simulate the response of DNA sequences to driving with THz radiation using the dynamical model of Ref. [1]. Homogeneous sequences of AT base-pairs experience an amplitude response that is distinct from homogeneous GC sequences in the parameter space of driving amplitude and frequency. Heterogeneous sequences with the same number of AT and GC pairs, but different ordering, also exhibit distinct responses in some regions of parameter space. Results indicate that THz driving is selective between different DNA sequences. [1] R. Tapia-Rojo, J. J. Mazo, and F. Falo, “Thermal and mechanical properties of a DNA model with solvation barrier,” Physical Review E 82, 031916 (2010).

*This work was supported by the National Science Foundation, grant No. PHY1725118.

1:03PM B64.00010: Surprising Charge Transport in DNA  
ROMAN ZHURAVEL (Presenter), Hebrew University of Jerusalem — The field of Nano-electronics concentrates a lot of interest from technological and scientific points of view. While charge transport in the solid state has been widely researched, for large single molecules many fundamental questions remain unsolved.

DNA is a good model molecule for many polymeric systems. Charge transport along DNA molecules has attracted scientific interest for over half a century. However, due to the many free parameters concerning these experiments, a variety of results were achieved, triggering an ongoing scientific debate on the DNA molecule conductivity. Our goal in this research is to reveal the charge transport mechanisms by controlled elucidation of the affecting parameters.

We have developed an experimental system for measurements of individual DNA molecules in a very precise and well defined manner with minimum number of experimental uncertainties. Preliminary measurements of 100bp dsDNA molecules with random and ordered sequences show unusually high currents and complex temperatures dependence, leading to new insights regarding the transport mechanism, which will be presented here.
RNA structure and kinetics including pseudoknots through complete landscape enumeration

OFER KIMCHI (Presenter), Harvard University; TRISTAN CRAGNOLINI, Chemistry, University of Cambridge; REES F GARMANN, VINOTHAN N MANOHARAN, MICHAEL PHILLIP BRENNER, Harvard University; LUCY COLWELL, Chemistry, University of Cambridge — Kinetic barriers as well as non-nested loops (pseudoknots) still pose challenges in the accurate prediction of RNA secondary structure. We will (1) develop a physical model to estimate the entropies of complex pseudoknots; and (2) demonstrate that their NP-complete enumeration need not impede their study. Our novel polymer physics model can address arbitrarily complex pseudoknots using only two free parameters corresponding to concrete physical quantities — over an order of magnitude fewer than the sparsest state-of-the-art phenomenological methods. By coupling this model to exhaustive enumeration of the set of possible structures, we compute the entire free energy landscape of secondary structures resulting from a primary RNA sequence. Despite our model’s parametric sparsity, it performs on par or better than previously published methods in predicting both pseudoknotted and non-pseudoknotted structures on a benchmark dataset of RNA structures of ≤ 80 nucleotides. We discuss the implications of the complete enumeration procedure employed for the study of kinetics.

*National Science Foundation [DMR-1420570, DMREF grant DMR-123869]; Office of Naval Research [N00014-17-1-3029]. NDSEG fellowship (OK). M.P.B. is an investigator of the Simons Foundation.

Protamine progressively folds DNA before looping

OBINNA UKOGU, ADAM SMITH, LUKA DEVENICA, HILARY BEDIAKO, ASHLEY CARTER (Presenter), Amherst College — In sperm, protamine proteins cause a rapid condensation of the DNA to almost crystalline packing levels. Understanding the physical mechanism for this dramatic process is an important limiting case in biophysics. In addition, protamine condensation of DNA may be useful in biomaterials research to assemble or fold DNA nanostructures. Here our goal is to understand the first step in the pathway, the folding of the DNA into a single loop by protamine. To answer this question, we image single molecules of DNA with bound protamine using an atomic force microscope (AFM). We also directly measure DNA folding dynamics in real time using tethered particle motion (TPM) assays. We expected our measurements to show a single folding event as the loop forms, but both measurements showed the presence of multiple, long-lived (100 s) intermediates. Structurally, these intermediates are half-loops or “c-shapes” that become more folded over as the protamine concentration increases. This data suggests a new model for DNA looping whereby small molecules coat the DNA and progressively fold it before forming a loop.

*This work was supported by the Research Corporation (Award #23239), an NSF CAREER award (Project #1653501), and Amherst College.

DNA Base-Pairing Visualized by Liquid-Cell Transmission Electron Microscopy

HUAN WANG (Presenter), BO LI, YE-JIN KIM, OH-HOON KWON, STEVE GRANICK, IBS Center for Soft and Living Matter — We show that fragile biological samples including DNA can be imaged using in situ transmission electron microscopy (TEM) without metal staining. Reporting statistical analysis of large datasets concerning single-strand and double-stranded aqueous DNA trapped in creases between paired graphene sheets, we visualize individual molecules with ~1 nm spatial resolution and ~100 ms time resolution for up to ~3 min, apparently without significant perturbation from the electron beam. Inspecting the time-dependent base-pairing of single-stranded DNA base-pairing, some pathways are as anticipated while others are surprising.

*The authors thank taxpayers who supported this work through the Korean Institute for Basic Science, project code IBS-R020-D1.
1:51PM B64.00014: Zippering dynamics of an RNA hairpin: Role of helicity*  
HUAPING LI, ALKAN KABAKCIOGLU (Presenter), Koc University — Despite several computational studies on hairpin folding and some supporting experimental data, role of the helical geometry on hairpin folding dynamics remains mostly unexplored. We here address this question by means of extensive molecular dynamics simulations on helical and (non-helical) "ladder-like" coarse-grained models. It is known that the folding time (t) of a thermally quenched RNA hairpin depends on the number of base pairs (N) as $t \sim N^\alpha$, where $\alpha=1+\nu$ is found to fit the experimental data with $\nu \approx 0.6$ (Flory exponent in three dimensions). We find that $\alpha$ changes from 1.6 to 1.2 ($=2\nu$) in three dimensions when duplex helicity is removed. Simulations in two dimensions ($\nu = 0.75$) and with a ghost chain ($\nu = 0.5$) further support the hypothesis $\alpha=2\nu$ for a "ladder-like" hairpin. The contrast between the two models which have identical single-strand properties suggests that duplex dynamics is a relevant component of the folding process, hence contradicting the theoretical models focusing on the non-equilibrium behavior of the unpaired segments alone. We propose a new scaling argument for $\alpha=1+\nu$ in helical chains and an energy argument for $\alpha \geq 2\nu$.


*This work was supported by TUBITAK through the grant 114F348.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B65 DBIO: Physics of Behavior II  
BCEC 260 - Yuhai Tu, IBM T J Watson Res Ctr - Tag(s): Focus

11:15AM B65.00001: Collective mechanical adaptation of honeybee swarms* [Invited]  
ORIT PELEG (Presenter), University of Colorado, Boulder, JACOB PETERS, MARY SALCEDO, L MAHADEVAN, Harvard University — Honeybee swarms form large congested tree-hanging clusters made solely of bees attached to each other. How these structures are maintained under the influence of dynamic mechanical forcing is unknown. To address this, we created pendant clusters and subject them to dynamic loads of varying orientation, amplitude, frequency and duration. We find that horizontally shaken clusters adapt by spreading out to form wider, flatter cones that recover their original shape when unloaded. Measuring the response of a cluster to an impulsive pendular excitation shows that flattened cones deform less and relax faster than the elongated ones. Particle-based simulations of a passive assemblage suggest a behavioural hypothesis: individual bees respond to local variations in strain by moving up the strain gradient, which is qualitatively consistent with our observations of individual bee movement during dynamic loading. Together, our findings highlight how a super-organismal structure responds to dynamic loading by actively changing its morphology to improve the collective stability of the cluster at the expense of increasing the average mechanical burden of an individual.


*US NSF PoLS grant 1606895

11:51AM B65.00002: Unsupervised Classification of Behavior for Open Field Mouse Recordings*  
UGNE KLIBAITE (Presenter), JESSICA VERPEUT, MIKHAIL KISLIN, SAMUEL S WANG, JOSHUA SHAEVITZ, Princeton University — Advances in computer vision and deep learning have made it possible to explore animal behavior at fine temporal and spatial scales. In particular, new advances in automated pose detection make it possible to track fine-scale movements in mice, a model system for the study of many aspects of neural function, from locomotion and coordination to complex neurodevelopmental disorders such as autism. We combine the use of a deep-learning-based approach called LEAP (LEAP Estimates Animal Pose), which produces estimates of joint coordinates, with unsupervised classification in order to discover distinct behavioral bouts in 72 wild-type mice in an open field arena over five subsequent days. We use the resulting behavioral phenotypes to explore the evolution of behavior in individuals over time, as well as identify behavioral differences between wild-type individuals and genetic models of neurodegenerative disease. These differences elucidate complex phenotypes that arise from neuropathology, and capture greater complexity with fewer experimental constraints than simpler high-throughput behavioral assays.

*This work was supported by the National Institutes of Health (R01MH115750) and the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030)
Experimental testing of the model both analytically and through computer simulation. This model makes robust predictions that can be applied to various scenarios. The ratio of the rates of creation and evaporation of the pheromones is crucial. Here we map the phase diagram for the extended model to forage from both food sources equally. We extend this model to include indirect recruitment of ants forage bistably from the different food sources, but as the population size is increased over a certain critical population size, they will start to forage from one of two food sources, the ants exhibit this type of bistability. At small population sizes, the ants will forage from one of two food sources, but as the population size is increased over a certain critical population size, they will start to forage from both food sources equally. We extend this model to include indirect recruitment of ants to a food source via a pheromone laid out by other ants. The critical population size of this extended model depends on the ratio of the rates of creation and evaporation of the pheromones. Here we map the phase diagram for the extended model both analytically and through computer simulation. This model makes robust predictions that can be experimentally tested.

*Work done in collaboration with A.P. Vedurmudi and J. Christensen-Dalsgaard; partially supported by BCCN–Munich.
12:51PM B65.00007: Decompositions of Behavioral Modulations and Run Shapes in Drosophila Larvae  JOSEPH SHOMAR (Presenter), ANGGIE FERRER, JOSHUA FORER, TOM ZHANG, MASON KLEIN, University of Miami — With its small size and limited motor tool set, the Drosophila larva is a good system for studying how animals alter their behavior to reach optimal conditions. We aim to distinguish behavioral modulations caused by the physical effects of temperature from those due to sensory input and to decompose curved runs (bouts of forward crawling) into run-shape eigenvectors.

To decouple the causes of behavioral modulation, we use temperature-insensitive mutants and 3 different spatiotemporal stimulus environments; PID controllers maintain the different spatial and temporal gradients. Many larvae are recorded during free navigation and computer vision software segments trajectories into alternating sequences of runs and turns, analogous to classic 2D random walks. The turn rate is the dominant characteristic of diffusive processes and larvae primarily achieve navigation by modulating it. Monte-Carlo simulations allow for comparison with experimental data and for analysis of otherwise unfeasible experiments.

Our results suggest that larvae exhibit different average speeds due to physical changes, and exhibit different turn rates because of both physical changes and sensory input. Computational methods are currently being explored for use in decomposing runs into run-shape eigenvectors.

1:03PM B65.00008: Slingshot Spider: Ultrafast kinematics, biological function and physical models of an extreme arachnid  SYMONE ALEXANDER (Presenter), SAAD BHAMLA, Georgia Institute of Technology — The natural evolution of ultrafast motion in living systems has inspired physicists, biologists, and engineers to design biomimetic materials and fast-moving robots. In this work, we quantify kinematics of a tiny ‘slingshot spider’ native to the Peruvian Amazon Rainforest. This spider exploits a conical 3D web structure to slingshot itself at extreme speeds and achieve accelerations exceeding 600 m/s², an order of magnitude faster than a cheetah (13 m/s²). To the best of our knowledge, this is the fastest movement by an arachnid ever recorded. In this talk, we will discuss how slingshot spiders achieve ultrafast motion, and share insight about the biological function of this extraordinary prey capture strategy. We reveal how the motion is actuated by a trigger mechanism that happens under a millionth of a second (0.8 μs). Lastly, we extract the underlying physics of this motion and the role of the 3D web in power amplification using simple physical models constructed from elastic rubber bands. The physical models further shed insight into built-in safety structures in the web that rapidly dissipate excess energy and protect the spider against the large stresses generated during this extreme motion.

1:15PM B65.00009: Testing a thermodynamic approach to collective animal behavior in laboratory fish schools  JULIA A GIANNINI (Presenter), Physics, Syracuse University, JAMES PUCKETT, Physics, Gettysburg College — Social animals including insects, fish, birds, and even humans exhibit self-organized collective behavior. Macroscopic properties arise not only from interactions between individuals, but also from environmental cues. Here, we present results from a series of experiments that utilize high speed footage of 2D schooling events, particle-tracking, and projected static and dynamic light fields to observe and control the behavior of negatively phototaxic laboratory fish schools (Hemigrammus bleheri). First, we use static light fields consisting of dark circular regions to produce visual stimuli that confine the schools to a range of areas. Next, we use dynamic light fields where the radius of the dark region shrinks linearly with time to compress the schools. Through measuring global quantities analogous to density, temperature, and pressure in statistical mechanics, we find that the temperature-like parameter depends on the speed of the compression. We discuss the implications of our results on current models.

1:27PM B65.00010: Mechanics of Snow-diving Animals  LEENA PARK (Presenter), Department of Biological and Environmental Engineering, Cornell University, EMMANUEL VIROT, Harvard University, SUNGHWAN JUNG, Department of Biological and Environmental Engineering, Cornell University — Some fox species plunge-dive to catch prey (e.g. rodents) underneath a pile of snow. This hunting behavior is known as “mousing.” In this behavior, the diving speed can range between 2 and 4 m/s. Here, we investigate how foxes dive into snow without alerting prey. An important factor to consider in this mousing process is the impact on snow. Snow is a compressible fluid consisting of 1~10% ice and the rest of air. When a tapered object (in this case, a fox’s head) compresses or dives into the snow, the pressure/information front does not propagate fast enough for the prey to detect and escape. Animals that portray this mousing behavior, such as red foxes, arctic foxes, and even servals and other feline species, all generally share a slim, narrow facial structure. In this study, 3D printed fox heads and similar funnel-shaped objects are dropped into a pile of snow to understand the propagation of the pressure in snow and the drag on the object.
1:39PM B65.00011: How to jump without spinning  MADHUSUDHAN VENKADESAN (Presenter), ALEXANDER LEE, ERIC CHAN, Department of Mechanical Engineering and Materials Science, Yale University — The remarkable displays of jumping in animals like frogs have inspired many studies on how their muscles generate power. However, in their natural habitats, these animals typically push off against muddy and unpredictably compliant terrains that induce the feet to apply unequal forces on the ground. This may result in substantial angular momentum at take-off, and have dire consequences such as the animal's mouth pointing away from an intended prey, or landing in ways that prevent escaping a predator. We investigated whether morphological features of jumping animals may alleviate this critical problem and help them to jump without spinning. Our analyses and experiments with a brainless passive mechanical jumper focus on the dynamics within the frontal plane as it pushes off unequally using two legs. We find that a flexible pelvis is sufficient to reduce the angular momentum due to unequal leg forces by several orders of magnitude in both our experiments and mathematical analyses. A flexible pelvis acts like a whiffletree mechanism that can balance loads between the legs. Our scaling analyses of these jumpers suggest passive mechanical designs for robotic jumpers and point to the critical role of pelvis morphology in jumping animals for stability.

1:51PM B65.00012: Geckos reconfigure control modules to self-right on diverse substrates  BENJAMIN MCINROE (Presenter), University of California, Berkeley, THOMAS LIBBY, University of Washington, DANIEL E KODITSCHEK, University of Pennsylvania, ROBERT FULL, University of California, Berkeley — Animals synergistically employ multiple appendages and body segments to perform behaviors. We hypothesize that these controllable components can be represented by sets of simple models (templates), recruited in series or parallel to provide multiple strategies for executing a maneuver. As the physics of substrate-body interaction changes, these control modules may be reconfigured for new functions, enabling task completion in new environments. To further define our conjecture, we measured terrestrial self-righting in geckos. On flat, rigid surfaces, geckos self-righted with average righting times of 0.22 ± 0.03 s using dynamic motions including body torsion and tail-ground contact. When placed on a partially excavated surface where the tail could not make ground contact, average righting time increased by 40%. However, righting time decreased to 0.19 ± 0.02 s if the geckos used a new strategy, swinging the tail in a way similar to inertial air righting. Body-level behavior was invariant to the dichotomy in tail control. From our experiments, we begin to develop composable templates for terrestrial righting. Our results suggest that geckos employ the tail as a multifunctional control module in parallel with a body torsion template to increase robustness to challenging substrates.

2:03PM B65.00013: Tuning impulsive mechanisms to their environment*  SATHVIK DIVI (Presenter), Mechanical Engineering Department, Carnegie Mellon University, MARK ILTON, Department of Physics, Harvey Mudd College, XIAOTIAN MA, SARAH BERGBREITER, Mechanical Engineering Department, Carnegie Mellon University — Organisms like fleas and froghoppers achieve fast repeatable motions due to the presence of highly tuned impulsive mechanisms; a motor slowly loads a spring, and this stored energy is quickly released by a latch. In this work, we explore how the latch and spring parameters are tuned to their environments to maximize performance. An analytical model is constructed to include both impulsive system parameters (e.g., mass, spring, latch) as well as the compliance and inertia of the environment. Simulations are then performed across the design space to understand the tuning relationship between the latch, spring and substrate (environment) parameters. These results are validated experimentally using an 8-gram robot for which latch and spring parameters can be changed. This robot is then tested on multiple compliant substrates. Results demonstrate that the latch and spring parameters can be tuned to their environment to maximize take-off velocity. Certain combinations of latch/spring/environment parameters result in recovery of energy from the compliant substrate thereby resulting in higher performance, and ultimately efficient, fast, and repeatable motions.

*Supported by the U.S. Army Research Laboratory and the U.S. Army Research Office under contract/grant number W911NF-15-1- 0358.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B66 DBIO GSNP GSOFT: Morphogenesis II  BCEC 261 - Zi Chen, Dartmouth Coll - Tag(s): Focus
11:15 AM B66.00001: Self-repairing symmetry in jellyfish* [invited] LEA GOENTORO (Presenter), MENGSHA GONG, Division of Biology and Biological Engineering, California Institute of Technology, CHIN LIN GUO, Institute of Physics, Academia Sinica, Taiwan — Standing on a British shore a century ago, D’Arcy Thompson wondered whether the shape of a medusa can be likened to the equilibrium form of a gelatinous drop. While many study how animals get their shapes during development, less is understood about how or whether animal shape is regulated in adulthood. We pursue this question of animal shape regulation in the moon jellyfish, Aurelia aurita. Using grafting and mechanical modulations, we found that Aurelia shape is governed by a morphogenetic system with multiple equilibria – such that we can make jellyfish with various stable shapes, including oval, rectangular, and triangular. Further, combining experimental and mathematical analyses, we found evidence that the shape of a medusa is governed as a dynamic equilibrium of the underlying tissue mechanics. Thus, as Thompson envisioned, belying its calm majesty, the shape of jellyfish is not statically encoded, but rather a continual balancing act.

*National Science Foundation
National Institute of Health
James S. McDonnell Foundation

11:51 AM B66.00002: On “irreversible” torsion in early chick embryonic brain development* HAO ZHANG (Presenter), HANNAH GROVER, SHICHENG HUANG, GUANGCHAO WAN, ZI CHEN, Thayer Engineering, Dartmouth College — The rightward torsion of the chick embryonic brain tube is one of the earliest organ-level left-right asymmetry developmental events. Previous studies have shown that vitelline membrane (VM) exerts the necessary force on the chicken embryo brain that drives the torsion, and surface tension can replace the mechanical role of VM resulting in a similar degree of torsion at a comparable stage. However, recent experiments show that when the surface tension is removed the torsion does not fully reverse suggesting that there are other overlooked mechanical factors in this process. Here, we show through a combination of in vivo experiments and a physical model of the embryonic morphology that the twisting of the chick embryonic brain tube is partially reversed when the surface tension is removed and the deformation of the early brain can be path dependent. We also studied the effect of embryonic curvature and shape on the degree of torsion, and identified how buoyancy may play a mechanical role in in this “irreversible” brain torsion process.

*Z.C. acknowledges the support by the Society in Science-Branco Weiss fellowship, administered by ETH Zurich.

12:03 PM B66.00003: Motility and adhesion gradient induced vertebrate body axis elongation and somite formation ANUPAM GUPTA (Presenter), LAKSHMINARAYANAN MAHADEVAN, Harvard University — The body of vertebrate embryos forms by posterior elongation from a terminal growth zone called the Tail Bud (TB). The TB produces highly motile cells that eventually constitute the presomatic mesoderm (PSM), a tissue playing an important role in elongation movements. PSM cells establish an anterior-posterior cell motility gradient which parallels a gradient associated with the degradation of a specific cellular signal (Fgf8) known to be implicated in cell motility. As Fgf8 degrades over time, anteriorly positioned cells move less, before eventually coming to a rest as they aggregate into epithelial somites. We show that simple microscopic and macroscopic mechano-chemical models for tissue extension that couple Fgf activity, cell motility, cell density and tissue rheology at both the cellular and continuum levels suffice to capture the speed and extent of elongation. These model qualitatively capture the condensation of cells into somites due to the effect of adhesion in the anterior region. These observations explain how the continuous addition of cells that exhibit an increase in cell density and a gradual reduction in motility combined with lateral confinement can be converted into somite formation in the anterior region and an oriented movement and drive body elongation.

12:15 PM B66.00004: Biomechanics of anteroposterior axis elongation in the chicken embryo ARTHUR MICHAUT (Presenter), Genetics, Harvard Medical School, KARINE GUEVORKIAN, PCC, Institut Curie, OLIVIER POURQUIE, Genetics, Harvard Medical School — In vertebrate embryos, anteroposterior axis elongation is a crucial developmental process resulting in the establishment of the basic body plan and the growth of the embryo from the tail region. In chicken, it has been proposed that a gradient of random cell motility along the presomitic mesoderm (PSM), rather than directed cell movements, drives axis elongation (Bénazéraf et al, Nature 2010). In order to access the physical mechanisms that could explain this process, we study the rheological properties of the PSM and the forces produced due to posterior PSM expansion. Both micropipette aspiration, as well as rounding experiments, show a liquid-like behavior for the PSM, and allow us to measure its viscoelastic properties. In addition, we have developed a novel cantilever-based system to measure the force of axis elongation and we relate it to the cell movements along the axis. We demonstrate that an isolated PSM explant elongates autonomously and contributes to the total elongation force of the embryo, highlighting its role in axis elongation. Taken together, our results provide a first quantitative description of the mechanics of the tail region in the chicken embryo, which will be essential for future modeling of axis elongation.
12:27 PM B66.00005: Actomyosin-mediated cytoplasmic flows synchronize the cell cycle in *Drosophila* embryos

AVANEESH NARLA (Presenter), University of California, San Diego, VICTORIA E. DENEKE, Department of Cell Biology, Duke University, ALBERTO PULIAFITO, Laboratory of Cell Migration, IRCCS (Istituto di Ricerca e Cura a Carattere Scientifico), STEFANO DI TALIA, Department of Cell Biology, Duke University, MASSIMO VERGASSOLA, University of California, San Diego — The synchronous cleavage divisions of early embryogenesis require coordination of the cell cycle oscillator, the dynamics of the cytoskeleton and the cytoplasm. As yet, it remains unclear how spatially restricted biochemical signals are integrated with physical properties of the embryo to generate collective cell cycle dynamics. Biochemical oscillations are initiated by local Cdk1 inactivation close to the nuclei and spread through the activity of mitotic phosphatase PP1 to generate cortical myosin II gradients. These gradients generate cortical and cytoplasmic flows that control proper nuclear positioning. Despite being in the very low Reynolds number regime, we find that Stokes flow does not adequately describe these flows. We will describe the physical properties of the flows, its role in nuclear migration and synchronization of the cell cycle in *Drosophila* embryos.

12:39 PM B66.00006: Quantifying the forces associated with body elongation in a chicken embryo

FENGZHU XIONG (Presenter), CHON U CHAN, WENZHE MA, Harvard University, BERTRAND BÉNAZÉRAF, Centre de Biologie Intégrative, Université Toulouse, L MAHADEVAN, OLIVIER POURQUIE, Harvard University — The role of mechanical forces in the context of morphogenesis and growth regulation in an embryo is now well accepted. Yet, it is still a challenge to perform mechanical measurements and manipulations on a whole embryo to obtain quantitative insights. Here we use chick embryos in the gastrulation stage to study how the tissues that form the body axis coordinate their rates of elongation. We found that the coordination and axis straightness are achieved via a positive feedback loop involving mechanics, as revealed by surgical implantation of soft gels and mechanical manipulation with magnetic pins. We also show that cell movement is required for the generation of, and can be a response to, the tissue forces. Finally, we deploy custom tools to apply force-clamps on the embryo over long times to affect both the growth and form of the embryo.

*The authors acknowledge the National Institutes of Health (NIH) for funding support*

12:51 PM B66.00007: Patterns make patterns: how hierarchical self-organization couples cell geometry to biochemical dynamics - Experiment

TZER HAN TAN (Presenter), Physics, Massachusetts Institute of Technology, MANON WIGBERS, FRIDTJOF BRAUNS, Physics, Ludwig Maximilian University of Munich, ZAK SWARTZ, Whitehead Institute, Massachusetts Institute of Technology, ERWIN FREY, Physics, Ludwig Maximilian University of Munich, NIKTA FAKHRI, Physics, Massachusetts Institute of Technology — Many cellular and developmental processes rely crucially on self-organization of protein patterns in space and time. When these protein patterns are coupled to force generation pathways, they can precisely pattern mechanical stress during processes such as cell division or tissue folding. Importantly, these mechanical processes generate shape deformations and cytoplasmic flows, which can modulate intracellular reaction-diffusion dynamics. This suggests a close coupling between cell mechanics and biochemical dynamics. But how do these protein patterns respond to a mechanically changing environment? Here, we use the Rho GTPase driven surface contractions waves in starfish oocytes as a model system to study these effects. By constraining oocytes in microfabricated shape chambers, we found that the behavior of the Rho waves can be qualitatively modulated. Further experiments show that the upstream regulator Cdk1 forms a cytosolic gradient which is modulated by cell geometry, forming a template for downstream pattern formation. We demonstrate that the surface contraction wave is a result of a cascade of coupled protein patterns, which we call ‘hierarchical self-organization’.

1:03PM B66.00008: Patterns make patterns: how hierarchical self-organization couples cell geometry to biochemical dynamics - Theory

MANON WIGBERS (Presenter), Ludwig-Maximilians University Munich (LMU), TZER HAN TAN, Massachusetts Inst of Tech-MIT, FRIDTJOF BRAUNS, Ludwig-Maximilians University Munich (LMU), NIKTA FAKHRI, Massachusetts Inst of Tech-MIT, ERWIN FREY, Ludwig-Maximilians University Munich (LMU) — Many cellular and developmental processes rely crucially on self-organization of protein patterns in space and time. When these protein patterns are coupled to force generation pathways, they can precisely pattern mechanical stress during processes such as cell division or tissue folding. Importantly, these mechanical processes generate shape deformations and cytoplasmic flows which, in turn, can modulate intracellular reaction-diffusion dynamics. This suggests a close coupling between cell mechanics and biochemical dynamics. But how do these protein patterns respond to a mechanically changing environment? Here, we use the Rho GTPase driven surface contractions waves in starfish oocytes as a model system. We combine experimental results with a reaction-diffusion model and show how a cascade of coupled protein patterns creates a feedback loop between the Rho membrane dynamics and the cell shape. We posit that such hierarchical self-organization is a general mechanism for cells to sense changes in its global geometry.
1:15PM B66.00009: Tuning biochemical patterns by dynamic mechanical deformations  MELIS TEKANT (Presenter), PETER FOSTER, NIKTA FAKHRI, Massachusetts Institute of Technology — Throughout embryonic development biochemical patterns are crucial for initiating and guiding vital cellular processes. As the geometry of the biological system evolves, patterns also adapt to reflect the new geometry, suggesting that patterning and geometrical deformations are closely coupled. Yet the mechanisms underlying this coordination are not fully understood. Here, we use cortial Rho activity in the oocytes of the starfish *Patricia miniata* as a model system to explore such coupling in evolving mechanochemical systems. In addition to being highly deformable, the oocyte exhibits versatile and tunable dynamical patterns on the membrane. Through the use of micropipette aspiration, we impose geometrical constraints on the oocyte that can be actively tuned. The evolution of the pattern in response to the changing geometry is probed in real time, revealing the underlying properties of the dynamics. This method provides a novel approach to studying the interplay between biochemical patterning and mechanically evolving biological systems.

1:27PM B66.00010: Active mechanics of starfish oocytes  PETER FOSTER (Presenter), NIKTA FAKHRI, Massachusetts Institute of Technology — During meiosis, starfish oocytes exhibit a dramatic surface contraction wave characterized by a band of large-scale deformation traveling from the vegetal pole to the animal pole. This inherently mechanical process is driven by active stresses generated by actomyosin contraction. What are the mechanical properties of these oocytes? How can modulating cytoskeletal organization affect the emergent mechanics and the contraction wave dynamics? Here, we present experimental results beginning to address these questions. Using micropipette aspiration, we find that the mechanical properties are well described by a modified Maxwell model, allowing us to quantitatively measure the viscosity, surface tension, and elastic modulus. These mechanical measurements are complemented by work combining quantitative light microscopy and pharmacological inhibition to assess cytoskeletal contributions to the emergent contraction wave dynamics. For example, using the actin inhibitor cytochalasin D, we find a dose dependent decrease in the magnitude of the contraction. This work represents a step towards understanding cytoskeletal contributions to the emergent dynamics and mechanics in starfish oocytes and in actin cortices more generally.

1:39PM B66.00011: Steady-state contractile actin flow in *Xenopus* egg extract droplets  JIANGUO ZHAO (Presenter), KENGO NISHI, Faculty of Physics, University of Gottingen, CHRISTOPH F. SCHMIDT, Department of Physics, Duke University — The actin cytoskeleton of eukaryotic cells is a highly dynamic viscoelastic “active material”. A typical cell maintains a cortex lining that supports the cell membrane, a polymer network consisting of actin, myosin motors and a plethora of regulatory proteins. Actin turns over between polymeric and monomeric forms on a time scale of minutes. Myosin motors generate active contractile stresses that can induce large-scale actin flow, which is essential for the transport of cytoplasmic components, locomotion as well as shape changes of cells. How exactly so many interacting biochemical processes result in static or dynamic steady states is unclear. Using water-in-oil droplet containing cytoplasmic extract of *Xenopus laevis* eggs as a model system for an active cytoskeleton, we could produce radially convergent continuous flow of polymerized actin that persist over time scales much longer than the turn-over time of a single actin filament. We mapped the spatiotemporal distribution of this contractile persistent actin flow. Interestingly, we found that macromolecular cargo present in the extract gets transported into the center of the droplet and compacted into a jammed state. We demonstrated this by tracking embedded IR fluorescent single-walled carbon nanotubes as mechanical probes.

1:51PM B66.00012: Mechanical competition leads to dynamic instabilities and heterogeneity in stem-cell derived cardiomyocytes*  DANIEL HÄRTTER (Presenter), TIL DRIEHORST, Third Institute of Physics-Biophysics, University of Göttingen, WOLFRAM ZIMMERMANN, Institute for Pharmacology, University of Göttingen Medical School, CHRISTOPH F. SCHMIDT, Department of Physics, Duke University — Cooperative and synchronized contraction of sarcomeres is important for the optimal function of cardiomyocytes. Theories of collective molecular motor dynamics, however, predict the possibility of emergent phenomena such as dynamic instabilities and spontaneous oscillatory motion due to non-monotonic force-velocity relations. We have tracked the contractions of individual sarcomeres in stem-cell derived cardiomyocytes by endogenous fluorescent labeling of α-actinin 2 using CRISPR/Cas9 technology. Cardiomyocytes were attached to micropatterned elastic substrates with various Young’s moduli between 7 and 60 kPa. On soft substrates, sarcomeres in one cell contracted coherently, whereas contractions became increasingly incoherent and heterogeneous with increasing substrate stiffness. These findings suggest that competition between sarcomeres, enforced by rigid mechanical boundary conditions, perturbs dynamic coherence. Using a simple dynamic model, we show that elastic coupling of z-lines to the substrate in conjunction with a non-monotonic force-velocity relation can account for many of the observed features.

*ERC
2:03PM B66.00013: Cilia coordinated temporal-spatial flow in the mammalian brain* YONG WANG (Presenter), Fluid Physics, Pattern Formation and Biocomplexity, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany, SHOBA KAPOOR, Genes and Behavior, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany, CHRISTIAN WESTENDORF, Fluid Physics, Pattern Formation and Biocomplexity, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — The walls of the ventricular system of mammalian brain are lined with ependymal cells, each of which sprouts a bundle of cilia that constantly beat and thereby maintain directional cerebrospinal fluid (CSF) flow. A transport network driven by coordinated motile cilia inside the ventral third ventricle (v3V) was reported recently. This network contains several CSF flow streams, generates flow patterns such as separatrix and whirl, and may coordinate the delivery of CSF components to different target sites within the ventricle. Particle tracking showed that in mouse brain this flow network locally differs between the two sides of the v3V and changes with age, which implies an age-dependent complex delivery system for CSF constituents. We also studied numerically the contribution of the temporal-spatial flow pattern to the overall CSF flow within the 3D ventricular cavity, and uncover likely physiological consequences of the flow pattern.

*We thank the Max Planck Society for financial support.

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B67 APS/SPS: Undergraduate Research II B67.00001: Visualizing Contact Area Growth in Frictional Interfaces* THOMAS PILVELAIT (Presenter), SHMUEL RUBINSTEIN, School of Engineering and Applied Sciences, Harvard University, SAMUEL DILLAVOU, Physics, Harvard University — Seemingly static interfaces between two solids are in fact dynamic. These multicontact interfaces (MCIs) exert enormous stresses on tiny contact areas, causing time-dependent deformation, also known as aging. Though these phenomena are ubiquitous in engineering and the sciences (e.g. from micromachines to plate tectonics), their underlying mechanisms are not yet well understood. Quantitative, 2D measurements of the real contact area between a polymer solid and a glass plate are obtained over a variety of normal loads and time steps. By varying geometric and elastic properties of our samples, we induce variations in the 2D structure of contact growth, which give insight into the mechanisms that produce aging in frictional interfaces.

*T.P. acknowledges support from the Harvard College Research Program.

B67.00002: Ultrafast Laser Ablation of Graphene under Water Immersion* ETHAN RICHMAN (Presenter), MAC SELESNICK, YU-TIEN CHOU, YANPEI DENG, LOGAN KAEBLING, ZIWEI LIANG, GREY MCALAINE, CAMERON MILLER, CHRISTOPHER LAFRATTA, PAUL CADDEN-ZIMANSKY, Bard College — We report on a technique to pattern 2-D materials by ultrafast laser ablation. This resist-free method is performed in single step using a Ti:sapphire laser coupled to a microscope with a programmable x-y stage. While close examination of samples ablated in ambient air revealed persistent defects, a novel modification to the technique by carrying out the ablation under water immersion dramatically reduced the observed defects. In addition to using this technique to create submicron graphene wires, its application to other 2-D materials, such as hexagonal boron nitride, is detailed.

*We thank the Sherman Fairchild Foundation for funding, as well as the Bard Summer Research Institute.

B67.00003: Theoretical Study of Amorphous Graphene* VICTOR BARONE (Presenter), BLAIR TUTTLE, Penn State Erie — Amorphous graphene is a two-dimensional sheet of carbon atoms with three fold coordination. The atoms in amorphous graphene mostly form hexagons but there are regions of interconnected 5, 6, 7 and 8 sided objects with carbon atoms at the vertices. Here we use density functional calculations to explore the mechanical and electronic properties of amorphous graphene.

*Research supported by Tuttle’s NSF RUI-DMR 1506403. This research was conducted using Advanced Cyber Infrastructure computational resources provided by The Institute for Cyber Science at The Pennsylvania State University.
**11:51 AM B67.00004: Mechanism to Generate Larger Strain in Two-Dimensional Materials**

MELISSA BOWMAN (Presenter), ANGELA COE, GUOHONG LI, EVA ANDREI, Rutgers University, New Brunswick — Two-dimensional (2D) materials, especially graphene, are very sensitive to strain due to every atom residing at the surface. Theory predicts that when graphene experiences large strain, its electronic properties change dramatically. In particular for strain in excess of 20% a strain-dependent gap is expected to develop in its band structure, providing a mechanism to switch its transport properties on and off. Thus far however strain levels achieved with standard techniques could not exceed a few percent. We present a piezoelectrically controlled technique that can introduce, in a controlled way, a continuously variable amount of uniaxial strain in 2D materials reaching up to ~25% where graphene ruptures.

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

**12:03 PM B67.00005: Effect of Lattice Mismatch Strain in Oxygen Deficient Strontium Titanate Films**

FRANCIS WALZ (Presenter), JOSEPH CARTELLI, AZRIEL WEINREB, ANTON WIGGINS, JEFFREY SIMPSON, RAJESWARI M KOLAGANI, Towson University, OLEKSIY SVITELSKI, Physics, Gordon College — SrTiO3 (STO) is a quantum paraelectric material which exhibits electronic phenomena that are interesting for technological applications. Applications of STO include its use as a dielectric layer in semiconductor devices, and as a photocatalytic material. Varying the oxygen content in STO affects the crystal structure and electronic properties which are important for such applications. In oxygen deficient STO (SrTiO3-y), the valence of the titanium ion and the average ionic sizes are different from those of the stoichiometric form (SrTiO3), leading to structural and electronic changes. Our study focuses on the structure and electronic properties of oxygen deficient epitaxial thin films of STO grown by Pulsed Laser Deposition on substrates with varying degrees of lattice mismatch. Previous work in our laboratory has shown that tensile strain promotes oxygen deficiency in epitaxial thin films of another perovskite oxide CaMnO3-y. Such coupling may be employed to engineer novel phases in thin films. We explore whether a similar coupling between strain and oxygen stoichiometry is present in STO. We will present the results of x-ray diffraction, electrical conductivity, Raman spectroscopy and atomic force microscopy studies.

*NSF Grant DMR 1709781 and the FCSM Fisher Endowment grant

**12:15 PM B67.00006: Annealing and Characterization of Niobium Oxide Films Deposited With Atomic Layer Deposition**

ANDREW H. ROWLEY, ZACHARY ROBINSON (Presenter), SUNY Brockport, ALEXANDER C. KOZEN, ASEE Postdoctoral Fellow residing at U.S. Naval Research Laboratory, MARK TWIGG, SHARKA PROKES, U.S. Naval Research Laboratory — Niobium oxides have seen a rise in interest due to their potential usefulness in optical, electronic, and memristive devices. Specifically, Nb2O5 and NbO2 have bandgaps of ~3.5 eV and ~1.2 eV, respectively. Nb2O5 is a high-k dielectric (k~41) and has a high refractive index (n~2.2). Both materials have the potential to be used in nonvolatile or volatile memristor devices. Amorphous thin-films of Nb2O5 and NbO2 were grown with atomic layer deposition on 4" Si(110) wafers with native oxide. The wafers were diced into 1 cm squares, and annealed in both inert and reducing environments in an atmospheric pressure tube furnace. The anneals were performed for up to 120 minutes, with temperatures ranging from 550 °C up to 1000 °C. It was found with X-ray diffraction and Raman spectroscopy that the amorphous Nb2O5 crystallizes at 550 °C, and nucleates crystalline NbO2 islands at 750 °C. Anneals performed at 1000 °C were found to be fully recrystallized as NbO2. As-deposited amorphous NbO2 was found to crystallize at similar temperatures. For both NbO2 and Nb2O5, trends were observed in the sample morphology, indicating that annealing temperature and duration are important in the reduction and recrystallization of as-grown Nb2O5 and NbO2 on SiO2.

**12:27 PM B67.00007: Perovskite Films on Plasmonic Metamaterials**

ASSATA ACEY (Presenter), Physics, Bryn Mawr College, GIORGIO ADAMO, HARISH KRISHNAMOORTHY, CESARE SOCI, Physics and Applied Physics, Nanyang Technological University, MICHAEL LIM, Physics and Astronomy, Rowan University — Perovskites are of rising importance for current applications in the field of sustainable energy. Of particular interest are the optical properties of patterned perovskite films. The properties of these gratings have been studied with simulations in COMSOL, providing predictions of how the reflection and absorption at different wavelengths may be tuned by varying the configuration of perovskite-coated gratings. Using inputs values for n and k determined through ellipsometry of the perovskite film, this work has led to promising grating designs that are now candidates for testing. One fabricated grating did not perform according to prediction, implying degradation in the material over time that was later confirmed.

*The authors acknowledge support from NSF-IRES 1559410.
12:39PM B67.00008: Optical properties of AlAu alloyed and intermetallic thin films* ABDUL QADEER REHAN (Presenter), MARIAMA REBELLO SOUSA DIAS, University of Richmond — Noble metal alloys have been widely investigated as an alternative to pure metals for improving the optical response of optoelectronic devices operating in the visible range of the electromagnetic spectrum. However, their use is hardly extended to the ultra-violet (UV) range. As an alternative, aluminum-based alloys could expand the functionality of photonic devices into the UV range of the spectrum. In this work, we fabricated and measured the optical response of a binary mixture of gold (Au) and aluminum (Al) thin films. The thin films were deposited on a glass substrate via the co-sputtering method. The dielectric functions were measured using spectroscopic ellipsometry. Also, we investigated how the optical response of the thin films changed under a wide range of temperatures, from 25°C to 200°C. We demonstrate that, in some cases, a bimetallic material can outperform their pure metal counterparts after the temperature treatment, e.g., Al0.15Au0.85 shows an increased quality factor of its localized surface plasmon (QLSP) than pure Au and Al. Moreover, we observe that Al-rich thin films are stable, no significant changes were noticed in its dielectric function, as temperature increased.

*University of Richmond Arts & Sciences Summer Fellowship.

12:51PM B67.00009: Exploring the effects of bismuth clustering on the energy band gap of GaBi\textsubscript{x}As\textsubscript{1-x} semiconductors* JOHN CARLTON (Presenter), ARTHUR LIN, GARNETT BRYANT, University of Maryland, College Park, JQI, NIST — Substituting Bi anions in place of As allows for effective tuning of the energy band gap of GaBi\textsubscript{x}As\textsubscript{1-x}. Such band gap control has applications in spintronics (quantum computing) and optoelectronics (photovoltaics). The energy band gap of dilute GaBi\textsubscript{x}As\textsubscript{1-x} alloys is dependent on the alloy configuration, in addition to the alloy concentration. In order to explore the effects of Bi configuration in dilute GaBi\textsubscript{x}As\textsubscript{1-x} alloys, an atomistic, nearest-neighbor, sp\textsuperscript{3}d\textsuperscript{*} tight-binding Hamiltonian is used to determine the energy levels for statistically constructed alloy supercells with random, clustered, and gaussian weighted distributions. By correlating these energies to both qualitative and quantitative measures of Bi clustering, the effects of Bi clustering are explored. From our theoretical calculations, we show that increases in Bi clustering correlate with greater decrease in band gap energies. Additionally, in more densely clustered configurations, we see higher total Bi probability for hole states and faster Bi band broadening congruent with the band anti-crossing model for GaBi\textsubscript{x}As\textsubscript{1-x}.

*This project is funded by the National Science Foundation under DMR – 1505628.

1:03PM B67.00010: Effects of Temperature on the Vibrational Mode Dynamics of Cubane* ANTHONY FROEHLICH (Presenter), GUOPING ZHANG, Indiana State University — Ab initio calculations and the Boltzmann distribution are utilized to determine the effects of temperature on the vibrational modes of cubane. Attention is paid to the propagation of energy throughout the normal modes as temperature changes, providing information about chemical and physical characteristics of cubane and their relationship to temperature. The order in which the energy levels of normal modes increase, the effect of this energy on the movement of atoms in a molecule, and the effects of this movement on chemical characteristics are the desired results of this project.

*US Department of Energy, contract no. DE-FG02-06ER46304 Indiana State University Department of Chemistry and Physics
Monte-Carlo Simulations of Magnetic Ising Models for Sodium Cobaltate*

JOSEPH LANIER (Presenter), Xavier University, PATRICK T GEMPERLINE, Physics, Auburn University, DAVID MORRIS, Xavier University — Sodium cobaltate is a material whose physical properties depend strongly on the concentration of sodium. It is unique because it acts as a thermoelectric material, and a superconductor at different concentrations of sodium. The sodium ions move within layers sandwiched between CoO2 layers. The sodium ions can occupy two different types of site; one low energy and one high energy. These sites neighbor each other, and by representing the two sites as pseudospin vectors pointing to the occupied site, we can study the ordering of sodium ions by simulating how the pseudospins interact with each other via the Ising Hamiltonian. This is done with the use of a Monte-Carlo Metropolis simulation with the results being presented here. The code is used to study the lowest energy structure of sodium cobaltate at different sodium concentrations.

*Hauck Foundation


Specific heat of Pr1-xNdxOs4Sb12*

YEH-CHIA CHANG (Presenter), SHOJI D HISHIDA, PEI-CHUN HO, California State University, Fresno, M BRIAN MAPLE, UC San Diego, TATSUYA YANAGISAWA, Hokkaido University — Filled skutterudites are the compounds that show the formula RM4X12. R is the rare earth metal, M is the transition metal, and X is the pnictogen. They will show rich varieties of strongly correlated electron behaviors, which attract our interest. The sample we focus on is a doping system, Pr1-xNdxOs4Sb12. PrOs4Sb12 show unconventional superconductivity, while NdOs4Sb12 exhibit ferromagnetism at low temperature. Therefore, there is a competition between two properties. In order to understand the compound better, we do the heat capacity measurement from 11K to 300K. From the curve of the specific heat of Pr1-xNdxOs4Sb12, parameters can be extracted out by the curve fitting with a combination of the Debye, Einstein, and Sommerfeld models. These parameters include Debye temperature, Einstein temperature, and electronic specific heat coefficient and can show the properties of the materials, such as the stiffness of the crystal structure, the rattling effect of the rare earth metal, and electron correlation. From the data analysis, we try to find out the trend of parameters depending on Nd concentration.

*Research at CSU-Fresno is supported by NSF DMR-1506677; at UCSD by US DOE DE-FG02-04ER46105 and NSF DMR-1810310; at Hokkaido U. by JP15H05885 and JP18H04297.

Investigating the Far-IR Optical Properties of Hg1-xCdxSe Semiconductor Alloys*

JOHN W LYONS (Presenter), FRANK C PEIRIS, Kenyon College, GREGORY N BRILL, U.S. Army Research Laboratory — Far-IR reflectivity was used to analyze phonon modes and obtain dielectric functions of a series of Hg1-xCdxSe thin films deposited on both ZnTe/Si(112) and GaSb(112) substrates. The data were supplemented by ellipsometric scans in the mid-IR to visible range to assist in modeling the dielectric functions. The combination and simultaneous modeling of these data allowed the determination of not only the phonon and free-carrier activity but also the complex dielectric function over an extremely large range of energies.

*The work at Kenyon is funded by DMR-1609245

Floquet Hofstadter Butterfly on the Kagome and Triangular Lattices*

ARIEL BARR (Presenter), LIANG DU, QI CHEN, AARON BARR, GREGORY FIEITE, University of Texas at Austin — Recently, the interactions of materials with light have attracted considerable interest from the materials science community. "Hofstadter's butterfly" refers to a fractal energy spectrum which occurs when a perpendicular magnetic field of extreme magnitude distributes the electronic energy levels of a lattice in a pattern resembling a butterfly. Lattices with a Hofstadter spectrum exhibit quantum Hall conductance, and under the influence of periodic driving, produce pairs of counter-propagating chiral edge modes which are robust against static disorder. We use Floquet theory to theoretically study the influence of a periodic driving potential provided by monochromatic circularly and linearly polarized light on the Hofstadter butterfly energy spectrum and Chern numbers of Kagome and triangular lattices. We find that as the lattices are exposed to driving, dramatic changes in the energy spectrum occur: reflection symmetry is broken, band width is altered, band inversion is observed, and polarization directional dependence can be identified. Further, we identify polarization-directional dependence of the Chern numbers. This work is currently under review at Phys Rev B, and can be found on Arxiv: arXiv:1808.02057

*We gratefully acknowledge funding from the Army Research Office and NSF.
2:03PM B67.00015: Cytoskeletal Dynamics of Neurons Measured by Combined Fluorescence and Atomic Force Microscopy*  PETER MOORE (Presenter), CRISTIAN STAII, Tufts University — Mechanical properties of neurons represent a key factor that determines the functionality of neuronal cells and the formation of neural networks. The main source of mechanical stability for the cell is a biopolymer network of microtubules and actin filaments that form the main components of the cellular cytoskeleton. This biopolymer network is responsible for the growth of neuronal cells as they extend neurites to connect with other neurons, forming the nervous system. Here we present experimental results that combine atomic force microscopy (AFM) and fluorescence microscopy to produce systematic, high-resolution elasticity and fluorescence maps of cortical neurons. This approach allows us to apply external forces to neurons, and to monitor the dynamics of the cell cytoskeleton. We measure how the elastic modulus of neurons changes upon changing the ambient temperature, and identify the cytoskeletal components responsible for these changes. These results demonstrate the importance of taking into account the effect of ambient temperature when measuring the mechanical properties of cells.

*Mutus Faculty Research Award

Monday, March 4, 2019 11:15 AM - 2:15 PM

Session B69 FED: The Role of Physics Departments in Educating Teachers BCEC 052A - Monica Plisch, American Physical Society APS - Tag(s): Education, Invited, Undergraduate

11:15AM B69.00001: The national landscape for STEM teacher education [invited]  MICHAEL MARDER (Presenter), University of Texas at Austin — For 35 years, STEM education for secondary students in the US has been in a state of crisis. Less than 40% of US high school students take physics, when in most of Europe and Asia 4 years of physics are customary. Computer science is in such shortage that states do not even try to require it, and we scarcely know how many students take it.

The story of the last 35 years is not as bad as it seems. There has been steady progress in some areas, and in some states and at some times strong improvement that went unrecognized. The key to the future is more and better teachers. Through programs such as PhysTEC from the American Physical Society and UTeach, physicists are helping lead the way.

11:51AM B69.00002: Get the Facts Out: Changing the conversation around physics teacher recruitment* [invited]  WENDY ADAMS (Presenter), Physics, Colorado Sch of Mines — The Get the Facts Out campaign is a joint effort between four societies and the Colorado School of Mines to change the conversation about high school and middle school physics, chemistry, and math teaching careers. We have developed a toolkit, based on pilot interventions that show positive results in shifting perceptions among students and faculty, and which have been shown to outperform traditional recruitment efforts, which is designed to be customizable and adaptable to the local situation. The materials and strategies include: (1) both student-facing and faculty-facing resources and a how-to guide for running interactive events, including but not limited to slide decks, clicker questions, and handouts with national survey data on retention, job satisfaction, and student loan forgiveness; (2) sample informational handouts on teacher salaries, comparisons of teacher and faculty salaries, and retirement benefits, with instructions on how to customize these with local data; and (3) brochures and posters that incorporate tested messaging strategies. In this presentation both the tools and the research and development behind them will be shared.

*This work is supported by the National Science Foundation IUSE and Noyce programs DUE-1821710/1821462.

12:27PM B69.00003: Improving undergraduate physics instruction and physics teacher preparation through the use of Learning Assistants* [invited]  VALERIE OTERO (Presenter), University of Colorado Boulder — Undergraduate Learning Assistants (LAs) help faculty make changes to their courses by encouraging active engagement. Through their work with students along with a special pedagogy course, LAs establish empathy for their peers as they learn physics, and they help them navigate large amounts of course material and motive students to persist. Through this process, students, their professors, and the LAs become more attuned to research-based strategies for teaching physics and to the complexities of building equitable learning environments that lead to student success. This sets the stage for better prepared physics teachers and for physics majors to find their way to physics teacher certification programs. In addition, the presence of LAs in courses leads to better learning outcomes, decreased failure rates, and improved outcomes for students from groups traditionally underrepresented in physics. The LA program will be described and program outcomes will be discussed. Conjectures about the mechanisms that are effecting change will also be discussed.

*Partially funded by NSF (#0302134, #0537870, #1557351), the University of Colorado Boulder, PhysTEC, Amgen, HHMI, Ball Aerospace, and Halliburton.
1:03PM B69.00004: A thriving physics teacher preparation program at Rowan University* [Invited]  KARENMagee-Sauer (Presenter), TREVOR I. Smith, PATRICK CHESTNUT, PHILIP LA PORTA, DAVID R. Klassen, Rowan University — The Department of Physics & Astronomy at Rowan University received a 3-year (2015 – 2018) Comprehensive Grant from the PhysTEC program. As part of this grant, Rowan attempted to build a sustainable framework for recruiting, retaining, training, inducting and mentoring future high school physics teachers. Rowan closely followed PhysTEC's “Key Components” for successful high school physics teacher education programs. A strong emphasis at the Rowan PhysTEC site was creating student research opportunities in Physics Education Research, early teaching experiences in a high school setting, an LA program to help recruit interest to teaching, and creating a vibrant high school physics teacher network in the South Jersey region. Another notable aspect was Rowan's success in creating a community within the department dedicated to supporting PhysTEC activities and leveraging our PhysTEC experience into helping gain other external grant opportunities. In this talk, we will present ideas and actions that were particularly successful in sustaining our PhysTEC activities. Rowan University is a Carnegie-classified Doctoral University (Moderate Research Activity) with approximately 19,000 students. Its main campus is located in Glassboro, N.J., 20 miles southeast of Philadelphia.

*This work was supported by a grant from the PhysTEC program. The PhysTEC program is led by APS in partnership with the American Association of Physics Teachers, with support from the National Science Foundation and the APS Campaign for the 21st Century.

1:39PM B69.00005: Next Gen PET: An effective, NGSS-aligned curriculum for future elementary teachers* [Invited] EDWARD PRICE (Presenter), California State University, San Marcos — The physical science preparation of prospective elementary school teachers has the potential for long-lasting and far-reaching impact. To this end, the Next Generation Physical Science and Everyday Thinking (Next Gen PET) curriculum has been designed to provide students with learning experiences aligned with the Next Generation Science Standards. Versions of the research-based, guided-inquiry materials are available for either small or large enrollments, and covering either physics or physical science content. These options provide instructors with flexibility regarding content and implementation format, as documented by case studies of faculty members' course designs. An extensive online instructor's guide* includes student and instructor materials, homework activities, videos of experiments and demonstrations, classroom video clips of student interactions, test banks, and more. An associated online faculty learning community** provides an opportunity for faculty to collaboratively improve their instruction, study student thinking and conduct classroom-based research using the Next Gen PET curriculum. The materials are in use by over 50 faculty around the U.S., and a study of over 1,500 students found significant improvements on multiple-choice and constructed-response tasks following the course. This talk will describe the curriculum, instructor resources, student learning outcomes, and online faculty community.

* http://nextgenpet.iat.com
** http://www.ngpfolc.org

*Supported by grants from the National Science Foundation NSF DUE-1626496 and the Chevron Foundation

Monday, March 4, 2019 11:45 AM - 2:15 PM

Session B80 APS/SPS: Meet Your Future: Careers in the Private Sector Westin Grand Ballroom B -

Tag(s): Careers, Industry, Undergraduate

11:45AM B80.00001: Meet Your Future: Careers in the Private Sector — FIAP and APS Careers will host a special lunchtime session in which representatives from industry will briefly describe their career path and answer questions about physics careers in the private sector. Topics will include work opportunities for physicists in industry, strategies for successfully pursuing industrial jobs, and advice on how to thrive in this exciting and challenging work environment.

The panelists this year are:
Scott Davis, Analog Devices Senior Manager, Electro-Optical System Development
Rachael Floyd Janis Research, Senior Cryogenic Physicist and Applications Engineer
Amy Herhold, ExxonMobil Director, Physics and Mathematical Sciences
Audra Macie, BAE Systems Senior Principal Systems Engineer
Matthew Thompson, BAE Systems, Technology Development Manager

Note that this session will be held in the Westin Hotel, not the Convention Center. Join us for a slice of pizza and gain many useful insights into this career path.
2:30PM C01.00001: Temperature Dependence of Charge Transport in an Undoped Weyl Semimetal – Y₂Ir₂O₇*
PATRICK LABARRE (Presenter), University of California, Santa Cruz, LIANYANG DONG, Florida State University, JENNIFER TRINH, University of California, Santa Cruz, THEO SIEGRIST, Florida State University, ARTHUR P RAMIREZ, University of California, Santa Cruz
— An undoped Weyl Semimetal (WSM) is predicted to exhibit resistivity varying with temperature as $\rho \propto T^{-4}$ in the presence of a random Coulomb potential screened by thermally generated charge carriers. Here we show that, in hydrothermally grown polycrystalline samples of the WSM Y₂Ir₂O₇, $\rho = \rho_0 T^{-4}$ over four orders of magnitude in $\rho$. The prefactor, $\rho_0$, agrees with theoretical estimates within the random potential model using reasonable materials parameters. The model works well beyond its range of applicability, extending into the high-resistivity region where the Ioffe-Regel parameter, $k_T l \ll 2\pi$.

The importance of strong electron correlations suggests this is behavior characteristic of a "bad-WSM".

*This work was supported by NSF-DMR 1534741 (P.G.L., A.P.R.), NSF DGE-1339067 (J.T.), and NSF-DMR 1534818 (T.S., L.D.).

2:42PM C01.00002: Higher-Order Symmetry Enriched Topological Phases*
CIARÁN HICKEY (Presenter), VATSAL DWIVEDI, TIM ESCHMANN, SIMON TREBST, University of Cologne — Higher-order topological insulators (TIs) exhibit boundary physics typically associated with lower dimensional TIs, e.g. 2-d second-order TIs exhibit localized 0-d zero energy corner modes. This physics is topologically protected as long as certain lattice symmetries are preserved, akin to topological crystalline insulators. So far, these phases have largely been explored in the context of non-interacting fermion systems. However, we know that symmetries may also "enrich" the physics of interacting topological phases, such as quantum spin liquids or fractional quantum Hall states. Is it possible to realize "higher-order" boundary physics in strongly interacting topological phases? In this talk, we discuss exactly such higher-order symmetry enriched topological phases, including an example of an exactly solvable spin model with a quantum spin liquid ground state that indeed exhibits topologically protected corner modes, a hallmark of second-order TIs.

*We acknowledge partial support from the Deutsche Forschungsgemeinschaft (DFG) within the CRC network TR 183 (projects B01 and B03) and SFB 1238 (project C03).

2:54PM C01.00003: Topological Phases of the Interacting SSH and Kitaev Models on the Bethe Lattice
PATRICK J WONG (Presenter), ANDREW K MITCHELL, School of Physics, University College Dublin — Topological phases of matter have been intensely studied in recent years, but there still remain a number of open questions regarding the interplay of topology and strong interactions in condensed matter systems, including the role of topological invariants. Two prototypical models in one dimension exhibiting non-trivial topological phases are the SSH model and the Kitaev chain. Here we study generalizations of these models on the Bethe lattice, showing that topological phases with bulk zero-modes can be realized in higher dimensions. We then consider interacting versions of these Bethe SSH and Kitaev models with local Hubbard interactions, $U$. These topological Hubbard models are solved exactly in infinite dimensions at $T=0$ using dynamical mean field theory with the numerical renormalization group as an impurity solver.

For the Bethe SSH Hubbard model with interactions $U<U_c$ below a critical strength, bulk gapped sites at $U=0$ develop a power-law pseudogap density of states, while sites with topological zero-mode poles at $U=0$ are augmented by power-law diverging quasiparticle Kondo peaks. A bulk Mott insulating phase is realized for $U>U_c$. A method of characterizing the topological phases of the systems in the presence of interactions based on their Green's functions is discussed.
3:06PM C01.00004: Interacting multi-channel topological boundary modes in a quantum Hall valley system
MALLIKA RANDERIA (Presenter), KARTIEK AGARWAL, Princeton University, BENJAMIN EZEKIEL FELDMAN, Stanford University, HAO DING, HUIWEN JI, ROBERT CAVA, SHIVAJI SONDHI, Princeton University, SIDDHARTH A PARAMESWARAN, University of Oxford, ALI YAZDANI, Princeton University — Quantum Hall ferromagnets (QHFMs) are two-dimensional electronic phases with spontaneously broken spin or pseudospin symmetry whose wavefunctions also have topological properties. Domain walls between distinct broken symmetry QHFM phases are predicted to host gapless one-dimensional (1D) modes that emerge due to a topological change of the underlying electronic wavefunctions at such interfaces. Although a variety of QHFMs have been identified in different materials, probing interacting electronic modes at these domain walls has not yet been accomplished. Here we use a scanning tunneling microscope (STM) to directly visualize the spontaneous formation of boundary modes, within a sign-changing topological gap, at domain walls between different valley-polarized quantum Hall phases on the surface of bismuth. By changing the valley occupation and the corresponding number of modes at the domain wall, we can realize different regimes where the valley-polarized channels are either metallic or develop a spectroscopic gap. This behavior is a consequence of Coulomb interactions constrained by the symmetry-breaking valley flavor, which determines whether electrons in the topological modes can backscatter, making these channels a unique class of interacting Luttinger liquids.

3:18PM C01.00005: Interesting behavior of magnetoresistance in single crystals of CeBi*
BRINDA KUTHANAZHI (Presenter), NA HYUN JO, LI XUANG, YUN WU, SERGEY BUDKO, ADAM KAMINSKI, PAUL CANFIELD, Physics, Iowa State University/Ames Laboratory — Cerium monopnictides, CeX (X= Sb, Bi) have gained renewed interest as potential candidates to host non-trivial topological band structure along with magnetism. High quality single crystals of CeBi were grown out of Bi self-flux. Systematic measurements of temperature and magnetic field dependent resistivity and magnetization were conducted on CeBi. A rich H-T phase diagram was mapped out. Interestingly, extremely large magnetoresistance was observed at low temperature, and large negative magnetoresistance was detected at the intermediate temperature regime. To obtain a better understanding of the system, the electronic structure is also being studied.

*This work is supported by the US DOE, Basic Energy Sciences, Materials Science and Engineering Division under contract no. DE-AC02-07CH11358. This work was supported by the Center for Advancement of Topological Semimetals, an Energy Frontier Research Center funded by the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences, through the Ames Laboratory. L. X. was supported, in part, by the W. M. Keck Foundation. N. H. J. is supported by the Gordon and Betty Moore Foundation EPiQS Initiative (Grant No. GBMF4411).

3:30PM C01.00006: Orbital Edelstein effect from spontaneous symmetry breaking*
GEREMIA MASSARELLI (Presenter), BRYCE WU, ARUN PARAMEKANTI, University of Toronto — Coupling between charge and spin, and magnetoelectric effects more generally, have been an area of great interest for several years, with the sought-after ability to control magnetic degrees of freedom via electric currents serving as an impetus. The orbital Edelstein effect is a magnetoelectric effect consisting of a bulk orbital magnetization induced by an electric current. It is the orbital analogue of the spin Edelstein effect, in which the carriers’ spin gives rise to the magnetization. The orbital Edelstein effect has recently been investigated in the context of Weyl materials. Motivated by these developments, we examine a toy model in which a crystal exhibits such an orbital Edelstein effect upon symmetry breaking via density-wave order which reduces it to a gyrotrropic crystal class.

*We acknowledge funding from the Natural Sciences and Engineering Research Council of Canada and from the Canadian Institute for Advanced Research. G. M. is supported by the Fonds de recherche du Québec - Nature et technologies.
3:42PM C01.00007: Observation of Double Weyl Phonons in Parity-Breaking FeSi*  
HU MIAO, Brookhaven National Laboratory, TIANTIAN ZHANG, LE WANG, Institute of Physics, DEREK MEYERS, Brookhaven National Laboratory, AYMAN SAID, Argonne National Laboratory, YILIN WANG, Brookhaven National Laboratory, YOUNGUO SHI, HONGMING WENG, ZHONG FANG, Institute of Physics, MARK DEAN (Presenter), Brookhaven National Laboratory — Condensed matter systems have now become a fertile ground to discover emerging topological quasiparticles with symmetry protected modes. While many studies have focused on fermionic excitations, the same conceptual framework can also be applied to bosons yielding new types of topological states. Motivated by Zhang et al.’s recent theoretical prediction of double Weyl phonons in transition metal monosilicides [Phys. Rev. Lett. 120, 016401 (2018)], we directly measure the phonon dispersion in parity-breaking FeSi using inelastic x-ray scattering. By comparing the experimental data with theoretical calculations, we make the first observation of double Weyl points in FeSi, which will be an ideal material to explore emerging bosonic excitations and its topologically nontrivial properties. 

*This work was supported by the Department of Energy, Office of Basic Energy Sciences, Early Career Award Program under Award No. 1047478. Work at Brookhaven National Laboratory was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE- SC0012704.

3:54PM C01.00008: Berryogenesis: self-induced Berry flux and spontaneous non-equilibrium magnetism*  
MARK RUDNER (Presenter), Niels Bohr Institute, JUSTIN SONG, Nanyang Technological University — Spontaneous symmetry breaking is central to the description of interacting phases of matter. In this talk I will discuss a new mechanism through which a driven interacting system subject to a time-reversal symmetric driving field can spontaneously magnetize [1]. Strong internal ac fields of a metal driven close to its plasmon resonance may enable Berryogenesis: the spontaneous generation of a self-induced Bloch band Berry flux. The self-induced Berry flux supports and is sustained by a circulating plasmonic motion, which may arise even for a linearly polarized driving field. Berryogenesis relies on feedback due to interband coherences induced by internal fields, and may readily occur in a wide variety of multiband systems. We anticipate that graphene devices, in particular, provide a natural platform to achieve Berryogenesis and plasmon-mediated spontaneous non-equilibrium magnetization in present-day devices.


*This work was supported by the European Research Council (ERC) under the European Union Horizon 2020 Research and Innovation Programme (Grant Agreement No. 678862), the Villum Foundation, and NRF fellowship award NRF-NRFF2016-05.

4:06PM C01.00009: Higher angular momentum band inversions in two dimensions  
JORN W F VENDERBOS (Presenter), YICHEN HU, CHARLES KANE, Physics and Astronomy, University of Pennsylvania — This talk discusses a special class of topological phase transitions in two dimensions described by the inversion of bands with relative angular momentum higher than 1. A band inversion of this kind, which is protected by rotation symmetry, separates the trivial insulator from a Chern insulating phase with higher Chern number, and thus generalizes the quantum Hall transition described by a Dirac fermion. Higher angular momentum band inversions are of special interest, as the non-vanishing density of states at the transition can give rise to interesting many-body effects. We introduce a series of minimal lattice models which realize higher angular momentum band inversions. Interaction effects are considered, focusing on the possibility of electron-hole condensation, which breaks rotational symmetry. We further describe how the notion of higher angular momentum band inversions can be generalized to time-reversal invariant systems. Such band inversions can be viewed as transitions to a topological insulator protected by rotation and inversion symmetry, and provide a promising venue for realizing correlated topological phases such as fractional topological insulators.

4:18PM C01.00010: Real-space recipes for interacting topological crystalline states  
CHEN FANG (Presenter), ZHIDA SONG, Chinese Academy of Sciences, YANG QI, Fudan University — We present a unified scheme for constructing all topological crystalline states, bosonic and fermionic, free and interacting, from real-space building blocks and connectors. Building blocks are finite-size pieces of lower dimensional topological states protected by onsite symmetries alone, and connectors are “glue” that complete the open edges shared by two or multiple pieces of building blocks. The resulted assemblies are selected against two physical criteria we call the “no-open-edge condition” and the “bubble equivalence”, which, respectively, ensure that each selected assembly is gapped in the bulk and cannot be deformed to a product state. The scheme is then applied to obtaining the full classification of bosonic topological crystalline states protected by several onsite symmetry groups and each of the 17 wallpaper groups in two dimensions and 230 space groups in three dimensions. We claim that our real-space recipes give the complete set of topological crystalline states for bosons and fermions, and prove the boson case analytically using a spectral sequence expansion of group cohomology.
4:30PM C01.00011: Non-Topological Majorana Zero Modes in Inhomogeneous Spin Ladders* ROBERT KONIK (Presenter), Brookhaven National Laboratory, NEIL ROBINSON, University of Amsterdam, ALEX ALTLAND, Universitat zu Koln, REINHOLD EGGER, Heinrich-Heine-Universitat, NIKLAS GERGS, Utrecht University, WEI LI, Beihang University, ALEXEI TSVELIK, ANDREAS WEICHSELBAUM, Brookhaven National Laboratory — We show that the coupling of homogeneous Heisenberg spin-1/2 ladders in different phases leads to the formation of interfacial zero energy Majorana bound states. Unlike Majorana bound states at the interfaces of topological quantum wires, these states are void of topological protection and generally susceptible to local perturbations of the host spin system. However, a key message of our work is that in practice they show a high degree of resilience over wide parameter ranges which may make them interesting candidates for applications.

*Work at BNL (N.J.R., A.M.T., A.W., R.M.K.) was supported by the CMPMS Division funded by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-SC0012704. N.J.R. was supported by the EU Horizon 2020 program, grant agreement No. 745944. A.W. acknowledges support from the Deutsche Forschungsgemeinschaft (DFG), Grant Nos. WE4819/2-1 and WE4819/3-1. D.S. is member of the D-ITP consortium of the Netherlands Organisation for Scientific Research. A.A. and R.E. acknowledge DFG support via Grant No. EG 96/11-1 and CRC TR 183 (project C4). R.M.K. and A.M.T. acknowledge the hospitality of LMU Munich and of HHU Dusseldorf where parts of this work have been done.

4:42PM C01.00012: Symmetry-protected exceptional rings in two-dimensional correlated systems* TSUNEYA YOSHIDA (Presenter), Department of Physics, University of Tsukuba, ROBERT PETERS, NORIO KAWAKAMI, Department of Physics, Kyoto University, YASUHIRO HATSUGAI, Department of Physics, University of Tsukuba — Emergence of exceptional points in two-dimensional systems is one of the characteristic phenomena in non-Hermitian systems. In this talk, we elucidate the impacts of symmetry on the non-Hermitian degeneracies. In particular, we analyze correlated systems with chiral symmetry in equilibrium where the imaginary-part of the self-energy induces the non-Hermitian phenomenon. Intriguingly, our analysis discover novel topological degeneracies which we call symmetry-protected exceptional rings (SPERs). Furthermore, we demonstrate that SPERs emerge in a correlated honeycomb lattice by employing the dynamical mean-field theory combined with the numerical renormalization group.

*This work is partly supported by JSPS KAKENHI Grants No. JP15H05855, No. JP16K05501, No. JP16K13845, No. JP17H06138, No. JP18H01140, No. JP18H04316, No. JP18K03511, and No. JP18H05842. The numerical calculations were performed on supercomputer at the ISSP in the University of Tokyo, and the SR16000 at YITP in Kyoto University.

4:54PM C01.00013: Large magneto-elastoresistance in WTe2* NA HYUN JO (Presenter), Department of Physics and Astronomy, Iowa State University/Ames Laboratory, LIN-LIN WANG, Ames Laboratory, PETER P. ORTH, GIL DRACHUCK, SERGEY L. BUD'KO, PAUL CANFIELD, Department of physics and astronomy, Iowa State University/Ames Laboratory — Elastoresistance is the relative change of a material's resistance under strain. Its value depends on two contributions: one coming from changes in the sample's geometry and another from changes of the electronic properties such as carrier densities or scattering rates. In common metals like copper, the geometric contribution dominates a temperature-independent elastoresistance with a value of about 2. In other materials, including Bi, changes in the electronic properties dominate. We find that WTe2 is a member of the second group exhibiting an elastoresistance as large as -20. Moreover, we discover that the magnetic field has a dramatic effect on the elastoresistance in WTe2, resulting in values of elastoresistance in applied magnetic field between -80 to 120. We present a detailed analysis of this phenomenon combining results from DFT calculations and quantum oscillation measurements. We conclude that such large magneto-elastoresistance can be realized in other semimetals with crystal structures similar to WTe2.

*This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358; Gordon and Betty Moore Foundation EPiQS Initiative (Grant No. GBMF4411). Peter P. Orth acknowledges support from Iowa State University Startup Funds.

5:06PM C01.00014: Topological Order and Subsystem Symmetry JULIAN MAY-MANN (Presenter), TAYLOR HUGHES, University of Illinois at Urbana-Champaign — When a system is invariant under a subsystem symmetry, it is as if it has a "gauge" symmetry on particular subregions. Motivated by this observation, we show that subsystem symmetries can lead to topological features reminiscent of those found in topological gauge theories. This is done by considering a subsystem symmetry generalization of a Chern-Simons field theory. Because of the subsystem symmetry, this model has a robust ground state degeneracy on torus and localized zero energy corner modes.
The concept of topology in condensed matter physics has been widely recognized since the theoretical discovery of topological insulators by Kane and Mele. Recently, the electron correlation effects on topological properties have attracted much attention because of nontrivial features that do not emerge in weakly correlated electron systems, such as topological Kondo insulators, magnetic orders in topological insulators, etc.

In the previous study, it has been elucidated that in the presence of spin U(1) symmetry, even ferromagnetic (FM) systems can acquire topological properties; system with spin U(1) symmetry can have a spin-selective gap which results in nontrivial topological properties. In general, however, spin U(1) symmetry is considered to be broken in heavy-fermion systems because of their strong spin-orbit coupling (SOC). This fact motivates us to ask whether the above topological phases can be realized in the presence of SOC.

In this study, we demonstrate that even in the absence of spin U(1) symmetry, ferromagnetic phases with mirror symmetry can have the topological properties. In particular, we analyze an effective model describing a thin film of SmB$_6$, and find the topological state in a half-metallic FM phase characterized by a mirror Chern number.

**Monday, March 4, 2019 2:30 PM - 5:30 PM**

**Session C02 DMP DCOMP GMAG: Dielectric & Ferroic Oxides -- Magnetolectric Effects**

2:30PM C02.00001: Multiferroics: hidden functionalities beyond magnetolectric coupling [Invited]  MANFRED FIEBIG (Presenter), Department of Materials, ETH Zurich — Requirements to “good multiferroics” are tough. They are supposed to have a spontaneous magnetization and polarization, preferably parallel to each other, with a strong magnetolectric coupling between them. Inevitably, this leads to a multiferroic state that is described by a very complex set of order parameters – complex enough to provide the symmetry degrees of freedom to fulfil so many requirements at once [1]. With the focus on electric-field-controlled magnetic order, it goes unnoticed that these degrees of freedom will permit many functionalities other than a refined magnetolectric coupling. In my talk, I will describe the quest for such functionalities in our group. I will discuss up to four cases. (i) For the multiferroic hexagonal manganites I will show that amplitude and phase of the order parameter may exhibit different coherence length. Taking this into account, we resolve the long-standing controversial question of how exactly the topological ferroelectric state in this system arises [2]. (ii) The emergence of a magnetic bulk phase transition out of the spin structure in the domain walls is shown for (Tb,Dy)FeO$_3$. (iii) Inversion of a ferroelectric and a ferromagnetic multi-domain state in homogeneous external fields is demonstrated: In each domain, the direction of the order parameter is reversed but the domain pattern as such is left untouched [3].


3:06PM C02.00002: Theory of orbital magnetic quadrupole moment and magnetolectric susceptibility* ATSUO SHITADE (Presenter), RIKEN Center for Emergent Matter Science, HIKARU WATANABE, YOUICHI YANASE, Department of Physics, Kyoto University — We derive a quantum-mechanical formula of the orbital magnetic quadrupole moment (MQM) in periodic systems by using the gauge-covariant gradient expansion. This formula is valid for insulators and metals at zero and nonzero temperature. We also prove a direct relation between the MQM and magnetolectric (ME) susceptibility for insulators at zero temperature. It indicates that the MQM is a microscopic origin of the ME effect. Using the formula, we quantitatively estimate these quantities for room-temperature antiferromagnetic semiconductors BaMn$_2$As$_2$ and CeMn$_2$Ge$_{2-x}$Si$_x$. We find that the orbital contribution to the ME susceptibility is comparable with or even dominant over the spin contribution.


*This work was supported by Grants-in-Aid for Scientific Research on Innovative Areas “JPhysics” (Grant No. JP15H05884) and “Topological Materials Science” (Grant No. JP16H00991) from the Japan Society for the Promotion of Science (JSPS), and by JSPS KAKENHI (Grants No. JP15K05164 and No. JP15H05745).
3:18PM C02.00003: Inelastic Neutron Scattering measurements on phonon-magnon coupling in BiFeO3
GUANGYONG XU (Presenter), ZHIJUN XU, National Institute of Standards and Technology, JOHN A. SCHNEELOCH, University of Virginia, JINSHENG WEN, Nanjing University, MASAKI MATSUDA, BARRY L. WINN, DANIEL PAJEROWSKI, Oak Ridge National Lab, YANG ZHAO, National Institute of Standards and Technology, CHRIS STOCK, Univ of Edinburgh, PETER M GEHRING, National Institute of Standards and Technology, T. USHIYAMA, Y. YANAGISAWA, Y. TOMIOKA, TOSHIMITSU ITO, AIST, Japan, ROBERT J BIRGENEAU, Univ. of California, Berkeley — We use inelastic neutron scattering to study phonons in multiferroic BiFeO3. When the low energy optic phonon is probed, an intensity enhancement is observed when the system enters the antiferromagnetic phase at TN=640K. It is interpreted as a possible dynamic coupling between phonons and magnons through the DM interaction. Polarized neutron measurements are performed to confirm the lattice nature of this enhancement, in other words, to show that this is more a “magneto-phonon” mode rather than a “electro-magnon” mode. We will also discuss neutron scattering measurements on higher energy phonons that could also be affected by the proposed dynamic coupling.

3:30PM C02.00004: RIXS excitations of polar magnet Fe2Mo3O8
HSIAO-YU HUANG (Presenter), AMOL SINGH, National Synchrotron Radiation Research Center, ABHISHEK NAG, KEJIN ZHOU, ANDREW WALTERS, MIRIAN GARCIA-FERNANDEZ, Diamond Light Source, JUN OKAMOTO, ASHISH CHAINANI, National Synchrotron Radiation Research Center, YU-MIIN SHEU, Department of Electrophysics, National Chiao Tung University, TAKASHI KURUMAJI, YOSHINORI TOKURA, Department of Applied Physics, University of Tokyo, CHIEN-TE CHEN, DI-JING HUANG, National Synchrotron Radiation Research Center — Cross control of magnetization (electric polarization) by an external electric (magnetic) field, i.e. magnetoelectric (ME) effect, is a key in designing novel multiferroic devices. The polar magnet Fe2Mo3O8 has been demonstrated to be a promising multiferroic material recently. The ME coupling is not only strong but also compositionally tunable. Upon Zn doping higher than 12.5%, the antiferromagnetic ground state becomes ferrimagnetic state accompanying a change in ME coefficient. To study the electronic structure of (Fe1-xZnx)2Mo3O8, we carried out comprehensive measurements including Hard X-ray photoemission, soft x-ray absorption and resonant inelastic X-ray scattering. Our results disentangle the electronic properties of octahedral and tetrahedral Fe2+ and provide spectroscopic evidence that the doped Zn favors to replace tetrahedral Fe in the doped compound. We observed peculiar temperature and polarization dependences of low-energy RIXS excitations across the phase transition of Fe2Mo3O8.

3:42PM C02.00005: Local magneto-electric response of Cr2O3 investigated with spin polarized positive muons*
MARTIN DEHN (Presenter), Department of Physics & Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia, DONALD J ARSENEAU, SARAH R DUNSIGER, BASSAM HITTI, TRIUMF, STEFAN HOLENSTEIN, Physik-Institut, Universität Zürich, MICHAEL FECHNER, Max Planck Institute for the Structure and Dynamics of Matter, HUBERTUS LUETKENS, Paul Scherrer Institut, W ANDREW MACFARLANE, RYAN M. L. MCFADDEN, Department of Chemistry, University of British Columbia, QUINTIN N MEIER, Department of Materials, ETH Zürich, GERALD D MORRIS, TRIUMF, ZAHER SALMAN, Paul Scherrer Institut, NICOLA SPALDIN, Department of Materials, ETH Zürich, ROBERT F KIEFL, Department of Physics & Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia — The bulk properties of the prototypical linear magneto-electric antiferromagnet Cr2O3 have been extensively studied. Here, we report on a muon spin rotation (μSR) study using spin polarized muons to probe the local magneto-electric response in order to investigate magnetoelectricity on a microscopic level. We find that the muon, a light interstitial probe, occupies several distinct stopping sites in Cr2O3, and displays a rich dynamic behavior that we interpret in the context of local muon hopping and thermally activated site transitions. Furthermore, when Cr2O3 is prepared in a single magnetic domain, a shift in the local magnetic field is observed in response to an applied electric field, with the sign of the shift depending both on the field direction and domain state. The origin of this apparent magneto-electric effect is discussed.

*NSERC Canada and Stewart Blusson Quantum Matter Institute
3:54PM C02.00006: Magnetoelectric Effect in Type II Multiferroic HoFeWO$_6$  MOEIN ADNANI TAKANTAPEH (Presenter), HUNG-CHENG WU, NARAYAN POUDEL, MELISSA GOOCH, LIANGZI DENG, ZHENG WU, PAUL C. W. CHU, Texas Center for Superconductivity and Department of Physics, University of Houston — In type II multiferroics, the ferroelectricity originates from the magnetic ordering as it breaks the inversion symmetry. In this work, we investigated multiferroicity in HoFeWO$_6$ which belongs to the RFeWO$_6$ (R=Rare-earth) system recently suggested to be type II multiferroic [1]. We found that this compound orders antiferromagnetically below $T_N$ ~17 K. Observation of an anomaly in dielectric constant and dielectric loss, as well as a polarization switchable by an electric field at the same temperature, reveal the ferroelectric nature of this transition.

We further found that below the temperature $T_C2$ ~5 K there appears a polarization ($P_2$) in opposite direction of the ($P_1$) at $T_C1$ ~17 K. While external magnetic field suppresses the polarization in the first transition ($P_1$), at a critical field $H_C1$ ~1T we observe a flipping of the direction of $P_2$. In addition, magnetic field dependent dielectric constant measurements show a magneto-dielectric effect of ~ 1.5% at 2 K for a critical field $H_C1$ ~1T. The metamagnetic behavior at low temperature with similar critical field indicates their direct relationship and the field induced nature of this observation.


4:06PM C02.00007: Electric-field control of magnetization, Jahn-Teller distortion and orbital ordering in ferroelectric ferromagnets* LAN CHEN, CHANGSONG XU, Physics Department, University of Arkansas, HAO TIAN, Department of Materials Science and Engineering, Nanjing University, HONGJUN XIAO, Physics Department, Fudan University, JORGE INIGUZ, Materials Research and Technology Department, Luxembourg Institute of Science and Technology, YURONG YANG (Presenter), LAURENT BELLAIChE, Physics Department, University of Arkansas — Controlling the direction of the magnetization by an electric field in multiferroics that are both ferroelectric and strong ferromagnetic will open the doors to the design of next generation of spintronics and memory devices. Unfortunately, this has never been achieved so far mostly because these materials are very scarce and/or may not have a large enough magnetoelectric coupling. Here, using first-principles simulations, we report the discovery that PbTiO$_3$/LaTiO$_3$ (PTO/LTO) superlattice does possess such highly-desired control, as evidenced by the electric-field-induced rotation of 90° and even full possible reversal of its magnetization in some cases. Moreover, such “wunderbar” systems also exhibit Jahn-Teller distortions, as well as orbital orderings, that are switchable by electric field, therefore making PTO-LTO of importance for the tuning of electronic properties too. Other possible materials possessing such couplings are also discussed, which further renders the presently reported electric controls to be a new general strategy to tune various properties of functional materials.

*This work was supported by ONR Grant No. N00014-17-1-2818.

4:18PM C02.00008: Multiferroic Behavior in Fe doped BaTiO$_3$ single crystals* PETER FINKEL (Presenter), MARGO STARUCH, United States Naval Research Laboratory, HATEM ELBIDWEIHY, ECE Department, US Naval Academy, MARKYS CAIN, Electrosciences, Ltd, PAUL THOMPSON, ESRF — Single crystals of BaTiO$_3$ (BTO) that have been doped at the titanium site with Fe$^{3+}$ or Mn$^{3+}$ have previously been shown to demonstrate large and recoverable electrostrains of up to 0.8 % that is thought to be due to the alignment of defects (i.e. O$^{2-}$ vacancies) with the crystallographic symmetry in the ferroelectric state when the samples are aged.[1,2] There is also the possibility that the incorporation of a magnetic ion could give rise to a magnetic signature and even potentially multiferroic coupling in these doped samples, the possibility of which has not been previously investigated. This would be of great interest as a new path to single phase multiferroic materials. In this presentation, results from magnetic and ferroelectric measurements will be presented for a 0.5% Fe doped BTO crystal. Anomalies in the magnetization at the ferroelectric-ferroelectric phase transitions, magnetocapacitance effects, and changes in the polarization with applied magnetic field confirm the existence of magnetoelectric coupling. The potential origins of this phenomenon will be discussed.

References:

*Office of Naval Reserach
4:30PM C02.00009: Magnetodielectric effect in ErFeO$_3$ single crystals  DONG GUN OH (Presenter), HWAN YOUNG CHOI, YOUNG JAI CHOI, NARA LEE, Yonsei Univ — We investigated magnetodielectric effect of orthoferrite single crystals of ErFeO$_3$, synthesized by the flux method using PbO flux. The canted antiferromagnetic order of Fe$^{3+}$ moments arises below $T_N \approx 640$ K and a spin reorientation transition occurs at $T_{SR} \approx 93$ K, which accompanies the rotation of weak net magnetic moments from the c- to a-axis. As the temperature is further decreased, a long-range magnetic order of $\text{Er}^{3+}$ spins emerges at $T_{ER} \approx 4$ K. From our investigation of anisotropic dielectric constant measurements, the magnetodielectric effect, described as the variation in the dielectric constant by applying external magnetic fields, is found in a broad range of temperature. Especially, the temperature dependence of dielectric constant exhibits a sharp anomaly at $T_{ER}$, as similarly observed in magnetic susceptibility along the c axis. In addition, a nonlinear variation in the isothermal dielectric constant, with a similar hysteretic behavior of the magnetic-field derivative of magnetization, is observed. The simultaneous non-linear variations of isothermal magnetization and dielectric constant below $T_{ER}$ suggest the important role of magnetic rare earth ions in magnetoelectric characteristics of the orthoferrite compound.

4:42PM C02.00010: Magnetoelectric properties in antiferromagnets composed of square cupolas $A$(TiO)Cu$_4$(PO$_4$)$_4$ ($A = \text{Ba, Sr, Pb}$)  YASUYUKI KATO (Presenter), YUKITOSHI MOTOME, University of Tokyo — We study the magnetoelectric properties in a newly synthesized series of quasi-two-dimensional magnets $A$(TiO)Cu$_4$(PO$_4$)$_4$ ($A = \text{Ba, Sr, Pb}$), by the cluster mean-field theory for a minimal quantum spin model [1,2]. The important building block of these compounds is Cu$_4$O$_{12}$ forming antiferromagnetic square cupolas where the local inversion symmetry is absent, and the Dzyaloshinskii-Moriya interaction is activated. By this antisymmetric interaction, the so-called quadrupole type spin configuration is stabilized at zero magnetic field. For nonzero magnetic fields, the magnetization curves are experimentally obtained up to above the saturation field for all $A$, and several anomalies are observed depending on the magnetic field directions. Our analysis well reproduces the full magnetization curves by tuning model parameters. Elaborating the phase diagram of the model, we show that the anomalies are explained by magnetoelectric phase transitions. Our theory also accounts for the dielectric anomaly observed in experiments. Furthermore, we show that the magnetoelectric behavior is well explained by the cluster multipole decomposition of complex spin configurations stabilized under the magnetic field.


4:54PM C02.00011: Realizing Magnetoelectric Coupling with Hydroxide as a Knob$^*$  JINYANG NI (Presenter), Department of physics, Fudan University — Materials with a coexistence of magnetic and ferroelectric order (i.e., multiferroics) provide an efficient route for the control of magnetism by electric fields. Unfortunately, a long-sought room temperature multiferroic with strongly coupled ferroelectric and ferromagnetic (or ferrimagnetic) orderings is still lacking. Here, we propose that hydrogen intercalation in antiferromagnetic transition metal oxides is a promising way to realize multiferroics with strong magnetoelectric coupling. Taking brownmillerite SrCoO$_{2.5}$ as an example, we show that hydrogen intercalated SrCoO$_{2.5}$ displays strong ferrimagnetism and large electric polarization in which the hydroxide acts as a new knob to simultaneously control the magnetization and polarization at room temperature. We expect that ion intercalation will become a general way to design magnetoelectric and spintronic functional materials.

$^*$This work is supported by the Special Funds for Major State Basic Research (Grant No. 2015CB921700), the Qing Nian Ba Jian Program, and the Fok Ying Tung Education Foundation.

5:06PM C02.00012: Magnetoelectric coupling effect in a new multiferroic RbFe(SO$_4$)$_2$  JUNJIE YANG (Presenter), Central Michigan University — In the past decade, intense efforts have been directed at the discovery of new multiferroic materials. To search new multiferroic materials, a lot of researches have been focusing on frustrated magnets which usually have complicated magnetic structure. For example, multiferroicity has been discovered in a triangular lattice antiferromagnet RbFe(MoO$_4$)$_2$. Recently we successfully grew high quality single crystals of RbFe(SO$_4$)$_2$ which is isostructural to the multiferroic RbFe(MoO$_4$)$_2$. In this work, we will discuss the ferroelectric polarization, dielectric constant and strong magnetoelectric coupling effect in RbFe(SO$_4$)$_2$ single crystals.
5:18PM C02.00013: Loss of spin polarization of tunnelling currents due to electrostatic screening at magnetoresistive ferromagnet/ferroelectric tunnel junctions*  IBRAHIM MISIRIOGLU (Presenter), CANHAN SEN, WAEL ALDULAIMI, OMID MORADI, Sabanci University — Magnetoelectric coupling inherent to the bulk of multiferroic films or control of spin orientation in magnetic layers via piezoelectric strain in composite layers have been two forthcoming approaches to enable electric control of magnetic order. Spin-dependent screening occuring at dielectric/ferromagnetinterfaces is another magnetoelectric effect important for spin selective tunnel junctions. Here, we analyze the spin-dependent screening of ferroelectric polarization in a film interfacing ferromagnetic electrodes using the continuity equations. We show that local spin population (LSP) in spin subbands near the interfaces can dramatically deviate from bulk, which is in qualitative agreement with recent first principles results. We compute the tunneling currents for majority and minority spins using the Wentzel-Kramers-Brillouin approximation and demonstrate that spin polarization tends to disappear for increasing values of ferroelectric polarization in direct connection with the increase in subband LSP for minority spins. We argue that the reduction in TMR due to spin mixing at the interfaces will be much more prominent in comparison to defect scattering and magnon-driven losses in spin polarization.

*Tübitak 116F207 and Tübitak 117F042

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C03 DCMP: Novel Topological Systems BCEC 107B - Haiming Deng, City College of New York

2:30PM C03.00001: Observation of topological edge modes via smart patterning*  DAVID J. APIGO (Presenter), KAI QIAN, CAMELIA PRODAN, New Jersey Institute of Technology, EMIL PRODAN, Yeshiva University — In this talk we present a novel quasi-periodic system supporting topological edge modes made of magnetically coupled mechanical spinners. The system is patterned such that it possesses a naturally multi-gapped phonon spectrum where energy cannot propagate. This behavior occurs solely due to the system’s patterning, no fine tuning of the system is required. Typically, fine tuning in periodic systems is required to break topological symmetry classes; however, due to its unique structure, the reported pattern displays topological behavior. We present experimental results that demonstrate the mapping of chiral bands within the large gaps of the system’s phonon spectrum by scanning over phason shifts in the pattern. By varying the phason, bulk behavior remains unchanged; however, the edge states shift connecting two bulks bands they reside in. This study demonstrates the robust nature of the edge states in the reported quasi-periodic system and suggests that they are novel platforms for studying these unique properties.

*All authors acknowledge support from the W.M. Keck Foundation.

2:42PM C03.00002: Electric tuning of topological properties in a symmetric broken gap quantum well  TIAGO DE CAMPOS, University at Buffalo, The State University of New York, MARCELO A. TOLOZA SANDOVAL (Presenter), Universidade Federal da Bahia, LEOVILDO DIAGO-CISNEROS, Departamento de Física Aplicada, Universidad de La Habana, GUILHERME M SIPahi, Instituto de Física de São Carlos, Universidade de São Carlos — A mainstream within topological insulators, GaSb/InAs quantum wells (QWs) present a broken gap alignment for the energy bands which supports the quantum spin Hall insulator phase [1,2] and forms an important building block in the search of exotic states of matter [3]. Such QWs have electrons and holes are confined in different layers, leading to a wide range of possibilities to tune the topological properties. In this work, we study the inverted band structure of a symmetric GaSb/InAs QWs under the influence of an electric field applied along the growth direction, using the 8-band k.p model and the envelope function approximation. Without external fields, the collapse of the energy gap occurs in ~10 nm for the InAs layer (where the conduction and valence states become degenerate) and the application of an electric field opens the gap with an inverted band structure. The behavior of the hybridization gap and of the corresponding edge states are investigated considering a gradual increasing of the electric field modulus, which shows that they can be externally tuned in this system.

2:54PM C03.00003: In-situ Fermi level tuning of semiconductor thin films on graphene during scanning tunneling microscopy studies*  
YULIA MAXIMENKO (Presenter), ZHENYU WANG, CHARLES STEINER, DAVIDE IAIA, VIDYA MADHAVAN, University of Illinois at Urbana-Champaign — Doping can often drive the system into interesting quantum phases such as superconductivity or the pseudo-gap phase. Typically, doping is controlled during fabrication by adjusting the dopant impurity ratios or tuning the chemical composition of the main elements. For a detailed atomically-resolved study of a material with a complex phase diagram, it is beneficial to implement in-situ Fermi level (EF) tuning that can be done by gating. Gating is a somewhat robust technique in transport measurements, but combining it with epitaxial film growth and scanning tunneling microscopy (STM) presents many technical challenges. Here, we report the design of a robust back-gating device for a versatile thin film growth and subsequent EF tuning inside STM. Graphene serves as the platform for epitaxial growth, while a range of materials can be used as an insulating gate depending on the particular experiment. We demonstrate successful EF tuning in both Bi$_2$Te$_3$ and SnTe films in STM. We study the strength of the effect in terms of Schottky barriers between materials, film thickness, and quality of the gate and report a magnetic field study of back-gated thin films of topological insulators.

*STM work was supported by US Dept. of Energy, Scanning Probe Division under Award#DE-SC0014335.

3:06PM C03.00004: Thermodynamic probe of the bulk gap in the quantum spin Hall insulator 1T'-WTe$_2$*  
SERGIO DE LA BARRERA (Presenter), QINGRUI CAO, Department of Physics, Carnegie Mellon University, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, BENJAMIN MATTHEW HUNT, Department of Physics, Carnegie Mellon University — Single-layer 1T'-phase WTe$_2$ has recently drawn great interest as a candidate material for hosting an intrinsic quantum spin Hall insulator state at low temperature, a highly attractive property for numerous studies and applications. Such a state requires topologically-protected helical edge states coincident with a bulk band gap. Initial calculations of the 1T'-WTe$_2$ electronic structure predicted semimetallic bands, however, several studies have shown simultaneous experimental evidence of edge states and a bulk gap in photoemission, tunneling spectroscopy, and electron transport. The nature of this gap, however, is not fully resolved, with disagreements between predicted gaps from first-principles calculations and spectroscopic measurements in various conditions. Here, we probe the thermodynamic properties of fully-encapsulated single-layer 1T'-WTe$_2$ using low-temperature capacitance to illuminate the discussion of this gap and its single-particle or interaction-driven origin.

*Funding for this work was provided by the Charles E. Kaufman Foundation, a supporting organization of The Pittsburgh Foundation, via Young Investigator research grant KA2016-85226.

3:18PM C03.00005: Quantifying charge-to-spin conversion efficiency in magnetically-doped topological insulator heterostructures*  
QUANJUN PAN (Presenter), XIAOYU CHE, QIMING SHAO, Electrical and Computer Engineering Department, University of California, Los Angeles, YABIN FAN, Microsystems Technology Laboratories, Massachusetts Institute of Technology, LEI PAN, HAO WU, PENG ZHANG, MOHAMMAD MONTAZERI, KANG L. WANG, Electrical and Computer Engineering Department, University of California, Los Angeles — We deployed a magneto–optical mangetometer and an electrical loop shift method to directly quantify the charge-to-spin conversion efficiency in a magnetically-doped topological insulator heterostructure. While these two approaches are essentially different in their experimental principles, quantitative agreements are found in values obtained by the two approaches. This consistency strongly suggests both methods can accurately estimate the charge-to-spin conversion efficiency without some ambiguity reported previously with other approaches. The charge-to-spin conversion efficiency, which is parameterized by the spin Hall angle tangent, is estimated to be 0.46 and 0.38 at 12K by the magneto–optical mangetometer and the electrical loop shift method, respectively. This value is at least one order larger than those of conventional heavy metals. Our results also reveal that magneto–optical mangetometer and loop shift methods are both reliable and easily accessible for investigation of magnetization dynamics in TI-based magnetic structures.

*We acknowledge the funding support from SHINES, MURI, TANMS, and the Army Research Office (ARO)
3:30PM C03.00006: Investigating the ferromagnetism-induced surface gap formation and effects of optical excitations in Cr-doped topological insulators (TIs)*

Adrian Llanos (Presenter), Department of Materials Science, California Institute of Technology. Chien-Chang Chen, Marcus Teague, Department of Physics, California Institute of Technology. Peng Zhang, Lei Pan, Koichi Murata, Kang Wang, Department of Electrical Engineering, University of California, Los Angeles. Nai-Chang Yeh, Department of Physics, California Institute of Technology — Despite the exciting observation of the quantum anomalous Hall effect (QAHE) in Cr-doped (BixSb1-x)2Te3 compounds, the microscopic origin of ferromagnetism (FM) and the temperature (T) evolution of the anomalous Hall (AH) resistance in these magnetic TIs remain poorly understood. We perform scanning tunneling spectroscopic and electrical transport studies on MBE-grown magnetic TIs, including uniformly 10% Cr-doped (BixSb1-x)2Te3 and bilayer systems consisting of a layer of pure (BixSb1-x)2Te3 on top of a 10% Cr-doped (BixSb1-x)2Te3 layer. In the STS studies on the bilayer system, a surface gap Δ opens up at T_{C2D} ~ 180 K, much higher than the bulk Curie temperature T_{C3D} ~ 35 K determined from the onset of AHE. The spatial distribution of Δ is largely homogeneous, and Δ increases with decreasing T, reaching Δ = (59±7) meV at 147K. Additionally, longitudinal (R_{xx}) and AH (R_{xy}) resistance are measured both with and without light. An increase in R_{xy} and decrease in R_{xx} is observed in the bilayer system under circularly polarized (CP) light (wavelengths λ =1600 ~ 1700 nm). In contrast, both R_{xx} and R_{xy} are suppressed under CP light for uniformly Cr-doped (BixSb1-x)2Te3. The physical implications of these findings will be discussed.

*This work is supported by Army Research Office.

3:42PM C03.00007: Interfaces and superlattices of the topological insulator Bi2Se3*

Niraj Aryal (Presenter), Efstratios Manousakis, Physics, Florida State University and National High Magnetic Field Laboratory — Interface states of topological materials are important for both emergent fundamental phenomena and for their potential application in future electronics and computing devices. Here, we propose different ways of manipulating the position of the energy of the surface Dirac states in the topological insulator (TI) Bi2Se3 relative to the bulk Fermi level, their linearity, their location, etc., by making contact with different materials. Our predictions are made by using density functional theory and model Hamiltonians. For example, in the case of an interface of a TI with a band insulator (BI) we find that the location of the interfacial topological state moves out of the topological insulator boundary to the BI side. When a TI forms an interface with a metal we find that the topological surface states can show oscillatory behavior which propagates inside the metal. We also present results for superlattices formed of a topological insulator with a band insulator.

*This work was supported in part by the U.S. National High Magnetic Field Laboratory, which is funded by NSF DMR-1157490 and the State of Florida.

3:54PM C03.00008: Microwave Impedance Microscopy of WTe2

Joshua Kahn (Presenter), University of Washington, Yanmeng Shi, University of California, Riverside, Zaiyao Fei, University of Washington, Brian A Francisco, Ben Niu, University of California, Riverside, Xiaodong Xu, University of Washington, Yongtao Cui, University of California, Riverside, David Henry Cobden, University of Washington — WTe2 is a van der Waals layered material that behaves as a 2D topological insulator when exfoliated down to a monolayer, supporting edge modes that should be topologically protected. Microwave impedance microscopy (MIM) is a technique that allows real-space mapping of conductivity with a resolution of < 50 nm, and is thus a powerful tool for studying these edge modes that reveals many features that are not accessible to transport measurements alone. Using MIM we observe that the edge is gapless and the edge conduction path conforms to microscopic corners and cracks in the edge and features internal to the monolayer flake. This is consistent with their topological nature and has important consequences for interpreting transport measurements and for making devices employing the 1D helical modes. We also study the behavior of multilayer WTe2, twisted bilayer WTe2, and monolayer WTe2 combined with other materials, such as different capping layers and 2D ferromagnets.

4:06PM C03.00009: Topological Classification Table Implemented with Classical Passive Meta-Materials*

Yafis Barlas (Presenter), Physics, Yeshiva University — Topological condensed matter systems from class A and class AII of the classification table have received classical electromagnetic and mechanical analogs. They topological phases exhibit protected wave-guiding which has been demonstrated experimentally. In this talk, we introduce a map which generates classical analogs for all entries of the classification table, using only passive elements. Physical mechanical models can be realized for all strong topological phases in dimension 2, as well as for three classes in dimension 3. As an example, we will show how the Kitaev topological super-conducting chain and it's braiding properties can be realized in classical systems.

*Keck Foundation
4:18PM C03.00010: Non-Local Spin Transport in Topological Insulator Nanowires  
POK LAM TSE (Presenter), GRACE LU, University of Southern California — The momentum and spin of charge carriers in Topological Insulators (TI) are constrained to be perpendicular due to spin-orbit coupling. Sb$_2$Te$_3$ is a TI material with a bulk band gap of 0.28 eV and surface states consisting of a single Dirac cone in the band gap. Single crystalline Sb$_2$Te$_3$ nanowires were synthesised. E-beam lithography were used to pattern two outer Au leads and two magnetic tunnel junctiion (MTJ) inner leads on individual Sb$_2$Te$_3$ nanowires. The MTJ leads consist of a free Py (Ni$_{80}$Fe$_{20}$) layer, whose magnetization determines the magnitude and direction of spin current injected into nanowire.

The two-point resistance between Au contacts under magnetic field sweep showed positive magneto-resistance, originating from weak anti-localization of carriers in nanowire induced by spin-orbit interaction, serves as evidence of a strong impact of spin orbit interaction in nanowires.

The symmetry of non-local spin valve (NLSV) signal is dramatically different from that of a NLSV with a channel that lacks spin-momentum locking (SML) (e.g. graphene). Two parallel states of the injector and detector magnetic moments give rise to different NLSV voltage values, which is never observed in conventional NLSVs. This unusual symmetry is a signature of SML in Sb$_2$Te$_3$ nanowire surface state.

4:30PM C03.00011: Numerical signatures of topology in disordered insulators*  
DOMINIC REISS (Presenter), ALBERT BROWN, FENNER HARPER, XU LIU, RAHUL ROY, Physics and Astronomy, University of California, Los Angeles — We investigate a number of numerical signatures which distinguish the topological and trivial phases of disordered insulators. In particular, we consider three dimensional systems with time-reversal symmetry (class AII) and numerically construct a set of maximally commuting spin-like operators using local unitary circuits. The properties of the resulting spin operators may be used to identify the topology of the underlying phase. Using similar methods, we also construct analogues of Wannier functions for disordered systems with symmetry. Finally, we discuss extensions of this approach to other spatial dimensions and symmetry classes.

*D. R., A. B., F. H., X. L. and R. R. acknowledge support from the NSF under CAREER DMR-1455368 and the Alfred P. Sloan Foundation.

4:42PM C03.00012: Scattering from Monolayer and Bilayer Step Edges on Topological Sb(111)*  
ADITYA MAHADEVAN (Presenter), Physics, Harvard University, HAIMEI ZHANG, Physics, Wellesley College, JIANFENG GE, YANG HE, Physics, Harvard University, ANJAN SOUMYANARAYANAN, ASTAR, SHIANG FANG, JENNIFER HOFFMAN, Physics, Harvard University — The topological semimetal antimony (Sb) has a layered structure that cleaves easily along the 111 plane, typically exposing large, atomically flat terraces separated by bilayer steps. Reflection and transmission of 2D surface states from these step edges can be used to quantify the topological protection against backscattering. Here we use scanning tunneling microscopy (STM) to image the cleaved surface of Sb(111). In addition to the expected bilayer steps, we occasionally find monolayer steps, as well as a combination of mesa, stair, and valley terraces. We use spectroscopic STM to probe the quantized energy levels of surface states on each of these terraces, and compare to the energy quantization that would be expected from the visible terrace width. Our analysis indicates that surface states are more easily transmitted under adjacent terraces, i.e. there is less backscattering from upward step edges.

*Experiments were supported by National Science Foundation DMR-1410480.
Quantized anomalous Hall conductance in a bulk dilute Mn-doped topological insulator Bi$_2$Te$_3$ at high temperatures

4:54PM C03.00013: HAIMING DENG (Presenter), ZHIYI CHEN, SHIHUA ZHAO, City College of New York, SIMON TURKEL, ABHAY PASUPATHY, Physics, Columbia University, LUKASZ PLUCINSKI, Physics, Forschungszentrum Juelich, MARCIN KONCZYKOWSKI, LSI, Ecole Polytechnique, AGNIESZKA WOLOS, Physics, University of Warsaw, KYUNGWHA PARK, Physics, Virginia Tech, LIA KRUSIN-ELBAUM, City College of New York — Thus far Quantized anomalous Hall (QAH) has only been realized in the mK range in ultra-thin (5-10nm) MBE films of heavily Cr- or V-doped (Bi,Sb)$_2$Te$_3$, where the Curie $T_c$ could be as high as 60 K but the onset of Anomalous Hall effect (AHE) was at a much lower $T$. Here we report achieving Hall conductance quantization in the Kelvin range in dilute (2%) Mn-doped thick (50-300 nm) single crystals of Bi$_2$Te$_3$ by taking a different approach to tune the Fermi level $E_F$ into the Dirac gap. Our technique employs high energy-electron beams (2.5MeV) to create charged defect states in the bulk and thermal annealing protocols to control both $E_F$ and the surface bandstructure of the initially n-type Mn-doped Bi$_2$Te$_3$. In contrast to previous work, the magnetization $M$ was found to be mean-field-like and carrier independent, with $M$ and AHE onsetting at the same $T_c$ ~ 13 K. We observe conductance quantization $G_{xy} = 1.0098 \ h/e^2$ not in the bulk gap but on the bulk conduction band where, remarkably, conduction electrons do not contribute to AHE. We will discuss the correlation of surface and bulk AHE with magnetism in this dilute system. The cross-correlation of transport data with STM and ARPES will be discussed.

*NSF-DMR-1420634, NSF-DMR-1312483-MWN, and NSF HRD-1547830

In gap states in topological Kondo insulators: Optical properties evidence

5:06PM C03.00014: ROBERTO FRANCO PEÑALOZA (Presenter), EDWIN RAMOS, JERESON SILVA VALENCIA, National University of Colombia, MARCOS SERGIO FIGUEIRA DA SILVA, Instituto de Fisica, Universidade Federal Fluminense — We investigate optical properties: ARPES, PES and optical conductivity of topological Kondo insulators; in particular we study the manifestation of In gap states in the ARPES and PES results, taking into account the presence of antiferro-magnetic short range correlations. We consider an additional narrow band to the otherwise completely localized f-electrons, by adding a term to the periodic Anderson model which allows a small hopping of the localized electrons between neighboring sites of the lattice. This new model is adequate to study a novel class of intermetallic 4f and 5f orbitals materials: the Kondo topological insulators. For simplicity, we consider a version of the periodic Anderson model on a two dimensional square lattice. Previously we shows that the anti ferro-magnetic correlations plays an important role on the gap opening of the topological Kondo insulators (1); in this work we discuss the manifestation of the in gap states in the ARPES and PES results, our results for the different symmetry points are similar to the reported for SmB$_6$ (2).

(2) M. Neupane et al, Nature Communications, DOI:10.1038/ncomms3991 (2013)

*Colciencias - Colombian National Science Agency
CNPq- Brazilian National Science Council

Engineering topological superlattices: Phase diagrams and electronic properties

5:18PM C03.00015: DEEPTI JAIN (Presenter), PAVEL P SHIBAYEV, ELIO KOENIG, MARYAM SALEHI, JISOO MOON, Rutgers University, New Brunswick — So far, the majority of topological materials being investigated have been bulk crystals or thin films. A much less-explored area is combining different topological materials with trivial insulators and creating a new topological phases with distinct electronic properties, in the form of topological superlattices. We have studied a topological superlattice composed of topological insulator Bi$_2$Se$_3$, and normal insulator In$_2$Se$_3$ of different thickness. In this talk, we will discuss the low-temperature magnetotransport measurements and field theoretical calculations which show how the electronic properties of topological superlattices evolve with unit-layer thicknesses. We will further discuss if it is plausible to implement other more complex topological phases such as artificial 3D Dirac and Weyl semimetals from TI superlattices

*Gordon and Betty Moore foundation

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C04 DMP: Dirac/Weyl Semimetals -- Nodal-line Semimetals and Beyond BCEC 107C - Lu Li, University of Michigan - Tag(s): Focus
2:30PM C04.00001: Electronic structure of topological nodal semimetals [Invited] TAY-RONG CHANG (Presenter), Physics, National Cheng Kung University, GUANG BIAN, Physics, U. of Missouri, SUYANG XU, Physics, MIT, GUOQING CHANG, Physics, Princeton U., ARUN BANSIL, Physics, Northeastern U., ROBERT CAVA, Chemistry, Princeton U., HSIN LIN, Physics, Academia Sinica, ZAHID HASAN, Physics, Princeton U. — Topological phases in condensed matter physics have attracted intense worldwide interest in the past decade because these phases lie outside the framework of Landau's spontaneous symmetry breaking paradigm. The early period of the field explored topological insulators (TIs). Three-dimensional (3D) TIs are distinct from the conventional band insulators in that they feature a bulk energy gap driven by spin-orbit coupling effects, and gapless surface states protected by time-reversal symmetry. In the last few years, the focus has shifted from insulators to topological semimetals (TSMs). Three types of TSMs have been identified, namely, Dirac, Weyl, and nodal-line semimetals. Dirac and Weyl semimetals are 3D analogs of graphene in which the bulk band structure disperses linearly from the nodal point in all three momentum directions, while the nodal-line semimetals display 1D nodal loops in the 3D Brillouin zone. In addition to the graphene-type (type-I) TSMs, the novel type-II TSMs where the band dispersion strongly violates Lorentz symmetry have also been studied extensively. In this talk, we will review a range of materials predictions including type-II Dirac semimetals [1], tunable Weyl semimetals [2], and nodal-line semimetals [3-5] by using first-principles calculations, and discuss various exotic phenomena observed experimentally in these compounds.


3:06PM C04.00002: Topological nodal line semimetals without drumhead surface states* QIU-BO CHENG (Presenter), Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, CHING-KAI CHIU, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, HONGMING WENG, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences — Topological nodal lines are protected by reflection symmetry or space-time inversion symmetry. The symmetries can quantize Berry phase in a proper basis and the π Berry phase stems from the presence of the protected topological lines. However, it has been shown that the only π Berry phase cannot lead to the presence of the stable drumhead surface states, which connect the bulk nodal lines. The other essential condition for the drumhead surface states is that no atoms should be located at the symmetry centers in the crystal structure. However, in condensed matter systems most of the topological nodal line semimetals fail this requirement and possess the drumhead surface states. In this talk, we show several concrete topological nodal line materials not possessing any drumhead surface states. The examples demonstrate that the bulk-boundary correspondence has very strict conditions for crystalline symmetries.

*the Strategic Priority Research Program of the Chinese Academy of Sciences, Grant No. XDB28000000 National key R&D Program of China, Grant No. 2016YFA0300600 NSFC, Grant No. 11421092

3:18PM C04.00003: Material realization of Z2 monopole nodal lines in ABC-stacked graphdiyne JUNYEONG AHN, Department of Physics and astronomy, Seoul National University, DONGWOOK KIM (Presenter), YOUNGKUK KIM, Department of Physics, Sungkyunkwan University, BOHM-JUNG YANG, Department of Physics and astronomy, Seoul National University — A topological nodal line semimetal refers to a topological state of matter characterized by protected one-diemsional gapless excitations in momentum space. Z2 Berry phase nodal line semimetal is one of the most widely studied topological nodal line semimetals with many material realizations. Here, another class of nodal line semimetal exists, referred to as Z2 monopole nodal line semimetals. This class of nodal line semimetal is remained widely unexplored without a suggested material realization yet. Using first-principles calculations, we show that a three-dimensional carbon allotrope, ABC-stacked graphdiyne (ABC-GDY), realizes the Z2 monopole nodal line semimetal [1]. We characterize a Z2 Stiefel-Whitney number and a linking number that dictate the Z2 monopole nodal line semimetal phase in ABC-GDY. We also show that ABC graphdiyne hosts two-dimensional Stiefel-Whitney insulating phase in two-dimensional subsystems of the Brillouin zone, which can be considered as a fragile topological insulator phase. We present nested wilson loop spectrum and hinge state to show the higher order band topology of ABC-GDY as well. Our findings suggest that ABC graphdiyne should serve as a new venue for the study of topological semimetals.
3:30PM C04.00004: Nodal surface semimetals: Theory and materials realization
WEIKANG WU (Presenter), YING LIU, Singapore University of Technology and Design, SI LI, Beijing Institute of Technology, CHENGYONG ZHONG, Chongqing University of Posts and Telecommunications, ZHI-MING YU, Singapore University of Technology and Design, XIAN-LEI SHENG, Beihang University, YUXIN ZHAO, Nanjing University, SI LI, Beijing Institute of Technology, CHENGYONG ZHONG, Chongqing University of Posts and Telecommunications, ZHI-MING YU, Singapore University of Technology and Design — We theoretically study the three-dimensional topological semimetals with nodal surfaces protected by crystalline symmetries. Different from the well-known nodal-point and nodal-line semimetals, in these materials, the conduction and valence bands cross on closed nodal surfaces in the Brillouin zone. We propose different classes of nodal surfaces, both in the absence and in the presence of spin-orbit coupling (SOC). In the absence of SOC, a class of nodal surfaces can be protected by spacetime inversion symmetry and sublattice symmetry, and characterized by a $Z_2$ index, while another class of nodal surfaces are guaranteed by a combination of nonsymmorphic two-fold screw-rotational symmetry and time-reversal symmetry. We show that the inclusion of SOC will destroy the former class of nodal surfaces but may preserve the latter provided that the inversion symmetry is broken. We further generalize the result to magnetically ordered systems and show that protected nodal surfaces can also exist in magnetic materials without and with SOC, given that certain magnetic group symmetry requirements are satisfied. Several concrete nodal-surface material examples are predicted via the first-principles calculations. The possibility of multi-nodal-surface materials are discussed.

3:42PM C04.00005: Possible pressure-induced topological quantum phase transition in the nodal line semimetal ZrSiS
DERRICK VANGENNEP (Presenter), Department of Physics, University of Florida, TIFFANY PAUL, Department of Applied Physics, Stanford University, CHASE W. YERGER, Department of Physics, University of Florida, SAMUEL T WEIR, Physics Division, Lawrence Livermore National Laboratory, YOGESH KUMAR VOHRA, Department of Physics, University of Florida at Birmingham, JAMES J. HAMLIN, Department of Physics, University of Florida — ZrSiS has recently gained attention due to its unusual electronic properties: nearly perfect electron-hole compensation, large, anisotropic magneto-resistance, multiple Dirac nodes near the Fermi level, and an extremely large range of linear dispersion of up to $\sim 2$ eV. We have carried out a series of high pressure electrical resistivity measurements on single crystals of ZrSiS. Shubnikov-de Haas measurements show two distinct oscillation frequencies. For the smaller orbit, we observe that the phase of the oscillations changes by $\sim 0.5$ between $\sim 0.16-0.5$ GPa. This change in phase is accompanied by an abrupt decrease of the cross-sectional area of this Fermi surface. We attribute this change in phase to a possible topological quantum phase transition. The phase of the larger orbit exhibits a Berry phase of $\pi$ and remains roughly constant up to $\sim 2.3$ GPa. Resistivity measurements to higher pressures show no evidence for pressure-induced superconductivity to at least 20 GPa.

*This work was supported by National Science Foundation (NSF) CAREER award DMR-1453752 as well as a National High Magnetic Field Laboratory (NHMFL) User Collaboration Grant. The NHMFL is supported by the NSF via Cooperative agreement No. DMR-1157490, the State of Florida, and the U.S. Department of Energy.

3:54PM C04.00006: Observation of Dirac nodal lines in rutile oxide IrO$_2$
JOICENNE NELSON (Presenter), LUCA MORESCHINI, Cornell University, JASON KAWASAKI, University of Wisconsin, Madison, ELI ROTENBERG, Advanced Light Source, Lawrence Berkeley National Laboratory, DARRELL G. SCHLOM, KYLE M SHEN, Cornell University — The complex oxide IrO$_2$ is predicted to be a dirac nodal line semimetal protected by nonsymmorphic symmetry. Some of its intriguing physical properties include a large spin hall effect, significant magnetoresistance, and a hall effect where the sign of the carrier may be controlled by an external magnetic field. Previously there has been no direct evidence of the topological features of the band structure. This is a non trivial prediction because the relevant orbitals Ir 5d and O 2p are known to often host strong electron correlations and spin orbit coupling. Using a combination of reactive oxide molecular beam epitaxy and Angle-Resolved Photoemission Spectroscopy we show that IrO$_2$ is a Dirac nodal line semimetal in agreement with the predictions of Sun et. al. This is the first experimental observation of nodal lines protected by nonsymmorphic symmetry. Significantly the crossing points are protected even in the case of large spin orbit coupling characteristic of iridates. Furthermore they cross the fermi level making IrO$_2$ an ideal system to study the low energy properties of Dirac nodal line materials.
4:06PM C04.00007: Multiple topologically non-trivial bands in non-centrosymmetric YSn$_2$  
YANGLIN ZHU (Presenter), Tulane University, TIANTIAN ZHANG, Institute of Physics CAS, JIN HU, Department of Physics, University of Arkansas, JAMIN KIDD, Tulane University, DAVID E GRAF, National High Magnetic Field Laboratory, XIN GUI, WEIWEI XIE, Department of Chemistry, Louisiana State University, MENGZE ZHU, XIANGLIN KE, Department of Physics and Astronomy, Michigan State University, HUIBO CAO, Quantum Condensed Matter Division, Oak Ridge National Laboratory, ZHIQIANG MAO, Tulane University — We show that, in non-centrosymmetric compound YSn$_2$, the slightly distorted square lattice of Sn generates multiple topologically non-trivial bands, one of which likely hosts nodal line and tunable Weyl semimetal state induced by the Rashba spin-orbit coupling (SOC) and proper external magnetic field. The quasiparticles described as relativistic fermions from these bands are manifested by nearly zero mass and non-trivial Berry phases probed in de Haas–van Alphen (dHvA) oscillations. The dHvA study also reveals YSn$_2$ has a complicated Fermi surface (FS), consisting of several 3D and one 2D pockets. Our first principle calculations show the point-like 3D pocket at Y point on the Brillouin zone boundary hosts the possible Weyl state. Our findings establish YSn$_2$ as a new interesting platform for observing novel topological phases and studying their underlying physics.

4:18PM C04.00008: Unraveling the Topological Nature of ZrSiTe using Scanning Tunneling Microscopy*  
BRANDON STUART (Presenter), JISUN KIM, SEOKHWAN CHOI, University of British Columbia, LESLIE SCHOOP, Chemistry, Princeton, DOUGLAS BONN, SARAH BURKE, University of British Columbia — 3D topological Dirac semimetals have been a topic of immense study since their experimental realization in 2014. The family of materials ZrSiX (X = S, Se, Te) are topological nodal-line Dirac semimetals, which exhibit a nodal-line band crossing encircling the Γ-point, and two Dirac cones at the X-point protected by a non-symmorphic symmetry. From this family, ZrSiS was the first material to be experimentally studied, and was shown to have two Dirac cones at ± 0.5 V [1]. It was predicted that due to the size difference, substituting S with Te would result in a uniaxial strain along the c-axis, shifting the upper Dirac cone towards the Fermi level [2]. Using low temperature scanning tunneling microscopy and spectroscopy we uncover the surface structure of ZrSiTe, which cleaves easily between ZrTe layers. We observe several unique defects, some of which span multiple lattice sites. Furthermore, by employing quasiparticle interference (QPI), we can resolve the scattering properties of the electrons, and unravel the complex topological nature of the band structure.

*Work funded by the following agencies: CFI, CFREF, NSERC, and MPI.

4:30PM C04.00009: Topological Phases of Zintl Compounds Ba$_3$X$_2$Y$_4$ (X=Zn, Cd; Y=As, Sb)*  
TAN ZHANG (Presenter), Chinese Academy of Sciences, SI-MIN NIE, Department of Materials Science and Engineering, Stanford University, HONGMING WENG, ZHONG FANG, Chinese Academy of Sciences — Based on first-principles calculations and effective k.p model analysis, we have studied three Zintl compounds, including Ba$_3$Zn$_2$As$_4$, Ba$_3$Cd$_2$As$_4$ and Ba$_3$Cd$_2$Sb$_4$, to reveal their electronic band topology under different conditions, such as including and not including spin-orbit coupling (SOC) and different external strains. We find that these family materials are close to the boundaries of several topological phases. When SOC is ignored, there are topological nodal lines around Fermi energy due to band inversion between valence and conduction bands at one or two time-reversal invariant momenta, which can be tuned by proper strain. When SOC is further included, these nodal lines are gaped and these materials become weak or strong topological insulators (TIs). They are suitable for studying topological phase transition.

*We acknowledge the supports from the Ministry of Science and Technology of China (Grants No. 2016YFA0300600 and 2018YFA0305700) the National Natural Science Foundation (Grant No. 11674369) and the Chinese Academy of Sciences (Grant No. XDB07000000).
4:42PM C04.00010: Topological hourglass Dirac semimetal in $\text{Ag}_2\text{BiO}_3$  

BAHADUR SINGH (Presenter), Shenzhen University, Shenzhen, China, BARUN GHOSH, Indian Institute of Technology Kanpur, India, CHENLIANG SU, Shenzhen University, Shenzhen, China, HSIN LIN, Academia Sinica, Taipei, Taiwan, AMIT AGARWAL, Indian Institute of Technology Kanpur, India, ARUN BANSIL, Northeastern University, Boston (MA), USA — Materials with tunable charge and lattice degrees of freedom provide excellent platforms for investigating multiple phases that can be controlled via external stimuli. We show how the charge-ordered ferroelectric oxide $\text{Ag}_2\text{BiO}_3$, which has been realized experimentally, presents a unique exemplar of a metal-insulator transition under an external electric field. Our first-principles calculations combined with a symmetry analysis, reveal the presence of a nearly ideal hourglass-Dirac-semimetal state in the nonpolar structure of $\text{Ag}_2\text{BiO}_3$. The low-energy band structure consists of two hourglass-like nodal lines located on two mutually orthogonal glide-mirror planes in the absence of spin-orbit coupling (SOC) effects. These lines cross at a common point and form an interlinked chain-like structure, which extends beyond the first Brillouin zone. Inclusion of the SOC opens a small gap in the nodal lines and results in two symmetry-enforced hourglass-like Dirac points on the $C_2\gamma$ screw rotation axis. Our results indicate that $\text{Ag}_2\text{BiO}_3$ will provide an ideal platform for exploring ferroelectric-semiconductor to Dirac-semimetal transition by the application of an external electric field.

4:54PM C04.00011: Pseudo Dirac-Nodal-Sphere Semimetal  

JIANFENG WANG (Presenter), Beijing Computational Science Research Center, FENG LIU, University of Utah, BING HUANG, Beijing Computational Science Research Center — Topological semimetals (TSMs) in which conduction and valence bands cross at zero-dimensional (0D) Dirac nodal points (DNPs) or 1D Dirac nodal lines (DNLs), in 3D momentum space, have recently drawn much attention due to their exotic electronic properties. Here we generalize the TSM state further to a higher-symmetry and higher-dimensional Dirac nodal sphere (DNS) or pseudo DNS (PDNS) state, with the band crossings forming a 2D closed or approximate sphere at the Fermi level. Such TSM state can exhibit unique electronic properties, such as peculiar collective plasmons, making DNS/PDNS a new type of fermion beyond DNP/DNL paradigm. Despite the difficulties to achieve the ideal DNS state in realistic crystals, we successfully demonstrate two possible types of PDNS states underlied by different crystalline symmetries, which are characterized with a spherical backbone consisting of multiple crossing DNLs and approximate band degeneracy in between the DNLs. Importantly, we identify all the possible band crossings with pairs of 1D irreducible representations to form the PDNS states in 32 point groups. Furthermore, we discover that strained $\text{MH}_3$ ($M = \text{Y, Ho, Tb, Nd}$) and $\text{Si}_3\text{N}_2$ are materials candidates to realize these two types of PDNS states, respectively.

5:06PM C04.00012: Exceptional lines in topological semimetals and superconductors*  

ALEXANDER ZYUZIN (Presenter), Aalto University, KRISTOF MOORS, University of Luxembourg, RAKESH P. TIWARI, McGill University, THOMAS L SCHMIDT, University of Luxembourg — We consider the impact of the disorder on the spectrum of three-dimensional Weyl and nodal-line semimetals. We show that the combination of disorder and a tilted spectrum leads to a non-Hermitian self-energy contribution that can split a Weyl node and nodal line into a single nodal ring and pair of exceptional lines, respectively. In nodal-line semimetals, these exceptional lines form the boundary of an open and orientable bulk Fermi ribbon in reciprocal space on which the energy gap vanishes. We find that the surface of such a disorder-induced bulk Fermi ribbon in general lies orthogonal to the direction of the tilt, which can be exploited to realize a bulk Fermi ribbon with nontrivial topology by means of a tilt vector that twists along a nodal loop.

We also consider the dispersion of the quasiparticles excitations in nodal superconductors in presence of weak disorder. Similarly to the semimetals, the complex self-energy correction to the Green function of quasiparticles due to disorder gives rise to the non-Hermitian BdG Hamiltonian describing the quasiparticle spectrum with exceptional points and lines.

*KM and TLS acknowledge the support by the National Research Fund Luxembourg with ATTRACT Grant No. 7556175. AZ acknowledges the support by the Academy of Finland.
Two-dimensional nonsymmorphic Dirac semimetal in chemically modified group-VA Monolayer with Black Phosphorene structure

KYUNG-HWAN JIN (Presenter), HUAQING HUANG, University of Utah, ZHENGFEI WANG, University of Science and Technology of China, FENG LIU, University of Utah — The symmetry-protected 2D Dirac semimetals have attracted intense interest due to their intriguing properties. Here, we investigate the 2D nonsymmorphic Dirac semimetal state by chemically modified group-VA 2D puckered structure. Based on first-principles calculations, we demonstrated 2D Dirac fermionic states not only exist, but in fact occur with two different types: one is a Dirac nodal line (DNL) structure in one-side modified phosphorene structure with negligible SOC; the other is a hourglass fermion protected by nonsymmorphic symmetry for the heavy elements with strong SOC. In the absence of SOC, the DNL exhibits anisotropic behavior and unique electronic properties, such as constant density of states. The Dirac node is protected from gap opening by nonsymmorphic symmetry. With the inclusion of SOC, the DNL states are split to form the hourglass dispersion due to broken inversion symmetry and Rashba SOC interaction. Moreover, around certain high symmetry points in the Brillouin zone, the spin orientation is enforced to be along a specific direction. The essential physics of 2D nonsymmorphic Dirac states is further analyzed by effective tight-binding models and group theory.

*This work is supported by DOE-BES under Grant No DE-FG02-04ER46148.

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C05 DMP: Topological Superconductivity: Twisted Layers, Heterojunctions, Interfaces

BCEC 108 - Arun Bansil - Tag(s): Focus

2:30PM C05.00001: Topological Chiral Superconductor with Spontaneous Vortices and Supercurrent in Twisted Bilayer Graphene

FENGCHENG WU (Presenter), Condensed Matter Theory Center, University of Maryland, IVAR MARTIN, Argonne National Laboratory — We present a study of d-wave superconductivity in twisted bilayer graphene within mean-field theory, and demonstrate new phenomena that arise due to the moire superlattice. In the d-wave pairing, the relative motion (RM) of two electrons in a Cooper pair can have either $d_x$ or $d_y$ symmetry, which carry opposite angular momenta. Due to the enlarged moire superlattice, the center-of-mass motion (COMM) can also carry a finite angular momentum without breaking the moire periodicity. By matching the total angular momentum, which has contributions from both the RM and the COMM, $d_x$ and $d_y$ RMs are intrinsically coupled in a way such that the COMM associated with one of the RMs has a spontaneous vortex-antivortex lattice configuration. Another new phenomenon is that the chiral d-wave state carries spontaneous bulk supercurrent. We also discuss the superconductivity gap structure. The chiral d-wave superconductors are gapped and also topological as characterized by quantized Chern number. Nematic d-wave superconductors, which could be stabilized when the six-fold rotational symmetry of the twisted bilayer graphene is broken, for example by uniaxial strain, are gapless with point nodes.

2:42PM C05.00002: Theory of Superconductivity in Magic-Angle Twisted Bilayer Graphene

NOAH BRAY-ALI (Presenter), Physics, CSU Dominguez Hills — Superconductivity in graphene bilayers occurs at certain “magic angles” of relative orientation between the layers. At these angles, the Moire-Bloch bandstructure becomes nearly flat at the Fermi energy. To describe superconductivity in these flat-band graphene bilayers, we extend the theory of superconductivity previously developed for single-layer graphene doped away from the Dirac point to the saddle point in the bandstructure on the edge of the Brillouin zone. The dominant channel for condensation is still spin-singlet Cooper pairing with $d_x+i d_y$ pair wavefunction, as we show using a perturbative renormalization group argument. Going beyond perturbation theory, we compute the entanglement spectrum using the Bardeen-Cooper-Schrieffer wavefunction and compare the result to the spectrum expected from the conformal field theory of a pair of free massless chiral Majorana fermions confined to the edge.

*The author acknowledges support from the California State University, Dominguez Hills Faculty Research Initiative and computational facilities provided by the campus computing center.
Flat bands and superconductivity in twisted bilayer graphene: insights from full scale Bogoliubov-de Gennes solutions.*

TOMAS LOTHMANN (Presenter), JOHANN SCHMIDT, FARIBORZ PARHIZGAR, ANNICA M BLACK-SCHAFFER, Uppsala University — The recently experimentally observed, possibly unconventional, superconducting state in twisted bilayer graphene (TBLG) opens up a highly tunable playground for correlated systems and exotic orders, where optimal conditions for exotic superconductivity are believed to result from a twist induced flattening of the electronic bands. Here we test the distinctive role of the flat bands in the formation and enhancement of superconductivity in TBLG and we detail the resulting implications for unconventional chiral $d+id$ superconductivity. We show these results from the self-consistent solutions of the complete Bogoliubov-de Gennes (BdG) equations of the full tight-binding Hamiltonian of TBLG, which in the case of magic twist angle TBLG with its long wavelength moiré interference pattern poses a formidable computational challenge that we rigorously address with a novel numerical approach.

*This work was supported by the Knut and Alice Wallenberg Foundation (KAW), the Swedish Research Council (Vetenskapsrådet), the Göran Gustafsson Foundation, the Swedish Foundation for Strategic Research (SSF), and by computation resources at UPPMAX provided by Swedish National Infrastructure for Computing (SNIC).

A unified numerical approach to topological semiconductor-superconductor heterostructures

GEORG W. WINKLER (Presenter), ANDREY ANTIPOV, BERNARD VAN HECK, Station Q, Microsoft, ALEXEY A SOLUYANOV, University of Zurich, LEONID GLAZMAN, Yale University, MICHAEL WIMMER, Delft University of Technology, ROMAN LUTCHYN, Station Q, Microsoft — We develop a unified numerical approach for modeling semiconductor-superconductor heterostructures and apply it to topological Majorana nanowires. Our approach takes into account on equal footing important key ingredients: proximity-induced superconductivity, orbital and Zeeman effect of an applied magnetic field, spin-orbit coupling as well as the electrostatic environment. As a model system, we consider indium arsenide (InAs) nanowires with epitaxial aluminum (Al) shell and demonstrate qualitative agreement of the obtained results with the existing experimental data. Finally, we characterize the topological superconducting phase emerging in a finite magnetic field and calculate the corresponding topological phase diagram.

Spin-resolved Andreev transport in quantum Hall edges of a proximitized van der Waals heterostructure*

&OUML;NDER G&OUML;L (Presenter), YUVAL RONEN, BRENNAN DIZDAR, SI YOUNG LEE, YOUNG JAE SHIN, Harvard University, DANIAL HAEI NAJAFBADI, University of Massachusetts Lowell, ZEYU HAO, JONATHAN ZAUBERMAN, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, PHILIP KIM, Harvard University — Topological superconductivity is a phase of matter that hosts non-Abelian quasiparticles, the building blocks for error-protected quantum computation. A well-known example is the Majorana quasiparticle. While several materials have been demonstrated to support topological superconductivity, most of them do not allow for the implementation of a universal set of protected logic gates. Van der Waals materials present a unique playground for topological superconductivity because they readily provide the ingredients to realize the quasiparticles suitable for universal topological quantum computation. Here, we show experiments on van der Waals heterostructures towards engineering non-Abelian quasiparticles from the quantum Hall state with induced superconductivity. Local electrostatic control of the graphene device enables spin-resolved Andreev transport. Advanced heterostructures including atomically flat (graphite) gates that fully encapsulate graphene significantly bring down the magnetic fields required for symmetry-broken and fractional quantum Hall states.

*Ö.G. acknowledges support by a Rubicon Grant of the Netherlands Organization for Scientific Research (NWO).

Electronic structure of semiconductor/superconductor interfaces from angle-resolved photoemission experiments

SERGEJ SCHUWALOW, Center For Quantum Devices and Microsoft Quantum Materials Lab - Copenhagen, Niels Bohr Institute, University of Copenhagen, NIELS SCHRÖTER (Presenter), Paul Scherrer Institute, CANDICE THOMAS, Department of Physics and Astronomy, Station Q Purdue, and Birck Nanotechnology Center, Purdue University, ALLA CHIKINA, MARCO CAPUTO, JONAS KRIEGER, Paul Scherrer Institute, GEOFFREY GARDNER, Department of Physics and Astronomy, Station Q Purdue, and Birck Nanotechnology Center, Purdue University, VLADIMIR STROCOV, GABRIEL AEPPLI, Paul Scherrer Institute, MATTHIAS TROYER, Microsoft Quantum, MICHAEL MANFRA, Department of Physics and Astronomy, Station Q Purdue, and Birck Nanotechnology Center, Purdue University, PETER KROGSTRUP, Center For Quantum Devices and Microsoft Quantum Materials Lab - Copenhagen, Niels Bohr Institute, University of Copenhagen — Hybrid epitaxial semiconductor/superconductor heterostructures have recently shown promise as a platform to realize Majorana zero modes. To pave the way towards the engineering of such heterostructures for quantum information applications, it is imperative to obtain information about their electronic properties at the semiconductor/superconductor interface. Here, we report on recent soft X-ray angle-resolved photoemission experiments to obtain key electronic material parameters for III-V semiconductor/aluminium interfaces, such as effective mass, charge density, and band offset.
3:42PM C05.00007: Topological Superconductivity on Moire Superlattices* [Invited] CENKE XU (Presenter), LEON BALENTS, CHAO-MING JIAN, University of California, Santa Barbara — Surprising correlated phenomena such as superconductor and insulator at fractional electron fillings have been observed in systems with Moire superlattice. We study the nature of these correlated phenomena, and explore the possibility of topological superconductivity in these systems using different approaches. The Dirac valley degree of freedom allows these system to form either spin triplet or spin singlet topological superconductor, depending on the sign of an effective “Hund’s coupling”. Experimental predictions such as magnetic flux quantization can be made based on the particular type of pairing. We will also investigate the nature of the observed insulators, and map the effective spin-valley physics of the insulator at both 1/2 and 1/4 filling to the boundary of a higher dimensional symmetry protected topological (SPT) state. The spin-valley physics of the insulators is governed by a Lieb-Shultz-Mattis theorem which can be interpreted as the boundary ’t Hooft anomaly of the higher dimensional SPT state.

*NSF Grant DMR1506119, DMR1151208, and the David and Lucile Packard Foundation

4:18PM C05.00008: Transparent Contacts between Quantum Anomalous Hall Insulators and Superconductors* MORTEZA KAYYALHA (Presenter), DI XIAO, RUOXI ZHANG, JAEHO SHIN, JUE JIANG, FEI WANG, YIFAN ZHAO, LING ZHANG, CHAO-XING LIU, QI LI, MOSES H. W. CHAN, NITIN SAMARTH, CUI-ZU CHANG, Pennsylvania State University — A quantum anomalous Hall (QAH) insulator coupled to an s-wave superconductor is predicted to harbor a chiral topological superconducting phase, the elementary excitations of which (i.e. chiral Majorana fermions) upon non-Abelian braiding operations can form topological quantum qubits. Here, we fabricated the QAH/Nb hybrid heterostructures and first studied their two-terminal conductance. We found that the two-terminal conductance constantly shows a half-quantized value in the entire range of the magnetic field where the magnetization is well-aligned. Next, we studied the contact transparency between the QAH and Nb films. When the QAH layer is tuned to the metallic regime by gating, we observed Andreev reflections, i.e., a large enhancement of the resistance when a DC bias voltage across the magnetic TI/Nb junction is increased above the Nb superconducting gap. This observation indicates a transparent interface between the QAH and Nb layers. Our study provides a more comprehensive understanding of the relation between the superconducting proximity effect and the observation of the half quantized two-terminal conductance in the QAH/Nb hybrid structure.

*This work is supported by ARO grant (W911NF1810198), Alfred P. Sloan Research Fellowship, 2DCC-MIP, ONR, and ARO MURI.

4:30PM C05.00009: Coherent single-electron transport in hybrid superconductor-semiconductor Coulomb islands* ALEXANDER WHITICAR (Presenter), ANTONIO FORNIERI, EOIN C O’FARRELL, ASBJORN C. C. DRACHMANN, Center for Quantum Devices and Station Q Copenhagen, University of Copenhagen, TIAN WANG, CANDICE THOMAS, SERGEI GRONIN, GEOFFREY GARDNER, MICHAEL MANFRA, Department of Physics and Astronomy and Station Q Purdue, Purdue University, CHARLES M MARCUS, FABRIZIO NICHELE, Center for Quantum Devices and Station Q Copenhagen, University of Copenhagen — The spatial separation of Majorana modes is expected to allow coherent transport of single electrons through a Coulomb blockaded one-dimensional topological superconductor [1]. Here we investigate phase coherent transport in a hybrid Al-InAs Coulomb island embedded in an Aharonov-Bohm interferometer. When a magnetic field is applied, the energy of a discrete sub-gap state is lowered below the charging energy and conductance oscillations are observed with a magnetic flux period of h/e (h is the Planck constant and e is the elementary charge), which indicates coherent transport of single electrons. The oscillation amplitude is maximized when the Coulomb peaks are 1 electron (1e) periodic, while the interference signal is suppressed when transport is 2e periodic or the island is in the normal state. The observation of phase-coherent transport enables us to investigate the coupling of Majorana modes from two separated topological wires with the goal of creating a topological qubit.


*This research was supported by Microsoft, and the Danish National Research Foundation
4:42PM C05.00010: Nonreciprocal charge transport at topological insulator/superconductor interface  KENJI YASUDA (Presenter), HIRONORI YASUDA, Department of applied physics, The University of Tokyo, TIAN LIANG, RYUTARO YOSHIMI, Center for Emergent Matter Science, RIKEN, ATSUSHI TSUKAZAKI, Institute for Materials Research, Tohoku University, KEI TAKAHASHI, Center for Emergent Matter Science, RIKEN, NAOTO NAGAOSA, MASASHI KAWASAKI, Department of applied physics, The University of Tokyo, YOSHINORI TOKURA, Center for Emergent Matter Science, RIKEN — Topological superconductor (TSC) is attracting growing interest for its potential application to topological quantum computation. The superconducting proximity effect on the topological insulator (TI) surface state is one promising way to yield the topological superconductivity. The superconductivity realized at the interface between TI Bi2Te3 and non-superconductor FeTe is one of such candidates because the mutual interaction between superconductivity and topological order is expected. Here, to detect the effect of spin-momentum locking in the Cooper pair, we investigate nonreciprocal transport; i.e. current-direction dependent resistance, which is sensitive to the broken inversion symmetry of the electronic state. The largely enhanced nonreciprocal phenomenon is detected in the Bi2Te3/FeTe heterostructure associated with the superconducting transition. The emergent nonreciprocal signal at low magnetic fields is attributed to the current-induced modulation of supercurrent density under in-plane magnetic fields perpendicular to current, exemplifying the close connection between the superconductivity and the topological electronic state at the interface.

4:54PM C05.00011: Transport in Superconductor-Topological Insulator-Superconductor 2D Arrays*  VINCENT HUMBERT (Presenter), GREG MACDOUGALL, NADYA MASON, University of Illinois at Urbana-Champaign — Once coupled to s-wave superconducting material, three-dimensional topological insulators (TIs) – providing spin momentum locking of the electrons and spin polarized current at the surface – are expected to show novel properties and unconventional superconductivity. To probe the interplay between TI surface properties and superconductivity, we fabricated 2D superconducting island arrays on exfoliated flakes of the 3D TI Bi2Se3. Such two-dimensional junction arrays have been shown to undergo Kosterlitz-Thouless transitions toward a superconducting state. Transport and Fraunhofer spectroscopy measurements carried out on our devices show unusual, asymmetric behavior. In particular, the measurements provide evidence of charged vortices on the topological surface.

*This work was supported by the DOE Basic Energy Sciences under DE-SC0012649 and NSF DMR 17-10437

5:06PM C05.00012: Uniaxial Strain Effect on Superconductivity in LaAlO3/SrTiO3 Nanostructures*  XINYI WU (Presenter), MEGAN BRIGGEMAN, JOSEPH ALBRO, JIANAN LI, Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, Materials Science and Engineering, Univ of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Physics and Astronomy, University of Pittsburgh — We investigate the effects of uniaxial strain on superconductivity in nanowires created at the LaAlO3/SrTiO3 interface using conductive atomic force microscope (c-AFM) lithography [1]. C-AFM-written areas are associated with Z-oriented ferroelastic domains, surrounded by in-plane insulating regions [2]. Application of external uniaxial stress is expected to displace the ferroelastic domain boundaries, either inward or outward, depending on the sign. Our initial experiments indicate that tensile and compressive strains profoundly affect the superconducting state at milli-Kelvin temperatures. Uniaxial stretching of the nanowire in the parallel direction is found to completely suppress the superconducting state, while reversal of the applied strain restores superconductivity. We discuss implications for understanding possible role of ferroelastic domain walls in electron-pairing mechanisms.


Monday, March 4, 2019 2:30 PM - 4:54 PM

Session C06 DCMP: Electronic States in S and Te Chalcogenides  BCEC 109A - Rico Schoenemann, National High Magnetic Field Laboratory
2:30PM C06.00001: Physical Properties of Low Dimensional Ternary Transition-Metal Sulfides* SHERMANE BENJAMIN (Presenter), ALISA DRENNER, MITCH BAKER, MICHAEL SMITH, JOHN J NEUMEIER, Montana State University, Bozeman — Transition-metal sulfides exhibit behaviors such as metal-insulator transitions, superconductivity, and magnetism. They provide an interesting class of compounds for comparison to transition-metal oxides. In this work, polycrystalline SrTa2S5 and BaTa2S5 samples were synthesized. Large (15 x 15 x 0.25 mm3) single crystals of BiNbS3 were grown by chemical vapor deposition. SrTa2S5 and BaTa2S5 superconduct at Tc=2.14 K and 3.2 K, respectively. BiNbS3 shows no signs of superconductivity above ~0.4 K. The magnetic properties, specific heat, electrical resistivity, structural analysis, and compositional analysis will be discussed. The influence of hydrostatic pressure on the electrical resistivity will be presented.

*Work at Montana State University was conducted with financial support from the US Department of Energy (DOE) DE-SC0016156.

2:42PM C06.00002: Bulk and topological effects on the optical conductivity of BaNiS2* RICARDO LOBO (Presenter), ESPCI Paris, CNRS, Sorbonne University — The BaCo1-xNi2S2 system forms a solid solution with an almost Mott like insulating phase when x=0 to a weakly correlated conductor in the Ni end member. This weakly correlated material has a series of interesting topological properties such as a hidden spin polarization due to a Rashba coupling and three dimensional Dirac-like cones close to the Fermi level. Here, I will discuss the temperature dependence of the optical conductivity (σ) of this material. The room temperature real part of σ shows a Drude like peak followed by a linear-in-frequency region. Upon cooling the material there is a spectral weight transfer from about 0.1 eV to 0.3 eV. Interestingly the linear region remains unchanged as a function of temperature. Combining the optical measurements with first principle calculations shows that this spectral weight transfer is a competition between regular carriers and Dirac-like bands.

*Collaborators: D. Santos-Cottin, A. Gauzzi, Y. Klein, L. de' Medici, M. Casula.

2:54PM C06.00003: Photoemission study on a special type of multiferroics: GaV4S8 & GeV4S8 AMOL SINGH (Presenter), National Synchrotron Radiation Research Center, JUNG-HAN LI, Department of Physics, National Tsing-Hua University Taiwan, YEN-FA LIAO, HSIAO-YU HUANG, YEN-YI CHU, JING CHANG, KU-DING TSUEI, National Synchrotron Radiation Research Center, LUNYONG ZHANG, Laboratory for Pohang Emergent Materials and Max Plank POSTECH Center for Complex Phase Materials, Pohang University of Science and Technology, Pohang 790-784, Korea, SANG-WOOK CHEONG, Department of Physics and Astronomy, 136 Frelinghuysen Road, Piscataway, New Jersey 08854, USA, Rutgers Center for Emergent Materials, MICHEL A VAN VEEENDAAL, Department of Physics, Northern Illinois University, DeKalb, IL 60115, USA, DI-JING HUANG, National Synchrotron Radiation Research Center — The lacunar spinels (AV4S8) with A=Ga and Ge, consisting of tetrahedral (AS4)n- and weakly linked cubane (V4S4)n+ are unique in known skyrmions because of a sizable ferroelectric polarization of ~ 1 μC/cm2 and polar crystal structure. Their electronic properties depend on the special degrees of freedom of the basic electronic units of V4S8. These materials are classified as a special class of Mott insulators in which strong electron correlations arise from weak intercluster hybridization. From the viewpoint of ionic formula, average valency of V is 3.25+ in GaV4S8 and 3+ in GeV4S8, yet exact valency of V in these compounds is not known. We conducted hard X-ray photoemission to study the electronic structure of GaV4S8 & GeV4S8 single crystals and to investigate the valency of V in these compounds. The V 2p photoemission spectra are best explained with (V4S4)5+ and (V4S4)6+ for GeV4S8 and GaV4S8 respectively. Further S 2p XPS spectra shows results consistent with the scenario of dynamical Jahn-Teller distortion in the paraelectric phase.

3:06PM C06.00004: Orbital-Order Driven Ferroelectricity and Dipolar Relaxation Dynamics in Multiferroic GaMo4S8 KORBINIAN GEIRHOS (Presenter), STEPHAN KROHNS, Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, HIROYUKI NAKAMURA, TAKESHI WAKI, YOSHIKAZU TABATA, Department of Materials Science and Engineering, Kyoto University, ISTVÁN KÉZSMÁRKI, PETER LUNKENHEIMER, Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — GaMo4S8, a compound of the lacunar spinel family, was recently shown to exhibit non-canonical, orbitally-driven ferroelectricity [1]. Our dielectric spectroscopy measurements on this multiferroic material reveal complex relaxation dynamics, above as well as below its Jahn-Teller transition at TJT= 47 K [2]. Above the Jahn-Teller transition, two types of coupled dipolar-orbital dynamics were found: On the one hand, relaxations within cluster-wise regions with strong-range polar order, as known from relaxor ferroelectrics. On the other hand, critical fluctuations of only weakly interacting dipoles, resembling the typical dynamics of order-disorder type ferroelectrics. Below TJT, the system is driven into long range ferroelectric order by the onset of orbital order and dipolar dynamics within the ferroelectric domains is observed: The found marked differences to the skyrmion host GaV4S8 seem to be related to the different structural distortions in these systems.

3:18PM C06.00005: Noise spectroscopy study of metal-insulator transition in CuIr$_2$S$_4$ DASHARATH ADHIKARI

(Presenter), AHMED ALI, ALI M ALSAQQA, COLIN P KILCOYNE, Physics, University at Buffalo, NOBUHIRO MATSUMOTO, National Metrology Institute and Chemical Measurement Laboratory, SAMBANDAMURTHY GANAPATHY, Physics, University at Buffalo — Single crystals of the CuIr$_2$S$_4$ exhibit a metal-insulator transition (MIT) at a critical temperature ($T_c$) ~ 231 K, accompanied by simultaneous charge ordering and spin dimerization, making it an interesting system to study the interplay of interaction among many degrees of freedom. By employing low-frequency electrical noise spectroscopy, we observe that the power spectral density (PSD) of the resistance fluctuations peaks around $T_c$ likely due to the formation of domains of opposite phase. The ultra-low frequency window of our measurements serves as a tool to measure the increased scattering of charge carriers near $T_c$ due to nucleation, pinning and/or propagation of domains. The probability density function (PDF) of the fluctuations in the transition region shows a significant deviation from the expected Gaussian behavior further supporting the intermixing of phases near $T_c$. In addition, an abrupt phase transition with a threshold behavior can also be triggered electrically from the insulating phase. The analysis of the PSD, PDF and 1/f behavior suggests a significant role of the domains in the electrically driven case too.

3:30PM C06.00006: Anomalous conductivity near percolative metal-insulator transition in monolayer MoS$_2$

BYOUNG HEE MOON (Presenter), JUNG JUN BAE, GANG HEE HAN, HYUN KIM, HOMIN CHOI, YOUNG HEE LEE, Center for Integrated Nanostructure Physics, Institute for Basic Science (IBS) — Conductivity of the insulating phase increases generally upon increasing a drain-source voltage due to the field-enhanced hopping or heating effect. Here, we report the opposite behavior, and anomalous metallic to insulating phase transition driven by a voltage at low voltage regime in monolayer molybdenum disulfide. We ascribe these features to the inhomogeneous state of the system in which the transport is governed by a percolation. At the higher voltage regime, the insulating phase is transformed further to the metallic phase, exhibiting unique multi-phases in this system. In this talk, we discuss these anomalous behaviors and their implications in a metal-insulator transition in two-dimension.

3:42PM C06.00007: Optical Thermal Measurements of Thermal Diffusivity in 1T-TaS$_2$

ERIK KOUNTZ (Presenter), JIECHENG ZHANG, AHARON KAPITULNIK, Physics, Stanford University — Thermal response of electronic materials can detect phase transitions and transport processes. Moreover, micron-scale measurements avoid sample imperfections such as dislocations, grain boundaries, and other defects, and allow for proper averaging on macroscopic samples. We use a photo-thermal microscope for high resolution thermal diffusivity and optical reflectivity measurements. A laser beam is focused at the surface of the targeted sample; the laser power is modulated to create a periodic, point-like heat source. A nearby laser measures the local reflectivity. In this talk we focus on 1T-TaS$_2$, a quasi-2D Mott insulator with various competing charge density wave (CDW) orders and a proposed quantum spin liquid phase at low temperature [1]. We study the nature of the phase transitions through anomalies in differential reflectivity (dR/dT) and the transport behavior though measurements of thermal diffusivity ($D_Q$). In particular, anomalies in dR/dT at the 180K- and 345K-CDW transitions are discussed in terms of the nature of the phase transitions and $D_Q$ is discussed in terms of its implications on transport mechanisms.

[1] 10.1103/PhysRevLett.121.046401

*Supported by Gordon and Betty Moore Foundation, EPIQS Initiative, Grant GBMF4529.

3:54PM C06.00008: Real space imaging of tuneable magnetic order in Fe$_{1+x}$Te with $x>0.12$

CHRISTOPHER TRAINER (Presenter), CHI MING YIM, PETER WAHL, University of St Andrews — Magnetism is thought to play an important role in the development of the superconductivity in the Iron chalcogenide superconductors. In the parent material, FeTe, the magnetic phase diagram is very complex with unusual magnetic states developing as a function of excess Iron doping [1]. We have conducted a spin-polarized scanning tunnelling microscopy study on samples of FeTe with different levels of excess Iron concentrations by in-situ prepared magnetic tips [2]. Using a ferromagnetic tip in a cryogenic STM in a vector magnetic field [3,4], we have been able to map out the magnetic order at the surface on an atomic scale in all three spatial directions. By collecting Fe atoms from the surface with the STM tip the excess Fe concentration of the surface can be tuned locally. For samples of Fe$_{1+x}$Te with $x>0.12$ our results reveal a magnetic transition from a single-q to a multi-q order as a function of local excess iron concentration [4]. I will discuss these results and compare them with the neutron scattering measurements.

4:06PM C06.00009: Visualizing uniaxial-strain-manipulation of antiferromagnetic domains in Fe$_{1+y}$Te using spin-polarized scanning tunneling microscope*  JOEL FRIEDMAN (Presenter), MARIAM KAVAI, IOANNIS GIANNAKIS, JUSTIN LESEN, Binghamton University, PAWEL ZAJDEL, Institute of Physics, University of Silesia, PEGOR AYNAJIAN, Binghamton University — The quest to understand correlated electronic systems has pushed the frontiers of experimental measurements towards development of new experimental techniques and methodologies. Here we use a novel home-built uniaxial-strain device integrated into our variable temperature scanning tunneling microscope (STM) that enables one to controllably manipulate in-plane uniaxial strain in the samples and probe their electronic response at the atomic scale. Using STM with spin-polarization techniques, we visualize antiferromagnetic (AFM) domains and their atomic structure in Fe$_{1+y}$Te, the parent compound of iron-based superconductors, and demonstrate how these domains respond to applied uniaxial-strain. We observe the bi-directional AFM domains in the unstrained sample, with an average domain size of ~ 50-150 nm, to transition into a single unidirectional domain under applied uniaxial-strain. Our findings open a new direction to utilize a valuable tuning parameter in STM as well as other spectroscopic techniques both for tuning the electronic properties as well as inducing symmetry breaking in quantum material systems.

*We acknowledge support from the U.S. National Science Foundation (NSF) CAREER under award No. DMR-1654482.

4:18PM C06.00010: Dimensional crossover in a van der Waals ferromagnet detected by spin correlation driven distortions  ALON RON (Presenter), Department of Physics, California Institute of Technology, ELI ZOGHLIN, Materials Department, University of California, Santa Barbara, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, STEPHEN WILSON, Materials Department, University of California, Santa Barbara, DAVID HSIEH, Department of Physics, California Institute of Technology — Magneto-elasticity – the structural deformation of a crystal in response to a change in its magnetic energy – is commonly detected across magnetic long-range ordering (LRO) transitions and yields insight into magnetic ground state energetics. In principle, distortions are also induced by magnetic short-range ordering (SRO), which provide complementary information about short-range correlations and energetics that are essential for understanding how LRO is established. However these distortions are difficult to resolve because the associated atomic displacements are exceedingly small and do not break symmetry. Here we demonstrate high-multipole nonlinear optical polarimetry as a sensitive and mode selective probe of SRO induced distortions using CrSiTe$_3$ as a testbed. This compound is composed of van der Waals bonded sheets of ferromagnetically interacting Heisenberg spins that, in isolation, would be impeded from LRO by the Mermin-Wagner theorem. Our results show that CrSiTe$_3$ evades this law via a two-step crossover from two- to three-dimensional magnetic SRO above its Curie temperature ($T_c=31$K), manifested through two previously undetected totally symmetric distortions at $T_{2D} \sim 110$K and $T_{3D} \sim 60$K, respectively. Such data open new avenues for mechanical control of magnetism.

4:30PM C06.00011: Thermal Expansion in Ba$_3$Zr$_2$S$_7$*  NATHAN KOOCHER (Presenter), Materials Science and Engineering, Northwestern University, RYAN KLEIN, ALISON ALTMAN, DANNA FREEDMAN, Chemistry, Northwestern University, JAMES M RONDINELLI, Materials Science and Engineering, Northwestern University — Ferroelectric perovskite oxides have recently been used in solar applications because their polarity allows for the separation of photocarriers when under illumination to generate a photocurrent. Oxides, however, often have band gaps that are beyond the solar-optimal regime (>3.3 eV); for this reason, perovskite-structured chalcogenides have been proposed as suitable candidate materials owing to their lower band gaps (= 2 eV). An understanding of the thermal expansion behavior of photovoltaic materials is important so as to prevent large stresses and strains during fabrication and operation of the photovoltaic device. Here, we evaluate the structural, lattice dynamical, and thermodynamic properties of Ruddlesden-Popper chalcogenide Ba$_3$Zr$_2$S$_7$ using the self-consistent quasi-harmonic approximation within density functional theory. These properties are compared to the thermal expansion of other Ruddlesden-Popper compounds, which allows us to suggest guidelines for engineering thermal expansion in the Ruddlesden-Popper structure type with diverse chemistries.

*This work was supported by the National Science Foundation's MRSEC program (DMR-1720139.) at the Materials Research Center of Northwestern University.
THOMAS KOEHLER (Presenter), SEBASTIAN PAAECKEL, SALVATORE MANMANA, University of Gottingen — We describe the formation of charge-density patterns induced by spin-selective photoexcitations of interacting fermionic systems with an underlying magnetic microstructure. Using tensor-network methods for one-dimensional model systems, we find stable charge-density patterns for a wide range of parameters. We discuss a generic mechanism explaining this effect for systems that possess a periodic modulation of local observables in any dimension. Realizations in pump-probe experiments on materials and by experiments with ultracold gases on optical lattices are proposed.

*Financial support from the Deutsche Forschungsgemeinschaft (DFG) through SFB/CRC1073 (project B03) and Research Unit FOR 1807 (project P7) and computational resources made available by the Department of Applied Theoretical Physics, Clausthal Technical University, are gratefully acknowledged.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C07 DCMP: Heavy Fermion and Correlated Electron Metals BCEC 109B - James Hamlin, University of Florida

2:30PM C07.00001: Spin-orbit interaction and quasiparticle bands in locally non-centrosymmetric heavy-fermion systems* GERTRUD ZWICKNAGL (Presenter), Inst. f. Mathemat. Physik, TU Braunschweig, Braunschweig, Germany, SEUNGYUN KHIM, MANUEL BRANDO, CHRISTOPH GEIBEL, MPI for Chemical Physics of Solids, Dresden, Germany — Non-centrosymmetric heavy-fermion systems (HFS) have gained much interest in the past decade. In these materials, the lack of inversion symmetry in combination with strong spin-orbit interaction and magnetic interactions can lead to novel phenomena. In this talk, we present calculations of the heavy quasiparticle bands in Ce- and Yb-based HFS from the tetragonal 122-family. This class of materials comprises compounds with the inversion-symmetric ThCr2Si2 structure as well as systems with the locally non-centrosymmetric CaBe2Ge2 structure. The calculations are performed by means of the Renormalized Band method which proceeds from a Dirac-relativistic description of the electronic structure and accounts for Crystalline Electric Field effects and the mass renormalization due to strong local correlations. We discuss results for YbIr2Si2 which crystallizes in both structures depending on preparation condition. Further on, we present results on the new HFS CeRh2As2.

*This work was supported by the ANR-DFG project Fermi-NESt.

2:42PM C07.00002: The high-field/high-pressure relationship of magnetic order and nematicity in the heavy fermion superconductor CeRhIn5* TONI HELM (Presenter), High Magnetic Field Laboratory, Helmholtz Zentrum Dresden Rossendorf, AUDREY GROCKOWIAK, Tallahassee, National High Magnetic Field Laboratory, FEDOR BALAKIREV, JOHN SINGLETON, Los Alamos, National High Magnetic Field Laboratory, KENT SHIRER, MARKUS KOENIG, Max Planck Institute for Chemical Physics of Solids, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory, STANLEY W TOZER, Tallahassee, National High Magnetic Field Laboratory, PHILIP MOLL, Institute of Materials, Ecole Polytechnique Federale de Lausanne — Recently, a nematic signature, i.e. a sudden resistivity anisotropy above a critical field \( B^* \ = 28 \) T, has been observed in CeRhIn5[1]. This heavy fermion antiferromagnet (\( T_N = 3.85 \) K) superconducts under pressure above \( p_c \ = 23 \) kbar, associated with an antiferromagnetic quantum critical point (QCP). The reported nematic behavior survives at ambient pressure only until magnetic order is suppressed at a critical field of \( B_c = 51 \) T, associated with a second QCP[2,3]. An open question is if and how the two QCPs, \( B \)-induced nematicity and \( p \)-induced superconductivity (SC) are related. Here we report high-field (up to 65 T) / high-pressure (up to 40 kbar) studies of magnetotransport in CeRhIn5. The combination of plastic diamond-anvil-cells, pulsed magnets, and focused-ion-beam microstructures enabled us to investigate this region in the \((p,T,B)\) phase diagram. We show that nematicity and SC reside in distinct regions. Our experiments reveal a surprising enhancement of magnetic order in high fields with pressure.


*We acknowledge the Max Planck Society; the DFG— MO 3077/1-1; the US DOE, BES, MSE; the NSF DMR-1157490 and DMR-1644779; and the State of Florida.
Quantum confinement of electronic states in a bulk heavy fermion crystal

NICOLAS GAUTHIER
(Presenter), JONATHAN SOBOTA, MAKOTO HASHIMOTO, ZHIXUN SHEN, Stanford University — Electronic states become quantized when confined in a potential well. This well-known phenomenon is observed for example in quantum dots or thin films [1]. In these cases, the confinement is created artificially by the microscopic dimensions of the system. Surprisingly, we recently observed the presence of confined electronic states in a bulk crystal of CeCoIn$_5$, a prototypical heavy fermion superconductor [2]. Our recent ARPES results revealed multiple electronic bands that were not observed previously [3-5] and are not predicted by theory [6]. Interestingly, the energy position of these bands follows the simple relation expected for a quantum well. In comparison to thin films, the origin of the confinement potential creating these quantized states in CeCoIn$_5$ is still unclear and requires more investigations.


Structural and Physical Properties of CeAu$_2$Bi: a New Frustrated Antiferromagnet Candidate

MARIO MODA PIVA (Presenter), Universidade Estadual de Campinas, FILIP RONNING, JOE D THOMPSON, Los Alamos National Laboratory, PASCOAL PAGLIUSO, Universidade Estadual de Campinas, PRISCILA ROSA, Los Alamos National Laboratory — Ce-based compounds often display emergent phenomena due to the interplay between competing magnetic interactions, crystalline electrical field (CEF) effects, and the Kondo effect. Here we report the structural and physical properties of the new heavy-fermion compound CeAu$_2$Bi. CeAu$_2$Bi crystallizes in a hexagonal structure (P6$_3$/mmc) with lattice parameters of $a = 4.8867(5)$ Å and $c = 9.3748(13)$ Å. This structure presents Ce planes containing a triangular lattice, which has the potential of displaying geometrical frustration. Antiferromagnetic ordering, however, takes place at $T_N = 3.1$ K, and is enhanced as a function of pressure, reaching 4.2 K at 18 kbar. We discuss our experimental results in the light of band structure calculations.

*This work was supported by FAPESP grants: 2015/15665-3, 2017/25269-3, 2017/10581-1; CAPES and CNPq, Brazil. Work at Los Alamos was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering. P. F. S. R. acknowledges support from the Laboratory Directed Research and Development program of Los Alamos National Laboratory under project number 20190076ER.

Theory of multipolar order and unconventional superconductivity in heavy fermion systems; importance of nonlocal vertex corrections

RINA TAZAI (Presenter), HIROSHI KONTANI, Nagoya University — In heavy-fermion systems, higher-rank multipole operators are active thanks to the strong spin-orbit interaction (SOI). Therefore, multipole fluctuations cause rich quantum critical phenomena, such as unconventional superconductivity and hidden-order phase. However, the microscopic pictures of these phenomena have not been fully understood. To solve these issues, we study higher-rank multipole fluctuations by considering the vertex corrections (VCs), which represent higher-order many body effects, on the basis of multi-orbital Periodic Anderson Model [1]. We find that the significant effects are given by Aslamazov-Larkin process, which originate from strong interference between multipole fluctuations. Due to the AL-VC, various types of multipole fluctuations develop simultaneously near the magnetic QCP. Especially, some electric multipole (quadrupole or hexadecapole) fluctuations are drastically enlarged, which remain small in mean field theories. Thus, various interesting phase due to the electric multipole fluctuations are expected to be realized in heavy fermion systems. In this talk, we discuss both the s-wave superconductivity in CeCu$_2$Si$_2$ [1] and the hidden-order phase in CeB$_6$, which are reported by recent improved experiments. [1] R. tazai and H. kontani, arXiv:1807.11427.
Recent experiments on heavy fermion materials have revealed a range of compounds that are both metallic and have local magnetic moments that reside on geometrically frustrated lattices. An interesting example of frustration, realized in a number of materials, is provided by systems with a valence bond solid ground state, which exhibit a magnetic transition in the same universality class as Bose-Einstein condensation (BEC) in an applied magnetic field. Moreover, recent experiments on YbAl$_3$C$_3$ suggest that this compound may realize a magnon BEC transition in the presence of an itinerant conduction band. Motivated by these observations, we consider a one-dimensional two-leg spin ladder with a valence bond solid ground state doped with itinerant fermions. Using the Density Matrix Renormalization Group we study the system as a function of Kondo coupling, magnetic field and the density of itinerant fermions. In addition, we use analytical techniques to map out the phase diagram and study the critical properties, and compare limiting cases with the numerically exact DMRG results. We also discuss the application of our results to 2D and 3D systems.

*P. Volkov is supported by a Rutgers CMT Postdoctoral Fellowship.

Reducing dimensionality is a powerful approach to increasing the influence of quantum fluctuations. Not only do quantum fluctuations become stronger in two- and one-dimensions, recent theoretical work using tools from quantum information science (tensor networks, etc.) allow exceedingly accurate studies of correlated electron systems in 1d. With this motivation we investigate quasi-1D 4f and 5f-based metallic compounds possessing non-trivial magnetic order. Using transport and thermodynamics we investigate the electronic and magnetic correlations in these systems and compare with theoretical understanding.

*Work at Los Alamos was performed under the auspices of the US DOE, Division of Materials Sciences and Engineering.

When the temperature drops below a characteristic temperature $T^*$, heavy electrons gradually emerge with further enhanced effective electron mass. The coexistence of ferromagnetism and HF state can be well interpreted by the dual properties (itinerant and localized) of 3d electrons. This work expands the limit of ferromagnetic HF materials from f- to d-electron systems and illustrates the positive correlation between ferromagnetism and HF state in the 3d-electron material, which is quite different from the f-electron systems.

*Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund, for support of this research under contract 56764-UNI10.
4:18PM C07.00010: Charge dynamics and untapped redox potential in a Mn$^{1+}$- based electrode.*
DIVYANSHI SAR (Presenter), S. ALEXANDER BREITWEISER, New York University, RUMIN QIAO, ALI FIROUZI, Natron Energy, LIN MIAO, ROURAV BASAK, New York University, SHAHROKH MOTALLEBI, CHRISTIAN VALENCIA, MAI FUJIMOTO, COLIN WESSELLS, HANNAH ISRAEL, YI-DE CHUANG, WANLI YANG, LEWIS A WRAY, Natron Energy — Manganese hexacyanomanganate (MnHCMn) with an unusual Mn$^{1+}$ charged valence state has recently been identified as a promising sodium ion anode material, in spite of what appears to be an unfavorable closed-shell electron configuration. I will present an analysis of MnHCMn charge dynamics with bulk- and surface-sensitive soft X-ray absorption spectroscopy (sXAS) and resonant inelastic X-ray scattering (RIXS) at the Mn L3 edge. A charge transfer collective mode is observed, and found to represent the likely energy of the next charging redox plateau, which is yet unachieved in redox experiments. This reveals a unique capability that RIXS can provide for strongly correlated battery electrode materials, and suggests a significant untapped potential for MnHCMn anodes.

*D. Sar acknowledges fellowship support from Natron Energy.

4:30PM C07.00011: Scanning Tunneling Microscopy and Spectroscopy on the Metallic Delafossite PdCoO$_2$*
DIBYASHREE CHAKRABORTI (Presenter), School of Physics and Astronomy, University of St Andrews, SEUNGHYUN KHIM, ANDREW MACKENZIE, Physics of Quantum Materials, Max Planck Institute of Chemical Physics of Solids, PETER WAHL, School of Physics and Astronomy, University of St Andrews — The metallic delafossite PdCoO$_2$ has risen to the limelight in the past few years [1]. Due to unusually long mean free paths, the electron fluid exhibits hydrodynamic effects [2]. The anisotropic crystal structure leads to a quasi-2D character of the electronic states making the material suitable for surface sensitive techniques. Because of the polar nature of the surface, exciting physics is observed such giant Rashba spin-splitting [3] and itinerant ferromagnetism [4]. In our study, we have investigated the different surface terminations of PdCoO$_2$ with low temperature Scanning Tunneling Microscopy. We will discuss their assignment and spectroscopic signatures.

1. SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, KY16 9SS, UK
2. Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany

4:42PM C07.00012: Collective Modes in SrTi$_{1-x}$Nb$_x$O$_3$ Measured with meV-Resolution EELS*
SAMANTHA RUBECK (Presenter), MELINDA RAK, MATTEO MITRANO, ALI HUSAIN, JIN CHEN, University of Illinois at Urbana-Champaign, ALEXANDER EDELMAN, PETER B LITTLEWOOD, University of Chicago, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — The emergence of superconductivity in low carrier solids does not follow the behavior of conventional BCS superconductivity. Niobium doped strontium titanate, SrTi$_{1-x}$Nb$_x$O$_3$, which becomes a superconductor at densities as low as 5.5×10$^{17}$ cm$^{-3}$ [1], is theorized to come about due to the hybridization of the longitudinal optic phonons with the plasmons. In this talk, I will present measurements of the collective charge excitations of SrTi$_{1-x}$Nb$_x$O$_3$ using momentum-resolved inelastic electron scattering (M-EELS). We observed a variety of acoustic and optic phonons in the range 0-200 meV that have been implicated in the superconducting pairing in this material. In addition, we observed an electronic mode at 25 meV that we identify as a valence plasmon from the Nb free carriers. I will discuss evidence for hybridization of these modes for different Nb concentration, $x$.


*This work was supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF - 4542 and by the National Science Foundation Graduate Research Fellowship under Grant No. DGE - 1746047.

4:54PM C07.00013: Infrared nano-imaging of Luttinger liquid plasmons in single walled carbon nanotubes
SHENG WANG (Presenter), FENG WANG, University of California, Berkeley — Quantum-confined electrons in one dimension (1D) constitute a Luttinger liquid, which features charge spin separation and other intriguing properties distinctly different from the Fermi liquid. Single walled carbon nanotubes (SWNTs) provide the ideal platform to explore such Luttinger liquid physics due to strong lateral quantum confinement and the presence of nanotubes of different species. But a systematic study of how the Luttinger liquid behaviors in carbon nanotubes depend on intrinsic and extrinsic factors such as chirality and doping has been lacking. We performed comprehensive infrared nano-imaging of Luttinger liquid plasmons in carbon nanotubes with different parameters and provide novel insights into Luttinger liquid physics in carbon nanotubes. This in-depth understanding of Luttinger liquid physics in SWNTs is not only of fundamental interests, but also pave the way for various nanophotonic applications based on carbon nanotubes.
5:06PM C07.00014: Investigation of Broken Time Reversal Symmetry in the Pr-rich side of Pr$_{1-x}$Nd$_x$Os$_4$Sb$_{12}$

PEI-CHUN HO (Presenter), Physics, California State University, Fresno, DOUGLAS E MACLAUGHLIN, Physics, University of California, Riverside, M BRIAN MAPLE, Physics, University of California, San Diego, LEI SHU, Physics, Fudan University, ADRIAN HILLIER, ISIS Neutron and Muon Sources, Science & Technology Facilities Council, OSCAR BERNAL, Physics, California State University, Los Angeles, TATSUYA YANAGISAWA, Physics, Hokkaido University, P. K. BISWAS, ISIS Neutron and Muon Sources, Science & Technology Facilities Council, JIAN ZHANG, CHENG TAN, Physics, Fudan University, SHOJI D HISHIDA, TAYLOR MCCULLOUGH-HUNTER, Physics, California State University, Fresno — One of the intriguing features that indicate unconventional superconductivity (SC) in the filled skutterudite compound PrOs$_4$Sb$_{12}$ is the broken time reversal symmetry (TRS). The preliminary analysis of our most-recent results of µSR experiments in Pr$_{1-x}$Nd$_x$Os$_4$Sb$_{12}$ of x=0.05, 0.1, 0.15 and 0.2, at 0 magnetic field, a combined exponential and Gaussian relaxation behavior was found. As T decreases, the exponential rate λ increases, while the Gaussian rate Δ has a slight decrease below $T_c$. The increase of Δ below $T_c$, previously observed in PrOs$_4$Sb$_{12}$, is not seen for x≥0.05, indicating that TRS is no longer broken. λ here is expected to be mainly dynamic in nature and has a strong temperature dependence below $T_c$. λ grows with increasing x, which may be due to a quantum critical point or transition below 0.05K. The origin of the anomalous shape of λ(T) in TF-µSR below $T_c$ for of x=0.15 and 0.2 is currently unknown.

*Research at CSU-Fresno is supported by NSF DMR-1506677; at UCSD by US DOE DE-FG02-04ER46105 and NSF DMR-1810310, at CSU-LA by NSF DMR-1523588; at Fudan U. by Chinese NSF-1147060; at Hokkaido U. by JSPS KAKENHI 26400342, 15K05882, and 15K21732.

5:18PM C07.00015: Tilted Weyl-Kondo Semimetal in Heavy Fermion Systems

SARAH GREFE (Presenter), HSIN-HUA LAI, Rice University, SILKE PASCHEN, Vienna University of Technology, QIMIAO SI, Rice University — Recently we have introduced a time-reversal-symmetry (TRS) invariant periodic Anderson model on a noncentrosymmetric and nonsymmorphic lattice and demonstrated a Weyl-Kondo semimetal (WKSM) [1]. This strongly correlated, Kondo driven, topological semimetal phase has been evidenced in the recently discovered heavy fermion semimetal Ce$_3$Bi$_4$Pd$_3$ [2]. In condensed matter systems without Lorentz invariance, a term that tilts the Weyl nodes is naturally present. In this study, we generalize the periodic Anderson model to realize a Tilted Weyl-Kondo Semimetal (TWKSM). We show how the tilted Weyl nodes allow for measurable properties that probe the topological nature of the TWKSM.


*NSF Grant No. DMR-1611392, the ARO Grant No. W911NF-14-1-0525, the Robert A. Welch Foundation Grant No. C-1411, and a Smalley Postdoctoral Fellowship at the Rice Center for Quantum Materials

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C08 DMP DCMP: Superconductivity: Copper Oxide - Pseudogap

BCEC 150 - Pengcheng Dai, Rice University

2:30PM C08.00001: Field-induced transitions from superconductors to Bose metal in La$_{1.875}$Ba$_{0.125}$CuO$_4$* JOHNN TRANQUADA (Presenter), YANGMU LI, GENDA GU, QIANG LI, ALEXEI TSVELIK, Brookhaven National Laboratory, JASMINKA TERZIC, PAUL G. BAITY, DRAGANA POPOVIC, National High Magnetic Field Lab — What happens to the pairing correlations in a cuprate superconductor when superconducting order is suppressed with a magnetic field? We have studied this problem in LBCO x=1/8, where 2D superconductivity appears below 40 K, but 3D order only occurs below 5 K, presumably due to pair-density-wave order intertwined with the spin- and charge-stripe orders. At $T = 0.35$ K, a c-axis magnetic field initially induces finite dissipation near 10 T, followed by re-entrant 2D superconductivity between 18 and 22 T [1]. The resistance per CuO$_2$ plane rises to $h/(4e^2)$ near 31 T, but then saturates at $2h/(4e^2)$ at higher fields. The saturation of the resistance indicates metallic behavior, but the fact that the Hall coefficient is ~ 0 indicates a lack of quasiparticles. We conclude that conduction is by incoherent hopping of pairs between charge stripes, indicating that stripes are good for pairing, but not phase coherence.


2:42PM C08.00002: The Valence Transition Model of Pseudogap, Charge-Order and Superconductivity in Electron- and Hole-Doped Copper Oxides. SUMITENDRA MAZUMDAR (Presenter), University of Arizona — I propose an integrated theoretical approach to spatial broken symmetries and superconductivity in electron- and hole-doped cuprates, as well as many other strongly correlated systems [1]. I propose that there occurs a discrete jump in ionicity Cu(2+)-to-Cu(1+) at optimal doping in the conventionally prepared electron-doped compounds and at the pseudogap phase transition in the hole-doped materials; the unusually high ionization energy of the closed shell Cu(1+)-ion, taken together with the doping-driven reduction in the 3D Madelung energy drives the transition. The undoped states behave as effective 1/2-filled Cu-band with the closed shell electronically inactive O(2-) ions; the doped states behave as correlated two-dimensional geometrically frustrated 1/4-filled oxygen hole-bands, now with electronically inactive closed-shell Cu(1+) ions. The charge-ordered state in the frustrated O-band is a period 4 paired Wigner crystal of spin singlets with broken C4 symmetry. Correlated-electron superconductivity results from the destabilization of the paired Wigner crystal. The theory gives the simplest yet most comprehensive understanding of experiments in the normal states, and is easily extended to many other unconventional superconductors.


2:54PM C08.00003: The Effect of Uniaxial Pressure on the High-Temperature Superconductor YBa2Cu3O7−x MARK E BARBER (Presenter), Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, TOSHINAO LOEW, HUN-HO KIM, Max Planck Institute for Solid State Research, Stuttgart, Germany, MARCIN KONCZYKOWSKI, Laboratoire des Solides Irradies, Ecole Polytechnique, France, BERNHARD KEIMER, Max Planck Institute for Solid State Research, Stuttgart, Germany, ANDREW MACKENZIE, CLIFFORD HICKS, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — The phase diagram of the high-temperature cuprate superconductors encompasses a variety of intertwined phases. Typically the phase diagram is traversed using chemical doping or magnetic field, but uniaxial pressure offers an alternative clean tuning parameter. Recently, large a-axis uniaxial pressures in YBa2Cu3O6.67 have been shown to stabilise a three-dimensional long-range-ordered charge density wave, analogous to that achieved with large c-axis magnetic fields, but at zero field [1]. Using GaAs-based Hall probe susceptometers, we have investigated the strain dependence of ∼1/8-doped YBCO with high spatial precision, up to pressures of at least 1.5 GPa, crossing the transition into long-range CDW order.


3:06PM C08.00004: Investigations of the pseudogap phase in overdoped Bi2+xSr2−xCaCu2O8+δ with μSR* SHAYAN GHEIDI (Presenter), KOLAWOLE ABAYOMI AKINTOLA, Simon Fraser University, ANDRE COTE, Kwantlen Polytechnic University, ALEX FANG, Simon Fraser University, SARAH R DUNSGER, TRIUMF, JEFF SONIER, Simon Fraser University — A recent μSR study of Bi2+2Sr2−CaCu2O8+δ (Bi2212) single crystals revealed the presence of weak quasi-static magnetism in the pseudogap (PG) phase [A. Pal et al., Phys. Rev. B 97, 060502(R) (2018)]. However, it is unclear whether the magnetism is associated with the PG, as muon diffusion above T ~ 160 K prevented determination of an onset temperature. In an attempt to circumvent this limitation, we have carried out sensitive muon Knight-shift and new zero-field muon spin relaxation (ZF-μSR) measurements of overdoped Bi2212. The temperature dependence of the muon Knight shift in the normal state exhibits a saturation below a temperature that scales with Tc, whereas the ZF-μSR relaxation rate appears to track the hole-doping dependence of the PG temperature T*. In addition, our measurements of highly overdoped Bi2212 provide evidence for phase separation. The results suggest the presence of two distinct phases above Tc.

*This work is supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Canadian Institute for Advanced Research (CIFAR).
Magnetic Excitations in Highly Underdoped Superconducting HgBa₂CuO₄₊δ*

ZACHARY ANDERSON (Presenter), YANG TANG, University of Minnesota, VIKAHM NAGARAJAN, University of California, Berkeley, MUN CHAN, Los Alamos National Laboratory, CHELSEY J DOROW, University of California, San Diego, GUICHUAN YU, University of Minnesota, DOUGLAS L ABERNATHY, ANDREW D CHRISTIANSON, Oak Ridge National Laboratory, LUCILE MANGIN-THRO, PAUL STEFFENS, Institut Laue-Langevin, YVAN SIDIS, PHILIPPE BOURGES, Laboratoire Léon Brillouin, CEA-CNRS, MARTIN GREVEN, University of Minnesota — Antiferromagnetic (AF) spin correlations are prominent across the phase diagram of the cuprate superconductors, and it has been proposed that they mediate Cooper pairing and are responsible for various pseudogap phenomena. HgBa₂CuO₄₊δ (Hg1201) is a simple-tetragonal compound with a single CuO₂ plane per unit cell and the highest optimal Tc among single-layer cuprates, and thus a model system for the study of the AF response of the quintessential CuO₂ planes. Our previous work has shown that the AF excitations in moderately to optimally-doped Hg1201 are distinctly different from what had been observed in other cuprates; namely, the low-energy response is commensurate and gapped, resulting in a 'Y'-shaped, rather than 'X'-shaped dispersion. Here we present our recent inelastic neutron scattering measurements of the AF excitations in heavily underdoped Hg1201.

*The work at the University of Minnesota was funded by the Department of Energy through the University of Minnesota Center for Quantum Materials under DE-SC-0016371.

Tracing the origin of charge density waves in cuprates*

FRYDERYK LYZWA (Presenter), Department of Physics and Fribourg Center of Nanomaterials, University of Fribourg, Chemin du Musée 3, 1700 Fribourg, Switzerland, MILAN ORLITA, LNCMI, CNRS-UGA-UPS-INSA, 25, Avenue des Martyrs, 38042 Grenoble, France, BING XU, CHRISTIAN BERNHARD, Department of Physics and Fribourg Center of Nanomaterials, University of Fribourg, Chemin du Musée 3, 1700 Fribourg, Switzerland — Since the discovery of the so-called pseudogap phenomenon in the 1990’s, the origin of the state properties of the underdoped cuprate high TC superconductors have been intensively studied [1]. An important step towards the identification of the HTSC pairing mechanism was the discovery, that a charge density wave (CDW) exists in large parts of the underdoped phase diagram [2-5]. It was shown, that in zero magnetic field (B=0) the short-ranged, static CDW is induced by defects, while a long-range CDW can be induced for high B-fields along the c-axis (perpendicular to the CuO₂ layers).

Here we aim to search for the origin of this CDW, its role in the pseudogap phenomenology and its relationship with superconductivity (competing or interwined order). We performed reflection experiments from THz-NIR region (50cm⁻¹-6000cm⁻¹) while applying high magnetic fields up to B=30Tesla.


*This study was funded by the LNCMI-CNRS, member of the European Magnetic Field Laboratory (EMFL) and by the Schweizerischen Nationalfonds (SNF) through project 200020-172611.
An outstanding challenge in high-Tc cuprates is to understand how charge density wave order is related to the pseudogap and superconducting phases [1]. To address this issue it is important to extract the energy scale $\Delta_{CDW}$ associated with the charge modulations, and to compare it with the pseudogap (PG) $\Delta_{PG}$ and the superconducting gap $\Delta_{SC}$. However, while $T_{CDW}$ is well-characterized from earlier works [2] little has been known about $\Delta_{CDW}$ until now. We will report the extraction of $\Delta_{CDW}$ for several cuprates using electronic Raman spectroscopy [3]. We observe that $\Delta_{CDW}$ increases in a manner similar to the doping dependence of $\Delta_{PG}$ and $\Delta_{SC}$. This reveals that the three phases have a common microscopic origin. In addition, we find that $\Delta_{CDW} \approx \Delta_{SC}$ over a substantial doping range, which suggests that CDW and superconducting phases are intimately related, for example intertwined or connected by an emergent symmetry [1, 4-6].


The nature of the pseudogap phase of cuprate superconductors remains a mystery. In that phase, the Fermi surface is transformed even though translational symmetry is not broken [1]. A possible explanation is a spin-liquid-like state with topological order [2].

The thermal Hall conductivity $\kappa_{xy}$ has recently emerged as a powerful probe of insulators with unusual forms of magnetism, such as quantum spin liquids [3] and quantum spin ice [4].

We report extensive measurements of the thermal Hall conductivity $\kappa_{xy}$ in several families of cuprates across a wide range of dopings. We observe a large and negative thermal Hall response at temperatures below the pseudogap temperature $T^*$, which appears immediately below the pseudogap critical doping $p^*$. The negative $\kappa_{xy}$ contrasts with the positive electrical Hall conductivity $\sigma_{xy}$ and, moreover, the magnitude of $\kappa_{xy}$ increases as doping is reduced towards $p = 0$, whereas $\sigma_{xy}$ vanishes as the material becomes an insulator.

The negative $\kappa_{xy}$ is therefore due to neutral heat carriers and it points to spin chirality [5], or perhaps topological excitations.

Pressure induced suppression of the Pseudogap in the cuprate superconductor Nd-LSCO probed by thermoelectric measurements

ADRIEN GOURGOUT (Presenter), AMIRREZA ATAEI, MARIE-EVE BOULANGER, SVEN BADOUX, Universite de Sherbrooke, DAVID E GRAF, National High Magnetic Field Laboratory, Florida State University, JIANSHI ZHOU, Mechanical Engineering, University of Texas, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, Universite de Sherbrooke — In cuprate superconductors, one of the most mysterious phase is the Pseudogap (PG). It seems linked to the superconducting dome, but the nature of their connection remains unknown. It onsets at a doping p* and is characterized by a drop in carrier density n from n=1+p above p* to n=p below. In resistivity and Hall effect, an upturn is seen at low temperature in both quantities[1]. In Nd_{0.4}La_{1.6-x}Sr_{x}CuO_{4} (Nd-LSCO), at ambient pressure, p*=0.23. A recent study from our group showed that by applying hydrostatic pressure, one can suppress the PG in Nd-LSCO and move p* to a lower doping[2]. At p=0.22, the upturns in resistivity and Hall effect are fully suppressed with 2GPa. The underlying mechanism for this effect is rooted in the Fermi Surface (FS), which imposes that the PG cannot open on an electron-like FS. Here we present a confirmation of these results, by means of Seebeck and Nernst effect measurements under pressure up to 2GPa and in magnetic fields up to 31.2T. In both quantities, the increase due to the PG is strongly suppressed by pressure at p=0.22, but shows only a weak effect at p=0.24, which further supports our interpretation that pressure tunes the pseudogap critical point p* to lower dopings in Nd-LSCO.


Interwined orders in the ground state of the Emery model in the underdoped regime*

ETTORE VITALI (Presenter), California State University, Fresno, SHIWEI ZHANG, ADAM C CHICIAK, Physics, College of William and Mary — We perform extensive Auxiliary-Field Quantum Monte Carlo (AFQMC) calculations for the three-band Hubbard (Emery) model in the underdoped regime, in order to study the ground-state properties of Copper-Oxygen planes in the cuprates. Interfacing generalized Hartree-Fock calculations with cutting-edge AFQMC techniques, we are able to resolve small energy scales, which is crucial for determining the complex candidate orders in such a system. We will present results as a function of hole-doping and charge-transfer energy.

*Supported by NSF and Simons Foundation

Coexistence of Superconductivity and Antiferromagnetism in the Hubbard model for cuprates*

ALEXANDRE FOLEY (Presenter), SIMON VERRET, ANDRE-MARIE TREMBLAY, DAVID SENECHAL, Universite de Sherbrooke — Antiferromagnetism and d-wave superconductivity are the most important competing ground-state phases of cuprate superconductors. Using cellular dynamical mean-field theory (CDMFT) for the Hubbard model, we revisit the question of the coexistence and competition of these phases in the one-band Hubbard model with realistic band parameters and interaction strengths. Using an exact diagonalization solver, we improve on previous works with a more complete bath parametrization which is carefully chosen to grant the maximal possible freedom to the hybridization function for a given number of bath orbitals. Compared with previous incomplete parametrizations, this general bath parametrization shows that the range of microscopic coexistence of superconductivity and antiferromagnetism is reduced for NCCO and confined to electron-doping with parameters relevant for hole-doped YBCO and LSCO.

*This work has been supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) under grants RGPIN-2014-04584 and RGPIN-2015-05598, the Canada First Research Excellence Fund, by the Research Chair in the Theory of Quantum Materials and by FRQNT (Quebec). Computing resources were provided by Compute Canada and Calcul Quebec.

Superconducting phase fluctuations and gap-filling phenomenology in the underdoped cuprates*

MIGUEL ANTONIO SULANGI (Presenter), JAN ZAANEN, Leiden University — We revisit the role of superconducting phase fluctuations in the cuprates as probed by various spectroscopic methods. We assume that the fluctuations of the phase of the d-wave superconducting order parameter are governed solely by a two-dimensional classical XY model and that no amplitude fluctuations are present. We find that much of the “filling-of-the-gap” phenomenology seen in the cuprates is captured by this simple model. At temperatures below the Kosterlitz-Thouless transition, the system behaves as a spatially uniform d-wave superconductor whose gap is proportional to the modulus of the spatial average of the order parameter. Above the KT transition, the vortex-dominated phase exhibits behavior that becomes more normal-like with increasing temperature. Fermi arcs in the spectral function are present near the KT transition. We also examine the effect of spatial inhomogeneity in the classical XY model and consider how the coexistence of superconducting and pseudogap-like regions seen in the cuprates can be reproduced using this model.

*This work was supported by the Netherlands Organisation for Scientific Research (NWO/OCW).
In order to further investigate the relationship between magnetism and superconductivity we have performed measurements of ultrasonic velocity and attenuation in LSCO. Around p=1/8, several anomalies are observed in the sound velocity and attenuation, associated with superconductivity and magnetic freezing. The competition between the two orders parameters is tuned with a magnetic field which enhances magnetic correlations at the expense of superconductivity.

2:30PM C09.00001: Numerical study of the momentum and doping dependence of “hot spots” and single-particle spectra in electron-doped cuprates*  
BRIAN MORITZ (Presenter), SLAC National Accelerator Laboratory, YAO WANG, Harvard University, EDWIN HUANG, Stanford University, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory — We present a systematic study of the single-particle spectral function in electron-doped cuprates determined from state-of-the-art numerical calculations using cluster perturbation theory. By comparing the appearance of the “hot spots” as a function of momentum and electron filling, we conclude that the Hubbard model with an intermediate interaction U can well capture recent experimental observations from photoemission in Nd$_{2-x}$Ce$_x$CuO$_4$. This work suggests that microscopic mechanisms similar to the hole-doped cuprates may drive the short-ranged anti-ferromagnetism, and ultimately superconductivity, even on the electron doped side, and set the stage for further theoretical explorations.

*This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515. The computational work was performed using the resources of the National Energy Research Scientific Computing Center (NERSC).

2:42PM C09.00002: Phenomenological Theory for Pseudogap and Superconducting Phases of High-Temperature Superconductors  
JIANHAO ZHANG (Presenter), SEN LI, Institute for Advanced Study, TSINGHUA UNIVERSITY, YAO MA, Department of Applied Physics, Xi’an Institute of Technology, ZHENG-YU WENG, Institute for Advanced Study, Tsinghua University — We present a phenomenological Green’s function to characterize the superconducting and pseudogap phases of the cuprates based on a microscopic theory of doped Mott insulators. In this framework, the “Fermi arc” and “superconducting kink” phenomena in ARPES experiments can be systematically obtained as a function of doping. We demonstrate that the phase-string-induced fractionalization plays a crucial role in leading to this exotic Green’s function paradigm.

2:54PM C09.00003: Intrinsic Pair Density Waves in CDMFT Improve Agreement with Cuprates*  
SIMON VERRET (Presenter), ALEXANDRE FOLEY, Institut quantique, RQMP, Université de Sherbrooke, JYOTIRMROY ROY, Université de Sherbrooke. Present address, University of Toronto, MAXIME CHARLEBOIS, Institut quantique, RQMP, Université de Sherbrooke. Present address, University of Tokyo, Applied Physics, DAVID SENSECHAL, ANDRE-MARIE TREMBLAY, Institut quantique, RQMP, Université de Sherbrooke — Cluster dynamical mean-field theory (CDMFT) is one of the most successful methods to treat strongly correlated electrons systems. It is well known, however, that CDMFT leads to an artificial breaking of translational invariance. Here, we investigate how this manifests itself. We report artificial density waves taking the shape of the cluster (cluster density waves) in all our CDMFT solutions. In particular, we report pair density waves in the superconducting solution. We discuss how these artificial density waves help the agreement of CDMFT with the low-energy spectra of cuprate high temperature superconductors. Namely, we find subgap structures similar to those found in tunnelling experiments and a related separation between nodal and anti-nodal gaps in the spectral weight, as observed in photoemission experiments. This agreement with cuprates suggests that spatial inhomogeneity is an important ingredient to explain the low-energy spectrum of cuprates, even in the strongly correlated case.

*Canada First Excellence Research Fund, NSERC Grant RGPIN-2014-04584, RGPIN-2015-05598, Research Chair in the Theory of Quantum Materials, Compute Canada, Calcul Québec, CIFAR.

3:06PM C09.00004: FLEX+DMFT approach for superconductivity in multi-band systems: A study on bilayer Hubbard model  
DAISUKE OGURA (Presenter), KAZUHIKO KUROKI, Osaka University — Broadly speaking, to enhance the superconducting transition temperature $T_c$, a strong paring interaction and a light electron effective mass are favorable. However, the strong pairing interaction not only enhance superconductivity, but also results in the strong quasi-particle renormalization in general. As a way to circumvent this dilemma, we can consider the multi-band Hubbard model as discussed in the previous studies [1, 2]. In multi-band systems, spin fluctuations with finite energy arising from interband scattering channels can develop and act as an effective pairing interaction. Finite energy fluctuations do not cause an abovementioned strong competition between the quasi-particle renormalization and superconductivity. To treat both local and non-local correlations, we have applied the FLEX (fluctuation exchange) + DMFT (dynamical mean-field theory) method [4, 5] to the bilayer Hubbard model. In the presentation, we will discuss the correlation effects and the superconductivity arising from the interband pair scattering.

with our previously reported results [2] where Ω is a constant below $\pi$. The inclusion of the variation of penetration lengths, and critical current and normalized superfluid densities as functions of temperature and of doping $\delta$.

We compare our current results for the condensation energy, the upper and lower critical fields, the coherence and superconducting gap as functions of temperature and of doping $\delta$.

4:06PM C09.00009: Influence of the variation of the number of Cooper pairs on the properties of underdoped YBa$_2$Cu$_3$O$_{6+x}$ cuprates

PATRICIA SALAS CASALES (Presenter), MIGUEL SOLIS, Instituto de Física, Universidad Nacional Autónoma de Mexico — We extend the Layered Boson-Fermion Model of superconductivity [1] to include the increase of the number $f(T)$ of Cooper pairs as temperature decreases from $T_\alpha$ to $T = 0$, for underdoped cuprate superconductors YBa$_2$Cu$_3$O$_{6+x}$.

We compare our current results for the condensation energy, the upper and lower critical fields, the coherence and superfluid densities as functions of temperature and of doping $x$, with our previously reported results [2] where $f(T) = f$ is a constant below $T_\alpha$. The inclusion of the variation of $f$ substantially improves our results when compared with the experimental results.

*We thank partial support form grants CONACyT 221030, DGAPA-PAPIIT IN107616 and DGAPA-PAPIIT IN110319.
4:18PM C09.00010: Vortex structure and Hall conductivity in d-wave superconductors  
VLADIMIR KALNITSKY (Presenter), NETANEL LINDNER, Physics, Technion - Israel Institute of Technology, EREZ BERG, Physics, University of Chicago, SEBASTIAN D HUBER, Physics, ETH Zurich — The Hall conductivity $\sigma_{xy}$ serves as an important experimental probe for determining the sign of charge carriers in materials. In type II superconductors models of vortex dynamics predicted $\sigma_{xy}$ to have the same sign as in the normal state; that is, the same as the charge carriers. However, Hall measurements showed that $\sigma_{xy}$ changes sign as a function of temperature in YBCO and other cuprates, in contradiction to these predictions. Recently it was shown that a sign reversal of $\sigma_{xy}$ occurs in a generic model for an s-wave superconductor, due to a topological transition in the vortex core. We show that a similar effect occurs in a model for a d-wave superconductor, and find a rich phase diagram of $\sigma_{xy}$ as a function of interaction strength and doping $p$: in addition to a sign reversed phase, we find a phase in which $\sigma_{xy} \sim p$. While such a relation implies a small Fermi surface, the model does not exhibit a bulk Fermi surface reconstruction.

4:30PM C09.00011: Electronic States Induced by Doping a Mott Insulator in the Presence of Antiferromagnetic Order  
MASANORI KOHNO (Presenter), National Institute for Materials Science — Recent theoretical studies on the Mott transition suggest that magnetically excited states emerge in the Mott gap in the single-particle spectrum with the dispersion relation shifted by the Fermi momenta following the doping of a Mott insulator [1--4]. This characteristic is difficult to explain in terms of mean-field quasiparticles in antiferromagnetic order. Here, by taking into account spin fluctuation in the random-phase approximation, electronic states exhibiting momentum-shifted spin-wave dispersion relation are shown to emerge in the Mott gap following the doping of a Mott insulator even though antiferromagnetic order persists [5]. The results imply that the emergence of electronic states exhibiting momentum-shifted magnetic dispersion relation is a general and fundamental characteristic of the Mott transition regardless of whether antiferromagnetic order exists or not.


4:42PM C09.00012: High Tc superconductivity in strong electron-phonon interacting systems with frustrated charge order  
ZIXIANG LI (Presenter), MARVIN L COHEN, DUNGHAI LEE, University of California, Berkeley — In this talk, I will discuss how geometric frustration inhibits charge order and allows superconductivity to benefits from strong electron-phonon coupling. We perform sign-problem-free Quantum Monte Carlo simulation to study Holstein model with strong electron-phonon coupling on triangular and square lattices. Our simulation indicates that geometric frustration of charge density wave enables strong superconductivity to exist under much wider conditions in temperature and electron-phonon coupling strength. In particular, under geometric frustration a novel coexistence phase where superconducting coherence develops within a charge ordered state exists in a strong electron-phonon coupling regime.

4:54PM C09.00013: Continuing search for the origin of HTSC: DFT studies of selected copper oxide proxy structures reviewed and paths forward suggested  
PAUL GRANT (Presenter), IBM RSM Emeritus & Principal, W2AGZ Technologies — In this presentation, we review our past attempts to uncover the pairing mechanism underlying high temperature superconductivity in copper oxide compounds and suggest possible paths forward.\footnote{Paul Grant, http://meetings.aps.org/link/BAPS.2016.MAR.R25.8} \footnote{P.M. Grant, Journal of Physics: Conference Series 129 (2008) 012042, doi:10.1088/1742-6596/129/1/012042} \footnote{C. Starr, Phys. Rev. 60, 241 (1941)} \footnote{Paul Grant, https://meetings.aps.org/Meeting/FWS17/Session/B2.10} One such path would be to derive and generalize pairing coupling functions to apply to DFT + U computed eigenstates in order to estimate Cooper pair coupling strengths arising from a combination of both lattice and spin excitations. Interestingly, such interactions were found in transition metal alums some 78 years ago as manifested in linking their respective Debye and Curie temperatures.\footnote{C. Starr, Phys. Rev. 60, 241 (1941)} We suggest repeating such experiments today on the copper oxide compounds as a function of hole/electron concentration, along with a possible computational strategy to pursue in the interpretation of the results\footnote{Paul Grant, https://meetings.aps.org/Meeting/FWS17/Session/B2.10} to finally resolve the fundamental origin of high temperature superconductivity.
Singlet $s^{\pm}$-wave pairing in quasi-one-dimensional ACr$_3$As$_3$ (A=K, Rb, Cs) superconductors

LI-DA ZHANG (Presenter), Beijing Institute of Technology, XIAOMING ZHANG, Institute for Advanced Study, Tsinghua University, JUAN-JUAN HAO, Beijing Institute of Technology, WEN HUANG, Institute for Advanced Study, Tsinghua University, FAN YANG, Beijing Institute of Technology — The recent discovery of quasi-1D Cr-based superconductivity has generated much excitement. We study in this work the superconducting instabilities of a representative compound, the newly synthesized KCr$_3$As$_3$ superconductor. Based on inputs from DFT calculations, we first construct an effective multi-orbital TB Hamiltonian to model its low-energy band structure. We then employ standard RPA calculations to investigate the superconducting instabilities of the resultant multi-orbital Hubbard model. We find the leading pairing symmetry realized in this material is singlet $s^{\pm}$-wave pairing. This singlet pairing is driven by spin-density wave fluctuations enhanced by FS. We design a phase-sensitive measurement to identify the $s$-wave pairing. The $s^{\pm}$-wave pairing in KCr$_3$As$_3$ shall also exhibit a subgap spin resonance mode near the nesting vector, which can be tested by inelastic neutron scattering measurements. We also propose further application of KCr$_3$As$_3$ by utilizing it to induce TRI TSC via proximity effect. Our study shall be of general relevance to all superconductors in the family of ACr$_3$As$_3$ (A=K, Rb, Cs). Reference: arXiv: 1809.07117

Superconductivity in systems exhibiting the Altshuler-Aronov anomaly*

RICHARD HLUBINA (Presenter), Comenius University in Bratislava, BRANISLAV RABATIN, Department of Physics, Florida State University — Dirty superconductors close to the metal-insulator transition frequently exhibit a pseudogap in the normal state due to the Altshuler-Aronov (AA) effect. In this talk we show that, making use of generalized Eliashberg equations, the AA effect and superconductivity can be described on equal footing. We derive explicit expressions for the Coulomb pseudopotential in 3D, taking into account also the anomalous diffusion. We present a full numerical solution for two normal-state and two anomalous self-energies. In the normal state, we amend the known results for the purely electronic AA effect; with electron-phonon coupling turned on, we find additional anomalies in the density of states close to the phonon energy. We study how the critical temperature and density of states of strongly disordered 3D superconductors change with normal-state resistivity. We find that the type of transition from the superconducting to the insulating state depends on the strength of electron-phonon coupling: at weak coupling there exists an intermediate normal state, whereas at strong coupling the transition is direct.

*This work was supported by the Slovak Research and Development Agency under Contract No. APVV-15-0496.

Monday, March 4, 2019 2:30 PM - 5:06 PM

Session C10 DMP: Fe-based Superconductors III

Phase diagram of a hetero-structured iron-based superconductor Sr$_2$VO$_3$FeAs [Invited]

JUN SUNG KIM (Presenter), Physics, Pohang University of Science and Technology — The interplay of spin and orbital degrees of freedom induces various magnetic or nematic phases, coexisting with the superconductivity, and leads to rich phase diagrams in iron-based superconductors (FeSCs). Among various iron-based superconductors, Sr$_2$VO$_3$FeAs holds a unique position as a naturally-assembled heterostructure of a FeSC and a Mott-insulating vanadium oxide, in which the unusual $C_4$ symmetric phases are recently identified and found to be highly distinct from those found in other FeSCs. In this talk, I will present our experimental explorations on these unusual phase transitions in the FeAs layers of Sr$_2$VO$_3$FeAs, and discuss the possible role of the magnetic proximity coupling and the resulting frustration of the otherwise dominant Fe stripe and V Neel fluctuations for stabilizing hidden orders in FeSCs.

Self-induced magnetic flux structure in magnetic superconductor*

VITALII VLASKO-VLASOV (Presenter), ALEXEI E KOSHELEV, JINKE BAO, DUCK YOUNG CHUNG, MERCOURI KANATZIDIS, ULRICH WELP, WAI-KWONG KWOK, Argonne National Laboratory — We image the temperature evolution of the distribution of the magnetic induction in single crystals of the magnetic superconductor EuRbFe$_4$As$_4$. In contrast to the traditional Meissner flux expulsion, the samples cooled in constant magnetic fields show unusual vortex patterns revealing a strong enhancement of the internal magnetic flux density upon approaching the magnetic transition temperature. The observed patterns demonstrate a cooperative response of the magnetic subsystem, which acts as an internal pump of the magnetic flux, and the superconducting system, which controls the delivery of vortices into the bulk of the sample. We suggest possible current distributions responsible for the observed flux patterns.

*The work was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division.
3:18PM C10.00003: STM/STS study of superconducting properties modified by Ca deposition on Ca$_{10}$(Pt$_4$As$_8$)$_5$*(Fe$_2$As$_2$)$_5$* JISUN KIM (Presenter), SEOKHWAN CHOI, BRANDON STUART, AMY QU, Stewart Blusson Quantum Matter Institute, University of British Columbia, SILU HUANG, RONGYING JIN, Department of Physics and Astronomy, Louisiana State University, DOUGLAS BONN, SARAH A. BURKE, Stewart Blusson Quantum Matter Institute, University of British Columbia — Ca$_{10}$(Pt$_4$As$_8$)$_5$ contains both superconducting building blocks (Fe$_2$As$_2$ layers) and conducting spacers (Pt$_4$As$_8$ layers), unlike insulating spacers in other Fe-based superconductors. Prior work showed the important role played by the charge environment and surface structures in its superconducting properties: evidence for superconductivity is absent in bare Pt$_4$As$_8$ surface but recovers when Ca atoms are atop [1]. Different surface reconstructions also lead different superconducting features. We use scanning tunneling microscopy and spectroscopy (STM/S) to directly confirm the role of charge balance and surface structures on superconductivity in this compound. Cleaving provides large areas of bare Pt$_4$As$_8$ layer, which originally does not show superconducting features. Depositing additional Ca atoms on the bare Pt$_4$As$_8$ surface, while the sample is on the STM scanning stage, results in changes in spectral features. We will discuss the relationship between surface structures and superconducting features based on the Ca structures formed by controlling the deposition temperature.


*Funded by NSERC, CFREF, USNSF

3:30PM C10.00004: Prediction of (Li$_{0.8}$Co$_{0.2}$OH)CoSb as A New Superlatticed Superconductor* PING CUI (Presenter), M. USMAN MUZAFFAR, WENJUN DING, JIANG ZENG, WEI QIN, ZHENYU ZHANG, ICQD, University of Science and Technology of China — We study theoretically the superlattice material of (Li$_{0.8}$Co$_{0.2}$OH)CoSb as a new candidate superconductor, in which the superconducting layer CoSb has the same crystal structure as FeSe, but with stronger spin-orbit coupling (SOC). Through density functional theory calculations, we find that substitution of Li by Co in the spacing layer not only minimizes the lattice mismatch between the spacing and superconducting layers in the ab plane, but also helps to stabilize the overall structure of the system. Moreover, we have investigated the detailed nature of charge transfer and found that Co in the spacing layer can significantly enhance the interlayer charge transfer, which is essential for achieving superconductivity. The predicted system is not only likely to add a new member into the superconducting family, but may also offer new opportunities for realizing topological superconductivity because of the stronger SOC.

*Supported by NNSF of China and MOST.

3:42PM C10.00005: Temperature- and pressure-dependent electronic structure evolution of quasi-one-dimensional iron chalcogenide ladder compounds, BaFe$_2$S$_3$, and BaFe$_2$Se$_3$: optical studies and DFT calculations JUNGSEEK HWANG (Presenter), SEULKI ROH, SOOHYEON SHIN, JAEKYUNG JANG, Sungkyunkwan University, ZHENXIAN LIU, George Washington University, G LAWRENCE CARR, Brookhaven National Laboratory, JOO YULL RHEE, TUSON PARK, Sungkyunkwan University — Since the discovery of a pressure-induced iron-based superconductor, BaFe$_2$S$_3$ (BFS), intensive studies have been performed on BFS and a similar compound BaFe$_2$Se$_3$ (BFSe). Both compounds are antiferromagnetic insulators, with increasing pressure they show metallic phases and eventually become superconductors under very high pressure. We measured reflectance spectra of those two compounds by controlling two experimental tuning parameters: temperature and pressure. From our temperature-dependent measured reflectance spectra of both samples using polarized lights, we obtained anisotropic optical conductivity along two crystal axes. We observed bandgaps in both samples along the ladder direction at low temperature. We also observed pressure-induced insulator-metal transitions (IMT) in both samples from our pressure-dependent measured mid-infrared reflectance spectra of both samples at 300 K using diamond anvil cells. The density functional theory calculations were also performed to understand the measured experimental spectra. In this presentation, we will present our results and discuss on them.
Melting of vortex lattice in magnetic iron-pnictide superconductor RbEuFe₄As₄*  
ALEXEI E KOSHELEV (Presenter), KRISTIN WILLA, ROLAND WILLA, MATTHEW SMYLIE, JINKE BAO, DUCK YOUNG CHUNG, MERCOURI KANATZIDIS, ULRICH WELP, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory — The iron-based superconductors are characterized by sizable thermal fluctuations due to high transition temperatures and small coherence lengths. We report calorimetric and transport observations for the vortex-lattice melting in the magnetic iron-pnictide superconductor RbEuFe₄As₄ with Tc ≈ 37K and dHc²/dT ≈ 4T/K. The melting transition is seen as a sharp drop of the resistivity and a step of the specific heat at the magnetic-field-dependent temperature. The typical step height is ∼ 4-5% of the zero-field jump, similar to YBa₂Cu₃O₇ and in agreement with theoretical estimates. The specific-heat peak due to the latent heat expected for very clean materials, however, was not observed. The melting line lies in the temperature/magnetic-field plane noticeably below the upper-critical-field line, and the vortex-liquid state occupies a significant portion of the phase diagram. The location of the melting transition is in quantitative agreement with theoretical predictions without fitting parameters.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. K.W. and R.W. acknowledge support from the Swiss National Science Foundation through an Early Postdoc Mobility fellowship.

Influence of magnetic ordering on the vortex matter in RbEuFe₄As₄ single crystals*  
MATTHEW SMYLIE, ULRICH WELP, WAI-KWONG KWOK, JINKE BAO, DUCK YOUNG CHUNG, MERCOURI KANATZIDIS, YILMAZ SIMSEK, KRISTIN WILLA, ALEXEI E KOSHELEV, Materials Science Division, Argonne National Laboratory, LEONARDO CIVALE (Presenter), MPA-Condensed Matter and Magnet Science, Los Alamos National Laboratory — Eu-containing Fe-based superconductors are ideal systems to study the interplay of superconductivity and magnetic order. The superconductor RbEuFe₄As₄ has Tc~37K and undergoes a magnetic ordering of the Eu at Tm~15K. We studied vortex pinning and dynamics in RbEuFe₄As₄ single crystals as a function of temperature (T), magnetic field and orientation (Θ) by angular dependent magnetization. The critical current density (Jc) of the pristine crystals is low, indicative of small disorder, and weakly anisotropic. Introduction of aligned columnar defects (CDs) by heavy ion irradiation increases Jc, but produces almost no changes in Tc and Tm. In the crystals with CDs, Jc(Θ) exhibits a lockin phase, the fingerprint of correlated pinning. Both pristine and irradiated crystals show clear evidence of the influence of the magnetic order on the vortex matter. In pristine crystals, the rate of decrease in Jc with T slows down in the proximity of Tm. Irradiation enhances this effect, with Jc(T) becoming nonmonotonic and developing a local maximum near Tm. In both cases, flux creep rates exhibit local minima around the magnetic transition, indicating an increase in the vortex pinning energy.

*Work supported by U.S. DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

Comparison of S- and Te-substitution effects in FeSe thin films*  
FUYUKI NABESHIMA (Presenter), TOMOYA ISHIKAWA, NAOKI SHIKAMA, ATSUTAKA MAEDA, University of Tokyo — We have successfully grown single crystalline films of FeSe₁₋ₓSₓ with x ≤ 0.43 via pulsed laser deposition. As x increases, the structural transition temperature decreases and the superconducting transition temperature, Tc, shows a gradual decrease even when the structural transition disappears. We observed a new kink structure in the resistivity-temperature curves for films with large x, which is likely due to a magnetic transition. The obtained phase diagram of FeSe₁₋ₓSₓ is in contrast to that of FeSe₁₋yTeₓ films, which shows a sudden increase of Tc at the composition where the structural transition disappears[1]. These results demonstrate that the relationship between the nematicity and the superconductivity is not universal in FeSe, suggesting that the nematicity does not play a primary role in the superconductivity in this system[2].


*This work was supported by JSPS KAKENHI Grant Number 18H04212 and The Murata Science Foundation.
Verwey-like Transition in $\beta$-Fe$_{4+\delta}$Se$_5$ Nanowires of Fe-vacancy Ordering

TUNG-SHENG LO (Presenter), KUNG-YU YEH, CHUNG-CHIEH CHANG, PHILLIP WU, Institute of Physics, Academia Sinica, KUEI-SHU CHANG-LIAO, Department of Engineering and System Science, National Tsing Hua University, MING-JYE WANG, Institute of Astronomy and Astrophysics, Academia Sinica, MAW-KUEN WU, Institute of Physics, Academia Sinica — The magnetotransport and the source-drain frequency dependence of $\beta$-Fe$_{4+\delta}$Se$_5$ nanowires are investigated. The nanowires feature Fe-vacancy ordering and mixed valence of Fe. The resistance shows a first-order metal-insulator transition of transition temperature at ~30K in the absence of magnetic fields. Colossal positive magnetoresistance is observed at temperatures around 30K. The metal-insulator transition presents uniaxial anisotropy with the c-axis in field-orientation dependence. The frequency dependence in resistance below the metal-insulator transition temperature is similar to features in magnetite nanowires at temperatures lower than the Verwey temperature. Our results reveal that the Fe-vacancy-ordered $\beta$-Fe$_{4+\delta}$Se$_5$ nanowires undergo a magnetic first-order phase transition strongly involving spin-orbital coupling with $d_{z^2}$ orbitals.

Observation of low-energy phonon anomalies in Ca$_{0.73}$La$_{0.27}$FeAs$_2$

ZHENZHONG SHI (Presenter), SACHITH DISSANAYAKE, Department of Physics, Duke University, DIPANSHU BANSAL, Department of Mechanical Engineering & Materials Science, Duke University, WENLI BI, AHMET ALATAS, Advanced Photon Source, Argonne National Laboratory, STEPHEN J KUHN, BRODIE POPOVIC, Department of Physics, Duke University, EVE EMMANOUILIDOU, NI NI, Department of Physics and Astronomy, University of California, Los Angeles, OLIIVER DELAIRE, Department of Mechanical Engineering & Materials Science, Duke University, AYMAN SAID, Advanced Photon Source, Argonne National Laboratory, SARA HARAVIFARD, Department of Physics, Duke University — Couplings between lattice and charge or spin degrees of freedom underpin a wide range of phenomena in strongly correlated electronic systems. Fe-based superconductors provide an important platform in probing the phonon effect on high temperature superconductivity, where spin-phonon interaction is expected to dominate. Ca$_{0.73}$La$_{0.27}$FeAs$_2$, considered as a parent compound of the 112 family, has an antiferromagnetic ground state, which gives way to a superconducting state at high pressure. We have performed a systematic inelastic X-ray scattering study on single crystals of Ca$_{0.73}$La$_{0.27}$FeAs$_2$, at both ambient and high pressure, and compared the results with density functional theory (DFT) calculations. A low-energy phonon anomaly was observed, and its nature will be discussed.

STM and Nernst measurements on tetragonal and orthogonal phase of Fe(Se$_{1-x}$S$_x$)

MASAHIRO HAZE (Presenter), WEN-KAI HUANG, DAIKI SANO, SHIGERU KASAHARA, MASAHIRO NARITSUKA, TOMOKA SUEMATSU, TOMOYA TANIGUCHI, YUICHI KASAHARA, Department of Physics, Kyoto University, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, University of Tokyo, YUJI MATSUDA, Department of Physics, Kyoto University — The crossover from the Bardeen-Cooper-Schrieffer (BCS) state for weakly paired fermions to the Bose Einstein condensation (BEC) state of tightly-bound pairs has attracted much attention as a new paradigm of superconductivity. In the BCS-BEC crossover regime, exotic phenomena, such as pseudogap formation owing to preformed pairs above superconducting transition temperature $T_c$, have been predicted.

It has been reported that multiband iron-based superconductor FeSe with the small Fermi energies is located at the BCS-BEC crossover regime. Moreover, very recent heat capacity and ARPES measurements have suggested a possibility that the tetragonal phase of Fe(Se$_{1-x}$S$_x$) ($x > 0.17$) is located at the state closer to the BEC limit. Pairing fluctuation and pseudogap formation above $T_c$, however, have not been reported so far.

In this study, we perform STM and Nernst measurements on FeSe$_{0.87}$S$_{0.13}$ and FeSe$_{0.75}$S$_{0.25}$, which are in the orthogonal and tetragonal phases, respectively. In our Nernst measurements, well exceeding Gaussian fluctuations are observed above $T_c$ in FeSe$_{0.75}$S$_{0.25}$, while pseudogap formation is not observed by the STM measurements. We will discuss the present results in terms of the BCS-BEC crossover in multiband superconducting systems.

Monday, March 4, 2019 2:30 PM - 5:06 PM

Session C11 DMP DCOMP FIAP: Defects in Semiconductors -- Energy Materials

Lyons, United States Naval Research Laboratory - Tag(s): Focus
2:30PM C11.00001: Bright triplet excitons in cesium lead halide perovskites [Invited] ALEXANDER EFROS (Presenter), United States Naval Research Laboratory — The observation of a ground optically forbidden “dark” exciton state in semiconductor nanocrystals was first reported in the seminal paper of Nirmal et al. in 1995. ¹ Later research in nanowires, nanorods, and nanoplatelets has shown that the ground exciton state in all these semiconductor structures is a dark exciton, leading us to believe that the ground exciton must be dark. Because dark excitons release photons slowly, hindering emission, semiconductor nanostructures that disobey this rule have been sought. Three years ago however cesium lead halide perovskite (CsPbX₃, with X = Cl, Br or I ) nanocrystals were grown, which demonstrated very bright photoluminescence (PL) with quantum yield 50-90% at room temperature. This bright emission was traced to a very short radiative decay time. The nanocrystals emit light about 20 and 1,000 times faster than any other semiconductor nanocrystal at room and cryogenic temperatures, respectively. The increase of the decay time with temperature is inconsistent with a dark ground state exciton suggesting that in these nanocrystals the ground exciton state is bright. We use an effective-mass model and group theory to demonstrate the possibility of such a ground bright state existing, which can occur when the strong spin–orbit coupling in the conduction band of perovskites is combined with the Rashba effect.² We then apply our model to CsPbX₃ nanocrystals, and measure size- and composition-dependent fluorescence at the single-nanocrystal level. The bright triplet character of the lowest exciton explains the anomalous photon-emission rates of these materials. The existence of this bright triplet exciton is further confirmed by analysis of the fine structure in low-temperature fluorescence spectra.


3:06PM C11.00002: Formation of DY Defect Centers in Bi-Doped Hybrid Halide Perovskites SUHUAI WEI (Presenter), JINLING LI, JINGXIU YANG, Beijing Computational Science Research Center — The DX center is a major killer defect that limits the n-type doping in some four-fold coordinated semiconductors. It is a deep negatively charged defect complex converted from a nominal shallow donor defect, which can serve as a trap center of electrons, thus is detrimental to the performance of optoelectronic devices. Similar to the DX center, we find that a donor-yielded complex center (DY center) also exists in six-fold coordination semiconducting materials. For example, Bi is commonly used as n-type dopant in perovskite APbX₃. However, our first-principles calculations show that the DY centers are formed in Bi doped MAPbBr₃ when the Fermi level is high in the gap, but, interestingly, it does not form in MAPbI₃. The reason that the DY center is formed in MAPbBr₃ instead of MAPbI₃ is attributed to the high conduction band minimum (CBM) of MAPbBr₃. Our results are able to explain recent puzzling experiment observations and the thorough discussions of the formation and the properties of the DY center in perovskites provide enlightening insights to the defect study in six-fold coordinated semiconductors.

3:18PM C11.00003: Significantly Different Solubility of Li, Na and K Dopants in Cu(In,Ga)Se₂ and Cu₂ZnSn(S,Se)₄ Solar Cells XIAN ZHANG, MENGLIN HUANG, SHIYOU CHEN (Presenter), East China Normal University — The doping of alkaline elements such as Na, K, Rb and Cs in Cu(In,Ga)Se₂ (CIGS) and Cu₂ZnSn(S,Se)₄ (CZTSSe) thin film solar cells had been intensively studied for decades and was shown to be critical for achieving high photovoltaic efficiency. However, the doping of the light alkaline element Li has been much less studied. Using the first-principles calculations, we show here that the formation energy of Li dopants is very low in CIGS and CZTSSe, while the formation energies of Na and K dopants are much higher, so the doping concentration (solubility) of Li can be very high in the CIGS and CZTS lattices at room temperature, much higher than those of Na and other heavier alkaline elements. Na and K may be doped into the CIGS and CZTSSe lattices with a high solubility at high temperature, but the dopants will diffuse out of the grains and prefer staying on the grain boundaries at room temperature because of the low solubility in the lattice. The concentration increase of the hole carriers after the alkaline doping will be discussed based on the calculated solubility.
3:30PM C11.00004: Modeling of disorder in II-IV-V2 semiconductors for tuning of novel properties  JACOB CORDELL (Presenter), Materials Science, Colorado School of Mines/National Renewable Energy Laboratory, JIE PAN, Materials Science, National Renewable Energy Laboratory, GARRITT TUCKER, Mechanical Engineering, Colorado School of Mines, STEPHAN LANY, Materials Science, National Renewable Energy Laboratory — The customization of multinary semiconductors has attracted great interest in the science community for a diverse set of novel applications. The properties of these materials can be fine-tuned by controlling composition and atomic ordering. However, an understanding of the structure-synthesis-property relationship is essential for a rational design. In this contribution, we use two II-IV-V2 materials: ZnSnN2 and ZnGeN2 as examples to illustrate the ordering effects. Model Hamiltonian based Monte Carlo simulations were used to create structures with different degrees of disorder. The energies and electronic structures were estimated from first principles calculations. We find that energies of ZnSnN2 can be well approximated by a Motif Hamiltonian which incorporates only short-range ordering. We demonstrate that, only with the consideration of disorder and oxygen contamination, the net doping level in ZnSnN2 can be lowered to agree with experiments (10^{17} cm^{-3}). However, for ZnGeN2, long-range ordering effects step in, and thus, we use the Cluster Expansion Hamiltonian to create disordered structures. The thermodynamics and optoelectronic properties of disordered ZnGeN2 will be discussed.

3:42PM C11.00005: Sulfur Vacancies as the Origin of n-type Doping in Unintentionally Doped Pyrite FeS2 Single Crystals*  BRYAN VOIGT (Presenter), WILLIAM MOORE, MICHAEL MANNO, JEFF WALTER, CHRIS LEIGHTON, University of Minnesota, ERAY S. AYDIL, New York University — Pyrite FeS2 has long been considered an ideal semiconductor for low-cost solar cells as it is composed of earth-abundant, non-toxic, inexpensive elements, has a suitable band gap (0.95 eV), and absorbs sunlight strongly. Disappointing power conversion efficiencies, however, have plagued pyrite solar cells. An important unanswered question is the origin of the n-type behavior seen in unintentionally-doped pyrite single crystals and thin films. Here, we present the first substantial electronic transport evidence that sulfur vacancies are this n-type dopant by varying sulfur vapor pressure (P_S) during single crystal growth. Crystals grown under high P_S exhibit semiconducting behavior, with transport activation energies of 225 meV and 300 K electron densities (n_{300K}) of 10^{16} cm^{-3}. Decreasing P_S increases n_{300K} to >10^{17} cm^{-3} and decreases the activation energy ten-fold, evidencing an evolution towards an insulator-metal transition. These trends are independent of metal impurity concentrations and, moreover, n_{300K} is too large to be explained by these impurities.

*Work supported by Xcel Energy through the Renewable Development Fund, and by the NSF through the UMN MRSEC.

3:54PM C11.00006: The nature of band gap of Co3O4 – a revisit from first-principles*  TYLER SMART (Presenter), Physics, University of California, Santa Cruz, TUAN ANH PHAM, Quantum Simulations Group, Lawrence Livermore National Laboratory, YUAN PING, Chemistry and Biochemistry, University of California, Santa Cruz, TADASHI OGITSU, Quantum Simulations Group, Lawrence Livermore National Laboratory — Cobalt Oxide (Co3O4) has emerged as a highly promising material for a wide variety of energy technologies, including hydrogen generation through solar-water-splitting and Li ion batteries. Yet, a detailed understanding of the electronic properties of this material is largely lacking. For example, contradicting experimental results have been reported for the optical gap, leading to two commonly reported values of 0.8 eV and 1.6 eV. Here we have employed hybrid functional calculations compliant with the generalized Koopmans' theorem, to demonstrate that the intrinsic band gap of Co3O4 is ~1.6 eV. Meanwhile, the ~0.8 eV transition found experimentally is due to the presence of polaron or defect states. In particular, our calculations predict the spontaneous formation of electron and hole polarons, that in turn exhibit significant contribution to the absorption spectra of the material and are responsible for the optical excitation at 0.8 eV. Finally, we resolve the nature of the stable spin states of electron and hole polarons, and we discuss how the interaction between polarons with n-type dopants (carbon) could improve the electrical conductivity of this intrinsic p-type material.

*NSF under grant No. DMR-1760260. Part of this work was preformed at LLNL under the DOE EERE.
Grain-size dependent carrier compensation in Cu$_2$O*  

GARIMA AGGARWAL (Presenter), SANDEEP KUMAR MAURYA, BALASUBRAMANIAM KAVAIPATTI RAMANATHAN, Energy Science and Engineering Department, Indian Institute of Technology Bombay, India — Cuprous oxide (Cu$_2$O) is an absorber material for low cost solar cells and various fundamental phenomena have been explained using this material. Phase pure Cu$_2$O samples with different grain sizes, in the range of 400 µm to 3 mm, were obtained by thermal oxidation of a Cu sheet. The temperature dependent carrier concentration of all samples follows the compensated semiconductor model. In this model, two independent monovalent acceptors (N$_{A1}$, N$_{A2}$) are assumed with one compensating donor level (N$_D$) and the carrier concentration is obtained from charge neutrality condition. It is observed that the difference in energy levels between two acceptors is ~80 meV, pertaining to a normal and a split Cu-vacancy in Cu$_2$O as acceptor defects. Interestingly, the concentration of donor defects increases with increasing grain boundary cross section (Λ$_{GB}$), from 5.8×10$^{13}$ cm$^{-3}$ for a sample with Λ$_{GB}$=0.22×10$^{-3}$ µm$^{-1}$ to 3.0×10$^{14}$ cm$^{-3}$ for a sample with Λ$_{GB}$=0.45×10$^{-3}$ µm$^{-1}$. It indicates that the grain boundaries act as source of compensating donor defects in Cu$_2$O. This study suggests that the increment in grain size of Cu$_2$O can improve the performance of electronic devices based on it.

*KRB acknowledges IRCC, IIT Bombay for providing funding (Grant No. 12IRCCSG014).

Structural and electronic properties of amorphous In$_2$O$_3$:Li,Na from first principles  

IVAN ZHURAVLEV (Presenter), JULIA MEDVEDEVA, Physics, Missouri University of Science and Technology — Amorphous oxide semiconductors (AOS) have found wide application in consumer electronic devices due to their unique properties, namely, high carrier mobility and transparency in the visible. Among the AOS materials, indium-based oxides show best overall performance. Additional cations, such as Zn, Ga, or Sn, allow one to tune the structural, electronic, and optical properties of ternary and quaternary AOS over wide ranges [1-2].

Here we present a thorough systematic analysis of the structural, electronic, and optical properties of amorphous In$_2$O$_3-x$ doped with Li and Na. From the theory of glass formation, it is known that alkali metal oxides such as Li$_2$O and Na$_2$O serve as structural modifiers, increasing the materials density. We employ ab-initio molecular dynamics liquid-quench simulations and accurate density-functional calculations to understand how addition of Li or Na affects the local In-O structure as well as medium-range In-In structure that determines the morphology of the amorphous network. The resulting electronic and optical properties of Li and Na doped amorphous indium oxide are investigated as a function of density, quench rates, cation composition, and oxygen stoichiometry.


Probing the Electronic States in GaAsNBi Alloys*  

ANDRA CHEN (Presenter), JORDAN M OCCENA, Materials Science and Engineering, University of Michigan, CAGLIYAN KURDAK, Physics, University of Michigan, RACHEL GOLDMAN, Materials Science and Engineering, University of Michigan — Although solar energy is the most abundant renewable energy source, an approach to combine energy harvesting and energy storage is urgently needed. Recently, solar to hydrogen (STH) conversion using photoelectrochemical cells (PEC) has emerged as a promising approach to harvest and store solar energy. Indeed, record STH efficiency is predicted for a tandem PEC which includes a 1.05 eV bandgap junction.  

Recently, we synthesized a novel alloy, gallium arsenide nitride bismide, which is nearly lattice-matched to gallium arsenide, with bandgaps tunable from 0.87 to 1.34 eV. To determine the energy bandoffsets and electronic states of GaAsNBi alloys, we are examining GaAs/GaAsNBi/GaAs single quantum well structures with dilute concentrations of N and Bi. Using a combination of photoluminescence spectroscopy, in conjunction with capacitance-voltage measurements and 1D-Schrödinger-Poisson simulations, we determine the band offsets and deep levels in GaAs/GaAs$_{1-x,y}$N$_x$Bi$_y$/GaAs heterostructures.


*We gratefully acknowledge support of the NSF, DMR 1810280.
4:42PM C11.00010: A theoretical study of the out-of-plane electrical transport of n-type thermoelectric SnS*  JUAN CUI (Presenter), Mechanical Engineering, The University of Hong Kong, JIAQING HE, Department of Physics, Southern University of Science and Technology, YUE CHEN, Mechanical Engineering, The University of Hong Kong — As a promising thermoelectric material containing non-toxic and abundant elements, SnS has attracted significant research focus in recent years. To further improve the thermoelectric energy conversion efficiency of SnS, it is critical to have a thorough understanding of its electronic structure. In this work, we have calculated the band structure of SnS from first principles using the HSE06 hybrid functional to unveil the detailed valence band features. We have then compared the band features of SnS with those of the analogue SnSe, which was recently shown to have a very high thermoelectric figure of merit. By further investigating the doping effects of n-type impurities on the electronic structure and electrical transport properties of SnS, we identify resonant states near the bottom of the conduction band and find a considerable increase of electron delocalization along the out-of-plane direction of the layer crystal structure. Boltzmann transport calculations show that these effects on the electronic structure may result in enhanced electrical transport properties.

*This work is supported by the Research Grants Council of Hong Kong under project numbers 27202516, 17200017 and F-HKU703/16T. We are grateful for the research computing facilities offered by ITS, HKU.

4:54PM C11.00011: scanning tunneling microscopy of defects in SnS2  MANOJ SINGH (Presenter), BISHNU SHARMA, BONING YU, Physics, Clark University, LYUBOV TITOVA, Physics, WPI, RONALD GRIMM, Chemistry, WPI, MICHAEL C BOYER, Physics, Clark University — We present our room- temperature scanning tunneling microscopy measurements of SnS2, a quasi-two dimensional layered semiconductor. SnS2 is a material of interest due to its high carrier mobility and its potential use in applications including in photonics, electronics, and solar energy conversion. Understanding the surface properties of SnS2 are particularly important for its incorporation and optimization in applications. Here we present our surface characterization of SnS2 and detail several surface features including surface/subsurface defects which locally distort the crystal lattice.

Monday, March 4, 2019 2:30 PM - 5:30 PM


2:30PM C12.00001: Indirect bandgap measured in β'-phase In2Se3 crystals by angle-resolved photoemission spectroscopy*  MICHAEL FUHRER (Presenter), JAMES COLLINS, CHUTIAN WANG, ARC Centre of Excellence in Future Low-Energy Electronics Technologies, ANTON TADICH, Australian Synchrotron, YUEFENG YIN, ARC Centre of Excellence in Future Low-Energy Electronics Technologies, SHUJIE TANG, SUNG-KWAN MO, Advanced Light Source, Lawrence Berkeley National Laboratory, CHANG LIU, CHANGXI ZHENG, NIKHIL MEDHEKAR, MARK T EDMONDS, ARC Centre of Excellence in Future Low-Energy Electronics Technologies — In2Se3 is a widely studied van der Waals (vdW) layered material and its many structural phases have attracted attention for their promise as semiconducting platforms for photovoltaics, use as an isostructural buffer layers in topological insulator superlattices, and recently as room temperature ferroelectrics1,2. The details of its electronic structure however have not been fully elucidated by experiments. We report on a combined angle-resolved photoemission spectroscopy and density functional theory study which reveals an indirect bandgap with highly anisotropic conduction and valence bands in bulk crystals of commercially obtained β'-phase In2Se3. The n-doped crystals exhibit large effective mass hole bands with maxima slightly offset from Γ, as well as small effective mass electron valleys which sit at M/M' points, with minima at M/M' lower in energy by about 0.3eV, resulting in an indirect bandgap of 1.41eV, and a direct bandgap at Γ in excess of 1.7eV.

1Y. Zhou et al., Nano Letters 17, 5508 (2017)

*This work was supported by the ARC Centre of Excellence in Future Low Energy Electronics Technologies and ARC grant DP150103837.
2:42PM C12.00002: Theory of “Emergence of excitonic superfluid at topological-insulator surfaces”*  
RUI WANG (Presenter), Shanghai Jiao Tong University, YASEN HOU, RUI XIAO, LUKE MCCLINTOCK, HENRY CLARK TRAVAGLINI, JOHN PAULUS FRANCIA, University of California, Davis, HARRY FETSCH, Harvey Mudd College, ONUR ERTEN, Arizona State University, SERGEY SAVRASOV, University of California, Davis, BAIGENG WANG, Nanjing University, ANTONIO ROSSI, INNA VISHIK, University of California, Davis, ELI ROTENBERG, Lawrence Berkeley National Laboratory, DONG YU, University of California, Davis — We study the BCS condensation of excitons on topological-insulator surfaces. With presence of a screened Coulomb interaction between excited electrons and holes, the BCS excitons can be formed with predicted transition temperature up to 40K. The thermal fluctuation is found to disturb the long-range order by creating vortex excitations. It lowers the mean-field estimation of the transition temperature and drives the transition into the Kosterlitz-Thouless type. The BCS condensation of excitons forms ground state with quantum coherence that leads to the experimentally observed long-range transport of photocurrent. We also discuss possible generation of the topological p+ip excitonic insulators at topological-insulator surfaces.

*This work was supported by National Science Foundation Grant DMR-1838532 and DMR-1710737. S.Y.S was supported by National Science Foundation Grant DMR-1411336. This research used the Molecular Foundry and the Advanced Light Source, which are US Department of Energy Office of Science User Facilities under contract no. DE-AC02-05CH11231. H.F. acknowledges the U.S. National Science Foundation Research Experiences for Undergraduates (REU) program under Grant No. PHY-1560482.

2:54PM C12.00003: Optical Selection Rules and Optical Nonlinearities of Excitonic States in Monolayer MoS2*  
DANIEL SOH (Presenter), Sandia National Laboratories California, ERIC CHATTERJEE, Ginzton Laboratory, Stanford University, CHRISTOPHER ROGERS, Sandia National Laboratories California, DODD J GRAY, HIDEO MABUCHI, Ginzton Laboratory, Stanford University — The monolayer MoS2 exhibits a strong optical response from the stable excitonic states even at room temperature, due to the large binding energy of the reduced dimension. We present that the topological chirality in MoS2 binding the valleys and the spins determines not only the linear but also the nonlinear optical responses. Using the massive Dirac Hamiltonian to provide efficient handling of the nonlinear processes, we perform a perturbative calculation in the low-temperature and weakly excited limit. We then derive the linear and the nonlinear optical susceptibilities. We calculated those for particularly the second- and the third-harmonic generations, two-photon absorption, and optical Kerr effect, based on the prescribed optical selection rules. We compare the optical responses of the monolayer MoS2 with our previous results on graphene, adopting the Keldysh-type wave functions and the S-matrix treatment. We also present the figure of merit for efficient optical Kerr device applications.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the DOE's National Nuclear Security Administration under contract DE-NA0003525.

3:06PM C12.00004: Photoluminescence studies of monolayer WSe2 in proximity with BiFeO3 thin films.  
ANIL RAJAPITAMAHUNI (Presenter), NEREA ONTOSO, CIC nanoGUNE, SAEDEH FAROKHPOOR, University of Groningen, JOSE IGNACIO PASCUAL, CIC nanoGUNE, BEATRIZ NOHEDA, University of Groningen, REYES CALVO, CIC nanoGUNE — We have studied the photoluminescence (PL) properties of 1-layer WSe2 in proximity with multiferroic BiFeO3 (BFO) thin films. Using pulsed laser deposition, we have grown epitaxial single crystalline BFO films of 20 -80 nm thick on SrRuO3 buffered (001) SrTiO3 substrates. X-Ray and AFM characterizations show the films have high crystallinity and smooth surface. Piezo-response force microscopy studies show that the as-grown PZT films have uniform polarization pointing away from the substrate. We then transferred WSe2 flakes onto 300 nm SiO2 and BFO using elastic film assisted micro-mechanical exfoliation. Optical microscopy combined with Raman spectroscopy is used to identify and determine the layer number of WSe2 flakes. Spatially-resolved PL spectroscopy measurements are performed using a scanning confocal microscope to investigate the valley excitonic properties of WSe2 in proximity with BFO. When compared to SiO2, we observed a quenching in PL signal for WSe2 on BFO at 300 K. We have also studied the effect of temperature and magnetic fields on the valley polarization of monolayer WSe2 in proximity with multiferroic BFO thin films.
3:18PM C12.00005: Tunable Optical Absorption by Excitons in Xenes via an External Electric Field*  MATTHEW BRUNETTI (Presenter), CUNY Graduate Center, OLEG BERMAN, ROMAN KEZERASHVILI, Physics, CUNY - City Tech — We study the binding energies and optical properties of direct and indirect excitons in monolayers and double-layer heterostructures of Xenes: silicene, germanene, and stanene. The exciton eigenenergies, optical transition energy, oscillator strength, and absorption coefficient are calculated [1]. An external electric field tunes the eigenenergies and optical properties of excitons by changing the effective mass of charge carriers. The Schrödinger equation with field-dependent exciton reduced mass is solved by using the Rytova-Keldysh (RK) potential for direct excitons, while both the RK and Coulomb potentials are used for indirect excitons. For indirect excitons, we show that the choice of interaction potential can cause significant changes in the eigenenergies. Finally, our results show that the choice of material parameters has a significant effect on the binding energies and optical properties of direct and indirect excitons. These calculations contribute to the rapidly growing body of research regarding the excitonic and optical properties of this new class of two-dimensional semiconductors.


*This work is supported by U.S. Department of Defense under Grant No. W911NF1810433

3:30PM C12.00006: Emergence of excitonic superfluid at topological-insulator surfaces* YASEN HOU (Presenter), University of California, Davis, RUI WANG, Shanghai Jiao Tong University, RUI XIAO, LUKE MCCLINTOCK, HENRY CLARK TRAVAGLINI, JOHN PAULUS FRANCIA, University of California, Davis, HARRY FETSCH, Harvey Mudd College, ONUR ERTEM, Arizona State University, SERGEY SAVRASOV, University of California, Davis, BAIGENG WANG, Nanjing University, ANTONIO ROSSI, INNA VISHIK, University of California, Davis, ELI ROTENBERG, Lawrence Berkeley National Laboratory, DONG YU, University of California, Davis — Excitons are spin integer particles that were predicted to condense into a coherent quantum state at sufficiently low temperature more than 50 years ago. Nonetheless, transport of exciton condensates is not yet understood and it is unclear whether an exciton condensate is a superfluid or an insulating electronic crystal. Topological insulators (TIs) with massless particles and unique spin textures have been theoretically predicted as a promising platform for achieving exciton condensation. Here we report experimental evidence of excitonic superfluid phase at the surface of three-dimensional (3D) TIs. We unambiguously confirmed that electrons and holes are paired into charge neutral bound states by the electric field independent photocurrent distributions. And we observed a millimetre-long transport distance of these excitons up to 40 K, which strongly suggests dissipationless propagation. The robust macroscopic quantum states achieved with simple device architecture and broadband photoexcitation at relatively high temperature are expected to find novel applications in quantum computations and spintronics.

*This work was supported by National Science Foundation Grant DMR-1838532 and DMR-1710737.

3:42PM C12.00007: Interlayer exciton diffusion in MoSe2/WSe2 heterostructures* JUNHO CHOI (Presenter), WEI-TING HSU, Department of Physics, University of Texas at Austin, TX 78712, United States, LI-SHUAN LU, HUI-YU CHENG, Department of Electrophysics, National Chiao Tung University, Hsinchu 30010, Taiwan, LIUYANG SUN, KHA TRAN, ANDRÉ ZEPEDA, MARSHALL CAMPBELL, MATTHEW STAAB, KAYLEIGH R JONES, Department of Physics, University of Texas at Austin, TX 78712, United States, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute of Material Science, 1-1 Namiki, Tsukuba, Ibaraki 205-0044, Japan, CHIH-KANG SHIH, XIAOQIN (ELAINE) LI, Department of Physics, University of Texas at Austin, TX 78712, United States, WEN-HAO CHANG, Department of Electrophysics, National Chiao Tung University, Hsinchu 30010, Taiwan — Excitons with large binding energy are formed in atomically thin semiconductors because of the insufficient dielectric screening outside of the 2D layers. In a vertical heterostructure consisting of MoSe2 and WSe2 monolayers, the type-II band alignment leads to the rapid transfer of electron to the MoSe2 layer and hole to the WSe2 layer, forming interlayer excitons with drastically different properties than excitons confined within one monolayer. We investigate the interlayer exciton diffusion in MoSe2/WSe2 heterostructures. We compare a mechanically stacked heterostructure with hexagonal boron nitride (hBN) encapsulation and one grown by chemical vapor deposition (CVD). Spatially and time-resolved photoluminescence measurements are performed at low-temperature. Interlayer exciton diffusion length and coefficient are extracted in both heterostructures and found to be rather different.

*We gratefully acknowledge funding from NSF MRSEC program DMR-1720595, NSF DMR-1808042, EFMA-1542747, and Welch Foundation F-1662.
Valley Selective Optical Routing in Hyperbolic Metamaterials

SRIRAM GUDDALA (Presenter), MANDEEP KHATONIAR, NICHOLAS YAMA, VINOD M MENON, Department of Physics, City College of New York, New York-10031, USA. — At the monolayer limit, the 2D transition metal dichalcogenides materials such as WS$_2$, WSe$_2$, and MoS$_2$ etc., are endowed with direct bandgap and high binding energy excitons at individually addressable two degenerate valleys in momentum space at K and K’ points in the first Brillouin zone. In recent years, there has been growing interest in achieving control over the selective valley excitation/emission by means of optical, electrical, and magnetic fields and explore this valley degree of freedom as an efficient way of data transfer, computing and storage technology, called valleytronics. We describe and experimentally demonstrate the optical control on selective valley excitation and emission routing through spatially confined subwavelength electromagnetic modes in an anisotropic metamaterial with hyperbolic dispersion. The directionality of selective valley exciton emission depends on the handedness of that valley’s circular polarization emission. The demonstrated capability of our hyperbolic metamaterial -TMD hybrid system is free from precise nanoscale structural dimensions and most importantly broadband response and shows great potential to develop prototype devices such as valley filters or valley-based qubits for quantum computing/communications.

*ARO, NSF-DMR, and DARPA.

Non-adiabatic effects in exciton-mediated Raman scattering from first principles

SVEN REICHARDT (Presenter), Department of Materials, University of Oxford, LUDGER WIRTZ, Physics and Materials Science Research Unit, University of Luxembourg, ANDREA MARINI, Division of Ultrafast Processes in Materials (FLASHit), Istituto di Struttura della Materia of the National Research Council Italy — We present a fully quantum mechanical, _ab initio_ approach for the calculation of optical properties of solids, in particular resonant Raman scattering. Starting from the fundamental observable, we derive a fully general description of light scattering by matter beyond the commonly used semi-classical approximations for the electron-nuclei interaction. Our approach captures both direct and phonon-mediated light absorption as well as inelastic light scattering.

We provide a concrete computational recipe for the calculation of resonant Raman intensities beyond the approximation of static (adiabatic) phonons and including excitonic effects. Applying our approach to several materials, we discuss the effects of non-adiabaticity on the Raman intensity. The latter are not captured by frozen-phonon-based approaches [1,2] and so far could only be described by neglecting excitonic effects [3,4], which, however, are predominant in low-dimensional semi-conductors.

References:

Probing the nonlinear response of strongly coupled plasmon-WSe$_2$ system

CHENTAO LI (Presenter), HAYK HARUTYUNYAN, XIN LU, AJIT SRIVASTAVA, Emory University — Two-dimentional transition metal dichalcogenides (TMDs) have recently emerged as a class of material that shows a great potential for strong light-matter interaction at the nanoscale. Signatures of strong coupling, such as Rabi-splitting in the linear optical spectra, have been observed by placing TMDs in optical nanocavities. Typically, plasmonic nanocavities and nanostructures are used to reach the appropriate parameters for the observation of strong coupling regime. However, most studies utilize dark field (DF) scattering experiments rather than photoluminescence (PL) for the demonstration of strong coupling phenomena, whereas the observation of PL splitting in this system has rarely been reported. Thus, more convincing evidences of strong coupling are still needed.

We have successfully assembled gold nanoparticles and TMD materials (WSe$_2$) to investigate the strong light-matter interaction in TMDs. Interestingly, our simulation based on a two-oscillator toy model predicts that second harmonic generation will show a pronounced spectral splitting in this regime. Thus, we suggest that probing of these systems in the nonlinear regime may give clearer evidence of strong coupling that could not be observed in the linear measurements.

*This work is supported by NSF EFMA – 1741691.
**4:30PM C12.00011: Probing the phonon scattering in the strong light-matter coupling regime**

XIAOZE LIU (Presenter), JUN YI, SUI YANG, University of California, Berkeley, ERH-CHEN LIN, National Tsing-Hua University, YUE-JIAO ZHANG, JIAN-FENG LI, Xiamen University, YUAN WANG, University of California, Berkeley, YI-HSIEN LEE, National Tsing-Hua University, ZHONG-QUN TIAN, Xiamen University, XIANG ZHANG, University of California, Berkeley — The strong light-matter coupling is the core of cavity quantum electrodynamics (CQED), which leads to discoveries of fascinating phenomena in solid state system such as Bose-Einstein condensation and photon blockade. Indirect evidence indicates non-fluorescence processes such as phonon scattering are critical to these phenomena. However, the understanding of such processes remains elusive due to their non-radiative nature smeared by the overwhelming fluorescence in cavities. Here we directly probe phonon scattering based on Raman spectroscopy in the strong coupling regime in a plasmonic cavity embedded with a monolayer MoS2. The studied non-fluorescence process is significantly modified by the hybrid properties of the newly formed half-light half-matter quasiparticles, i.e., polaritons. For the first time, we observe nonlinearly enhanced valley-dependent phonon modes, involved with stimulated lattice vibrations and inter-valley scatterings. This work provides a new perspective to investigate fundamental quantum processes in the strong coupling regime.

**4:42PM C12.00012: Ultra-long wavelength Dirac plasmons in graphene capacitors**

DAVID MELE (Presenter), HOLGER GRAEF, MICHAEL ROSTICHER, Laboratoire Pierre Aigrain, CNRS - Ecole Normale Supérieure, LUCA BANSZERUS, CHRISTOPH STAMPFER, JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, ERWANN BOCQUILLON, GWENDAL FÊVE, JEAN-MARC BERROIR, Laboratoire Pierre Aigrain, CNRS - Ecole Normale Supérieure, EDWIN HANG TONG TEO, School of Electrical and Electronic Engineering, Nanyang Technological University, BERNARD PLAÇAIS, Laboratoire Pierre Aigrain, CNRS - Ecole Normale Supérieure — Graphene is a recognized 2D platform for plasmonics in the THz and mid-IR domains. These high-energy plasmons couple to the dielectric surface modes, giving rise to hybrid plasmon-polariton excitations. The ultra-long wavelength GHz range addresses the low energy end of the spectrum, where Dirac plasmons are damped by ohmic losses but essentially decoupled from environment. Using hBN encapsulated graphene [1], we demonstrate a plasma resonance capacitor [2] showing a quarter-wave plasmon mode, at 40 GHz, with a quality factor Q=2. The resolution of the resonant technique yields precise determinations of the electronic compressibility, kinetic inductance, and mean free-path, in good agreement with theory. The 100µm-long wavelength allows engineering of doping-modulated devices where plasmons are controlled by Klein tunneling. Downscaling for room temperature operation opens up perspectives in microwave detection for wireless communication and sensing [3].


*Funding from the European Union ‘Horizon 2020’ research and innovation programme under grant agreement No.785219 ‘Graphene Core’ and from the ANR-14-CE08-018-05 ‘GoBN’.

**4:54PM C12.00013: Strong coupling in metal-WS2 hybrid system**

JINWEI SHI (Presenter), DAHE LIU, Physics, Beijing Normal University, CHIH-KANG SHIH, Physics, University of Texas at Austin, YI-HSIEN LEE, SHANGJR GWO, National Tsing-Hua University — Metallic particle array as an effective plasmonic cavity has attracted great interest. Coupling between such plasmonic cavity and gain materials have been reported. In this work, we studied two kinds of polaritons in such system. First, we studied the strong coupling between groove localized surface plasmon resonance (LSPR) and lattice surface plasmon polariton in a metallic groove array. We found that the optical response of such system is different from the ordinary weak coupling surface lattice resonance. A giant Rabi splitting of ~440 meV was observed, both angle and pitch tuning. The underlying mechanism is analyzed. Next, we studied the coupling between the metallic grating and the exciton in WS2 monolayer. LSPR was used. The parallel electric field within the groove can provide an effective coupling to the excitons of monolayer WS2. To overcome the problem of angle tuning reported in previous work, we developed a depth chirped grating to realize the resonance tuning. A moderate Rabi splitting of 56 meV was observed. These works demonstrate the potential application in strong coupling devices based on plasmonic cavity.

*NSF of China (11774035, 11674032), and Beijing Cooperative Construction Project.
5:06PM C12.00014: Optical absorption spectra of monolayer transition metal dichalcogenides at high doping levels

MINDA DENG (Presenter), CHUN-LAN WU, Stanford University, ZILIANG YE, Stanford University & University of British Columbia, YI CUI, Stanford University, TONY F HEINZ, Stanford University & SLAC — The absorption spectra of semiconducting transition metal dichalcogenides (TMDCs) at monolayer thickness are dominated by excitonic transitions due to the strong Coulomb interactions associated with the materials’ reduced screening and dimensionality. It has been shown that the excitons in these materials can be tuned electrically by using a Si back gate to achieve carrier density up to several times $10^{12}$ cm$^{-2}$. Here we extend these studies to higher carrier densities through the use of electric double layer gating technique with the ionic solid conductor LaF$_3$ as the electrolyte. In this fashion, we are able to electrostatically gate monolayer WSe$_2$ to a density of a few $10^{13}$ cm$^{-2}$. While earlier investigations showed shifts in exciton (and charged exciton) energies and binding energies, the excitonic absorption features remained relatively strong and distinct. At carrier densities in the $10^{13}$ cm$^{-2}$ range, however, we find that the excitonic absorption features are no longer observable. The progression of the measured absorption spectra with increasing doping density is compatible with the behavior expected for a Mott transition from the excitonic regime to an electron–hole plasma regime, as was previously reported for the case of strong photodoping of TMDC monolayers.

5:18PM C12.00015: Nonperturbative nonlinear effects in the dispersion relations for TE and TM plasmons on two-dimensional materials

VERA ANDREEVA (Presenter), MITCHELL LUSKIN, School of Mathematics, University of Minnesota, DIONISIOS MARGETIS, Department of Mathematics, University of Maryland — We analytically obtain the dispersion relations for transverse-electric (TE) and transverse-magnetic (TM) surface plasmon-polaritons in a nonlinear two-dimensional (2D) conducting material with inversion symmetry lying between two Kerr-type dielectric media. To this end, we use Maxwell’s equations within the quasielectrostatic, weakly dissipative regime. We show that the wavelength and propagation distance of surface plasmons decrease due to the nonlinearity of the surrounding dielectric. In contrast, the effect of the nonlinearity of the 2D material depends on the signs of the real and imaginary parts of the third-order conductivity. Notably, the dispersion relations obtained by naively replacing the permittivity of the dielectric medium by its nonlinear counterpart in the respective dispersion relations of the linear regime are not accurate. We apply our analysis to the case of doped graphene and make predictions for the TM-polarized surface plasmon wavelength and propagation distance.

*We acknowledge support by ARO MURI Award No. W911NF-14-0247 (V.A., M.L., D.M.) and NSF Grant No. DMS-1412769 (D.M.).

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C13 DMP GMAG: 2D Materials (General) -- Magnetic and Thermal Properties

2:30PM C13.00001: Magnetic order in the cleavable van der Waals crystal Fe$_2$GeTe$_2$ *ANDREW MAY (Presenter), Oak Ridge National Laboratory, DMITRY OVCHINNIKOV, University of Washington, QIANG ZHENG, RAPHAEL HERMANN, STUART CALDER, Oak Ridge National Laboratory, BEVIN HUANG, ZAIYAO FEI, University of Washington, YAOHUA LIU, Oak Ridge National Laboratory, XIAODONG XU, University of Washington, MICHAEL A MCGUIRE, Oak Ridge National Laboratory — Van der Waals bonded materials with intrinsic magnetism play a key component in several aspects of present-day materials physics. In this study, we report the structure and properties of Fe$_{5-x}$GeTe$_2$. The average crystal structure obtained from single crystal x-ray diffraction contains disorder associated with occupation of Fe/Ge split sites. Atomic-resolution STEM has been utilized to inspect the local crystal structure and has revealed local ordering. The magnetism has been characterized using magnetization measurements on single crystals, as well as powder neutron diffraction and Mössbauer spectroscopy on a polycrystalline sample. The crystals have been successfully exfoliated, and Hall effect measurements on nanoflakes confirm magnetic order near room temperature. These results demonstrate that Fe$_{5-x}$GeTe$_2$ will be a promising material for incorporation into van der Waals heterostructures and devices.

*This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
2:42PM C13.00002: Single Crystal Neutron Diffuse Scattering on Nonstoichiometric Quasi-2D Ferromagnetic Fe₃₋ₓGeTe₂*  
YAOHUA LIU (Presenter), STUART CALDER, Neutron Scattering Division, Oak Ridge National Laboratory, ANDREW MAY, Materials Science and Technology Division, Oak Ridge National Laboratory, YAWEI HUI, Computer Science and Mathematics Division, Oak Ridge National Laboratory — Two-dimensional (2D) van der Waals magnetic materials hold great potential for spintronics. Particularly, the recent discovery of gate-tunable room-temperature ferromagnetism in atomically thin Fe₃₋ₓGeTe₂ makes it a promising candidate toward voltage-controlled low-dispersion devices. However, the magnetic properties of Fe₃₋ₓGeTe₂ show a considerable dependence on the stoichiometry. To better understand the role of the Fe-deficiency, we have performed single crystal neutron diffuse scattering at the CORELLI spectrometer at the Spallation Neutron Source to investigate the local structure. The nonstoichiometric sample shows highly structured diffuse scattering patterns in the HK plane with a weak q dependence along the L direction. As revealed from the cross-correlation analysis with the statistical chopper, the observed diffuse scattering is mainly of a static origin. The L dependence can be partially attributed to the stacking faults. To produce the HK plane diffuse scattering features, we have performed Monte Carlo simulations to model the short-range order of the Fe vacancies and considered the lattice relaxation around the Fe vacancies.

*This research used resources at Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

2:54PM C13.00003: Skyrmions in the Moire of van der Waals 2D Magnets*  
QING TONG (Presenter), Physics and Electronics, Hunan University, FEI LIU, Physics, The University of Hong Kong, JIANG XIAO, Physics, Fudan University, WANG YAO, Physics, The University of Hong Kong — We explore the skyrmion formation and control possibilities in 2D magnets from the ubiquitous moiré pattern in vdW heterostructures. Using the example of a ferromagnetic monolayer on an antiferromagnetic substrate, we demonstrate a new origin of skyrmions in the 2D magnets, from the lateral modulation of interlayer magnetic coupling by the locally different atomic registries in moiré. The moiré skyrmions are doubly degenerate with opposite topological charge, and trapped at an ordered array of sites with the moiré periodicity that can be dramatically tuned by strain and interlayer translation. At relatively strong interlayer coupling, the ground states are skyrmion lattices, where magnetic field can switch the skyrmion vorticity and location in the moiré. At weak interlayer coupling limit, we find metastable skyrmion excitations on the ferromagnetic ground state that can be deterministically moved between the ordered moiré trapping sites by current pulses.


*The work is supported by the Croucher Foundation, the Research Grants Council and University Grants Committee (17303518P, AoE/P-04/08) of Hong Kong SAR.

3:06PM C13.00004: Design and discovery of van der Waals magnets toward room temperature devices* [Invited]  
FAZEL FALLAH TAFTI (Presenter), MYKOLA ABRAMCHUK, KENNETH BURCH, GAVIN B OSTERHOUDT, SAMANTHA JASZEWSKI, YIPING WANG, Boston College — Chromium trihalides were recognized as magnetic Van der Waals materials since 1920s. They were studied vigorously during 1950s to 70s when fundamental theories of magnetic ordering, exchange interactions, and magnetic anisotropy were developing. Recent advances in device fabrication and magneto-optical measurements lead to the discovery of 2D magnetic ordering in CrI₃ monolayers with great potential for atomically thin devices. CrCl₃, CrBr₃, and CrI₃ are stable in air and easy to exfoliate, therefore ideal for applications. Here, we present the chemical pathway to tune all the physical properties of these materials by mixing different halide species. We use CrCl₃₋ₓBrₓ as a benchmark to show the design principles of mixed halides where isovalent substitution of Br for Cl occurs during a chemical vapor transport process. Remarkably, all physical properties including the van der Waals gap, the magnetic ordering temperature, the ferromagnetic exchange coupling, the optical gap, and the magnetic anisotropy are tuned linearly as a function of x. Our results demonstrate unprecedented control over the magneto-optical properties of CrCl₃₋ₓBrₓ required for a range of applications from spintronics to biomedical industries.

*The authors acknowledge funding by the National Science Foundation under awards DMR-1708929 and DMR-1709987.
Transition metal dichalcogenides (TMDs) are atomically thin semiconductors of the type MX$_2$ with M being a transition metal (such as Mo, W etc.) and X being a chalcogen atom (such as S, Se and Te). TMDs have recently attracted considerable attention because of their novel electronic and optical properties. Little attention is given to the synthesis and characterization of chromium dichalcogenides. Here, we introduce a new method for obtaining Cr$_2$S$_3$ via vapor-solid growth mechanism. Polycrystalline Cr-sulfide sample was synthesized by heating a mixture of Cr and S in a sealed and evacuated silica tube (<10$^{-5}$ mbar) at 500°C for 24 hours and then 800°C for another four days. At 800 °C, with the help of Ar as carrier gas, we deposited Cr$_2$S$_3$ on sapphire samples. AFM images showed only quasi-two-dimensional triangular islands on otherwise flat samples. The phase and structural analysis of as synthesized powder were examined by a powder X-ray diffractometer. Some of the XRD peaks match well with the calculated XRD data for Cr$_2$S$_3$ confirming the quasi-2D nature of the islands observed in the AFM images.

This work was supported by the following grant: NDEPSCoR #UND0021231.

Integrating two-dimensional(2D) magnet with topological insulator is an exciting topic. Other than the possible proximity induced magnetic ordering inside topological insulator, the 2D magnet/ topological insulator heterostructure can also lead to more efficient spin orbit torque switching, or the formation of magnetic skyrmions. The recent discovery of room temperature ferromagnetic ordering in 2D material MnSe$_2$ and VSe$_2$ further brings more potential in such heterostructure systems. In this talk, we report the synthesis and characterization of 2D magnet MnSe$_2$ and VSe$_2$ on topological insulator Bi$_2$Se$_3$. Monolayer and few layers of MnSe$_2$ and VSe$_2$ are grown on Bi$_2$Se$_3$ with molecular beam epitaxy. The material quality and magnetic property are characterized with RHEED, XRD, XPS, and SQUID. Furthermore, the 2D magnet/ topological insulator heterostructures are characterized with STM to study their atomic structure and local electronic properties. Finally, recent progress of measuring the local magnetic properties of these films with spin-polarized STM will also be discussed.

This project is mainly supported by the US Department of Energy (Grant No. DE-SC0018172).

Synthesis, Raman scattering and transport studies of quasi-two-dimensional magnetic Cr$_2$S$_3$ nanoplates

The recent discovery of intrinsic ferromagnetism in atomically thin crystals has sparked a growing effort in synthesizing two-dimensional magnetic materials for new spintronic applications. In this work, we synthesized quasi-two-dimensional Cr$_2$S$_3$ nanoplates via a facile sulfurization approach, in which Cr metal was annealed in sulfur atmosphere. Depending on the thickness of Cr layers, the Cr$_2$S$_3$ nanoplates were grown either epitaxially or non-epitaxially (i.e. randomly oriented) on the sapphire substrates. Raman scattering studies suggest that both types of nanoplates have a rhombohedral R3 structural phase, which in its bulk form shows weak ferromagnetism below a metal-insulator transition (MIT) temperature (~120K). Density-functional calculations clearly identified most of the Raman-active peaks and their vibrational patterns. The epitaxially grown nanoplates exhibit an enhanced MIT up to ~260 K, while the non-epitaxial sample shows an insulating behavior that can be described by the variable-range-hopping model.

Work supported in part by NSF DMR-1506460, CAREER Grant No. DMR- 1760668, and NSF DMR 1709781
4:18PM C13.00008: Electron Spin Resonance of Magnetic Two-Dimensional Covalent Organic Frameworks* ABIGAIL FIRM (Presenter), VALERIE A. KUEHL, JOSEPH MURPHY, JOHN O. HOBERG, WILLIAM RICE, University of Wyoming — Two-dimensional (2D) materials have generated significant interest because of their unique electrical, optical, and magnetic single-layer behaviors. However, the inability to add electrical or magnetic dopants to a substantial set of 2D materials hinders their ability to be incorporated into device architectures. Here, we synthesize 2D covalent organic frameworks (COFs) that have a lattice of nanopores, which we are able to synthetically fill with magnetic ions (Mn$^{2+}$) that are hexagonally arranged. We use a host of characterization techniques, such as x-ray diffraction, TEM, NMR, and FTIR, to demonstrate that our COFs are ordered, nanoporous, and 2D. Magnetic ion filling is empirically shown through electron spin resonance measurements. Unlike the unfilled COFs, which have a single peak at $g=2.0$, the Mn-filled COFs show a hyperfine-split, sextet of peaks with a spin relaxation time of ~0.5 ns and a 19 G exchange splitting. The ability to chemically change the nanopore spacing and the inter-ion distance, combined with our confirmation of the hexagonal Mn$^{2+}$ ion arrangement, suggests the possibility of using these 2D COFs for potential quantum spin liquids or in magneto-optical devices.

*We acknowledge support from the UW School of Energy Resources and the A&S Dean’s Office.

4:30PM C13.00009: Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface x-ray scattering* I-CHENG TUNG, Argonne National Laboratory, ARAVIND KRISHNAMOORTHY, University of Southern California, SRIDHAR SADASIVAM, HUA ZHOU, QI ZHANG, Argonne National Laboratory, KYLE SEYLER, GENEVIEVE CLARK, University of Washington, Seattle, EHREN MANNEBACH, CLARA M NYBY, FRIEDERIKE ERNST, Stanford University, DILING ZHU, JAMES M GLOSSNIA, MICHAEL E KÖZINA, SANGHOON SONG, SILKE NELSON, SLAC National Accelerator Laboratory, HIROYUKI KUMAZOE, FUYUKI SHIMOJO, Kumamoto University, RAJIV KALIA, PRIYA VASHISHTA, University of Southern California, PIERRE DARANCET, Argonne National Laboratory, TONY F HEINZ, Stanford University, AIICHIRO NAKANO, University of Southern California, XIAODONG XU, University of Washington, Seattle, AARON M LINDENBERG, Stanford University, HAIDAN WEN (Presenter), Argonne National Laboratory — The direct structural characterization of nonequilibrium processes within a monolayer crystal remains a challenge due to significantly reduced scattering volume. In this work, we demonstrate femtosecond surface x-ray diffraction in combination with crystallographic model-refinement calculations to measure the ultrafast structural dynamics of monolayer WSe$_2$ crystals on a substrate. We found the absorbed photon energy is preferably coupled to the in-plane lattice vibrations within 2 picoseconds while the out-of-plane lattice vibration amplitude remains unchanged during the first 10 picoseconds. The model-assisted fitting suggests an asymmetric intralayer spacing change upon excitation. The demonstrated methods unlock the benefit of x-ray scattering to quantitatively measure ultrafast structural dynamics in atomically thin materials and across interfaces.


4:42PM C13.00010: Vibrational Properties of van der Waals Materials SABINE NEAL (Presenter), Department of Chemistry, University of Tennessee, HEUNG SIK KIM, Department of Physics and Astronomy, Rutgers University, AMANDA HAGLUND, Department of Materials Science and Engineering, University of Tennessee, KEVIN SMITH, Department of Chemistry, University of Tennessee, MICHAEL CROCKER MARTIN, HANS BECHTEL, Lawrence Berkeley National Laboratory, G LAWRENCE CARR, Brookhaven National Laboratory, DAVID VANDERBILT, KRISTJAN HAULE, Department of Physics and Astronomy, Rutgers University, DAVID GEORGE MANDRUS, Department of Materials Science and Engineering, University of Tennessee, JANICE LYNN MUSFELDT, Department of Physics and Astronomy, Department of Chemistry, University of Tennessee — Single sheet van der Waals materials have become increasingly important over the last decade because of their broad range of applications in areas such as catalysis, energy storage, and microelectronics. These single/few layer constructs have been thoroughly analyzed by Raman spectroscopy but all infrared spectroscopy to date has been unsuccessful due to the inability to overcome the diffraction limit. The investigation of characteristic ungerade infrared modes is, however, crucially important in understanding material functionality. Synchrotron infrared nanospectroscopy, a fusion of near-field optical microscopy with high brightness infrared synchrotron radiation, has overcome this fight for photons and enabled a better understanding of size-induced effects, including quantum confinement and symmetry breaking which lead to distinctive chemical, electronic, optical, and thermal properties that are quite different from the single crystal. This approach will be illustrated with the complex magnetic semiconductor, MnPS$_3$. 

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4:54PM C13.00011: Phonons and thermal transport in hafnium disulphide (HfS$_2$)*  JIE PENG (Presenter), PETER CHUNG, Mechanical Engineering, University of Maryland, College Park, SINA NAJMAEI, MADAN DUBEY, Sensors and Electron Devices Directorate, United States Army Research Laboratory — Recent studies have shown that hafnium disulphide (HfS$_2$) exhibits many desirable properties such as high room-temperature mobility, finite bandgap, and high on-off current ratio that are favored by electronic devices. Despite the large number of existing studies of HfS$_2$, thermal transport properties have not been fully explored and the related question of how temperature affects the thermal properties remain unanswered. In this work, we report anharmonic phonons in HfS$_2$ via first-principle calculations. Key calculated properties include the fully anisotropic Gruneissen parameters, specific heats, coefficients of thermal expansion, and anisotropic thermal conductivity. The study of thermal expansion found interesting behaviors that suggest the structure of HfS$_2$ gives rise to negative Gruneissen parameters where the frequency or energy of a mode can decrease with applied pressure. The associated phonon lifetimes and specific heats also are used to examine mode contributions to the anisotropic thermal conductivity. Our results also confirm that the overall out-of-plane thermal conductivity of HfS$_2$ is small, on the order of 1 W/mK, suggesting the promise of HfS$_2$ application to thermoelectric devices.

*ARO(#W911NF-14-1-0330), ARL-CISD and SEDD Center for Engineering Concepts Development

5:06PM C13.00012: Anisotropic thermal conductivity of printed films made of 2D-materials based inks  MIZANUR RAHMAN (Presenter), Department of Physics and Astronomy, York University, Toronto, ON, Canada, KHALED PARVEZ, CHAOCHAO DUN, CINZIA CASIRAGHI, School of Chemistry, University of Manchester, United Kingdom, SIMONE PISANA, Department of Electrical Engineering and Computer Science, York University, Toronto, ON, Canada — Graphene and other 2-dimensional (2D) materials are the subject of intense research due to their distinct properties, particularly for electronic and optoelectronic applications. Solution-processed 2D materials can accelerate the progress even further due to their compatibility with flexible substrates, large scale and low-cost device fabrication. In addition, printed films of such inks, could have potential use in thermal and thermoelectric applications. However, very little is known about the thermal properties of 2D-materials based inks due to the challenge and complexity associated with measuring their thermal properties, which are highly anisotropic. To develop applications based on the thermal properties of 2D-materials based inks, it is of fundamental importance to understand the relation between structure and property, and to determine how electron and heat transport relate in 2D materials.

Here, we present the electrical conductivity and in-plane and out-of-plane thermal conductivity of graphene and other 2D-materials thin films, produced by ink-jet printing of water-based 2D-materials inks. Thermal anisotropies of 40:1 are observed together with ultra-low cross-plane thermal conductivity well below 1 W/mK.

5:18PM C13.00013: Temperature Dependent Phonons of Transition- Metal Dichalcogenides Calculated from Spectral Energy Density: Thermal Lattice Conductivity as an Application*  ARASH MOBARAKI, Bilkent University, CEM SEVIK, Eskisehir Technical University, DENIZ ÇAKIR, Department of Physics and Astrophysics, University of North Dakota, OGUZ GULSEREN (Presenter), Bilkent University — Predicting the mechanical and thermal properties of quasi two dimensional transition metal dichalcogenides (TMDs) is an essential task necessary for their implementation in device applications. Although, rigorous density functional theory (DFT) based calculations are able to predict mechanical and electronic properties, mostly they are limited to zero temperature. Classical molecular dynamics (MD) facilitates the investigation of temperature dependent properties, but its performance is highly depend on potential used for defining interactions between atoms. In this study, we calculated temperature dependent phonon properties of single layer TMDs, namely MoS$_2$, MoSe$_2$, WS$_2$, and WSe$_2$, by utilizing Stillinger-Weber (SW) type potentials with optimized sets of parameters with respect to the first principle results. The phonon lifetimes and contribution of each phonon mode in thermal conductivities in monolayer MoS$_2$, MoSe$_2$, WS$_2$, and WSe$_2$ are systematically investigated by means of spectral energy density (SED) method. The obtained results from this approach are in good agreement with previously available results from Green-Kubo (GK) method.

*We acknowledge the support from The Scientific and Technological Research Council of Turkey, TUBITAK, (Grant No. 115F024).

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C14 DMP: 2D Materials (Metals, Superconductors, and Correlated Materials) -- Superconductivity  BCEC 153C - Eric Spanont, University of California, Santa Barbara - Tag(s): Focus
Probing the Superfluid Density and the Superconducting Gaps under Pressure in 2H-NbSe2

ZURAB GUGUCHIA (Presenter), Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, FABIAN VON ROHR, Department of Chemistry, University of Zürich, ORAIN JEAN CHISTOPHE, RUSTEM KHASANOV, ALEX AMATO, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, ABHAY PASUPATHY, Department of Physics, Columbia University, ZAHID HASAN, Laboratory for Topological Quantum Matter & Advanced Spectroscopy, Princeton University, HUBERTUS LUETKENS, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, YASUTOMO J UEMURA, Department of Physics, Columbia University — We report on high-pressure (pmax = 2.1 GPa) muon spin rotation experiments probing the temperature-dependent magnetic penetration depth λ(T) in the layered superconductor 2H-NbSe2. Upon increasing the pressure, we observe a substantial increase of the superfluid density nS/m* ∼ 1/λ2, which we find to scale linearly with Tc. This linear scaling is considered a hallmark feature of unconventional superconductivity, especially in high-temperature cuprate superconductors. Our current results, along with our earlier findings on 1T'-MoTe2 [1], demonstrate that this linear relation is also an intrinsic property of the superconductivity in transition metal dichalcogenides, whereas the ratio Tc/TF is approximately a factor of 20 lower than the ratio observed in hole-doped cuprates. We, furthermore, find that the values of the superconducting gaps are insensitive to the suppression of the quasi-two-dimensional CDW state, indicating that the CDW ordering and the superconductivity in 2H-NbSe2 are independent of each other.


Exponential decrease of the collective vortex state energy with layer number in 2H-NbSe2

AVISHAI BENYAMINI (Presenter), EVAN TELFORD, DA WANG, DANTE KENNES, KENJI WATANABE, Columbia University, TAKASHI TANIGUCHI, ANDREW MILLIS, National Institute of Materials Science, JAMES HONE, CORY R DEAN, ABHAY PASUPATHY, Columbia University — In the last years, a new generation of superconductors truly in the two-dimensional limit has been discovered in van der Waals materials. Recently, it has been shown that these type-II SCs can be extremely sensitive to external perturbation which pushes the system into a non-equilibrium steady state exhibiting metallic-like behavior [1]. Here we study the equilibrium and non-equilibrium phase diagrams of few-layered 2H-NbSe2 with minimal external perturbations. At finite magnetic field we observe a current-induced crossover to a non-activated metallic-like regime with a critical current that reduces with layer number. We discuss our results both phenomenologically and in the vortex picture which we compare with time-dependent Ginzburg-Landau simulations. In the vortex-picture we attribute the crossover to a transition from a pinned to unpinned vortex liquid. Finally, we demonstrate that by spreading non-uniform currents, we stabilize different vortex steady states in different spatial locations, potentially leading to novel interfaces.


Strongly enhanced Andreev reflection in ultra-transparent NbSe2/ bilayer graphene junctions

JING LI (Presenter), National High Magnetic Field Laboratory, Los Alamos National Lab, HAILONG FU, Department of Physics, The Pennsylvania State University, HAN-BING LENG, Department of Physics, Huazhong University of Science and Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, CHAOXING LIU, Department of Physics, The Pennsylvania State University, XIN LIU, Department of Physics, Huazhong University of Science and Technology, JUN ZHU, Department of Physics, The Pennsylvania State University — Van der Waals (vdW) layered materials with diverse properties provide an alternative route to construct future generations of miniaturized electronic devices. The prospect of constructing superconducting circuits from all vdW materials is attractive from many different viewpoints. Making transparent superconductor to normal conductor (S-N) junctions is a critical step in this endeavor. Here we present measurement and simulations of Andreev reflection (AR) in ultra-transparent NbSe2/ bilayer graphene (BLG) S-N junctions constructed via vdW stacking. The resistance across the junction is as low as 13 Ω, indicating a highly transparent NbSe2/ BLG interface. In these devices, the proximity effect penetrates to the BLG side for at least 500 nm. We observe strongly enhanced AR in the differential conductance measurement across the junction. The zero-bias conductance peak reaches up to 1.7 times the normal value. We present a comprehensive study of the AR by systematically varying the carrier density and temperature in different devices. A model is constructed to capture the rich features of the experimental data. Important factors include the spatial decay of the superconducting gap, the effect of the carrier density profile near the interface and the interface transparency.
3:06PM C14.00004: Dynamically-created Josephson Junctions in thin layers of NbSe2

STEVEN TRAN (Presenter), University of Maryland, College Park — Niobium Diselenide (NbSe2) is a member of the transition metal dichalcogenides (TMDs) family which displays superconducting properties and is host to charge density waves (CDWs) down to its monolayer limit. These properties alongside its hexagonal structure make it an interesting material to study physics within its two dimensional limit. Here, we report on fabrication and low-temperature transport measurements of atomically-thin layers of NbSe2 in four-terminal configurations. We observe the formation of phase slip lines across our NbSe2 sheets which appear as non-zero resistances in the superconducting state. The formation of the phase slip lines dynamically creates Josephson junctions (JJs). We interact with these dynamically-created JJs through the application of RF and magnetic fields. Interestingly, we observe a deviation from the conventional behavior of JJs in the presence of RF and a skewed Fraunhofer pattern in the presence of a magnetic field. We model our observations in the presence of RF by assuming a coupling of a JJ to a CDW. We found that the dynamics of the CDW influence the behavior of the JJ to produce results that qualitatively agree with our experiment.

3:18PM C14.00005: Thinning-Induced Metastable Superconductivity in a Correlated 2D Material: 1T-IrTe2

MASARO YOSHIDA (Presenter), RIKEN Center for Emergent Matter Science, KAZUTAKA KUDO, MINORU NOHARA, Research Institute for Interdisciplinary Science, Okayama University, YOSHIHIRO IWASA, Department of Applied Physics, The University of Tokyo — Recently, reduced thickness was found to dramatically impact not only the static electronic structure (e.g. graphene, MoS2), but also the dynamic ordering kinetics (e.g. 1T-TaS2) [1]. The ordering kinetics of first-order phase transitions becomes significantly slowed with decreasing thickness, and metastable supercooled states can be realized by thinning alone. We therefore focus on layered iridium ditelluride (IrTe2), a charge-ordering system that is transformed into a superconductor by suppressing its first-order transition. Here, we discovered a persistent superconducting zero-resistance state in mechanically-exfoliated IrTe2 thin flakes [2]. The maximum superconducting critical temperature was identical to that of the bulk crystal which is chemically optimized, and the emergent superconductivity was revealed to have a metastable nature. The discovered robust metastable superconductivity suggests that 2D material is a new platform to induce, control, and functionalize metastable electronic states that are inaccessible in bulk crystals. [1. M. Yoshida et al. Sci. Adv. 1, e1500606 (2015); 2. M. Yoshida et al., Nano Lett. 18, 3113 (2018)]

3:30PM C14.00006: Dynamic phase diagram at zero magnetic field in 2D superconducting MoS2

YU SAITO (Presenter), University of California, Santa Barbara — Recent discoveries of two-dimensional (2D) crystalline superconductors [1] have led to clarifications of various intrinsic nature in magnetic fields. For example, 2D crystalline superconductors with weak pinning are very fragile against out-of-plane magnetic fields, and thus show a quantum metallic state due to quantum fluctuations [2] (though this phenomenon is still under debate [3]). However, there has been no report for how the BKT state at zero magnetic field evolves into the normal state through the dynamic states with increasing current in such systems. In this talk, we report on transport properties at zero magnetic field in ion-gated MoS2 as a function of current and temperature. We show a clear BKT transition and anomalous kinks observed in resistance-temperature and current-voltage curves, and discuss the dynamic phase diagram based on these data, which contains a variety of current-induced nonequilibrium states originating from not only thermal but also quantum dissociation of vortices and antivortices.


3:42PM C14.00007: Superconductivity in WTe2

JOSHUA FOLK (Presenter), University of British Columbia — tbd

4:18PM C14.00008: Quantum and classical vortex ratchets in a trigonal 2D superconductor

YUKI ITAHASHI (Presenter), YU SAITO, TOSHIYA IDEUE, Department of Applied Physics, University of Tokyo, TSUTOMU NOJIMA, Tohoku University, YOSHIHIRO IWASA, University of Tokyo — One of the unique features of recently emerging 2D superconductors is the quantum metallic state, which is a temperature-independent finite resistive state that appears once finite magnetic field is switched on [1, 2]. This quantum metallic state exhibits a sharp contrast with the conventional superconductor-insulator transition in conventional 2D systems, where the metallic state appears only at a single critical point. To investigate the vortex dynamics which governs the resistance in the quantum metallic state, we have investigated the nonreciprocal transport in gated MoS2, an archetypal noncentrosymmetric 2D superconductor with trigonal symmetry. We found that the second harmonic resistance $R_{xx}^{2\omega}$ appears when the vortex motion is controlled by the classical vortex flow, while $R_{xx}^{2\omega}$ is substantially suppressed when the vortex motion is in quantum creep region. The present result indicates that the trigonal 2D superconductor is a new model system for investigation of quantum and classical ratchets.

4:30PM C14.00009: Superconductivity in TaSe₂ epitaxial thin films  

YUKI TANAKA (Presenter), HIDEKI MATSUOKA, MASAKI NAKANO, YOSHIHIRO IWASA, University of Tokyo — Transition metal dichalcogenides (TMDs) draw much attention because of their intriguing properties emerging at two-dimensional (2D) limit. Nowadays, some groups have succeeded in exfoliation of metallic TMDs such as NbSe₂ and TaS₂ down to a monolayer limit, unveiling new aspects of 2D physical properties. One remarkable example is unconventional superconductivity achieved by combination of large spin-orbit coupling and broken inversion symmetry, where spin-momentum-locked Cooper pairs play an important role in their superconducting states. Another unique feature is the relationship between superconductivity and charge-density wave (CDW), which has been discussed both in NbSe₂ and TaS₂. In this work, we focus on TaSe₂, which has also been known to have similar electronic structure and exhibit both superconductivity and CDW in its bulk form. There is one paper reporting electronic structure of monolayer TaSe₂ [1], but electrical transport properties of TaSe₂ ultrathin films have not been investigated so far. In this presentation, we report on fabrication of high-quality TaSe₂ thin films by molecular beam epitaxy, and show their transport properties with reduced dimensions.


4:42PM C14.00010: Sign reversing Hall effect in atomically thin high temperature superconductors  

SHU YANG FRANK ZHAO (Presenter), NICOLA POCCIA, MARGARET G. PANETTA, CYNDIA YU, JEDEDIAH W. JOHNSON, HYOBIN YOO, Harvard University, RUIDIAN ZHONG, GENDA GU, Brookhaven National Laboratories, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, SVETLANA POSTOLOVA, Institute for Physics of Microstructures, VALERII VINOKUR, Argonne National Laboratory, PHILIP KIM, Harvard University — We fabricate van der Waals heterostructure devices using few unit cell thick Bi₂Sr₂CaCu₂O₈₊δ for magnetotransport measurements. The superconducting transition temperature and carrier density in atomically thin samples can be maintained close to that of the bulk samples. As in the bulk sample, the sign of the Hall conductivity is found to be opposite to the normal state near the transition temperature but with a drastic enlargement of the region of Hall sign reversal in the temperature-magnetic field phase diagram as the thickness of samples decreases. Quantitative analysis of the Hall sign reversal based on the excess charge density in the vortex core and superconducting fluctuations suggests a renormalized superconducting gap in atomically thin samples at the two-dimensional limit. Preprint available at arXiv:1809.06944.

4:54PM C14.00011: Spatially Resolved Electronic Structure of Bi₂Sr₂₋ₓLaₓCuO₆₊δ in the Two-dimensional Limit  

HENGSHENG LUO (Presenter), LIGUO MA, PENG CAI, Physics Department, Fudan University, DONGJOON SONG, National Institute of Advanced Industrial Science and Technology, RUIDIAN ZHONG, Brookhaven National Laboratory, JIAN SHEN, Physics Department, Fudan University, GENDA GU, Brookhaven National Laboratory, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, XIANHUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Physics Department, Fudan University — Dimensionality plays a fundamental role in high-temperature superconductivity; all high-temperature superconductors adopt a layered crystal structure, and much of high-temperature superconductor theory is based on purely two-dimensional (2D) models. Here we exfoliate Bi₂Sr₂₋ₓLaₓCuO₆₊δ (referred to as La-Bi₂2201) single crystals down to monolayers (half unit cell) at liquid nitrogen temperature under ultra-high vacuum. A monolayer La-Bi₂2201 contains only a single layer of CuO₂ plane, and therefore represents a cuprate superconductor in the ultimate 2D limit. We study the electronic structure of monolayer La-Bi₂2201 at atomic scale using scanning tunnelling microscopy and spectroscopy.

5:06PM C14.00012: Visualizing the electronic structure of monolayer Bi₂Sr₂CaCu₂O₈₊δ  

LIGUO MA (Presenter), YIJUN YU, PENG CAI, Physics Department, Fudan University, RUIDIAN ZHONG, Brookhaven National Laboratory, CUN YE, JIAN SHEN, Physics Department, Fudan University, GENDA GU, Brookhaven National Laboratory, XIANHUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Physics Department, Fudan University — Although high-temperature superconductors are a complex and diverse family of materials, they all adopt a layered crystal structure, in which two-dimensional lattices stack together to form the three-dimensional bulk. This curious fact begs the question: does high-temperature superconductivity (HTS) exist in an isolated monolayer, and if so, is the two-dimensional HTS—and various other correlated phenomena related to HTS—different from its three-dimensional counterpart? The answer to these questions may provide important insights on the role of dimensionality in HTS. Here, we fabricate atomically thin cuprate Bi₂Sr₂CaCu₂O₈₊δ that retains HTS down to monolayer (i.e. half unit cell) limit. The electronic structure of monolayer Bi₂Sr₂CaCu₂O₈₊δ is probed with scanning tunneling microscopy and spectroscopy. Survey of the electronic phases – superconductivity, pseudogap, charge order and Mott insulating state – reveals that they are indistinguishable from those in the bulk. Out results, therefore, indicates that essential physics of HTS is contained in a monolayer Bi₂Sr₂CaCu₂O₈₊δ.
Tunable high-temperature superconductivity in monolayer Bi\textsubscript{2}Sr\textsubscript{2}CaCu\textsubscript{2}O\textsubscript{8+δ}  

YIJUN YU (Presenter), LIGUO MA, PENG CAI, Fudan University, RUIDAN ZHONG, Brookhaven National Lab, CUN YE, JIAN SHEN, Fudan University, GENDA GU, Brookhaven National Lab, XIANGHUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Fudan University — Dimensionality plays a central role in high-temperature superconductivity (HTS). Layered cuprate superconductors hold the record of $T_c$ at ambient pressure. Cuprates in the two-dimensional (2D) limit would provide valuable insights on the nature of HTS and offer unprecedented tunability in their material properties. Half-unit-cell-thick single crystal of Bi\textsubscript{2}Sr\textsubscript{2}CaCu\textsubscript{2}O\textsubscript{8+δ} (referred to as monolayer Bi-2212) is such an ideal 2D system. Here we fabricate transport devices from monolayer Bi-2212 samples obtained by exfoliation and study the evolution of superconductivity as the dimensionality and doping level is varied. We find that superconductivity remains intact in monolayer Bi-2212. Finite size scaling analysis at superconductor-to-insulator transition (SIT) reveals distinct critical behaviors at different disorder levels. Our study leads to a unified picture of SITs previously reported in cuprate systems.

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C15 DMP: 2D Materials (Semiconductors) -- Multilayers & Heterostructures II BCEC

2:30PM C15.00001: Electronic and thermoelectric transport in two-dimensional layered-structure material  

SHI-JUN LIANG (Presenter), JUNWEN ZENG, Nanjing University, XIN HE, LIJUN ZHANG, Jinlin University, DAVID SINGH, University of Missouri, FENG MIAO, Nanjing University — Electronic and thermoelectric transport properties have been the extensively studied topics in the two dimensional materials. Hicks and Dresselhaus predicted that the reduction in dimensionality of materials can enhance the thermopower power factor. However the observation of confinement-induced enhancement of thermoelectric power factor predicated by Hicks and Dresselhaus has been challenging. In this work, we firstly studied the electronic transport mechanism of InSe nanoflakes in the presence of the magnetic field and gate voltage. We observed the gate-tunable weak antilocalization phenomenon and a very long coherent length of up to 320 nm at 1.7 K. The scattering mechanisms were analysed in details. Furthermore, we investigated the thermoelectric properties in the InSe thin film and revealed that the Seebeck coefficient and power factor can be enhanced by the enhanced DOS arising from the size confinement effect when the thickness of InSe thin film is thinned down. Most importantly, we experimentally identified the condition for drastically enhancing the thermoelectric power factor in the 2D layered-structure materials.

2:42PM C15.00002: Moiré Valleytronics: Realizing Dense Arrays of Topological Helical Channels*  

CHEN HU (Presenter), VINCENT MICHAUD-RIOUX, Center for the Physics of Materials and Department of Physics, McGill University, WANG YAO, Department of Physics and Center of Theoretical and Computational Physics, University of Hong Kong, HONG GUO, Center for the Physics of Materials and Department of Physics, McGill University — In hexagonal 2D crystals, the valley degree of freedom is characterized by non-trivial Berry curvatures. Valley-dependent topological helical channels are novel conducting states without back scattering, which can benefit to low power consumption in practical applications. We propose a general, robust and experimentally-feasible platform, the moiré valleytronics, to realize high-density arrays of 1D topological helical channels in real materials at room temperature. We demonstrate the idea using a long-period 1D moiré pattern of graphene on hBN by first-principles calculation. Through calculating the Berry curvature and topological charge of the electronic structure associated with various local graphene/hBN stackings in the moiré pattern, it is revealed that the helical channel arrays originate intrinsically from the periodic modulation of the local topological orders by the moiré pattern.

*This work is financially supported by the Natural Science and Engineering Research Council (NSERC) of Canada (H. G.) and the Research Grants Council of Hong Kong (HKU17302617). We thank Compute Canada and the High Performance Computing Center of McGill University for substantial computational support.
2:54PM C15.00003: Guiding experimental investigation of a pentagonal layered material through theoretical modeling/simulation  LIANGBO LIANG (Presenter), KAI XIAO, ALEXANDER PURETZKY, GIANG NGUYEN, AN-PING LI, DAVID GEOHEGAN, BOBBY G SUMPTER, Oak Ridge National Laboratory — PdSe₂ is a new 2D layered material with an in-plane pentagonal network and stronger-than-vdW interlayer coupling. It offers great trade-off between carrier mobility, band gap, and air stability for 2D electronics [JACS, 139, 14090 (2017)]. Here I will highlight how first-principles modeling/simulation guided experiments to explore its electronic and vibrational properties. Because of strong interlayer coupling, its band gap varies significantly from 1.3 eV (monolayer) to 0.06 eV (bulk), based on both calculations and measurements. Our Raman scattering simulation revealed that, unlike graphene and MoS₂, the PdSe₂ layers are no longer quasi-rigid in low-frequency interlayer vibrations. Therefore, the thickness dependence of the interlayer Raman modes’ frequencies in PdSe₂ deviates significantly from the linear chain model (LCM), which was verified by Raman measurements. A revised LCM was developed to account for the layer non-rigidity [2D Materials, 5, 035016 (2018)]. Finally, according to our nudged elastic band calculations, the pentagonal structure and strong interlayer coupling lead to low diffusion barriers for defects, and hence both intralayer and interlayer hopping of defects can occur relatively easily, as observed by scanning tunneling microscope [PRL, 121, 086101 (2018)].

3:06PM C15.00004: Optical properties of monolayer MoSe₂/layered antiferromagnet heterostructures  MASARU ONGA (Presenter), YUSUKE SUGITA, TOSHIYA IDEUE, YUJI NAKAGAWA, RYUJI SUZUKI, YUKITOSHI MOTOME, YOSHIHIRO IWASA, University of Tokyo — Van der Waals heterostructure has attracted much interest because of its high extensibility by using various layered materials. Furthermore, the recent discovery of 2D magnets has provided us a new platform to investigate magnetic van der Waals heterointerfaces, leading to novel studies on spin-/valley-tronics [1]. Here we report a new type of magnetic van der Waals heterointerface using monolayer transition metal dichalcogenides (especially MoSe₂) and layered antiferromagnets. We fabricated the samples by using all-dry-transfer method in inert atmosphere and performed photoluminescence measurements at low temperature. The characteristic spectra are observed below the transition temperature of the magnets, which suggests that the magnetic ordering can affect the exciton property of MoSe₂ directly.


3:18PM C15.00005: Mobility and quantum mobility of a 2DEG in modern GaAs/AlGaAs heterostructures  MICHAEL SAMMON (Presenter), Physics, University of Minnesota, TIANRAN CHEN, Physics, West Chester University, MICHAEL ZUDOV, BORIS SHKLOVSKI, Physics, University of Minnesota — In modern GaAs/AlGaAs heterostructures with record high mobilities, a two-dimensional electron gas (2DEG) in a quantum well is provided by two remote donor δ-layers placed on both sides of the well. Each δ-layer is located within a narrow GaAs layer, flanked by narrow AlAs layers which capture excess electrons from donors but leave each of them localized in a compact dipole atom with a donor. These excess electrons minimize their Coulomb energy and screen the random potential of charged impurities. We developed a theory of this screening and used it to calculate both the mobility and the quantum mobility of the 2DEG.[1,2] Our results show that the remote donor limited mobilities strongly increase with the filling fraction of excess electrons, and the calculated mobilities drastically exceed the measured values. This suggests that the mobilities are limited either by background charged impurities, or the weakening of screening by additional disorder in the doping layer such as roughness at the GaAs/AlAs interface or spreading of the donors outside of the δ-layer. [1] M. Sammon, M. A. Zudov, B. I. Shklovskii, Phys. Rev. Materials 2, 064604 (2018). [2] M. Sammon, Tianran Chen, B. I. Shklovskii, Phys. Rev. Materials 2, 104001 (2018).

3:30PM C15.00006: Atomic interaction through two-dimensional materials governed by competitive energy fluctuations  *HUASHAN LI (Presenter), Sino-French Institute of Nuclear Engineering and Technology, Sun Yat-Sen University, WEI KONG, JEEHWAN KIM, JEFFREY C GROSSMAN, Massachusetts Institute of Technology — The rapid development of hybrid 2D materials has unveiled its potential to achieve complex functionality. The impact of 2D materials on intermolecular interactions of crystalline materials has not been fully understood. In this study, we computationally investigated a variety of heterojunctions with 2D materials sandwiched by 3D crystal layers.[1] The results suggest that transparency of 2D interlayer is governed by competition between the substrate potential energy fluctuation attenuated, and the binding energy fluctuation generated by 2D interlayer. Although the potential field from covalent-bonded materials is screened by a monolayer of graphene, that from ionic-bonded materials is strong enough to penetrate through a few layers of graphene. Such field penetration is substantially attenuated by 2D hBN, which itself has polarization in its atomic bonds. The insight has been verified by our experiments and further employed to control the transparency via modulating the nature and thickness of 2D interlayer, which eventually leads to the successful remote epitaxial growth of single-crystalline materials across the periodic table.


*We thank the support from the NSFC (11804403) and the GD-NSF (2018B030306036).
Two-dimensional van der Waals (vdW) layered materials have attracted great attention for their applications in flexible electronics and optoelectronics. In this work, we report a comprehensive theoretical study of graphene/graphyne (Gyne/Gyne), graphyne-like BN/graphyne-like BN (BNyne/BNyne) and graphene/graphyne-like BN (Gyne/BNyne) bilayers by density functional theory. These bilayers exhibit distinct stacking dependent characteristics in the ground state electronic structure and have different responses to external strain and electric field. For Gyne/Gyne and Gyne/BNyne bilayers, a biaxial tensile strain increases the band gap while biaxial compressive strain or uniaxial strain, reduces it. For the BNYne/BNyne bilayer the trend is opposite. Under a vertical electric field, the band gap decreases in homo-bilayers Gyne/Gyne and BNYne/BNyne. For the hetero-bilayer Gyne/BNyne, band gap decreases under a positive electric field but remain almost constant in negative electric field. These properties are understood by analyzing the calculated electronic density and potential.

**References**


**Microscopic theory of band gap opening and spin-orbit splitting in graphene/TMDC heterobilayers**

Theoretical ab initio calculations have shown a gap opening and an induced spin-orbit splitting in the band structure of graphene from the TMDC layer [1, 2]. These results have been experimentally confirmed by recent magnetotransport experiments showing weak antilocalisation (WAL) [2, 3]. Using perturbation theory, we propose a microscopic model to explain the origin of the gap and of the spin-orbit splitting. We also consider the dependence of the spin-orbit splitting on the misalignment of graphene and TMDC layers.

**Graphene-Oxide-Semiconductor photodetector**

The photodetection properties of a graphene-oxide-semiconductor (GOS) diode have been extensively investigated by measuring current-voltage characteristics under illumination with light-emitting diode (LED). We demonstrate that the newly developed GOS heterostructure, with graphene as a transparent gate electrode to form the inversion layer at the oxide-semiconductor interface, can function as a GOS field-effect transistor (GOSFET) operable at low temperature (T) down to 1.5 K. By studying the gate tunneling current in the GOSFET, we find that the dark current is below ~ 0.1 nA, which is almost two orders of magnitude smaller than that in graphene-Si (GS) Schottky detector diode. Our work paves the way for the implementation of hybrid photodetectors devices fabricated by two-dimensional materials and conventional semiconductors with CMOS integrability.

**Coexistence of Different Charge Transfer Mechanisms in the Hot Carrier Dynamics of Hybrid Plasmonic Nanomaterials**

Plasmon induced hot-electron dynamics at the interfaces of metallic nanostructures and semiconductors is of significant importance for photovoltaic and photocatalytic applications. Plasmon-driven charge separation processes were considered to be only dependent on the type of donor-acceptor interactions, i.e., conventional hot electron transfer mechanism for van der Waals interactions and plasmon-induced interfacial charge-transfer transition pathway for chemical bonds. Here we demonstrate the two mechanisms can coexist in a typical metal-semiconductor hybrid plasmonic nanomaterials, both happen on a faster time scale than carrier relaxation process. The origin of the two mechanisms is attributed to the spatial vertical and parallel modes of excited plasmon, where the vertical mode couples to semiconductors much strongly than the parallel one. Our findings provide a new insight into the photoinduced plasmonic carrier dynamics, which is relevant for many potential applications including solar energy conversion, efficient water splitting and photocatalysis.
We discuss the 2D prototype system of hexagonal BN (hBN), a wide bandgap insulator with strong excitonic effects and UV luminescence properties. We investigate the optical properties of few layer hBN, focusing on the Davydov splitting of the lowest bound exciton, which dominates the absorption. We use \textit{ab initio} methods and a model mapping the Bethe-Salpeter equation onto an effective tight-binding Hamiltonian with few parameters. We thus obtain a precise characterization of the symmetries of the excitonic states and their optical selection rules.

We discuss the splitting of excitonic states in systems of \( N \) layers, and construct a simple model for the absorption spectrum as a function of \( N \). We show that for \( N>2 \), one can distinguish between surface and inner excitons. The former are found to be lower in energy and can be optically active. 

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4:42PM C15.00012: Rapid bimolecular and defect-assisted carrier recombination in hexagonal Boron Nitride

\textsc{Ioannis Chatzakis (Presenter)}, \textsc{Roderick Davidson II}, \textsc{Adam Dunkelberger}, \textsc{Andrea Grafton}, United States Naval Research Laboratory, \textsc{Joshua D Caldwell}, Electrical and Mechanical Engineering, Vanderbilt University, \textsc{Song Liu}, Tim Taylor Dept. of Chemical Engineering, Kansas State University, \textsc{Jaime A. Freitas}, Jr., \textsc{James Clifford Culbertson}, United States Naval Research Laboratory, \textsc{James H. Edgar}, Tim Taylor Dept. of Chemical Engineering, Kansas State University, \textsc{Daniel Ratchford}, \textsc{Chase Ellis}, \textsc{Alex Giles}, \textsc{Joseph G Tischler}, \textsc{Jeffrey Owrutsky}, United States Naval Research Laboratory — Hexagonal boron nitride (hBN) is an indirect wide band gap semiconductor that holds great promise for optoelectronic devices in the ultraviolet regime. Here we report the dynamics of photoexcited charge carriers at room temperature in exfoliated monoisotopic \(^{10}\text{B}\) enriched hBN. Two recombination mechanisms were identified, and their associated time scales measured, using ultrafast two-photon pump, infrared probe transient transmission spectroscopy. Initially, when the free carrier density is high, bimolecular decay dominates recombination with a rate constant of \((1.33 \pm 0.09) \times 10^{-7} \text{ cm}^{-3}/\text{s}\). At later times, the recombination of the free carriers is characterized by an exponential decay with a time constant on the order of a nanosecond, determined by the density of the impurities/defects in the lattice.

4:54PM C15.00013: Understanding the electrical behaviors in van der Waals heterostructure field-effect transistor based on band alignment

\textsc{Seonyeong Kim (Presenter)}, \textsc{Taekwang Kim}, \textsc{Somyeong Shin}, \textsc{Hyewon Du}, \textsc{Minho Song}, \textsc{Hansung Kim}, \textsc{Dain Kang}, Sejong University, \textsc{Chang-Won Lee}, Hanbat university, \textsc{Sunae Seo}, Sejong University — Van der Waals heterostructures based on 2D layered materials have been extensively studied because their unique electronic properties, which can be controlled by optimally selecting the band alignments. Although the rectifying behavior is usually observed in output characteristics of these heterostructures, the underlying transport mechanism have not been fully understood. Here, we investigate transport properties of multilayer \( \text{MoTe}_2/\text{SnS}_2 \) heterostructure field-effect transistor (hetero-FET) fabricated by exfoliating each material and manually stacking them and observe gate-tunable diode-like current rectification. With the qualitative band analysis, we noticed that the interfacial barrier by band bending plays a crucial role to realize the transport properties of hetero-FETs, especially rectification behavior. Our experimental study offers the inspiration for understanding the transport behavior and reference to novel hetero-FETs.
Demonstrating Band Design in Two-Dimensional Covalent Organic Frameworks*

HALLEH BALCH (Presenter), Physics, University of California, Berkeley, AUSTIN EVANS, Chemistry, Northwestern University, RAGHUNATH DASARI, SIMIL THOMAS, KAITLIN SLICKER, HONG LI, Chemistry, Georgia Tech, RUOFAN LI, DAN RALPH, Physics, Cornell University, JEAN-LUC E BREDAS, SETH R. MARDER, Chemistry, Georgia Tech, WILLIAM DICHTEL, Chemistry, Northwestern University, FENG WANG, Physics, University of California, Berkeley — Two dimensional covalent organic frameworks (COFs) are periodic lattices whose rational design can yield novel optoelectronic properties and new heterostructure devices. Analogous to graphene and the inorganic family of 2D materials, 2D COFs are covalently bonded in-plane with out-of-plane bonding through Van der Waals interactions. To date, 2D COF properties are limited by large molecular bandgaps, low intermolecular coupling, and poor control of the material morphology. Here, we report the rational design and characterization of a new, highly conjugated, semiconducting 2D framework. We characterize the structure by X-ray scattering, TEM, and AFM, and demonstrate facile manipulation onto arbitrary experimental platforms. We further employ broadband optical and vibrational spectroscopies to observe electronic behavior emergent in this highly conjugated system.

*Army Research Office grant number W911NF-15-1-0447

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C16 DMP: Transport in Nanostructures -- Quantum dots, nanocrystals, and nanowires

BCEC 155 - Jeremy Levy, University of Pittsburgh - Tag(s): Focus

2:30PM C16.00001: Three-dimensional imaging of material functionality through nanoscale tracking of energy flow* [Invited] MILAN DELOR, HANNAH L WEAVER, QINQIN YU, NAOMI GINSBERG (Presenter), University of California, Berkeley — The ability of energy carriers to move within and between atoms and molecules underlies virtually all biochemical and material function. Understanding and controlling energy flow, however, requires observing it on ultrasmall and ultrafast spatiotemporal scales, where energetic and structural roadblocks dictate the fate of energy carriers. We therefore developed a universal, non-invasive optical scheme that leverages interferometric scattering to track tiny changes in material polarizability created by energy carriers. Our approach enables mapping energy transport trajectories in four dimensions of spacetime with few-nanometer precision and directly correlating them to material morphology. We visualize exciton, charge, and heat transport in polyacene, silicon and perovskite semiconductors and elucidate, in particular, how grain boundaries impact energy flow through their lateral- and depth-dependent resistivities. We reveal new strategies to interpret energy transport in disordered environments that will direct the design of defect-tolerant materials for the semiconductor industry of tomorrow.

*This work has been supported by STROBE, A National Science Foundation Science & Technology Center under Grant No. DMR 1548924. Q.Y. acknowledges a National Science Foundation Graduate Research Fellowship (DGE 1106400). N.S.G. acknowledges an Alfred P. Sloan Research Fellowship, a David and Lucile Packard Foundation Fellowship for Science and Engineering, and a Camille and Henry Dreyfus Teacher-Scholar Award.

3:06PM C16.00002: Levy statistics in quasi one-dimensional percolation paths in nano-patterned quantum dot solids TAMAR MENTZEL (Presenter), Physics, Harvard University — Quantum dot (QD) solids hold promise as a tunable platform for applications such as quantum computation and spintronics, and for exploring many-body physics. However, the predicted, novel electronic properties in QD solids have been obscured by disorder caused by structural defects, variability in electronic energy levels of the QDs and charge traps on the QD surfaces. We nano-pattern QD solids with dimensions ~10−100 nm that are free of structural defects found in many larger superlattices. The QDs are strongly coupled (≤1 nm inter-dot spacing), which offsets inhomogeneities in the electronic energy levels in the QD. We find current noise that increases linearly with the average current at high temperatures, and we find random telegraph noise at low temperatures. We show that charge is transmitted along quasi-one-dimensional channels, which open and close at a rate given by Levy statistics. The trapping and release of charge in the QD matrix is the likely cause for these fluctuations. These nano-patterned QD solids enable measurement of the charge transport mechanism intrinsic to the QDs; and, they offer a direct measurement of the influence of charge trapping on the charge transport mechanism.
3:18PM C16.00003: Triplet excitons on the interface of Colloidal Quantum Dots and organic molecules*  TAMAR GOLDZAK (Presenter), ALEXANDRA MCISAAC, TROY VANVOORHIS, Massachusetts Institute of Technology — Colloidal Quantum Dots (QDs) have been long-standing candidates for optoelectronic devices and applications, such as solar photovoltaic, light emitting diodes, detectors, and biological sensing. They are composed of semi-conductor materials, and are synthesized from solution. Their optical and electronic properties change with their size, shape, composition, and surface. In the up-conversion (UC) process two low frequency photons are converted into one high energy photon, this can broaden the absorption spectrum and increase the efficiency of optoelectronic devices. One of the steps in the UC process is the transfer of high energy triplet exciton across the interface of colloidal QD/organic molecule. Using electronic structure calculations combined with experimental observations, we study and try to characterize triplet excitons on various QD structures ligated with organic molecules to get a better understanding of the transfer mechanism. We also use Molecular Dynamics simulations to study the morphology of these interfaces.

*This work was supported by the Center for Excitonics, an Energy Frontier Research Center funded by the U.S and the MIT-Technion post doctorate fellowship.

3:30PM C16.00004: Layer-Dependence of Charge Transfer Kinetics in Hybrids of 2D MoS2 and PbS/CdS Quantum Dots*  JIA-SHIANG CHEN (Presenter), Department of Materials Science and Chemical Engineering, Stony Brook University, MINGXING LI, MIRCEA COTLET, Center for Functional Nanomaterials, Brookhaven National Laboratory — Two-dimensional (2D) layered transition metal dichalcogenides (TMDs) have attracted tremendous attention owing to their unique optical and physical properties. However, weak photon absorption due to their atomically thin thickness prohibits their spectral sensitivity. Here, 2D-MoS2 with different layers are combined with core/shell PbS/CdS quantum dots (QDs) to produce hybrids with improved photoresponsivity by interfacial charge transfer. The charge transfer kinetics in the hybrids of MoS2 and PbS/CdS QDs has been revealed by time-resolved photoluminescence (PL) microscopy, showing that the charge transfer rate increases with the layer of MoS2 increased due to the increased driving force in between conduction band edge of MoS2 and QDs. We have evaluated the results with the theoretical model of Marcus theory, which is in good agreement with our observation. Understanding the interfacial charge transfer kinetics between QDs and 2D materials is crucial and useful for improving photon-to-current conversion efficiency in next-generation optoelectronics.

*This work was carried out in part at the Center for Functional Nanomaterials, Brookhaven National Laboratory (BNL), which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-SC0012704.

3:42PM C16.00005: Charge Kondo effects in a quadruple quantum dot in spinless and spinful regimes.  JUHO CHOI (Presenter), GWANGSU YOO, HEUNG-SUN SIM, KAIST — We theoretically study charge Kondo effects in a quadruple quantum dot, whose shape is such that three dots A,B,C are located at the three corners of a triangle respectively and the other dot D is at the center of the triangle. Here, the dots A and B are coupled to reservoirs. We consider a spinless regime under an external magnetic field and a spinful regime in the presence of electron tunneling between the dots A and B, when the system has two-fold degenerate ground-state charge configurations (n_A=1,n_B=1,n_C=1,n_D=0) and (0,0,0,1). In the spinless regime, a single-channel charge Kondo effect occurs. In this case, the two charge configurations act as the pseudospin states of the Kondo effect. In the spinful regime, electrons of the dots A and B in the charge configuration (1,1,1,0) form a spin singlet state, and the system is described by an anisotropic two-channel Kondo Hamiltonian. Because the channel anisotropy is large, the quadruple dot shows a single-channel charge Kondo effect. We compute electron transport through the quadruple dot for the two regimes.
3:54PM C16.00006: Metal-insulator transition in a semiconductor nanocrystal network* BENJAMIN L GREENBERG, Mechanical Engineering, University of Minnesota, ZACHARY ROBINSON (Presenter), YILIKAL Z AYINO, Physics, University of Minnesota, JACOB T HELD, Chemical Engineering and Materials Science, University of Minnesota, TIMOTHY A PETERSON, Physics, University of Minnesota, K. ANDRE MKHOYAN, Chemical Engineering and Materials Science, University of Minnesota, VLAD S PRIBIAG, Physics, University of Minnesota, ERAY S. AYDIL, Chemical Engineering and Materials Science, University of Minnesota, UWE RICHARD KORTSHAGEN, Mechanical Engineering, University of Minnesota — In bulk semiconductors, the metal-insulator transition is described by the well-known Mott criterion. A recent theory proposes a more stringent criterion condition in nanocrystal (NC) networks, dependent on the electron density \( n \) and the inter-NC facet radius \( \rho \): \( n\rho^3 \approx 0.3 \). Here we use plasma-synthesized ZnO NCs coated with Al\(_2\)O\(_3\) via ALD to study the electronic properties of a NC network as a function of \( n \) and \( \rho \). Through a xenon-flashlamp annealing process, we selectively sinter/dope the NC network by flashing the film before/after the ALD infill, allowing independent control of \( \rho \) and \( n \). While we observe large changes in the mobility and \( n \), we do not see finite conductivity \( (\sigma) \) as \( T \to 0 \)K. To cross the transition, prior to the Al\(_2\)O\(_3\) ALD infill we coat the NCs with 8 cycles of ZnO ALD. This changes \( \rho \) from ~1.5 nm to ~2.8 nm and increases the packing density from 33% to 47%. By then tuning \( n \) we achieve a transition from the semiconducting to metallic state, with finite \( \sigma \) as \( T \to 0 \)K. At the transition we see power law conductivity of the unusual form \( \sigma(T) \propto T^{1/5} \), and observe critical scaling behavior when scaling \( \sigma \) by the \( n\rho^3 \) criterion. This is the first conclusive evidence for metallic behavior in a NC network.

*This work was supported by UMN MRSEC program of the NSF under grant DMR-1420013

4:06PM C16.00007: Manipulation of non-linear heat currents in dissipative quantum dot systems BITAN DE (Presenter), BHASKARAN MURALIDHARAN, Electrical Engineering, Indian Institute of Technology Bombay — The anomalous behavior of phonon transport due to finite electron-phonon interaction is investigated using an Anderson-Holstein based dissipative quantum dot setup in two relevant cases: (a) electron flow stimulated by the voltage bias in the absence of an electronic temperature gradient and (b) electron flow driven by the electronic temperature gradient at zero voltage. We explain the observation of the cumulative effect of voltage and electronic temperature gradient on the non-linear phonon current with the aid of a new transport coefficient called electron induced phonon thermal conductivity. It is demonstrated that under suitable operating conditions in Case (a), the dot can pump in phonons into the hotter phonon reservoir and in Case (b), the dot can extract phonons out of the colder phonon reservoirs. Finally, we elaborate how the non-linear electronic heat current can be stimulated and controlled by engineering the temperatures of the phonon reservoirs.

References:

4:18PM C16.00008: Measurement of the Kondo cloud length via a quantum dot coupled to a 1d interferometer: Theory (1/2) JEONGMIN SHIM (Presenter), Physics, Korea Advanced Institute of Science and Technology, IVAN BORZENETS, Physics, City University of Hong Kong, JASON CHEN, Applied Physics, The University of Tokyo, MICHIHISA YAMAMOTO, SEIGO TARUCHA, CEMS, RIKEN, H.-S. SIM, Physics, Korea Advanced Institute of Science and Technology — The Kondo effect, known as the archetype of many-body correlations, arises from the interaction between a localized magnetic moment and surrounding conducting electrons. Advances of nanotechnology allow us to study the Kondo effect for a single magnetic impurity confined in a semiconductor quantum dot in contact with electron reservoirs. This development also makes it possible to embed a Kondo correlated state into an interferometer. However, the special extent of the Kondo cloud has yet to be measured.

Here, we demonstrate that the Kondo cloud length \( \xi_K \) can be measured in a system of a Kondo correlated quantum coupled to a 1D Fabry-Perot (F-P) interferometer. Using numerical renormalization group and poor man's scaling methods in parallel we characterize the oscillations in Kondo temperature with respect to resonances of the F-P interferometer. We show that the amplitude of the temperature oscillations can be described by the interferometer length as well as the coupling strength. Thus, we demonstrate a system where an experimentally defined length can be used to infer the Kondo length.
4:30PM C16.00009: Measurement of the Kondo cloud length via a quantum dot coupled to a 1d interferometer: Experiment (2/2) IVAN BORZENETS (Presenter), Physics, City University of Hong Kong, JEONGMIN SHIM, Physics, Korea Advanced Institute of Science and Technology, JASON CHEN, Applied Physics, The University of Tokyo, H.-S. SIM, Physics, Korea Advanced Institute of Science and Technology, MICHIHISA YAMAMOTO, SEIGO TARUCHA, CEMS, RIKEN — We have developed an all-solution processed transparent conductor, known as the archetype of many-body correlations, arises from the interaction between a localized magnetic moment and surrounding conducting electrons. Advances of nanotechnology allow us to study the Kondo effect for a single magnetic impurity confined in a semiconductor quantum dot in contact with electron reservoirs. This development also makes it possible to embed a Kondo correlated state into an interferometer. However, the special extent of the Kondo cloud has yet to be measured.

In this work, we perform direct experimental measurement of the Kondo cloud length $\xi_K$ by coupling a Kondo correlated quantum dot to ballistic, multi-channel quantum wires, one of which couples more strongly to the dot and works as a 1D Fabry–Perot (F-P) interferometer defined on a GaAs/AlGaAs heterostructure. We demonstrate that the measured Kondo temperature undergoes resonances with respect to the F-P fluctuations. By looking at the strength of the resonances versus the interferometer lengths, we are able to access the length of the Kondo cloud. We back up our results by comparing the behavior of the interferometer in the Kondo as well as the Coulomb Blockade Regimes.

4:42PM C16.00010: Phonon backscatter, trapping, bottlenecking, and misalignment effects on thermal conductivity of Si Nanostructures FRANCIS VANGESSEL (Presenter), PETER CHUNG, University of Maryland, College Park — Nanostructured systems offer the ability to reduce thermal conductivity which, for instance, may be used to improve the thermoelectric efficiency. The internal surfaces of these nanostructures significantly curtail the ballistic free flight of phonons, and thus resist thermal transport. In this talk, we present a recent investigation of a simple one-parameter geometry that simultaneously modulates backscattering and trapping effects to enable directed study of controlling phonons. The geometry is a simple sequence of chambers offset from one another by a defined distance. We use the geometry to study the effects of phonon backscatter, trapping, bottlenecking, and corner-turning on the thermal conductance in Si nanowires (NWs). By creating a geometry that maximizes backscatter, a roughly 8-fold reduction in thermal conductance below the Casimir limit can be achieved at room temperature which is a factor of four smaller than the nearest reported value in the literature. The geometry is also useful for systematic investigation of other means of controlling phonons and affecting thermal transport. Specifically, we investigate the induced misalignment between the phonon flow and thermal flux due to the shape of the geometry as well as phonon filter-like behavior of the geometry.

5:06PM C16.00012: All-solution processed micro/nano-wires as transparent conducting electrodes CHAOBIN YANG (Presenter), JUAN M. MERLO, LUKE D’IMPERIO, AARON H ROSE, YITZI M CALM, VICTORIA GABRIELE, MARK SCHILLER, KRZYSZTOF KEMPA, MICHAEL J NAUGHTON, Boston College — We have developed an all-solution processed transparent conductive electrode with sheet resistance an order of magnitude smaller than conventional nanowire-based transparent conductors. This is achieved by integrating all-solution-produced microwires1 with nanowires and electroplate welding. As a result, the advantages of these transparent conductors are indium-free, vacuum-free, lithographic-facility-free, metallic-mask-free, with small domain size, high specific conductivity and mechanical flexibility, thus making them an excellent replacement for ITO.

**Session C17 DCOMP: Matter in Extreme Environments: Melting and Melts**

**Monday, March 4, 2019 2:30 PM - 5:06 PM**

**5:18PM C16.00013: Formation of Interfacial Dipole Formations during Contact Electrification**

JAMES CHEN (Presenter), MOHAMAD IBRAHIM CHEIKH, University at Buffalo, The State University of New York, TYLER J HIEBER, ZAYD C LESEMAN, Mechanical and Nuclear Engineering, Kansas State University — This study introduces a plausible origin of the driving force for electron transfer in contact electrification and triboelectrification for dielectric materials. As two material approaches each other, surface lattices of both materials form a weak interaction, the perturbed states of each surface lattice can be approximated a dipole. These surface dipoles induce a potential field in the proximity and provides a driving force for electron transfer. A tribopair of barium titanate and magnesia are investigated as an example. The simulation results show that such tribopair can generate up to 104 V/cm², which is comparable with the experimental measurements in published literature.

*This work is supported by NSF under Award 1662879*

**2:30PM C17.00001: Melting Under Extreme Conditions: Ab Initio Monte Carlo Simulations**

EDISON FLOREZ, CTCP, INMS, Massey University, Auckland, TRYGVE HELGAKER, University of Oslo, WIM KLOPPER, KIT, ANDREW TEALE, University of Nottingham, STELLA STOPKOWICZ, University of Mainz, ELKE PAHL (Presenter), CTCP, INMS, Massey University, Auckland — Melting results for rare gas clusters and solids under extreme pressures and magnetic fields are presented. Phase transitions are simulated by exploring phase space with classical (parallel-tempering) Monte Carlo methods combined with a very accurate computation of the interaction energy of the sampled configurations. We employ many-body expansions where the total interaction energy of the \( N \)-atom system is obtained by decomposing the total energy into two-, three- and higher-body fragments.

For rare gases, this approach works well for melting under ambient conditions\(^1\) and for argon for pressures up to 100 GPa, 1 Million times the atmospheric pressure\(^2\). We work in the isobaric, isothermal ensemble, allowing for atom displacements as well as cell volume adjustments employing periodic boundary conditions. Excellent agreement with experimental data is found up to very high pressures.

Neon clusters in high magnetic fields show elevated melting points and also give fascinating insight in the melting process itself. In a strong homogeneous magnetic field applied in \( z \)-direction the clusters get squeezed in the perpendicular plane as also observed for atoms. Around the melting temperature, we observe an additional squeezing parallel to the magnetic field due to perpendicular paramagnetic bonding responsible for the enhanced melting points. For these studies, dimer potential curves were computed on MP2 and coupled-cluster level depending on the magnetic field, the interatomic distance and the angle of the molecular axis with the magnetic field direction.


*We thank the Marsden fund, Royal Society of New Zealand (MAU1409), the Centre for Advanced Study at Norwegian Academy of Science and Letters and the MacDiarmid Institute for Advanced Materials and Nanotechnology for financial support.*
**3:06PM C17.00002: Fast determination of melting curves at high pressure**

JOHANN BOUCHET (Presenter), VANINA RECOULES, FRANCOIS BOTTIN, MARC TORRENT, CEA, DAM, DIF — Determination of accurate melting curves of materials is an old problem. In the past twenty years, reliable results have been obtained with ab-initio molecular dynamics (AIMD). These simulations are usually based on molecular dynamics of the solid or the liquid (one phase approach), or the direct simulation of the solid-liquid interface (two phases approach) [1]. Unfortunately, AIMD can be very time consuming, and prevent applications on complex systems or heavy elements. Fast alternative methods are necessary, at least to give a starting point for more complex calculations.

The famous phenomenological Lindeman [2] approach based on the comparison of the amplitude of thermal vibrations of atoms with the interatomic distance and proposed more than 100 years ago is still widely used [3]. We have tested its validity for several metals (Au, Al, Fe...) on a large pressure scale. We will also discussed applications on MgO and U in regard to our recent calculations of vibrational frequencies in temperature [4].


**3:18PM C17.00003: Critical point, liquid-vapor coexistence, and melting of Mg$_2$SiO$_4$ from *ab-initio* simulations**

THOMAS R MATTSSON (Presenter), Sandia National Laboratories, GIL SHOHET, Department of Aeronautics & Astronautics, Stanford University, JOSHUA TOWNSEND, LUKE SHULENBURGER, MICHAEL PAUL DESJARLAIS, Sandia National Laboratories — We report density functional theory-based molecular dynamics calculations (DFT-MD) of Mg$_2$SiO$_4$ liquid and vapor across the liquid-vapor coexistence boundary that spanned 0.22-3.22 g/cc in density and 5000-10000 K in temperature. The critical point was estimated through a bootstrap analysis of a collection of DFT-MD isotherms above and below the critical point. Additionally, we describe the structure and composition of the liquid and vapor around the critical point. Finally, we discuss melting behavior at P=1 bar.

*This work was supported by the Z Fundamental Science Program (ZFSP) at Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

**3:30PM C17.00004: Chain melting simulations in dense potassium from a machine-learned atomic potential**

ANDREAS HERMANN (Presenter), HONGXIANG ZONG, VICTOR NADEN ROBINSON, GAVIN WOOLMAN, GRAEME ACKLAND, University of Edinburgh — Compressed potassium forms a host-guest structure above 19 GPa, K-III, where the host and guest structures have incommensurate lattice constants $c_h$ and $c_g$ [1]. The guest structure comprises a linear set of chains with long range order at low temperature and has been observed to de-correlate or “melt” upon heating, while the host structure remains solid [2]. We studied this motion and onset of inter- and intra-chain de-correlation, which lead to the disappearance of guest structure diffraction peaks, by ab initio molecular dynamics (AIMD) using approximants of the incommensurate crystal. The system sizes that can be simulated with AIMD are limited, so a forcefield was trained on the AIMD data set. The trained potential was used to produce potassium’s PT phase diagram up to 60 GPa and 1000 K, correctly predicting the stable solid phases, the chain melt and the full melting line [3].


*Research funding from the ERC (grant HECATE) and computational resources provided through EPSRC (EP/P020194 and EP/P02256/1) are acknowledged.
3:42PM C17.00005: Pre-melting hcp to bcc Transition in Beryllium by First-Principles Phonon Quasiparticle Approach  
DONG-BO ZHANG (Presenter), College of Nuclear Science and Technology, Beijing Normal University, Beijing 100875, China, YONG LU, Beijing Computational Science Research Center, Beijing 100193, China, TAO SUN, Key Laboratory of Computational Geodynamics, University of Chinese Academy of Sciences, Beijing 100088 China, PEIHONG ZHANG, Department of Physics, University at Buffalo, State University of New York, 14260, USA, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics; Department of Earth and Environmental Sciences and Lamont-Doherty Earth Observatory, Columbia University, 10027, USA — Beryllium (Be) is an important material with wide applications ranging from aerospace components to x-ray ray equipment. Yet a precise understanding of its phase diagram under extreme conditions remains elusive. We have investigated the phase stability of Be using a recently developed hybrid free energy computation method that accounts for anharmonic effects by invoking phonon quasiparticles. We find that the hcp → bcc transition occurs near the melting curve at 0 < P < 11 GPa with a positive Clapeyron slope of $41(4)$ K/GPa, which is more consistent with recent experimental measurements. This work also demonstrates the validity of this theoretical framework based on the phonon quasiparticle to study the structural stability and phase transitions in strongly anharmonic materials.

3:54PM C17.00006: Direct Observation of Shock-Induced Melt Kinetics in a Porous Solid Using Time-Resolved X-Ray Diffraction*  
ANIRBAN MANDAL (Presenter), BRIAN JENSEN, Shock and Detonation Physics (M-9), Los Alamos National Laboratory, Los Alamos, NM 87545, USA, MATTHEW HUDSPETH, SETH ROOT, Dynamic Material Properties, Sandia National Laboratories, Albuquerque, NM 87185, USA, RYAN CRUM, MINTA C AKIN, Physics Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA — Time-resolved x-ray diffraction was used to obtain direct (real time) evidence of shock-induced melting and associated kinetics in a porous solid (aluminum (Al) powder). Broadening of the Debye-Scherrer ring corresponding to the (111) peak of Al provided unambiguous evidence of melting. Our data showed that complete bulk melting of the powder could take in excess of 450 ns even when it is shocked to equilibrium pressure-temperature states above the melt boundary. Information on the melt kinetics obtained from our work provide insight into the thermal equilibration time and thermal diffusivity of the material under high-pressure dynamic loading, which are essential to developing well-constrained heat transfer and melting models for Al powder and other porous materials (LA-UR-18-30166).

*Acknowledgments to A.M. and B.J.J. acknowledge financial support from Los Alamos National Laboratory's Science Campaigns, Joint Munitions Program (JMP), and MaRIE concept, and National Security Technologies' Shock Wave Physics Related Diagnostic programs. M.H. and S.R. acknowledge financial support provided by the Truman fellowship (LDRD) and Science Campaigns within Sandia National Laboratories. R.C. and M.C.A were supported by Lawrence Livermore National Laboratory's LDRD program (tracking no. 16-ERD-010).

4:06PM C17.00007: In situ X-ray diffraction of Ce melting under shock loading  
MATTHEW T BEASON (Presenter), BRITTANY BRANCH, BRIAN JENSEN, Los Alamos National Laboratory — With 7 observed crystalline phases below 20 GPa, cerium exhibits a complex phase diagram. In particular, the γ-α phase transition exhibits a large volume collapse (13%-16%) resulting in a low melting pressure for a metal. Sound speed measurements have shown that Hugoniot intersects the melt boundary at 10 GPa with complete melting near 18 GPa; however, the processes and timescales involved are not yet known. This work presents experiments performed at the Dynamic Compression Sector examining the phase evolution of γ-Ce under shock loading. The results indicate that γ-Ce and α-Ce coexist with liquid Ce at pressures near the onset of melt. With increasing pressure, α-Ce is no longer observed; however, γ-Ce persists after impact at pressures beyond 18 GPa. The results indicate significant kinetics, with complete melting observed 200 ns after impact. An experiment performed below the melting pressure shows that the γ-α transition occurs over a similar timescale, with visible peaks for γ-Ce and α-Ce observed over 50 ns after impact. As a result, the γ-α transition appears to exhibit occurs over a relatively long timescale, which is surprising for an isostructural phase transition, and appears to be a significant barrier to melting. (LA-UR-18-30167)
suggest a melting temperature, with diffuse X-ray scattering and visual changes in the sample before and after laser-heating. At POPOV, ROSTISLAV HRUBIAK, High Pressure Collaborative Access Team (HP-CAT), Argonne National Laboratory, NIKOLA DRAGANIC, Shock and Detonation Physics (M-9), Los Alamos National Laboratory, YOGESH KUMAR VOHRA, Department of Physics, University of Alabama at Birmingham, NENAD VELISAVLJEVIC, Shock and Detonation Physics (M-9), Los Alamos National Laboratory — Robust modeling of shock phenomena requires accurate and precise experimental measurements of equations of state and phase diagrams. Zirconium is of particular interest in nuclear applications because of its low neutron cross section. Here, we present the thermal equation of state and melting curve of ultra-high purity Zr in the body-centered cubic (bcc) phase measured using the laser-heated diamond-anvil cell (LHDAC) coupled with in situ synchrotron-based X-ray diffraction (XRD). From quasi-hydrostatic room-temperature compression to pressure ($P$) = ~70 GPa using helium as a pressure transmitting medium, we constrain the bcc-Zr bulk modulus, $K_0 = 120(7)$ GPa and its pressure derivative, $K_0' = 3.0(1)$. Additionally, we have collected LHDAC XRD data over a range of $P = \sim 10 - 40$ GPa and temperature ($T$) = ~1400 – 2200 K to further constrain the bcc-Zr thermal equation of state parameters. Within a separate set of experiments, we have observed melting of bcc-Zr between $P = \sim 10 – 20$ GPa based on plateaus in the $T$ versus laser-power curves coupled with diffuse X-ray scattering and visual changes in the sample before and after laser-heating. At $P = \sim 10$ GPa, initial results suggest a melting temperature, $T_m = 2270(50)$, that implies a melting curve slope of ~14 K/GPa.

2:30PM C17.00009: Melting Line and Structure of Hot dense Fluids probed by X-ray diffraction [Invited] GUNNAR WECK (Presenter), DIF, CEA, FRÉDÉRIC DATCHI, IMPMC, Université Pierre et Marie Curie, GASTON GARBARINO, ESRF, SANDRA NINET, IMPMC, Université Pierre et Marie Curie, JEAN-ANTOINE QUEYROUX, THOMAS PLISSON, PAUL LOUBEYRE, MOHAMED MEZOUAR, DIF, CEA — Warm dense simple molecular fluids constitute a large fraction of planetary interiors. Their current microscopic understanding is essentially based on ab-initio calculations. Novel states are predicted such as: ionic water and ammonia, metallic oxygen and hydrogen, or polymerized carbon dioxide and nitrogen with possible first-order transition. These remain to be tested by experiment. In this contribution, we will present some developments which have enabled to perform structural measurements on dense simple molecular fluids in the 100 GPa range and few thousand Kelvin. An elaborate sample environment has been implemented to homogeneously laser heat the molecular system. A multichannel collimator is used to filter the overwhelming x-ray diffraction background contribution from the diamond anvils. A careful data analysis is applied to extract the liquid structure factor and the radial distribution function. Observing the liquid diffraction is essential to unambiguously determine the occurrence of melting. Measurements on laser heated nitrogen, gold and xenon will be presented to illustrate this experimental approach.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C18 DCOMP DCMP DAMOP: Machine Learning Quantum Many-body Models BCEC 156B - Yi Zhang, Cornell University - Tag(s): Focus

2:30PM C18.00001: Quantum Loop Topography for Machine Learning Transport [Invited] YI ZHANG (Presenter), Department of Physics, Cornell University, CARSTEN BAUER, PETER BROECKER, Institute for Theoretical Physics, University of Cologne, PAUL GINSARG, Department of Physics, Cornell University, SIMON TREBST, Institute for Theoretical Physics, University of Cologne, EUN-AH KIM, Department of Physics, Cornell University — Despite the rapidly growing interest in harnessing machine learning in the study of quantum many-body systems, there remains a central challenge in efficiently extracting information from the model simulations of the quantum states and turning the information into formats compatible with the machine learning architecture, such as an artificial neural network. Here we introduce quantum loop topography (QLT): a feature-selection machine learning procedure by evaluating correlators' loop products of the microscopic models at independent Monte Carlo steps. Following the contribution of the current-current correlations, we demonstrate that QLT can probe the distinctive transport properties of diverse states of matter, which are sometimes challenging to access directly. To showcase this approach, we study the emergent superconducting fluctuations as well as the topological phases with quantized Hall transport. We find that the QLT approach detects a change in transport in very good agreement with their established phase diagrams. We also demonstrate that our pre-selection of features relevant to transport allows us to work with a simple neural network, and then offer an interpretation of such a neural network for the analytical decision criteria. The high fidelity and numerical efficiency of our machine learning algorithm also point a way to identify hitherto elusive transport phenomena such as the non-Fermi liquids.
Recent advances in the study of frustrated magnetism with Neural-Network quantum states
KENNY CHOO, TITUS NEUPERT, University of Zurich, GIUSEPPE CARLEO (Presenter), CCQ, Flatiron Institute — Neural-Network quantum states are an actively explored route to solve challenging interacting quantum problems. Early representations of many-body quantum states in terms of artificial neural networks were based on shallow, restricted Boltzmann Machines [1-3]. The benefits of using deeper networks are however emerging in latest research, where the use of suitably adapted deep networks to the quantum domain is proving rewarding. During this talk I will discuss our strategy to represent quantum states using deep convolutional networks. The advantages of this representation will be shown in the particularly challenging case of frustrated magnets in two dimensions. Here, I will show latest applications to the frustrated J1-J2 model on the square lattice. In this case, neural-network quantum states achieve results that are comparable or better than existing state of the art variational methods developed in the past decade.

Symmetries and Many-Body Excitations with Neural-Network Quantum States* KENNY JING CHOO (Presenter), Physik Institut, University of Zurich, GIUSEPPE CARLEO, Center for Computational Quantum Physics, Flatiron Institute, NICOLAS REGNAULT, Laboratoire Pierre Aigrain, Ecole normale superieure, TITUS NEUPERT, Physik Institut, University of Zurich — Artificial neural networks have been recently introduced as a variational ansatz for representing many-body wave functions. While previous efforts have been focused on obtaining ground states, in this work we extend the method to the study of excited states, which is an important task for many condensed matter applications. First, we give a prescription that allows us to target the lowest energy state within a symmetry sector of the Hamiltonian. Second, we give a simple algorithm to compute the low-lying states without symmetries. We demonstrate this approach on the one-dimensional spin 1/2 Heisenberg model and the one-dimensional Bose-Hubbard model and found good agreement where exact results are available. We applied our approach using both the restricted Boltzmann machine (RBM) and the feedforward neural network (FFNN). Interestingly, we obtained more accurate results using a deeper FFNN as compared with a shallower RBM with comparable number of variations parameters.

*European Unions Horizon 2020 research and innovation program (ERC-StG-Neupert-757867- PARATOP)

Learning Quantum Models from Symmetries ELI CHERTKOV (Presenter), BENJAMIN VILLALONGA, BRYAN CLARK, University of Illinois at Urbana-Champaign — Inverse method algorithms that learn models from data, such as machine learning algorithms, have been successful in solving complicated engineering tasks and are increasingly being applied to study quantum systems. Moreover, inverse methods have the potential to automate the discovery of quantum materials with desired properties. With this goal in mind, we present an inverse method algorithm for learning quantum models, i.e., Hamiltonians, from symmetries or integrals of motion. The forward problem of starting from a given Hamiltonian and finding its symmetries, is generically difficult both analytically and numerically. Yet, despite the difficulty of the forward problem, we show that this method can efficiently solve the inverse problem of starting from a desired set of symmetries and finding Hamiltonians obeying those symmetries. In this talk, we describe this inverse method and give examples of its application.

Parent hamiltonians of restricted Boltzmann machine wavefunctions* SAMUEL LEDERER (Presenter), EUN-AH KIM, Cornell University — Wavefunctions based on the restricted Boltzmann machine (RBM) architecture have recently been found to be highly effective in variational calculations on interacting spin models. The promise of RBMs for compactly encoding quantum states motivates study of the structure underlying RBM wavefunctions. Here we tackle the question of what hamiltonians take RBM wavefunctions as eigenstates. Using a recently developed framework for identifying local hamiltonians from wavefunctions, we consider a select set of RBM states, and comment on the features of their parent hamiltonians.

*Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-SC0018946
Learning a local Hamiltonian from local measurements

EYAL BAIREY (Presenter), ITAI ARAD, NETANEL LINDNER, Physics, Technion - Israel Institute of Technology — Recovering an unknown Hamiltonian from measurements is an increasingly important task for certification of noisy quantum devices and simulators. Recent works have succeeded in recovering the Hamiltonian of an isolated quantum system with local interactions from long-ranged correlators of a single eigenstate. Here, we show that such Hamiltonians can be recovered from local observables alone, using computational and measurement resources scaling linearly with the system size. In fact, to recover the Hamiltonian acting on each finite spatial domain, only observables within that domain are required. The observables can be measured in a Gibbs state as well as a single eigenstate; furthermore, they can be measured in a state evolved by the Hamiltonian for a long time, allowing to recover a large family of time-dependent Hamiltonians. We derive an estimate for the statistical recovery error due to approximation of expectation values using a finite number of samples, which agrees well with numerical simulations.

Accelerating Density Matrix Renormalization Group Computations with Machine Learning

JACOB MARKS (Presenter), Physics, Stanford University, HONG-CHEN JIANG, THOMAS DEVEREAUX, SIMES, SLAC, and Stanford University — Density Matrix Renormalization Group (DMRG) has achieved great success as a technique for simulating one-dimensional and quasi-two-dimensional quantum systems. One major bottleneck for these computations is the variational procedure for ground state approximation. We investigate the application of machine learning methods to this problem and improve convergence time for various classes of strongly correlated systems.

Observation of topological phenomena in a programmable lattice of 1,800 qubits

JUAN CARRASQUILLA (Presenter), Vector Institute — Here we demonstrate a large-scale quantum simulation of this phenomenon in a network of 1,800 in situ programmable superconducting flux qubits arranged in a fully-frustrated square-octagonal lattice. Essential to the critical behavior, we observe the emergence of a complex order parameter with continuous rotational symmetry, and the onset of quasi-long-range order as the system approaches a critical temperature. We use a simple but previously undemonstrated approach to statistical estimation with an annealing-based quantum processor, performing Monte Carlo sampling in a chain of reverse quantum annealing protocols. Observations are consistent with classical simulations across a range of Hamiltonian parameters. We anticipate that our approach of using a quantum processor as a programmable magnetic lattice will find widespread use in the simulation and development of exotic materials.

Self-learning with neural networks in determinant quantum Monte Carlo studies of the Holstein model.

SHAOZHI LI, Physics, University of Michigan, PHILIP DEE (Presenter), University of Tennessee, EHSAN KHATAMI, Physics, San Jose State University, STEVEN JOHNSTON, University of Tennessee — Machine learning techniques have recently occupied the focus of many investigators in computational many-body physics. In particular, some practitioners of quantum Monte-Carlo have considered the efficacy of various "Self-Learning" techniques which aim to reduce CPU runtime associated with updates and autocorrelation times. We have used artificial neural networks (NN) within determinant quantum Monte-Carlo to improve the scaling of CPU runtime with typical system parameters. This work focuses on a singleband Holstein Hamiltonian, which models Einstein phonons coupled to on-site electrons. We have implemented both fully connected and convolutional NN and used them to study the metallic and insulating phases of this model. To close, we will assess the generality of this approach to other model systems.

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering. P.D. acknowledges support from the U.S. Department of Energy, SCGSR program administered by ORISE for the DOE under contract No. DE-SC0014664. E.K. acknowledges support from the NSF under Grant No. DMR-1609560.
4:42PM C18.00010: Unsupervised manifold learning of ground state wave functions*  MICHAEL MATTY (Presenter), YI ZHANG, Cornell University, SENTHIL TADADRI, Massachusetts Institute of Technology, EUN-AH KIM, Cornell University — Quantum many-body wave functions are complex objects that encode much information, but it can be challenging to back out the information. In particular, there is no good way to assess whether a given wave function can be a ground state of some local Hamiltonian. Here we employ an unsupervised machine learning algorithm well-suited for discovering trends in high-dimensional space: manifold learning. We apply our approach to a band insulator and the toric code and demonstrate that our approach can separate ground state wave functions from excited state wave functions without any prior knowledge.

*This work was partially supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875). This work also acknowledges support by the National Science Foundation (Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)) under Cooperative Agreement No. DMR-1539918.

4:54PM C18.00011: Machinery representation of physics models via structured self-attention network  JUNWEI LIU (Presenter), Hong Kong University of Science and Technology, YANG ZHANG, Max Planck Institute for Chemical Physics of Solids, YUJUN ZHAO, Hong Kong University of Science and Technology — Recently machine learning techniques, especially deep neural networks, are widely used to identify phases and phase transition and speed up the simulations in variety of physical models. However, deep neural networks are often required to model the energy or partition function, which results in heavy computational cost and also limits the application to large system. In this work, we proposed a structured self-attention neural network approach, inspired by mean field theory, to represent the original Hamiltonian via well-structured neural layers. We experiment with the ring exchange Ising model and double exchange model, and show these two models can be well represented by pseudo spin layers and local field layers. Quite different from the sequential neural network, which stores all the information in every single layer, the separation strategy achieves significantly less training time, higher accuracy and straightforward application to large system. We therefore believe the new structural network would also be highly efficient to identify different phases and accelerate the numerical simulations for even complex models.

5:06PM C18.00012: Neural Network Renormalization Group*  SHUO-HUI LI (Presenter), LEI WANG, Institute of Physics — We present a variational renormalization group (RG) approach using a deep generative model based on normalizing flows. The model performs hierarchical change-of-variables transformations from the physical space to a latent space with reduced mutual information. Conversely, the neural net directly maps independent Gaussian noises to physical configurations following the inverse RG flow. The model has an exact and tractable likelihood, which allows unbiased training and direct access to the renormalized energy function of the latent variables. To train the model, we employ probability density distillation for the bare energy function of the physical problem, in which the training loss provides a variational upper bound of the physical free energy. We demonstrate practical usage of the approach by identifying mutually independent collective variables of the Ising model and performing accelerated hybrid Monte Carlo sampling in the latent space.

*The work is supported by the Ministry of Science and Technology of China under the Grant No. 2016YFA0300603 and the National Natural Science Foundation of China under Grant No. 11774398.

5:18PM C18.00013: Learning density functional theory mappings with extensive deep neural networks and deep convolutional inverse graphics networks*  KEVIN RYCZKO (Presenter), Department of Physics, University of Ottawa, DAVID STRUBBE, Department of Physics, University of California, Merced, ISAAC TAMBLYN, National Research Council of Canada — In this work, we show that deep neural networks (DNNs) can be used in conjunction with Kohn-Sham density functional theory (KS-DFT) for two-dimensional electron gases in simple harmonic oscillator and random potentials. Using calculations from the Octopus real-space DFT code we show that extensive DNNs (EDNNs) can learn the mappings between the electron density and exchange, correlation, external, kinetic and total energies simultaneously. Our results hold for local, semi-local, and hybrid exchange-correlation functionals. We then show that the external potential can also be used as input for an EDNN when predicting the aforementioned energy functionals, bypassing the KS scheme. Additionally, we show that EDNNs can be used to map the electron density calculated with a local exchange-correlation functional to energies calculated with a semi-local exchange correlation functional. Lastly, we show that deep convolutional inverse graphics networks can be used to map external potentials to their respective self-consistent electron densities. This work shows that EDNNs are generalizable and transferable given the variability of the potentials and the ability to scale to an arbitrary system size with an O(N) computational cost.

*The authors would like to thank NSERC.
2:30PM C19.00001: Quantum Monte Carlo Study of Strongly Interacting Fermi Gases in Two Dimensions: BCS-BEC Crossover, Spin-orbit Coupling, and Dynamical Response Functions* [Invited] HAO SHI (Presenter), Simons Foundation, PETER ROSENBERG, SIMONE CHIESA, ETTORE VITALI, College of William and Mary, SHIWEI ZHANG, Simons Foundation — We describe recent advances in auxiliary-field quantum Monte Carlo techniques, which enable calculations on large lattices to reliably compute ground-state and excited-state properties in the thermodynamic limit. Exact calculations are performed on the two-dimensional strongly interacting, unpolarized, uniform Fermi gas with a zero-range attractive interaction. An equation of state is obtained, with a parametrization provided, which can serve as a benchmark and allow accurate comparisons with experiments. The pressure, contact parameter, and condensate fraction are determined systematically vs. the interaction strength. Rashba spin-orbit coupling is then included to examine its interplay with superfluidity and the resulting pairing and spin structures and correlations. The imaginary-time propagation of Slater determinants is used to compute the pairing gap in the two-dimensional Fermi gas. The spectral functions, and the density and spin structure factors are then obtained using analytic continuation to provide unique tools to visualize the BEC-BCS crossover. We will also discuss briefly calculations in optical lattice systems and comment on the prospect for precision calculations in spin-imbalanced systems.

*Supported by NSF, DOE, and the Simons Foundation.

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3:06PM C19.00002: "Quasielectrons in Lattice Moore–Read Models" SOURAV MANNA (Presenter), Quantum Many-Body Systems, Max Planck Institute for the Physics of Complex Systems, D-01187, Dresden, Germany, JULIA WILDEBOER, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky, 40506-0055, USA, ANNE E. B. NIELSEN, Quantum Many-Body Systems, Max Planck Institute for the Physics of Complex Systems, D-01187, Dresden, Germany — Anyons are fractionally charged quasiparticles which are neither fermions nor bosons. Anyons exhibit fractional statistics and important for topological quantum computation. Anyonic Moore–Read states provides a well explored description for the insertion of quasiholes in the continuum. However, quasielectron insertion creates a singularity in the continuum state which further complicates the problem. In this work we show that the singularity problem can be avoided by placing quasielectrons in fractional quantum Hall lattice systems. We construct Moore–Read Pfaffian states for filling fraction 5/2 and incorporate quasiholes and quasielectrons. We investigate density profile, charge, size and braiding properties of the anyons by means of a Metropolis Monte Carlo simulation. Further we derive a few body parent Hamiltonian for the states. Additionally we investigate density profile, charge and shape of the anyons in the Kapit–Mueller model by employing an exact diagonalization technique. We compare our results for the analytical states with the anyons in the Kapit–Mueller model.

3:18PM C19.00003: Dispersion Relation of the GMP Mode in the Nematic Phase of Fractional Quantum Hall States* UMANG MEHTA (Presenter), DAM THANH SON, Physics, University of Chicago — We compute the dispersion relation for the GMP mode of the fractional quantum Hall effect in the nematic phase for Jain sequences at large N using Golkar, Nguyen, Roberts and Son’s ‘higher-spin theory’ for magnetorotons. The dispersion relation is computed to all orders in the momentum expansion and is valid wherever the momentum expansion holds. It captures the magnetoroton minimum at finite momentum in the regime where the momentum expansion still holds.

*This work is supported, in part, by DOE grant No. DE-FG02-13ER41958 and a Simons Investigator grant from the Simons Foundation.
3:30PM C19.00004: Interacting Chern insulators: Diagrammatics well beyond the lowest order*  
IGOR TUPITSYN (Presenter), NIKOLAI PROKOF’EV, University of Massachusetts Amherst — We study phase diagram of the interacting spin-1/2 Haldane model with chiral phase $\varphi=\pi/2$ at half-filling. Both on-site and long-range Coulomb repulsive interactions (Haldane-Hubbard-Coulomb model) are considered. The problem with on-site interaction $U$ alone was addressed in the past by a variety of approximate and finite size methods that produced results in disagreement with each other both quantitatively and qualitatively. Conventional Quantum Monte Carlo methods, capable of dealing with "reasonable" system sizes, are ineffective here due to the fermionic sign problem. We employ the Diagrammatic Monte Carlo (DiagMC) technique to (i) accurately locate topologically nontrivial phases in the $(\triangle, U)$-plane ($\triangle$ is the inversion symmetry breaking on-site energy) and (ii) demonstrate the strong effect of typically discarded in theoretical considerations long-range part of the Coulomb interaction. The DiagMC technique is not subject to the conventional fermionic sign problem and allows one to deal with arbitrary shape of interaction potential in an approximations free manner. Final results with controlled accuracy are obtained by computing vertex corrections from higher-order diagrams until convergence is reached.

*We thank the Simons Collaboration on the Many Electron Problem for support.

3:42PM C19.00005: Critical torus spectrum of the Gross-Neveu-Yukawa field theory*  
MICHAEL SCHULER, Institute for Theoretical Physics, University of Innsbruck, STEPHAN HESSELMANN (Presenter), Institute for Theoretical Solid State Physics, RWTH Aachen University, SETH WHITSITT, Joint Quantum Institute, NIST and the University of Maryland, THOMAS C LANG, Institute for Theoretical Physics, University of Innsbruck, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University, ANDREAS LÄUCHLI, Institute for Theoretical Physics, University of Innsbruck — We compute the low-energy critical torus spectrum of the Gross-Neveu-Yukawa universality class, which features $N=4$ component Dirac spinors that spontaneously break a $Z_2$ chiral symmetry, in $D=(2+1)$ dimensions. A possible lattice realization of such Dirac fermions is provided by the interacting $t$-$V$ model of spinless fermions on the honeycomb lattice. We use a combination of Exact Diagonalization and Quantum Monte Carlo simulations to compute the energy spectrum on finite-size clusters with periodic boundaries, and perform an extrapolation to the thermodynamic limit. We show that the interaction between the spinor field and the scalar order-parameter field strongly influences the torus spectrum at the critical point, and propose the critical spectrum as a universal fingerprint of the critical Gross-Neveu-Yukawa field theory. Moreover, we estimate the renormalization of the Fermi velocity in the Dirac phase from the interaction induced corrections to the energy spectrum, and extrapolate the observed linear renormalization up to the critical point. Finally, we contrast the Fermi velocity renormalization in the spinless $t$-$V$ model with the situation in the spinful Hubbard model.

*FWF project I-2868-N27, FWF project F4018, DFG project RTG 1995 and DFG project FOR 1807.

3:54PM C19.00006: Unconventional pairing symmetry of interacting Dirac fermions on a π-flux lattice  
HUAIMING GUO (Presenter), Department of Physics, Beihang University — The pairing symmetry of interacting Dirac fermions on the π-flux lattice is studied with the determinant quantum Monte Carlo and numerical linked-cluster expansion methods. The $s^*$- (i.e., extended s-) and d-wave pairing symmetries, which are distinct in the conventional square lattice, are degenerate under the Landau gauge. We demonstrate that the dominant pairing channel at strong interactions is an unconventional $ds^*$-wave phase consisting of alternating stripes of $s^*$- and d-wave phases. A complementary mean-field analysis shows that while the $s^*$- and d-wave symmetries individually have nodes in the energy spectrum, the $ds^*$ channel is fully gapped. The results represent a new realization of pairing in Dirac systems, connected to the problem of chiral d-wave pairing on the honeycomb lattice, which might be more readily accessed by cold-atom experiments.
4:06PM C19.00007: Universal trends in interacting two-dimensional Dirac materials* SAIKAT BANERJEE (Presenter), Condensed Matter Physics, University of Augsburg, Germany, DAVID ABERGEL, Condensed Matter Physcis, Nordic Institute for Theoretical Physics, HANS AGREN, Theoretical Chemistry and Biotechnology, KTH Royal Institute of Technology, Sweden, GABRIEL AEPLLI, Condensed Matter Physcis, Paul Scherrer Institute, ALEXANDER BALATSKY, Condensed Matter Physcis, Nordic Institute for Theoretical Physics — We investigate the extent to which the category of Dirac materials provides general statements about the behavior of both fermionic and bosonic Dirac quasiparticles in the interacting regime. For both quasiparticle types, we find common features in the renormalization of the conical Dirac spectrum by interactions. This feature motivates us to declare that Dirac materials form a separate and well-defined category with universal properties. To support this view, we compute the self-energy for both types of quasiparticles with different interactions and collate previous results from the literature whenever necessary. The computations are performed both at zero and finite temperature. Guided by the systematic presentation of our results in Table I, we conclude that long-range interactions generically lead to an increase of the slope of the single particle Dirac cone, whereas short-range interactions lead to a decrease. The quasiparticle statistics does not impact the self-energy correction for long-range repulsion but does affect the behavior of short-range coupled systems, giving rise to different thermal power-law contributions.

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KAW-2013.0096, KAW-2013.0020
VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744)

4:18PM C19.00008: Universal Fermi-surface anisotropy renormalization for interacting Dirac fermions with long-range interactions* SHAFFIQUE ADAM (Presenter), Yale-NUS College, JIA NING LEAW, HO KIN Y TANG, MAXIM TRUSHIN, National University of Singapore, FAKER ASSAAD, Universität Würzburg, SANKAR DAS SARMA, University of Maryland — Recent evidence suggest an intriguing universal relationship between the Fermi surface anisotropy of the non-interacting parent two-dimensional electron gas and the strongly correlated composite Fermi liquid formed in a strong magnetic field close to half-filling. Inspired by these observations, we explore more generally the question of anisotropy renormalization in interacting 2D Fermi systems. Using a recently developed [1] non-perturbative and numerically-exact projective quantum Monte Carlo simulation as well as other numerical and analytic techniques, only for Dirac fermions with long-range Coulomb interactions do we find a universal square-root decrease of the Fermi-surface anisotropy [2]. Our proposed universality can be tested in several anisotropic Dirac materials including graphene, topological insulators and organic conductors.


*Supported by the Singapore Ministry of Education (MOE2017-T2-1-130)

4:30PM C19.00009: Energy scales and quasi-particle behavior of fermions in the normal state of flat-band systems* PRAMOD KUMAR (Presenter), Department of Applied Physics, Aalto University, VANHALA TUOMAS, Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig Maximilians-University, Munich, Germany, SEBASTIANO PEOTTA, PAIVI TORMA, Department of Applied Physics, Aalto University — We explore the energy scales and quasi-particle behavior in the paramagnetic normal state of the repulsive Hubbard model on the Lieb lattice. The special geometry of the Lieb lattice, a face-centered 2D square lattice, has a flat dispersion, which leads to various novel electronic phases with the inclusion of many-body interactions [1, 2]. Singularity in the density of states can lead to the breakdown of quasi-particle behavior at finite temperature. The interplay of the singularity and the interaction determine the energy scale to observe such non-Fermi liquid behavior. We address this using dynamical mean field theory (DMFT), a very well-established methodology for correlated many-body systems. We have used continuous-time quantum Monte Carlo (CTQMC), an exact impurity solver, within DMFT. We also comment on particle-hole mapping between attractive and repulsive Hubbard model with a unitary transformation and the corresponding electronic properties.


*Academy of Finland and European Research Council
It is demonstrated by explicit construction that the intricate links among short-range-entangled (SRE) states across different dimensions have a vivid embodiment in the realm of symmetry protected topological (SPT) phases with crystalline symmetry. We systematically study three-dimensional bosonic topological phases protected by any space group symmetry $G$. We prove that these phases are classified by $H_{\varphi}^5(G;\mathbb{Z}) \times H_{\varphi}^1(G;\mathbb{Z})$, where $\varphi$ indicates $g \in G$ acting on $\mathbb{Z}$ as multiplying $\varphi(g)=\pm 1$ depending on whether orientation is preserved by $g$ or not. The factor $H_{\varphi}^5(G;\mathbb{Z})=H_{\text{Borel}}^4(G;U(1))$, known as the group cohomology proposal for classifying bosonic SPT phases, corresponds to only the phases presented by some SRE 2-skeleton without presence of $E_8$ state or its multiples (i.e., two-dimensional chiral bosonic phases characterized by quantized thermal Hall effect). The extra factor $H_{\varphi}^1(G;\mathbb{Z})$ describes inequivalent $E_8$ state configurations and can be easily read off directly from the international (Hermann-Mauguin) symbol for $G$. Moreover, our result supports the Generalized Cohomology Hypothesis in the case of crystalline symmetries.

*H.S. acknowledges financial support from the Spanish MINECO grant FIS2015-67411, the CAM research consortium QUITEMAD+ S2013/ICE-2801, and Grant FEI-EU-17-14 PICC.
Transferable screened range-separated hybrids for layered materials  
ASHWIN RAMASUBRAMANIAM (Presenter), Mechanical & Industrial Engineering, University of Massachusetts Amherst, DAHVYD WING, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science — The optoelectronic properties of layered semiconductors can vary significantly between bulk (3D) phases and their single- or few-layer, 2D counterparts. In particular, the vastly different asymptotic behavior of dielectric screening in 2D and 3D structures poses a challenge for designing screened range-separated hybrid (SRSH) functionals that are accurate for both bulk and low-dimensional systems. We present a simple yet effective approach for simultaneously tuning the fraction of short-range exact exchange and the range-separation parameter that delivers tuned SRSH functionals for 2D sheets and 3D bulk phases of layered semiconductors. The ground-state SRSH eigenvalues are found to be in excellent agreement with bandstructures from accurate, manybody GW calculations. Excited state properties are predicted using time-dependent DFT calculations, based on the SRSH functional, and are also found to be in good agreement with absorption spectra obtained from GW and Bethe-Salpeter (BSE) calculations. The ability to develop SRSH functionals that are only material- but not structure-specific opens up avenues for systematic and accurate studies of layered materials and their nanostructures at a fraction of the cost of many-body calculations.

First-principles study of bioinspired perylene diimide molecular nanowires*  
ALIYA MUKAZHANOVA (Presenter), Division of Materials Science and Engineering, Boston University, NATHAN FREY, Department of Physics, Boston University, KASIDET TRERAYAPIWAT, Department of Chemistry, Boston University, AMIR MAZAHERIPOUR, ANDREW BARTLETT, HUNG NGUYEN, ALON A. GORODETSKY, Department of Chemical Engineering and Materials Science, University of California, Irvine, SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University — Perylene-3,4,9,10-tetracarboxylic diimide (PTCDI) has excellent electrochemical and photophysical properties that makes it a promising material for optoelectronic devices. Molecular nanowires consisted from PTCDI derivatives can be placed in DNA like base by standard automated oligonucleotide synthesis. Here, we study the electronic and optical properties of a series of recently synthesized bioinspired perylene diimide molecular nanowires by first-principles density functional theory (DFT) spectroscopy and molecular dynamics (MD). We apply time-dependent DFT with Franck-Condon analysis to study our material. Initial structures are taken from MD and the final vibronic spectra is an average over many structures. By stacking the molecules along a DNA-like backbone and varying the number of stacked molecules from one to four, we determine the role of inter-molecular interactions on the excited-state energetics, as well as vibrational excitations within the molecules. We demonstrate that strong inter-molecular interactions lead to distinct vibrational, electronic, and optical properties for design of new electronic and optoelectronic nanowires.

Phase stability of MnSe, MnTe, and VO2 from total energies in the random phase approximation*  
STEPHAN LANY (Presenter), National Renewable Energy Laboratory — While the limitations (semi-)local density functionals for the electronic structure are widely acknowledged, total energies are usually considered to be rather accurate. However, in transition metal compounds, standard density or even hybrid functionals often predict the wrong ground state structure. Total energy calculations in the random phase approximation (RPA) greatly improve the phase stability prediction, e.g., rock-salt vs wurtzite in MnO, but quantitative predictions are still sensitive on input wavefunction for the RPA energy [1]. Here, we calculate the phase stability for MnSe and MnTe in the rocksalt, nickeline, and wurtzite structures, for the "negative-pressure" phase in MnSeTe alloys [2]. To account for the wavefunction dependence, we perform a variational minimization of the RPA energy with respect to the onsite potentials U and V [1]. In VO2, the failure of standard DFT to produce a band gap can be remedied by simple DFT+U calculation, at the expense of the incorrect prediction that the undistorted antiferromagnetic phase is lower in energy than the experimentally known nonmagnetic monoclinic phase. We further discuss results based on the SCAN functional.


*DOE-SC-BES (EFRC)
3:54PM C20.00006: Can exact (local) Kohn-Sham potential reproduce band gaps?: Analysis using an analytically solvable two- and three-body models*  YU-ICHIRO MATSUSHITA (Presenter), Tokyo Institute of Technology, TAICHI KOSUGI, The University of Tokyo — We have clarified whether the exact (local) Kohn-Sham(KS) potential reproduces the exact band gap or not [1]. We have investigated the analytically solvable interacting two- and three-body models and calculated the exact electron levels through the one-particle Green's function of the two-body system analytically. Subsequently, we constructed the exact KS potential analytically and compared the obtained KS levels with exact ones. Then, we have found that KS-DFT even with the exact (local) KS potential does not reproduce the exact band gaps.


*This research was supported by MEXT as “Exploratory Challenge on Post-K computer” (Frontiers of Basic Science: Challenging the Limits).

4:06PM C20.00007: Wannier Koopmans method for band gap calculations of extended systems*  LIN-WANG WANG (Presenter), Lawrence Berkeley National Laboratory, MOUYI WENG, FENG PAN, School of Advanced Materials, Peking University, Shenzhen Graduate School — We have developed a method to correct the density functional theory band gap problem, especially for extended systems. In this method, the Wannier functions are generated and the Hamiltonian is required to satisfy the Koopman theory (the total energy is linearly dependent on the occupation number) when a Wannier function is partially occupied. The resulting Hamiltonian gives a correction term for the Kohn-Sham eigen equation. This method can be considered as an extension of the delta DFT method to bulk systems. We have used this method to study common semiconductors, alkali halides, 2D materials, organic crystals, as well as oxides. We found in general, the accuracy of this Wannier Koopman method (WKM) is on a par with the GW results.


*This work was supported by SC/BES/MSED under Contract No. DE-AC02-05CH11231, through the Material Theory program.

4:18PM C20.00008: WITHDRAWN ABSTRACT

4:30PM C20.00009: High-Harmonic Gereration with quantized fields: Minimal coupling of Pauli Spinors to quantized electromagnetic fields  MARY-LEENA MARTINE TCHENKOE DJOUOM (Presenter), DAVIS DAVE WELAKUH, MICHAEL RUGGENTHALER, HEIKO APPEL, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter — Interaction between classical light and matter lies at the heart of a broad range of applications, such as the generation of spatially and temporally coherent ultraviolet light using the technique of high harmonic generation(HHG)[1]. The semi-classical treatment of HHG is, however, not able to capture the quantum features of light. In the present work, we consider Pauli spinors minimally coupled to quantized electromagnetic fields and investigate HHG with quantized fields. In this talk we will present a numerical implementation of the Pauli-Fierz Hamiltonian and first results for one-dimensional model systems and highlight differences to the usual semi-classical treatment.

Polaritonic chemistry: The influence of mass renormalization

DAVIS DAVE WELAKUH (Presenter), MARY-LEENA MARTINE TCHENKOU DJOUM, MICHAEL RUGGENTHALER, HEIKO APPEL, ANGEL RUBIO, Theory, Max Planck Institute for the Structure and Dynamics of Matter (MPSD) — If molecules are placed inside a cavity or near a plasmonic surface strong light-matter interaction can occur that mixes matter and photon degrees of freedom [1]. This can modify properties of molecules [2] and can even alter chemical reactions due to the changed electromagnetic vacuum. The theoretical descriptions of such novel chemical situations is usually done with simplified few-level models and only recently more advanced ab-initio methods [4] have been developed and applied [5]. However, so far all these considerations have neglected the influence of the changed electromagnetic vacuum on the masses of the particles. That is, while the mass of electrons and nuclei are usually defined with respect to the bare electromagnetic vacuum, in the above cases the electromagnetic vacuum is changed considerably. Here we present first ab-initio studies of how multi-mode fields influence the total mass of the particles and thus change physical observables.


First principles approaches to strong light-matter coupling

JOHANNES FLICK (Presenter), PRINEHA NARANG, Harvard University — In recent years, research at the interface of chemistry, material science, and quantum optics has surged, now opens new possibilities to study strong light-matter interactions at different limits [1,2]. In this new regime, correlated electron, nuclear and photon interactions have to be treated on the same quantized footing [3] and towards this overarching goal, we have introduced a general time-dependent density-functional theory.

In this talk, we review recent developments and show how collective Rabi splitting under strong light-matter coupling emerges for CO2 molecules in optical cavities. Further, we use this novel framework to study how the potential-energy surfaces (PES) of a CO bond stretching in an ensemble of Formaldehyde molecules is modified under collective strong-light matter coupling, demonstrating the novel abilities to alter and open new chemical reaction pathways as well as to create new hybrid states of light and matter in this regime [4].


Time evolution methods for matrix-product states *

SEBASTIAN PAECKEL (Presenter), Georg-August-Universität Göttingen, Institut für Theoretische Physik, ANDREAS SWOBODA, München, Ludwig-Maximilians-Universität, THOMAS KOEHLER, SALVATORE MANMANA, Georg-August-Universität Göttingen, Institut für Theoretische Physik, ULRICH JOSEPH SCHOLLWOECK, München, Ludwig-Maximilians-Universität, CLAUDIUS HUBIG, Garching, Max-Planck-Institut für Quantenoptik — Matrix-product states (MPS) have become the de facto standard for the investigation of one-dimensional quantum many body systems, also out-of-equilibrium. Various approaches have been introduced for computing the time evolution of MPS, e.g., a time-dependent variational principle (TDVP) for MPS as well as matrix product operator (MPOs) representations of the time evolution operator. In this talk I review important developments and compare four commonly used methods applied to five representative examples, including systems with long-ranged interactions or in 2D.

These results give insights to the state-of-the-art treatment of MPS out-of-equilibrium and a guideline for which method to choose for a problem at hand.

*Financial support via Research Unit FOR1807 (project P07) and SFB/CRC (project B03) from the Deutsche Forschungsgemeinschaft (DFG) is gratefully acknowledged.
Calculating Quantum Corrections to Electronic Transport in Disordered Nanostructures

CHENYI ZHOU (Presenter), HONG GUO, Physics, McGill University — Electronic transport in nanostructures shows strong dependencies on disorder and related quantum effects. The leading-order quantum corrections to the diffusive transport were identified as the weak-localization (WL) and the Altshuler-Aronov (AA) effects. An important issue is to develop a numerical method for computing these quantum corrections starting from the atomistic arrangement. To this end, a diagrammatic scheme based on nonequilibrium Green functions is put forward. We employ a nonlocal expansion technique to generate Cooperon diagrams in order to capture WL. We implement this approach using a tight-binding Anderson model to simulate finite wires containing disorder. In WL regime, our computed conductance agrees well with the exact numerical solution, and the WL corrected resistance shows a nonlinear scaling versus the channel length. The WL induced negative magnetoresistance is also investigated. For AA correction, we extend the numerical GW method by dressing interaction vertices with diffusons, and we apply it to a finite Anderson-Hubbard model. Density of states anomalies are found at energies corresponding to bias voltages, and their size dependence is analyzed. The AA effect in nonlinear transport will also be reported.

*We acknowledge support by NSERC Canada (H.G.).

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C21 DCOMP DBIO DMP GSOFT: Exploring Free Energy Landscapes in Biology and Materials Science II

Direct and universal bounded entropy evaluation in complex simulations

RAM AVINERY (Presenter), ROY BECK, Tel Aviv University — Complex physical simulations are ubiquitously employed to characterize thermodynamics in diverse systems; free-energy, or related quantities, are often their goal. While enthalpy is calculable using the apriori choice of interactions (i.e., force-field, coupling parameters), entropy remains a challenge to quantify directly. Typically, methods for free-energy estimation are based on thermodynamic relations (e.g., Jarzynski's equality) rather than the independent statistics of the target ensembles.

We have previously demonstrated a universal entropy calculation scheme using loss-less compression algorithms which delivers a tight upper-bound estimate [1]. In this talk, I will describe another novel information-based approach for estimation of entropy. This new approach establishes tight lower and upper entropy bounds for complex simulations. Our novel method, based on counting statistics, is inherently universal and provides a direct estimate for entropy along with margins of error. Given this method's universality and statistical guarantees, we expect it to be highly useful for both simulated and experimentally recorded systems.


*This work is supported by the Israeli Science Foundation (550/15) and NSF/BSF grant (201696)

Predicting shear transformation events in glasses via energy landscape sampling

BIN XU (Presenter), Beijing Computational Science Research Center, MICHAEL FALK, Johns Hopkins University, JINFU LI, LINGTI KONG, Shanghai Jiaotong University — Shear transformation (ST) events, as the elementary process for plastic deformation of glasses, are of vital importance to understand the mechanical behavior of glasses. Here, by characterizing first-order saddle points in the potential energy landscape, we develop a framework to characterize and to predict the triggering (i.e. locations, triggering strains, and local structural transformations under different shear protocols) of ST events. Verification undertaken with a model Cu-Zr glass reveals that the predictions agree well with athermal quasistatic shear simulations. The proposed framework is believed to provide an important tool for developing a quantitative understanding of the deformation processes that control mechanical behavior of metallic glasses.

*B. X. and L. T. K. acknowledge financial support by the National Key R&D Program of China (2017YFB0701501), the National Natural Science Foundation of China (NSFC, Grants No. 51620105012 and No. 51271114), and MaGIC of Shanghai Jiao Tong University. M. L. F. acknowledges support provided by NSF Grants No. 1408685 and No. 1409560. Computing facility from the rr cluster at Shanghai Jiao Tong University is also acknowledged.
2:54PM C21.00003: Utilizing finger prints to construct the disconnectivity graph. DEB DE (Presenter), BASTIAN SCHEFER, SANTANU SAHA, DANIELE TOMERINI, STEFAN A C GOEDECKER, University of Basel — Theoretical studies have identified the dodecahedron of Si20 H20 as the lowest energy structure among many competing configurations several years ago. However this ground state structure has never been observed experimentally. The characteristics of an energy landscape are ultimately the key to understand the existence of a particular configuration. We employ a fingerprint distance (FP)-based exploration of the Potential Energy Surface, to establish relationships between the minima and their connecting transition states (saddle points of the PES). We apply this in a comparative investigation of Si20H20 with two existing structures, namely the C60 and C20H20 fullerenes. The striking differences between the PES of these three systems are used to understand why the global minimum is experimentally observed only for C60 and C20H20. We show that the complex pathways between different metastable configurations and the ground state of the Si20H20 cluster explain the lack of observation of the global minima configuration in experiment.

3:06PM C21.00004: Three birds with one stone: reaction coordinate, thermodynamics and kinetics from all-atom molecular simulations* PRATYUSH TIWARY (Presenter), University of Maryland, College Park — Many molecular systems involve processes with intertwined spatio-temporal resolutions ranging from femtoseconds to days, making it hard to probe them completely using traditional experimental tools. It has been a holy grail to simulate these in all-atom resolution using molecular dynamics methods, but these can go up to only a few hundred microseconds even with the most powerful and custom-built supercomputers. Thankfully, over the decades several sampling algorithms have been proposed that can simulate these complex systems in an accelerated but controllable manner. However, a large class of these methods (arguably all!) need an a priori sense of a low-dimensional reaction coordinate (RC) even before performing the sampling. This has severely limited the usefulness of such sampling methods. In order to deal with this cyclic problem where one needs extensive sampling of the rare events to know the RC, but also needs to know the RC in the first place to perform sampling, it is thus extremely desirable to construct methods that learn the RC as they perform the sampling. Here we will describe two such methods, namely SGOOP [1,2] and RAVE [2] developed by us that use flavors of statistical mechanics and deep learning to solve this problem. We will demonstrate the generality and power of these methods by showing how they give direct predictive insight into biologically important problems such as mechanisms of ligand-protein (including T4L99A lysozyme and tyrosine kinases), and transcription factor-DNA (including Epstein Barr virus binding domain) interactions. Our findings includes an all-atom characterization of metastable and transition states, their stabilities, various rate constants, as well as prediction of deleterious point mutations in the system which could upend the functioning of the protein, DNA or the ligand.

3:42PM C21.00005: Nucleation Kinetics using Generalized Ensemble Simulations* MURALIKRISHNA RAJU, DEEPTI BALLAL, Ames Laboratory, Iowa State University, Ames, XUEYU SONG (Presenter), Department of Chemistry and Ames Laboratory, Iowa State University, Ames, IA50011 — The recently developed generalized replica exchange method (gREM) is employed to sample various coexistence phases efficiently, especially the crystal cluster coexisting with its liquid phase. Namely, the gREM method facilitates comprehensive sampling of phase-transition regions by transforming metastable or unstable energy states in the canonical ensemble to stable ones in the generalized ensemble. Using weighted histogram analysis method (WHAM) analysis, the Gibbs energy as a function of temperature curves can be constructed for the liquid, crystal and various coexisting states. Thus, the nucleation barrier can be extracted without using the classification scheme of liquid and crystal particles. Using the classical nucleation theory, applications to the nucleation kinetics of mW water model and NaCl melt demonstrate that the nucleation rate obtained from our simulation method agrees well with the direct measured nucleation rate from simulations with the same model.

*This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering. The research was performed at the Ames Laboratory. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358.
3:54PM C21.00006: Understanding inverted solubility through specialized patchy particle models*  
IREM ALTAN (Presenter), Duke University, AMIR KHAN, Trinity College Dublin, SUSAN JAMES, MICHELLE QUINN, Maynooth University, PATRICK CHARBONNEAU, Duke University, JENNIFER MCMANUS, Maynooth University — The high specificity and anisotropy of protein-protein interactions give rise to remarkably rich phase and assembly behaviors. A thorough understanding of these interactions is notably key to forming crystals for protein structure determination. Despite the inherent complexity of these biomolecular systems, coarse-grained patchy models can be used to elucidate the physico-chemical processes that govern protein self-assembly. Here, we consider crystal formation in certain mutants of human γD-crystallin, which remarkably form assemblies that become less soluble as temperature increases. We find that using a minimal patchy model with temperature-deactivated patches recapitulates this inverted solubility trend and provides microscopic insights into the origin of this unusual behavior. This finding provides physical constraints for the observation of retrograde solubility in soft matter more generally.

*National Science Foundation Grant No. DMR-1749374  
Extreme Science and Engineering Discovery Environment (XSEDE)  
Open Science Grid

4:06PM C21.00007: Spikes to Hills: A Continuation of Sticky Hard Sphere Clusters to Long Range Clusters*  
ANTHONY TRUBIANO (Presenter), MIRANDA HOLMES-CERFON, Math, Courant Institute of Mathematical Sciences — Energy landscapes for particles with short range interactions are notoriously difficult to explore computationally. To study the sensitivity of these landscapes to parameters of the interaction potential, we start with the most rugged landscape, the set of sticky hard sphere clusters, and use a continuation procedure to evolve the clusters as the range of the potential increases. This procedure captures most local minima of the smoother landscapes, with those missing being mostly high energy clusters. As the potential smoothens, we characterize the merging of clusters by a graph with tree structure. We find these graphs to be insensitive to the interaction strength at short range, but the graphs corresponding to a Lennard-Jones potential vary more than those for a Morse potential at longer range.

*Anthony Trubiano was supported in part by the Research Training Group in Modeling and Simulation funded by the National Science Foundation via grant RTG/DMS – 1646339.

4:18PM C21.00008: Surveying the Free Energy Landscape of Attractive Colloidal Spheres  
SHANGHUI HUANG (Presenter), Chemistry and Biochemistry, University of Notre Dame, JONATHAN WHITMER, Chemical and Biomolecular Engineering, University of Notre Dame — Controlling the assembly of colloidal particles into specific structures has been a long-term goal in the soft materials community. Much can be learned from the process from the self-assembly by examining the early stage assembly into clusters. For the simple case of hard-spheres with short-range attractions, the small-N rigid structures have been enumerated theoretically and tested experimentally. Less is known, however, about how the free energy landscapes are altered when the interparticle potential is long-ranged. In this work, we demonstrate how adaptive biasing in molecular simulations may be used to pinpoint shifts in the stability of colloidal clusters as the interparticle potential is varied. We also discuss the generality of our techniques and strategies for applications to related molecule systems.

4:30PM C21.00009: Resolving the Interfaces in C₆₀-SubPC Organic Solar Cells Using Molecular Dynamics Simulations*  
JACOB TINNIN (Presenter), Department of Physics, University of Houston, PENGZHI ZHANG, Center for Advanced Computing and Data Science, University of Houston, EITAN GEVA, Department of Chemistry, University of Michigan, BARRY DUNIETZ, Department of Chemistry and Biochemistry, Kent State University, MARGARET CHEUNG, Department of Physics, University of Houston — Organic photovoltaic cells (OPVs) are still associated with relative low efficiencies despite recent advances. As the performance depends on the molecular dynamics (MD) and structure, it is crucial to understand this relationship at a quantitative level. To do this we analyzed the well-studied dyad of boron subphthalocyanine chloride (SubPC) and C₆₀ using MD simulations to understand the effects of device fabrication scheme on the materials interfaces. We developed order parameters to resolve the interface at the molecular level. Using importance sampling, we find an additional interfacial geometry over the two primary configurations addressed in the previous studies. In addition, we show that, due to an energy barrier between basins, the population of structures depends on the initial set-up which is used to differentiate between the fabrication schemes. We expect that the insight we provide will enhance efforts to design effective OPVs.

*This project utilized the computational resources from NERSC, a U.S. DOE Office of Science User Facility operated under Contract No. DE-AC02-05CH11231, as well as the uHPC cluster managed by the University of Houston and acquired through NSF Award 1531814. We are also grateful to the DOE (DE-SC0016501) and the NSF (PHY-1427654) for their support.
4:42PM C21.00010: Bivariate Transition Matrix Monte Carlo Method for Joint Density of States Calculations* YONG HWAN LEE (Presenter), DAVID YEVICK, University of Waterloo — While most thermodynamic variables of a statistical system can be evaluated at all temperatures from the density of states, if a phase transition is present, quantities such as Landau free energy and the probability distribution of the order parameter must instead be determined from the joint density of states which is a function of both the energy and a second variable, typically the order parameter. This talk demonstrates that by combining the transition matrix Monte Carlo method with the bivariate multicanonical sampling the joint density of states can be efficiently and accurately computed. The procedure is then applied to the Ising and Potts models as well as to Ising spin glasses. The Landau free energies, the probability distribution of the order parameter and the Binder cumulants are calculated. Finally, we discuss the implications of our results with regard to the existence of a nonzero temperature phase transition in the two-dimensional Ising spin glass.

*The Natural Sciences and Engineering Research Council of Canada is acknowledged for financial support.

4:54PM C21.00011: Policy-guided Monte Carlo: Reinforcement-learning Markov chain dynamics TROELS BOJESEN (Presenter), University of Tokyo — We introduce Policy-guided Monte Carlo (PGMC), a computational framework using reinforcement learning to improve Markov chain Monte Carlo (MCMC) sampling. The methodology is generally applicable, unbiased and opens up a new path to automated discovery of efficient MCMC samplers. After developing a general theory, we demonstrate some of PGMC’s prospects on an Ising model on the kagome lattice, including when the model is in its computationally challenging kagome spin ice regime. Here, we show that PGMC is able to automatically machine learn efficient MCMC updates without a priori knowledge of the physics at hand.

5:06PM C21.00012: Integrating cluster algorithms and transition matrix methods* DAVID YEVICK (Presenter), YONG HWAN LEE, University of Waterloo — The transition matrix procedure accumulates in a single matrix all accepted and rejected transitions generated during biased sampling of statistical systems, increasing the accuracy of calculations of the density of states relative to standard methods that ignore rejected transitions. However, the efficiency of the transition matrix algorithm is limited by the requirement that the system realizations adequately sample the entire physically accessible configuration space. In the Ising model, the slow diffusion of the single spin-flip procedure through this space severely limits the computation speed, especially for large systems.

This talk introduces a more efficient sampling procedure that combines the Wolff and Metropolis algorithms. [1] In particular, the Metropolis acceptance rule is employed at temperatures that slowly increase (or decrease) as the calculation proceeds. Near the critical temperature, however, one or more Wolff cluster flips are periodically performed before reverting to the single spin-flips that are required to populate the transition matrix. Potential methods for extending this strategy to more complicated systems are then proposed.


*NSERC is acknowledged for financial support

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C22 DCOMP DBIO DPOLY DCMP: Building the Bridge to Exascale: Applications and Opportunities for Materials, Chemistry, and Biology III BCEC 157C - Jack Deslippe, Lawrence Berkeley Natl Lab - Tag(s): Focus
OpenAtom: massively-parallel simulations for molecular and electronic dynamics

MINJUNG KIM (Presenter), SUBHASISH MANDAL, Yale Univ, ERIC MIKIDA, KAVITHA CHANDRASEKAR, QI LI, ERIC BOHM, NIKHIL JAIN, LAXMIKANT KALE, University of Illinois at Urbana-Champaign, GLENN MARTYNA, Pimpernel Science, Software and Information Technology, SOHRAB ISMAIL-BEI GI, Yale Univ — OpenAtom (OA) is an open-source, massively parallel software application that performs ab initio molecular dynamics simulations (AIMD) and ground and excited states calculations utilizing a plane-wave basis set. OA shows excellent scaling performance on thousands of compute nodes by employing overdecomposition and asynchrony strategies that the Charm++ parallel framework upon which OA is built provides.

Here, we describe recent advances in OA capabilities: 1) Path-integral Car-Parinello MD simulations implementation and performance results of a hydrogen adsorption in a metal-organic framework (MOF) and 2) release of a GW method implementation for quasiparticle properties and the scaling results up to 32K cores on Mira and Blue Waters. We will also discuss our collaborative efforts and ongoing development in OA concerning the projector augmented wave method, reduced order $O(N^3)$ GW calculations, porting to next generation machines with multiple GPGPUs per node, and extreme scale platform concerns for post-petascale and exascale environments.

*This work is supported by National Science Foundation through grants NSF ACI-1339804 and ACI-1339715.

Automated Discovery of Chemical Mechanisms using Reactive Molecular Dynamics

JAMES KOVAL, AHMED ISMAIL (Presenter), Chemical and Biomedical Engineering, West Virginia University — Reactive molecular dynamics simulations allow for changes in chemical computation through the dynamic calculation of bond orders between atoms. This can allow for the determination of large-scale reaction mechanisms if sufficiently large numbers of reaction events can be captured. Determination of "critical pathways" and elimination of closed "unstable loops" that return to the original reactants therefore requires the study of large systems of potentially tens of thousands of atoms for tens of nanoseconds—creating a large "data science" problem analyzing gigabytes or even terabytes of data. We demonstrate a recently developed algorithm that can construct such reaction mechanisms and pathways as well as provide inputs for quantum mechanical calculations to determine reaction rates. As examples, we apply this approach to the combustion mechanism of non-petroleum-based alternative fuel candidates.

Molecular Dynamics Simulations of an Entire HIV Virion

JUAN PERILLA (Presenter), Chemistry & biochemistry, University of Delaware, TYLER REDDY, Los Alamos National Laboratory — The HIV viral particle contains all the necessary components to infect a human cell. The so-called virion is made of glycoproteins, lipids, the Gag polyprotein, viral RNA and other essential proteins. After budding, several biological process occur inside the virion, including a major re-arrangement of the virion's cargo commonly referred as maturation. Here, we present the steps performed towards the construction of an atomistic model of a mature and immature virion. Our model includes all major components, including glycosylated proteins, twenty-four lipid types and capsid protein. Our effort constitutes one of the major efforts to construct a realistic HIV virion at atomic resolution. In addition, we discuss the techniques developed to prepare the system and the steps required to simulate and analyze our atomistic HIV virion model, which contains over 800 million atoms.

*This work was supported by the NIGMS and NIAID (P50GM082251).

Co-design in molecular dynamics for exascale

SAM REEVE (Presenter), JAMES BELAK, Lawrence Livermore Natl Lab — The continuing push towards exascale computing capabilities and accompanying shift toward heterogeneous hardware has highlighted the need for rethinking of even well-established computational methods. We focus here on molecular dynamics, assessing common algorithmic choices (e.g. ordering of computation and data layout in memory) and discussing new choices for novel machines. This talk will primarily explore how changes in data structure, particularly use of hybrid array-of-structs-of-arrays (AoSoA), i) both enable and require changes to compute kernels and ii) map well to multiple hardware architectures (e.g. both CPU and GPU). This exploration is enabled through the Co-design center for Particle Applications (CoPA) Cabana library for particle-based simulation methods.

*Work performed under the auspices of the U.S. DOE by LLNL under contracts DE-AC52-07NA27344 and supported by the Exascale Computing Project (17-SC-20-5C), a collaborative effort of the U.S. DOE Office of Science and the NNSA.
3:18PM C22.00005: Extending the accuracy, size, and duration of atomistic simulations on exascale hardware*
DANNY PEREZ (Presenter), ARTHUR F. VOTER, ANDERS NIKLASSON, CHRISTIAN NEGRE, MARC CAWKWELL, BLAS PEDRO UBERUAGA, Los Alamos National Laboratory, STEVEN JAMES PLIMPTON, AIDAN THOMPSON, MITCHELL A WOOD, MARY ALICE CUSENTINO, Sandia National Laboratories, BRIAN WIRTH, LI YANG, University of Tennessee, Knoxville — Because of its unparalleled predictive power, molecular dynamics (MD) has established itself as a workhorse of computational materials science. However, the limited strong-scalability of conventional MD combined with the exponential increase in parallelism currently leaves wide swaths of the theoretically-accessible simulation space inaccessible in practice, by only allowing for the simulation of larger systems but not of longer times. Fulfilling the promises of the exascale era will therefore require exposing new levels of parallelism in order to make the whole Accuracy/Size/Time simulation space accessible. The EXAALT project aims at addressing this challenge for systems that evolve through sequences of rare, thermally activated, events. By combining conventional domain decomposition with replication, speculation, and localization approaches, we show that novel computational techniques deployed at the exascale have the potential to dramatically extend the simulation space that will be accessible to MD over the next decade.

*This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations, the Office of Science and the National Nuclear Security Administration.

3:30PM C22.00006: Large-Scale Simulations of Protein Self-Assembly*
JENS GLASER (Presenter), SHARON GLOTZER, University of Michigan — Despite steady advances in computing methodology and in the accuracy of all-atom force fields, large scale simulations of biological self-assembly processes still defy the current capabilities of computer simulation. However, with simplified models it is sometimes possible to extract the important physics on the relevant time and length scales. Here we present results of our efforts to simulate the nucleation of protein crystals on the Titan supercomputer, employing large-scale simulations of rigid protein models to form the experimentally observed crystal structure. It has been hypothesized that biological crystallization occurs non-classically via an intermediate of a liquid droplet, to overcome the large barriers to nucleation via critical fluctuations. Using a model with an artificially tunable specificity, we test this hypothesis. We outline how more powerful simulations of biological self-assembly can be achieved on upcoming pre-exascale architectures using HOOMD-blue with support for NVLINK node-local communication.

*ARO W911NF-15-1-0185
This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

3:42PM C22.00007: First-principles simulations of electronic excitations and real-time dynamics on high-performance super computers*
[Invited] ANDRE SCHLEIFE (Presenter), University of Illinois at Urbana-Champaign — Excited electronic states and their ultrafast dynamics are foundational to how we interact with or probe many materials. Thanks to advanced experimentation, electronic excitations are accessible with high accuracy and time resolution, however, solid theoretical understanding is crucial for a detailed interpretation of experimental results. To this end, first-principles electronic-structure methods, such as many-body perturbation theory and time-dependent density functional theory, are powerful tools that provide highly accurate insight.

In this talk, I will discuss recent examples where we used real-time time-dependent density functional theory and Ehrenfest dynamics to study non-equilibrium electron dynamics coupled to classical ions. We performed simulations for highly energetic projectile ions impacting semiconductors and metals, that, however, suffer from high computational cost owing to small time steps during numerical integration. Massive parallelization and high-performance super computers such as Blue Waters and ALCF are needed, motivating our recent work on evaluating efficient and accurate numerical integrators within the Qb@ll code, e.g. using the PETSc library.

I will also discuss examples for using many-body perturbation theory to predict photon absorption and to establish the connection between structural and optical properties of semiconductors and their nanocrystals. In this context, the accurate computation of exciton binding energies is particularly demanding because it relies on eigenvalues of large dense matrices. I will illustrate how fast iterative eigensolvers help us tackle these problems on Blue Waters and broaden the applicability of many-body perturbation theory towards more diverse material systems.

*This work is supported by NSF (OAC-1740219, DMR-1555153) and used resources of the Argonne Leadership Computing Facility under Contract DE-AC02-06CH11357 and the Blue Waters sustained-petascale computing project (NSF OCI-0725070, ACI-1238993).
4:18PM C22.00008: Massively-parallel time-dependent density functional theory calculations for optical near-field excitations in silicon  
MASASHI NODA (Presenter), Center for Computational Sciences, University of Tsukuba, KENJI IIDA, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, MAIKU YAMAGUCHI, Graduate School of Engineering, The University of Tokyo, KAZUYA ISHIMURA, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, TAKASHI YATSUI, Graduate School of Engineering, The University of Tokyo, KATSUYUKI NOBUSADA, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, KAZUHIRO YABANA, Center for Computational Sciences, University of Tsukuba —

In current frontiers of optical science, electron dynamics in nano-materials has been explored in time domain using ultrashort light pulse. To describe such phenomena, we have been developing a program package SALMON (Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience) that is based on first-principles time-dependent density functional theory. SALMON solves time-dependent Kohn-Sham equation in real time using three-dimensional grid representation. The code is efficiently parallelized with respect to spatial grids, orbitals, and k-points. We have applied the code to wave vector excitations in three silicon bilayers with a Si(111) surface terminated by hydrogen atoms by optical near fields (ONF). To describe electronic excitations accompanying wave vector changes that are promoted by the ONF, we calculated the system composed of 10,240 atoms. The calculation costs 13 hours using 4096 nodes on the K computer at RIKEN Center for Computational Science. We have found that the excitation by ONF is a few orders of magnitude larger than that by the far field. We also find the lowering of the absorption edge by the ONF excitation that is attributed to direct interband transitions with finite wave vector differences.

4:30PM C22.00009: Combined Next-Generation Neutron Vibrational Spectroscopy and High-Accuracy Massively Parallel DFT Calculations Benchmark Electronic Descriptions of Complex Organic Molecular Systems  
ANUP PANDEY (Presenter), ADA SEDOVA, LUKE DAEMEN, YONGQIANG CHENG, ANIBAL J. RAMIREZ-CUESTA, Oak Ridge National Laboratory —

Vibrations in crystals govern their fundamental properties. In organic molecular crystals, low frequency vibrations depend on intermolecular interactions which are difficult to describe accurately with density functional theory (DFT) and must be carefully benchmarked. Inelastic neutron scattering (INS), complemented by accurate theoretical studies, can provide vital information on vibrations and molecular forces. Next-generation INS instruments measure THz and far-IR regions with excellent resolution; the VISION spectrometer is unique in providing high signal allowing for high-quality low-frequency data. Impressive agreement with experimental spectra is obtained using DFT calculations, however, discrepancies still exist. Frequency errors lead to incorrect Helmholtz free-energy estimates used in predictions of the relative stability of crystals, and incorrect intensities indicate poorly described intermolecular forces. By exploiting the parallel nature of finite-displacement methods, we can calculate the spectra of complex pharmaceutical and bio-organic solids using very large basis sets and a number of DFT functionals and dispersion descriptions in a few hours using the Titan supercomputer. Such benchmarks can transform theoretical studies of organic materials.

4:42PM C22.00010: ExaAM: Additive manufacturing process modeling at the fidelity of the microstructure*  
JAMES BELAK (Presenter), Lawrence Livermore Nat Lab, JOHN TURNER, Oak Ridge National Laboratory —

In FY17, the USDOE Exascale Computing Project (ECP) initiated projects to design and develop simulation codes to use exascale computing, including the Exascale Additive Manufacturing Project (ExaAM), a partnership between LLNL, LANL, and ORNL. Exascale Computing will enable AM process modeling at the fidelity of the microstructure. Here we discuss what this means, in particular, tight coupling of Process-Structure-Property calculations. Macroscopic continuum codes are used to simulate the metal melt-refreeze, within which mesoscopic codes (PF and CA) are used to simulate the development of microstructure. This microstructure is then used by crystal plasticity codes to calculate local properties. Here we focus on in situ coupling so that the calculated microstructure is relevant to the complex thermo-mechanical conditions of AM processing. Examples will be given for the SLM process of metal additive manufacturing along with comparison to experimental observations.

*Work performed under the auspices of the U.S. DOE by LLNL, LANL and ORNL under contracts DE-AC52-07NA27344, DE-AC52-06NA25396, DE-AC05-00OR22725, and supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. DOE Office of Science and the NNSA.
Cross-scale atomistic simulations of crystal plasticity*

VASILY BULATOV (Presenter), Lawrence Livermore Natl Lab — Predictions of crystal plasticity directly from the atomic motion have been regarded as unthinkable given the severe limits on time- and length-scale accessible to direct MD simulations. We will discuss our recent direct MD simulations of compressive straining of single crystals of Ta and Al. One of our simulations, Livermore BigBig (LBB) simulation, is by far the largest MD simulation ever performed: it generated a fully dynamic trajectory of over 2.1 billion atoms over 5 microseconds of simulated MD trajectory. LBB generated nearly 80 exabytes of recordable trajectory data only a tiny fraction of which was saved on disk in a highly compressed/post-processed form available for further analysis. As opposed to multiscale, LBB and other simulations of its magnitude can be regarded as cross-scale being sufficiently large to be statistically representative of collective action of dislocations resulting in macroscopic crystal flow and yet fully resolved to every atomic “jiggle and wiggle”. We will discuss new insights into physics of crystal plasticity brought about by our simulations and discuss challenges and strategies for on-the-fly learning on immense data generated in such simulations.

*Supported by NNSA ASC Program, LLNL Computing Grand Challenge Program and DOE INCITE Program.

Beyond Petascale: HPC and Polymeric Materials Design*

MONOJOY GOSWAMI (Presenter), Oak Ridge National Laboratory — Designing advanced polymeric materials for novel applications is challenging due to the experimental complexity associated with each and every polymer. Achieving success in polymeric materials design consequently relies on trial-and-error experimental techniques that often fail to achieve the predetermined goal. Computational modeling along different experimental techniques, therefore, has become the forefront of research in materials design. Recent developments in HPC, particularly from Petascale to Exascale supercomputing, are quickly shaping the precise design principles of polymeric materials. In this talk, I will highlight the importance of beyond-petascale computing in advanced manufacturing, polyelectrolyte complexation and phase change materials using molecular dynamics simulations that can help achieve future materials design goal.

*This material is based upon work supported by the U.S. DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division. The research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, Contract # DE-AC05-00OR22725. A portion of this research was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a DOE Office of Science User Facility.

Towards Exascale Quantum Transport Calculations

WENCHANG LU (Presenter), EMIL BRIGGS, JERRY BERNHOLC, North Carolina State University — Beyond Moore's law devices will approach nanometer dimensions and operate in the regime where quantum and atomic-scale effects become important. In this regime, classical concepts of device design cease to be predictive and need to be augmented by quantum simulations of key parts of devices and circuits. Based on the non-equilibrium Green's function (NEGF) methodology within the density functional theory, we have developed a NEGF module within the real-space multigrid (RMG) suite of codes (www.rmgdft.org) by which the quantum transport properties can be studied for nanoscale devices containing tens of thousands of atoms. Multilevel parallelization with MPI, threads and/or Cuda programming is implemented to enable adaptation to future exascale supercomputers. The module can be used to simulate and design new quantum devices at the atomic level. For a system with ten thousand atoms, the NEGF module's performance scales linearly from 100 to 1000 nodes on the Summit supercomputer at ORNL. With an efficient implementation of GPU acceleration using the new Cuda-managed memory capability, our benchmark calculations show a 3.5 to 4.5 speed-up over CPU-only calculations.
2:30PM C23.00001: Arctic cloud and sea ice feedbacks from satellite observations and a global climate model*  
[Invited] ARIEL MORRISON (Presenter), Atmospheric and Oceanic Sciences, University of Colorado Boulder — Over the next century, the Arctic Ocean is projected to become seasonally sea ice-free. Assessing feedbacks between clouds and sea ice as the Arctic loses sea ice cover is important because of clouds’ radiative impacts on the Arctic surface. Here, present and future Arctic cloud-sea ice relationships are assessed using spaceborne lidar observations and a fully-coupled global climate model that incorporates a lidar simulator. Using a novel surface mask that restricts the analysis to where sea ice concentration varies, we isolate the influence of sea ice cover on Arctic Ocean clouds during summer and fall. Summer cloud structure and fraction are nearly identical over sea ice and over open water, but more clouds are observed over open water than over sea ice in the fall. With future sea ice loss, modeled summer cloud fraction, vertical structure, and optical depth barely change, while the boundary layer deepens and clouds become more opaque over open water during fall. There is little evidence for a summer cloud-sea ice feedback but strong evidence for a positive cloud-sea ice feedback that emerges during non-summer months as the Arctic warms and sea ice disappears.  

*This work was funded by NASA grant 15-CCST15-0025, CloudSat/CALIPSO grant 13005376, NSF grant 1554659 and the Chateaubriand Fellowship from the Office for Science & Technology of the Embassy of France in the United States.

3:06PM C23.00002: Spatiotemporal Dynamics of Lake Patterns in a Changing Arctic Tundra Landscape*  
THAO N. NGUYEN (Presenter), Department of Physics and Environmental Science, St. Mary's University, IVAN A SUDAKOV, Department of Physics, University of Dayton — The evolution of Arctic tundra lakes exhibits percolating properties. More specifically, there exists a threshold where initially disjoint lakes gradually transition into a network of complex, interconnected structures on a macroscopic level when the value of some parameter exceeds a critical value. Behaviors of these lakes, primarily characterized by the lake area fraction and fractal dimension of the system, are significant to statistical physics due to their analogous nature to phase transitions. On account of similarities in geographical characteristics of the Arctic tundra landscape and that of slow immiscible fluid invasion processes in porous media, we developed our model based on a standard invasion percolation model under the influence of changing temperature. This model helps to explain the critical percolation threshold in the lake system in order to understand long-term lake dynamics and its contribution to climate change.  

*Funding for this research was provided in part by the University of Dayton College of Arts and Sciences and the Department of Physics.

3:18PM C23.00003: Homotopy Importance Sampler For Noisy Dynamics*  
JUAN RESTREPO (Presenter), ANDREW JENSEN, ROBERT MILLER, Oregon State University — We propose a Bayesian estimation method for moments of a state vector that obeys stochastic nonlinear dynamics and its observations. The method uses a homotopy procedure to improve the convergence of an MCMC importance sampler. Designed to sample non-Gaussian statistics, the method can also be used to sample very low uncertainty Gaussian statistics dynamics. In this talk I will describe the method and show comparisons that suggest that the method is efficient and comparatively accurate on a variety of practical and challenging problems.  

*This research is supported by NSF OCE1434198.

3:30PM C23.00004: Application of the Rayleigh-Debye-Gans (RDG) theory for determining optical properties of biomass burning aerosols.*  
EMMANUEL SARPONG (Presenter), DAMON SMITH, SOLOMON BILILIGN, North Carolina Agricultural and Technical State University — Biomass burning emissions are a major source of fractal aggregates which are clusters of spherules forming aerosols of non-spherical shape. Both the developed and developing world are subject to biomass burning events through agricultural burning, wildfires, and domestic burning applications. Accurate quantification of their optical properties is important both for their measurement and for predicting their radiative effect on climate. RDG assumes that each monomer in the aggregate interacts independently with radiation, by neglecting multiple scattering and shadowing. Absorption is an incoherent process and as a result the absorption of the aggregate is equal to the number of monomers, N, times the absorption of a single monomer. TEM images are used to determine the size parameters of the fractal aggregates. We report use of the RDG theory to fit experimentally measured optical properties to extract the refractive indices of biomass burning aerosols.  

*The Authors acknowledge the support from the National Science Foundation under grant number 1555479
3:42PM C23.00005: A theory for global precipitation change  NADIR JEEVANJEE (Presenter), Princeton University, DAVID ROMPS, EPS, UC Berkeley — Global warming simulations robustly show that mean precipitation increases at 1-3% per Kelvin, but we do not know what sets these values. Mean precipitation is constrained by radiative cooling, however, and we demonstrate here that radiative cooling profiles exhibit a certain invariance under warming when plotted in temperature coordinates. This invariance can then be leveraged to derive simple analytical equations for precipitation change with warming. These equations are validated in cloud-resolving simulations of the tropics, and give intuition for why precipitation changes at a rate of 1-3% per Kelvin.

3:54PM C23.00006: Estimation of Hourly and Daily Clearness Indices and Diffuse Fraction, over Port Harcourt and Kano using National Centre for Environmental Prediction and National Centre for Atmospheric Research Satellite Data  OPEYEMI OMOLE (Presenter), Physics Department, College of Education Ikere Ekiti Nigeria, BABATUNDE ADEYEMI, Physics Department, Federal university of Technology Akure — Estimation of clearness index (KT) and diffuse fraction (KD) were calculated using satellite data obtained from National Centre for Environmental Prediction and National Centre for Atmospheric Research data base covering a period of 10 Years (2005 - 2014) for Port Harcourt and Kano stations which are Coaster and Sahel regions respectively. Direct solar data and diffuse solar data collected were added to give the Global solar radiation. The computed clearness index values were used to characterize the sky conditions into clear skies and overcast skies. Port-Harcourt with low clearness index indicated low global solar radiation while Kano with large clearness index indicated high global solar radiation. The implications of these results on the effective utilization of solar energy are discussed. The results also serve as very useful for solar energy collectors in designing and estimation of solar application systems

4:06PM C23.00007: Threshold dependence in the flip-flop model  DOUGLAS KURTZE (Presenter), Saint Joseph's University — The flip-flop salt oscillator model\(^1\) is a simplified dynamical model describing buoyancy-induced oscillations in the ocean. In this model, coupling to the atmosphere can increase the density of water at the surface to the point that it becomes denser than the water beneath, at which point vigorous vertical convection sets in and restores stable stratification. One parameter in this model quantifies the strength of the atmospheric forcing; the dependence of the amplitude and period of the oscillations in vertical mixing on this parameter has been well studied. However, in order for the model to produce oscillations at all, it must allow convective mixing to begin when the stratification is still slightly stable; a “threshold” parameter must be given to specify how close to unstable the stratification must be for convection to begin. The geophysical significance of this parameter is unclear, and typically it is set to some arbitrary small value. We show, however, that the amplitude and period of oscillations in the model depend strongly on this parameter, being proportional to its value and its square root, respectively. Thus numerical results from the flip-flop model need to be interpreted with care.


4:18PM C23.00008: Threshold phenomena in the marine carbon cycle*  DANIEL ROTHMAN (Presenter), Massachusetts Institute of Technology — The history of the marine carbon cycle is punctuated by transient disruptions. These events are typically attributed to anomalous inputs of carbon from external sources or changes in the rates at which carbon is buried in sediments. The magnitude of the events is commonly assumed to scale proportionately to the size of the disturbance. Here I show, via construction and analysis of a 2-dimensional dynamical system, how carbon-cycle disruptions can instead result from nonlinear amplification of relatively small perturbations that exceed a threshold. When the solitary fixed point is stable, small but finite perturbations of the steady state can result in a large-amplitude excitation that precedes the return to the fixed point. The excitation represents runaway ocean acidification. Similar events are observed in the paleoclimate record. In particular, the model’s disruptions exhibit a characteristic size and rate of growth consistent with observations. The threshold for initiating an excitation is also consistent with results inferred from previous disruptions. The modern oceanic uptake of carbon will likely exceed this threshold by the end of the present century.

*This work was supported by NASA Astrobiology grant NNA13AA90A and NSF grant EAR-1338810.
**4:30PM C23.00009: Implications of Lorenz-Mie scattering by cloud droplets in an absorbing atmosphere for cloud feedbacks* WILLIAM COLLINS (Presenter), DANIEL R. FELDMAN, CHAINCY KUO, Lawrence Berkeley National Laboratory — There is still considerable uncertainty as to the magnitude of cloud feedbacks to anthropogenic climate change. The magnitude is determined by changes in the bulk cloud radiative effects (CREs) on both solar and terrestrial radiation in response to changes in the Earth's average surface temperature. The range of CRE responses of low-altitude liquid clouds is one of the dominant sources of uncertainty. To date, the CREs for these clouds have been computed using variants of classical far-field Mie theory applied to spherical particles (i.e., water droplets) embedded in a non-absorbing medium. At many wavelengths where water vapor is the predominant radiatively active gas, the assumption of a non-absorbing medium is manifestly violated, for example in the near-infrared near the primary and overtone absorption bands of H₂O. For this reason, it is important to redo the calculation of CREs using new, generalized Lorenz-Mie scattering in an absorbing atmosphere (Mishchenko et al, 2017 and 2018). We quantify differences in reflection, transmission, and absorption of sunlight and terrestrial radiation by liquid clouds and the impacts of these differences on low-cloud feedbacks to increasing surface temperatures.  

*DOE Contracts DE-AC02-05CH11231 and DE-AC02-05CH11231 to LBNL.

**Monday, March 4, 2019 2:30 PM - 5:30 PM**

**Session C24 DAMOP DCMP: Non-Equilibrium Physics in AMO Systems I** BCEC 159 - Norman Yao, University of California, Berkeley - Tag(s): Focus

**2:30PM C24.00001: Making Matter from Light: Photon Mott Insulators and Topological Fluids* [Invited] JONATHAN SIMON (Presenter), University of Chicago — Recent developments in quantum optics have enabled strong interactions between individual photons. I will describe work at the University of Chicago harnessing these tools to assemble quantum matter from light: in a collaboration between the Simon and Schuster labs, we have demonstrated dissipative stabilization of a Mott insulator of microwave photons, trapped in an array of transmon qubits; in the Simon lab we have demonstrated that a twisted optical resonator generates artificial magnetic fields for photons trapped within it; we have now employed Rydberg atoms to mediate interactions between these photons and are exploring topological fluids of light. From thermodynamics of driven equilibria to microscopy of entangled systems, photonic materials provide unique opportunities in few-to-many body physics.  

*This work was supported by Army Research Office grant W911NF-15-1-0397; and by the University of Chicago Materials Research Science and Engineering Center (MRSEC), which is funded by National Science Foundation (NSF) under award number DMR-1420709. It was also supported by Air Force Office of Scientific Research MURI grant FA9550-16-1-7-0323.

**3:06PM C24.00002: Dynamically Tuning One Dimensional Systems Across Quantum Phase Transitions: Classical and Quantal Defects.* ANDREW MILLIS (Presenter), Columbia University, DANTE KENNES, Fachbereich Physik, Freie Universität Berlin — Infinite-system time dependent density matrix renormalization group and Loschmidt-amplitude methods are used to analyse the physics occurring when a one dimensional system is dynamically tuned across a quantum phase transition, either by an ac (`Floquet') drive with time vary amplitude or a simple ramp in Hamiltonian parameters. Tuning the XXZ model between two points in the gapped phase introduces classical defects leading to exponentially decaying correlations as expected; tuning between two points in the gapless phase produces excitations which do not destroy the long-distance power-law behavior, and tuning across the phase transition produces quantum phase slips which appear in pairs and then annihilate. Loschmidt methods are used to interrogate the wave function obtained after (one or multiple) ramps across the critical point of the transverse field quantum Ising model, leading to new understanding of the population of the defects created and of the importance of quantum coherence. Portions of this work were performed in collaboration with A. Ron. A. della Torre, D. Hsieh and C. Karrasch.  

*This work was funded by the Basic Energy Sciences program of the US Department of Energy under grant DE-SC-0018218
3:18PM C24.00003: Nonequilibrium Mass Transport in the 1D Fermi-Hubbard Model* JAN STOLPP (Presenter), Institute for Theoretical Physics, Universität Göttingen, SEBASTIAN SCHERG, THOMAS KOHLERT, Fakultät für Physik, Universität München, JACEK HERBRYCH, Department of Physics and Astronomy, University of Tennessee, PRANJAL BORDIA, Fakultät für Physik, Universität München, ULRICH SCHNEIDER, Cavendish Laboratory, University of Cambridge, FABIAN HEIDRICH-MEISNER, Institute for Theoretical Physics, Universität Göttingen, IMMANUEL FELIX BLOCH, MONIKA AIDELSBURGER, Fakultät für Physik, Universität München — We report on the results of a combined experimental and numerical study of nonequilibrium dynamics of ultracold fermions in a 1d lattice induced by quenching the trapping potential to zero [1]. This leads to an expansion of the cloud in a homogeneous lattice under the influence of interactions. For initial states with a significant admixture of doublons in a sea of singlons, we observe a dynamical demixing of fast expanding singlons from doublons that remain in the center of the system. We interpret this as evidence for fermionic quantum distillation [2]. For initial product states of one fermion per site and random spin orientations, we study the asymptotic expansion velocity. Compared to bosons [3], these velocities depend only very weakly on the interaction strength. We explain this observation by the fact that the Pauli principle significantly limits the amount of interaction energy that can be generated for fermions as compared to bosons.


*European Commission (UQUAM, AQuS) and the Nanosystems Initiative Munich (NIM). DFG (Deutsche Forschungsgemeinschaft) Research Unit FOR 1807 and SFB 1073.

3:30PM C24.00004: Universal Aspects of Operator Thermalization in Hamiltonian Dynamics* DANIEL PARKER (Presenter), XIANGYU CAO, EHUD ALTMAN, University of California, Berkeley — The long-time behavior of observables in thermalizing quantum systems can often be captured through hydrodynamics, involving just a few local quantities. A key question in quantum dynamics is to derive such behavior from the microscopic behavior and predict quantities such as diffusion coefficients or conductivities. We describe a conjectural form for super-operator Green's functions in thermalizing systems at infinite temperature in any dimension. The conjecture is supported by numerical calculations for a broad range of thermalizing many-body models and exact analytic results for large-q SYK models. The universal asymptotic form of the Green's function suggests an efficient numerical technique for extracting diffusion coefficients of operators in strongly interacting systems. Additionally, the conjecture implies some 'universal' behavior of operators under Hamiltonian dynamics.

*D.E.P. received support from the NSF GRFP, DGE 1752814. X.C. acknowledges support from a Simons Investigatorship. E.A. acknowledges ERC synergy grant UQUAM.

3:42PM C24.00005: Observation of Dynamical Quantum Phase Transition in Antiferromagnetic Spinor Bose-Einstein Condensates in a short time region LIYUAN QIU (Presenter), HAOXIANG YANG, TIAN TIAN, HAIYU LIANG, ANJUN CHU, YANBIN YANG, Center for Quantum Information, IIIS, Tsinghua University, YINGMEI LIU, Oklahoma state university, LUMING DUAN, Center for Quantum Information, IIIS, Tsinghua University — In this work, we show direct evidence of the dynamical quantum phase transition (DQPT) in antiferromagnetic spin-1 Na Bose-Einstein condensate system. Initially, the spinor-1 BEC is at its ground state with quadratic Zeeman coefficient $q=11.2$Hz where all atoms are in $|F=1, m_F=0\rangle$ state, i.e. the fraction of spin-0 atoms $\rho_0$ is 1, then at $t=0$, the $q$ suddenly changed to a $q_f$ and the BEC will evolve variable times at this $q_f$. To observe DQPT, first minimum dip depth (Adip) of $\rho_0(t)$ is chosen to be a new order parameter. The experimental result shows that once the final quadratic Zeeman coefficient $q_f$ crossed the transition point, $\rho_0(t)$ will shows large fluctuation and $A_{\text{dip}}$ will arise abruptly. Further, the dip depths $A_{\text{dip}}$ under different quenched parameters $q_f$ shows similar behavior with the long time average $\rho_0(t)$ which indicates the dynamical quantum phase transitions across the critical point.
We demonstrate analytically and numerically that in isolated quantum systems of many interacting particles, the number of many-body states participating in the evolution after a quench increases exponentially in time, provided the eigenstates are delocalized in the energy shell. The rate of the exponential growth is defined by the width $\Gamma$ of the local density of states (LDOS) and is associated with the Kolmogorov-Sinai entropy for systems with a well defined classical limit. In a finite system, the exponential growth eventually saturates due to the finite volume of the energy shell. We estimate the time scale for the saturation and show that it is much larger than the characteristic decay time of the initial state $1/\Gamma$. Numerical data obtained for a two-body random interaction model of bosons and for a dynamical model of interacting spin-1/2 particles show excellent agreement with the analytical predictions.

*NSF Grant No. DMR-1603418.

Dark states are stationary states of a dissipative, Lindblad-type time evolution with zero von Neumann entropy, therefore representing examples of pure, steady quantum states. Non-equilibrium dynamics featuring a dark state recently gained a lot of attraction since their implementation in the context of driven-open quantum systems represents a viable possibility to engineer unique, pure states. In this work, we discuss a driven many-body spin system, which undergoes a transition from a dark steady state to a mixed steady state as a function of the driving strength. This transition connects a zero entropy (dark) state with a finite entropy (mixed) state and thus goes beyond the realm of equilibrium statistical mechanics and becomes of genuine nonequilibrium character. We discuss the relevant long wavelength fluctuations driving this type of transitions and bring it into context with other nonequilibrium phenomena, such as self-organized criticality and bistability.

The transport of spin, instead of charge, is the basis of the field of spintronics. Besides in condensed matter, spin transport has recently been explored in experiments with ultracold atoms which allow spin-selective control. A central phenomenon in the transport of spin current is spin drag, where a chemical potential bias on one spin component induces the transport of the other component via interactions. For attractive contact interactions, the ground state of fermions in one dimension is a singlet superfluid, and spin drag is due to pairing of fermions with opposite spin. This was recently observed in a quantum point contact setup [1]. Motivated by recent transport experiments with ultracold atoms [1, 2], we investigate analytically and numerically the possibility of spin drag of repulsively interacting fermions in a one-dimensional wire, where the ground state is a spin density wave.

References


The concept of quantum many-body scars -- atypical, nonergodic energy eigenstates of an otherwise ergodic many-body system -- was recently introduced to explain the surprising long-lived oscillations observed in an interacting, constrained spin chain following a quantum quench. Here, we provide numerical evidence that a suitable, quasi-local deformation of the system leads to a dramatic increase of the lifetime of the oscillations, even possibly allowing them to last for an indefinitely long time. We show that this seemingly perfect oscillatory dynamics can be understood via an emergent large SU(2)-spin undergoing precession, contained within a special subspace of the many-body Hilbert space, while the rest of the system remains ergodic. The presence of such dynamics severely constrains the structure of certain energy eigenstates in the thermodynamic limit. Furthermore, we introduce a toy model which captures the salient features of quantum many-body scarring.
4:42PM C24.00010: Cooperative Breakdown of the Oscillator Blockade in the Dicke Model  FLORENTIN REITER (Presenter), Department of Physics, Harvard University, THANH LONG NGUYEN, JONATHAN HOME, Institute for Quantum Electronics, ETH Zürich, SUSANNE F YELIN, Department of Physics, Harvard University — Spin-boson models provide an interaction between atoms and harmonic oscillators and lie at the heart of quantum science. The superradiant phase transition in the Dicke model [1] constitutes a prime example of a non-equilibrium phase transition which has recently been realized experimentally [2].

In addition to these steady-state phases, we observe a second dissipative phase transition to a nonstationary phase, which can be understood as a breakdown of the photon blockade which is known from the single-particle context [3]. We demonstrate that our many-body breakdown effect is of cooperative nature and study its dependence on the system size [4]. The model can be realized using standard experimental platforms; in particular we discuss a realization based on trapped ions.


4:54PM C24.00011: Computing Thermalizing Quantum Dynamics without Matrix Product States*  XIANGYU CAO (Presenter), EHUD ALTMAN, University of California, Berkeley — Quantum dynamics of many-body systems is hard to simulate because of the exponentially large Hilbert space. Getting around it and capturing the classical hydrodynamics emerging at large scales presents an actively sought after goal. Based on this idea, we present a new numerical method that represents the variational quantum state by a consistent set of reduced density matrices on overlapping small blocks (increasing block size improves precision, at higher computational cost). Assuming that all other connected correlations vanishes, we obtain a time-dependent variational principle scheme that can be used to approximate generic short-range Hamiltonian evolution/quantum circuits. Like existing methods based on matrix product state/operator, the new approach also respects all local conservation laws, but has the advantage that it can be readily generalized to higher dimensions.

*We acknowledge support from a Simons Investigatorship (XC) and ERC Synergy Grant UQUAM (EA)

5:06PM C24.00012: Hydrodynamic behavior of non-interacting quantum particles in presence of dephasing  OLES SHTANKO (Presenter), SETH LLOYD, Massachusetts Institute of Technology — In quantum transport problems, thermal environment plays an important role. We demonstrate that additionally to suppressing transport via dephasing, the environment is able to induce new dynamic effects absent in an isolated system. In particular, we show that single particle or gas of free particle in presence of stochastic environment exhibits a formation of vortices and Poiseuille flow, the effects mainly considered as hydrodynamic behavior. We provide a detailed analysis of the phenomenon and derive equations for quasi-viscous flow. The environmentally induced quantum viscosity suggests new possible transport regimes accessible in solid-state devices, isolated atomic systems, and photonic quantum simulators.

5:18PM C24.00013: Scalling theory of quantum ratchet in low temperature limit*  KEITA HAMAMOTO (Presenter), TAKAMORI PARK, HIROAKI ISHIZUKA, University of Tokyo, NAOTO NAGAOSA, RIKEN — Directionality of responses in noncentrosymmetric materials is a central issue in condensed matter physics. The quantum dynamics of particles in an asymmetric washboard potential with dissipation is a typical system. Previous study on the 2nd order mobility have shown the rich physics in this system, the sign reversal of the rectified current and quantum to classical crossover, for instance. However, the relations with the quantum phase transition taking place at certain strength of the dissipation above which the system goes to a localized state, is still a nontrivial issue. Here, we clarified the detailed low temperature behavior of the steady velocity and mobility of a particle under the ratchet potential both analytically and numerically. The exponent in the power law dependence for arbitrary order mobility is determined and summarized in simple scaling forms. The relations to the quantum phase transition is also discussed.

*N.N. was supported by Ministry of Education, Culture, Sports, Science, and Technology Nos. JP24224009 and JP26103006, the Impulsing Paradigm Change through Disruptive Technologies Program of Council for Science, Technology and Innovation (Cabinet Office, Government of Japan), and Core Research for Evolutionary Science and Technology (CREST) No. JPMJCR16F1.
Simulations provide molecular insight into the mechanism of phase separation in these mixtures. The (1-butyl-3-methylimidazolium) cation, [BMMIM] (ternary 1-butyl-2,3-dimethylimidazolium) on the phase diagram. The method we have recently developed. We explore the influence of PEO molecular weight and the C2 methylation of [BMIM] behavior a mixture of poly(ethylene oxide) (PEO) and imidazolium-based ionic liquids using a new molecular simulation solution properties. There are fundamental questions regarding the LCST phase behavior: The critical point is at high importance for use in polymer solid state batteries and temperature sensors, where the ionic liquid allows a tuning of the solvent quality. SAXS and liquid-phase TEM demonstrate that between the B block and the IL were explored in four different ILs. Equilibration occurs after annealing, and the relaxation scattering, small-angle X-ray scattering, and liquid-phase transmission electron microscopy. The effects of solvent quality decrease in size. Exploration of the equilibration kinetics for BEO in ILs is being conducted using temperature-jump light scattering (SANS) to measure the radius of gyration of varying chain lengths of perdeuterated poly(ethylene oxide) in imidazolium-based ILs, which vary in both cation and anion identity. The dependence of coil size on molecular weight yields Flory exponents (χ) for 4 different IL-based solvent systems. For all the solvents studied, the exponents lie within 0.55 and 0.6, indicating moderately good to very good solvent behavior. However, greater expansion of d-PEO coils is observed in ILs comprising cations with longer alkyl chains and less basic anions. Interestingly, variation of the anion has a stronger effect on coil dimensions than the cation. Additional relevant parameters such as temperature and lithium salt addition on the coil dimensions of d-PEO chains in ILs are also explored.

*This work was supported by the National Science Foundation DMR-1707578

Phase behavior of polymer/ionic liquids mixture: a molecular dynamics study* HYUNTA JUNG (Presenter), ARUN YETHIRAJ, University of Wisconsin - Madison — The phase behavior of polymers in ionic liquids is of practical importance for use in polymer solid state batteries and temperature sensors, where the ionic liquid allows a tuning of the solution properties. There are fundamental questions regarding the LCST phase behavior: The critical point is at high polymer concentrations, and the critical temperature is insensitive to molecular weight. In this work, we study the phase behavior a mixture of poly(ethylene oxide) (PEO) and imidazolium-based ionic liquids using a new molecular simulation method we have recently developed. We explore the influence of PEO molecular weight and the C2 methylation of [BMIM] (1-butyl-3-methylimidazolium) cation, [BMIM] (ternary 1-butyl-2,3-dimethylimidazolium) on the phase diagram. The simulations provide molecular insight into the mechanism of phase separation in these mixtures.

*This research was supported by US Department of Energy, Basic Energy Sciences Contract DE-SC0017877 and used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility Contract DE-AC05-00OR22725.

Kinetics of Block Copolymer Micelle Fragmentation in Ionic Liquids* JULIA EARLY (Presenter), TIMOTHY LODGE, University of Minnesota — Recently, more attention has been directed to quantifying the relaxation kinetics of block copolymer micelles. However, there are very few experimental studies quantifying the rates of fragmentation in block copolymer micelles. The micelle radius for poly(1,2-butadiene)-block-polyethylene oxide (BEO) in EO-selective ionic liquids (ILs) depends on the solution preparation method. When BEO is dissolved directly into an IL, the spherical aggregates are large and disperse in size. Upon high temperature annealing, these micelles equilibrate and decrease in size. Exploration of the equilibration kinetics for BEO in ILs is being conducted using temperature-jump light scattering, small-angle X-ray scattering, and liquid-phase transmission electron microscopy. The effects of solvent quality between the B block and the IL were explored in four different ILs. Equilibration occurs after annealing, and the relaxation times exhibit a significant dependence on concentration and solvent quality. SAXS and liquid-phase TEM demonstrate that the core radius decreases by 5 nm after annealing. These experiments demonstrate that relaxation mechanisms other than individual chain exchange dominates in these highly amphiphilic systems.

*This work was supported by the National Science Foundation DMR-1707578

Effect of Solvent Selectivity on Chain Exchange Kinetics in Block Copolymer Micelles EN WANG (Presenter), DAN ZHAO, TIMOTHY LODGE, FRANK BATES, University of Minnesota — Block copolymer (BCP) micelles in selective solvents are useful for a variety of applications, such as nanolithography, drug delivery, and viscosity modification. The solvent quality is an important factor for both thermodynamics and dynamics of BCP micelles. Previous work revealed the effect of solvent selectivity on thermodynamic properties of BCP micelles formed by poly(styrene-b-ethylene-alt-propylene) (PS-PEP) diblock copolymers in mixed solvents of squalane and 1-phenyldecane. The systematic change of solvent composition tunes the interfacial tension between the core and corona-solvent matrix, embodied in the Flory-Huggins interaction parameter χ. This should also affect the kinetics of chain exchange between micelles. This presentation will describe the consequences of varying the solvent composition on the rate of chain exchange using time-resolved small-angle neutron scattering (TR-SANS). An independent method, static light scattering (SLS), was performed to estimate χ between the core block and the solvent as a function of solvent composition and temperature. Based on TR-SANS and SLS results, the dependence of the chain exchange rate on χ can be quantified.
3:18PM C25.00005: Probing Polymer Solution Conformation along Microparticle Formation Pathways with SANS*  
WILLIAM SHARRATT (Presenter), MARCO ADAMO, JOAO CABRAL, Imperial College London — Polymeric microparticles are ubiquitous in encapsulation and targeted release applications. Their function is predicated on their microstructure, shape and interactions, which determine stability, phase behaviour and release profiles. Polymer solution droplet extraction is an attractive route to control their formation, and understanding the thermodynamic and non-equilibrium pathways involved is crucial for their predictive design. Here, we show microfluidic droplet formation and selective solvent exchange to yield porous polymer microparticles [1] with tunable morphologies [2]. We systematically explore the process with model poly(vinyl alcohol), varying polymer functionality, size, concentration, and droplet size [3]. We map polymer solution conformation with small angle neutron scattering (SANS) and microfluidic-SANS to resolve how chain dimensions evolve with mixed solvent/non-solvents during solidification. Our study elucidates, for the first time, the spatio-temporal evolution of polymer solutions into particles, from molecular to micron scales.


*We thank the EPSRC for funding.

3:30PM C25.00006: Arrested Mobility Effects on the Spinodal Decomposition of Ternary Polymer Solutions*  
JAN ULRIC GARCIA (Presenter), University of California, Santa Barbara, DOUGLAS R. TREE, Brigham Young University, KRIS T DELANEY, GLENN FREDRICKSON, University of California, Santa Barbara — Many polymer membranes are made by immersion precipitation: a polymer solution film is immersed in a nonsolvent bath, inducing phase separation of the film into a polymer-rich phase that becomes the membrane matrix and a polymer-poor phase that becomes the membrane pores. Microstructure formation of these membranes is still not fully understood, given the interdependence of the processes involved: the mass transfer through the film-bath interface, the phase separation of the film, the coarsening of domains, and finally the glass transition that arrests the microstructure. In this work, we use phase-field models of the ternary system to solve the coupled convection-diffusion and momentum equations that describe membrane formation. We model the glass transition using mobility and viscosity contrasts between the polymer-rich and polymer-poor phases. We report how the glassy dynamics changes the microstructures formed by bulk spinodal decomposition. We also study how mass transfer between the bath and film changes with the formation of a glassy interface.

*We acknowledge support from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1720256) and NSF CNS-1725797. We also thank Asahi Kasei Corp. for support. JUG acknowledges support from the NSERC PGS-D program.

3:42PM C25.00007: SANS study of the thermodynamics and demixing of highly interacting PaMSAN/dPMMA blends  
YUTAKA AOKI (Presenter), WILLIAM SHARRATT, HAOYU WANG, Chemical Engineering, Imperial College London, SARAH ROGERS, ROBERT DALGLIESH, ISIS-STFC, Rutherford Appleton Laboratory, JULIA HIGGINS, JOAO CABRAL, Chemical Engineering, Imperial College London — Spinodal decomposition of partially miscible polymer blends has the potential to generate well-defined polymeric nanostructured materials. While the Cahn-Hilliard (CH) theory prediction for the initial spinodal lengthscale generally holds, phase sizes attained by thermally-induced demixing are, however, stubbornly much greater that $R_g$. Using Small Angle Neutron Scattering (SANS), we investigate a series of LCST poly(a-methyl styrene-co-acrylonitrile) and deuterated poly(methyl methacrylate) (PaMSAN/dPMMA) blends which exhibit a remarkably steep temperature dependence of $G''$ (and thus $c$), the driving force for demixing [1,2]. We explore the role of PMMA molecular mass ($MW = 40$-$130$ kg/mol), tacticity, composition, and temperature and to map $G''$ and $c$ as a function of these parameters in the one-phase region, employing Random Phase Approximation theory. We then carry out a series of rapid jumps into the unstable and metastable regions, establishing a comprehensive map of lengthscales achieved and theoretically expected, and limits and opportunities for bicontinuous nanostructure design by this approach.

3:54PM C25.00008: Single molecule studies of comb polymer dynamics in semi-dilute solutions*  SHIVANI PATEL (Presenter), CHARLES SCHROEDER, Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign — We study the dynamics of single branched polymers in non-dilute solutions using single-molecule fluorescence microscopy (SMFM). In particular, we use a hybrid enzymatic-synthetic approach to synthesize DNA-based branched polymers (comb polymers) that contain a long backbone with multiple side branches grafted at various positions. Following synthesis, we directly study the transient stretching dynamics of single comb polymers in semi-dilute solutions in extensional flow. We compare the transient dynamics of single comb polymers in semi-dilute solutions of linear unlabeled polymers to the dynamics of comb polymers in ultra-dilute solutions. Interestingly, the transient stretching dynamics and relaxation behavior of comb polymers is markedly different in non-dilute polymer solutions, which reveals changes in molecular-scale dynamics due to chain branching and chain-chain intermolecular interactions. We further study the effects of background concentration and polymer topology on comb polymer dynamics in order to elucidate the non-equilibrium behavior of topologically complex polymers. Overall, our work shows that single polymer dynamics can be used to provide a direct link between polymer microstructure and bulk rheological properties.

*We thank NSF CCF 1807526 for funding.

4:06PM C25.00009: Thermodynamics and conformation of PPPO in mixed solvents: towards nanoporous polymeric gas sensors  ROISIN O’CONNELL (Presenter), JOAO CABRAL, JULIA HIGGINS, ALEXANDRA PORTER, Imperial College London — Poly(2,6-diphenyl-p-phenylene oxide) (PPPO) can be processed into high performance nanoporous materials, with applications ranging from gas separations to sensing. An attractive design route involves demixing from solution, generally via spinodal decomposition induced by non-solvent addition, and followed by phase inversion and kinetic arrest. In this work, we investigate the thermodynamics and phase separation of the ternary PPPO/solvent/non-solvent system, combining light and Small Angle Neutron Scattering, and electron microscopy.

We determine the polymer conformation and interaction parameters in binary and ternary solutions across the concentration range relevant for porous polymer formation. Combined with viscosimetry measurements, we establish overlap and concentrated crossovers, $c^*$ and $c^{**}$, and obtain radii of gyration $R_g$ and its dependence on concentration in mixed solvents, as well as the respective $\chi$ parameters. We then determine the demixing pathway for the polymer-rich phase, approaching the glass transition and resulting in its kinetic arrest. Based on these results, we establish a predictive and versatile design strategy for PPPO nanoporous gas adsorbers.

4:18PM C25.00010: Conformations of bottlebrush polymers in dilute solution  SARIT DUTTA (Presenter), MATHEW WADE, DYLAN WALSH, DAMIEN GUIRONNET, SIMON ROGERS, CHARLES SING, University of Illinois at Urbana-Champaign — Bottlebrush polymers are a class of highly branched polymers consisting of a central backbone chain with a large number of side chains emanating from it. As the overall structure and stiffness deviates considerably from that of a linear chain, it is important to understand the role of various architectural parameters that determine the conformations of a bottlebrush molecule. We present results that highlight the effects of backbone length, side chain length, and grafting density on the equilibrium static and near-equilibrium dynamic properties of bottlebrushes in dilute solution. Our results are based on a combination of viscometric measurements and computer simulations. The experiments were performed on a series of low polydispersity bottlebrushes comprising of poly(norbornene) backbone and poly(lactic acid) side chains. The simulations were performed on a coarse-grained bead-spring model using a combination of Brownian Dynamics and Monte Carlo. The simulation predictions show quantitative agreement with experimental results, enabling us to probe further structural details not easily amenable to experiments.
4:30PM C25.00011: Diffusion Driven Nonsolvent Induced Phase Separation  DOUGLAS R. TREE (Presenter), Brigham Young University, LUCAS FRANCISCO DOS SANTOS, Universidade Estadual de Maringa, CADEN B WILSON, TIMOTHY R SCOTT, Brigham Young University, JAN ULRIC GARCIA, GLENN FREDRICKSON, University of California, Santa Barbara — Nonsolvent induced phase separation (NIPS) occurs when a polymer solution is brought into contact with a miscible nonsolvent, leading to the precipitation of a polymer-rich phase. Because of its simplicity, NIPS processes are widely used to generate a variety of microstructures in polymer materials such as membranes and micro/nanoparticles. Despite its prevalence, predicting and controlling the microstructure generated by NIPS remains a difficult challenge, owing to the complex interactions between the diffusive transport, hydrodynamics and phase-separation kinetics in the process. In our approach, we use simulations of a "multi-fluid" phase-field model of a ternary polymer solution that incorporates all of these kinetic processes. In the case of NIPS driven by purely diffusive solvent/nonsolvent exchange, we find two regimes capable of generating microstructure via spinodal decomposition: one at times much shorter than the diffusion time of the nonsolvent and one at much longer times. We then use our model to predict (i) which compositions of polymer solution will lead to microstructure formation at both short and long times and (ii) what microstructures emerge as composition is varied.

4:42PM C25.00012: Effects of Side-Chain Deuteration of Poly(N-isopropylacrylamide) on the Thermal Transition Behaviors in Water*  DONGSOOK CHANG (Presenter), KUNLUN HONG, Oak Ridge National Laboratory — Polymers with lower critical solution temperature (LCST) in water are promising building blocks in designing temperature-responsive materials. The thermal transition of polymer and proteins in water is known to depend on deuteration (either of solvent or of polymer/protein), but a full understanding of this phenomenon remains elusive. In this study, we focus on the fact that although partially deuterated poly(N-isopropylacrylamide) (PNIPAm) has been widely used in many studies due to its facile synthesis, its thermal transition behavior has not been independently characterized. We investigate the effect of side-chain deuteration of PNIPAm on its electronic structure, hydrogen bonding, and hydration in water. The thermal transition of PNIPAm with its isopropyl side chain deuterated (d7-PNIPAm) is broader and approximately 2 °C higher than that of h-PNIPAm in dilute solution when measured by microcalorimetry. While the underlying mechanisms are complex, our results currently point to weaker hydrogen bonding of d7-PNIPAm due to a small destabilization of the negative dipole in the amide nitrogen, which results in a weaker cooperativity in hydration.

*This work was performed at the Center for Materials Sciences which is a US Department of Energy (DOE) Office of Science User Facility.

4:54PM C25.00013: Increasing block copolymer dispersity leads to more uniform micelles*  SRITEJA MANTHA (Presenter), SHUANHU QI, Institute of Physics, Johannes Gutenberg University of Mainz, Germany, MATTHIAS BARZ, Institute for Organic Chemistry, Johannes Gutenberg University of Mainz, Germany, FRIEDERIKE SCHMID, Institute of Physics, Johannes Gutenberg University of Mainz, Germany — Synthetic polymers possess some inherent dispersity in their length due to the mechanism of the underlying polymerization reaction. Since nearly every property of the polymers depend strongly on the length of the chain, it is expected that the polymer chain dispersity effects different structural, dynamic and their self-assembly properties in the solution as well as in the melt conditions. In this work we investigate the effect of amphiphilic diblock copolymer chain length dispersity on the size distribution of the spherical micelles formed by them in the solution. Using self-consistent field theory calculations, we show that the monodisperse diblock copolymers form micelles of different sizes in the solution, whereas polydisperse diblock copolymers form micelles which are uniform in size. We attribute this to the fact that the packing of the solvophobic monomers in the micellar core can be optimized if the constituent polymers have different length.

*German Science Foundation - SFB 1066 (Project Q1), SFB 146 (Project C1)
5:06PM C25.00014: Particle Packings in Bidisperse Diblock Copolymer Blends*  
AARON LINDSAY (Presenter), RONALD LEWIS, BONGJOON LEE, MICAH J. HOWARD, TIMOTHY LODGE, FRANK BATES, University of Minnesota - Twin Cities — Recent investigation into the phase behavior of compositionally asymmetric diblock copolymers has resulted in the discovery of a host of previously unanticipated particle packings, including a dodecagonal quasicrystal and several Frank-Kasper (FK) phases. Conformational asymmetry has been shown to favor these fascinating morphologies. However, the number of sufficiently conformationally asymmetric systems available for study is limited. An alternative approach, simply blending two diblocks, has been predicted by self-consistent field theory to allow access to these FK phases, potentially enabling study of these morphologies in a wider range of systems. In this work, we investigated the phase behavior of bidisperse blends of polystyrene-b-poly(1,4-butadiene); the nominally single component diblock copolymer melts show no evidence of FK phase formation. The core block length and relative volume fraction of each polymer was varied, keeping constant the length of the corona block. Small angle X-ray scattering and transmission electron microscopy revealed a rich phase behavior, providing a new means of accessing various particle-packings in diblock copolymer melts.

*NSF: DMR-1104368 and 1801993; GRFP 00039202

5:18PM C25.00015: Investigating the Properties and Phase Behavior of Ionic Liquid and Polymer Blends*  
CAITLIN DONOVAN (Presenter), OSCAR MORALES, MALGORZATA CHWATKO, AARON A BURKEY, ALYSHA HELENIC, SEUNGMIN OH, JOAN BRENNECKE, NATHANIEL A LYND, Chemical Engineering, The University of Texas at Austin — Atmospheric carbon dioxide (CO2) traps heat and increases global temperatures. Both ionic liquids (ILs) and polymers have been investigated for use in CO2 capture technologies. However, composite polymer/IL materials could enhance capture and maintain favorable physical properties for industrial usage. Previously, we identified 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([hmim][Tf2N]) as an IL with excellent physical CO2 solubility. We are interested in polyether and ionic liquid composite materials specifically because of the favorable interactions polyethers have with CO2. It is a necessary first step to investigate the phase behavior and properties of these blends.

We present results of the phase behavior of [hmim][Tf2N] blends with hydrophobic polyethers that have appreciable CO2 solubility. The polymers studied include poly(n-butyl glycidyl ether), poly(allyl glycidyl ether), and poly(isopropyl glycidyl ether). Phase behavior was probed using DSC, microscopy and turbidimetry. The effect of the pendant functional groups in the glycidyl ether polymers (isopropyl vs. n-butyl, and the presence of the double bond in the allyl version) was investigated using 2D NMR and FTIR spectroscopies.

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Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C26 DQI: Superconducting Circuits: Josephson Amplifiers and Non-reciprocal Devices  
BCEC 160B - Jose Aumentado

2:30PM C26.00001: Broadband design of parametric non-reciprocal devices  
OFER NAAMAN (Presenter), Google Inc - Santa Barbara, JOSE AUMENTADO, NIST, Boulder CO., JOHN M MARTINIS, Google Inc - Santa Barbara — There has been significant recent progress in understanding parametric non-reciprocal devices such as circulators and directional amplifiers based on superconducting Josephson circuits. However, these devices remain of limited practical utility due to their narrow bandwidths - typically in the 10's of MHz. To be useful for multiplexed readout in intermediate scale quantum processors, we must engineer these devices to meet prescribed bandwidth and transmission characteristics. In this talk, we outline a procedure for designing parametric devices with bandwidths up to ~1 GHz. We give design examples for a broadband parametric circulator with better than 20 dB isolation over a 500 MHz band, and a non-reciprocal parametric amplifier with broadband reverse isolation and 20 dB forward gain. We illustrate the devices' predicted performance with simulation of their S-parameters.
Quantum discord in squeezed microwaves

KIRILL FEDOROV (Presenter), STEFAN POGORZALEK, MINXING XU, MICHAEL RENGER, MICHAEL FISCHER, EDWAR XIE, QI-MING CHEN, ACHIM MARX, FRANK DEPPE, RUDOLF GROSS, Walther-Meißner-Institut, Munich, Germany — Quantum discord is known as a general measure for quantum correlations in bipartite systems. It encompasses all nonclassical correlations including entanglement. Quantum discord has many intriguing fundamental properties many of which require experimental verification such as the asymptotic robustness towards environmental noise. We experimentally investigate quantum discord in propagating two-mode squeezed (TMS) microwave states generated with the help of superconducting Josephson parametric amplifiers. We exploit asymmetric noise injection into these TMS states which allows us to demonstrate the robustness of quantum discord as opposed to the sudden death of entanglement. Finally, we discuss the relevance of quantum discord as a resource in quantum communication and sensing, in particular with respect to remote state preparation and quantum radar protocols.

We acknowledge support by the German Research Foundation through FE 1564/1-1, Elite Network of Bavaria through the program ExQM, EU Quantum Flagship project QMiCS, and Excellence Cluster MCQST.

Proposal for a novel directional parametric amplifier requiring no external nonreciprocal components

ANDREW LINGENFELTER (Presenter), VOLODYMYR SIVAK, SHYAM SHANKAR, MICHEL H. DEVORET, Yale Univ — Quantum-limited Josephson parametric amplifiers are an important part of most superconducting qubit readout systems. Parametric amplifiers typically operate in reflection and require external nonreciprocal devices to spatially separate the input and output fields of the amplifier and to protect the qubit from noise propagating from the output field. To achieve this without additional external components, the parametric amplifier should have a matched input port, large forward gain from input to output, ideally zero reverse gain from output to input, a matched output port, and an auxiliary port which provides amplified quantum noise to the output. We propose a novel four-port phase-preserving parametric amplifier that satisfies all of the above requirements. This proposal is a natural extension of the previously realized three-port directional amplifier, but does not require an isolator on its output. We discuss the properties of this proposal, and we present a possible experimental implementation.

Work supported by: ARO and YINQE

Theoretical study of nonreciprocal microwave transmission based on Gebhard-Ruckenstein hopping

SHUMPEI MASUDA (Presenter), Tokyo Medical and Dental University, SHINGO KONO, KEISHI SUZUKI, The University of Tokyo, YUUKI TOKUNAGA, NTT Secure Platform Laboratories, NTT Corporation, YASUNOBU NAKAMURA, The University of Tokyo, KAZUKI KOSHINO, Tokyo Medical and Dental University — Several types of quantum information processing schemes and many of superconducting quantum optics experiments require routing of microwaves in a cryostat. Thus, cryogenic circulator is an important tool, and the loss at the circulators is detrimental especially for quantum information processing. This has been urging many researchers to experimental and theoretical works devoted to lossless on-chip microwave circulators.

In this presentation, we theoretically investigate the nonreciprocal microwave transmission based on the Gebhard-Ruckenstein hopping. We consider a superconducting device that consists of microwave resonators and a coupler. The Gebhard-Ruckenstein hopping between the resonators gives rise to a linear energy dispersion, which manifests chiral propagation of microwaves in the device. This device can work as a microscopic circulator when transmission lines are attached. It is shown that our microwave circulator can be robust against detuning of incident microwaves.

We acknowledge the support from JST ERATO (JPMJER1601) and JSPS KAKENHI (16K05497 and 18K03486).

Exploiting the Kerr-free point of a SNAIL for improvement of dynamic range in parametric amplifiers

VOLODYMYR SIVAK (Presenter), ANDREW LINGENFELTER, NICHOLAS E. FRATTINI, VIDUL JOSHI, WEI DAI, SHYAM SHANKAR, MICHEL H. DEVORET, Yale Univ — Quantum-limited Josephson parametric amplifiers are an important component for most superconducting qubit readout methods. While being well optimized for the noise performance, the scalability of resonant parametric amplifiers is determined predominantly by the ability to boost their dynamic range and bandwidth. The dynamic range of the state-of-the-art "paramps" is limited by the spurious Kerr-induced Stark shifts which detune the paramp from its operating point, leading to the reduction of gain with increased signal power. We show that using a Superconducting Nonlinear Asymmetric Inductive eLement (SNAIL) as an active element, we are able to tune to a Kerr-free sweet spot in the presence of the pump, which exhibits significantly improved 1 dB compression power.

ARO, ONR, AFOSR, and YINQE
Towards a SQUID-based Traveling Wave Parametric Amplifier

LUCA PLANAT (Presenter), KARTHIK SRIKANTH BHARADWAJ, OLIVIER BUISSON, REMY DASSONVILLE, JOVIAN DELAFOREST, FARSHAD FOROUGHI, WIEBKE GUICHARD, SÉBASTIEN LÉGER, VLADIMIR MILCHAKOV, CECILE NAUD, JAVIER PUERTAS, NICOLAS ROCH, Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France — Superconducting Parametric Amplifiers are key to research fields involving microwave signals in the quantum regime, such as superconducting qubits or NEMs because of the large gain they provide and their noise performance. Large interaction time between a weak microwave signal, a strong coherent pump tone and a non-linear medium is required to obtain enough gain. Up to now, this was achieved by coupling the non-linear medium to a resonator. But this is also possible by using distributed non-linear media and working in transmission, thus overriding issues of limited bandwidth due to resonant cavities. When the medium is a Josephson junction, this new class of amplifier is called Josephson Traveling Wave Parametric Amplifier (J-TWPA) [1]. We will present our on-going effort to develop a SQUID-based TWPA. It will allow to tune in situ the characteristic impedance of the TWPA to have a perfect impedance match with the rest of the electronic setup, despite the uncertainty of the electrical properties of the device due to the fabrication process.


*This work was supported by the French Agence Nationale de la Recherche (ANR CLOUD project No. ANR-16-CE24-0005)

Design and Fabrication of Broadband Parametric Amplifiers for Quantum Applications

JOEL GREBEL (Presenter), AUDREY BIENFAIT, ETIENNE DUMUR, HUNG-SHEN CHANG, MING-HAN CHOU, CHRISTOPHER CONNER, Institute for Molecular Engineering, University of Chicago, GREGORY A PEAIRS, Department of Physics, University of California, Santa Barbara, RHYS G POVEY, Institute for Molecular Engineering, University of Chicago, KEVIN SATZINGER, Department of Physics, University of California, Santa Barbara, YOUPENG ZHONG, ANDREW N CLELAND, Institute for Molecular Engineering, University of Chicago — Josephson parametric amplifiers (JPAs) provide a straightforward means for the quantum-limited amplification of signals, with noise approaching 1/2-photon for phase-independent gain [1]. These are an important resource for the single-shot readout of superconducting qubits, allowing high fidelity measurements of single as well as multiplexed qubits. I will describe the circuit designs and fabrication process for JPAs developed at the University of Chicago, fabricated in a new nanofabrication facility. The process includes low-loss dielectric deposition, superconducting crossovers, and a Dolan-bridge based Josephson junction definition. We will present data on lumped-element JPA devices with state-of-the-art gain, saturation power, and bandwidth [2], and describe different circuit designs for achieving large bandwidths [3].


*Supported by AFOSR MURI FA9550-15-1-0029, UChicago MRSEC (NSF DMR-1420709), DOE, UChicago PNF SHyNE NNCI NSF EECS-1542205, ARL W911NF-15-2-0058, and ANL.

Development of all aluminum Josephson Travelling Wave Parametric Amplifiers (TWPA)

SHAHID NAWAZ (Presenter), University of California, Berkeley, KEVIN O’BRIEN, Research Laboratory of Electronics – MIT, IRFAN SIDDIQI, University of California, Berkeley — Josephson parametric amplifiers (JPA) have demonstrated high measurement fidelity in qubit readout applications, and near quantum-noise-limited operation in many fundamental physics experiments. While conventional single junction JPAs have limited bandwidth and low saturation power, traveling wave devices can operate with GHz of instantaneous signal bandwidth and the power handling capacity needed for multiplexed readout. We report on progress toward developing an all-aluminum traveling wave parametric amplifier (TWPA) utilizing aluminum oxide capacitor technology. Such devices would require significantly less dielectric material than current silicon dioxide capacitors, potentially reducing the insertion loss observed in state-of-the-art niobium amplifiers.

*This work was supported by the Army Research Office and the Department of Energy.
reciprocal qubit-qubit interactions.

under proper magnetic shielding. We will describe our ongoing progress towards a 3D circuit QED platform with non-
below saturation magnetization of YIG), allowing for direct coupling to transmons qubits and superconducting cavities

A circulator can be converted into a multi-mode cavity, which enables detailed study of hybridized magnon-photon spectra

The single crystalline yttrium iron garnet (YIG) in a waveguide-based package, we realize a microwave circulator with insertion

loss of ~1% and isolation of >20 dB in the quantum regime (at single-photon power and 20 mK temperature). The

non-reciprocal interactions between qubits or cavities to stabilize entanglement or novel many-body states. Here, using

control the information flow while maintaining high fidelity. Moreover, such directional channels can be used to mediate

switching. Josephson junction-based switches can be designed for dissipation-free operation with fast switching, and can be more readily integrated with superconducting quantum circuits, providing a very appealing alternative to semiconductor switches. Here, we present the design and characterization of a lossless single pole double throw (SPDT) superconducting switch based on tunable DC SQUIDs. The switch features fast switching times, large

bandwidth, and a large on/off ratio. Applications for this device include coherent switch of itinerant photons for

applications in quantum information, including quantum computation.

*E.I.R acknowledges support from the ARO QuaCGR fellowship. This work is supported by the ARO under contract

W911NF-14-1-0079 and the National Science Foundation under Grant Number 1125844.

4:18PM C26.00010: A Fast Tunable, Large Bandwidth Superconducting Microwave Switch* HUNG-SHEN CHANG

(Presenter), University of Chicago, KEVIN SATZINGER, UC Santa Barbara; University of Chicago, YOUPENG ZHONG, AUDREY

BIENFAIT, MING-HAN CHOU, CHRISTOPHER CONNER, ETIENNE DUMUR, JOEL GREBEL, University of Chicago, GREGORY A

PAIRS, UC Santa Barbara; University of Chicago, RHYS G POVEY, ANDREW N CLELAND, University of Chicago — Fast controlled

switches are a key feature in classical communication architectures, and likely will play an analogous role in quantum

communication applications. Conventional semiconductor-based microwave switches have been used with

superconducting quantum circuits, enabling for example the in-situ measurement of multiple devices via a common

readout chain. However, these switches dissipate energy when switched, making them unsuitable for applications

requiring rapid, repeated switching. Josephson junction-based switches can be designed for dissipation-free operation

with fast switching, and can be more readily integrated with superconducting quantum circuits, providing a very appealing alternative to semiconductor switches. Here, we present the design and characterization of a lossless single pole double throw (SPDT) superconducting switch based on tunable DC SQUIDs. The switch features fast switching times, large

bandwidth, and a large on/off ratio. Applications for this device include coherent switch of itinerant photons for

applications in quantum information, including quantum computation.


MRSEC (NSF DMR-1420709), and UChicago PNF ShyNe NNCI (NSF ECCS-1542205)

4:30PM C26.00011: Low-loss ferrite waveguide circulator for non-reciprocal circuit QED* YINGYING WANG

(Presenter), THOMAS CONNOLLY, CHEN WANG, Dept. of Physics, Univ. of Mass. Amherst — In a quantum information

processing network, it is highly desirable to have low-loss directional transmission channels with circulators/isolators to

control the information flow while maintaining high fidelity. Moreover, such directional channels can be used to mediate

non-reciprocal interactions between qubits or cavities to stabilize entanglement or novel many-body states. Here, using

single crystalline yttrium iron garnet (YIG) in a waveguide-based package, we realize a microwave circulator with insertion

loss of ~1% and isolation of >20 dB in the quantum regime (at single-photon power and 20 mK temperature). The

circuit can be converted into a multi-mode cavity, which enables detailed study of hybridized magnon-photon spectra

and the internal loss of various modes. The circulator operates at a relatively low magnetic field of 25 mT (significantly

below saturation magnetization of YIG), allowing for direct coupling to transmons qubits and superconducting cavities

under proper magnetic shielding. We will describe our ongoing progress towards a 3D circuit QED platform with non-

reciprocal qubit-qubit interactions.

*This research is supported by the U.S. Army Research Office.

4:42PM C26.00012: Broadband superconducting switches for integrated quantum networks ERIC ROSENTHAL

(Presenter), JILA, University of Colorado, Boulder, CHRISTIAN M.F. SCHNEIDER, Institute for Experimental Physics, University of

Innsbruck, BENJAMIN J. CHAPMAN, Departments of Physics and Applied Physics, Yale, LEILA R. VALE, GENE C. HILTON, National

Institute of Standards and Technology, K. W. LEHNERT, JILA, National Institute of Standards and Technology and the University of

Colorado, Boulder — Switching elements are a generally useful tool in superconducting circuit experiments. They may be

used to reconfigure the connectivity of a network, multiplex qubit readout, and create non-reciprocal devices. In particular,
broadband switches allow for the construction of a broadband, on-chip microwave circulator. For integration with

superconducting qubits, however, these switches must be low-loss and dissipate negligible heat when switching.

Engineering such switches requires reactive circuit elements that tune rapidly between low and high impedance. To

achieve these effects, we develop widely tunable SQUID arrays and present measurements of their performance. We then
describe a new generation of broadband superconducting switches.
4:54PM C26.00013: Josephson Junction-Based Components for Scalable Quantum Computing* BRITTANY RICHMAN (Presenter), Joint Quantum Institute, University of Maryland, College Park, COSMIC RAJ, University of Tokyo, JACOB TAYLOR, NIST — The physical realization of larger quantum computing schemes will require highly scalable signal processing architectures for precise qubit control. Various microwave components are needed for signal routing and isolation, but the size and design of commercially available components are not always feasible for on-chip solutions. With this motivation, we examine how arrays of Josephson junctions in external magnetic fields provide the potential to replace larger devices using the ordering of flux degrees of freedom in the arrays. As a key example, we consider models of circulators, non-reciprocal devices that enable isolation of quantum circuits.

*This research was partially supported by the NSF-funded Physics Frontier Center at the Joint Quantum Institute.

5:06PM C26.00014: Efficient qubit measurements with a nonreciprocal microwave amplifier FLORENT LECOCQ (Presenter), National Institute of Standards and Technology Boulder, LEONARDO M RANZANI, Raytheon BBN Technologies, GABRIEL PETERSON, KATARINA CICAK, JOHN TEUFEL, JOSE AUMENTADO, National Institute of Standards and Technology Boulder — In typical circuit quantum electrodynamics and microwave optomechanics system, the measurement of the observable of interest — the state of a quantum bit or the position of a mechanical oscillator — hinges on the efficient detection of the phase shift that it imparts on a microwave field. Ideal measurement efficiency can only be achieved with a lossless single quadrature measurement apparatus and has been a longstanding challenge. Nonreciprocal parametric amplifiers could enable such high measurement efficiency as they can be directly integrated with the quantum system, avoiding common technical losses due to circulators, cables and connectors used in state-of-the-art amplification chains.

In this talk we will discuss the measurement of a 3D transmon qubit with a Field-Programmable Josephson Amplifier (FPJA, [1]). The FPJA is programmed in situ by a set of microwave drives to perform reciprocal or nonreciprocal frequency conversion or amplification. For each mode of operation, we will monitor the qubit coherence and lifetime, as well as measurement efficiency and backaction.


5:18PM C26.00015: Anomalous Supercurrents in exciton-condensate/normal-barrier/exciton-condensate (EC/N/EC) junctions JUNG-JUNG SU (Presenter), Electrophysics, National Chiao Tung University, YA-FEN HSU, Physics Division, National Center for Theoretical Sciences — The exciton-condensate/normal-barrier/exciton-condensate (EC/N/EC) junction in a bilayer consist of a normal barrier sandwiched between two exciton condensates (ECs), while the two ECs retain a relative phase of $\phi_0$. It is a setup inspired by the superconducting Josephson junction but with a special ingredient – the interlayer tunneling. In EC/N/EC junctions of short-barrier, fractional solitons with topological charge $Q = \phi_0/2\pi$ are predicted to occur. In this paper, however, we focus on the case that the barrier length $d_J$ is larger than the excitonic coherence length $\xi$. We find that the supercurrent occurs because of a distinctive mechanism – an Andreev reflection occurs in one of the EC/N interfaces along with the interlayer tunneling in the barrier. This exotic mechanism gives rise to only a half portion of a fractional soliton that carries a doubled topological charge $2Q = \phi_0/\pi$ (for the same relative phase $\phi_0$). The distinction in topology between the EC/N/EC junctions of short- and long-barrier is reflected in the supercurrents and their current phase relations, which can be observed directly by experiments.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C27 DQI: Quantum Thermodynamics and Resource Theories BCEC 160C - Bo Sun, HRL Laboratories - Tag(s): Focus
Quantum to ‘classical’ behaviour in closed-systems thermodynamics: an analysis of the quantum work distribution in driven fermionic chains

KRISSIA ZAWADZKI (Presenter), Department of Physics, Northeastern University, MARCELA HERRERA, ROBERTO MENEZES SERRA, Department of Physics, Federal University of ABC, IRENE D'AMICO, Department of Physics, University of York — The role of many-body interactions in work and entropy production at nanoscales has become a trend topic mainly boosted by increasing interest of probing the laws of thermodynamics for few particle systems. When we turn to the case of strongly correlated systems, one might be interested in probing phase transitions by means of thermodynamical quantities and their statistics, as, for instance, the moments of the so-called quantum work distribution P(W). We propose to examine this question in the context of out-of-equilibrium Hubbard chains by inspecting the extracted work \( W \) and the first four central moments \( \langle W - \langle W \rangle \rangle^k \), \((k=1,2,3,4)\) of P(W).

Our analysis inspects the interplay between coupling and dynamical regimes, i.e., we analyse the thermodynamical quantities from non-interacting to the strongly coupled limits when the driving external field is turned on adiabatically or as a sudden quench. Our results indicate a high sensibility of the third momentum (skewness) to the Mott insulator transition and we discuss how it could be used as an order parameter to probe quantum phase transitions in experimental nanoscopic strongly correlated systems.

*Royal Society (NA140436); CNPq (PVE-401414/2014-0); CAPES (PDSE-88881.135185/2016-01); (INCT-IQ).

Local superfluid distillation of Bose liquids

TYLER VOLKOFF (Presenter), YONGKYUNG KWON, Physics, Konkuk University — By introducing a localized resource theory of quantum coherence, we discuss limits to local distillation of complete superfluidity from imperfect superfluid states. To define the local maximal superfluid resource, we develop a theory of local superfluidity from first principles using local Galilei transformations, and demonstrate the framework in effective and microscopic models of Bose liquids. The combined theoretical framework of local superfluidity and localized resource theory of quantum coherence allows quantum information-based design and analyses of spatially structured superfluid quantum devices.

*This work was supported by the Korea Research Fellowship Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (Grant No. 2016H1D3A1908876) and by the Basic Science Research Program through the NRF funded by the Ministry of Education (Grant No. 2015R1D1A1A09056745).

Work Extraction from a Single Energy Eigenstate

KAZUYA KANEKO (Presenter), EIKI IYODA, TAKAHIRO SAGAWA, Department of Applied Physics, The University of Tokyo — Work extraction from the Gibbs ensemble by a cyclic operation is impossible, as represented by the second law of thermodynamics. On the other hand, recent studies revealed that a thermal equilibrium state can be represented not only by the Gibbs state, but also by a single energy eigenstate. This is referred to as the eigenstate thermalization hypothesis (ETH). We attempt to unify these two perspectives by examining the possibility of extracting work from a single energy eigenstate. Specifically, we performed numerical exact diagonalization of a quench protocol of local Hamiltonians and evaluated the number of work-extractable energy eigenstates. We found that it becomes exactly zero in a finite system size, implying that a positive amount of work cannot be extracted from any energy eigenstate, if one or both of the pre- and the post-quench Hamiltonians are non-integrable. This result suggests that the second law of thermodynamics is true even at the level of individual energy eigenstates if the system is non-integrable (i.e., quantum chaotic), which is analogous to the ETH.


*This work is supported by JSPS KAKENHI Grant No. JP16H02211, No. JP15K20944, and No. JP17J06875.
3:06PM C27.00004: DFT protocols for quantum thermodynamics of out-of-equilibrium systems* AMY SKELT, Department of Physics, University of York, KRISIA ZAWADZKI (Presenter), Departamento de Fisica e Ciencia Interdisciplinar, Instituto de Fisica de Sao Carlos, University of Sao Paulo, MARCELA HERRERA, Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, IRENE D'AMICO, Department of Physics, University of York — Quantum thermodynamics strives to understand quantum fluctuations at the nanoscale, with an emphasis on the determination of thermodynamic properties of out-of-equilibrium quantum systems. This already challenging task becomes significantly more complex when many-body interactions give rise to strongly correlated systems. Inspired by the Kohn-Sham approach to Density Functional Theory (DFT), we propose to tackle this problem in a framework where the system is effectively described by non-interacting particles, and extend the protocol introduced in M. Herrera, R.M. Serra, I. D'Amico, Scientific Reports 7, 4655 (2017). Considering all dynamic regimes, from adiabatic to sudden quench, we study the work extraction and entropy production in finite Hubbard chains up to 8 sites, and compare results from various driving potentials. We examine the competition between the evolution time, interaction strength, and thermal regimes, benchmarking approximate results against the exact ones. Our results reveal that the DFT-inspired protocol performs well, with deviation of less than 10%, compared to the exact results up to moderate coupling regimes and, surprisingly for a ground state DFT protocol, up to intermediate temperatures of KT~2-3 J, J the hopping parameter.

*We thank EPSRC for support.

3:18PM C27.00005: Absolute irreversibility and continuous quantum measurement: a fluctuation theorem perspective* SREENATH KIZHAKKUMPURATH MANIKANDAN (Presenter), CYRIL ELOUARD, ANDREW N JORDAN, Department of Physics and Astronomy, University of Rochester — The out-of-equilibrium fluctuations of thermodynamic quantities like entropy production for a small system in contact with a thermal reservoir are constrained beyond the second law using relations known as fluctuation theorems. Here we show that, in the absence of a thermal reservoir, the dynamics of continuously measured quantum systems can also be described by a fluctuation theorem, where the fluctuations originate from inherently probabilistic quantum measurement dynamics. This theorem captures the emergence of an arrow of time in the measurement process, from microscopically reversible quantum state dynamics in continuous quantum measurements. We also demonstrate that the measurement-induced wave-function collapse exhibits absolute irreversibility, such that Jarzynski and Crooks-like equalities are violated. We apply our results to different continuous measurement schemes on a qubit: dispersive measurement, homodyne and heterodyne detection of qubit's fluorescence.

*This work was supported by the John Templeton Foundation Grant ID 58558, the US Army Research Office grant No. W911NF-15-1-0496, the National Science Foundation grants No. DMR-1506081 and NSF PHY-1748958, and the US Department of Energy grant No. DE-SC0017890

3:30PM C27.00006: Thermodynamics of fast quantum gates* CYRIL ELOUARD (Presenter), Department of Physics and Astronomy, University of Rochester, MASSIMILIANO ESPOSITO, University of Luxembourg, ALEXIA AUFFÈVES, Institut Néel - CNRS, ANDREW N JORDAN, Department of Physics and Astronomy, University of Rochester — Quantum computation gates rely on the possibility to perform qubit rotations in the Bloch sphere faster than decoherence. Strikingly, a thermodynamic description analyzing the coherent energy exchanges between the qubit and the driven field is still missing. Previous studies have focused on long timescales [1-2], much larger than one Rabi period, blurring out any coherent phenomenon, and are therefore inadequate to study e.g. the work cost of fast gates. Here we propose a thermodynamic description that is valid at short time-scales, where the dynamics is captured by the Optical Bloch Equations, featuring coherent excitation exchanges between qubit and the field. We identify the first and second law and their quantum components. The derivation of an integral and a detailed Crooks quantum fluctuation theorems ensures the thermodynamic consistency of our theory. Predictions from earlier Floquet-based (long time-scale) approaches are recovered in relevant regimes. Our results contribute to bridge the gap between quantum thermodynamics on the one hand, and quantum optics and quantum computation on the other hand.


3:42PM C27.00007: Quantum of information and its fluctuations in a conductor heat current* [Invited] YASUHIRO UTSUMI (Presenter), Physics Engineering, Mie University — Mesoscopic quantum conductors have been tools to investigate thermodynamics in the quantum regime [1]. They also offer a playground to think about entanglement and information transmission. In a quantum conductor, by applying a source-drain bias voltage, entangled electron-hole pairs can be created [2]. Moreover one bit of information content can be conveyed by the arrival or non-arrival of an electron [3]. We revisit this problem by analyzing a novel quantity, the distribution of fluctuating information, particle and heat currents, which is closely related to the Rényi entanglement entropy [4]. Our approach is the full-counting statistics based on the multi-contour Keldysh Green function developed recently [4,5].

To quantify the particle-hole entanglement, one has to remove the contribution from superpositions of different particle number eigenstates, which cannot be created and measured locally [2]. For this purpose, we account for the local electron number constraint and discuss the condition that the maximum accessible entanglement is realized [4].

The quantum physics limits the performance of communication through a conductor [3]. The optimum channel capacity, the maximum rate at which information can be transmitted under a given signal power, i.e. heat current, relates theory of communication and thermodynamics. We demonstrate a universal relation connecting the fluctuation of information, the Rényi entropy of order zero and the optimum capacity [4].

[5] YV Nazarov, PRB 84 205437 (2011); MH Ansari and YV Nazarov, ibid. 91 104303 (2015); ibid. 91 174307 (2015); ibid. 95 174302 (2017)

*This work was supported by JSPS-KAKENHI17K05575 and JP26220711

4:18PM C27.00008: Work extraction and Landauer's principle in a quantum spin Hall device INANC ADAGIDELI (Presenter), AHMET MERT BOZKURT, BARIS PEKERTEN, Sabanci University — Landauer’s principle states that erasure of each bit of information in a system requires at least a unit of energy kBT ln2 to be dissipated. In return, the blank bit may possibly be utilized to extract usable work of the amount kBT ln2, in keeping with the second law of thermodynamics. While in principle any collection of spins can be utilized as information storage, work extraction by utilizing this resource in principle requires specialized engines that are capable of using this resource. In this work, we focus on heat and charge transport in a quantum spin Hall device in the presence of a spin bath. We show how a properly initialized nuclear spin subsystem can be used as a memory resource for a Maxwell’s Demon to harvest available heat energy from the reservoirs to induce charge current that can power an external electrical load. We also show how to initialize the nuclear spin subsystem using applied bias currents which necessarily dissipate energy, hence demonstrating Landauer’s principle. This provides an alternative method of “energy storage” in an all-electrical device. We finally propose a realistic setup to experimentally observe a Landauer erasure/work extraction cycle.

4:30PM C27.00009: The dramatic impact of non-energetic coherences on heat flows* CAMILLE LOMBARD LATUNE (Presenter), ILYA SINAYSKIY, FRANCESCO PETRUCCIONE, University of KwaZulu-Natal — We show that the heat flow between a system and a stationary reservoir (under Born-Markov approximation) is dramatically affected by coherences between degenerate levels of the system. To assess the resulting effects of coherences on heat flows we introduce a concept of apparent temperature [1] which crucially takes into account coherences, by contrast with the virtual temperature [2]. It provides an intuitive picture in which non-energetic coherences behave as populations, enabling one to recover seminal results on phaseonium, thermally entangled atoms, and lasing without inversion. Moreover, we predict new effects like the dramatic increase of apparent temperature due to delocalised excitations. One of its manifestations, testable experimentally, is the “apparent thermalization”, where an ensemble of indistinguishable subsystems equilibrates at a much lower (or higher) energy than when interacting separately (or distinguishably) with the bath. Such phenomena stem from the mixture of the dynamics of the populations and coherences, which happens only in presence of degeneracy and is unique to quantum thermodynamics.


*South African Research Chair Initiative
Quantum thermalization and optimal control are compatible in a many-body system

FERNEY RODRIGUEZ (Presenter), FERNANDO GÓMEZ-RIUZ, LUIS QUIROGA, Physics, Universidad de Los Andes, NEIL F JOHNSON, Physics, George Washington University — We propose a novel protocol for characterizing and ultimately controlling collective matter-radiation effects that emerge when a many-body quantum system is driven through a critical value of the interaction coupling strength. There are many possible ways to use our scheme to achieve quantum computing and information processing, including controlling superconducting qubits or color defects in diamond by means of quantum light in cavities. We show that apparently disparate phenomena such as thermalization, excited state quantum phase transitions and orthogonality catastrophes can be present in the system when subject to a finite pulsed coupling with the light field. In particular, we demonstrate a connection between the thermalization through entanglement of the global quantum pure system reached at the middle of the pulse, and the controlled production of an orthogonal global state at the end of the pulse. Our results should prove useful in a variety of contexts including the preparation of phases of condensed matter in quantum simulators and the engineering of states in quantum protocols.

Critical point behaviour of a measurement-based quantum heat engine

SUMAN CHAND, ASOKA BISWAS (Presenter), Indian Institute of Technology Ropar — At the critical point (CP), pertaining to quantum phase transition (QPT), the long-range quantum correlation (e.g., entanglement) becomes dominant. We show, in case of an ion-based quantum Otto engine, that such correlation does not necessarily enhance the efficiency of the engine, in the neighborhood of the CP. We choose two trapped ions as the working system, subject to a magnetic field and an internal energy-exchange coupling J1. During the expansion stage of the engine cycle, the adiabatic decrease of the magnetic field from B_H to B_L leads to certain work. The cooling of the system during the exhaust stage is mimicked by a projective measurement of the system into the ground state. During the compression stage, the magnetic field is adiabatically restored to B_H. We find that the critical point B_L=J1/2 poses as a minimum threshold for the system to work as a heat engine. Further, the efficiency of the engine increases with increase of the interaction strength J_1. On the contrary, the coupling to any ancillary system deteriorates the efficiency at the critical point, though such coupling enhances entanglement into the system. Our result suggests that long-range correlation may not be beneficial for an efficient quantum heat engine in the realm of QPT.

Topological work in nonequilibrium quantum thermodynamics

CHARLES STAFFORD (Presenter), Physics, University of Arizona, ABHAY SHASTRY, Chemistry, University of Toronto, YIHENG XU, Physics, U.C. San Diego, MARCO ANTONIO JIMENEZ VALENCIA, Physics, University of Arizona — As a model open quantum system out of equilibrium, we consider a system of electrons coupled to multiple (typically 3) macroscopic electron reservoirs and threaded by an Aharonov-Bohm flux φ. For the noninteracting case, we determine the exact nonequilibrium steady-state density matrix and entropy. We prove that the Nernst theorem (3rd law of thermodynamics) holds without exception for an open quantum system, even for the nonequilibrium case. The general principles are illustrated for the case of a quantum thermocouple. Both the chemical work due to electron exchange between the reservoirs and the topological work due to the Aharonov-Bohm effect must be included in applying the 1st law. The effect of electron-electron interactions on the thermoelectric device performance beyond linear response are investigated.

Observable Thermalization

FABIO ANZA (Presenter), Physics, University of California, Davis — To understand under which conditions thermodynamics emerges from the microscopic dynamics is the ultimate goal of statistical mechanics. Despite the fact that the theory is more than 100 years old, we are still discussing its foundations and its regime of applicability. A point of crucial importance is the definition of the notion of thermal equilibrium, which is given as the state that maximises the von Neumann entropy. Here we argue that it is necessary to propose a new way of describing thermal equilibrium, focused on observables rather than on the full state of the quantum system. We characterise the notion of thermal equilibrium, for a given observable, via the maximisation of its Shannon entropy and highlight the thermal properties that such a principle heralds. Eventually, we bring to light an intimate connection with the Eigenstate Thermalisation Hypothesis.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C28 DQI: Topological Quantum Information with Majorana Nanowires

Angela Kou, Yale Univ
2:30PM C28.00001: Probing coherent coupling of Majorana modes via single-electron photon assisted tunneling:
Part 1* DEIVIDAS SABONIS (Presenter), DAVID VAN ZANTEN, JUDITH TABEA SUTER, University of Copenhagen, DMITRY PIKULIN, Microsoft Corp, JUKKA VAYRYNEN, Univ of California - Santa Barbara, TORSTEN KARZIG, Microsoft Corp, EOIN C O’FARRELL, DAVYDAS RAZMADZE, University of Copenhagen, KARL D PETERSSON, PETER KROGSTRUP, Microsoft Corp, CHARLES M MARCUS, University of Copenhagen — The coherent coupling between Majorana zero modes localized in distinct topological islands mixes the 1e charge states of islands. This coherent superposition of even and odd parity states is a necessary condition for the operation of topological qubits. We demonstrate the coherent coupling of zero modes in a superconducting double island created in a InAs/Al nanowire. This is achieved by tracking microwave induced charge transitions between the islands. The dispersion of photon assisted tunneling features is 1e periodic and shows the presence of an anti-crossing between even and odd parity charge states.

In this talk we will first characterize the coupling between islands using microwave spectroscopy in the absence of magnetic field and finally discuss the transition into the topological regime.

*Research supported by Microsoft Station Q and Danish National Research Foundation.

2:42PM C28.00002: Probing coherent coupling of Majorana modes via single-electron photon assisted tunneling:
Part 2* DAVID VAN ZANTEN (Presenter), DEIVIDAS SABONIS, JUDITH TABEA SUTER, University of Copenhagen, DMITRY PIKULIN, JUKKA VAYRYNEN, TORSTEN KARZIG, Station Q, Microsoft, EOIN C O’FARRELL, DAVYDAS RAZMADZE, KARL D PETERSSON, University of Copenhagen, PETER KROGSTRUP, Station Q, Microsoft, CHARLES M MARCUS, University of Copenhagen — The coherent coupling between Majorana zero modes localized in distinct topological islands mixes the 1e charge states of islands. This coherent superposition of even and odd parity states is a necessary condition for the operation of topological qubits. We demonstrate the coherent coupling of zero modes in a superconducting double island created in a InAs/Al nanowire. This is achieved by tracking microwave induced charge transitions between the islands. The dispersion of photon assisted tunneling features is 1e periodic and shows the presence of an anti-crossing between even and odd parity charge states.

In this talk we will discuss microwave spectroscopy measurements in the presence of magnetic field and show that the 1e periodicity results from discrete zero-energy states which emerge in magnetic field.

*Research supported by Microsoft Station Q and Danish National Research Foundation.

2:54PM C28.00003: Single-shot readout of spin-orbit-split Andreev doublets: motivation and setup* VALLA FATEMI (Presenter), MAX HAYS, KYLE SERNIAK, Department of Applied Physics, Yale University, DANIËL BOUMAN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, GIJS DE LANGE, Microsoft Station Q Delft, Delft University of Technology, SPENCER DIAMOND, Department of Applied Physics, Yale University, PETER KROGSTRUP, JESPER NYGÅRD, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, ATTILA GERESDI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, MICHEL H. DEVORET, Department of Applied Physics, Yale University — Modern efforts towards constructing exotic superconducting qubits such as Andreev spin qubits and Majorana bound states hinges on spin-orbit coupling. The physics of these unique quantum systems may be explored using the well-developed microwave techniques of circuit QED, which can yield sharp spectral resolution and time-domain information. Here we report on measurements of long InAs-nanowire Josephson junctions embedded in a circuit QED architecture. The Andreev bound state spectrum includes transitions which correspond to the transfer of a single quasiparticle between two spin-orbit-split Andreev doublets. Some of these transitions exhibit large coupling to the on-chip resonator. Thus, fast, time-domain measurement of the many-body state of the junction can be achieved through dispersive readout. In this first part of a joint presentation, we will present the background and motivation, as well as the experimental setup and a theoretical model for our system.

*Work supported by ARO, ONR, NSF, and AFOSR
(Presenter), VALLA FATEMI, KYLE SERNIAK, Applied Physics, Yale University, DANIËL BOUMAN, Qutech and Kavli Institute of Nanoscience, Delft University of Technology, GIJS DE LANGE, Microsoft Station Q Delft, Delft University of Technology, SPENCER DIAMOND, Applied Physics, Yale University, PETER KROGSTRUP, JESPER NYGÅRD, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, ATILIA GERESDI, Qutech and Kavli Institute of Nanoscience, Delft University of Technology, GIJS DE LANGE, Microsoft Station Q Delft, Delft University of Technology, SPENCER DIAMOND, Applied Physics, Yale University — Modern efforts towards constructing exotic superconducting qubits such as Andreev spin qubits and Majorana bound states hinges on spin-orbit coupling. The physics of these unique quantum systems may be explored using the well-developed microwave techniques of circuit QED, which can yield sharp spectral resolution and time-domain information. Here we report on measurements of long InAs-nanowire Josephson junctions embedded in a circuit QED architecture. The Andreev bound state spectrum includes transitions which correspond to the transfer of a single quasiparticle between two spin-orbit-split Andreev doublets. Some of these transitions exhibit large coupling to the on-chip resonator. Thus, fast, time-domain measurement of the many-body state of the junction can be achieved through dispersive readout. In this second part of a joint presentation, we will describe the experimental data and discuss the outlook.

*Works supported by ARO, ONR, NSF, and AFOSR

3:18PM C28.00005: Entangling Spins in Double Quantum Dots and Majorana Bound States  MARKO RANCIC
(Presenter), SILAS HOFFMAN, Department of Physics, University of Basel, CONSTANTIN SCHRADE, Massachusetts Institute of Technology, JELENA KLINOVAJA, DANIEL LOSS, Department of Physics, University of Basel — We theoretically investigate the coupling between a singlet-triplet (ST) spin qubit realized in a double quantum dot and a topological qubit composed of Majorana bound states. First, we derive an effective Hamiltonian which facilitates an entangling gate between the two individual qubits, thereby enabling a CNOT gate and, subsequently, a SWAP gate. Using standard readout and single qubit operations of the ST qubit, we show how the former gate can be used to readout the state of Majorana qubit while the latter gate enables universal quantum computation of the topological qubit. We estimate the fidelity of the entangling and SWAP gate operations to be 0.9997 and 0.993, respectively, using parameters that are consistent with realizing both of the qubits within a nanowire. Furthermore, we find that the coupling between the ST qubit and a single Majorana bound state induces an oscillation between the two singlet-triplet levels which has the utility to (1) perform single qubit operations on the singlet-triplet around the x axis without a need for a gradient of Zeeman fields and (2) provide a signature for the presence of zero energy bound states. Lastly, we propose a scheme to extend our setup to a scalable network using the ST-Majorana bound state qubit as the atomic unit.

3:30PM C28.00006: Quasiparticle Poisoning in a Proximitized Semiconductor Nanowire Qubit*  WILLEMIJNTJE UILHOORN (Presenter), ARNO BARGERBOS, JAMES KROLL, JASPER VAN VEEN, QuTech, Delft University of Technology, CHUNG-KAI YANG, Station Q Delft, Microsoft, JESPER NYGÅRD, Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, PETER KROGSTRUP, Station Q Lyngby, Microsoft, LEO KOUWENHOVEN, ANGELA KOU, GIJS DE LANGE, Station Q Delft, Microsoft — Topological qubits are predicted to have very long coherence times due to their inherent protection against local perturbations. However, non-parity preserving processes such as quasiparticle poisoning (QPP) set the bandwidth requirements for controlling topological qubits. Quasiparticle poisoning rates have been recorded in conventional superconducting transmon qubits [1, 2] and in hybrid proximitized semiconductor nanowire junctions [3] at zero magnetic field.

Here we perform QPP measurements on nanowire transmons in a magnetic field by monitoring parity-dependent shifts of the transmon's readout resonator. We investigate the magnetic field dependence of the QPP up to magnetic fields required to reach the topological phase.


*This work was supported by Microsoft and the Netherlands Organisation for Scientific Research (NWO/OCW).
Little-Parks effect in a semiconducting nanowire-based superconducting qubit with \textit{in-situ} switching between transport and cQED* 

ANDERS KRINGHØJ (Presenter), THORVALD W LARSEN, OSCAR ERLANDSSON, DEIVIDAS SABONIS, Center for Quantum Devices and Microsoft Quantum Lab–Copenhagen, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark, BERNARD VAN HECK, Center for Quantum Devices and Microsoft Quantum Lab–Copenhagen, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark, and Microsoft Quantum, Microsoft Staq.

We demonstrate \textit{in-situ} switching between coherent cQED measurements and transport measurements based on a full-shell nanowire using a Josephson junction as a gate tuneable switch. These field-compatible devices show flux-dependent lobe spectra in both transport and cQED measurements associated with the Little-Parks effect. Coherent operations are performed both around zero applied field and around 90 mT, corresponding to one flux quantum being threaded through the wire, with a destructive regime in between.

This opens the possibility of detecting the presence of MZMs in one-flux-quantum regime by cQED measurements.


Cavity-based readout and control of Majorana qubits

THOMAS SMITH (Presenter), ARNE GRIMSMO, STEPHEN D BARTLETT, ANDREW C DOHERTY, Univ of Sydney — We discuss readout and control protocols based on coupling Majorana bound states to cavities. In particular, we consider hybrid superconductor-semiconductor nanowires where the Majorana-cavity coupling is mediated by a quantum dot. The resulting qubit-cavity interaction can be operated in the dispersive regime, familiar from circuit QED. Alternatively, a longitudinal interaction can be activated by parametric modulation of the qubit-cavity coupling strength [1]. We explore how these interactions can be used for readout of Majorana qubits, as well as their use for cavity-mediated entangling gates.


Nonlinear quantum optics for the characterization of Majorana qubits*

SAMUEL BOUTIN (Presenter), Institut quantique and Département de Physique, Université de Sherbrooke, ANQI MU, Department of Physics, University of Toronto, PEDRO LOPES, Stewart Blusson Quantum Matter Institute, University of British Columbia, UDSON MENDES, ION GARATE, Institut quantique and Département de Physique, Université de Sherbrooke — Recent developments in the design of Majorana qubits have focused on devices with significant charging energy. In this parameter regime, methods from circuit QED can be used to study topological qubits. In particular, the toolbox of quantum optics opens new possible schemes for the characterization, measurement, and control of Majorana qubits. As a step in this direction, we investigate how the phenomenon of bifurcation in nonlinear cavities, commonly used for measuring qubits, is altered in the presence of Majorana bound states. Our preliminary results indicate that bifurcation could help characterize quasiparticle poisoning events in quantum wires-based Majorana qubits.

*This research has been funded by the Natural Sciences and Engineering Research Council of Canada, the Fonds de Recherche du Québec - Nature et Technologies, and Canada's First Research Excellence Fund.
On-chip microwave spectroscopy of an InAs nanowire Cooper-pair transistor

DOMINIQUE LAROCHE (Presenter), ALEXANDER PROUTSKI, BAS VAN ‘T HOOFT, QuTech, Delft University of Technology, JESPER NYGÅRD, PETER KROGSTRUP, Center for Quantum Devices and Station Q Copenhagen, University of Copenhagen, LEO P KOUWENHOVEN, ATTIKA GERESDI, QuTech, Delft University of Technology — Controlling both the charging and the Josephson energies of superconducting islands is a crucial requirement for the operation and readout of prospective Majorana-based topological qubits. Here, we present the study of Cooper-pair transistors (CPTs) fabricated from InAs nanowires with superconducting Al shell, a promising platform for the physical realization of topological qubits. By utilizing on-chip microwave spectroscopy, we are able to induce excitations between energy levels of the CPT in a parity conserving manner. We map both the charge- and the photon-like excitations of the system, and show that it is possible to tune the CPT from a Coulomb-blockaded to a transmon-like regime by adjusting the system parameters. The quantum system is exhaustively modeled, allowing us to extract the effective charging and Josephson energies of the CPT. In addition, we study the ground state charge occupation of the CPT and attribute the observed temperature dependence of the even-odd parity structure to the presence of a sub-gap state on the superconducting island.

Rapid single-shot detection of coherent tunneling in an InAs nanowire double quantum dot through dispersive gate sensing

DAMAZ DE JONG (Presenter), JASPER VAN VEEN, LUCA BINCI, AMRITA SINGH, Delft University of Technology, JESPER NYGÅRD, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, PETER KROGSTRUP, Center for Quantum Devices and Microsoft Quantum Lab Copenhagen, Niels Bohr Institute, University of Copenhagen, LEO P KOUWENHOVEN, WOLFGANG PFAFF, JOHN WATSON, Microsoft Station Q Delft, Delft University of Technology — Dispersive gate sensing can enable scalable and high-fidelity readout of solid-state quantum bits. In particular, it has been proposed for fast non-demolition readout of topological qubits that can be measured by single electrons tunneling through zero-energy modes [1, 2]. Such a readout requires resolving the coherent charge tunneling amplitude from a quantum dot in a Majorana zero-mode host system faithfully on short time scales. Here we demonstrate rapid detection of single-electron tunneling between InAs nanowire quantum dots. To this end we have engineered a sensitive dispersive detection circuit by connecting a microwave resonator to a high-lever arm gate. This circuit translates charge tunneling between the dots into a dispersive shift on the resonator [3]. At charge degeneracy the phase shift of a reflected probe signal approaches its maximal possible value of 180 degrees, enabled by the large dot-resonator coupling. This allows us to detect the charge tunneling amplitude with an SNR exceeding two in a microsecond [4]. Our result paves the way for fast high-fidelity measurements of fermion parity in topological qubits.

Dispersive gate-sensing of a quantum dot coupled to a superconducting island

JASPER VAN VEEN (Presenter), DAMAZ DE JONG, LIN HAN, CHRISTIAN PROSKO, QuTech and Kavli Institute of NanoScience, Delft University of Technology, TORSTEN KARZIG, Station-Q, Microsoft Research, PETER KROGSTRUP, JESPER NYGÅRD, Center for Quantum Devices and Station-Q Copenhagen, Niels Bohr Institute, University of Copenhagen, LEO P KOUWENHOVEN, JOHN WATSON, WOLFGANG PFAFF, Microsoft Station-Q at Delft University of Technology — Combining superconductivity with quantum dots in proximitized, semiconducting nanowires has led to many novel phenomena ranging from $\pi$-junctions to Cooper-pair splitters. Currently, these hybrid systems are of interest in the context of Majorana-zero modes (MZMs). In particular, it has been proposed that a topological qubit can be made by coupling a superconducting island hosting MZMs to a dot. However, to date, even trivial superconducting island-dot systems are not yet fully understood.

To increase this understanding, we experimentally study the coupling between a quantum dot and a superconducting island. Dispersive gate-sensing is used to readout because it is directly sensitive to the coupling amplitude between the two systems. We focus on two regimes characterized by their coupling to the leads. For weak, but finite, lead coupling, we identify the relevant charge-transfer processes by comparing a phenomenological model to our data. For a closed system without lead coupling, we can access quasiparticle states allowing us to extract the free energy difference of the island.

Combined, these experiments set the stage for future dot-MZMs experiments. This is necessary for distinguishing dot-trivial superconductor coupling from dot-MZM coupling.
Observation of quantized conductance in quantum point contacts on near surface InAsSb quantum wells* MIHIR PENDHARKAR (Presenter), JOON SUE LEE, MICHAEL A SEAS, ANTHONY MCFADDEN, TAOZHI GUO, CONNOR DEMPSEY, SEAN HARRINGTON, DANIEL J PENNACHIO, TOBIAS BROWN-HEFT, HADASS INBAR, CHRIS PALMSTROM, University of California, Santa Barbara — Topological protection in Majorana Zero Mode (MZM) based quantum computation depends on the induced topological energy gap in the host superconductor-semiconductor hybrid system. Induced topological gap is in turn directly proportional to the spin-orbit coupling in the host system. Certain compositions of InAsSb are expected to have an enhanced spin-orbit coupling as compared to InAs and InSb, thus making InAsSb an ideal platform for robust and scalable topological networks. In this work, top gate control of electron density in near surface InAsSb 2DEGs has been demonstrated. Full depletion can be observed at relatively low top gate voltages, at 2K. Additionally, quantum point contacts on InAsSb 2DEGs show quantized conductance at zero-field at 2K. This work paves the way for coupling superconductivity and enabling the use of near surface InAsSb quantum wells as a host material system for MZM-based topological quantum computation.

Majorana fermions in nanowire-superconductor systems in periodic magnetic fields and their resonant manipulation* VIKTORIA KORNICH (Presenter), University of Wisconsin - Madison, XIAOLI HUANG, TU Delft, MAXIM VAVILOV, MARK G FRIESEN, M. A. ERIKSSON, SUSAN COPPERSMITH, University of Wisconsin - Madison, Y. V. NAZAROV, TU Delft — The nanowire-superconductor structures with a helical magnetic field are known to host Majorana fermions. We show that the structures built in Si can support Majorana fermions even for the field shapes that are very different from helical ones. We discuss various shapes and imperfections of the magnetic field, and present phase diagrams for a wide range of experimental parameters.

Robust micro-magnet geometries for Majorana modes in low g-factor materials SARA TURCOTTE (Presenter), SAMUEL BOUTIN, JULIEN CAMIRAND LEMYRE, ION GARATE, Institut quantique, Université de Sherbrooke, MICHEL PIORO-LADRIERE, Institut quantique, Université de Sherbrooke and Canadian Institute for Advanced Research — Signatures of Majorana bound states (MBS) have been widely reported in semiconductors materials with large spin-orbit coupling and proximity-induced superconductivity [1]. In principle, MBS can also emerge in weakly spin-orbit coupled materials subjected to inhomogeneous magnetic fields [2]. However, in practice small g-factors make it difficult to reach the topological phase. In this work, we explore a versatile approach where spin-orbit coupling arises from a non-uniform magnetic field produced by a micro-magnet array [3]. Using the recently developed RGF-GRAPE algorithm [4], we optimize realistic micro-magnet geometries to find suitable conditions for the emergence of MBS in a one-dimensional wire without intrinsic spin-orbit coupling. In addition, we study robustness of MBS against possible micro-magnet nanofabrication errors. Finally, we identify suitable low g-factor materials commonly used in the microelectronic industry as promising candidates for experimental implementations.

We introduce an ultra-high-impedance superconducting circuit where the role of phase difference across a Josephson junction is replaced by quasi-charge. This Hamiltonian is dual to that of the transmon, in which the kinetic energy term associated with the charging energy is replaced by the inductive energy. Our circuit consists of a small-area Josephson junction shunted by a large linear inductance exceeding one micro-Henry. In such a circuit, the sensitivity of the ground to the first excited state transition is virtually flux insensitive while the flux-tunability of the transitions to higher excited states is largely preserved. Proper circuit design and choice of the fabrication techniques enable the mitigation of the parasitic capacitance previously associated with such large shunting inductances. In this talk, we demonstrate how the device spectra can be adequately described by the dual Hamiltonian and show that the flux dispersion of the qubit transition is reduced down to less than 100 MHz across the entire flux quantum. We also put a limit on the loss tangent of the inductor to be $5 \times 10^{-6}$.

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Tunable Josephson phase-slip qubits (JPSQs) present the possibility of constructing effective spin-1/2 Hamiltonians with arbitrary 2-local interactions using superconducting technology. Here, we discuss how this mapping is made, presenting a Pauli-operator breakdown of the current and voltage dipoles of a JPSQ along a qubit annealing path that allows for preparation and readout in addition to the engineered couplings. As an example of the possibilities inherent in these devices, we present a system of JPSQs that adiabatically encodes or decodes a logical qubit in a $[[4,1,2]]$ Bacon-Shor code.

The Josephson phase-slip qubit (JPSQ) [1] is a superconducting circuit that emulates a vector quantum $S=1/2$ system, with an effective dipole moment nearly independent of applied field, even near zero. This makes JPSQs ideal for emulating vector spin interactions, such as non-Stoquastic $+XX$ of interest for quantum annealing. We describe the design and operation of a JPSQ implementation. Using dispersive readout, we demonstrate the predicted periodic tuning with both flux and charge, and measure lifetimes in the microsecond regime. We also characterize the influence of charge jumps on the circuit’s operation. These results confirm the operating principles of the JPSQ and suggest that it could play an important role in a variety of quantum device architectures.


*This research is funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the U.S. Government.
3:18PM C29.00005: Characterization of Josephson phase-slip qubits, Part 2: Annealing* ROBERT HINKEY (Presenter), MOE KHALIL, SERGEY NOVIKOV, DAVID CLARKE, JAMES I. BASHAM, STEVEN DISSELER, ALEXANDER MARAKOV, JEFFREY GROVER, Northrop Grumman - Mission Systems, DAVID K KIM, MIT Lincoln Laboratory, ZACHARY A STEGEN, Northrop Grumman - Mission Systems, ALEXANDER MELVILLE, BETHANY M. NIEDZIELSKI, JONILYN YODER, MIT Lincoln Laboratory, DANIEL A LIDAR, University of Southern California, KENNETH M. ZICK, DAVID FERGUSON, Northrop Grumman - Mission Systems — Josephson phase slip qubits (JPSQs) have been identified as a promising qubit with which to build next-generation quantum annealers. These qubits have charge tunability through the Aharanov-Casher effect. This charge tuning is a signature of their ability to achieve “strong” non-stoquastic XX couplings with “strong” indicating couplings that are large relative to residual single qubit fields. This coupling regime is not known to be possible to achieve with conventional flux qubits. In this talk we present initial characterization measurements of JPSQs that are annealing-compatible and have a large charge dispersion.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) through the Army Research Office (ARO) Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).

3:30PM C29.00006: Classically reversible logic gate coupled to a superconducting qubit: Problem definition (pt. 1) KEVIN DANIEL OSBORN (Presenter), WALTRAUT WUSTMANN, LPS at the University of Maryland, College Park — New research is starting on a digital logic that uses physical and logical reversibility to achieve higher energy efficiency than commercial digital gates which are irreversible. After describing resonant dynamics of topological solitons in classical reversible superconducting gates, we discuss the theoretical coupling to a superconducting qubit. The solitons in this classical logic are fluxons in Long Josephson Junctions (LJJs), and the fluxon polarity (fluxon or antifluxon) represents a bit state. Gate structures consist of input and output LJJs, and a JJ circuit interface in-between is such that an incoming fluxon temporarily exchanges energy with a localized mode, before an output fluxon emerges with operation-defined polarity. This scattering is efficient and fast in 1- and 2-bit gates. While quantum fluctuations are intentionally negligible for classical gate operations, we study fluxon gates coupled with a qubit, as a possible resource for qubit readout. We analyze the gates with a quasiparticle model for the LJJ fields. Depending on the exact interface design, different types of elastic scattering occur. In a quantum regime, with a qubit embedded across the central interface JJ, a quantized version of the quasiparticle model should be a convenient approximation.

3:42PM C29.00007: Classically reversible logic gate coupled to a superconducting qubit: Qubit simulation (pt. 2) WALTRAUT WUSTMANN (Presenter), KEVIN DANIEL OSBORN, LPS at the University of Maryland, College Park — We theoretically study a classically reversible logic gate coupled to a superconducting qubit for potential applications in quantum computing. The classical gate consists of a Josephson junction circuit interface between long Josephson junctions, and the input of the gate is a ballistically traveling fluxon (a topological sine-Gordon soliton). Depending on the gate definition, a fluxon can undergo different types of resonant elastic scattering, e.g., forward scattering as fluxon or antifluxon. Here we report on how the scattering outcome can depend on the state of a qubit that is embedded in the interface, thus potentially allowing the readout of the qubit from the fluxon dynamics. We specifically will show the effect for a fluxonium qubit galvanically coupled through a junction in the gate interface. This presents a large 4pi-phase difference seen by the qubit. Different fluxon scatterings are found in the classical dynamics of the coupled system for the fluxonium qubit states with macroscopically different phases. We will further use a quantized version of a quasiparticle model, originally developed for classical gates, and take into account few fluxonium levels. The newer analysis should allow us to predict state evolution of a qubit strongly coupled to a topological soliton.
3:54PM C29.00008: Quantum information processing using 3D multimode circuit QED* SRIVATSAN CHAKRAM (Presenter), RAVI NAIK, AKASH DIXIT, YAO LU, ALEXANDER ANFEROV, NELSON LEUNG, ANDREW ORIANI, DAVID SCHUSTER, University of Chicago — Multimode superconducting microwave cavities provide a hardware efficient means of engineering a large, high-coherence Hilbert space suitable for quantum information processing. When coupled to a superconducting transmon circuit, they can be used to construct random access quantum processors in which logic gates can be performed between arbitrary pairs of cavity modes via sideband transitions with the transmon [1]. We present our progress toward realizing such a processor using a seamless rectangular 3D multimode cavity - the quantum flute, with a tailored mode dispersion and decay times around a millisecond for tens of cavity modes. To eliminate coherent errors arising from multimode state dependent Stark shifts of the transmon, we introduce an intermediate single-mode 'manipulate' cavity with a tunable coupling to the multimode cavity.


*This research was supported by Samsung Advanced Institute of Technology Global Research Partnership.

4:06PM C29.00009: Towards Developing a Graphene Josephson junction based qubit device KYLE MCELROY (Presenter), The Johns Hopkins University Applied Physics Laboratory, JESSE E THOMPSON, BRANDON T BLUE, Department of Physics and Nanoscience Technology, University of Central Florida, LAFE SPIETZ, Spietz Applied Sciences, LLC, JACOB EPSTEIN, The Johns Hopkins University Applied Physics Laboratory, MASA ISHIGAMI, Department of Physics and Nanoscience Technology, University of Central Florida, JOAN A HOFFMANN, The Johns Hopkins University — Construction of Josephson weak links is an integral part of superconducting quantum devices. New junction structures have various potential applications as new qubits or sensors. We will discuss the preliminary development of a transmon with a graphene based Josephson junction. The devices are fabricated using epitaxially grown graphene, transferred to a sapphire base with standard lithographic techniques used for junction and antenna layout. The junctions are designed to have 0.3-0.85 nA critical currents and antenna geometry for device resonances between 2-6 GHz and are imbedded in a high Q 3D cavity at 7.7 GHz.

4:18PM C29.00010: Quantum coherent control of graphene-based transmon qubit* JOEL WANG (Presenter), Research Laboratory of Electronics, Massachusetts Institute of Technology, USA, CHARLOTTE BOETTCHER, Dept. of Physics, Harvard University, USA, LANDRY BRETHEAU, Laboratoire des Solides Irradiés, Ecole Polytechnique, France, DANIEL CAMPBELL, Research Laboratory of Electronics, Massachusetts Institute of Technology, USA, BHARATH KANNAN, Research Laboratory of Electronics, Dept. of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, USA, DAVID D OLIVER, Dept. of Physics, Research Laboratory of Electronics, and Lincoln Lab, Massachusetts Institute of Technology, USA, MORTEN KJÆRGAARD, PHILIP KRANTZ, Research Laboratory of Electronics, Massachusetts Institute of Technology, USA, GABRIEL O. SAMACH, Lincoln Lab, Massachusetts Institute of Technology, USA, FEI YAN, Research Laboratory of Electronics, Massachusetts Institute of Technology, USA, JONILYN L YODER, Lincoln Lab, Massachusetts Institute of Technology, USA, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, NIMS, Japan, TERRY PHILIP ORLANDO, Research Laboratory of Electronics, Dept. of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, USA, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, USA, PABLO JARILLO-HERRERO, Dept. of Physics, Massachusetts Institute of Technology, USA, WILLIAM D OLIVER, Dept. of Physics, Research Laboratory of Electronics, and Lincoln Lab, Massachusetts Institute of Technology, USA — Van der Waals (vdW) materials—a family of layered crystals with various functionalities, can be assembled in specific arrangements to create new electronic devices called vdW heterostructures. The extraordinary and versatile electronic properties of these heterostructures, in combination with their epitaxial precision, make vdW-based devices a promising alternative for constructing key elements of novel solid-state quantum computing platforms. We demonstrate quantum coherent control of a superconducting circuit incorporating graphene-based vdW heterostructures. We show that this device can be operated as a voltage-tunable transmon qubit, whose spectrum reflects the electronic properties of massless Dirac fermions traveling ballistically. In addition to the potential for advancing extensible quantum computing technology, our results represent a new approach to studying vdW materials using microwave photons in coherent quantum circuits.(arXiv:1809.05215)

*This research was funded in part by the ARO grant No. W911NF-17-S-0001, and by the Department of Defense via MIT Lincoln Laboratory under AF Contract No. FA8721-05-C-0002.
4:30PM C29.00011: Resonator Cavities Compatible with Epitaxial InAs-Al Heterostructures* JOSEPH YUAN (Presenter), MATTHIEU DARTIAILH, WILLIAM ANDREW MAYER, ERIC SONG, KAUSHINI WICKRAMASINGHE, JAVAD SHABANI, Physics, New York University — Epitaxial Al-InAs structures are prime candidates for tunable superconducting qubits, the so-called “gatemon” where the Josephson energy can be tuned in-situ with an applied electric field to an InAs Josephson junction, eliminating the need for flux tuning in superconducting qubits [1]. Here we have characterized microwave cavities needed for coupling to superconducting gatemon qubits. We present resonator quality factors for a fixed design on various levels of the buffer layers used as substrates. We make a comparison to bare InP and Si to establish a comparative baseline.


*We acknowledge support from the US Army Office of Research, ARO: W911NF-18-1-0067

4:42PM C29.00012: Superconducting gatemon qubits based on selective-area-grown semiconductor materials* ALBERT HERTEL (Presenter), LAURITS ORHEIM ANDERSEN, Center for Quantum Devices, Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, NATAIL PEARSOR, Theoretische Physik, ETH Zürich, Zürich, Switzerland, MALCOLM R CONNOLLY, Center for Quantum Devices, Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, VALENTINA ZANNIER, LUCIA SORBA, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Pisa, Italy, LIU YU, PETER KROGSTUP, Center for Quantum Devices, Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, GEOFFREY C. GARDNER, MICHAEL MANFRA, Purdue University, Station Q Purdue, KARL PETERSSON, CHARLES M MARCUS, Center for Quantum Devices, Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen — Semiconductor-superconductor hybrid gatemon qubits offer a promising path to large scale quantum processors. In contrast to conventional transmon qubits that are controlled using currents, gatemons allow complete control using only gate voltages [1], potentially alleviating challenges to scaling superconducting qubits [2]. Here, we present a novel approach to building gatemons utilizing selective-area-grown InAs structures on an InP substrate [3,4]. This approach allows deterministic placement and straightforward fabrication of the gatemon qubits. We characterize the material and perform first proof-of-principle measurements to demonstrate coherent qubit oscillations. Further work is needed to understand the dominant loss mechanisms and improve coherence times.


*This work was supported by Microsoft, the U.S. Army Research Office, and the Danish National Research Foundation.

4:54PM C29.00013: Control of topological properties in the Kitaev chain by quantum microwave radiation* FABIO MÉNDEZ-CÓRDOBA (Presenter), FERNANDO GÓMEZ-RUIZ, JUAN MENDOZA-ARENAS, FERNEY RODRIGUEZ, Physics, Universidad de Los Andes, CARLOS TEJEDOR, Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, LUIS QUIROGA, Physics, Universidad de Los Andes — We investigate observable signatures coming from the light-matter coupling of a Kitaev chain embedded in a microwave cavity. We study and describe the quantum phases of the system, and the transitions between them, for two different composite fermion-photon model, namely a cavity homogeneously coupled to the whole chain as well as the case of a microwave selectively coupled to an edge site of the chain only. Our results are based on two complementary approaches, an analytic mean-field theory and numerical matrix product state simulations. We find that as a consequence of the interaction between the matter-radiation subsystems, a topological non-trivial phase of the Kitaev chain can be increased and identified by following the behavior of different photon observables such as the mean photon number and the Fano factor. Our analysis reveals a second order phase transition for different types of microwave-fermion couplings. The observed phenomena and the control of the quantum state of the chain assessed with the cavity, make it a potential candidate for further experimental investigations that seek the presence of Majorana fermions in solid-state systems.

*Financial support from 10th call for Projects Cooperation UAM-Santander-UniAndes, 2017-2018, is acknowledged.
Ultra low-loss single-crystalline material platform for high-Q quantum devices

ILYA RODIONOV
(Presenter), ALEKSANDR BABURIN, ILYA A. RYZHIKOV, AIDAR R. GABIDULLIN, DMITRIY O. MOSKALEV, ALINA
DOBRONOSOVA, ALEXEY MATANIN, Functional Micro/Nanosystems, Bauman Moscow State Technocal University — Quantum
technologies is a rapidly grown research area, which have the potential to lead the revolution in supercomputing, sensing,
global communications and security. The leading quantum computing concepts of design like superconductive qubits,
optical quantum computing devices, solid-state and hybrid quantum systems are based on traditional semiconductor
technology platform. However, new materials and nanoscale structures fabrication techniques are needed to explore the
underlying physics and fulfill the subsequent specifications. Losses in thin films, surface, structure and interfaces quality
are coming into the fore.

Here we present a new approach for high vacuum deposition of single-crystalline metallic films with extremely low losses,
which we name the SCULL (Single-crystalline Continuous Ultra-smooth Low-loss Low-cost) process. Fabricated films show
perfect crystallinity (FWHM for \( \omega \)-scan is better than 0.3), best published optical, superconductive, electrical properties and
sub-0.5nm roughness. We demonstrate perfect silver/gold plasmonic films and superconductive aluminum films. With
SCULL films the longest SPP propagation length (200 \( \mu \)m at \( \lambda = 780 \) nm) and the brightest single-photon source (over 35
million photons per second) at room temperature is demonstrated.

Monday, March 4, 2019 2:30 PM - 4:54 PM

Session C30 GSOFT: Liquid Crystals II

BCEC 162B - Nasser Abukhdeir, University of Waterloo - Tag(s): Focus

2:30PM C30.00001: Nanocomposites of Ferroelectric Liquid Crystals and Magnetic Nanoparticles: Potential
Application as a MRI Contrast Agent*

LUZ MARTINEZ-MIRANDA (Presenter), University of Maryland, College Park, PATRICIO
N ROMERO-HASLER, EDUARDO A SOTO-BUSTAMANTE, University of Chile, LYNN K. KURIHARA, NextFED, LAMAR O MAIR,
IRVING N WEINBERG, Weinberg Medical Physics, Inc. — Nanocomposites of ferroelectric liquid crystals in combination with
FeCo magnetic nanoparticles are considered as a MRI contrast agent, by creating a magnetic field as a function of the
body's electric field. The rotational viscosity of the sample needs to be reduced in order to reduce the electric field
strength required for liquid crystal rotation to the values observed in many live biological states. This is achieved by having
the nanoparticles act as lubricants to the ferroelectric liquid crystal. The magnetic field depends on the concentration of
nanoparticles, which cannot be toxic to the biological environment. The concentrations used form aggregates that tend to
exist in stable spherulites, that are also reversible with temperature. We find a relation between the magnetic field and the
number of spherulites per unit area that align as a function of the electric field in the presence of a very small sample such
as our model system. Finally, we present a model of how the electric field rearranges the spherulites and produces the
magnetic field.

*Fulbright Scholarship (USA), and FONDECYT No. 1130187 and CONICYT No. 21130413 (Chile) projects.

2:42PM C30.00002: Can a minimum principle describe shear alignment of liquid crystals?*

XINGZHOU TANG
(Presenter), JONATHAN SELINGER, Kent State University — When a static perturbation is applied to a liquid crystal, the
director configuration changes to minimize the free energy. When a shear flow is applied to a liquid crystal, one might ask:
Does the director configuration change to minimize any effective potential? To address that question, we derive the Leslie-
Ericksen equations for dissipative dynamics, and determine whether they can be expressed as relaxation toward a
minimum. The answer may be yes or no, depending on the number of degrees of freedom. Using theory and simulations,
we consider two specific examples, reverse tilt domains under simple shear flow and dowser configurations [1] under
plane Poiseuille flow, and determine whether each example shows relaxation toward the minimum of an effective
potential.


*This work is supported by NSF Grant No. DMR-1409658.
2:54PM C30.00003: Surface reconstruction of chiral liquid crystalline oligomers under the action of volatile organic compounds  
PETR SHIBAEV (Presenter), Fordham University — Significant changes in surface morphology as well as in chiral fingerprint structure are discovered in solid chiral oligomers and their compositions with low molar mass liquid crystals affected by volatile organic compounds. The changes are manifested by inversion of chiral pattern and surface periodic structure. Surprisingly, the changes are reversible with a relaxation time of several days at room temperature. This reversibility of the effect underscores the importance of chiral structure beneath the surface and not affected by the volatile compounds in restoration of initial morphology. The importance of underlying chirality is also confirmed by the absence of this effect in replicas of chiral surface created by means of common polymers (polystyrene, polyvinylpyridine). The discovered effect is also modelled by means of computer simulations and a simple theoretical model is presented. The discovered effect can find applications in gas detectors and optical devices.

3:06PM C30.00004: High order nonlinear electrophoresis in nematic liquid crystal*  
MOJTABA RAJABI (Presenter), Department of Physics, Kent State University, TARAS TURIV, Advanced Materials and Liquid Crystal Institute, Chemical Physics Interdisciplinary Program, Kent State University, O D LAVRENTOVICH, Department of Physics, Advanced Materials and Liquid Crystal Institute, Chemical Physics Interdisciplinary Program, Kent State University — Electrophoresis is motion of particles relative to a surrounding fluid in a uniform electric field. In anisotropic fluids such as liquid crystals (LC) the particle's velocity growth with the square of the electric field strength [1]. As a result, reversing polarity of the electric field does not change the direction of propulsion, which makes it possible to drive a sustained transport by an alternating-current (AC) field [2]. Here we report a higher-order nonlinear electrophoresis in which the velocity acquires a component proportional to the fourth power of the electric field strength. The effect is observed in a nematic LC with negative anisotropy of dielectric permittivity. The electric field realigns the director around the colloidal particle and thus modifies the geometry of spatial charge separation and the viscous drag; as a result, the velocity dependence on the field acquires higher-order nonlinearities.


*The work was supported by NSF DMREF grant DMS-1729509.

3:18PM C30.00005: Comparison of material parameters among flexible dimer, trimer, tetramer of nematic mesogens*  
ZEINAB PARSOUZ A.SH (Presenter), GRETA BABAKHANOVA, RONY SAHA, MOJTABA RAJABI, TARAS TURIV, Kent State University, CHRIS WELCH, GEORG H MEHL, Department of Chemistry, University of Hull, Hull, UK, JAMES GLEESON, ANTAG ISTVAN JAKLI, O D LAVRENTOVICH, SAMUEL SPRUNT, Kent State University — We compare the temperature dependencies of the birefringence, elastic constants and orientational viscosities for four homologous nematic liquid crystal oligomers: dimer (DTC5C9), its associated trimer and tetramer. These materials all exhibit the twist-bend nematic (NTB) phase. The magnitudes of the splay (K11), twist (K22) and bend (K33) elastic constants, as well as the corresponding orientational viscosities are determined by dynamic light scattering measurements. Interestingly K33 in the dimer and tetramer shows the monotonic decrease with temperature below the nematic-isotropic transition followed by a pretransitional increase close to the nematic to NTB transition. The trimer, in contrast, shows essentially no pretransitional change in K33. This behavior can be attributed to odd-even effect associated with the number of monomer unites in oligomers. The orientational viscosities associated with splay, twist and bend fluctuations in the N phase of dimer, trimer and tetramer are comparable to those of nematics formed by rod-like molecules. All three show strong temperature dependence, increasing sharply near the N – NTB transition.

References

*The work was supported by NSF grants DMR-1410378 and DMR-1307674.
3:30PM C30.00006: Enhanced Dissipation Behavior of Main-Chain LCE Networks  CRISTINA MARTIN LINARES  (Presenter), ALEJANDRO MARTIN LINARES, Mechanical Engineering, Johns Hopkins University, NICHOLAS TRAUGUTT, UC DENVER, THAO NGUYEN, Mechanical Engineering, Johns Hopkins University, CHRISTOPHER YAKACKI, UC DENVER — Liquid Crystal Elastomers (LCEs) are composed of mesogens bound to an elastomeric network of polymer chains. The orientation of mesogens relative to the polymer network leads to reversible actuation at the nematic-isotropic transition (Tni), soft-elasticity, and enhanced dissipation. Instead of a peak at Tg, the tan-delta curve for LCEs is elevated over Tg-Tni, indicating enhanced dissipation. At large strains, the material exhibits rate-dependent soft-elasticity with hysteresis[1]. We hypothesize that the enhanced dissipation behavior arises from the motion of the mesogens relative to the polymer network and measure the effect of mesogen ordering and network orientation. We developed uniaxial tension tests using 3D-DIC to measure the rate-dependent load-unload response and hysteresis for 3 main chain LCE networks with different microstructures, including polydomain and monodomains. The modulus and hysteresis increased significantly with strain rate for all networks. The modulus for a monodomain stretched parallel to the director was an order of magnitude higher than that of a polydomain. The monodomain stretched perpendicular to the director had the greatest dissipation.


3:42PM C30.00007: Defect nucleation in quenched freely suspended smectic liquid crystal films*  ADAM GREEN  (Presenter), CHEOL PARK, JOSEPH E MACLENNAN, MATTHEW GLASER, NOEL ANTHONY CLARK, University of Colorado, Boulder — Freely suspended films of smectic liquid crystals, which can be as thin as two molecular layers, are a natural choice for studying ordering and phase transitions in 2D. One 2D system of ongoing interest is that of the XY-model, which describes the U(1) symmetry group of rotations, broken by either a complex number or 2D vector. The XY-model gives rise to topological defects, or vortices, with interesting implications for phase transitions in two dimensions eg. Kosterlitz-Thouless transitions. Here, we describe our recent experiments focusing on the nucleation of topological defects in the quasi-2D system of freely-suspended smectic films. By rapidly quenching a film (inducing a rapid phase transition from an ordered to a disordered phase), and studying the evolution of the dynamics with a high-speed video camera, we are able to visualize defect nucleation in smectic C (tilted) films, and we will discuss the role that islands (pancake-like, circular regions with additional smectic layers bounded by an edge dislocation) play in mediating the creation of these defects.

*This work was supported by NASA Grants No. NNX-13AQ81G and No. NNX17AC74G and by the Soft Materials Research Center under NSF MRSEC Grants No. DMR-0820579 and DMR-1420736.

3:54PM C30.00008: Shaping nanoparticle fingerprints at the interface of cholesteric emulsions*  LISA TRAN  (Presenter), Columbia University, HYE-NA KIM, University of Pennsylvania, NINGWEI LI, University of Massachusetts, Amherst, SHU YANG, KATHLEEN STEBE, RANDALL D KAMIEN, University of Pennsylvania, MARTIN HAASE, Rowan University — In this work, we balance the interfacial energy of nanoparticles against the elastic energy of cholesteric liquid crystals to dynamically shape nanoparticle assemblies at a fluid interface. By adjusting the concentration of surfactant that plays the dual role of tuning the nanoparticle hydrophobicity and altering the anchoring of liquid crystals, we pattern nanoparticles at the interface of cholesteric liquid crystal emulsions. Interfacial assembly is tempered by elastic patterns that arise from the geometric frustration of confined cholesterics. Patterns are tunable by varying both surfactant and chiral dopant concentrations. Adjusting the particle hydrophobicity more finely by regulating the surfactant concentration and solution pH further modifies the rigidity of assemblies, giving rise to surprising assembly dynamics dictated by the underlying elasticity of the cholesteric. Because assembly occurs at the interface with the desired structures exposed to the surrounding water solution, particles can be readily cross-linked and manipulated. This study serves as a foundation for better understanding inter-nanoparticle interactions at interfaces by tempering their assembly with elasticity.

*National Science Foundation, American Association of University Women, Simons Foundation
4:06PM C30.00009: Twist fluctuations and rotational diffusion of the director near hedgehog defects in nematic droplets
ALEXIS DE LA COTTE (Presenter), OLAF STENULL, Department of Physics and Astronomy, University of Pennsylvania, PETER COLLINGS, Department of Physosc and Astronomy, Swarthmore College, TOM C LUBENSKY, A. G. YODH, Department of Physics and Astronomy, University of Pennsylvania — When strong homeotropic boundary conditions are set at the interface of emulsion droplets containing a nematic liquid crystal (NLC), the spherical confinement combined with the system bulk elasticity is known to produce a point-like defect called a radial hedgehog with topological charge +1. We measure the director fluctuations about this state and compare them to the predictions of a theoretically calculated normal mode analysis. Three distortion modes are evident experimentally using two different optical microscopy techniques. Using polarizing microscopy, we observe the motion of the two extinction axis and identify two angular diffusions: a fast one, following the angle the axes make in respect to each other, and a slow one, tracking the angle they make in respect to the polarizers' orientations. In bright field, we are also able to measure the translational motion of the hedgehog. Analysis of these distortion modes indicates the possibility of an instability toward a twisted hedgehog configuration in droplets of the NLC 5CB.

*We gratefully acknowledge funding support from NSF-DMR16-07378, the NSF-MRSEC-DMR17-205030, and NASA NNX08AO0G grants.

4:18PM C30.00010: Artificial spin (and Potts) ice of skyrmions in liquid crystals
AYHAN DUZGUN (Presenter), CRISTIANO NISOLI, Los Alamos National Lab — Artificial spin ices [1] are engineered arrays of mutually interacting, frustrated, single domain magnetic nano-islands that can be characterized at the degree of freedom level and designed in different arrangements for different emergent behaviors [2]. Beyond magnets, similar ideas have been exported to trapped colloids [3] and vortices in pinned superconductors [4]. In this work, we present a proposal to realize them in a new platform: Liquid crystals. Liquid Crystals possess various advantages as a spin ice platform. Skyrmions in liquid crystals [5], can be confined in traps made of light or field gradients where their preferential position in the trap can mimic a binary Ising spin or a Potts variable. By solving partial differential equations for chiral nematic liquid crystals in the presence of constraints, we demonstrate that skyrmions can reproduce the ice-state of square ice and honeycomb ice. We then extend these simulations to Potts systems.


4:30PM C30.00011: Two-Dimensional Hexagonal Boron Nitride Nanosheet as the Planar-Alignment Agent in a Liquid Crystal-Based Electro-Optic Device
RAJRATAN BASU (Presenter), LUKAS ATWOOD, United States Naval Academy — The planar-alignment agent in an electro-optic liquid crystal (LC) device plays an essential role for the LC’s electro-optical characteristics. Rubbed polyimide (PI) layers are conventionally used as the planar-alignment agent in traditional liquid crystal displays (LCDs). Here we experimentally demonstrate that the 2D hexagonal boron nitride (h-BN) nanosheet can serve as the planar-alignment agent in an LC cell. Two h-BN-covered indium tin oxide (ITO) glass slides are placed together to fabricate an LC cell. A nematic LC inside this h-BN-based cell exhibits uniform planar-alignment. This planar-alignment at the molecular scale is achieved due to the coherent overlay of the benzene rings of the LC molecules on the hexagonal BN lattice. This h-BN-based LC cell shows the typical electro-optical effect when an electric field is applied via ITO electrodes. The dielectric measurement across this h-BN-based electro-optic cell shows a standard Fréedericksz transition of the LC, confirming that the 2D h-BN, as the planar-alignment agent, supplies adequate anchoring energy. Finally, we show the h-BN-based LC cell exhibits more optical transparency than a regular PI alignment layer-based LC cell.

*This work was supported by ONR (N0001418WX01842; N0001418WX01543)
4:42PM C30.00012: Peculiar Nonlinear Elasticity of Liquid Crystal Elastomers Revealed by Biaxial Stretching*  
ASAKA TAKEBE, HARUKI TOKUMOTO, KENJI URAYAMA (Presenter), Dept. Macromol. Eng. Sci., Kyoto Institute of Technology —  
Liquid crystal elastomers (LCE) are a combination of liquid crystal and elastomer. The coupling of liquid crystal alignment  
and rubber elasticity results in a unique mechanical property which is often called soft elasticity. The stretching in the  
direction normal to the initial director requires very small mechanical work due to the director rotation along the  
stretching axis. This is clearly observed as a finite plateau region with very low stress in the stress-strain curve. Most of the  
earlier characterizations of finite deformation of LCEs have been conducted using uniaxial stretching. In general, uniaxial  
stretching, however, provides a limited basis for comprehensive understanding of nonlinear elasticity of elastomers,  
because it is only a particular one among all physically accessible deformations. Present work investigates the biaxial  
stress-strain behavior of polydomain nematic elastomers with varying the strains independently in the two directions. We  
have found the peculiarity in nonlinear elasticity of LCEs which has not been characterized by uniaxial stretching  
measurements.  
*This work was partly supported by MEXT KAKENHI Grant Number JP18H02034.  

Monday, March 4, 2019 2:30 PM - 4:54 PM  
Session C31 DCP: DFT, Embedding, and, Beyond (ES1) BCEC 203 - Timothy Berkelbach, University of Chicago - Tag(s):  
Focus  
2:30PM C31.00001: Projection-based quantum embedding for periodic systems* [Invited]  JASON GOODPASTER  
(Presenter), University of Minnesota — Quantum embedding methods are ideal for describing surface chemistry of large  
periodic systems by using a higher level of theory—such as wave function (WF) theory—for the smaller active site, while  
still accounting for the quantum mechanical interactions with the electrons in the surrounding environment with a more  
computationally tractable level of theory such as density functional theory (DFT). We have developed a projection-based  
quantum embedding approach for the embedding of periodic systems that is numerically exact compared to Kohn-Sham  
DFT. Furthermore, we show that our method can accurately and efficiently reproduce adsorption and reaction energies  
from canonical WF methods and experiments.  
With Huzinaga projection-based embedding, we have shown that the exact KS-DFT calculations and accurate WF-in-DFT  
ergies can be reproduced if both systems are described using the basis set of the full system. However, we find that  
 improved accuracy and efficiency can be obtained for WF-in-DFT if the subsystems are only described in basis functions  
associated with that subsystem. This allows for periodic embedding where the smaller active site is described using non-  
periodic basis functions, and the large environment is treated using periodic basis functions. We have found this approach  
to be highly accurate and significantly cheaper due to the use of a much reduced basis set for the WF region, and it is  
broadly applicable to a large number of chemical systems. With this method, we will be able to accurately describe  
chemistry at interfaces.  
*This research was carried out within the Nanoporous Materials Genome Center, which is supported by the U.S.  
Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences under  
Award DE-FG02-17ER16362.  
3:06PM C31.00002: Density Matrix Embedding Theory for Strongly Correlated Solids  HUNG PHAM (Presenter), LAURA  
GAGLIARDI, University of Minnesota — Density matrix embedding theory (DMET) [Phys. Rev. Lett. 2012, 109, 186404] has  
offered a promising wave function-in-wave function embedding method to treat electron correlation for large and  
extended systems. DMET has been gaining some successes for several lattice models and molecular systems. Herein, we  
present an extension of DMET to treat strongly correlated periodic systems, namely pDMET. In our implementation, a unit  
cell is considered as an impurity embedded in the environment made up by other unit cells in the computational supercell.  
The Wannier functions, i.e. the real-space presentation of the wave function, are used to perform the embedding  
calculation. The correlation potential is augmented in the k-space one-electron Hamiltonian to self-consistently minimize  
the difference between the one-electron density matrix at the mean-field level and that at the high-level. We test our  
method using different quantum chemical solvers (e.g. FCI, DMRG-CI, CCSD) on variety of systems, such as one-  
dimensional structure (hydrogen chain), covalent crystal (crystalline silicon), and ionic crystal (magnesium oxide). Finally,  
we discuss the feasibility of extending the method to compute electronic band structures of materials.
Embedded cluster density approximation for exchange-correlation energy: a natural extension of the local density approximation*  
CHEN HUANG (Presenter), Department of Scientific Computing, Florida State University — We developed a local correlation method in the framework of Kohn-Sham density functional theory (KS-DFT). The method is termed embedded cluster density approximation (ECDA) and is a logical extension of the local density approximation. In ECDA, an embedded cluster is defined for each atom based on the finite-temperature density-functional embedding theory. The clusters' XC energy densities are calculated using high-level XC functionals. The system's XC energy is then constructed by patching these locally computed, high-level XC energy densities in the system in an atom-by-atom manner. A key result is the derivation of the relationship between the embedding potential and system's KS potential, based on which we show how to efficiently compute the system's XC potential following the optimized effective potential procedure. The accuracy of ECDA is examined by patching the exact exchange (EXX) and the random phase approximation (RPA) correlation energies in a one-dimensional hydrogen chain, as well as by patching EXX energies in several molecules. We expect ECDA to be a simple, yet effective method to scale up high-level KS-DFT calculations in large-scale strongly correlated systems.

*Florida State University (start-up fund) and NSF under CHE-1752769

Polaron Modulated Electronic Structures of Doped La$_2$CuO$_4$ by Self-Interaction Corrected Density Functional Theory Approach  
QIUSHI YAO (Presenter), QIANG LIU, Department of Physics, Southern University of Science and Technology — Single-particle ab-initio approaches, e.g., density functional theory (DFT) with standard exchange-correlation functionals, is notorious for its poor treatment of the electronic structures of cuprate superconductors, not to mention their properties upon doping. Here, taking La$_2$CuO$_4$ (LCO) as an exemplar, with both $T$ and $T'$ phase, we show that self-interaction corrected DFT accurately produces the experimentally observed insulator to metal transition, as a function of hole and electron doping concentration, respectively. Based on our calculations, doped carriers form localized polarons under low doping concentration dissolving into extended states upon high doping concentration, thus making the system conducting. The correct description of LCO provides us a practical route to the doping problems of strong correlated materials within Kohn-Sham DFT framework, which is capable to treat a larger supercell than the methods beyond DFT.

Head-to-head comparison of spectral properties of transition-metal oxides using DFT and beyond-DFT methods*  
SUBHASISH MANDAL (Presenter), G.L. PASCUT, KRISTJAN HAULE, KARIN RABE, DAVID VANDERBILT, Physics and Astronomy, Rutgers University, Piscataway, NJ, United States — The development of computational tools for the accurate prediction of the electronic structure of strongly correlated materials has been an active field of research for several decades. As a result, a variety of methods, including density functional theory (DFT), DFT+U, hybrid functionals, meta-GGAs, GW quasiparticle approaches, and DFT-embedded dynamical mean field theory (DMFT), are now available. Among these, the beyond-DFT methods have been instrumental for understanding the electronic structure of strongly correlated systems, but it is unclear how reliable are those methods when applied to typical strongly correlated solids. It is thus of pressing interest to compare the quality of these methods as they apply to different categories of materials. Here we begin by systematically testing these methods on transition-metal oxides (TMOs) such as FeO, CoO, MnO, and NiO, which provide a suitable platform since conventional DFT methods are known to fail to predict their electronic structure accurately. We present a head-to-head comparison of spectral properties as obtained using the listed methods, and compare with experimental photoemission data where available.

*This research is supported by NSF DMREF DMR-1629059 and NSF-DMR-1629346

Bridging molecular dynamics and correlated wave-function methods for accurate finite-temperature properties*  
DARIO ROCCA (Presenter), ANANT DIXIT, MICHAEL BADAWI, SÉBASTIEN LEBÊGUE, Université de Lorraine and CNRS, Nancy (France), TIM GOULD, Griffith University, Nathan (Australia), TOMÁŠ BUČKO, Comenius University and Slovak Academy of Sciences, Bratislava (Slovakia) — We introduce the "$\;`\;selPT`\;" perturbative approach, based on ab initio molecular dynamics (AIMD), for computing accurate finite-temperature properties by efficiently using correlated wave-function methods. We demonstrate the power of the method by computing a prototypical molecular enthalpy of adsorption in zeolite (CH$_4$ on protonated chabazite at 300 K) using the random phase approximation. Results are in excellent agreement with experiment. The improved accuracy provided by selPT represents a crucial step towards the goal of truly quantitative AIMD prediction of experimental observables at finite temperature.

*This work was supported by Agence Nationale de la Recherche under grant number ANR-15-CE29-0003-01.
4:06PM C31.00007: Towards a molecular-level understanding of metal-like conductivity in bacterial protein nanowires*  
PETER DAHL (Presenter), Molecular Biophysics and Biochemistry, Yale Univ, ATANU ACHARYA, Chemistry, Yale Univ,  
SIBEL EBRU YALCIN, SOPHIA YI, J. PATRICK O'BRIEN, Molecular Biophysics and Biochemistry, Yale Univ, VICTOR BATISTA,  
Chemistry, Yale Univ, NIHIL MALVANKAR, Molecular Biophysics and Biochemistry, Yale Univ — Protein appendages of Geobacter sulfurreducens exhibit metal-like conductivity and transport electrons at rates rivaling to those of metallic carbon nanotubes. Our recent experiments have revealed an increase in \( \pi \)-stacking upon lowering the pH of nanowires leading to a 100-fold increase in conductivity and carrier density. We employed molecular dynamics simulations to obtain a molecular-level understanding of the enhanced \( \pi \)-stacking obtained under highly acidic pH. Electronic structure calculations were also performed using QM/MM technique to elucidate the frontier orbitals and the energy gap between them. Our MD simulations suggest that under highly acidic pH significant structural rearrangement of the protein structure leads to the enhanced \( \pi \)-stacking. Electronic structure calculation reveals that the enhanced \( \pi \)-stacking results in higher coupling between the carrier states. Hence, conductivity is increases by several fold at highly acidic pH. Our results suggest that significant orbital overlap between adjacent charge carriers is pivotal in the observed conductivity of these nanowires.

*Funded by NIH New Innovator and NSF CAREER Awards.

4:18PM C31.00008: A finite-field approach to performing GW calculations and solving the Bethe-Salpeter equation  
[Invited] GIULIA GALLI (Presenter), University of Chicago — We describe a finite field approach to compute density response functions, and to compute optical spectra and exciton binding energies of molecules and solids based on the solution of Bethe-Salpeter equation. The approach allows for efficient G0W0 and G0W0\( \Gamma \) calculations as well as for the calculation of optical spectra beyond the random phase approximation.

In addition it utilizes localized orbitals obtained from Bloch states with bisection techniques, thus greatly reducing the complexity of the calculation and enabling the efficient use of hybrid functionals to compute input orbitals, when using a plane-wave representation.

Monday, March 4, 2019 2:30 PM - 5:06 PM

Session C32 DCP: Theory and Experiment for Complex Systems in Gas Phase (A) BCEC 204A -

2:30PM C32.00001: Theory meets experiment in gas-phase spectroscopy: the VMS bridge [Invited] VINCENZO BARONE  
(Presenter), Scuola Normale Superiore — The impressive advances in hardware developments, the availability of powerful graphical interfaces together with the set-up of effective and user-friendly software are leading to a new generation of virtual tools able to deal effectively with the complex systems and phenomena of current interest in the fields of molecular spectroscopy, chemistry (also astrochemistry) and biology. Moving from the presentation of theoretical results as a collection of numbers corresponding to models (often oversimplified) to the \textit{vis-à-vis} comparison between "in silico" and "in vitro" spectral outcomes, possibly combined with 3D renderings and natural interfaces, should at last overcome the diffidence of experimentalists towards theoreticians and bridge the gap between experiment and theory. Among the available virtual instruments, we focus here on the multifrequency spectrometer (VMS) our group has been developing in the last few years (see, V. Barone, WIREs Comput Mol Sci 6, 86-110 (2016)), which allows a \textit{vis-à-vis} comparison of experimental spectra with their simulated counterparts as well as the interpretation of the results in terms of the interplay among different well defined effects. The main building blocks of this tool are, apart from powerful 3D pre- and post-processing tools: (a) first-principle approaches based on composite schemes involving post-Hartree-Fock methods complemented by models based on the density functional theory for the proper description of stationary points and their local environment on the pertinent potential energy surfaces; (b) integrated perturbative/variational treatments for describing nuclear motions beyond the rigid rotor / harmonic oscillator level. In this presentation I will sketch the present status of VMS and the ongoing efforts toward increasing its range of application with special reference to different spectroscopies in the gas-phase. Some case studies will be selected to better illustrate the above concepts.
3:06PM C32.00002: Broadband Rotational Spectroscopy of Odorants and their Complexes: Experiment and Theory in Concert* [invited] MARI EUGENIA SANZ (Presenter), Chemistry, King's College London — Studies of large molecules and their complexes in gas phase using spectroscopic techniques provide experimental data on their structures and interactions that can be directly compared with predictions from theory. One of the most powerful methods for structural determination is rotational spectroscopy, which can identify different coexisting conformations and determine actual atom positions, thus enabling calculation of bond lengths and angles. The development of broadband rotational spectroscopy, allowing fast collection of broad segments of the spectrum at once, has dramatically extended the range and complexity of the molecular systems that can be tackled and opened new opportunities to benchmark theoretical methods.

In this talk we will present our results on the conformations and interactions of several odorants, and their complexes with water and mimics of amino acid residues. Using broadband rotational spectroscopy and quantum chemistry calculations, we have obtained detailed information on their structures and conformational preferences, identifying the global minimum for each system and the prevailing interactions. For the complexes, primary binding sites have been located and the interplay between intra- and intermolecular interactions has been characterised. Comparison between experimental and theoretical results allows evaluation of the theoretical methods used and indicates possible avenues to further improve the theoretical description of complex molecular systems.

*The authors would like to thank funding from the EU FP7 (Marie Curie grant PCIG12-GA-2012-334525), EPSRC and King's College London.

3:42PM C32.00003: Exploring conformational landscapes of chiral molecules in their solvation and self-aggregation clusters* [invited] YUNJIE XU (Presenter), University of Alberta — Our research program focuses on applying and developing new spectroscopic tools to bridge the gap of our understanding in terms of structural and dynamical properties of an isolated chiral molecule and of it in liquid phase and in solution. Using broadband rotational spectroscopy aided by high level ab initio calculations, we probe structural diversity and emerging bulk behavior in trimeric and tetrameric aggregates of the transiently chiral 2-fluoroethanol (FE). We show that the FE tetramer is an intriguing system at the interface between gas- and bulk-phase behavior, where the conformational specificity seen in the gas-phase is still experimentally relevant but plays a diminished role relative to the intermolecular topology and cooperative stability. In the second example, we examine conformational landscapes of tetrahydro-2-furoic acid (THFA), a chiral carboxylic acid, and its dimer and its complexes with water molecules in a jet expansion using rotational spectroscopy. We also apply vibrational circular dichroism and Raman optical activity to probe how intermolecular interactions with water and THFA itself influence the aforementioned conformational preference in condense phase directly. The interplay between experiment and theory is essential for all the work described.

*This research was funded by the Natural Sciences and Engineering Research Council of Canada, Canada Foundation for Innovation, Alberta Enterprise and Advanced Education, and by the University of Alberta. We gratefully acknowledge access to the computing facilities by the Shared Hierarchical Academic Research Computing Network, the Western Canada Research Grid (Westgrid), and Compute/Calcul Canada. YX holds a Tier I Canada Research Chair in Chirality and Chirality Recognition.

4:18PM C32.00004: Conformational Preferences of Gas Phase Peptides and Synthetic Foldamers: Challenges to Theory and Experiment* TIMOTHY ZWIER (Presenter), KARL N BLODGETT, CHRISTOPHER P HARRILAL, JOSHUA L FISCHER, JOHN T LAWLER, DEWEI SUN, Purdue University — This talk will describe combined experimental/computational studies of the conformational preferences of isolated, beta-peptide foldamers as neutrals, probing the development of mixed 10/12 helices with size. We will also describe our work on cryo-cooled protonated peptides in the gas phase, including a study of peptides capable of forming salt bridges. In both contexts, the need for accurate and fast exploration of the conformational landscape is crucial to success. The prospects and limits of both theory and experiment will be discussed.

*The authors gratefully acknowledge support for this work from the NSF under grant CHE-1764148.
On optical confinement to length scales arbitrarily smaller than the wavelength. Further discuss some computational progress with regard to coupling efficiency and some prospective technologies based on polarimetry measurements of a tightly focused vortex beam. We module into a near-field scanning optical microscope, we have built a confocal spectroscope for transmittance measurements in the VIS and SWIR, and we report on polarimetry measurements of a tightly focused vortex beam. We have previously reported our novel nanofabrication process, which leverages the conformal nature of atomic layer deposition (ALD), and which produces high aspect ratio nanocoaxes. In this work, we report in more detail some optical transmission measurements, particularly related to signatures of coupling into the fundamental mode. We have relatively few experimental works. To interrogate these structures, we have integrated an optical vortex generation module into a near-field scanning optical microscope, we have built a confocal spectroscopic module for transmittance measurements in the VIS and SWIR, and we report on polarimetry measurements of a tightly focused vortex beam. We further discuss some computational progress with regard to coupling efficiency and some prospective technologies based on optical confinement to length scales arbitrarily smaller than the wavelength.

4:30PM C32.00005: Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene  
YAIR LITMAN (Presenter), Theory, Fritz Haber Institute of the Max Planck Society, JEREMY OSCAR RICHARDSON, Physical Chemistry, ETH Zurich, TAKASHI KUMAGAI, Physical Chemistry, Fritz Haber Institute of the Max Planck Society, MARIANA ROSSI, Theory, Fritz Haber Institute of the Max Planck Society — The making and breaking of H-bonds on highly anharmonic potential energy surfaces involved in proton and hydrogen transfer reactions require a full-dimensional quantum mechanical treatment of not only electrons, but also of nuclei. Here we demonstrate that dealing with this complexity is necessary for achieving predictive simulations that can solve puzzling properties of these reactions by addressing the intramolecular double hydrogen transfer (DHT) in porphycene[1]. Our theoretical treatment combines dispersion corrected hybrid density-functional theory calculations and path-integral ring-polymer methods. Our simulations predict the position and width of the N-H stretching band of porphycene and DHT rates in excellent agreement with experiments, thus confirming our determination of the tunneling pathways and the anharmonic mode couplings that play a role in this reaction. They also confirm the importance of the usually ignored competition between concerted and stepwise DHT pathways for this system. Our general theoretical approach provides a quantitative framework for a deeper physical understanding of hydrogen transfer dynamics in complex systems. [1] Y. Litman, J. O. Richardson, T. Kumagai, M. Rossi. arXiv:1810.05681 (2018)

4:42PM C32.00006: A Stochastic Non-empirical approach in the problem of the reaction path seeking*  
IURII NAGORNOV (Presenter), RYOSUKE AKASHI, Department of Physics, University of Tokyo — In the atomistic simulation methods, the escaping trajectories, which is rendered rare because of the potential energy barrier, and free-energy landscape along them are usually calculated by applying artificial force and/or empirical collective variables. Our motivation is to develop the method free from such artificial forces and collective variables. We developed a non-empirical scheme to search for the minimum-energy escape paths from the minima of the potential surface to unknown saddle points nearby. This method employs only the local gradient and diagonal part of the Hessian matrix of the potential [R. Akashi, YSN, J. Phys. Soc. Jpn. 87, 063801 (2018)]. In our method we employ a stochastic equation, with which the distribution of the “walkers” representing atomic positions move up the potential surface through the valleys to the saddle points. The key to the successful tracking of the minimum-energy paths is the choice of the initial position. We designed a systematic method to generate initial atomic coordinates and efficiently simulate the paths to the saddle points starting from them. We demonstrate our method with several systems such as argon clusters.

*MEXT as Exploratory Challenge on Post-K computer (Frontiers of Basic Science: Challenging the Limits)

4:54PM C32.00007: N-Body networks for molecular simulation*  
BRANDON ANDERSON (Presenter), RISI KONDOR, TRUONG SON HY, Computer Science, University of Chicago — We introduce a novel deep learning architecture for learning molecular force fields. Our architecture, called CGnet, “bakes in” the underlying rotational invariance of the problem using the Clebsch-Gordan operator. We apply CGnet to the molecular N-Body problem of learning force-fields from ab-initio molecular dynamics simulations. We find state-of-the-art results when applied to the MD-17 dataset. We also train CGnets on QM9 and find competitive results. Finally, we provide a set of tools, called FastCG, along with an interface with PyTorch and Tensorflow, to allow for fast and efficient calculation of CG products, along with their analytical gradients.

*DARPA Young Faculty Award for Multiresolution Machine Learning for Molecular Modeling D16AP00112

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C33 FIAP: Applied Photonics BCEC 204B - Juan Merlo

2:30PM C33.00001: Optical Confinement in Nanocoaxial Waveguides: Coupling to the Fundamental TEM-Like Mode  
YITZI M CALM (Presenter), LUKE D'IMPERIO, NATE T NESBITT, JUAN M. MERLO, AARON H ROSE, MICHAEL J BURNS, KRZYSZTOF KEMPA, MICHAEL J NAUGHTON, Boston College — The nanocoax has demonstrated confinement of VIS and NIR light, and calculations show that extreme confinement can be achieved by coupling to the fundamental mode. We have previously reported our novel nanofabrication process, which leverages the conformal nature of atomic layer deposition (ALD), and which produces high aspect ratio nanocoaxes. In this work, we report in more detail some optical transmission measurements, particularly related to signatures of coupling into the fundamental mode. While there have been many computational works concerning the excitation of the fundamental mode at optical frequencies, to date there have been relatively few experimental works. To interrogate these structures, we have integrated an optical vortex generation module into a near-field scanning optical microscope, we have built a confocal spectroscopic module for transmittance measurements in the VIS and SWIR, and we report on polarimetry measurements of a tightly focused vortex beam. We further discuss some computational progress with regard to coupling efficiency and some prospective technologies based on optical confinement to length scales arbitrarily smaller than the wavelength.

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2:42PM C33.00002: Packaging of surface nanoscale axial photonic microresonators*  MATHIEU COUILLARD
(Presenter), PABLO BIANUCCI, Concordia University — Due to their high Q factor and small volume surface, nanoscale axial photonic (SNAP) resonators have been used to study nonlinear effects, sensing, optomechanics and many other applications. The best way to couple light into SNAP resonators is through the evanescent field of a tapered fiber. However, these tapered fibers are fragile, and SNAPs are very sensitive to their environment. These factors make SNAP resonators difficult to transport and keep intact for long periods of time without some kind of packaging. We present an inexpensive technique for packaging SNAP resonators as a pigtail device using a 3D printed housing and low index optical epoxy. We then report the effects of this packaging technique on the spectra and measure the change in spectra due to impact, heat and environmental impurities.

*We would like to acknowledge support from the National Science and Engineering Research Council (NSERC) of Canada, through the Discovery Grant program (grant 435875-2013).

2:54PM C33.00003: Time Stretch Single-shot Terahertz Analyzer  TIANWEI JIANG (Presenter), CEJO KONUPARAMBAN LONAPPAN, Department of Electrical and Computer Engineering, University of California, Los Angeles, CLÉMENT EVAIN, CHRISTOPHE SZWAJ, ELÉONORE ROUSSEL, MARC LE PARQUIER, SERGE BIELAWSKI, PIAM, Université Lille 1, BAHRAM JALALI, Department of Electrical and Computer Engineering, University of California, Los Angeles — Terahertz technology has important applications in security due to its penetration in common packaging material. Being able to measure bursts of THz signal in real-time has applications in medicine, data communication, compact radar, and particle accelerators. Unfortunately, the established terahertz instrumentation systems have a slow response and are not capable of real-time measurements. Photonic Time Stretch is a data acquisition method which enables continuous recording of fast single shot events over long record lengths. It has been successfully used to capture THz emission due to electron bunching in synchrotrons, and has led to the discovery of new phenomena in optics such as optical rogue waves and soliton molecule dynamics. In this talk we will provide an overview of Time Stretch technology with emphasis on its design for THz operation. We will describe several methods for overcoming the frequency fading phenomena including single sideband, phase diversity and inverse propagation methods as well as balanced detection for common mode rejection to achieve high sensitivity. We will also describe its implementation at optical frequencies.

3:06PM C33.00004: Excitation Dynamics of MoS2 Using Optical Pump-THz Probe Magneto-spectroscopy  ASHLYN BURCH (Presenter), ANDREW GARRISON LINN, BIPLOB BARMAN, Physics, University of Alabama at Birmingham, DENIS KARAISKAJ, Physics, University of South Florida, STEPHEN A MCGILL, National High Magnetic Field Laboratory, DAVID J. HILTON, Physics, University of Alabama at Birmingham — THz spectroscopy is a method that can be used to study transitional metal dichalcogenide material systems on ultrafast time scales by determining the quantum effect of emitted THz radiation and phase on the material under extreme conditions.1 Monolayer molybdenum disulfide (MoS2) has been broadly studied and displays electron-phonon interactions and exciton-exciton scattering that influence the coherence time and often are the driving component for the application of this material.2 These measurements were performed on bulk MoS2, using an optical pump-terahertz probe spectrometer that operated under high magnetic fields (< 25 T) at the National High Magnetic Field Laboratory in Tallahassee, Florida. The response of this material was measured under different constant magnetic fields using an air-biased coherent detection system (ABCD) by tracing optical pump delays while sitting at the peak of the transmitted THz pulse.


3:18PM C33.00005: Bragg Filters for Integrated Photonic Circuity*  QINGYING CHEN (Presenter), SCOTT HOLMSTROM, Department of Physics and Engineering, University of Tulsa, Tulsa 74104, United States, NATHAN TYNDALL, TODD STIEVATER, Optical Science Division, Naval Research Lab, Washington DC 20375, United States — We report the design, fabrication, and measurement of waveguide Bragg filters for use in integrated Raman- and fluorescence-based spectroscopy and sensing systems. A periodic effective index was produced by a series of silicon nitride (SiN) patches located adjacent to and on both sides of a straight SiN waveguide. A chirp was applied to the length and spacing of the patches to broaden the reflection bandwidth. The filters were simulated using an eigenmode expansion solver and manufactured at a photonic integrated circuit (PIC) foundry.

*This material is based on research sponsored by Air Force Research Laboratory under agreement number FA8650-15-2-5220.
Integrated spin wave AND gate using iron garnet film

TAICHI GOTO (Presenter), TAKUYA YOSHIMOTO, Toyohashi University of Technology, CAROLINE ANNE ROSS, Massachusetts Institute of Technology, KOJI SEKIGUCHI, Yokohama National University, ALEXANDER B. GRANOVSKY, Moscow State University, YUICHI NAKAMURA, HIRONAGA UCHIDA, MIHUTERU INOUE, Toyohashi University of Technology — Spin wave (SW) attracts many interest as a candidate of post-CMOS device. Previously we demonstrated XNOR or AND/OR logic gates using interference of forward volume (FV) SW propagating in a 10 μm thick yttrium iron garnet (YIG) film [1]. However the size of these gate is mm order because YIG and electrodes for excitation and detection of SW were fabricated discretely. Therefore, integration of electrodes on YIG and miniaturization of YIG waveguide is essential for demonstration of further functionality.

In this work, we fabricated ψ-shape spin wave waveguide to demonstrate electrodes integrated AND logic gate. A 200 nm thick YIG was fabricated on garnet substrate using liquid phase epitaxy. YIG film was etched into ψ-shape using electron beam lithography and wet etching. The width of YIG film was 14 μm. Then four coplanar waveguides (CPWs) for excitation and detection of FV SW were placed on YIG waveguide. To measure a field dependence of propagation properties of FV SW, CPWs and vector network analyzer were connected via micro-probe to measure the scattering parameters. Successfully, the AND gate using FV SW phase interference was demonstrated, comparable to the case using 10 μm thick YIG. This is the smallest AND gate using spin wave.


Demonstration of Inverse Designed Broadband Cavity-Waveguide Couplers*

JINHIE SKARDA (Presenter), KYOUL YANG, DRIES VERCRUYSSE, NEIL V. SAPRA, LOGAN SU, ALEXANDER Y. PIGGOTT, JELENA VUCKOVIC, Stanford University — The ability to control cavity-waveguide coupling over a wide wavelength span is necessary in a number of applications such as frequency conversion and frequency comb generation. However, achieving a specified target coupling at multiple wavelengths using the conventional approach of evanescent coupling is an outstanding challenge. In our approach, we instead treat the cavity-waveguide coupling region as a 2-input, 2-output port device and optimize the structure to produce the desired coupling spectrum. This inverse design method enables us to specify any coupling spectrum as our optimization objective, and the fabrication-constrained optimization produces coupler structures that are fully fabricable with standard lithography processes. We experimentally demonstrate our ability to control the coupling spectrum between a straight waveguide and racetrack resonator on 220 nm SOI while maintaining a Q factor of about 30,000. Our progress on efficient coupling over an octave span is an important step for integrated nonlinear photonics.

* Air Force Office of Scientific Research (FA9550-17-1-0002); Gordon and Betty Moore Foundation (GBMF4744, GBMF4743); National Science Foundation Graduate Research Fellowship (DGE-1656518); Nano- and Quantum Science and Engineering Fellowship

Electrostatically and Optically Gated Field Emission Transistors

WILLIAM JONES (Presenter), Jet Propulsion Laboratory, LUCIA DEROSE, AXEL SCHERER, Applied Physics, California Institute of Technology — Recently, several groups have demonstrated that plasmonically trapped light can optically stimulate ultra-fast field emission of electrons [1] [2] by taking advantage of the sub-wavelength confinement of light at the metal/air interface to generate the intense electric fields needed to tunnel an electron into vacuum. Nanoscale field emission transistors produce the same magnitude fields electrostatically by applying modest voltages over nanoscale distances [3]. We have combined both principles and produced nanoscale field emission transistors integrated into hybrid plasmonic waveguides on a SOI platform. These devices can be optically or electrostatically gated and may serve as building blocks for ultra-fast optoelectronic circuits.

modulated through gate voltage (Vg) applied to a reverse biased III-V Schottky diode [IEEE TED 61(4), pp.1006-1013, 2014].

The 2DEG density in Transistor (HEMT) used in high speed RF circuits and routinely operated at >100GHz frequencies. We present a modified rate beyond 100GBps [Nature 562, pp.101–104, 2018]. We propose a design inspired by III-V High Electronic Mobility heterostructures.

The bandwidth in electro-optic materials is limited by R-C time constants of the electrical contacts, resulting in high bit error rate beyond 100GBps [Nature 562, pp.101–104, 2018]. We propose a design inspired by III-V High Electronic Mobility Transistor (HEMT) used in high speed RF circuits and routinely operated at >100GHz frequencies. We present a modified Drude model to analyze the strength of the plasma dispersion effect of the 2DEG at the III-V interface. The 2DEG density is modulated through gate voltage (Vg) applied to a reverse biased III-V Schottky diode [IEEE TED 61(4), pp.1006-1013, 2014].

Plasma dispersion due to 2DEG is dominant as compared to free charge carriers in the AlGaN barrier. We obtain an analytical expression for the carrier induced electro refraction:

\[ \Delta n = \frac{-e\lambda^2\varepsilon_x (V_g - V_{th})}{8\pi^2c^2n_d(m^*_{2DEG})^2} \]

\( V_{th} \) is threshold voltage corresponding to pinch-off for the 2DEG and other symbols are per standard notation. As compared to multi-quantum well intersubband modulators, the structure we propose is easier to fabricate and analyze. The simple device structure enables several methods of coupling light, making a waveguide manifestation feasible.

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4:54PM C33.00013: Localization of light induced by pulling a fiber* TABASSOM HAMIDFAR (Presenter), PABLO BIANUCCI, Concordia University — Optical microresonators based on whispering gallery modes (WGM) can be potentially used in many areas of science and technology including telecommunications, microfluidics, optomechanics, and others. They are dielectric convex structures that confine light through total internal reflection. Out of the many available types of WGM microresonators, the surface nanoscale axial photonics (SNAP) platform enables fabrication of resonant ultralow loss photonics structures at the surface of an optical fiber. Due to their flexibility, and ultra-low loss, which lead to the creation of high-quality WGMs, they have great potential applications as photonic micro-devices in switching, slowing light, filtering, lasing and sensing with high precision. In this work, we propose a new technique for the creation of SNAPs, by using a regular hydrogen-oxygen torch, which requires less equipment than current techniques. We characterize our resonator by evanescent spectroscopy using a tapered fiber for coupling. The transmission spectra shows that light can be fully localized by pulling a fiber, with the potential to host very low loss resonant modes.

*National Science and Engineering Research Council (NSERC) of Canada (grant 435875-2013)

5:06PM C33.00014: Quantum Confined Stark Effect in Phase-Pure Thick-Shell CdSe/CdS Quantum Dots* LEI ZHANG (Presenter), HONGYU YANG, YUFEN YUAN, YIPING CUI, JIAYU ZHANG, Advanced Photonics Center, Southeast University — Colloidal semiconductor quantum dots (QDs) have recently attracted great attention in electric fields sensing via the quantum confined Stark effect (QCSE). Here, the QCSE in ensemble of phase-pure wurtzite CdSe/CdS QDs is studied by applying a uniform external electric field. We observe a clear field-dependent PL and absorption modulations, including the spectral shifts and broadening, as well as the changes in its intensity. The Stark shifts in ensemble emission and absorption are found to be typical quadratic function of the external field. Moreover, the multiexciton states also exhibit obvious optical responses to the electric field, with a decrease of 18% in emission intensities and an increase in the ultrafast lifetime from 25 to 31 ps. The results imply that the field-induced QCSE in the QD ensemble are attributed to the effective suppression of the primary source of local field in such thick-shell QDs, thus proving that an efficient field control over the optical properties (the changes in emission and absorption intensity, spectral shifts, and PL lifetime) in these nanoparticles is feasible and open the potential possibility of field-sensitive QDs to achieve real-time electro-optic sensing.

*The National Basic Research Program of China (2015CB352002)

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C34 GIMS: Keithley Session BCEC 205A - Tag(s): Invited
2:30PM C34.00001: Making the invisible visible: Spins probed with soft x-rays* [Invited] ELKE ARENHOLZ (Presenter), Lawrence Berkeley National Laboratory — The advancement of spintronics relies on our improved understanding spin based phenomena and our ability to engineer materials with specific magnetic and transport properties. In this talk, we will highlight the contributions optimized soft x-ray based characterization tools can make to this endeavour.

Chiral domain walls are promising candidates for low-energy consumption memory and logic devices. We engineered chiral domain wall arrays in Pt/Co/Cu multilayers and using resonant soft X-ray diffraction find that the chirality of the magnetic spin textures in the surface near region reverses as function of layer thickness due to the interplay of competing driving forces (DMI, magnetic anisotropy, magnetic dipole interaction). [1]

The recent discovery of magnetic long-range order in two-dimensional van der Waals materials opens up new opportunities for spintronics. We employed soft X-ray photoemission electron microscopy (PEEM) to image the domain configuration of Fe₃GeTe₂. We find that the magnetic long-range order in micron scale Fe₃GeTe₂ pattern leads to an unconventional out-of-plane stripe-domain phase that undergoes a transition to an in-plane vortex phase with increasing temperature. [2]

Spin currents are mostly detected indirectly through measurement of spin-torque driven magnetization precession, spin-current induced second harmonic optical effects, inverse spin Hall effect (ISHE), etc. We have succeeded in monitoring a pure ac spin current directly through a Py/Cu/Co multilayer with by X-ray detected ferromagnetic resonance (XFMR). [3]

In this talk, the powerful X-ray instrumentation optimized for these studies of spintronics phenomena will be discussed.

References

*Research at the Advanced Light Source is supported by the DOE Office of Science under contract DE-AC02-05CH11231.

3:06PM C34.00002: Resonant Inelastic X-ray Scattering of Energy Materials: from Fundamental Understandings to Practical Developments* [Invited] WANLI YANG (Presenter), Lawrence Berkeley National Laboratory — The pressing demand of improving the energy device performance calls for new concepts that require characterization techniques beyond conventional probes. With much improved throughput, ultra-high efficiency mapping of Resonant Inelastic X-ray Scattering (mRIXS) has opened up RIXS as such a powerful technique. This has become a timely and critical solution to characterize the novel electronic states of both transition-metals and oxygen involved in electrochemical devices, i.e., batteries, for energy applications.

In this presentation, we first show that the electrochemical performance of batteries is fundamentally defined by many intrinsic physics parameters of the materials, e.g., spin states, ionization energy, crystal field etc., which could be approached through conventional spectroscopy [1]. However, modern concepts based on novel states in batteries are often difficult to be clarified and require tools that are more incisive. We demonstrate that these unconventional states could be clearly addressed through mRIXS experiments [2]. In particular, mRIXS could distinguish the critical lattice oxygen activities in batteries, and precisely quantify its contributions, reversibility, and cyclability upon electrochemical cycling. mRIXS findings clarify many misunderstandings of the mysterious oxygen activities in battery electrodes and indicate independent oxygen behaviors that are intrinsically determined by the material physics, something that has been indiscreetly taken for granted [3]. At the end, we show that mRIXS results have gone beyond fundamental understandings and led to guidelines for future material developments and optimizations.

[1] Wu et al., JACS 139, 18358 (2017)

*ALS is a DOE Office of Science User Facility under contract No. DE-AC02-05CH11231.

3:42PM C34.00003: TBD [Invited] ZHIXUN SHEN (Presenter), Stanford University — TBD
Laser ARPES on High Temperature Superconductors and Quantum Materials

The mechanism of high temperature superconductivity in the copper-based and iron-based superconductors remains a prominent and challenging issue in condensed matter physics. Angle-resolved photoemission spectroscopy (ARPES), as a powerful technique to directly probe the electronic structure of materials, has played a key role in studying high temperature superconductors, as well as other quantum materials. In this talk, I will first briefly introduce ARPES technique, in particular, the latest development of vacuum-ultra-violet (VUV) laser-based ARPES systems. Then I will highlight some ARPES results on topological materials including Bi$_2$Se$_3$, monolayer silicene, and ZrTr$_5$. Finally, I will report some of our recent results in utilizing the state-of-the-art laser-based ARPES to study high temperature cuprate superconductors and iron-based superconductors.

3. Ya Feng et al., PNAS 133, 14656 (2016).

Joseph F. Keithley Award For Advances in Measurement Science Talk: Science Driven Instrumentation and Applications with Soft X-rays

Sharper and sharper experimental tools are often crucial for understanding of novel physical phenomena and making new discoveries. Today in condensed matter physics we are experiencing need for revolutionary new instrumentation for understanding interplay of many degrees of freedom interacting at different energy, length and time scales. These interactions lead to new phases of matter and emergent phenomena such as high temperature superconductors, topological insulators and two dimensional transition metal dichalcogenides, to name a few. The primary focus of my talk is to present some of the novel soft x-ray instrumentation developed during the last two decades at the Advanced Light Source and their science applications, through various examples for unraveling the emergent phenomena in quantum materials and energy related challenges. My talk will include advanced instrumentation for Angle-Resolved Photoemission Spectroscopy (ARPES), Ambient Pressure XPS and Resonant Inelastic X-ray Scattering (RIXS).

*The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 and DE-AC02-06CH11357. Development of qRIXS endstation and detector is partially funded by Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515. QERLIN is funded by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4630.

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C35 DQI: Hybrid Systems: Coupling Spin Qubits with Microwave Resonators

Coupling Spin Qubits with Microwave Resonators

Vanita Srinivasa, Sandia National Laboratories - Tag(s): Focus
2:30PM C35.00001: Circuit Quantum Electrodynamics with superconductor-semiconductor hybrid systems (Invited)
PASQUALE SCARLINO (Presenter), DAVID VAN WOERKOM, ETH Zurich, UDSON MENDES, Univ. of Sherbrooke, CLEMENS MUELLER, JONNE KOSKI, ANDREAS LANDIG, JANN HINNERK UNGERER, CHRISTIAN KRAYLUND ANDERSEN, SIMONE GASPARINETTI, CHRISTIAN REICHL, WERNER WEIGSCHERER, KLAUS ENSSSLIN, THOMAS IHN, ETH Zurich, ALEXANDRE BLAIS, Univ. of Sherbrooke, ANDREAS WALLRAFF, ETH Zurich — Semiconductor qubits rely on the control of charge and spin degrees of freedom of electrons or holes confined in quantum dots (QDs). Typically, semiconductor qubit-qubit coupling is short range, effectively limiting qubit distance to the spatial extent of the wavefunction of the confined particle (a few hundred nanometers). This is a significant constraint towards scaling of QD-based architectures to realize dense 1D or 2D arrays of QDs. Inspired by techniques originally developed for circuit QED, we recently demonstrated the strong coupling of individual electrons [1,2] confined in GaAs quantum dots to individual microwave photons, making use of the enhanced electric component of the vacuum fluctuations of a resonator with impedance beyond the typical 50 Ohm of standard coplanar waveguides. In this hybrid technology, we recently realized a proof of concept experiment, where the coupling between a transmon and a double QD (DQD) is mediated by virtual microwave photon excitations in a high impedance SQUID array resonator, which acts as a quantum bus enabling long-range coupling between dissimilar qubits [3]. Similarly, we achieved coherent coupling between two DQD charge qubits separated by approximately 50 um [4]. In the dispersive regime, we spectroscopically observed qubit-qubit coupling as an avoided-crossing in the energy spectrum of the DQD charge qubits. The methods and techniques developed in this work are transferable to QD devices based on other material systems and can be beneficial for spin based hybrid systems [5].


3:06PM C35.00002: Towards cavity-mediated coupling of spin-qubits (Invited)
FELIX BORJANS (Presenter), XANTHE CROOT, XIAO MI, JASON R PETTA, Department of Physics, Princeton University — While single-qubit gates with fidelities approaching superconducting qubits have been demonstrated [1] and two-qubit gates based on nearest-neighbour exchange are being realized with improved performance on length scales of a few hundred nanometers [2-4], cavity-mediated coupling of spin-qubits over ~1 cm distances remains an outstanding challenge. With the recent demonstration of strong-coupling of a single electron-spin to the electric field of a cavity photon [5, 6], this long-range entanglement between two spin-qubits is within reach. Here we present recent progress in our effort to complete this milestone.


3:18PM C35.00003: Multi-qubit entangling gates for spins in silicon (Invited)
MICHAEL GULLANS (Presenter), JASON R PETTA, Physics, Princeton University — Implementing large-scale algorithms on a quantum computer will require efficient gate compilation strategies to reduce overhead. We recently demonstrated an efficient CNOT gate for spins in Si [1]. The gate operates in a regime where the magnetic field gradient exceeds exchange. By turning on exchange, it is possible to implement a CNOT gate in a single step using resonant microwave excitation. We will discuss possible extensions of the resonant gate in more complex device architectures [2] and present a detailed analysis of multi-qubit gate fidelities.


*Research sponsored by ARO grant No. W911NF-15-1-0149 and the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant GBMF4535.
We present results on superconducting resonators made of thin titanium nitride, studied in an in-plane magnetic field. By implementing a lattice of penetration holes with sizes comparable to the superconducting penetration length, we observe the resonators remain resilient to small out-of-plane magnetic fields. The resonators are then combined with novel 2D materials to serve as a sensitive quantum-coherent probe of condensed-matter properties.

*This research was funded in part by the HRL Matisse program; and by the Department of Defense via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.

3:42PM C35.00005: Design of Multi-chip Module with High Impedance Microwave Resonators for cQED Experiments with Si/SiGe Quantum Dots

We describe in a general perturbation theory approach the origin of the couplings of a spin qubit to a superconducting cavity as a low-energy limit. Special attention is paid to the so-called curvature couplings related to qubit’s quantum capacitance, which is derived as a low-energy limit of a perturbation expansion to second order. We discuss the applicability of these couplings to current experiments with multi-dot spin-qubits, including single-, double, and triple-dot quantum dot qubits, as well as with superconducting qubits.

*This work supported in part by the DOD under H98230-15-C0453, ARO (W911NF-17-1-0274), and the Vannevar Bush Faculty Fellowship program under ONR grant number N00014-15-1-0029. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies or endorsements, either expressed or implied, of the ARO or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein.

3:54PM C35.00006: Integrating singlet-triplet qubits with superconducting resonators

*This work was supported by the Army Research Office Grants No. W911NF-15-1-0203 and No. W911NF-17-1-024.
In this work we explore this sweet-spot regime, which provides both resilience to charge noise and strong dipolar coupling to the resonator. We analyze the trade-offs between strong coupling, relaxation, dephasing, and leakage to the (0,2) singlet state, and we maximize the resulting gate fidelities. We identify a wide window in parameter space over which the qubit-resonator system can achieve two-qubit gate fidelities above 95%.

**4:30PM C35.00009: Two-qubit gates between quantum dot spins coupled by a resonator**† ADA WARREN (Presenter), EDWIN BARNES, SOPHIA ECONOMOU, Virginia Tech — Recent experimental work with silicon qubits has shown that it is possible, using an inhomogeneous magnetic field, to strongly couple the modes of a superconducting resonator to the spin of a single electron trapped within a double quantum dot. This suggests the possibility of realizing long-range spin-spin interactions mediated by cavity photons. We present here our theoretical calculation of the effective interaction between distant quantum dot spins coupled via a resonator and our proposed cavity-mediated two-qubit gate.

*This work is supported by the Army Research Office (W911NF-17-0287).

**4:42PM C35.00010: Highly coherent spin states in carbon nanotubes coupled to cavity photons**† TINO CUBAYNES (Presenter), MATTHIEU DELBECQ, MATTHIEU DARTIAILH, RÉOUVEN ASSOULY, MATTHIEU M DESJARDINS, LAURIANE CONTAMIN, Laboratoire Pierre Aigrain UMR 8551, Ecole normale Supérieure - PSL Research university, CNRS, Université Pierre et Marie Curie - Sorbonne Universités, Université Paris Dider, LAURE BRUHAT, Microtechnology and nanoscience, Chalmers University of Technology, ZAKI LEGHTAS, FRANCOIS MALLET, AUDREY COTTET, TAKIS KONTOS, Laboratoire Pierre Aigrain UMR 8551, Ecole normale Supérieure - PSL Research university, CNRS, Université Pierre et Marie Curie - Sorbonne Universités, Université Paris Dider — Circuit quantum electrodynamics allows one to probe, manipulate and couple superconducting quantum bits using cavity photons at an exquisite level. Mesoscopic-QED inherits the c-QED toolbox and applies it to quantum dot circuits. In this talk, I will present a spin-qubit encoded in a carbon nanotube based double quantum dot with non-collinear ferromagnetic contacts. Using the c-QED spin-photon interface, we drove a single electronic spin and performed microwave spectroscopy of it. From this measurement we identified a decay rate which can be tuned to be as low as 250kHz. The cooperativity of the spin-photon interface is also measured as a function of the detuning, allowing to identify an optimal working point. These coherence properties, which are attributed to the use of pristine carbon nanotubes stapled inside the cavity, should enable coherent spin-spin interaction via cavity photons and compare favorably to the ones recently demonstrated in Si-based circuit QED experiments.

*This work is supported by the ERC Starting Grant "CirQys" and by the ANR "FunTheme".

**4:54PM C35.00011: Magnon-photon coupling between a superconducting resonator and a thin film permalloy stripe**† YI LI (Presenter), Department of Physics, Oakland University, TOMAS POLAKOVIC, YONGLEI WANG, JING XU, SERGI LENDINEZ, ZHIZHI ZHANG, JUNJIA DING, TRUPTI KHAIRE, HILAL SAGLAM, Materials Science Division, Argonne National Laboratory, RALU DIVAN, Center for Nanoscale Materials, Argonne National Laboratory, JOHN E. PEARSON, WAI-KWONG KWOK, ZHILI XIAO, VALENTYN NOVOSAD, AXEL F HOFFMANN, Materials Science Division, Argonne National Laboratory, WEI ZHANG, Department of Physics, Oakland University — Coherent processing of magnetic excitations has received increasing attentions for spin-wave-based functionality such as magnonics, cavity spintronics and quantum information processing. They usually involve strong coupling of different excitations, such as magnons and photons, which leads to their hybridized modes.

In this work, we achieve strong magnon-photon coupling of a device ferromagnet of Ni$_{80}$Fe$_{20}$ (Py) to a high-quality NbN coplanar superconducting resonator. Microwave characterizations at 1.6 K show a high quality factor Q~10000. A Py 30 nm stripe was then fabricated on top of the resonator with a 10-nm MgO spacer. We observe a strong anti-cross between the superconducting resonator mode and the Kittel mode of the Py stripe. A maximum coupling strength of $g_{eff}$/f=100 MHz is obtained at about 5 GHz when the biasing field is orthogonal to the microwave field from the resonator. The anti-crossing is completely suppressed when the biasing field is parallel to the resonator microwave field. Our results provide new pathways for implementing on-chip magnonic devices with efficient and coherent information transducers.

*This work was supported by DOE-BES, Materials Science and Engineering Division, and CNM under Contract No. DE-AC02-06CH11357, and NSF-DMR-1808892
ANDREAS LANDIG, JONNE KOSKI, PASQUALE SCARLINO (Presenter), DAVID VAN WOERKOM, CHRISTIAN REICHL, WERNER WEGSCHEIDER, ANDREAS WALLRAFF, KLAUS ENSSLIN, THOMAS IHN, Department of Physics, ETH Zurich, Switzerland — A coherent link connecting different qubits over long distances is necessary to benefit from the advantages in gating or coherence times of different qubit implementations in a future quantum processor. We realize such a link between a spin qubit and a transmon qubit in a circuit quantum electrodynamics architecture [1] similar to a recent work that involved a charge qubit and a transmon qubit [2]. The spin qubit is a resonant exchange qubit [3] formed by three electrons in a gate defined triple quantum dot in a GaAs/AlGaAs heterostructure. The qubit states are split energetically by exchange interaction. Consequently, the spin qubit can be operated at zero magnetic field and exhibits a decoherence rate of $\gamma^2/2\pi \approx 10\text{MHz}$, limited by hyperfine interaction in the host material. The transmon qubit has $\gamma^2/2\pi \approx 0.7\text{MHz}$ limited by Purcell decay. Both qubits are capacitively coupled to a high impedance SQUID array resonator with coupling strengths of $g_{SQ}/2\pi \approx 50\text{MHz}$ and $g_{T}/2\pi \approx 180\text{MHz}$ for the spin and transmon qubit, respectively. We demonstrate resonant and dispersive interaction between the two qubits mediated by real and virtual microwave photons.


Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C36 DBIO: Statistical Physics of Large Populations of Cells: from Microbes to Tissues I

2:30PM C36.00001: A unifying theory of branching morphogenesis [Invited] BENJAMIN SIMONS (Presenter), Physics, University of Cambridge — Branching morphogenesis has been a subject of abiding interest. Although much is known about the underlying signaling pathways, it remains unclear how the macroscopic features of branched organs, including their size, network topology and spatial patterning, are encoded. Here we show that, in the mouse mammary gland, kidney and pancreas, these features can be explained quantitatively within a single unifying framework of branching and annihilating random walks. Based on large-scale organ reconstructions, genetic lineage tracing and proliferation kinetics, we show that morphogenesis follows from the collective proliferative activity of sublineage-restricted equipotent self-renewing progenitors localized at ductal tips that drive a process of ductal elongation and stochastic tip bifurcation. By correlating ductal termination with proximity to maturing ducts, this dynamics results in the specification of a complex network of defined density and statistical organization. These results show that branched epithelial structures in mammalian tissues develop as a self-organized process, reliant upon a strikingly simple, but generic, set of local rules, without recourse to a rigid and deterministic sequence of genetically programmed events.

3:06PM C36.00002: Diversity, dynamics and defense in microbial communities* [Invited] DEVAKI BHAYA (Presenter), Carnegie Institution for Science — Cyanobacteria are an ancient group of microbes that can carry out photosynthesis and nitrogen fixation. They are important members of microbial communities in terrestrial and aquatic environments. They thrive in moderate and harsh environments where they can adapt to desiccation stress and extremes of heat or cold. For several years we have focused on extremophile communities that form stratified biofilms or microbial mats in the hot springs of Yellowstone National Park. In these communities, 16S rRNA diversity has been correlated with environmental gradients of temperature and light. The genomes of two Synechococcus isolates that dominate at different temperatures in the mats, has provided key insights into genomic and metabolic diversity within these populations. Metagenomic data in combination with deep amplicon sequencing from these communities, revealed an unexpectedly high degree of genomic micro-diversity. We have also attempted to explore the co-evolution of host and cyanophage populations in the microbial mats, by creating viromes and exploiting CRISPR spacer information. Finally, we are also interested in probing the importance of phototaxis and motility in these structured communities. I will describe our findings in the context of how these moderately complex communities are ideally suited to probing how physical forces and chemical gradients in combination with genetic diversity shape microbial community structure and organization. The future of modeling complex interactions and the ability to test hypotheses in synthetic communities will be explored.

*This research is funded by the National Science Foundation and the Carnegie Institution for Science.
3:42PM C36.00003: Coevolutionary dynamics in the immune system [Invited] ARMITA NOURMOHAMMAD (Presenter), Max Planck Institute for Dynamics and Self-organization — The vertebrate adaptive immune system provides a flexible and diverse set of molecules to neutralize pathogens. Yet, viruses such as HIV can cause chronic infections by engaging in a coevolutionary arms race with the adaptive immune system: The B-cell receptors in the adaptive immune system diversify to neutralize the virus and HIV evolves to evade the immune response. While it is clear that HIV exerts strong selection on the adaptive immune system, the modes of immune response are still unknown. Here I introduce a non-equilibrium framework to characterize the rapid coevolution of immune cells and pathogens. By tracing the immune repertoire of HIV patients over time and reconstructing the history of the accumulated mutations within patients, I show evidence for strong co-adaptation of the immune repertoire and HIV. I argue that rapid affinity maturation of the immune system upon viral expansion and a quasi-stationary response during chronic infection characterize the B-cell response to HIV.

4:18PM C36.00004: Cooperative growth and cell-cell aggregation in marine bacteria* [Invited] OTTO X CORDERO (Presenter), Civil and Environmental Engineering, Massachusetts Institute of Technology — Bacterial cooperation, whereby cells secrete compounds that can facilitate the growth of neighboring cells, has been extensively studied through the lens of evolutionary biology. However, the environmental implications of cooperation and the ecological scenarios under which it takes place remain much less understood. In this talk I will discuss the conditions under which cooperative growth emerges in microbial populations that degrade complex organic materials in the ocean. I will show that organisms that are poor secretors of hydrolytic enzymes use chemotactic behavior to form cell-cell aggregates that enable individuals to increase local concentrations and efficiently uptake the solubilized organic matter. By contrast, when organisms secrete highly active enzymes dynamics turn competitive, cells avoid aggregation and the efficiency of carbon uptake drops. I will discuss the theoretical limits of aggregation and how bacterial isolates from the ocean can overcome these limits in the laboratory by developing multicellular behaviors. I will back up these results with theory, data from individual based models and experiments with natural isolates. Finally, I will discuss the potential role of social cheaters in the natural environment, based on a study with hundreds of micro-scale particle colonization experiments in natural seawater.

*This work was supported by a grant from the Simons Foundation (542395, O.X.C)

4:54PM C36.00005: How adaptive immunity constrains the composition and fate of large bacterial populations* [Invited] SIDHARTHA GOYAL (Presenter), MADELEINE BONSMA-FISHER, University of Toronto — Features of the CRISPR-Cas system, in which bacteria integrate small segments of phage genome (spacers) into their DNA to neutralize future attacks, suggest that its effect is not limited to individual bacteria but may control the fate and structure of whole populations. Emphasizing the population-level impact of the CRISPR-Cas system, recent experiments show that some bacteria regulate CRISPR-associated genes via the quorum sensing (QS) pathway. Here we present a model that shows that from the highly stochastic dynamics of individual spacers under QS control emerges a rank-abundance distribution of spacers that is time invariant, a surprising prediction that we test with dynamic spacer-tracking data from literature. This distribution depends on the state of the competing phage–bacterium population, which due to QS-based regulation may coexist in multiple stable states that vary significantly in their phage-to-bacterium ratio, a widely used ecological measure to characterize microbial systems.

*NSERC Discovery Grant (SG) and Vanier Canada Graduate Scholarship.(MB-F)

Monday, March 4, 2019 2:30 PM - 5:06 PM

Session C37 GMAG DCMP DMP: Spin Liquids: Alpha-RuCl3 BCEC 206A - Arnab Banerjee, Oak Ridge National Laboratory - Tag(s): Focus

2:30PM C37.00001: Kitaev spin liquids in spin-orbit coupled correlated materials* [Invited] HAE-YOUNG KEE (Presenter), University of Toronto — Recently, a new family of correlated honeycomb materials with strong spin-orbit coupling have been promising candidates to realize the Kitaev spin liquid. In particular, a half-integer quantized thermal Hall conductivity was reported in alpha-RuCl3 under the magnetic field. Using a generic nearest neighbour spin model with bond-dependent interactions, I will present numerical evidence of an extended regime of quantum spin liquids. I will also discuss how to achieve a chiral spin liquid near ferromagnetic Kitaev interaction in the presence of the magnetic field leading to the quantized thermal Hall conductivity.

*NSERC of Canada
3:06PM C37.00002: Field induced quantum spin liquid with spinon Fermi surfaces in the Kitaev model*  
HONG-CHEN JIANG, Stanford Institute for Materials and Energy Sciences, SLAC and Stanford University, CHANGYAN WANG (Presenter), Department of Physics, The Ohio State University, BIAO HUANG, Department of Physics and Astronomy, University of Pittsburgh, YUAN-MING LU, Department of Physics, The Ohio State University — Recent experimental evidence for a field-induced quantum spin liquid (QSL) in α-RuCl₃ calls for an understanding for the ground state of honeycomb Kitaev model under a magnetic field. In this work we address the nature of an enigmatic gapless paramagnetic phase in the antiferromagnetic Kitaev model, under an intermediate magnetic field perpendicular to the plane. Combining theoretical and numerical efforts, we identify this gapless phase as a U(1) QSL with spinon Fermi surfaces. We also reveal the nature of continuous quantum phase transitions involving this U(1) QSL, and obtain a phase diagram of the Kitaev model as a function of bond anisotropy and perpendicular magnetic field.

*This work is supported by NSF under award number DMR-1653769 (CYW,YML), by U.S.ARO (W911NF11-1-0230), AFOSR (FA9550-16-1-0006), MURI-ARO (W911NF17-1-0323) (BH), by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515 (HCJ), and in part by NSF grant PHY-1607611 (YML).

3:18PM C37.00003: Magnetic field induced intermediate gapless spin-liquid phase with a spinon Fermi surface*  
NIRAVKUMAR D. PATEL (Presenter), NANDINI TRIVEDI, The Ohio State University — Quantum spin liquids have generated considerable excitement in the condensed matter physics community. We employ the density matrix renormalization group to study the Kitaev model with a magnetic field in the H∥[111] direction. We show the presence of an intermediate phase, between the gapped Kitaev spin liquid and partially field polarized phase, that is a candidate spin liquid. We show that the spin-spin correlations in real-space obey power-law decay that is indicative of gapless spin excitations. Additionally, we present calculations of specific heat, entropy, and spin susceptibility at the finite temperature to provide further evidence of a gapless phase. Using the peaks of spin structure factor, we propose an existence of a spinon Fermi surface in the intermediate phase.

*Department of Energy, under grant DE-FG02-07ER46423

3:30PM C37.00004: Pristine graphene contacts to exfoliated α-RuCl₃ crystals  
JESSE BALGLEY (Presenter), BOYI ZHOU, Washington University, St. Louis, PAULA J KELLEY, DAVID GEORGE MANDRUS, Oak Ridge National Laboratory, ERIK HENRIKSEN, Washington University, St. Louis — The layered Mott insulator α-RuCl₃ has garnered significant attention as a candidate to host a Kitaev quantum spin liquid, harboring fractionalized excitations and Majorana fermion-like spin excitations. Though significant progress has been made toward understanding how these phenomena manifest in α-RuCl₃, experimental procedures to date have largely consisted of probes for pristine bulk samples. However α-RuCl₃ may be readily exfoliated down to monolayer thicknesses. We show that we can achieve good electrical contact to α-RuCl₃ using monolayer graphene, enabling direct measurement of the resistivity. In this talk, we present device configurations for interrogating exfoliated α-RuCl₃ crystals in the few-layer limit by the fabrication of graphene/α-RuCl₃ heterostructures. We further discuss measurements of the Mott gap via optical spectroscopy.

3:42PM C37.00005: Effect of pressure, stress and electronic modification on alpha-RuCl₃*  
SANANDA BISWAS (Presenter), STEPHEN WINTER, ROSER VALENTI, Physics, Goethe University Frankfurt — The honeycomb Mott insulator, α-RuCl₃, is being intensively studied as a candidate for realizing Kitaev physics. One of the areas of current research is to find routes to enhance Kitaev interactions in order to stabilize a possible spin liquid, by increasing exchange frustration by the application of external perturbations such as magnetic field, doping or pressure. We have explored these possibilities by applying stress and electronic modifications. In this talk, I will discuss effects of these perturbations on structural, electronic, vibrational and magnetic properties.

*SFB/TR 49
attention for a candidate of the Kitaev model, α-RuCl$_3$, showing spin liquid behaviour under magnetic field. Owing to the frustrated bond-dependent exchange interactions on a honeycomb spin lattice. The observation has recently attracted

4:30PM C37.00009: New Features in the Field-dependent Thermal Conductivity of α-RuCl$_3$ at Low Temperatures*

PETER CZAJKA (Presenter), TONG GAO, JINGJING LIN, Department of Physics, Princeton University, PAULA J KELLEY, ARNAB BANERJEE, CHRISTIAN BALZ, JIAQIANG YAN, DAVID GEORGE MANDRUS, STEPHEN NAGLER, Oak Ridge National Laboratory, NAI-PHUAN ONG, Department of Physics, Princeton University — α-RuCl$_3$ is currently the most promising and well-studied candidate for realizing the unique physics of the Kitaev model. Because the energy scale of the exchange interactions is understood to be quite high (J ~ 100K), measurements at low temperatures have been somewhat scarce and it’s behavior below 2K remains largely unexplored. This is especially true for thermal transport experiments, which have proven to be an incredibly powerful probe of excitations and phase transitions in insulating magnets. We present measurements of the thermal conductivity as a function of temperature and in-plane magnetic field that were performed between 0.4 and 1.7K. We identify several new features in $\kappa_{xx}(B)$ that occur between 7 and 11T, a regime located between the long range ordered and fully polarized states and where spin liquid behavior is thought to occur. Possible explanations for these new features as well as their relation to the recent observation of a half-integer quantized thermal hall conductance will be discussed.

*We acknowledge support from the Department of Energy (DE-SC0017863) and the Gordon and Betty Moore Foundation’s EPiQS Initiative (Grant No. GBMF4539).
4:42PM C37.00010: High Temperature Fermi Statistics from Majorana Fermions in an Insulating Magnet*  
YIPING WANG (Presenter), GAVIN B OSTERHOUDT, Boston College, YAO TIAN, Apple inc., PAULA J KELLEY, ARNAB BANERJEE, Oak Ridge National Lab, THOMAS A GOLDSTEIN, JUN YAN, umass Amherst, JOHANNES KNOLLE, Blackett Laboratory, Imperial College London, JOJI NASU, Tokyo Institute of Technology, YUKITOSHI MOTOME, University of Tokyo, STEPHEN NAGLER, DAVID GEORGE MANDRUS, Oak Ridge National Lab, KENNETH BURCH, Boston College — Majorana fermions, particles that are their own anti-particles, can emerge in insulating magnets as excitations with fractions of the constituent's quantum numbers. Interest in Majoranas is driven by their potential for quantum computation, and as evidence of novel topological states. Observations have been limited to liquid helium temperatures as edge modes in topological superconductors and quantum spin liquids (QSL) without combined evidence of particle-hole symmetry, Fermi statistics, and presence in the bulk. Here we report all three in α-RuCl3, at temperatures exceeding liquid nitrogen via new energy gain as well as loss Raman spectra and a unique framework to identify the statistical properties of the Kitaev QSL. α-RuCl3 is close to the Kitaev QSL, where bond-dependent Ising interactions produce excitations that are non-local in terms of spin flips. Consistent with particle-hole symmetric excitations obeying Paul-exclusion, the sum of the energy loss and gain responses are nearly temperature and energy independent. Our new method can be used to identify the unique properties of QSLs, and demonstrates the promise of α-RuCl3 for efforts in topological phases and quantum computation.

*NSF

4:54PM C37.00011: Origin of the saw-tooth torque in spin-orbital-coupled magnets: Application to α-RuCl3*  
ROSER VALENTI (Presenter), KIRA M. RIEDL, STEPHEN WINTER, Goethe University Frankfurt — Honeycomb Kitaev candidate materials based on 4d5 and 5d5 metals have been recently shown to commonly display a distinct saw-tooth angular dependence of the magnetic torque over a wide range of magnetic fields. By a combination of density functional theory calculations, exact diagonalization and semiclassical considerations, we show here that bilinear anisotropic interactions and/or g-anisotropy are each sufficient to explain the observed torque response, which may be distinguished on the basis of high-field measurements. We argue that these finding unify the understanding of magnetic torque experiments in a variety of Kitaev candidate materials.

*We acknowledge support by the DFG (Deutsche Forschungsgemeinschaft).

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C38 GMAG: Spin Chains and 1D Magnetism BCEC 206B - Roberta Sessoli, University of Florence - Tag(s):
Focus

2:30PM C38.00001: Thermal evolution of quasi-one-dimensional spin correlations within the anisotropic triangular lattice of α-NaMnO2  
REBECCA DALLY (Presenter), University of California, Santa Barbara, ROBIN CHISNELL, LELAND HARRIGER, NIST Center for Neutron Research, National Institute of Standards and Technology, YAOHUA LIU, Neutron Scattering Division, Oak Ridge National Laboratory, JEFFREY W LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology, STEPHEN WILSON, University of California, Santa Barbara — The temperature dependence of the magnetic order on the spatially anisotropic triangular lattice of α-NaMnO2 will be presented. Single crystals were studied via time-of-flight and triple-axis neutron diffraction measurements, which revealed the transition into a commensurate, collinear antiferromagnetic ground state with \( k = (0.5, 0.5, 0) \) occurs below \( T_N = 22 \) K. Above this temperature, the transition is preceded by the formation of a coexisting, short-range ordered, incommensurate state below \( T_{IC} = 45 \) K whose two dimensional propagation vector evolves toward \( k = (0.5, 0.5) \) as the temperature approaches \( T_N \). At high temperatures \( (T > T_{IC}) \), quasielastic scattering reveals one-dimensional spin correlations along the nearest neighbor Mn-Mn "chain direction" of the MnO6 planes. Our data are consistent with the predictions of a mean field model of Ising-like spins on an anisotropic triangular lattice, as well as the predominantly one-dimensional Heisenberg spin Hamiltonian reported for this material.
2:42PM C38.00002: Thermal control of spin excitations in the coupled Ising-chain material RbCoCl$_3$*  
CHRISTIAN RUEGG (Presenter), MATTIA MENA, Neutrons and Muons Research Division, Paul Scherrer Institute, NORA HAENNI, Department of Chemistry and Biochemistry, University of Bern, SIMON WARD, Neutrons and Muons Research Division, Paul Scherrer Institute, EVA HIR TENLECHNER, Institut Laue Langevin, ROBERT BEWLEY, ISIS Facility, Rutherford Appleton Laboratory, CLAUDIUS HUBIG, ULRICH JOSEPH SCHOLLWOECK, Arnold Sommerfeld Center, Ludwig Maximilians University, BRUCE NORMAND, Neutrons and Muons Research Division, Paul Scherrer Institute, KARL KRAEMER, Department of Chemistry and Biochemistry, University of Bern, DESMOND F MCMORROW, London Centre for Nanotechnology, University College London — We have used neutron spectroscopy to investigate the spin dynamics of the quantum ($S = 1/2$) antiferromagnetic Ising chains in RbCoCl$_3$. The structure and magnetic interactions in this material conspire to produce two magnetic phase transitions at low temperatures, presenting an ideal opportunity for thermal control of the chain environment. The high-resolution spectra we measure of two-domain-wall excitations therefore characterize precisely both the continuum response of isolated chains and the `Zeeman-ladder' bound states of chains in three different effective staggered fields in one and the same material. We apply an extended Matsubara formalism to obtain a quantitative description of the entire dataset, Monte Carlo simulations to model the magnetic order, and finite-temperature DMRG calculations to interpret the spectral features of all three phases, providing a complete understanding of the multi-faceted Ising physics of RbCoCl$_3$.

*This research was supported by the UK Engineering and Physical Sciences Research Council (EPSRC), by the European Research Council (ERC) under the EU Horizon 2020 research and innovation program, by the Bavarian Elite Network ExQM, and by the Swiss National Science Foundation (SNF).

2:54PM C38.00003: Spin dynamics in quasi-one-dimensional antiferromagnets*  
SYLVAIN CAPPONI (Presenter), Toulouse university, MAXIME DUPONT, UC Berkeley, EDMOND ORIGNAC, Ecole Normale Supérieure de Lyon, NICOLAS LAFLORENCIE, CNRS & Toulouse university — Theoretically challenging, the understanding of the dynamical response in quantum antiferromagnets is of great interest, in particular for both inelastic neutron scattering (INS) and nuclear magnetic resonance (NMR) experiments. In such a context, we theoretically address this question for quasi-one-dimensional quantum magnets, e.g., weakly coupled spin chains for which many compounds are available in nature. In this class of systems, the dimensional crossover between a three-dimensional ordered regime at low temperature towards one-dimensional physics at higher temperature is a nontrivial issue, notably difficult concerning dynamical properties. We present a comprehensive theoretical study based on both analytical calculations and numerical simulations which allows us to describe the full temperature crossover for the NMR relaxation rate $1/T_1$ or the dynamical structure factor probed by INS, from one-dimensional Tomonaga-Luttinger liquid physics to the three-dimensional ordered regime, as a function of interchain couplings [1].


*We thank the French ANR program BOLODISS (Grant No. ANR-14-CE32-0018) and Région Midi-Pyrénées for funding.
3:06PM C38.00004: Spin-1/2 antiferromagnetic chiral chains: the sine-Gordon model and beyond.* [Invited] PAUL GODDARD (Presenter), Department of Physics, University of Warwick, JUNJIE LIU, Department of Physics, University of Oxford, SHUNICHIRO KITAKA, Institute for Solid State Physics, University of Tokyo, ROGER JOHNSON, Department of Physics, University of Oxford, TOM LANCASTER, Centre for Materials Physics, Durham University, JOHN SINGLETON, National High Magnetic Field Laboratory, Los Alamos National Laboratory, TOSHIRO SAKAKIBARA, YOSHIMITSU KOHAMA, Institute for Solid State Physics, University of Tokyo, ROGER JOHNSON, Department of Physics, University of Oxford, ZACHARY MANSON, JAMIE MANSON, Department of Chemistry and Biochemistry, Eastern Washington University — The dramatic effect of an alternating local spin environment on the properties of the spin-1/2 antiferromagnetic chain was first discovered through high-field neutron scattering and heat capacity experiments on copper-benzoate, which revealed the development of an energy gap on application of magnetic field. This was perplexing until it was found that the behaviour of this system, and a handful of others, could be described by the sine-Gordon model of quantum-field theory. Under the influence of the applied field, the gap emerges thanks to the presence of internal staggered fields and DM interactions that are a direct result of the staggered Cu(II) octahedra.

Here, we report on the molecule-based chiral spin chain \([\text{Cu(pym)}(\text{H}_2\text{O})_4]\text{SiF}_6\cdot\text{H}_2\text{O}\) (pym = pyrimidine), which at first glance could be a sine-Gordon chain, but with an added twist: a 41 screw. Electron-spin resonance, magnetometry and heat capacity measurements reveal the presence of staggered g tensors, a rich low-temperature excitation spectrum, a staggered susceptibility and a spin gap that opens on the application of a magnetic field. These phenomena are reminiscent of those previously observed in non-chiral sine-Gordon materials. In the present case, however, the size of the gap and its measured linear field dependence do not fit with the sine-Gordon model as it stands. We propose that the differences arise due to additional terms in the Hamiltonian resulting from the chiral structure.

*This project has received funding from the European Research Council (grant no. 681260). We also thank the NHMFL, EPSRC, STFC, Royal Society, NSF (grant no. DMR-1703003, DMR-1157490), DoE and the State of Florida.

3:42PM C38.00005: Formation of a Longitudinal Mode in One Dimensional Yb$_2$Pt$_2$Pb* WILLIAM GANNON, Stewart Blusson Quantum Matter Institute, University of British Columbia, IGOR ZALIZNYAK, Brookhaven National Laboratory, LIUSUO WU, Southern University of Science and Technology, ALEXEI TSVELIK, Brookhaven National Laboratory, FRANZ DEMMEL, ISIS Neutron Source, Rutherford Appleton Laboratory, GEORG EHLERS, ANDREI PODLESNYAK, Oak Ridge National Laboratory, MEIGAN ARONSON (Presenter), Stewart Blusson Quantum Matter Institute, University of British Columbia — The low energy magnetic excitations measured with neutron scattering (NS) in Yb$_2$Pt$_2$Pb are spinons on one dimensional chains, in good agreement with the expectations of the XXZ Hamiltonian for nearly isotropic $S=\pm 1/2$ magnetic moments despite the large, rare earth Yb$^{3+}$ moments that make up the system [1]. In applied magnetic field, we observe spinon confinement into bound states coinciding with a longitudinally polarized interchain mode [2]. New NS measurements probe the dispersion of this mode as a function of field in the vicinity of the confinement transition. We find weak modifications to the quantum continuum for fields approaching the critical field of 0.7 T, with the mode growing in intensity as field is increased through the transition. Interestingly, the antiferromagnetic order is strongly pinned with periodicity that does not evolve smoothly as a function of field as seen previously in a different orientation [2]. Rather, there is an abrupt transition to a weak, completely incommensurate order at 1.3 T with the mode correspondingly returning spectral weight to the continuum, reflecting strong low dimensional fluctuations even at fields near saturation.


*Funding provided by NSF-DMR-1807451

3:54PM C38.00006: Thermal fluctuation in low dimensional systems - an experimental, computational and analytical study* NOAM KESTIN (Presenter), THIERRY GIAMARCHI, University of Geneva — We apply a near optimal density matrix renormalization group scheme (T-DMRG) to weakly coupled spin-half ladders. By doing so, one can reach sufficiently good resolution in the calculation of spin-spin correlations at finite temperature. We compare the results with analytic predictions such as the one of the Tomonaga Luttinger liquid, and experiments on compounds such as (\text{C}_{3}\text{H}_{12})_2 \text{Cu Br}_2 \text{Cl}_2.

*This work is supported by the Swiss National Science Foundation under Division II.
4:06PM C38.00007: Coercivity Dependence on Chain Length in a Low-Dimensional Magnetic System  THOMAS GREDIG (Presenter), KEVIN CANO, California State University, Long Beach — Single chain magnets deposited in the form of thin films can have tunable average chain lengths. A small molecule, iron phthalocyanine, is sublimed on a non-interacting substrate in the form of a thin film with a thickness of about 100 nm. The molecule's central ions form magnetic chains that are oriented parallel to the substrate surface. Furthermore, the average chain length is varied using the substrate deposition temperature in order to achieve a set of different magnetic responses as measured in magnetic hysteresis loops. The coercivity increases strongly with samples that have longer chain lengths. For comparison, a model with reduced dimensions based on single domain spherical magnetic particles in the superparamagnetic regime is developed and applied to this data set. The lower-dimensionality markedly extends the range of grain sizes over which the coercivity increases.

4:18PM C38.00008: Normal Modes of a Spin Cycloid or Helix* RANDY FISHMAN (Presenter), Oak Ridge National Laboratory, TOOMAS ROOM, National Institute of Chemical Physics and Biophysics, Estonia, ROGÉRIO DE SOUSA, Department of Physics and Astronomy, University of Victoria, Canada — Although spin cycloids and helices are quite common, remarkably little is known about the normal modes of a spin cycloid or helix with finite length on a discrete lattice. Based on simple one-dimensional lattice models, we numerically evaluate the normal modes of a spin cycloid or helix produced by either Dzyaloshinskii-Moriya (DM) or competing exchange (CE) interactions. The normal modes depend on the type of interaction and on whether the nearest-neighbor exchange is antiferromagnetic (AF) or ferromagnetic (FM). In the AF/DM and FM/CE cases, there is only a single Goldstone mode; in the AF/CE and FM/CE cases, there are three. For FM exchange, the spin oscillations produced by non-Goldstone modes contain a mixture of tangential and transverse components. For the DM cases, we compare our numerical results with analytic results in the continuum limit.

*Research by RF sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division. TR would like to acknowledge support from the Estonian Ministry of Education and Research with institutional research funding IUT23-3, and the European Regional Development Fund Project No. TK134. RdS acknowledges support from NSERC (Canada) through its Discovery program (RGPIN-2015-03938).

4:30PM C38.00009: The dynamic structure factor in impurity-doped spin chains in a magnetic field  IMKE SCHNEIDER (Presenter), KEVIN JÄGERING, University of Kaiserslautern, ANNABELLE BOHRDT, Physics, TU Munich, SOFIA BRENNER, DANIEL WESSEL, SEBASTIAN EGGERT, University of Kaiserslautern — We consider the dynamic structure factor in impurity doped spin-1/2 chains for general anisotropy, magnetic field and momentum. The impurities lead to effectively isolated finite chain segments with a discrete spectrum and characteristic correlations, which have a distinct effect on the dynamic structure factor. We present very accurate results for the low energy spectral weight obtained by numerical Density Matrix Renormalization Group techniques and identify the character of dominant excitations. We find that due to the impurities spectral weight is shifted away from the two-particle continuum into regions where no signal would be expected for undoped chains. Further, we compare with bosonization and find surprisingly good agreement with the numerical results. This has direct relevance for recent experiments on spin chains and ultracold gases and shows that, contrary to expectations, bosonization works especially well for short chains and in the vicinity of divergences.

4:42PM C38.00010: First-principles investigation of the complex lattice, charge, orbital, and spin structures in the spinel CuIr2S4* XILIANG JIN, Jilin University, China, WEIGUO YIN (Presenter), Brookhaven National Laboratory — The CuIr2S4 thiospinel undergoes a metal-insulator transition at 230K on cooling accompanied by very large variations in the Ir-Ir bond lengths and the loss of localized magnetic moments. This phenomenon has been interpreted in terms of a unique octamer model and orbitally driven one-dimensional Peierls transition. Here we report systematic first-principles studies of the crystal structures, electronic band structures, and phonon spectra of CuIr2S4, as well as the effects of electron-phonon, electron-electron, and spin-orbit interactions. Wannier function analysis is used to derive the effective low-energy Hamiltonian. Our results suggest a new way to understand this material.

*U.S. DOE-BES, Division of Materials Science and Engineering, under Contract No. DE-SC0012704.

4:54PM C38.00011: New spin-filtering mechanism through atomic chains without magnetic field: first-principles study  TOMONORI TANAKA (Presenter), YOSHIHIRO GOHDA, Tokyo Institute of Technology - Suzukakedai Campus — We investigated a new one-dimensional (1D) Rashba system, Bi-adsorbed in atomic chains, using first-principles calculations. One of the most stable structures in the system shows unconventional spin textures, which is the reversal of the spin polarization direction in Rashba bands. This result suggests a new spin-filtering mechanism through atomic chains. Similar mechanisms to ours, 1D spin filter, have been proposed already. However, our mechanism has a great advantage; previous spin-filtering mechanisms require the external magnetic field, whereas ours does not need the magnetic field. This feature is suitable for spintronic applications.
5:06PM C38.00012: Very slow spin dynamics in a ferromagnetic chain with three-body interactions  KEVIN BEACH
(Presenter), KHAGENDRA ADHIKARI, University of Mississippi — Projector Monte Carlo methods can be adapted to quantum spin models in which the Hamiltonian is a sum of local three-body operators. I discuss the case of spin-half chains whose interactions are pairwise ferromagnetic but contingent on the spin state at a third adjacent site. The resulting family of Hamiltonians, which includes the Fredkin spin chain and its t-deformed cousins, is frustration-free but highly nontrivial. The phase diagram includes states with large entanglement and unusually slow dynamics. Since the Monte Carlo can be carried out independently within each spin sector, I am able to present numerical data for the ground state and various low-lying excitations.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C39 GMAG DCMP DMP: Spin-orbit Coupling in Semiconductors  BCEC 207 - Vlad Pribiag

University of Minnesota - Tag(s): Focus

2:30PM C39.00001: Asymmetric g Tensor in Low-Symmetry Two-Dimensional Hole Systems* [Invited]  ROLAND WINKLER (Presenter), Northern Illinois University, C. GRADL, C. SCHUELLER, T. KORN, University of Regensburg — Zeeman coupling characterized by the g factor is a key ingredient to developing novel spin-based technologies such as quantum information protocols. In low-symmetry systems, the g factor becomes a second-rank tensor (a 3×3 matrix) that couples the spin to the magnetic field B. It has long been believed that this tensor g only affects the energy splitting in a magnetic field. We demonstrate [1] that it also encodes the direction of the axis about which the spins precess in the external field B. In general, this axis is not aligned with B. Using time-resolved Kerr rotation measurements performed on a sequence of low-symmetry two-dimensional hole systems in GaAs/AlAs quantum wells, we show that this feature of the tensor g manifest itself in unusual precessional motion as well as distinct dependencies of hole spin dynamics on the direction of the magnetic field B. A detailed theoretical analysis of these experiments allows us, for the first time, to determine the individual components of the full tensor g for [113]-, [111]- and [110]-grown samples. We also derive transparent analytical expressions for the components of the tensor g, complemented with accurate numerical calculations yielding very good agreement between experiment and theory.

Second-rank tensors characterizing materials properties such as electrical conductivity and dielectric constant are usually symmetric. In contrast, our study demonstrates that the tensor g is generally neither symmetric nor antisymmetric. Opposite off-diagonal components can differ in size by up to an order of magnitude. Consequently, the coupling of spins to the magnetic field varies drastically upon interchanging the direction of magnetic field and spin. This work extends the general concept of optical orientation to the regime of nontrivial Zeeman coupling.


*This work was supported by the NSF under Grant No. DMR-1310199.

3:06PM C39.00002: Enhancement of the Spin-Orbit Coupling in Silicon by Bismuth Doping  FABIEN RORTAIS (Presenter), SOOBEOM LEE, RYO OHSHIMA, SERGEY DUSHENKO, YUICHIRO ANDO, MASASHI SHIRAISHI, Kyoto University — Si possesses a low spin-orbit coupling, it allows a long spin lifetime but limits new device-designing possibilities in spintronics, particularly with the spin-charge conversion effects to create an all-Si spin devices. The purpose of this study is to create a sizable spin-orbit interaction in Si by implantation of a heavy element, bismuth (Bi).

To compare the spin-orbit coupling strength in the Si channel with and without Bi doping (SOI:P:B and SOI:P, respectively), we measured quantum corrections to the conductance in function of temperature. The elastic diffusion length (L_d), the spin-orbit coupling length (L_{so}) and the phase coherence length (L_{\phi}) can be extracted from the magnetoconductance data by using the Hikami-Larkin-Nagaoka model. L_d has the same order of magnitude (10 nm-25 nm) for both samples, however L_{so} decreased after the Bi doping (with the strongest decrease from 177 nm to 35 nm at 2 K). In the case of SOI:P:Bi, the Bi doping induced a spin-orbit coupling length of the same order of magnitude with the phase coherence length (L_{so} = 54 nm and L_{\phi} = 35 nm at 2K).

The increased spin-orbit coupling strength led to observe the crossover between the WL and the WAL. These results demonstrate a control over the strength of the spin-orbit coupling in Si channel using Bi doping.
3:18PM C39.00003: Strain engineering of Rashba-Dresselhaus spin-orbit coupling and intrinsic spin-Hall effect in Si
PAUL C LOU, ANAND KATAILLHA, RAVINDRA G BHARDWAJ, SANDEEP KUMAR (Presenter), University of California, Riverside —
The weak intrinsic spin-orbit coupling and centrosymmetric crystal structure are critical bottlenecks in the development of Si spintronics because it leads to insignificant spin-Hall effect (spin current generation) and inverse spin-Hall effect (spin current detection) even though it results into long spin diffusion length at room temperature. In this experimental study, we use strain gradient to break the structural inversion symmetry, which causes flexoelectric effect and charge separation. This leads to the Rashba-Dresselhaus spin-orbit coupling in the bulk of Si along with Si interface. The cubic Rashba-Dresselhaus spin-orbit coupling lifts the spin degeneracy of band structure introducing intrinsic spin-Hall effect, which is uncovered using spin-Hall magnetoresistance measurement in Ni$_{80}$Fe$_{20}$/MgO/p-Si freestanding thin film. The strain gradient effects are uncovered using piezoresistive behavior due to thermal expansion induced compressive stresses. The intrinsic spin-Hall effect is observed in both n-doped and p-doped Si thin films. This experimental study brings the Si spintronics closer to reality. This work demonstrates that strain gradient can be used for spin current generation, detection and control in Si.

3:30PM C39.00004: ABSTRACT WITHDRAWN

3:42PM C39.00005: Unidirectional magnetoresistance in a bulk Rashba ferromagnet
RYUTARO YOSHIMI (Presenter), CEMS, RIKEN, KENJI YASUDA, MIT, ATSUSHI TSUKAZAKI, IMR, Tohoku Univ., MINORU KAWAMURA, KEI TAKAHASHI, CEMS, RIKEN, MASASHI KAWASAKI, University of Tokyo, YOSHINORI TOKURA, CEMS, RIKEN — The Rashba effect is the spin band splitting due to broken inversion symmetry through spin-orbit coupling, typically observed at surfaces and interfaces. Recently, some noncentrosymmetric crystals have been found to have the bulk Rashba bands that are larger than surface/interface ones. Nonreciprocal transport of quantum particles such as electron, spin and phonon is known to occur by further breaking time reversal symmetry in such a material without inversion symmetry. In particular, the interplay with magnetism in spin-polarized bands may enhance the nonreciprocal charge transport. In this study, we investigated the unidirectional magnetoresistance in thin films of Ge$_{1-x}$Mn$_x$Te, which is a bulk ferromagnetic Rashba semiconductor. The magnitude of nonreciprocal transport shows a strong dependence on carrier density, which suggests that the scattering process on Fermi surface is essential for the nonreciprocal transport in the system.

3:54PM C39.00006: The temperature and doping dependence of inverse spin Hall effect in n-GaAs
ZHEN JIANG (Presenter), School of Physics and Astronomy, University of Minnesota, SAHIL PATEL, Departments of Electrical and Computer Engineering and Materials, University of California, Santa Barbara, PAUL CROWELL, School of Physics and Astronomy, University of Minnesota, CHRIS PALMSTROM, Departments of Electrical and Computer Engineering and Materials, University of California, Santa Barbara — We have carried out measurements of the inverse spin Hall effect (ISHE) in a series of n-GaAs epilayers doped near the metal-insulator transition. Spin currents are generated using epitaxial Fe/GaAs (001) Schottky tunnel barriers. The ISHE is detected in a simple Hall cross geometry, and precession in a static magnetic field (the Hanle effect) is used to separate the effect from background contributions. We find that the ISHE voltage at low temperatures is much larger than expected based on previous measurements of the direct spin Hall effect. The enhancement is accompanied by significant distortion of the Hanle curves, suggesting that hyperfine interactions play a significant role. Comparison with non-local spin valve measurements over the entire doping range (3 x 10$^7$ cm$^{-3}$ to 7 x 10$^7$ cm$^{-3}$) and at temperatures up to 110 K indicates that local inhomogeneities in the hyperfine field, which disappear as the temperature increases, may be responsible for the enhancement.

*This work was supported by NSF DMR-1708287 and the National Science Foundation NNCI program.
In this study, we employed ultrafast Time Resolved Differential Reflectivity (TRDR) and ultrafast time resolved Magneto-optic Kerr Effect (MOKE) on InAs$_x$P$_{1-x}$ ternary alloy. In recent years, InAs$_x$P$_{1-x}$ ternary alloys have attracted extensive attention due to the immense prospect for various optoelectronic applications including optical telecommunication, broadband photodetectors, mid-IR lasers, and also quantum communication devices.\textsuperscript{1,2} As the switching rates in devices are pushed to higher frequencies in optoelectronic and spintronic devices, it is required to perform comprehensive studies of the carrier and spin relaxation dynamics in semiconductors on a femto-second timescale. Here we report carrier and spin dynamics of n-type InAs$_x$P$_{1-x}$ films in a broad optical region (700 nm and 1000 nm). Also, we observed the generation of coherent oscillations which could be related to photo-induced coherent acoustic phonons. The InAs$_x$P$_{1-x}$ films are ~1.2 micron thick grown on semi-insulating InP (001) wafers and the carrier concentrations are estimated to be 1x10$^{17}$ cm$^{-3}$.

\textsuperscript{1} Journal of Applied Physics \textbf{115}, 193503 (2014).
\textsuperscript{2} Applied Physics Letters \textbf{102} (22), 222102 (2013).

*Supported by the Air Force Office of Scientific Research award FA9550-17-1-0341 and DURIP funding (FA9550-16-1-0358).
Ubiquitous Spin-Orbit Coupling in a Screw Dislocation with High Spin Coherency

LIN HU (Presenter), HUAQING HUANG, University of Utah, ZHENGFEI WANG, University of Science and Technology of China, WEI JIANG, XIAOJUAN NI, YINONG ZHOU, University of Utah, V ZIELASEK, University of Bremen, MAX G LAGALLY, University of Wisconsin, BING HUANG, FENG LIU, University of Utah — We theoretically demonstrate that screw dislocation (SD), a 1D topological defect widely present in semiconductors, exhibits ubiquitously a new form of spin-orbit coupling (SOC) effect. Differing from the widely known conventional 2D Rashba-Dresselhaus (RD) SOC effect that typically exists at surfaces or interfaces, the deep-level nature of SD-SOC states in semiconductors readily makes it an ideal SOC. Remarkably, the spin texture of 1D SD-SOC, pertaining to the inherent symmetry of SD, exhibits a significantly higher degree of spin coherency than the 2D RD-SOC. Moreover, the 1D SD-SOC can be tuned by ionicity in compound semiconductors to ideally suppress spin relaxation, as demonstrated by comparative first-principles calculations of SDs in Si/Ge, GaAs, and SiC. Our findings therefore open a new door to manipulating spin transport in semiconductors by taking advantage of an otherwise detrimental topological defect.

*Science Challenge Project (No. TZ2016003), China Postdoctoral Science Foundation (No. 2017M610754), NSFC (Grants No. 11574024 and No. 11704021), and NSAF (No. U1530401). U.S. DOE (No. DE-FG02-04ER46148).

Ubiquitous Spin-orbit Coupling in a Screw Dislocation of Semiconductors

BING HUANG (Presenter), LIN HU, Beijing Computational Science Research Center, FENG LIU, University of Utah — We demonstrate that screw dislocation (SD), a 1D topological defect widely present in semiconductors, exhibits ubiquitously a new form of spin-orbit coupling (SOC) effect. Differing from the widely known conventional 2D Rashba-Dresselhaus (RD) SOC effect that typically exists at surfaces/interfaces, the deep-level nature of SD-SOC states in semiconductors readily makes it an ideal SOC. Remarkably, the spin texture of 1D SD-SOC, pertaining to the inherent symmetry of SD, exhibits a significantly higher degree of spin coherency than the 2D RD-SOC. Moreover, the 1D SD-SOC can be tuned by ionicity in compound semiconductors to ideally suppress spin relaxation, as demonstrated by comparative first-principles calculations of SDs in Si/Ge, GaAs, and SiC.

Extreme asymmetry of 90-degree domain walls in multilayered films of (Ga,Mn)(As,P)

VITALII VLASKO-VLASOV, WAI-KWONG KWOK, Materials Sciences Division, Argonne National Laboratory, SINING DONG, XINYU LIU (Presenter), MALGORZATA DOBROWOLSKA, J K FURDYNA, Department of Physics, University of Notre Dame — We image the magnetic domain structure during remagnetization of MBE grown multilayered films of a diluted magnetic semiconductor (Ga,Mn)(As,P) with digital modulations of the phosphorus concentration. The samples show two in-plane easy magnetization axes corresponding to the <100> cubic and [110] uniaxial anisotropies, typical for the GaMnAs system. Their remagnetization occurs in two steps through the nucleation and growth of 90-degree domains. Unexpectedly, the domain boundaries align precisely with the easy axes in contrast to our micromagnetic calculations using the measured magnetic parameters of the samples. We discuss how such totally asymmetric Neel domain walls can appear due to Dzyaloshinskii-Moriya interactions enhanced by the multiple sharp interfaces in the multilayered films.

*Magnetic characterization of the films at Argonne was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division. Synthesis of the films at Notre Dame University was supported by the NSF Grant DMR14-00432.
Large perpendicular magnetic anisotropy and anisotropic electronic structure of the new ferromagnetic semiconductor (Ba,K)(Zn,Mn)2As2 single crystal studied by angle-dependent x-ray magnetic circular dichroism

SHOYA SAKAMOTO (Presenter), SLAC National Accelerator Laboratory, GUOQIANG ZHAO, Chinese Academy of Sciences, YOSUKE NONAKA, KEISUKE IKEDA, ZHENDONG CHI, YUXUAN WAN, MASAHIRO SUZUKI, The University of Tokyo, TSUNEHARU KOIDE, KEK, SADAMICHI MAEKAWA, JAEA, CHANGQING JIN, Chinese Academy of Sciences, ATSUSHI FUJIMORI, The University of Tokyo — (Ba,K)(Zn,Mn)2As2 is a new ferromagnetic semiconductor isostructural to 122-type Fe-based superconductors. The Curie temperature (Tc) reaches 230 K for polycrystalline samples exceeding the highest Tc = 200 K of (Ga,Mn)As. In relation to the anisotropic crystal structure, this material has large perpendicular magnetic anisotropy.

In the present study, we have investigated the origin of the perpendicular magnetic anisotropy by angle-dependent x-ray magnetic circular dichroism (AD-XMCD) measurements. The XMCD spectra were similar to those of (Ga,Mn)As and showed multiplet features. This indicates the localized nature of the Mn 3d electrons being consistent with the carrier-induced-ferromagnetism scenario. The angle-dependent measurements yielded the anisotropy field of 0.8 T. The XMCD spectra taken under the transverse geometry (TXMCD), where the spin aligns perpendicular to the x ray, showed finite dichroic signals. This originates from the aspherical distribution of 3d electrons, and indeed the TXMCD spectra were reproduced by the configuration interaction cluster-model calculation incorporating D4h crystal-field splitting. We suggest that degenerate p-dxz,yz hybridized orbitals at the Fermi level are responsible for the magnetic anisotropy of this compound.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C40 GMAG DMP: Magnetic Structure in Bulk Oxides

2:30PM C40.00001: Spin density wave order and its influence on the unconventional metallic states in carrier-doped Srnx+1IrnxO3n+1 systems*

STEPHEN WILSON (Presenter), University of California, Santa Barbara — The discovery of spin-orbit assisted or J_eff=1/2 Mott insulating states in select 4d and 5d transition metal oxides has fueled a number of predictions of novel electronic phases that emerge once the parent Mott phase is quenched. Depending on the structure type, examples of these phases span from unconventional superconductivity to new manifestations of correlated topological electronic states. The seminal examples of J_eff=1/2 Mott states found in the homologous Ruddlesden-Popper series Srnx+1IrnxO3n+1 are a versatile platform for understanding the mechanism for the collapse of the Mott state as the J_eff=1/2 band is driven away from half filling and for resolving the presence of nearby electronic instabilities. In this talk, I will present some of our recent work exploring the competing states accessed via chemically doping these compounds. Upon electron-doping into Sr2IrO4 and hole-doping into Sr3Ir2O7, spin density wave states emerge and provide clues to the nature of the unconventional metals that form in each. A “diagonal” spin density wave state analogous to those formed in the underdoped high-Tc cuprates appears in electron-doped Sr2IrO4 and suggests a link between the competing ground states of La2-xSrxCuxO4 and Sr2-xLa2xIrO4. In hole-doped Sr3Ir2O7, the slow collapse of the Mott state reveals an intermediate strange metal regime where spin density wave order survives beyond the collapse of the Mott charge gap. I will discuss these two examples and the implications of each in understanding the phase diagrams of more strongly correlated Mott states.

*SDW acknowledges funding from NSF Award DMR-1505549

3:06PM C40.00002: Evolution of Magneto-Orbital order Upon B-Site Electron Doping in Na1-xCa4Mn7O12 Quadruple Perovskite Manganites*

ROGER JOHNSON (Presenter), University of Oxford, FRANCESCO MEZZADRI, Istituto dei Materiali per Elettronica e Magnetismo, PASCAL MANUEL, DMITRY KHAYAVIN, ISIS Facility, STFC, EDMONDO GILJOLI, Istituto dei Materiali per Elettronica e Magnetismo, PAOLO G. RADAELLI, University of Oxford — We present the discovery and refinement by neutron powder diffraction of a new magnetic phase in the Na1-xCa4Mn7O12 quadruple perovskite phase diagram, which is the incommensurate analogue of the well known pseudo-CE phase of the simple perovskite manganites. We demonstrate that incommensurate magnetic order arises in quadruple perovskites due to the exchange interactions between A and B sites. Furthermore, by constructing a simple mean field Heisenberg exchange model that generically describes both simple and quadruple perovskite systems, we show that this new magnetic phase unifies a picture of the interplay between charge, magnetic, and orbital ordering across a wide range of compounds.

*We acknowledge financial support from the Royal Society (UK) and from EPSRC (UK), Grant No. EP/M020517/1, entitled “Oxford Quantum Materials Platform Grant.”
3:18PM C40.00003: Magnetic Properties of the Q1D Solid Solution Ca_{1-x}Na_{x}Cr_{2}O_{4} Studied with Neutrons and Muons

ELISABETTA NOCERINO (Presenter), OLA KENJI FORSLUND, Applied Physics, KTH Royal Institute of Technology, YASMIN SASSA, Physics and Astronomy, Uppsala University, DANIEL ANDREICA, Physics, Babes-Bolyai University, HIROSHI NOZAKI, Toyota Central research and Development Lab, GEDIMINAS SIMUTIS, JEAN-CHRISTOPHE ORAIN, Paul Sherrer Institut, HIROYA SAKURAI, National Institute for Materials Science, RUSTEM KHASANOV, Paul Sherrer Institut, JUN SUGIYAMA, IZUMI UMEGAKI, Toyota Central research and Development Lab, MARTIN MÅNSSON, Applied Physics, KTH Royal Institute of Technology — In this work we present the results of the measurements carried out by neutron powder diffraction and muon spin rotation/relaxation (μ+SR) in ambient and high pressure on the $x = 1$ (NaCr$_2$O$_4$) and $x = 0$ (CaCr$_2$O$_4$) members of the solid solution Ca$_{1-x}$Na$_x$Cr$_2$O$_4$ and on the intermediate compound $x = 0.5$ (Ca$_{0.5}$Na$_{0.5}$Cr$_2$O$_4$). The $x = 1$ results show a unique spin structure where the Cr moments in each zig-zag chain are aligned ferromagnetically along the c-axis, whereas antiferromagnetically along the a-axis between the adjacent zig-zag chains. The $x = 0$ results show the formation of a complex magnetic order below $T_N$, that is consistent with an incommensurate AF (IC-AF) order. The investigation on the intermediate compound Ca$_{1-x}$Na$_x$Cr$_2$O$_4$ shows a fast-relaxing component, possibly indicating a spin-glass state. Moreover, the magnetic order was shown to be almost completely unsensitive to pressures (up to $p \approx 25$ kbar), hereby revealing that the effect from the tuning of the spin density of the chains is clearly dominant.

*This research is fully funded by the Swedish Foundation for Strategic Research (SSF) within the Swedish national graduate school in neutron scattering (SwedNess).

3:30PM C40.00004: Experimental observation on Jeff=1/2 state in CuAl2O4

HWANBEOM CHO (Presenter), CHOONG HYUN KIM, Department of Physics and Astronomy, Seoul National University, ARA GO, Center for Theoretical Physics of Complex Systems, Institute for Basic Science (IBS), HOSUB JIN, Department of Physics, Ulsan National Institute of Science and Technology (UNIST), JE-GUEN PARK, Department of Physics and Astronomy, Seoul National University — The spin-orbit entangled pseudo-spin state, Jeff=1/2 has driven intriguing phenomena such as high-Tc superconductivity, quantum spin liquid, and topological semimetal. This studies have been conducted on 4d or 5d compounds but 3d systems haven’t been focused on. The Jeff=1/2 states in 3d systems including cuprates haven’t been considered to emerge in condensed matter physics. One reason is the spin-orbit coupling constant of 3d is smaller than that of Ru (4d) or Ir (5d) ions and the other is that many 3d systems have distorted-crystal structures which lead quenched orbital angular momentum. However, we suggest CuAl2O4 is a candidate material to induce Jeff=1/2 states. Cubic symmetry of the crystal structure verified by single crystal XRD supports Jeff=1/2 nature. Moreover, X-ray absorption spectroscopy also shows this nature following the electric dipole selection rule.

*Center for Correlated Electron Systems, Institute for Basic Science (IBS)

3:42PM C40.00005: Magnetism in spin-orbit coupled oxides

[Invited] ARUN PARAMEKANTI (Presenter), University of Toronto — Transition metal oxides with 4d and 5d ions provide a glimpse into unusual facets of spin-orbit coupled magnetism. In this talk, I will discuss how a theoretical study of resonant inelastic X-ray scattering enables us to extract single-site effective Hamiltonian parameters relevant to “bottom-up” modelling of such materials, including iridates, rhenates, and osmates. Such single-site Hamiltonians are useful to extract spin-exchange interactions, study its sensitivity to lattice distortions, and to understand bulk magnetism. We illustrate this via the exploration of frustrated Jeff=1/2 Mott insulators on the face-centered cubic lattice. These results are applicable to a wide class of materials called double-perovskites. Finally, we show how thin films of spin-orbit coupled metallic magnets may host tunable skyrmion crystals induced by strain and magnetic field, and potentially exhibit a phenomenon we term “topological quantum oscillations”.

*AP is funded by NSERC of Canada through a Discovery Grant, and was partly supported by the Canadian Institute for Advanced Research under the Quantum Materials programme.
4:18PM C40.00006: Magnetic properties of single crystalline Nd$_2$O$_3$^*  BINOD RAI (Presenter), Materials Science and Technology Division, Oak Ridge National Lab, GABRIELE SALA, Neutron Scattering Division, Oak Ridge National Lab, ANDREW D CHRISTIANSON, ANDREW MAY, Materials Science and Technology Division, Oak Ridge National Lab — Triangular-lattice magnets have recently attracted interest due to their exotic phases like frustrated magnetism, quantum spin liquids, and topological spin textures that originate from competing interactions. The nearest-neighbor and next-nearest-neighbor magnetic interactions are crucial to realizing these exotic phases. Nd$_2$O$_3$ is a triangular-lattice compound that crystallizes in the trigonal centrosymmetric space group $Pm1$. Very recently, long-range magnetic order below $T_N = 0.55$ K was revealed by studies on polycrystalline samples of Nd$_2$O$_3$ using neutron diffraction and thermodynamic measurements. The reported frustration ratio of $= 43$ suggests Nd$_2$O$_3$ is a frustrated system driven by competing interactions. We have synthesized single crystals of Nd$_2$O$_3$ to further characterize the intrinsic magnetic properties. This talk will emphasize the anisotropic magnetic properties of Nd$_2$O$_3$ single crystals and the temperature--magnetic field phase diagram.

^*This research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

4:30PM C40.00007: Muon spin rotation study of the rare-earth quantum dimer system Yb$_2$Si$_2$O$_7$  REDHA ROUANE (Presenter), ARASH AKBARI-SHARBAF, XAVIER BAZIER-MATTE, JEFFREY QUILLIAM, Département de Physique, Université de Sherbrooke, Sherbrooke, QC, Canada, GAVIN L HESTER, KATE A ROSS, Department of Physics, Colorado State University, Fort Collins, Colorado, USA — In quantum dimer systems, a zero-field singlet state can give way to Bose-Einstein condensation (BEC) of triplons under applied magnetic field [1]. We will present work on the material Yb$_2$Si$_2$O$_7$, an effective spin-1/2 antiferromagnet where Yb ions form an anisotropic honeycomb lattice with two different bonds length. It is expected that Yb spins form dimers on the shortest Yb-Yb bonds, and the resulting singlet-triplet gap has been observed with specific heat and inelastic neutron scattering. Between critical fields $H_{C1} = 0.4$ T and $H_{C2} = 1.4$ T, an antiferromagnetic phase reminiscent of a BEC of triplons is observed. We will present a low-temperature µSR investigation of this Yb-based quantum dimer system. Below the critical field $H_{C1}$, our measurements confirm the lack of magnetic order, yet also exhibit anomalous spin relaxation, which might be explained through hyperfine enhancement or a perturbation of the local environment by the implantation of a muon. At longitudinal magnetic fields near and above $H_{C1}$, a dramatic increase in muon spin relaxation, associated with antiferromagnetic order, is observed.


4:42PM C40.00008: Effects of Oxygen Deficiencies in CaMn$_2$O$_4$-δ  MELISSA GOOCH (Presenter), HUNG-CHENG WU, LIANGZI DENG, Physics, Texas Center for Superconductivity at the University of Houston, HUNG-DUEN YANG, Physics, National Sun Yat-sen University, PAUL C. W. CHU, Physics, Texas Center for Superconductivity at the University of Houston — Manganese oxides over the last few years have experienced a considerable increase in research interests due to their rich and complex phase diagrams, that are a result of the flexibility of the manganese ions oxidations states. The compounds in the Ca-Mn-O system provide an excellent platform, where theoretically predicted multiferroic behavior could exist. Many manganese oxides have already been thoroughly investigated; however, a potential candidate CaMn$_2$O$_4$ is still not well understood to date.

Polycrystalline CaMn$_2$O$_4$ samples were synthesized and annealed in oxygen and argon flows respectively to further explore the effect of oxygen deficiencies on the physical properties. From temperature dependent dc magnetization and heat capacity measurements, the previously reported antiferromagnetic ordering near 220 K was observed for both samples. However, a spontaneous polarization ($P_S$) was observed near 253 K for only the oxygen annealed sample without applied magnetic field, while no $P_S$ was observed for the argon annealed sample. In addition, the dielectric and loss measurements revealed anomalies above 260 K with the time and magnetic field dependent phenomena in both samples. Detailed measurements for both samples are ongoing to gain greater insight into this complex system.
Determined lattice distortion of Ba$_2$NaOsO$_6$  
RONG CONG (Presenter), RAVINDRA NANGUNERI, VESNA F MITROVIC, BRENDA RUBENSTEIN, Brown University — Exotic quantum phases have been proposed in magnetic Mott insulators with strong spin-orbit coupling. Our recent nuclear magnetic resonance (NMR) studies of the Mott insulator Ba$_2$NaOsO$_6$ established that local lattice distortions precede the onset of canted ferromagnetic order$^{1,2}$. It was suggested that lattice distortions are a manifestation of the orbital order that drives the magnetism in this class of materials$^3$. To decipher the microscopic nature of the putative orbital order, we investigate different lattice distortion models and calculate their associated NMR observables. Results of various distortion models will be discussed in this talk.


A strongly correlated polar metal LiOsO$_3^*$  
JIANSHI ZHOU (Presenter), JOHN GOODENOUGH, Mechanical Engineering, University of Texas at Austin, KAZUNARI YAMAURA, Superconducting Properties unit, National Institute for Materials Science, XIANG LI, Y. SHIRAKO, Mechanical Engineering, University of Texas at Austin — LiOsO$_3$ is metallic and undergoes a second-order transition to a polar phase at $T_c$=140 K. This unusual property provides a unique opportunity to study the interplay between itinerant electrons and electric dipoles. We report a suite of measurements of the properties of LiOsO$_3$ versus temperature, including resistivity and magnetoresistance on a single crystal sample down to 0.16 K; Seebeck coefficient, Hall coefficient, high-precision magnetization, and the specific heat were made on polycrystalline samples. The results indicate that electrons become strongly correlated in responding to ferroelectric ordering of dipoles.

We have monitored how the thermal conductivity is changed by dipole fluctuations at the transition and how it is influenced by ferroelectric domain boundaries at low temperatures to obtain information on interaction between the electrons and the dipoles. The observation of a transition from glassy to phonon-like thermal conductivity on cooling through $T_c$ provides a solid proof that the ferroelectric transition is an order-disorder, not a displacive transition.

$^*$This work was supported by the National Science Foundation NSF MRSEC DMR-1720595. KY was supported in part by JSPS KAKENHI Grant Numbers JP15K14133 and JP16H04501.

Ground state properties of Sr$_2$RuO$_4$: dynamical mean-field description based on spin-orbit entangled basis$^*$  
HYEONG JUN LEE (Presenter), Center for Theoretical Physics of Complex Systems, Institute for Basic Science, CHOONG HYUN KIM, Center for Correlated Electron Systems, Institute for Basic Science, ARA GO, Center for Theoretical Physics of Complex Systems, Institute for Basic Science — We investigate the ground state wavefunction and dynamical properties of Sr$_2$RuO$_4$ at zero temperature, using the density functional theory plus dynamical mean-field theory with the exact diagonalization solver. We especially focus on the interplay between the spin-orbit and Hund's coupling by considering the full rotationally invariant Kanamori interaction Hamiltonian.

Near the Fermi level, the quasi-particles and low-lying excitations are well described by spin-orbit coupled basis. They exhibit a distinguished self-energy behavior that reflects the signature of the magnetic response and the orbital dependent-correlations of the Hund's metal. We will discuss how these responses are related to the two-fold degeneracy of ground state.

$^*$This work was supported by Institute for Basic Science (IBS) in Korea (IBS-R024-D1 (HJL, AG) and Grant No. IBS-R009-D1 (CHK))

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C41 GMAG DMP: Spin Dynamics I  
BCEC 209 - Yu-Sheng Ou, University of Delaware - Tag(s): Focus
2:30PM C41.00001: Competing spin transfer and dissipation at Co/Cu(001) interfaces on femtosecond timescales

[Invited] ANDREA ESCHENLOHR (Presenter), Faculty of Physics, University Duisburg-Essen, Germany — Spin dynamics driven by optical excitation with femtosecond (fs) laser pulses offers fascinating possibilities in the ultrafast manipulation of spin-dependent microscopic processes in magnetically ordered materials and heterostructures. In particular, fs spin currents are very promising for future ultrafast spintronics applications. However, the role of the interface in fs spin dynamics is to date largely unexplored. By means of a combined experimental-theoretical approach, we identify the fundamental microscopic processes during optically induced, fs charge and spin transfer at a model epitaxial ferromagnet/paramagnet interface for technologically relevant ferromagnetic heterostructures. A comparison of fs time-resolved, interface-sensitive magneto-optical experiments with ab initio time-dependent density functional theory on the Co/Cu(001) interface demonstrates that the ultrafast spin dynamics originates from spin-dependent charge transfer, including resonantly excited minority spin back-transfer from Cu to Co. Already on timescales below 100 fs, this fs spin transfer competes with dissipation of spin angular momentum mediated by spin-orbit coupling [1].

Reference:

*Funding from the German Research Foundation within SPP 1840 QUTIF is gratefully acknowledged.

3:06PM C41.00002: Domain dynamics of a ferromagnetic CoFe/Ni multilayer in response to ultrafast optical pumping

DMITRIY ZUSIN (Presenter), University of Colorado, Boulder / JILA, EZIO IACOCCA, University of Colorado, Boulder, LOIC LE GUYADER, European X-Ray Free-Electron Laser Facility GmbH, ADAM BLONSKY, University of Colorado, Boulder / JILA, ALEX REID, WILLIAM F SCHLOTTER, SLAC National Accelerator Laboratory, Menlo Park, CA, United States, TIANMIN LIU, DANIEL J HIGLEY, Stanford University / LCLS, Menlo Park, CA, United States, PHOEBE TENGandin, CHRISTIAN GENTRY, University of Colorado, Boulder / JILA, SHEENA PATEL, ANATOLY SHABALIN, NELSON HUA, STJEPAN HRKAC, University of California San Diego, HANS T. NEMBACH, JUSTIN SHAW, Quantum Electromagnetics Division, NIST, Boulder, CO, United States, MARK A HOEFER, University of Colorado, Boulder, HENRY C KAPTEYN, MARGARET MARY MURNANE, University of Colorado, Boulder / JILA, ERIC FULLERTON, University of California San Diego, HERMANN DURR, Uppsala University, Sweden, THOMAS SILVA, Quantum Electromagnetics Division, NIST, Boulder, CO, United States — We studied a response of nanoscale magnetic domains in a 50 nm thick [Co90Fe10/Ni] multilayer to a femtosecond laser pulse by use of time-resolved soft X-ray resonant magnetic scattering (RMS) at the Linear Coherent Light Source. By collecting X-ray diffraction at high scattering angles, we observe the 1st, 3rd and 5th order RMS intensity peaks and thus capture the dynamics of fine magnetic features. We observe a rapid shift in the position of all diffraction orders towards smaller scattering angles and a simultaneous reduction of their magnitude. Surprisingly, higher orders start to decline relative to the 1st order only after a few picoseconds. With our data, we develop a method to extract real-space domain dynamics. We find that the dynamics across the domains are non-uniform, with smaller domains demagnetizing stronger than their larger neighbors. The domain walls remain relatively unchanged and start to broaden only after a few picoseconds. Using our models we attribute this behavior to a combined effect of non-uniform spin transport and a gradient in the absorption of the laser pump throughout the sample.

*The authors acknowledge support from the Department of Energy (DOE) Office of Basic Energy Sciences X-Ray Scattering Program Awards No. DE-SC0002002 and DE-SC0018237

3:18PM C41.00003: Simulations of all optical switching using TDDFT

PETER ELLIOTT (Presenter), J. KAY DEWHURST, Max Planck Institute for Microstructure Physics, SANGEETA SHARMA, Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, E.K.U. GROSS, Max Planck Institute for Microstructure Physics — Time dependent density functional theory (TDDFT) is an ab-initio method for studying the magnetization dynamics induced by strong laser pulses. We have previously applied TDDFT to study ultrafast demagnetization in simple ferromagnets[1,2] and optical inter sublattice spin transfer (OISTR)[3] where we found we could switch the magnetic ordering from AFM to a transient FM state[4]. In this work, we simulate RE-TM2 compounds in the C15 Laves geometry and ask whether OISTR plays a role in the all optical switching observed in such materials.

3:30PM C41.00004: High harmonic generation in ferromagnetic thin films as a tool to probe spin and charge dynamics* GUOPING ZHANG (Presenter), Indiana State University, MINGSU SI, Lanzhou University, MITSUKO MURAKAMI, YIHUA BAI, Indiana State University, THOMAS F GEORGE, University of Missouri-St. Louis — High-order harmonic generation (HHG) in solids has garnered worldwide attention [1-3]. The materials include metals, semiconductors, insulators, graphene, fullerenes, and topological insulators. However, this has never been explored for magnetic materials. This study represents the first investigation in the field. We show that HHG in Fe(110) and Fe(001) monolayers carries spin information. If a HHG signal is dispersed into the crystal momentum space, the harmonic peak can be assigned to a single transition, a key step to spin-resolved band structure detection. Different from the optical counterpart, the spin HHG only has even orders. Our findings thus predicts a new frontier of magneto-high-order harmonic generation [4].


*The U.S. Department of Energy under Contract No. DE-FG02-06ER46304.

3:42PM C41.00005: Absence of Correlation between Damping and Crystal Quality in Epitaxial Fe BEHROUZ KHODADADI (Presenter), MIN GAO, JIE-FANG LI, DWIGHT D VIEHLAND, SATORU EMORI, Virginia Tech — Most studies on ferromagnetic relaxation in metallic thin films are performed on polycrystalline structures, which makes it difficult to compare the experimental findings with theoretical calculations. Also it is unclear how microstructure – in addition to electronic properties – would affect damping in such polycrystalline metallic thin films. Our experimental study investigates the interplay between structure and damping in epitaxial thin films of pure Fe, grown on single-crystal MgO and MgAl₂O₄ substrates by magnetron sputtering. Our structural characterization by X-ray diffraction indicates significantly higher crystalline quality for Fe/MgAl₂O₄ as evidenced by pronounced Laue oscillations and an order of magnitude narrower rocking curve, compared to Fe/MgO. However, we find no difference in the value of Gilbert damping parameter α from broadband ferromagnetic resonance measurements up to 50 GHz, i.e., both Fe/MgAl₂O₄ and Fe/MgO consistently exhibit α ≈ 0.003. Our experimental observations are contrary to the expectations that structural disorder should impact ferromagnetic relaxation, and may provide insight into the fundamental mechanism of damping in metallic ferromagnets.

3:54PM C41.00006: Spin wave generator via oscillating vortex-antivortex core pairs at zero external field* LIANG-JUAN CHANG (Presenter), SHANG-FAN LEE, Institute of Physics, Academia Sinica — We demonstrate that the radiation of spin waves can be generated from an oscillating vortex-antivortex core pair. The emission of spin waves was produced by the oscillation of nanoscale magnetic vortex-antivortex core pair in a NiFe disk-film composite structure. The sample consists of a 20-nm-thick, 4 micron long and 1 micron wide NiFe magnonic waveguide, located at the gap of a single-end GS coplanar waveguide circuit, and magnetic disk with thickness 50 nm and diameter 500 nm on top. The vortex cores in the disk was excited by an out of plane radio frequency magnetic field. The dynamic behaviors of the magnetization were studied using a micro-focused Brillouin light scattering spectroscopy (BLS) setup. In addition to the discrete ferromagnetic resonance (FMR) signals above external dc saturation magnetic field, we observed clear signals at zero magnetic field where vortex cores are present. We have found an ultra-flexible mechanism for consistent excitation of propagating spin waves. The frequencies of the spin waves excited are coherently tunable by the driving frequencies from 5 GHz up to 15 GHz. The short wavelength down to 80 nm for 15 GHz was observed.

*The financial support from the Academia Sinica and the Ministry of Science and Technology, Taiwan is acknowledged.
4:06PM C41.00007: Ramsauer-Townsend Resonance for Spin Waves  PABLO BORYS (Presenter), NASER QURESHI, OLEG KOLONOTSEV, ICAT, Universidad Nacional Autonoma de Mexico — Spin waves are fluctuations about the stable configuration in a ferromagnet. As spin waves are free from Joule heating, they are interesting for technological applications. Controlling spin waves propagating in solids relies on the predefined, constant magnetic parameters. However, recently, it has been shown that it is possible to have a dynamic variation of these parameters. Using a laser, thermal landscapes are created in the magnetic medium that results in a modulation of the saturation magnetization[1].

We excite spin waves on a thin ferromagnetic film using micromagnetic simulations. The film has a region where saturation magnetization is decreased, creating a potential well. We calculate the spin wave reflection coefficient for different widths of the well. We found that there are resonances on the reflection coefficient. These resonances resemble the ones found in the quantum mechanical Ramsauer-Townsend (RT) effect.[2] The RT effect describes an electron wave propagating above a finite potential well and exhibits resonances for certain energies and well widths.

Our results may be of interest for magnonic applications by only varying the width of the well.


4:18PM C41.00008: Exchange Stiffness in pMTJ Free Layers by Magnetometry and Spin-Torque Ferromagnetic Resonance*  JAMILEH BEIK MOHAMMADI (Presenter), JINTING HANG, New York University, BARTEK KARDASZ, GEORG WOLF, MUSTAFA PINARBASI, Spin Transfer Technologies, ANDREW D KENT, New York University — Exchange interactions play a critical role in setting the scale of micromagnetic structure and the spin-wave excitation spectrum in nanometer scale magnetic elements. Specifically, in perpendicularly magnetized free layers of magnetic tunnel junction (pMTJ) nanopillars, exchange, magnetic anisotropy and dipolar interactions determine the spin-wave modes and magnetization reversal pathways. Here we report studies of the exchange stiffness $A$ in composite CoFeB free layers in pMTJ (extended) thin films. Vibrating sample magnetometry (VSM) was used to determine the free layer magnetization versus temperature, which is fit to Bloch's law to determine $A$. We further perform field modulated spin-transfer FMR (ST-FMR) measurements on 30 to 80nm diameter nanopillars to infer the confined spin-wave modes, providing, in principle, an independent means of determining $A$. We discuss the correspondence between these methods and the nature of the spin-transfer excited spin-wave modes in such pMTJ nanopillars.

*This project is supported by Spin Transfer Technologies Inc.

4:30PM C41.00009: Dynamics of 1D Magnetic Topological Structures*  MARTYNA SEDLMAYR (Presenter), NICHOLAS SEDLMAYR, Department of Physics and Medical Engineering, Rzeszow University of Technology, JAMAL BERAKDAR, Martin-Luther University Halle-Wittenberg, VITALII DUGAEV, Department of Physics and Medical Engineering, Rzeszow University of Technology — In one dimensional ferromagnetic wires domains of collinear ferromagnetic order can be separated by different types of topological, and non-topological, domain walls. Domains of opposite orientation are typically separated by either Bloch or Néel domain walls, whereas domains of the same orientation can be separated by magnetic impurities, or by a one dimensional equivalent of a skyrmion which may be found in quasi-one dimensional wires. We consider the different current induced dynamics and stability of these various magnetic deformations. We will go on to make a thorough investigation of the different magnetoresistance which can be caused by these various forms of domain walls, paying particular attention to the one dimensional skyrmion.

*This work was supported in Rzeszoow University of Technology by the National Science Center in Poland as research Project No. UMO-2017/27/B/ST3/02881.
4:42PM C41.00010: New spin excitations in metals*

VLADIMIR ANTROPOV (Presenter), ALEX WYSOCKI, MANH CUONG NGUYEN, Ames Laboratory, Ames, IA, 50010, USA, ANDREY KUTEPOV, Brookhaven National Laboratory, Upton, NY 11973, USA, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, Ames, IA, 50010, USA — The spin excitations in metals have been studied using density functional methods. First, we used linear response method with well converged basis set to obtain the spin excitations in para- and ferromagnetic phases of different d metals at all q-vectors and frequencies. Our calculations revealed the existence of new nearly localized in real space spin excitations in metals and we discuss their relation to the existing experiments. We further analyzed the spin correlations in these metals by using the fluctuation dissipation ratio and a corresponding quantum spin ‘noise’. The very large dynamic spin short range order has been identified and will be shown in paramagnetic Pd. These observed unusual features of spin dynamics and the exchange coupling will be discussed using the analysis of microscopical equations of motion for the charge, current and spin densities in the frame of corresponding density functional approach.

*This work was supported by the Office of Basic Energy Science, Division of Materials Science and Engineering. The research was performed at Ames Laboratory, which is operated for the U.S. DOE by Iowa State University under contract # DE-AC02-07CH11358.

4:54PM C41.00011: On and Off-Resonance Spin Wave/Surface Acoustic Wave Coupling Measured Using Brillouin Light Scattering*

KATHERINE E. NYGREN (Presenter), Department of Physics, Colorado State University, JOSEPH D. SCHNEIDER, QIANCHANG WANG, Mechanical and Aerospace Engineering Department, UCLA, DOMINIC LABANOWSKI, SAYEEF SALAHUDDIN, Department of Electrical Engineering and Computer Science, UC Berkeley, GREG CARMAN, Mechanical and Aerospace Engineering Department, UCLA, KRISTEN S. BUCHANAN, Department of Physics, Colorado State University — Surface acoustic waves (SAWs) have a much longer propagation distance than most spin waves, especially in metallic ferromagnets. If spin waves can be effectively coupled to SAWs they can travel farther and SAW/spin wave coupling also offers new opportunities for energy efficient spin wave generation. Here we have used an interdigital transducer (IDT) on a piezoelectric substrate to produce a SAW at 1.8 GHz and we have studied the coupling of the SAW to spin waves in a 20 nm thick Ni thin film using Brillouin light scattering (BLS). A strong signal is observed at the driving frequency \( f \) that varies in intensity as a function of the applied magnetic field. At fields where \( f \) overlaps with the spin wave manifold an additional peak is observed at 2f that is not present at higher fields, which indicates that nonlinear process are active. Measurements were also performed at multiple locations on the nickel pad to characterize how the spin wave decays with distance.

*This work is supported by NSF EFMA 1741666, NSF DEEC 1160504, and NSF EFRI NewLaw award no. 1641128.

5:06PM C41.00012: Spin wave excitations of magnetic metalorganic materials*

ROBERTO PÉREZ (Presenter), JOHAN HELLSVIK, RICHARD GEILHUGE, Nordic Institute for Theoretical Physics, MARTIN MÅNSSON, KTH Royal Institute of Technology, ALEXANDER BALATSKY, Nordic Institute for Theoretical Physics — The Organic Materials Database (OMDB) is an open database at Nordita that is hosting about 25,000 electronic band structures, density of states and other properties for synthesized 3-dimensional organic crystals. The web interface of the OMDB offers various search tools for the identification of novel functional materials such as band structure pattern matching and density of states similarity search. In this work we extend the OMDB to include magnetic excitation properties. For inelastic neutron scattering we focus on the dynamical structure factor \( S(Q, \omega) \) which contains information on the excitation modes of the material. We introduce a new dataset containing atomic magnetic moments and Heisenberg exchange parameters for which we calculate the spin wave spectra and dynamic structure factor with linear spin wave theory and atomistic spin dynamics. We thus develop the materials informatics tools to identify topological magnon spectra such as Dirac crossings within the class of organic molecular crystals, and reveal mechanisms for the topological protection of the crossings.

*Swedish Research Council (VR) 2016-06955 BIFROST, Villum Center of Excellence for Dirac Materials, and KAW 2013.0096.
Terahertz-frequency magnetization oscillations in an uncompensated ferrimagnet under a spin-transfer torque*  

IVAN LISENKOV, Winchester Technologies, LLC, ROMAN KHYMYN, JOHAN AKERMAN, Physics Dept., University of Gothenburg, NIAN XIANG SUN (Presenter), Northeastern University, BORIS IVANOV, National Taras Shevchenko University of Kiev — Current of spin-polarized electrons can interact with materials exhibiting a long-range magnetic order via a spin-transfer torque (STT). An STT of a sufficient magnitude may compensate damping and the spins come into a self-sustained precession [1]. In ferromagnetic materials the precession frequency is limited to tens of GHz by the value of the external magnetic field. In materials with more than one magnetic sublattice, the strong exchange interaction speeds up the precession frequency up to several THz [2], but due to magnetic compensation, in antiferromagnetic materials the THz frequency output power is small [3]. In our simulations we show that in easy-plane unbiased nearly compensated GdFeCo thin layers: (i) the precession frequency can be in over of THz and controlled by current, (ii) the precession of the Neel vector is conical, where the cone angle is defined by the non-compensation of the sublattices. The conical precession excites an AC spin-current, which can be converted to AC voltage by inverse spin-Hall effect.


*This work was funded by NSF TANMS ERC Award No. 1160504.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C42 DQI: Applications of Noisy Intermediate Scale Quantum Computers I

BCEC 210A - Timothy Hsieh, Perimeter Institute for Theoretical Physics - Tag(s): Focus

2:30PM C42.00001: Error-mitigated quantum computation with noisy superconducting qubits* [Invited]  

*This work was supported by the IBM Research Frontiers Institute.

3:06PM C42.00002: A quantum computing algorithm for the investigation of the molecular excited states  
PAULINE OLLITRAULT (Presenter), PANAGIOTIS BARKOUTSOS, STEFAN WOERNER, IVANO TAVERNELLI, IBM Research - Zurich Research Laboratory — Quantum computing is emerging as a new paradigm for the solution of quantum chemistry problems. Recently, the Variational Quantum Eigensolver (VQE) algorithm has been proposed and successfully applied to the simulation of the ground state properties of simple molecular systems in a real quantum device. The calculation of molecular excited state properties constitute an additional challenge for both classical and quantum electronic structure algorithms. In fact, in addition to the calculation of a well-converged ground state wavefunction, one needs to devise schemes for the evaluation of the higher energy states, which - in general - are not accessible through the simple optimization procedure. In this work, a perturbative approach is applied to the ground state wavefunction to derive a pseudo-eigenvalue problem, which size is characterized by a favorable scaling in the number of electrons. The different matrix elements are measured on the quantum hardware using the ground state wavefunction parametrized according to the UCC and the hardware efficient Ansätze described in [Barkoutsos et al., Phys. Rev. A 98, 022322]. The method is applied to the calculation of the excited states of simple molecules, including H₂, LiH and H₂O.
3:18PM C42.00003: Error Mitigation in the Presence of Spatially Correlated Noise  VICKRAM PREMAKUMAR (Presenter), EKMEK ERCAN, JOYDIP GHOSH, MARK G FRIESEN, MARK ALAN ERIKSSON, SUSAN COPPERSMITH, ROBERT JAMES JOYNT, University of Wisconsin - Madison — The most common error models for quantum computers assume the independence of errors on different qubits. However, most noise mechanisms have some correlations in space. We show how to improve quantum information processing for few-qubit systems when spatial correlations are present. This starts with strategies to measure the correlations. Once the correlations have been determined, we can define decoherence measures that are local in Hilbert space. These measures yield criteria to assess the ability of different candidate quantum circuits to carry out a given task with high fidelity. We show that these criteria work in few-qubit systems. Finally, we point out ways in which error mitigation in few-qubit systems can be extended to large-scale quantum information processing.

3:30PM C42.00004: Benchmarking error mitigation techniques on noisy quantum processors  CORENTIN BISOT, EMMANUEL LILETTE, THOMAS AYRAL (Presenter), Atos Quantum Lab — Several error mitigation techniques have been proposed in the recent years to compensate for the errors of noisy, intermediate-scale quantum (NISQ) devices before full-fledged, yet costly error correction methods can be implemented. Here, we present an implementation of a combination of these techniques, and a detailed benchmark based both on realistic noisy simulations and actual computations on current quantum architectures such as, for instance, superconducting transmon processors. We examine the link between the accuracy of the knowledge of the quantum hardware (via tomography), the accuracy on the final observable, and the overhead of mitigation. We also discuss the relevance of these methods for reaching high enough accuracies in applications such as quantum chemistry.

3:42PM C42.00005: Efficient scheduling of noise characterization protocols in quantum computing architectures  RIDDHI SWAROOP GUPTA (Presenter), MICHAEL JORDAN BIERCUK, Quantum Control Laboratory, The University of Sydney — Spectator qubits embedded in quantum computing architectures enable in situ detection of noise processes affecting quantum hardware. Common spatial correlations between processing and spectator qubits present a new resource which may be exploited in efficient scheduling of measurements. We present an algorithmic framework for 2D field mapping in quantum computing architectures using sparse measurements. We adapt classical simultaneous localisation and mapping (SLAM) techniques to enable spatial field characterization using idle qubits, where idle qubits are a static or a dynamically available resource. A Quantum SLAM (QSLAM) framework is implemented via a particle filter that shares information between neighboring qubits while discovering neighborhood sizes relevant to the physical system; an adaptive controller then schedules future measurements based on this algorithm. We use experimental measurements on a linear array of trapped ions subject to an observed but uncontrolled magnetic field gradient. Numeric simulations demonstrate that QSLAM outperforms a brute force approach for estimating the magnetic field gradient by over an order of magnitude across a range of operating parameter regimes. Extensions to incorporating time dynamics are discussed.

3:54PM C42.00006: Superfast encodings for fermionic quantum simulation*  KANAV SETIA (Presenter), Dartmouth College, SERGEY BRAVYI, ANTONIO MEZZACAPPO, IBM, JAMES WHITFIELD, Dartmouth College — Here we revisit the Superfast Encoding introduced by Kitaev and one of the authors. This encoding maps a target fermionic Hamiltonian with two-body interactions on a graph of degree d to a qubit simulator Hamiltonian composed of Pauli operators of weight O(d). A system of m fermi modes gets mapped to n=O(md) qubits. We propose Generalized Superfast Encodings (GSE) which require the same number of qubits as the original one but have more favorable properties. First, we describe a GSE such that the corresponding quantum code corrects any single-qubit error provided that the interaction graph has degree d≥6. In contrast, we prove that the original Superfast Encoding lacks the error correction property for d<6. Secondly, we describe a GSE that reduces the Pauli weight of the simulator Hamiltonian from O(d)to O(logd). The robustness against errors and a simplified structure of the simulator Hamiltonian offered by GSEs can make simulation of fermionic systems within the reach of near-term quantum devices. As an example, we apply the new encoding to the fermionic Hubbard model on a 2D lattice.

*AM and SB supported by: IBM Research Frontiers Institute and KS and JDW partly supported by: NSF awards DMR-1747426, 1820747.
4:06PM C42.00007: Experimental Implementation of Quantum Circuit Born Machines in Near-Term Quantum Devices
ALEJANDRO PERDOMO (Presenter), VICENTE LEYTON-ORTEGA, Rigetti Computing, OSCAR PERDOMO, Central Connecticut State University — Finding valuable machine learning that could benefit from noisy intermediate-scale quantum computers is one of the leading research efforts towards the milestone of practical quantum advantage. In this talk, we will focus in the one of most challenging tasks for the machine learning community: the case of generative modeling in unsupervised machine learning. In Ref. [1], a data-driven quantum circuit learning (DDQCL) approach was proposed as a hybrid quantum-classical algorithm capable of training shallow quantum circuits to prepare desirable quantum states. This resulting quantum state is referred as a Quantum Circuit Born Machine (QCBM) [1,2] and it exploits the probabilistic nature of the Born amplitudes from the computational basis states to capture correlations in the classical training data set. This QCBM model can be used to solve unsupervised generative modeling tasks such as image generation and reconstruction. We will discuss results of experimental implementations of QCBMs via DDQCL, as well as ideas for DDQCL variants that could be useful in, for example, quantum state preparation and noise mitigation.

References:

4:18PM C42.00008: Simulations of Real Time Scattering in the 1D Quantum Ising Model*
ERIK GUSTAFSON (Presenter), YANNICK MEURICE, University of Iowa, JUDAH F UNMUTH-YOCKEY, Department of Physics, Syracuse University — We will discuss the results of quantum simulating a real time scattering event in the 1D Quantum Ising spin models using a quantum simulator. We discuss how we can measure the phase shifts of scattering processes. We compare the results from exact diagonalization with those using a quantum simulator. We examine the errors introduced in our simulation by some of the noise that would be present on a real quantum computer. We discuss the efficacy of simulating this model on a quantum computer.

*We thank the Department of Energy for supporting this research under Award Number: DE-SC0019139

4:30PM C42.00009: Quantum Local Search for Graph Community Detection*
RUSLAN SHAYDULIN (Presenter), HAYATO USHIJIMA-MWESIGWA, ILYA SAFRO, Clemson University, SUSAN MNISZEWSKI, Computer, Computational, & Statistical Sciences Division, Los Alamos National Laboratory, YURI ALEXEEV, Computational Science and Leadership Computing Divisions, Argonne National Laboratory — We present Quantum Local Search (QLS) approach and demonstrate its efficacy by applying it to the problem of community detection in real-world networks. QLS is a hybrid algorithm that combines a classical machine with a small quantum device. QLS starts with an initial solution and searches its neighborhood, iteratively trying to find a better candidate solution. One of the main challenges of the quantum computing in NISQ era is the small number of available qubits. QLS addresses this challenge by using the quantum device only for the neighborhood search, which can be restricted to be small enough to fit on near-term quantum device. We implement QLS for modularity maximization graph clustering using QAOA on IBM Q Experience as a quantum local solver. We demonstrate the potential for quantum acceleration by showing that existing state-of-the-art optimization solvers cannot find a good solution to the local problems quickly and provide an estimate of how larger quantum devices can improve the performance of QLS. We apply QLS to the problem of clustering microbiome co-occurence networks and present the preliminary results.

*This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357

4:42PM C42.00010: Marginals optimization procedure: algorithmically extending the capability of near-term quantum computers
PETER JOHNSON (Presenter), MAX RADIN, AMARA KATABARWA, JHONATHAN ROMERO, YUDONG CAO, Zapata Computing — We are entering an era in which quantum computers can perform contrived tasks that classical computers cannot. However, these devices are far from being able to break RSA encryption or to simulate complex chemical reactions. A big question driving the field is: can we find a practical use for these near-term intermediate scale quantum (NISQ) devices? A promising approach is to explore “variational quantum algorithms”, which treat a quantum circuit much like an artificial neural network to solve optimization problems approximately. These optimization problems include estimating the ground state energy of a small molecule and understanding the structure of social networks.

Variational quantum algorithms have yet to outperform state-of-the-art classical optimization techniques. While improving quantum devices is necessary to achieve this so-called “quantum advantage”, improving quantum algorithms also brings us closer towards this goal. Based on a simple observation about the role of the quantum computer in these algorithms, we have developed a technique which algorithmically extends the depth of a quantum computer. We describe the marginals optimization procedure for improving variational quantum algorithms and demonstrate its performance in simulations and small experiments.
An analog quantum simulator does not employ digital gates with quantum error correction. Yet, one hopes such devices can achieve a "quantum advantage," i.e., enable the simulation of some property that cannot be simulated efficiently on a classical computer. Typically, one considers "universal" properties in condensed matter, as these are the quantities that are robust in the presence of perturbations [1]. What is the relationship between robustness and complexity? Are the robust properties efficiently simulatable on a classical computer, and the complex properties hyper-sensitive to perturbation? To address these questions, we seek to quantify the reliability of an analog quantum simulator while simulating complex systems and thereby identify these universal quantities. We study a "programmable" analog quantum simulator in the 16-dimensional Hilbert space based on optimal control of atomic spins in cesium [2], and study the basic paradigms such as the excited state quantum phase transitions [3] in the Lipkin-Meshkov-Glick (LMG) model [3].

References:

*National Science Foundation

5:06PM C42.00012: Experimental Methods for Improving Heuristic Quantum Algorithms on NISQ Devices*
BRADLEY MITCHELL (Presenter), RAVI NAIK, UNPIL BAEK, DAR DAHLEN, JOHN MARK KREIKEBAUM, University of California, Berkeley, KEVIN P O' BRIEN, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, VINAY RAMASESH, MACHIEL BLOK, University of California, Berkeley, WIM LAVRIJSEN, COSTIN IANCU, Lawrence Livermore National Laboratory, Berkeley CA, IRFAN SIDIQI, University of California, Berkeley — Heuristic quantum algorithms, such as QAOA (Quantum Approximate Optimization Algorithm) and VQE (Variational Quantum Eigensolver), have the potential for performing useful, classically intractable calculations on NISQ (Noisy Intermediate Scale Quantum) devices, with applications ranging from general optimization to quantum chemistry. Outstanding challenges in implementing these algorithms include error mitigation and minimizing costly calls to quantum hardware. We report experimental developments to identify and address these challenges on a superconducting quantum processor. To this end, we employ techniques including using an expanded Hilbert space of the transmon as a computational space and performing Pauli twirling operations.

*This work was supported by the Department of Energy.

5:18PM C42.00013: State-of-the-art Classical Tools to Benchmark NISQ Devices*
SALVATORE MANDRA (Presenter), Quantum Artificial Intelligence Lab (QuAIL) @ NASA Ames - Stinger Ghaffarian Technologies (SGT), BENJAMIN VILLALONGA, University of Illinois at Urbana-Champaign - Quantum Artificial Intelligence Lab (QuAIL) @ NASA Ames - USRA Research Institute for Advanced Computer Science (RIACS), SERGIO BOIXO, Google Inc., HELMUT KATZGRABER, Texas A&M University, ELEANOR RIEFFEL, Quantum Artificial Intelligence Lab (QuAIL) @ NASA Ames — In the race to show quantum advantage, early quantum devices must be compared to the state-of-the-art classical technology currently available. At the Quantum Artificial Intelligence Lab (QuAIL) at NASA Ames, we are continuously developing new classical algorithms to benchmark/validate quantum hardware and to raise the bar to claim quantum advantage. In my talk, I will present some of our latest state-of-the-art classical tools to optimize classical cost functions (in collaboration with Texas A&M University), including numerical results on hard benchmark problem sets. Moreover, I will present our optimized classical simulator for large quantum circuits (in collaboration with the Google AI team), including numerical simulations of the Google Bristlecone quantum processing unit.

*This research is based upon work supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via Interagency Umbrella Agreement IA1-1198, the AFRL Information Directorate under grant F4HBKC4162G001 and the NASA Ames Research Center, including the NASA Transformative Aeronautic Concepts program.
2:30PM C43.00001: Locating the missing superconducting electrons in overdoped cuprates* [Invited] PETER ARMITAGE (Presenter), Johns Hopkins University — Overdoped high-temperature cuprate superconductors have been widely believed to be described by the physics of d-wave BCS-like superconductivity. However, recent measurements indicate that as the doping is increased, the superfluid density decreases smoothly to zero rather than increasing as expected by BCS theory in the absence of disorder. Here, we combine time-domain THz spectroscopy with kHz range mutual inductance measurements on the same overdoped La$_{2-x}$Sr$_x$CuO$_4$ films to determine both the superfluid and the uncondensed carrier density as a function of doping. A significant fraction of the carriers remains uncondensed in a wide Drude-like peak even as $T_\text{c}$, which, when taken with the linear-in-temperature superfluid density, is inconsistent with existing theories for the role of disorder in suppressing the superfluid density in a d-wave superconductor. Our almost eight orders of magnitude in measurement frequency range gives us a unique look at the low frequency spectral weight distribution, which may suggest the presence of quantum phase fluctuations as the critical doping is approached.


*Work at JHU was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0019331. Film synthesis by molecular beam epitaxy and characterization was done at BNL and was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division. X.H. is supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4410 to IB.

3:06PM C43.00002: Density fluctuations in strange metals* [Invited] PETER ABBAMONTE (Presenter), University of Illinois at Urbana-Champaign — Metals exhibit plasmon excitations, which are collective modes one can think of as sound waves in the electron density (as opposed to the atomic density). The so-called "strange metals" are bizarre phases of matter that fail to exhibit well-defined quasiparticles but somehow are still good conductors, leading one to wonder what degree of freedom is actually carrying the charge. A sensible question to ask is, Do strange metals exhibit plasmons? In this talk I will describe momentum-resolved EELS (M-EELS) measurements of several strange metals, notably Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ which is also a high-temperature superconductor. I will show that plasmon excitations are barely defined in these materials, which instead exhibit an incoherent continuum of charge fluctuations with no particular length or time scale. These fluctuations obey a simple, power law form, suggesting some kind of scale-invariant phase is present, though the data are not consistent with a (textbook) quantum critical point. I will discuss efforts by theorists to explain this phenomenon using holographic approaches based on the AdS-CFT correspondence.

*M-EELS development was partly supported by DOE grant DE-AC02-98CH10886. Crystal growth was supported by DOE grant DESC0012704. P.A. acknowledges support from the EPiQS program of the Gordon and Betty Moore Foundation, Grant GBMF-4542.

3:42PM C43.00003: Universal superconducting precursor in perovskite-based oxides* [Invited] DAMJAN PELC (Presenter), ZACHARY ANDERSON, BIQIONG YU, CHRIS LEIGHTON, MARTIN GREVEN, University of Minnesota — A pivotal challenge posed by unconventional superconductors is to unravel how superconductivity emerges upon cooling from the generally complex normal state. Some of the most prominent unconventional superconductors are oxides: strontium titanate, strontium ruthenate, and the cuprates exhibit greatly different superconducting transition temperatures $T_c$, and although their respective superconducting pairing mechanisms remain unknown, they are thought to differ as well. We use nonlinear magnetic response – a probe that is uniquely sensitive to the superconducting precursor – to uncover remarkable universal behavior in these three distinct classes of oxide superconductors [1]. We find an unusual exponential temperature dependence of the diamagnetic response above the transition temperature $T_c$, with a characteristic temperature scale that strongly varies with $T_c$. We correlate this scale with the sensitivity of $T_c$ to local stress, indicating that the universal behavior is caused by intrinsic, self-organized structural inhomogeneity inherent to the oxides’ perovskite-based structure. Furthermore, the precursor can be strongly influenced by structural disorder, intentionally induced by uniaxial plastic deformation. The results show that structural inhomogeneity is prevalent in perovskite-related superconductors, with far-reaching implications for the interpretation of their electronic properties in general.


*This work was funded by the DOE through the University of Minnesota Center for Quantum Materials under DE-SC-0016371.
4:18PM C43.00004: NMR study of the effect of hydrostatic pressure on charge-density waves and superconductivity in YBa2Cu3Oy [Invited]  MARC-HENRI JULIEN (Presenter), CNRS Grenoble, Laboratoire National des Champs Magnétiques Intenses (LNCMI) — High-Tc superconductivity in the cuprates arises in close proximity to a charge-density wave (CDW) phase. A challenge in the field is to understand how both phenomena compete and whether, behind pure competition, there is a more involved relationship between them. To tackle this question, experiments have used temperature, magnetic field, hole-doping or uniaxial strain as tuning parameters. The effect of hydrostatic pressure, on the other hand, is controversial. Here, using nuclear magnetic resonance (NMR) in YBa2Cu3Oy, we find that the short-range CDW in the normal state as well as the long-range CDW in high fields are weakened only slightly at a pressure of 1.9 GPa. Quantitative analysis of the data supports the hypothesis that virtually all of the increase in Tc upon increasing pressure arises from a gradual decrease of CDW strength up to ~15 GPa. We propose explanations for some of the conflicting conclusions drawn from different experiments and suggest that they may actually shed light on the CDW.

Work done with I. Vinograd, R. Zhou, H. Mayaffre, S. Krämer (LNCMI Grenoble), R. Liang, W.N. Hardy, D.A. Bonn (University of British Columbia)

4:54PM C43.00005: Uniaxial Pressure Control of Competing Orders in a High Temperature Superconductor [Invited]  MATTHIEU LE TACON (Presenter), Karlsruhe Institute of Technology — External control of electronic phases in correlated-electron materials is a long-standing challenge of condensed-matter research. Layered cuprates exhibit antiferromagnetic, charge density-wave (CDW), and high-temperature superconducting ground states which can be tuned by doping and external magnetic fields. However, disorder generated by lattice defects and randomly pinned magnetic vortices greatly complicates the interpretation of these experiments.

Here, we report a high-resolution inelastic x-ray scattering study of the high-temperature superconductor YBa2Cu3O6.67 under uniaxial stress (1), and show that a three-dimensional long range-ordered CDW state can be induced by pressure along the a-axis, in the absence of magnetic fields. The amplitude of the CDW is strongly suppressed below the superconducting transition temperature, indicating strong thermodynamic competition with superconductivity. We also show that the transition is driven by the complete softening of an optical phonon mode.

The results provide new insights into the anomalous normal-state properties of high temperature superconductors and illustrate the potential of uniaxial-pressure control of competing orders in quantum materials.


Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C44 : Dynamics in Glassy Systems 8CEC 210C - Andrea Liu, University of Pennsylvania - Tag(s): Invited

2:30PM C44.00001: Connections between classical mean field models with glassy dynamics and quantum SYK models [Invited]  JORGE KURCHAN (Presenter), Ecole Normal Superieure Paris — TBD

3:06PM C44.00002: On the trap model description of glassy dynamics* [Invited]  M. BAITY-JESI, Chemistry, Columbia, NYC, GIULIO BIROLI, Physics, ENS, Paris, CHIARA CAMMAROTA (Presenter), Mathematics, King's College London, UK, ENZO MARINARI, Physics, Sapienza, Rome — The description of activated dynamics of glassy systems in the multidimensional configurational space is a long-standing open problem. In this talk I will discuss about recent studies of the equilibrium and out-of-equilibrium dynamics of a number of models with rough potential energy landscapes. These models provide examples of dynamics where typical relaxation channels go over finite potential energy barriers despite the presence of less-energy-demanding escaping paths in configurational space. This phenomenon is naturally expected to be relevant in the thermally activated regime of realistic models of glass-formers. The numerical and analytic results will show whether, and to what extent, due to this phenomenon the activated dynamics displayed by these models can be effectively described in terms of the fully solvable dynamics of thermally-activated systems like trap models.

*Simons Foundation for the collaboration “Cracking the Glass Problem” (No. 454935 to G. Biroli), ERC grant CIPHERASY (Grant No. 247328), ERC grant NPRGGLASS (No. 279950), ERC grant (No. 694925)
Understanding the geometrical properties of high-dimensional, random energy landscapes is a central problem in the physics of glassy systems, as well as in interdisciplinary applications to computer science, ecology and biology.

In this talk I will discuss a framework to compute the statistical distribution of stationary points of random landscapes, making use of a replicated version of the Kac-Rice formula. I will focus on models which provide a mean-field description of the glass transition, and discuss how to compute the statistics of the energy barriers between local minima of the landscape. I will discuss the dynamical implications on these results, especially for the activated regime of the dynamics.

*Simons Foundation collaboration Cracking the Glass Problem (No. 454935 to G. Biroli)

4:18PM C44.00004: Glassy dynamics: mean-field theory and beyond* [Invited] GRZEGORZ SZAMEL (Presenter), Colorado State Univ — The slowing down of a liquid's dynamics upon approaching the glass transition is accompanied by a number of novel dynamical phenomena: transient localization of particles' positions, strong spatial and temporal fluctuations of the dynamics of individual particles, etc. The description of these dynamics, even at the level of a mean-field theory, is still being developed. I will present a simple theory for the dynamics of mean-field-like models of glass forming liquids. Next, I will turn to the glassy dynamics of one particle moving in a frozen matrix and, in this simpler case, show how one can incorporate dynamic events neglected in the mean-field approach.

*NSF DMR-1608086

4:54PM C44.00005: New computational approaches to dynamics in complex landscapes [Invited] DAVID REICHMAN (Presenter), Columbia University — TBD

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C45 DCMP: Oxide Surfaces and Defects BCEC 211 - Christopher Homes, Brookhaven National Laboratory

2:30PM C45.00001: Surface reaction kinetics of dimethyl methylphosphonate (DMMP) on zirconium hydroxide using attenuated total reflection infrared (ATR-FTIR) spectroscopy* SEOKMIN JEON (Presenter), Chemistry Division at US Naval Research Laboratory, National Research Council Research Associateship Program, ROBERT B BALOW, GRANT C DANIELS, Chemistry Division, US Naval Research Laboratory, JESSE S KO, Chemistry Division at US Naval Research Laboratory, National Research Council Research Associateship Program, PEHR E. PEHRSSON, Chemistry Division, US Naval Research Laboratory — Amorphous zirconium hydroxide (ZH) attracts growing attention due to its high activity for decomposing toxic chemicals, especially chemical warfare agents (CWA). We synthesize zirconium hydroxide films using cathodic electrodeposition and investigate their surface chemistry to a CWA simulant, dimethyl methylphosphonate (DMMP), using attenuated total reflection infrared spectroscopy (ATR).

The ATR data show the accumulation of surface-bound decomposition products, including methoxy and phosphonate derivatives. Time-dependent IR absorption spectra reveal the adsorption, decomposition, and desorption kinetics. Growth of the IR absorption intensities for surface reaction products is evaluated with various adsorption and diffusion kinetic models. Thermodynamic parameters are derived from the adsorption isotherm. The dependence of the kinetic and thermodynamic parameters on reaction temperature will be discussed.

Calcination of amorphous zirconium hydroxide produces crystalline zirconia via a transition to amorphous zirconia. Reduced chemical activity upon calcination correlates with decreased surface area and loss of hydroxyl groups, as confirmed by XPS and ATR data.

*The work was supported by the Defense Threat Reduction Agency under award CB10123.
Microscopic investigation on surface structures and intrinsic defects of Cu$_2$O(111)*

LY TRINH (Presenter), Department of Physics, BRL, and EHSRC, University of Ulsan, Ulsan 44610, Korea (the Republic of), TAEHUN LEE, Department of Materials Science and Engineering, Yonsei University, Seoul 03722, Republic of Korea, GANBAT DUVJIR, SANGHWA KIM, Department of Physics, BRL, and EHSRC, University of Ulsan, Ulsan 44610, Korea (the Republic of), ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University, Seoul 03722, Republic of Korea, SE YOUNG JEONG, Department of Nanoenergy Engineering and College of Nanoscience and Nanotechnology, Pusan National University, Busan 46241, Korea (the Republic of), JUNGDAE KIM, Department of Physics, BRL, and EHSRC, University of Ulsan, Ulsan 44610, Korea (the Republic of) — Copper (I) oxide or cuprous oxide (Cu$_2$O) is known to be a p-type semiconductor with direct band gap of ~ 2.1 eV. Since most binary oxides exhibit n-type behavior originating from the donor nature of oxygen vacancies, Cu$_2$O has been considered as a p-type counterpart for oxide-based electronics. Although some theoretical studies reported about the origin of p-type nature in Cu$_2$O, atomistic experimental study on this issue has not been conducted yet. In this work, we investigate the surface structures and intrinsic defects of Cu$_2$O(111) via home-built low temperature scanning tunneling microscopy (STM). Thin Cu$_2$O(111) layer is prepared on top of Cu(111) film by ambient oxidation, and the surface of Cu$_2$O(111) is cleaned by Ar sputtering and annealing for STM experiments. STM topography reveals the stoichiometric oxygen-terminated surfaces of Cu$_2$O(111). We also directly observed two types of intrinsic defects which show different contrast in topography depending on bias polarity. These defects are identified by comparison with density functional theory (DFT) simulations. The electronic property of defects will be discussed during the presentation.

*This work was supported by the National Research Foundation of Korea [NRF-2015R1D1A1A01057271, NRF-2009-0093818, and NRF-2014R1A4A1071686].

Cu$_2$O island growth during Cu oxidation revealed by correlated in situ ETEM and multiscale simulations*

MENG LI, MATT CURNAN, University of Pittsburgh, XINYU LI, GRAEME HENKELMAN, University of Texas, Austin, WISSAM SAIDI, JUDITH YANG (Presenter), University of Pittsburgh — Fundamental understanding of the surface oxidation process is essential for controlling and predicting oxide growth for catalysts and electronic devices applications. Despite numerous studies on the bulk oxidation process, the initial oxide growth process is still less explored, especially at the atomic scale. In this work, by combining in situ Environmental TEM (ETEM) with multiscale atomistic simulation, the dynamic process of initial Cu$_2$O nano island growth was explored. Our ETEM result shows during Cu(100) oxidation, Cu$_2$O nano islands grow through a layer-by-layer adatom growth mechanism along Cu$_2$O(110) surface. Our simulation results show that comparing with Cu$_2$O(100), Cu$_2$O(110) has lower surface energy, lower Cu diffusion energy and more favorable Cu adsorption energy, leading to easier Cu$_2$O monolayer formation along Cu$_2$O(110) that ultimately caused the observed layer-by-layer oxide growth. These results will enhance the understanding of surface oxidation and will also provide insights into understanding initial oxide growth mechanisms of other metal/alloy systems.

*This work is supported by NSF DMR-1410055, NSF DMR-1508417, and NSF DMR-1410335.

First-principles study of Iridium oxide desorption from iridium low-index surfaces at high temperature

INSUNG SEO (Presenter), Materials Science and Engineering, Tokyo Institute of Technology, SHUNSUKE YOKOTA, YOUSUKE IMAI, ISHIFUKU Metal Industry, YOSHIHIRO GOHDA, Materials Science and Engineering, Tokyo Institute of Technology — Iridium is one of the noble metals. Although iridium has good chemical inertness and mechanical properties especially at high temperature, iridium has a problem to use, due to the desorption problem[1]. It is known that desorption occurs mainly the form of IrO$_3$ molecule below 1775K[2]. To investigate about iridium desorption problem, theoretical understanding of iridium surface oxide is needed. In this study, we investigate surface oxide of low-index iridium surface, such as Ir(100), Ir(110), and Ir(111) to find energetically favorable surface oxide by using first-principles calculations based on density functional theory. Also we use a thermodynamical approach, we can find energetic difference between the low temperature and high temperature.

3:18PM C45.00005: Atomic Structure and Nano-Fracture Mechanics of Semiconductor-Oxide Interfaces
Investigated by Transmission Electron Microscopy and Scanning Force Microscopy

DIPANWITA DUTTA (Presenter), Paul Scherrer Institute, DARIUSZ JARZABEK, Mechanics of Materials, Institute of Fundamental Technological Research, Polish Academy of Sciences, HELMUT SCHIFT, Paul Scherrer Institute, ZYGMUNT RYMUZA, Micromechanics and Photonics, Warsaw University of Technology, THOMAS JUNG, Paul Scherrer Institute — Quantitative Information on interface adhesion and fracture resistance is of importance for electronic and MEMS/NEWS device manufacturing. Here we focus on Scanning Force Microscopy derived methods [1] which reveal the mechanical properties and fracture thresholds of oxide with respect to semiconductor interfaces like SiO$_2$/Si and SiO$_2$/SiC. Load/unload cycles i.e. force vs. distance curves reflect the effect of structural defects on interface strength under the influence of fluids solubilising and modifying surface/interface layers [2]. Nanomechanic properties can be assessed at different time scales. Interface defects are characterized by complementary Microscopic and Spectroscopic Nanoanalysis using STEM and HR-TEM.


*EU-CH Scientific Exchange Programme (No. 10.021), the European Social Fund and the Nano-Aargovia Grant of the Swiss Nanoscience Institute and the Canton Aargau of Switzerland are acknowledged.

3:30PM C45.00006: Amorphous Networks at the Atomic-Scale: Comparing Two-Dimensional Silica and Germania

KRISTEN BURSON (Presenter), Physics, Hamilton College, ADRIAN LEWANDOWSKI, Chemical Physics, Fritz-Haber Institute of the MPG, PHILOMENA SCHLEXER, Materials Science, Università di Milano-Bicocca, CHRISTIN BUECHNER, Lawrence Berkeley National Laboratory, HANNAH BURRALL, Physics, Hamilton College, WOLF-DIETER SCHNEIDER, Chemical Physics, Fritz-Haber Institute of the MPG, GIANFRANCO PACCHIONI, Materials Science, Università di Milano-Bicocca, MARKUS HEYEDE, H J FREUND, Chemical Physics, Fritz-Haber Institute of the MPG — Recently, new insight into the atomic-scale structure of amorphous networks was established through the development of 2D thin-films of known glass formers using scanning tunneling microscopy (STM) in combination with density functional theory (DFT) [1-3]. Here we present a study of two prominent glass-formers, silica and germania, using high-resolution ultra-high vacuum STM to characterize structure. Both SiO$_x$ and GeO$_x$ films were grown on Ru(0001) by physical vapor deposition and subsequent annealing in oxygen, yielding either crystalline or amorphous structures. STM images reveal a hexagonal network with domain boundary structures in atomically flat monolayer films for both glass formers, with germania showing a greater variety of structures. Bilayer films provide for the development of amorphous structure and similar ring structures are seen for both materials. A few exceptions to the structural analogy are seen experimentally and described by DFT, which predicts a stronger interaction with the metal support for germania. This work reveals commonalities and species dependency for glassy structures.


3:42PM C45.00007: A non-invasive SOI gating method of probing pristine chemically-terminated silicon surfaces

LUKE ROBERTSON (Presenter), BRUCE E KANE, Laboratory for Physical Sciences — Silicon has a variety of surface terminations available to it in which surface states are passivated and where 2D electron inversion layers are possible through electrostatic gating. Here, Si(111) surfaces are terminated with hydrogen using a simple wet chemical treatment, and techniques to probe 2D transport on these passivated surfaces have been established. We are presently developing new techniques to probe pristine hydrogen-terminated Si surfaces using a non-invasive SOI flip-chip gating assembly in which all critical device fabrication is performed on the SOI end. Extremely high mobilities, in excess of 300,000 cm$^2$/Vs, have been demonstrated in our previous generation devices, and further refinement of these novel techniques to preserve the pristine nature of these passivated Si surfaces is expected to yield even higher mobilities. Until now, we have focused exclusively on H-Si(111), but are in process of extending our study to include H-Si(100) surfaces. Further, recent progress in halogen-terminated (Cl, Br, I) Si surfaces has provided new avenues for future investigation using our device platform. Architecture details and ohmic contact tests will be presented as well as ongoing low temperature device characterization measurements.

*The Laboratory for Physical Sciences
3:54PM C45.00008: DFT-MD simulations of reaction mechanisms between tricresyl phosphate and Fe₃O₄ (111) surface*  
NAOKI UEMURA (Presenter), SHUJI OGATA, Nagoya Institute of Technology, YOSUKE HARADA, Idemitsu Kosan Co., Ltd. — Tricresyl Phosphate (TCP), used, e.g., as an anti-wear additive reacts to form surface layers on metal and metal oxide under high pressure and high temperature. So far, many experimental and theoretical studies have suggested principal factors that affect the reaction: configurational orientations of P=O group of TCP on the surface, water molecules on the surface, and oxygen atoms of oxidized metal. In a recent DFT study [1], three decomposition mechanisms of TCP on pure iron surfaces was investigated. We here perform DFT-MD simulations of gradually pressurized (~10 GPa) TCP on Fe₃O₄ (111) surfaces to understand the effects of exposed oxygen atoms of the Fe₃O₄ surfaces and of TCP orientations initially relaxed on the Fe₃O₄ surfaces. We thereby find that: (i) the P-O bond that connect to the toluene base of TCP breaks in all cases, (ii) the P-O bond breaking is attributed to the attacking by either oxygen or iron atom of the Fe₃O₄ surfaces, (iii) the adsorption behavior of TCP varies depending on the initial TCP orientations and the amount of exposed oxygen atoms of the Fe₃O₄ surfaces.


*This work was funded by New Energy and Industrial Technology Development Organization of Japan (NEDO) Grant (P16010).

4:06PM C45.00009: Exceptional scaling relation exhibited by oxygen reduction reaction intermediates on TiO₂ surfaces  
YOSHIYUKI YAMAMOTO (Presenter), SHUSUKE KASAMATSU, OSAMU SUGINO, The Institute for Solid State Physics, The University of Tokyo — Enhancing the oxygen reduction reaction (ORR) is a major topic of electrocatalysis, and surfaces have long been designed to realize a full alignment of the adsorption energies of the reaction intermediates, O₂*, O*, OH* and OOH*. The alignment is not easy to realize because the adsorption energies often change obeying a linear relationship among them, known as the scaling relation, rather than change independently by modifying the surface. Pristine oxide surfaces tend to show the scaling relation [1], but defective TiO₂, attracted attention as the electrocatalyst beyond Pt, may behave exceptionally because of the measured high reactivity. Our density functional calculations have shown that OH* and OOH* on defective TiO₂ surfaces follow the same scaling relation found for typical pristine oxide surfaces, suggesting defective TiO₂ is not closer to the ideal catalyst. To our surprise, however, there are metastable surfaces whose pristine surfaces exhibit a significantly deviated relation. This exceptional behavior is related to the fact that those surfaces let OOH* dissociate into O* at a two-folded O site and OH* at a Ti. The deviation from the scaling relation suggests a possibility towards realizing an ideal catalyst.


4:18PM C45.00010: Structural and electronic coupling at the surface of SrTiO₃ (001)*  
MOHAMMAD SAGHAYEZHIAN (Presenter), Physics and astronomy, Louisiana State University, S. M. REZAEI, Institute for Research in Fundamental Sciences (IPM), JIANDI ZHANG, E WARD PLUMMER, Physics and astronomy, Louisiana State University — The surface of SrTiO₃ (001) is considered to be weakly polar and in this work, we study the validity of this notion. Using low energy electron diffraction at room temperature, a surface structural distortion was found. Structural analysis shows the presence of strong surface rumpling in the TiO₂ terminated surface with the Ti and O atoms move in and outward. Density functional calculations confirm the measured rumpling, and experimental data show the distortion is localized at the surface. Angle-dependent core-level X-ray photoemission spectroscopy (XPS) shows that the surface rumpling strongly impacts the electronic structure of the surface. Density functional theory demonstrates that the valence state of Ti at the surface is reduced while O is enhanced. In addition, we found the Ti-O bonds are more covalent near the surface. Changes in the XPS satellite structures at the surface are consistent with this picture of the change in bonding, indicating that the (001) surface of SrTiO₃ is not polar and charge rearrangement is a consequence of surface rumpling. We will also present our latest finding on the effect of cubic-tetragonal transition on the surface structure.

*This work was supported by the US Department of Energy (DOE) under Grant No. DOE DE-SC0002136.
Cryogenic force microscopy of Sketched LaAlO₃/SrTiO₃ Nanostructures

JOSEPH ALBRO (Presenter), JESSICA H MONTONE, FENG BI, MENGCHEN HUANG, Physics and Astronomy, University of Pittsburgh, JUNG-WOO LEE, HYUNGWOO LEE, CHANG-BEOM EOM, Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Physics and Astronomy, University of Pittsburgh —

Local probes can provide insight into the electronic properties of 2D oxide interfaces (in particular, LaAlO₃/SrTiO₃) that are hard to determine using bulk transport methods. Scanning SQUID microscopy has revealed enhanced transport along ferroelastic domain boundaries [1]. Recently, Frenkel et al showed [2] that local pressure applied to the LAO/STO interface can reveal enhanced transport along ferroelastic domain boundaries. We are interested in resolving electron transport in LaAlO₃/SrTiO₃ nanostructures that are “sketched” [3] using conductive-AFM lithography. We describe experiments performed both at room temperature and at low temperatures (<25 K) using a modified vacuum AFM.


Molecular Beam Epitaxy (MBE) Growth of Model Cathode to Study Interfacial Ion Diffusion

BILASH KC (Presenter), JAKE R JOKISAARI, ROBERT KLIE, University of Illinois at Chicago — High performance lithium transition metal oxide battery cathodes, such as LiMn₂O₄, remain a highly active research area. Single-crystals provide well-defined orientations, defect concentrations, homogeneity, and surface terminations that allow isolation of specific chemical and structural aspects of intercalation to be examined. These features make single crystals highly desirable for characterization of pristine and cycled cathodes, compared to polycrystals/particles.

Here we present single-crystal LiMn₂O₄ thin films grown using MBE as model cathodes. Pristine and electrochemically cycled films were characterized using X-ray diffraction (XRD), X-ray photoemission spectroscopy (XPS), transmission electron microscopy (TEM/STEM), and electron energy loss spectroscopy (EELS) to study the effects of surface orientation, Mn dissolution, defects, and solid electrolyte interface (SEI) on the structural changes in the films and interfaces during (de)intercalation.

The authors acknowledge funding from the Joint Center for Energy Storage Research (JCESR), funded by U.S. Department of Energy (DoE). The acquisition of the JEOL JEM-ARM200CF and Gatan Quantum GIF was supported by grants from National Science Foundation (DMR-0959470) and DMR-1626065 respectively.

Homoepitaxial growth of SrTiO₃ by Pulsed Laser Deposition: energetic vs thermal growth

JEFFREY ULBRANDT (Presenter), XIAOZHI ZHANG, University of Vermont, RUI LIU, MATTHEW DAWBER, Stonybrook University, RANDALL HEADRICK, University of Vermont — The role of energetic processes in homoepitaxial growth of SrTiO₃ (STO) by Pulsed Laser Deposition (PLD) was studied via Real-Time X-ray scattering. Two process were developed, an energetic process and a thermal process. Both processes utilized a background gas of 2 mTorr of O₂. The thermal process had an additional 300 mTorr of Helium to act as a buffer gas. Langmuir probe measurements verified the energies of the two process to be between 50-100 electron-volts (eV) and 0.02-0.05 eV respectively. Specular X-ray reflectivity, sensitive to inter-layer transport of material, was the same for both processes. Diffuse scattering, sensitive to the in-plane transport of material, was markedly different. In the thermal process, sharp peaks in the diffuse scattering arise with the growth of each successive layer indicating growth of well correlated islands with a well-defined mean spacing. In the energetic process, diffuse scattering peaks also arise at a similar wavevector, though much weaker and broader. These results suggest an energetic process, such as island breakup, may be responsible for the broadening of the diffuse scattering, in which material from the edges of growing islands is broken off into smaller islands.

This work was supported by NSF Grant: DMR-1506930

Surface Stress in nano-oxides and what it tell us

SIU-WAI CHAN (Presenter), Columbia University — Surface stress of solid surfaces and interfaces is ubiquitous, but has not often been modeled/calculated. In this short talk, experimental results definitely prove that surface stress exists in nanocrystals and can be modified with adsorbents affecting the material's basic properties such as stiffness and thermal expansion. It is particularly influential in surface/interface dominated systems such as thin films and nanoparticles. Whether we choose to deal with it, it will often spring surprises on us during processing for advanced architecture in novel device integration.

NSF DMR Funding 2012-2016
5:18PM C45.00015: Adsorption and destruction of nerve agent sarin and its simulant DMMP on zinc oxide* ROMAN TSYSHEVSKIY (Presenter), SCOTT HOLDREN, University of Maryland College Park, KENAN FEARS, JEFFREY OWRUTSKY, U.S. Naval Research Laboratory, BRYAN EICHHORN, MICHAEL ZACHARIAH, MAJJA M KUKLA, University of Maryland College Park — Discovery and design of new filter materials requires an atomistic level understanding of how these materials interact with toxic agents. High toxicity of chemical warfare agents (CWAs) is the main barrier for experimental study of these compounds which hinders the search for improved filter materials. To fill the gaps in the understanding of CWA interactions with existing and potential filter materials, relatively benign simulant compounds are usually used to replace toxic CWAs. Despite structural similarity of the simulants with real chemical agents the questions have been frequently raised about the reliability of the results obtained for CWA simulants and ability to extrapolate these results to real toxins. Here we report results of our joint DRIFTS, FTIR and DFT study of adsorption and destruction of dimethyl methylphosphonate (DMMP) simulant molecule on ZnO nanoparticles. The synergy between theory and experiment enables further DFT modeling of interactions of the nerve agent sarin with pristine and hydroxylated ZnO surfaces. Results of this work provide new important details on mechanisms and kinetics of destruction of these compounds on ZnO.

*This work was funded by DTRA (HDTRA11510005) R.T. acknowledges support from XSEDE, NERSC, MARCC and UMD supercomputing resources.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C46 DMP: 4d/5d Transition Metal Systems -- Chalcogenides and Nonoxides

2:30PM C46.00001: Electrical and Magnetic Properties of PdSb2 and PtBi2 with Multiple Band Degeneracy* RONGYING JIN (Presenter), Louisiana State University — The discovery of topological properties in condensed matter started a new era of physics. Many fermionic particles and phenomena predicted in high energy physics are now experimentally observed in topological materials such as Dirac, Weyl, and Majorana particles. Their nontrivial topology results from crossings of conduction and valence bands. Depending on crystal symmetry, such crossings can result in degeneracy (g) with g = 2, 3, 4, 6, and 8. It is known that g = 2 corresponds to Weyl fermions, and g = 4 corresponds to Dirac fermions. The cases of g = 3, 6, and 8 are of particularly interesting as they can only be found in condensed matter systems, having no high energy analogues as constrained by Poincare symmetry. In this talk, I will present our experimental investigations on a 4d compound PdSb2 with g = 6, and a 5d compound PtBi2 with g = 3. By analyzing both the de Haas-van Alphen and Shubnikov-de Haas oscillations observed in these compounds, we obtain topological properties of the bands. The implications of these findings will be discussed.

*This work was supported by DOE via DE-SC0012432 and DE-SC0016315.

3:06PM C46.00002: Confirmation of Semiconducting Behavior in TaIrGe ETERI SVANIDZE (Presenter), M BOBNAR, I ANTONYSHYN, MARKUS KOENIG, O SICHEVYCH, U BURKHARDT, F WAGNER, YURI GRIN, Max Planck Institute for Chemical Physics of Solids — Despite being exclusively composed of metallic elements, the half-Heusler compound TaIrGe has been predicted to be a semiconductor with a large indirect gap. Several experimental results, however, have shown metallic behavior. This discrepancy between theoretical prediction and experimental observation is assumed to be due to difficulties in material synthesis. Specifically, the presence of several neighboring phases prevents the synthesis of TaIrGe in single-phase form. With that in mind, we implement focused-ion-beam structuring to polycrystalline TaIrGe. This work does not only provide evidence for intrinsic semiconducting behavior of TaIrGe, but also serves as the first example of selective domain structuring in a polycrystalline material. This novel approach gives a rare opportunity to access materials that cannot be synthesized in single-phase form, sparing costly and time-consuming synthesis efforts, which are frequently futile.
SMITA SPEER (Presenter), HONG CHANG, XIN GUI, MADALYNN G. MARSHALL, WEIWEI XIE, RONGYING JIN, Louisiana State University — Transition-metal stannides are known to exhibit strong d-p hybridization, leading to narrow band gap semiconductors. We have successfully grown Ir$_3$Sn$_{7-x}$Mnx single crystals using the flux method. Single crystal x-ray diffraction refinement indicates that Ir$_3$Sn$_{7-x}$Mnx forms a cubic structure (space group Im3m), and the dopant Mn occupies the Sn site. For x = 0.1, the electrical resistivity shows metallic behavior and can be described by $\rho = \rho_o + aT^2 + bT$ between ~22 K and 300 K. An upturn is observed below 22 K, which is due to an antiferromagnetic (AFM) transition as reflected in the magnetization. Unexpectedly, the application of magnetic field results in negative magnetoresistance below the AFM transition. The effect of Mn doping will be discussed.

*This work is supported by the National GEM Consortium and the Department of Physics & Astronomy, LSU-BR

ZHEN WANG (Presenter), GUIXIN CAO, ZHENYU ZHANG, Louisiana State University, MYUNG-GEUN HAN, LIJUN WU, YIMEI ZHU, RONGYING JIN, 2Condensed Matter Physics and Materials Science Departement, Brookhaven National Laboratory, E WARD PLUMMER, Louisiana State University — Transition-metal dichalcogenide IrTe$_2$ has attracted extensive attention because of its intriguing structural transitions, abnormal resistivity, and superconductivity. While it forms a trigonal phase at room temperature, the structure below the phase transition at 280 K is still in debate. With in-situ transmission and scanning transmission electron microscopy (STEM), we study the phase transitions of IrTe$_2$ single crystal from room temperature down to 20 K. The electron diffraction and imaging results show that IrTe$_2$ below 280 K is phase separated, with the coexistence of the well-characterized 5 × 1 × 5 phase, an intergrowth phases with multiple modulated vectors, and the remaining trigonal phase. The 5 × 1 × 5 phase is present down to 20 K, but we never observe the 6 × 1 × 6 or 8 × 1 × 8 phase previously reported. The valence states of IrTe$_2$ for different phases have been investigated by electron energy loss spectroscopy. A clear picture of the temperature-dependent structural evolution of bulk IrTe$_2$, which is essential to understand the unique electric and magnetic behaviors, will be presented.

**Supported by U.S. NSF through grant No. NSF DMR-1504226

RESHEF TENNE (Presenter), Weizmann Institute of Science — Misfit layered compounds (MLC) of the form (MX)$_{1+y}$TX$_2$ (M=Pb, Sn, rare earth, etc.; X=S,Se,Te; T=Sn, Ta, V, etc.) are known since about 50 years and have been studied by various groups. They are made of an alternating lattice made of one layer of a distorted cubic (orthorhombic) sublattice, like PbS (MS), and hexagonal/octahedral lattice of, e.g. SnS$_2$ or NbS$_2$ (TS$_2$) in a periodic arrangement (denoted as MS.TS$_2$ for brevity). Van der Waals forces hold the MX and TX$_2$ layers together, as well as polarization forces which emanate from partial charge transfer from the MX to the TX$_2$ units. Modern techniques allow synthesizing more complex superstructures from the MX and TX$_2$ sublattices. In many cases, the unit length of the two sublattices coincide along the directions b & c and is incommensurate along a. The lattice mismatch between the MX and TX$_2$ sublattices is known to lead to the formation of microscopic cylindrical crystals for many years.

It was hypothesized that combining the lattice mismatch in the MX.TX$_2$ misfit structure and the general instability of nanocrystals from layered compounds, due to edge effects, will lead to nanotubes (and also nanoscrolls) of small diameter (<300 nm) and high aspect ratio (>10). Exploiting variety of solid state chemical techniques nanotubular structures from a large variety of misfit compounds, like SnS.SnS$_2$; PbS.NbS$_2$ and LnS.TaS$_2$ MLC were synthesized. Several CoO$_2$ based MLC tubes were synthesized and characterized as well. Their structure was studied mostly via transmission electron microscopy as well as some DFT calculations. Raman analysis indicate that the interlayer interactions are stronger in the tubular structures, compared with the bulk MLC. Transport properties of single LaS.TaS$_2$ tubes will be reported as well.

4:18PM C46.00006: Generalization of de Gennes factor for the strong spin-orbit coupled systems. HOSHIN GONG (Presenter), Department of Physics, Pohang University of Science and Technology, Pohang, 37673, Korea, KYOO KIM, SUNGDAE JI, MPPC_CPM, Pohang University of Science and Technology, Pohang, 37673, Korea, BONGJAE KIM, Department of Physics, Kunsan National University, Gunsan, 54150, Korea, BYUNG IL MIN, Department of Physics, Pohang University of Science and Technology, Pohang, 37673, Korea — The magnetic exchange interaction parameters of magnetic systems can be obtained from the consideration of energetics within density functional theory (DFT)-based approaches. Spin Hamiltonians, such as the Heisenberg model, are mainly used to fit the various total energies of magnetic configurations obtained from DFT band calculations, which can be directly compared to the experimental findings including spin-wave dispersions. However, for the strong spin-orbit coupled systems, these approaches often fail and predict wrong energy scales compared to the experimental values due to the entanglement of spin and orbital moments. By including the generalized de Gennes factor, which connects the spin and orbital moments to the total moment, we have found that the better description of exchange interaction parameters can be obtained for the strong spin-orbit coupled systems.

4:30PM C46.00007: A Non-Perturbative, Variational Technique of Calculating RIXS Spectral Response Functions KRZYSZTOF BIENIASZ (Presenter), Stewart Blusson Quantum Matter Institute, University of British Columbia — The field of strongly correlated electrons, and in fact condensed matter physics in general, makes heavy use of spectroscopic experiments to pry into the intricate details of the physical properties of solids. In order to explain the spectra measured in such an experiment a theoretical calculation has to be provided, often relying on some effective model of the physical system under consideration. To explain phenomena such as high-\(T_c\) superconductivity in cuprates or exotic magnetic and orbital phases in manganites, a wide range of spectroscopic measurements are performed, each requiring a different setup and apparatus. Among them, RIXS is a prominent technique which allows one to probe different degrees of freedom of a system with precise control over electron transitions. Our aim is to develop a simple yet accurate standard theoretical tool for calculating RIXS response functions, relying on the non-perturbative, variational (momentum average) approximation to calculate the relevant propagators. This approach should bridge between the exact diagonalization of small clusters vs. perturbative expansion techniques, which until now have dominated the theory of RIXS.

4:42PM C46.00008: Thermoelectric studies of Ir\(_{1-x}\)Rh\(_x\)Te\(_2\) (0 ≤ x ≤ 0.3)* YU LIU (Presenter), HECHANG LEI, KEFENG WANG, MILINDA ABEYKOON, JOHN WARREN, EMIL BOZIN, CEDOMIR PETROVIC, Brookhaven National Laboratory — We present the thermal transport properties of Ir\(_{1-x}\)Rh\(_x\)Te\(_2\) (0 ≤ x ≤ 0.3) alloy series where superconductivity emerges as the high-temperature structural transition (\(T_s\)) is suppressed. The isovalent Rh substitution in Ir\(_{1-x}\)Rh\(_x\)Te\(_2\) results in a slight reduction of lattice parameters and in an increase of number of carriers per unit cell. Positive thermopower \(S(T)\) values for all samples indicate the hole-type carriers. The decrease of \(S(T)\) in pure IrTe\(_2\) (x = 0) at \(T_s\) implies that the Fermi surface is related to partial localization of hole-type carriers below the structural transition. Phonon-related thermal conductivity in pure IrTe\(_2\) (x = 0) features a broad maximum around (50 – 60) K, which is significantly suppressed with Rh substitution. This is mostly contributed by the Rh/Ir doping disorder enhanced point defects scattering. Weak-coupled BCS superconductivity in Ir\(_{0.8}\)Rh\(_{0.2}\)Te\(_2\) that emerges at low temperature (\(T_c^\text{zero} = 2.45\) K) is most likely driven by electron-phonon coupling rather than dimer fluctuations mediated pairing.

*This work has benefited from using the X7B beamline at the NSLS at BNL. Thanks Jonathan Hanson for his help with the x-ray diffraction experiment setup. Work at BNL is supported by the US DOE under Contract No. DE-SC0012704.

4:54PM C46.00009: Magnetic Domains in the Strongly Correlated Weyl Semimetal Candidate CeBi* NATHAN DRUCKER (Presenter), YU LIU, CHRISTIAN MATT, HARRIS PIRIE, Department of Physics, Harvard University, NA HYUN JO, BRINDA KUTHANAZHI, SERGEY L. BUD'KO, PAUL C. CANFIELD, Department of Physics and Astronomy, Iowa State University, JENNIFER HOFFMAN, Department of Physics, Harvard University — Weyl Fermions can arise from Dirac semimetals when the degenerate massless states are split by broken time-reversal symmetry into two bands with opposite chirality. Recently, such states have been predicted in the strongly correlated cerium monopnictides, which develop band inversion as spin orbit coupling increases, and are known to host complex magnetic phase diagrams. Thus cerium monopnictides are ideal materials for studying the interplay of magnetism and topology. Here, we use spin-polarized scanning tunneling microscopy to map the magnetic phases of CeSb and CeBi on the atomic scale. We find distinct magnetic domains with differing spin periodicities, separated by abrupt domain walls. Furthermore, we observe quasiparticle scattering from the domain walls and defects in both materials. Control of these magnetic phases in cerium monopnictides provides the possibility of tuning the key energy scales and momentum splitting of Weyl fermions.

*STM work was supported by DOE EFRC, Center for the Advancement of Topological Semimetals. Work at Ames Lab was supported by the U.S. DOE, BES, DMSE Contract No. DEAC0207CH11358. HP and NHJ were funded by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grants GBMF4536 and GBMF4411.
5:06PM C46.00010: Probing band topology of Weyl-Kondo semimetal candidates CeSb and CeBi by quasiparticle interference imaging*  
YU LIU (Presenter), CHRISTIAN MATT, HARRIS PIRIE, NATHAN DRUCKER, Department of Physics, Harvard University, NA HYUN JO, BRINDA KUTHANAZHI, SERGEY L. BUD’KO, PAUL CANFIELD, Department of Physics & Astronomy, Iowa State University, JENNIFER HOFFMAN, Department of Physics, Harvard University — Topological materials are characterized by strong spin-orbit coupling and bulk band inversion, leading to protected surface states with momentum-locked spin or chirality. Meanwhile, Kondo systems often host rich magnetic phase diagrams because of their strong electron correlations. Materials with both strong spin-orbit coupling and strong electron correlations are predicted to host even more intriguing topological properties. Here we use scanning tunneling microscopy (STM) and quasiparticle interference (QPI) to image the band structure of the predicted Weyl-Kondo candidates CeSb and CeBi. We probe the dispersion of Ce $p$ and $d$ bands, and identify two accidental crossings, one below and one above the Fermi level. We search for topological surface states, by imaging their scattering from atomic defects and magnetic domain boundaries.

*STM work was supported by DOE EFRC, Center for the Advancement of Topological Semimetals. 
HP was funded by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4536 
Work at Ames Lab was supported by the U.S. DOE, BES, DMSE under Contract No. DE-AC02-07CH11358. 
NHJ was funded by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4411

5:18PM C46.00011: Evidence for a purely anionic charge density wave transition in LaAgSb$_2$  
ASHISH CHAINANI (Presenter), JUNG-HAN LI, AMOL SINGH, YEN-FA LIAO, YEN-YI CHU, KU-DING TSUEI, DI-JING HUANG, Condensed Matter Physics, National Synchrotron Radiation Research Center, CHIA-NUNG KUO, CHIN SHAN LUE, Department of Physics, National Cheng Kung University — We study the electronic structure of LaAgSb$_2$, using bulk-sensitive temperature(T)-dependent (20 K – 220 K) Hard X-ray photoemission spectroscopy (HAXPES). LaAgSb$_2$ exhibits two CDW transitions, one below T$_1$ = 207 K along the crystallographic a-axis, followed by a second CDW transition below T$_2$ = 186 K along the c-axis. Recent studies have identified a Dirac-cone band dispersion and nested Fermi surfaces at T = 16 K, but T-dependent measurements were not reported. We use HAXPES to investigate T-dependent changes in the electronic states of La, Ag and Sb in order to identify states responsible for the CDW transition in LaAgSb$_2$. HAXPES core level measurements show that the La 3d and Ag 3d core-levels show negligible changes across the CDW transitions. In contrast, Sb 3d core levels show a clear well-separated satellite formation below T$_1$, and the spectral intensity of the satellite progressively increases on lowering the temperature below T$_2$. The T-dependence of the Sb 3d satellite feature suggests a second order transition, consistent with the known BCS behavior of T-dependent superlattice reflections by x-ray diffraction. The results indicate a purely anionic character CDW transition, with no direct involvement of the La and Ag cationic derived states in the CDW transition.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C47 GERA: Electrochemical Interfaces BCEC 213 - Carlos Gutierrez, Sandia Natl Labs

2:30PM C47.00001: Lithium Electroreduction at Metal/Polymer Interfaces for Lithium Metal Batteries via Atomistic Molecular Dynamics Simulation  
JEONGMIN KIM (Presenter), THOMAS MILLER, Caltech — Understanding and stabilizing lithium electrodeposition is a major bottleneck for developing safe and cyclable lithium metal batteries. The process is complicated by the heterogeneous composition and structure of the solid electrolyte interphase (SEI). To establish a molecular understanding of lithium electroreduction, we employ atomistic molecular dynamics simulations to address ion solvation properties and electron-transfer kinetics of electrochemical reactions at a model SEI/metal interface. Our SEI model is a chemically and structurally well-defined homopolymer including poly (ethylene oxide) (PEO) and poly (ethylene carbonate) (PEC). Model electrodes are either pristine or structurally inhomogeneous with pre-existing deposits. Both the electrodes and deposited lithium are modeled using time-dependent induced-charge polarizability. In this talk, we discuss the effects of the SEI and surface-roughness on the kinetics and mechanism of interfacial lithium electroreduction.
Ab Initio Molecular Dynamics Study of the Effect of Lithium Salts on Lithium Superoxide Clustering in Lithium-Air Batteries

EMILY CRABB (Presenter), ARTHUR FRANCE-LANORD, GRAHAM MICHAEL LEVERICK, YANG SHAO-HORN, JEFFREY C GROSSMAN, Massachusetts Institute of Technology — Lithium-air batteries are an active area of research because of their potential to have a much higher energy density than traditional lithium-ion batteries. However, they are not yet commercially viable due to poor efficiency, high charging voltages, and low cycle lifetimes. Experimental studies of Li-air batteries with aprotonic solvents have shown that the O₂ reduction starts when superoxide (O₂⁻) forms in solvent and reacts with Li⁺ to form lithium superoxide (Li⁺-O₂⁻). Solid Li₂O₂ then forms as the final discharge product on the cathode. Recent experimental work has suggested that a better understanding of the factors governing the behavior of the lithium superoxide in solvent could help control the discharge at the cathode. We are therefore modeling systems of lithium salts and LiO₂ molecules in various common solvents such as dimethyl sulfoxide, acetonitrile, and 1,2-dimethoxyethane to examine how the interplay between solvents and salts affects properties such as LiO₂ clustering behavior. Results from these explicit solvent calculations performed using density functional theory calculations and ab-initio molecular dynamics simulations will be presented and discussed.

*This work is supported in part by a grant from Shell, as well as partial support from a DOE fellowship.

Operando soft x-ray spectroscopy characterization of interfacial charge transfer in energy materials and catalysis

JINGHUA GUO (Presenter), YI-SHENG LIU, Lawrence Berkeley National Laboratory — Soft x-ray spectroscopic techniques with operando capabilities offer the unique characterization in energy conversion/storage materials and catalysis in regards to the functionality, complexity, and interactions among constituents within. It has been found that the microstructure and composition of materials as well as the evolution process have a great influence on performances in a variety of fields, e.g., energy conversion and energy storage materials, chemical and catalytic processes. Operando soft x-ray characterization offers an opportunity to uncover the phase conversion, chemical environment change of elements and other very important information of solid/gas and solid/liquid interfaces in real time. We will overview a number of the experimental studies that successfully revealed the catalytic and electrochemical reactions in real time, e.g. solid (Au or hematite films)/liquid (water) electrochemical interface, Mg-ion batteries, and Li-S batteries. The experimental results demonstrate that the operando soft x-ray characterization provides the unique information for understanding the real reaction mechanism.

*This research used the ALS, a DOE Office of Science User Facility under contract no. DE-AC02-05CH11231. This work was supported by the JCESR and HyMARC of the DOE.

Probing Multiscale Ion Transport and Heterogeneities in High Capacity Battery Materials: From Meso to Micronscale

JAGJIT NANDA (Presenter), Oak Ridge National Laboratory — Majority of electrode materials used for advanced lithium based batteries have well defined chemical composition and particle morphology. The chemistry as well as the microstructure can undergo reversible or irreversible changes under continuous electrochemical charge-discharge cycles. These could have measurable impact on the battery capacity and life. The talk will cover the recent work related to applying x-ray transmission imaging combined with near edge absorption spectroscopy (XANES) to study the evolution of chemical oxidation state of the transition metal (TM) cations accompanied by changes in the particle morphology for lithium-manganese rich NMC cathodes (LMR-NMC). 2D XANES images collected for LMR-NMC cathodes at various stages of cycling (4.8-2.5V) can be reconstructed in 3D to measure bulk changes in TM concentration as well as monitor the change in morphology. The later part of the talk will highlight the various multiscale Raman imaging methods for studying electrode-electrolyte interfaces.

*Research done at Oak Ridge National Laboratory is supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U.S. Department of Energy.
KATHERINE HARMON (Presenter), FELIPE JIMENEZ-ANGELES, Northwestern University, SANG SOO LEE, Argonne National Lab, MICHAEL J BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University, PAUL FENTER, Argonne National Lab — A driving factor in electrochemical energy storage is the adsorption of ions in an electrical double layer (EDL) at the electrode-electrolyte interface. A complete understanding of the structure-property relationships among charged surfaces, ions, and solvents that give rise to the EDL is needed to optimize capacitive energy storage devices. Here, we present in situ X-ray reflectivity (XR) and resonant anomalous XR (RAXR) results of the atomistic, element-specific structure of the EDL at the interface of a graphene/SiC electrode and aqueous RbCl. RAXR data are analyzed using increasingly complex levels of theory of the EDL structure, starting from the simple Gouy-Chapman model of an exponentially decaying charge distribution, to assess the level of theory needed to describe the data. Classical MD simulations of the system qualitatively agree with the experimental structures. A quantitative analysis of the MD predictions is performed via direct comparison of the experimental data with RAXR signals expected from the predicted structures.

This work was supported by MICCoM, DOE/BES. KH gratefully acknowledges support from the DoD NDSEG program, and the Ryan Fellowship from the Northwestern IIN. XR measurements were performed at the Advanced Photon Source at ANL, a DOE/BES facility.

JUN HARUYAMA (Presenter), Institute for Solid State Physics (ISSP), The University of Tokyo, TAMIO IKESHOJI, MINORU OTANI, National Institute of Advanced Industrial Science and Technology (AIST) — Because charge transfer reactions at electrode/solution interfaces limits the performance of lithium-ion batteries (LIBs), it is considered that Li insertion/desorption reaction at the interface between graphite anode and electrolyte solution. Density functional theory + effective screening medium (ESM) method combined with reference interaction site model (RISM), ESM-RISM [1], is applicable to the charge transfer reaction because the chemical potential of electrons (\(\mu_e\)) corresponds to an electrode potential [2] and the distribution function of the solvation is automatically formulated for the solvation/desolvation structures. The reacting Li is moved from the stable site in graphite to the bulk solution region. The constant-\(\mu_e\) ESM-RISM simulations show that the assuming Li path is accompanied by an electron transfer process. The activation energy at equilibrium potential is approximately 0.6 eV[3], which is consistent with experiments. The dependences of the activation energy and the surface charge density according to the Li content x (LixC6, x=0, 0.5, 1) are further discussed. [1] S. Nishihara and M. Otani, PRB 96, 115429 (2017). [2] J. Haruyama, T. Ikeshoji, and M. Otani, PRM 2, 095801 (2018). [3] J. Haruyama, T. Ikeshoji, and M. Otani, J. Phys. Chem. C 122, 9804 (2018).

PRIYA SRIVASTAVA (Presenter), MONOJIT BAG, Indian Institute of Technology Roorkee — A lot of research has been done on the efficiency improvement of Perovskite Solar Cells by optimization of the film morphology using various techniques including electrochemical impedance spectroscopy (EIS) in a solid-state active device geometry.1 Recently, the optimization of the film morphology at liquid electrolyte interface by EIS is trending as a more simplified and accurate approach.2,3 Here, we have studied the charge transfer at the methylammonium lead tri-iodide (MAPbI3) perovskite-liquid electrolyte interface under the effect of applied bias. By applying the different dc bias from +1V to -1V, it was found that the ion diffusion at low-frequency regime changes significantly with bias. Also, the films show the same trend of change in impedance under positive and negative bias, which reveals the ambipolar nature of the hybrid perovskites. The ions migrate more under light and get accumulated at the interface in the dark as depicted by the Nyquist plot. We have simulated a model to explain the charge kinetics across the interface with different applied bias under dark and light.

References
Here we investigate the electrodeposition dynamics at a solid-solid interface. We find that the stress-field alters the conduction pathways in the electrolyte and gives rise to a non-monotonic ionic transport. Additionally, the strain-energy alters the reaction free-energy landscape and causes further complexations. The electrodeposition at the solid-solid interface turns out to be governed by both the bulk as well as surface characteristics.

The effects can be summarized by desorption of oxygen-containing species from the sample surface and by reactions within the film. Also presented is an estimate of the layer thickness’ time evolution during prolonged SR exposure.


4:18PM C47.00010: Decomposition of phosphorus-containing additives at a charged NMC surface: atomistic modeling insights  
HAKIM IDDIR, JUAN GARCIA (Presenter), ADAM TORNHEIM, Argonne National Laboratory, RITU SAHORE, Oak Ridge National Laboratory, IRA BLOOM, ZHENGCHENG ZHANG, Argonne National Laboratory — Stabilizing the cathode/electrolyte interface at high voltage is necessary to achieve higher capacities while still maintaining capacity retention in Lithium-ion batteries. One strategy is through the use of additives in the electrolyte: components in low concentration (<10%) that have a lower anodic stability than the baseline electrolyte, so that during the initial cycles, the additive will decompose on the charged cathode surface preferentially over the baseline electrolyte. This reaction will then yield a layer which will inhibit further reaction between the electrolyte and the cathode surface. However, the mechanism of improvement remains unclear. In the present work, Density Functional Theory is used to gain insights and understanding on experimental results using a potentiostatic hold technique to evaluate cathode/electrolyte reactivity for two families of additives: phosphites and phosphates. Simulations indicate the susceptibility of the various additives to electrochemical and chemical oxidation, showing chemical oxidation to be much more likely with the phosphite moiety. The identity of the ligands on the phosphorus-containing additive can dramatically affect both the decomposition current and the cathode surface film.

4:30PM C47.00011: Characterization of Electrical Energy Storage Interfaces with Advanced Optical, Electrochemical, and X-ray Probes  
JONATHAN LARSON (Presenter), HANS BECHTEL, ETHAN J CRUMLIN, ROBERT KOSTECKI, Lawrence Berkeley National Laboratory — Novel and improved methods for energy storage are urgently required to enable effective use of renewable energy sources and to facilitate energy demand-response management across time and length scales. While lithium-ion batteries meet many of the criteria required for portable electronics, they are insufficient to meet the requirements for emerging applications (e.g. aerospace) and grid scale storage. New electrical energy storage concepts are needed to meet these current and future demands. Central to the onset of transformational breakthroughs is the need to increase understanding of the fundamental physical and chemical processes that occur in these complex systems. To this end, we plan to impact this space by leveraging synchrotron-enabled scanning broadband nanoscopy and nano-FTIR spectroscopy for local information on permittivity and chemistry, scanning nanobattery probes for local nano-electrochemical testing, and ambient pressure X-ray photoelectron spectroscopy. Here we provide an operational overview, and the advantages of, these cutting-edge characterization techniques for advancing the basic science of electrical energy storage interfaces.

*Funding to support this work was provided by the Energy & Biosciences Institute through the EBI-Shell program.
Lithium-sulfur battery is considered as promising substitute of Li-ion battery for the next generation energy storage system. However, the intermediate process during charging and discharging cycles is not clear. It is believed that Li$_2$S$_2$ is one of the most important intermediate products which may present as insoluble solid phase in the system. In this talk, we considered three phases of crystalline Li$_2$S$_2$ (tetrahedra, triclinic and hexagonal) to investigate their thermodynamic and mechanical stability based on density functional theory. The results show that the hexagonal Li$_2$S$_2$ is relatively stable than the other two phases. The highly anisotropic mechanical characteristics of Li$_2$S$_2$ are shown to be due to the unique arrangement of S-S bonds in these crystalline structures.

Computational Development of an Artificial Solid Electrolyte Interphase for Rechargeable Multivalent Ion Batteries

JOSHUA YOUNG (Presenter), MANUEL SMEU, Physics, Binghamton University — Multivalent ion batteries (MVIB), or those utilizing Mg, Ca, Zn, and Al, are garnering increasing attention as alternatives to Li-ion batteries in non-portable applications such as grid storage, as they are energy dense, cost efficient, and safe. The development of such MVIBs, however, has been hindered by the inability of existing electrolytes to reversibly plate and strip metallic anodes. This is a particular problem in Ca ion batteries, as the solid-electrolyte interphase (SEI, the passivating layer which forms between the electrolyte and anode) does not allow for the migration of Ca$^{2+}$ ions. In this work, we develop an understanding of this SEI using a computational approach combining DFT and ab initio molecular dynamics (AbMD) simulations. First, we show that AIMD can be utilized to predict the decomposition products making up the SEI in a variety of systems containing different anodes and electrolytes. Second, we demonstrate that the use of an amorphous Al$_2$O$_3$ layer between the Ca metal anode and organic electrolyte prevents decomposition while allowing for the transport of Ca ions. We propose that this strategy can aid in the development of rechargeable Ca ion batteries by completely avoiding the formation of an ionically insulating SEI from electrolyte decomposition.

Predicting pseudocapacitve adsorption isotherms through quantum-continuum calculations

NATHAN KEILBART (Presenter), Pennsylvania State University, YASUAKI OKADA, SHINICHI HIGAI, Murata Manufacturing Co., Ltd., ISMAILA DABO, Pennsylvania State University — Pseudocapacitive electrodes function through redox reactions that occur on the surface of the electrode allowing for high charging/discharging rates. Complex interfaces cause much to be unknown about the pseudocapacitive process. Computational modeling has made progress in predicting the response of these systems but further research is needed to optimize performance. A theoretical approach is developed to study pseudocapacitive systems, focusing on ruthenium dioxide (RuO$_2$). Material properties from quantum-continuum simulations are combined with Monte Carlo sampling to predict adsorption isotherms. Computational findings for the RuO$_2$ (110) surface show good agreement with experimental data where the double-layer contribution is shown to be a small fraction of the overall electrochemical response but controls to a overall pseudocapacitive response of the electrode. By focusing on the double-layer contribution, different trends emerge based on the surface orientation. For RuO$_2$ (110), the double-layer capacitance from electronic-structure methods show a small spread while a downward trend is seen for (100) with increasing coverage. By using double-layer capacitance predicted from first principles, good agreement is reached with experiment along the (100) surface orientation.

Decoding the surface instability of perovskite oxides at the atomic level: Sr segregation in La$_{1-x}$Sr$_x$MnO$_{3-\delta}$ in SOFC electrodes

FRANZISKA HESS (Presenter), BILGE YILDIZ, Nuclear Science and Engineering, Massachusetts Institute of Technology — One of the most important and best-studied perovskite materials for energy conversion applications is La$_{1-x}$Sr$_x$MnO$_3$ (LSM). As the oxygen exchange at the surface is typically rate-limiting, tuning of the electrode surface is a key aspect in the development and optimization of materials for energy conversion applications. Sr-doped perovskite materials form passivating Sr-rich layers which inhibit the oxygen exchange at the surface, thus reducing the efficiency of the SOFC. We assess the stability of LSM surface and bulk using a combination of DFT calculations on the GGA+U level and DFT-based thermodynamics. We find the clean LSM(001) surface to be unstable and prone to reconstructions and defect segregation.

Considering a wide variety of near-surface defects, as well as the growth of SrO as clusters, particles or homoepitaxial layers, we come to the conclusion that Sr segregation should be self-limiting because the surface dipole moment is removed by SrO overlayers that do not cover the entire surface. These surface terminations are stable and not prone to further segregation of Sr.

These results allow us to develop a knowledge-based doping strategy that prevents Sr segregation in LSM. Our modeling strategy and principle findings are transferable to other perovskite oxides.
Monday, March 4, 2019 2:30 PM - 4:18 PM

Session C48 DFD GSNP: Fluid-Structure Interactions (FSI) II  BCEC 251 - Frederick Gosselin, Ecole Polytechnique de Montreal - Tag(s): Focus

2:30PM C48.00001: Vortex-induced vibration of a flexibly-mounted cylinder placed in the proximity of a stationary parallel cylinder*  MAHDI RIAZAT, RAMIN GHOREISHI, BRIAN VERMEIRE, MOJTABA KHEIRI (Presenter), Mechanical, Industrial and Aerospace Engineering, Concordia University — Some computational results on the vortex-induced vibrations (VIV) of a flexibly-mounted cylinder placed in the proximity of a stationary parallel cylinder will be presented. Simulations are performed at moderate Reynolds numbers (100<Re<1000), where VIV features of the non-stationary cylinder are examined for various gap sizes between the two cylinders and for different diameters of the stationary cylinder. An in-house fluid-structure interactions solver based on HORUS platform -- an open-source LES/DNS flow solver -- is used for simulations with two- and three-dimensional (2- and 3-D) cylinders. The results for 2-D cylinders of the same diameter at Re=150, the reduced velocity of 5 and for the centre-to-centre distance of 3.5D* (D* being the cylinder diameter) show a broken-symmetry vortex-shedding pattern behind the oscillating cylinder. This is caused by interactions between vortices shedding from the oscillating and stationary cylinders, as well as formation of a gap flow between them. Previous computational studies considered only 2-D cylinders and employed RANS flow solvers coupled with turbulence models.

*MR and MK appreciate support from Concordia University. BV and RG acknowledge support from NSERC, Calcul Quebec, WestGrid, SciNET, Compute Canada, and FRQNT.

2:42PM C48.00002: Modal Analysis of Strongly Coupled Fluid-Structure Interaction Problems*  ALEXANDRE COUTURE (Presenter), FREDERICK GOSSELIN, STÉPHANE ÉTIENNE, Department of Mechanical Engineering, Polytechnique Montreal — With recent trends in many energy markets, the use of hydroelectric turbines is shifting from base power delivery to grid regulators. The emergence of intermittent renewable energy sources is increasing the need for the use of turbines in off-peak conditions and frequent starts and stops. These cause transient phenomena that can be damageable to the fatigue life of the main turbine components. To tackle this issue, knowledge of the turbines vibration modes frequency and damping coefficient is essential. In this context, we developed a new modal analysis method for strongly coupled fluid-structure interaction (FSI) problems. The proposed technique couples linear elastic equations and linearized Navier-Stokes equations in a finite element formulation. This allows for the evaluation of the frequency and damping coefficient of the coupled modes of complex structures subject to important flows without the need for computationally heavy fully coupled non-linear time-integration FSI simulations. For now, a proof of concept has been elaborated using the 2D flag flutter problem and it was validated using 3D hydrofoil experiments.

*This work is supported by the Natural Sciences and Engineering Research Council of Canada (NSERC), FRQNT and the Trottier Energy Institute.

2:54PM C48.00003: Modal analysis of a spinning disk in a dense fluid as a model for high head hydraulic turbines*  MAX LOUYOT (Presenter), Laboratory for Multiscale Mechanics, Department of Mechanical Engineering, Polytechnique Montreal, BERND NENNEMANN, CHRISTINE MONETTE, Andritz Hydro Canada Inc., 6100 Trans Canada Hwy., Pointe-Claire, H9R 1B9, Québec, Canada, FREDERICK GOSSELIN, Laboratory for Multiscale Mechanics, Department of Mechanical Engineering, Polytechnique Montreal — In high head Francis turbines and pump-turbines in particular, RSI is an unavoidable source of excitation that needs to be predicted accurately. Precise knowledge of turbine dynamic characteristics, notably the variation of the rotor natural frequencies with rotation speed and added mass of the surrounding water, is essential to assess potential resonance and resulting amplification of vibrations. In these machines, the rotating disk-like structures of the runner crown and band as well as the head cover and bottom ring give rise to the emergence of diametrical modes and a mode split phenomenon for which no efficient solution method exists to date. Fully coupled FSI methods are too computationally expensive; hence, a simplified method based on the modal force approach would be a powerful tool for the design and expected life prediction of these turbines. This work presents the development of an analytical model for a rotating disk in a dense fluid, which accurately predicts the natural frequency split as well as the natural frequency drift that are observed in experiments. Additionally, the analytical model gives an explanation on the physical origin of the mode split phenomenon.

*We would like to thank the MITACS program and Andritz Hydro for funding this work.
3:06PM C48.00004: Force and wake observations for a circular cylinder undergoing forced 2-DOF motion in a free stream  JASON M DAHL (Presenter), ERDEM AKTOSUN, Ocean Engineering, University of Rhode Island — A series of forced motion experiments were performed for a circular cylinder undergoing combined in-line and cross-flow motion in a free stream. Variation of the in-line amplitude, cross-flow amplitude, reduced velocity, and phase between in-line and cross-flow motions were made for a Reynolds number of 7620, with a total of 9555 experiments. Forces were measured for all experiments and PIV visualization of the wake was made for select experiments. Specific phases between in-line and cross-flow motion are shown to have multiple possible wakes depending on the length of the experiment, with specific motion combinations being particularly sensitive to the conditions of the experiment. Although all forced motions were symmetric, asymmetry was observed in the wake for specific combinations of motion parameters, leading to asymmetric forcing and large mean lift. The measured forces and resulting wake are particularly sensitive to the phasing between in-line and cross-flow motion, indicating that if using forces derived through forced motion experiments for the prediction of 2-DOF vortex-induced vibrations, one should have sufficient resolution in the phase parameter in order to properly capture the variation in forces.

3:18PM C48.00005: Insights on the pressure distributions of controlled ice-induced vibration experiments ERSEGUN DENIZ GEDIKLI (Presenter), TORODD NORD, Norwegian University of Science and Technology — Increased need for energy pushed offshore wind, oil, and gas companies into deeper waters in the Arctic and Subarctic regions, bringing extra challenges with it. It is observed that dynamic interaction between the offshore structure and floating ice sheet might result in ice-induced vibrations, which can contribute to fatigue damage. To better understand this complex phenomenon, forced ice-induced vibration experiments are carried out in the ice tank at the Hamburg Ship Model Basin (HSVA), Hamburg, Germany. In the tests, different rigid structures are forced through the still ice by systematically changing the ice speed. Pressure distributions in the ice-structure interface and resulting structural motions are analyzed using two multivariate analysis methods: 1) proper orthogonal decomposition and 2) smooth orthogonal decomposition. Results indicate that both methods capture the dominant pressure variations successfully and result responses that are physically interpretable. For example, first pressure mode illustrates the ductile pressure variation on the structure, which varies in the ice drift direction, and some combinations of second and third pressure modes represent the oscillations in the cross-flow direction, which illustrate the complex nature of ice-induced vibrations.

3:30PM C48.00006: Burst-and-coast swimming in zebrafish  BENJAMIN THIRIA (Presenter), RAMIRO GODOY-DIANA, BILL FRANÇOIS, ESPCI ParisTech, FREDERIC LECHENAULT, Ecole Normale Supérieure — Swimming kinematics of small fish such as zebrafish are characterized by intermittent sequences consisting in an active swimming phase directly followed by a passive coast phase. These specific sequences are based on a coupling between sensing and decision: fish use the passive time to sense their environment and prepare their next move. Fish essentially use vision and the lateral line system to see and sense their surrounding environment. The mechanisms that govern this “sensing” to “decision-making” (S2D) process are still to be understood and detailed. This work is an attempt to characterize these sequences using several archetypal model experiments and models gathering hydrodynamics, statistics and behavioral sciences. We will focus on new results obtained from real fish experiments in free swimming and forced gait configurations (using a controlled swimming channel). We will show how the statistics of these S2D sequences evolve with the conditions of the experiment; the important parameters being here the external flow conditions and the size of the habitat, but also the species and the maturity state of the fish (larva, juvenile or adult). We believe that these results will have direct implications on the design and implementation of biomimetic robotic systems.

3:42PM C48.00007: Swimming via size-change: High efficiency propulsion using resonant fluid-structure interactions  GABRIEL WEYMOUTH (Presenter), Faculty of Engineering and Physical Science, University of Southampton — Cephalopods use large-scale structural deformation to propel themselves underwater, changing their internal volume by 20-50%. In this work, the hydroelastic response of a swimmer comprised of a fluid-filled elastic-membrane is studied via analytic, numerical, and experimental methods. The self-propelled soft-body fluid and solid dynamics are shown to benefit greatly from the irreversible jet flow, the reversible internal added-mass variation, and the pulsation in tune with the swimmer’s immersed fundamental frequency. It is shown that even a simplistic size-changing structure can utilize these physical mechanisms to achieve quasi-propulsive power ratios of greater than 100%, i.e. self-propulsion for these swimmers requires less energy than towing at the same speed.
3:54PM C48.00008: Breakdown of continuum models of fluid structure interaction in a nanoporous biological material* STEVEN HARRELLSON (Presenter), Department of Physics, Columbia University, MICHAEL DELAY, XI CHEN, Department of Biological Sciences, Columbia University, AHMET HAMDI CAVUSOGLU, Department of Chemical Engineering, Columbia University, OZGUR SAHIN, Department of Physics, Columbia University — Determining how porous materials interact with permeating fluids is important for understanding their mechanical properties. Existing approaches often treat the permeating fluid as a continuous medium, but for many materials the pore dimension can be on the order of a nanometer, close to the size of a single water molecule. It is not clear how the discreteness of the permeating fluid affects the macroscopic mechanical properties of these materials. Here we show the bacterial spore, a dormant biological nanoporous structure, exhibits mechanical properties that challenge theoretical models based on continuum treatment of water. We found a statistical mechanical treatment of the confined water correctly predicts a range of equilibrium and dynamic properties of the spore, including an extreme slowdown of relaxation kinetics and a highly nonlinear mechanical response. Because the underlying assumptions of this approach are based on the geometry and not specific to the spore chemistry, these findings could also be applicable to other nanoporous materials.

*Funding was provided by U.S. Dept. of Energy (DOE) Early Career Research Program, Office of Science, Basic Energy Sciences (BES), under award no. DE-SC0007999; as well as the David and Lucile Packard Fellows Program.

4:06PM C48.00009: Enhancing and controlling parametric instabilities in structures: Application to an electromagnetic pendulum. ARNAUD LAZARUS (Presenter), Department of Mechanical Engineering, Sorbonne Université, SUZIE PROTIÈRE, Institut Jean Le Rond d’Alembert, CNRS — Parametric instabilities are dynamical instabilities arising when the mechanical state of a structure is properly modulated in time. It is sometimes seen as a phenomenon to avoid for sailing ships (parametric rolling) or landing helicopters (ground resonance) but it has also been exploited in vibrating fluids (Faraday waves) or NanoElectroMechanical Systems (parametric amplification). One well-known limitation in fully exploiting classic parametric instabilities based on small periodic modulation of a mechanical state is that inherent friction forces rapidly cancel sub-harmonic parametric resonances. To overcome this drawback, we suggest to formerly modify the state of a mechanical system close to its diverging instability, so that it becomes possible to periodically modulate a system between a naturally oscillating and diverging state. This original way of enhancing and controlling parametric instabilities is illustrated here through the numerical and experimental implementation of an electromagnetic pendulum. Not only we find it is possible to greatly enhance the number of subharmonic instability regions, but it is feasible to control the width of those regions, opening a promising way for frequency filtering in NanoElectroMechanical Systems.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C49 DPOLY: Advanced Morphological Characterization of Polymer II: X-ray and Neutron Scattering BCEC 252A - Brian Collins, Washington State University - Tag(s): Focus

2:30PM C49.00001: Role of Chain Length in the Formation of Frank-Kasper Phases in Diblock Copolymers* FRANK BATES (Presenter), RONALD LEWIS III, AKASH ARORA, HALEY BEECH, BONGJOON LEE, AARON LINDSAY, TIMOTHY LODGE, KEVIN DORFMAN, University of Minnesota — Formation of the Frank-Kasper (FK) sigma phase in compositionally asymmetric A-B diblock copolymer melts has been shown using self-consistent mean-field theory (SCFT) to be associated with conformational asymmetry, \( b_A/b_B > 1 \), where \( b \) is the statistical segment length. Small-angle X-ray scattering and rheological measurements performed with narrow dispersity poly(styrene)-b-poly(butadiene) (PS-PB) diblocks show an absence of the FK sigma phase whereas poly(ethylethylene)-b-poly(lactide) (PEE-PLA) diblocks exhibit a wide composition window of this complex phase, where both systems have \( b_A/b_B = 1.3 \). This behavior is associated with block self-concentration expressed through the invariant degree of polymerization \( N(bar) = Nb^6/v^2 \) in which \( v \) is the statistical segment volume. A direct analogy will be drawn between the role of \( N(bar) \) in FK phase formation in diblocks and the value \( N_e(bar) \) that defines the universal crossover from Rouse to reptation dynamics in homopolymer melts, where the block values of \( N(bar) \) for PEE-PLA and PS-PB are less than and greater than \( N_e(bar) \), respectively.

*Support from NSF DMR-1104368 and DMR-1725272

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2:42PM C49.00002: PRISM Theory as an Accessible Model for Neutron and X-ray Scattering Experiments of Liquid-Like Polymer Systems  
TYLER MARTIN (Presenter), RONALD JONES, National Institute of Standards and Technology — Polymer Reference Interaction Site Model (PRISM) theory is able to predict the structure and thermodynamics of a wide range of liquid-like polymer systems including polymer melts, blends, solutions, polyelectrolytes, and nanocomposites. Using single-molecule, intra-molecular correlations as input, past studies have used PRISM to model the experimental scattering data of concentrated solutions and melts, including data from small-angle neutron scattering (SANS), small-angle X-ray scattering (SAXS), and wide-angle X-ray scattering experiments (WAXS). Despite its utility in these studies, PRISM theory has remained inaccessible to many scientists seeking to extract thermodynamic and structural information from their scattering data of liquid-like polymer systems. Recently, we have released a computational tool called pyPRISM which aims to reduce the barrier to accessing PRISM theory and allow users to calculate structure factors and total scattering intensities from single-molecule scattering functions. In this talk, we will discuss the features and limitations of using PRISM theory as a scattering model by highlighting our efforts in using pyPRISM to create new models for the scattering of several systems including worm-like micelles, monoclonal antibodies, and bottlebrush polymers.

2:54PM C49.00003: Phase Behavior of Hybrid Inorganic-Organic Diblock Copolymer Electrolytes  
GURMUKH SETHI (Presenter), University of California, Berkeley, IRUNE VILLALUENGA, Lawrence Berkeley National Laboratory, NITASH BALSARA, University of California, Berkeley — Solid polymer electrolytes are advantageous for applications in lithium batteries due to improved chemical stability compared to organic liquid electrolytes. Diblock copolymer electrolytes offer highly tunable nanostructures with both soft, ion-conducting domains and mechanically rigid non-conducting domains. The phase behavior of poly(ethylene oxide)-block-polyhedral oligomeric silsesquioxane acrylate (PEO-POS) mixed with lithium bis(trifluoromethane)sulfonimide (LiTFSI) salt is studied by varying the diblock composition and salt concentration. Using small angle X-ray scattering (SAXS), the morphology and Flory-Huggins interaction parameter is obtained to quantify the thermodynamic interactions. PEO-POS without salt exhibits a classical order-disorder transition. Adding salt dramatically changes the phase behavior and a disorder-order transition is observed upon heating. Upon further salt addition, a transition from lamellae to coexisting lamellae and hexagonally packed cylinders is observed. Our results suggest that the addition of salt plays a more complicated role in this hybrid organic/inorganic electrolytes in comparison to traditional all organic diblock copolymer electrolytes.

*This work was supported by a National Science Foundation Graduate Research Fellowship.

3:06PM C49.00004: In Situ Study of ABC Triblock Terpolymer Self-Assembly under Solvent Vapor Annealing  
SANGHO LEE (Presenter), LI-CHEN CHENG, Materials Science and Engineering, Massachusetts Institute of Technology, KEVIN G. YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory, MUHAMMAD MUMTAZ, KARIM AISSOU, Laboratoire de Chimie des Polymères Organiques, CNRS – ENSCPB – Université de Bordeaux, CAROLINE ANNE ROSS, Materials Science and Engineering, Massachusetts Institute of Technology — The morphological transition of core-shell cylinder-forming triblock terpolymers during solvent vapor annealing is monitored in situ using grazing-incidence small-angle X-ray scattering. We investigate the self-assembly behavior of two linear ABC triblock terpolymers, poly(1,1-dimethyl silacyclobutane-block-styrene-block-methyl methacrylate) (PDMSB-b-PS-b-PMMA or DSM) and poly(1,1-dimethyl silacyclobutane-block-styrene-block-lactide) (PDMSB-b-PS-b-PLA or DSL). The morphology, orientation, and period of the microdomains are characterized under a continuous vapor flow of CHCl₃ as a function of deswelling rate and swelling ratio. Films of DSM form in-plane core-shell cylinders, while DSL films predominantly form vertically oriented core-shell cylinders. A reversible order-order phase transformation between spheres and cylinders and a reorientation from in-plane to out-of-plane cylinders occur during the annealing process.

*This work was supported by NSF DMR-1606911. Shared experimental facilities of CMSE, an NSF MRSEC under award DMR-1419807, were used. This research used resources of the Center for Functional Nanomaterials, and the National Synchrotron Light Source II, which are U.S. DOE Office of Science Facilities, at Brookhaven National Laboratory under Contract No. DE-SC0012704.
**3:18PM C49.00005: In-situ Observation of Non-solvent-induced Phase Separation of Cellulose Cuprammonium Solution by Small-Angle X-ray Scattering**. KAZU HIROSAWA (Presenter), TATSUMI IWAMA, MAIKO YAMAGATA, NAOKI SAKAMOTO, AYUMI KUROHARA, YOSHIYUKI SHIOMI, TORU MORITA, Asahi Kasei Corporation — Phase separation caused by permeation of non-solvents into polymer solution is called non-solvent-induced phase separation (NIPS). NIPS are often applied to fabrication processes of polymer materials such as wet-spinning of fibers and porous membranes. For example, NIPS of cellulose cuprammonium solution in water has been utilized to manufacture regenerated cellulose fibers. Hence, understanding the mechanism of NIPS has crucial importance in chemical industries. However, study of NIPS is challenging because it is complicated process which includes time-dependent variation of composition of polymer, solvent, and non-solvent molecules. To understand the structure formation mechanism, we performed in-situ structural analysis on NIPS process of cellulose in cuprammonium solution by means of small-angle X-ray scattering (SAXS). From time-development of SAXS profiles of the cellulose solution, we characterized phase separation structure and the dynamics of structural growth. Eventually, we clarified that network structure having ~ 10 nm characteristic length is formed by desorption of ammonia from cellulose solution into water.

*The SAXS experiment was performed at the Frontier Soft Matter Beamline (FSBL; BL03XU), SPring-8, Hyogo, Japan (proposal No. 2017A7201, 2017B7251).

**3:30PM C49.00006: The Multi-Layered Structure of Novel Cellulose-Coated Oil-in-Water Emulsions Revealed by Contrast Variation Neutron Scattering**. YACHIN COHEN (Presenter), SOFIA NAPSO, DMITRY REIN, Chemical Engineering, Technion - Israel Institute of Technology, ZHENDONG FU, AUREL RADULESCU, Jülich Center for Neutron Science, Heinz Maier-Leibnitz Zentrum — Amphiphilic cellulose chains dissolve molecularly in the ionic-liquid 1-ethyl-3-methylimidazolium acetate. When the solution is mixed vigorously with oil and water a stable oil-in-water emulsion is formed, as water regenerates an amorphous cellulose coating on the oil droplets. Imaging by cryo-transmission electron microscopy indicated a unique multilayered structure of the cellulose coating. Small-angle neutron scattering from these emulsions was measured at three contrasts: full contrast (protiated oil and cellulose in D2O), shell contrast (oil matched to D2O) and core contrast (water matched to cellulose). The fitted model describes a spherical core with two concentric shells. The fitted parameters were the core diameter and thicknesses of the two shells, and the scattering length densities of the inner and outer shells, to account for their cellulose content. Particular attention was focused on whether the inner shell is imbibed by water or oil. It was concluded that the oil core (diameter 67±17 nm) is surrounded by a water-imbibed cellulose hydrogel (~3% cellulose), of thickness 34.5 nm an outer coating of a dense cellulose layer 3.5 nm thick. This novel structure may be utilized as a microreactor for cascade enzymatic reactions.

*the Israel Science Foundation and JCNS

**3:42PM C49.00007: Probing chemical pathways in polyamide reverse osmosis membranes**. ALEXANDRA PORTER (Presenter), Materials, Imperial College London — Reverse Osmosis (RO) membranes are widely used for sea water desalination applications. As the cost of installing desalination plants at sea is high it has become important to have a fundamental understanding of how the membranes work so that costs can be reduced. Much effort has gone into understanding the bulk properties of the membranes, but little effort on understanding the nanoscale interactions that control ion selectivity. The membranes are made from a polyester backing layer, a polysulfone (PSf) support and a polyamide (PA) membrane which is typically 100-500nm thick in a commercial membrane. Due to the membrane’s complex hierarchical structure, the controllability of ion selectivity remains unclear.

Recent work has suggested that although complex, the structure is actually made out of a single sheet of membrane about 10nm thick that has been ‘crumpled’. There is also evidence that the top and bottom surfaces of the membrane are terminated with different functional groups suggesting that ion permeation pathways across the membrane may be due to chemical variations. Because of the amorphous nature of the polymer it is impossible to visualize any physical or chemical pathways using conventional transmission electron microscopy or scanning TEM (STEM). The only method that can be used to investigate variations in chemistry on the sub nanometre scale is spatially resolved electron energy-loss spectroscopy (EELS).

Here we use monochromated EELS spectrum imaging to map differences in the spatial distribution of C, N and O across flat in-house fabricated 10nm membranes and rough commercially available membranes. Additionally we show clear changes in the fine structure of the C K edge in the different polymer layers (PSf, PA and resin) as well as changes across the membrane itself. The chemical pathways that can be deduced from these findings provide us with a much clearer understanding of the transport mechanisms through the membrane.

*BPICAM*
4:18PM C49.00008: Enzyme Immobilization in Mesoporous Metal-Organic Frameworks by SANS* LILIN HE (Presenter), Oak Ridge National Laboratory, XIAOLIANG WANG, Department of Chemistry, University of South Florida, SHUO QIAN, Oak Ridge National Laboratory, SHENGQIAN MA, Department of Chemistry, University of South Florida — Metal-organic frameworks (MOFs) are an emerging class of solid supports for enzyme immobilization owing to their high accessible pores and tunable pore size and surface for increasing affinity between enzymes and supports. Although the immobilization of enzymes by MOFs has shown improved catalytic efficiency, enzymes’ location in the hierarchical solid matrix, the relationship between enzyme dimension and pore size, and conformations of encapsulated enzymes remain elusive. In this work, we present a small-angle neutron scattering (SANS) characterization of cytochrome C (CyT. C) adsorbed into Tb-TATB under in-situ conditions. The scattering curve of unloaded Tb-TATB showed mass fractal feature arising from the network structure and a shoulder at ~0.03Å presumably corresponding to disordered building blocks or defects in the crystals. The correlation peaks located between 0.07 and 0.4 Å⁻¹ were attributed to ordered arrangement of two nanopores, 39 Å and 47 Å, respectively. Upon loading of the CyT. C, substantial decreasing intensities of Bragg peaks proved the entry of enzyme molecules into the MOF’s cages with entry windows that are smaller than the enzyme.

*The Bio-SANS beamline is supported by DOE BER office. X. W. and S. M. thank National Science Foundation (DMR-1352065).

4:30PM C49.00009: The Influence of Ionic Liquids on the Nanostructure of Polyimide based Aerogels SAMANTHA J. RINEHART (Presenter), University of Tennessee, BAOCRAU N. NGUYEN, Ohio Aerospace Institute, ROCCO P. VIGGIANO, MARY ANN B. MEADOR, NASA Glenn Research Center, MARK DADMUN, University of Tennessee — Aerogels are promising materials for many aerospace applications, including high performance antennae and flexible insulation because of their inherent low density-high surface area properties. Polymeric aerogels, more specifically polyimide aerogels (PIA), provide excellent mechanical properties beyond traditional silica aerogels while maintaining the required thermal stability. NASA has investigated PIA paired with ionic liquids to develop novel mechanically robust electrolyte systems for next generation batteries. PIA surface area, porosity, and pore volume are important properties; however, these measurements are traditionally conducted sans solvent. Because of this, the impact of the ionic liquid on the nanoscale structure of PIA is unclear. To determine the impact of solvent presence, we use small angle neutron scattering to determine solvated PIA skeletal size and composition. Our results indicate that the pores as well as the polyimide skeleton absorb solvent. The amount of solvent uptake in the struts is dependent upon ionic liquid structure as well as polyimide structure. These results broaden the characterization of polymeric aerogels and provide the ability to correlate structural characteristics to their performance.

4:42PM C49.00010: Effect of Electrostatic Interactions Between Nafion and Functionalized Nanoparticles on Ionomer Morphology and Nanoparticle Dispersion ALLISON JANSTO (Presenter), APOORVA BALWANI, Department of Chemical and Biomolecular Engineering, Clemson University, TYLER MARTIN, RONALD JONES, Center for Neutron Research, National Institute of Standards and Technology (NIST), ERIC DAVIS, Department of Chemical and Biomolecular Engineering, Clemson University — Ionomer nanocomposites have emerged as a promising replacement to traditional polymer electrolyte membranes for technologies like vanadium redox flow batteries as they curtail undesired vanadium ion crossover while maintaining high proton conductivity. However, the mechanism by which the introduction of silica nanoparticles (SiNPs) acts to increase ion selectivity remains elusive. Presently, SiNP surface chemistry was systematically altered to determine the relationship between SiNP dispersion, membrane morphology, and vanadium ion transport, via transmission electron microscopy, small-angle neutron scattering (SANS), and ultraviolet-visible spectroscopy, respectively. Results indicate that the SiNP surface chemistry plays a vital role in controlling their dispersion and resultant ionomer morphology, where changes in SANS data were observed as a function of both surface chemistry and SiNPs loading in the ionomer membrane. Further, it was observed that the SiNP dispersion state had a direct impact on the vanadium ion permeation: SiNP aggregation reduced vanadium ion crossover as compared to well-dispersed particles with the same end functionality. Additionally, the overall NP surface charge is a key factor in controlling vanadium ion permeation through these composite membranes.
Due to omniphobic nature of fluoropolymers, block copolymers (BCPs) having fluoropolymer block can be an excellent choice for self-assembly of multi-compartmented nanoparticles. However, the strong incompatibility between fluoroblock and solvent could pose high energy barrier for the exchange of BCPs, kinetically trapping the systems. Herein, we investigated the chain exchange dynamics of the self-assembled fluoroalkyl-BCP micelles as well as their structures using contrast-varied small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS). Time-resolved SANS revealed the effects of temperature and fluoroblock length on the exchange dynamics within spherical micelles. Despite of high energy barrier for the fluoroblock pullout from the core domain, the exchange is reasonably fast due to significantly small friction within fluoropolymers. However, as the fluoroblock molar mass approaches 100 kDa, the energy barrier becomes tremendous that the fluoroblocks are actually arrested at the core. Therefore, the chain size of fluoroblock should be wisely chosen to drive self-assembly towards equilibrium in such strongly segregated systems.

* This work was supported by the National Creative Research Initiative Program supported by the National Research Foundation of KOREA(2013R1A3A2042196).

The phase behavior of PVBA-b-PS with various volume fractions of PS block ($f_{PS}$) was investigated via small-angle X-ray scattering and transmission electron microscopy. With increasing $f_{PS}$ from 0.1 to 0.8, body-centered-cubic spheres of PS, hexagonally packed (HEX) cylinders of PS, lamellae, and HEX cylinders of PVBA were observed. Interestingly, PVBA-b-PS with $f_{PS} = 0.75$ showed asymmetric lamellar microdomains. We also prepared thin film of PVBA-b-PS on a substrate as a template for spatial arrangement of gold nanoparticles (AuNPs). When the surface of AuNPs was modified with thymine-containing polymer chains, AuNPs were selectively sequestered into PVBA microdomains through the complementary hydrogen bonding between thymine and adenine units.

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C50 DPOLY GSOFT DMP: Optically and Photonically Active Polymers BCEC 252B - Zhe Qiang, Northwestern University - Tag(s): Focus
Micro- and Nanoporous Polymer Coatings: A Diverse and Promising Platform for Optical and Thermal Regulation

JYOTIRMOY MANDAL (Presenter), YUAN YANG, NANFANG YU, Applied Physics and Applied Mathematics, Columbia University — Polymers vary widely in their intrinsic optical properties – for instance, poly(ethene) (PE) is highly transparent across the visible to far-infrared wavelengths, while poly(vinylidene fluoride-co-hexafluoropropene) (P(VdF-HFP)) is highly emissive in the long-wave infrared (LWIR). When made porous, polymers optically scatter sunlight. As a result, porous P(VdF-HFP) can attain solar reflectance ($R_{\text{solar}}$) > 96% and LWIR emittance ($\varepsilon_{\text{LWIR}}$) ~ 97%, which makes it a near-perfect radiative cooler for buildings. Meanwhile, the high $R_{\text{solar}}$ (~ 80%) and LWIR transmittance (~ 60%) of porous PE makes it useful in thermoregulation devices with tuneable $\varepsilon_{\text{LWIR}}$. Furthermore, by reversibly wetting and drying porous polymers with appropriate fluids, scattering efficiencies of the pores can be greatly altered to cause switching between solar reflective and transparent states (by 74%). Switching between LWIR transparent and absorptive/emissive states (by 60%) can also be achieved. Such optically switchable porous polymer coatings can control heat and light in buildings, and be used for camouflaging. Promisingly, porous polymers are already widely manufactured, making the stated applications viable.


Automated Platform for Investigating Aligned Carbon Nanotube Films

JOSH WALKER (Presenter), University of Wyoming, JEFFREY FAGAN, National Institute of Standards and Technology, HENRY WLAJKOWSKI, University of Wyoming, THOMAS A SEARLES, Howard University, ANGELA HIGHT WALKER, National Institute of Standards and Technology, WILLIAM RICE, University of Wyoming — The one-dimensional nature of single-wall carbon nanotubes (SWCNTs) creates highly directional properties. Utilizing this anisotropy for optoelectronic devices requires researchers to macroscopically align SWCNT ensembles. Recently, surfactant-dispersed SWCNTs were aligned using a manually operated, slow-filtration technique. Building off this method, we present in this work a new platform for reproducibly forming multiple aligned SWCNT films simultaneously. Our parallel filtration setup uses machine vision with pressure feedback control to produce aligned SWCNT films with areas ranging from 2.5 to 9.6 cm$^2$. SWCNT alignment is then determined by polarized optical measurements, such as linear dichroism and Raman spectroscopy. The ability to reproducibly create aligned films enables us to investigate parameters contributing to SWCNT alignment. Specifically, we show that for certain filtration conditions, meniscus pinning produces a spherulite pattern. Additionally, we tune the ionic strength across four orders of magnitude to show the effects of the inter-nanotube electrostatic environment on alignment. These results lead us to a deeper understanding of the physics behind SWCNT directional control.

*JSW, HVW and WDR acknowledge support from the UWyo School of Energy Resources.

Cold Plasma Effects on the Optical Properties of Salmon DNA Thin-films

MOSES NNAJI (Presenter), BEN JANG, HEUNGMAN PARK, Texas A&M University - Commerce — Fabrication of organic electronics is attractive due to the prospective lower cost when compared to inorganic devices. In particular, deoxyribonucleic acid (DNA) biopolymers show excellent promise for use in organic electronics due to their great electron-blocking capability and abundance in animal waste products. While DNA thin-films are often created by associating DNA with hexadecyltrimethylammonium chloride (CTMA) surfactant to promote DNA solubility in organic solvents and spin coat higher quality films, some success in reproducing uniform, water-based DNA thin-films on silicon and glass substrates has been achieved by incorporation of methanol as well as implementation of UV-ozone cleaning. Resulting DNA films were then subjected to cold plasma treatment to study the effects on the films via ellipsometry and spectrophotometry, where the refractive index and absorption coefficient have been characterized. Optical changes and potential novel resonance behavior induced by Ar plasma treatment encourage the continued use of Ar plasma under various conditions, as well as the use of other inert noble gases.

*This work is supported in part by the Physics and Astronomy Scholarship for Success (PASS) project funded by the NSF under grant No. 1643567 at Texas A&M University-Commerce.
3:06PM C50.00004: Optically active self-assembled pi-conjugated peptides* [Invited] CHARLES SCHROEDER (Presenter), University of Illinois at Urbana-Champaign — A major challenge in bioorganic electronics lies in the development of soft, deformable, and (opto)electronically active materials that can assemble into hierarchical structures. We use molecular design and engineering to develop new materials for organic electronics and photonics. In this talk, I discuss recent work that focuses on optically active, pi-conjugated peptides that can be engineered for precise supramolecular assembly. We consider both the kinetics and thermodynamics of assembly using a combination of experiments and modeling. Pi-conjugated peptides are guided to assemble under reaction- or diffusion-dominated conditions, such that the morphology and properties of assembled peptide fiber networks can be controlled by kinetics. A combined spectroscopy-microrheology technique is used to study the sol-gel transition of these materials during assembly, which enables direct measurement of modulus and photophysical properties during gelation. In situ confocal fluorescence microscopy and in situ fluorescence lifetime imaging microscopy (FLIM) are used to characterize peptides during the assembly process. We further demonstrate a facile strategy to macroscopically align supramolecular fibers using a templating method based on sacrificial colloidal microchannels that does not require photolithography. The structural and chemical properties of oligopeptide fibers are characterized using AFM-infrared spectroscopy (AFM-IR), photoinduced force microscopy (PiFM), fluorescence polarization microscopy, and electron microscopy. In addition, the charge transport properties of pi-conjugated peptides are determined under a wide range of applied voltages. Overall, this work illustrates simple yet robust strategies to pattern 1-D supramolecular fibers over large areas, thereby offering new routes for assembling functional organic materials.

*This work was supported by the U.S. DOE, Basic Energy Sciences (BES) under Award # SC-0011847

3:42PM C50.00005: Effect of Polymer Spacer Length in FRET-Based Fluorescent Donor-Acceptor Sensing System CHAN HO PARK (Presenter), BUMJOON KIM, KAIST — In contrast to traditional fluorescent resonance energy transfer (FRET) acceptors, two-dimensional (2D) materials potentially create the long-range energy transfer due to the strong dipole-surface energy transfer. Stimuli-responsive polymers can be an efficient tunable spacer between the FRET donor and 2D acceptor because of their conformational change to the diverse stimuli that allows the dynamic change of distance in a wide range (approximately 1-25 nm). Thus, controlling the length of polymer spacer is the most crucial to maximize the FRET signal in response to the stimuli, because FRET is dominantly distance dependent. In this paper, we present a fluorescent, thermo-responsive block copolymer grafted 2D nanosheets to retain dynamic fluorescence quenching through the change of grafted polymer length. Distance dependent FRET efficiency is studied according to the molecular weight and areal chain density of polymers. The relationship between thermally-responsive FRET and polymer behavior is theoretically calculated and elucidated by measurements of time-resolved fluorescence. Consequently, we first suggest the FRET distance between organic dye and 2D nanosheets and find optimum condition of grafting polymers to maximize the fluorescence response as a function of temperature.

3:54PM C50.00006: Nanostructured Polymer Films Exhibiting Solvent-Responsive Photonic Band Gaps YIFAN XU (Presenter), JACOB A LANASA, ROBERT HICKEY, Materials Science and Engineering and Materials Research Institute, Pennsylvania State University — Tunable and reversible photonic band gap materials generated from nanostructured block polymers have shown applications in displays, sensors and waveguides. Here, we present a way to rationally design the change in the photonic band gap of a lamellar-forming poly(1,2-butadiene)-block-poly(ethylene oxide) (1,2PBD-b-PEO) on the addition of solvents that are able to selectively swell one or both domains. A good solvent for both 1,2PBD and PEO domains, like tetrahydrofuran, leads to the largest increase in the domain spacing, and as a result, the largest change in the photonic band gap. For selective solvents like water and hexane, only one domain swells (PEO or 1,2PBD domain, respectively), leading to smaller changes in the photonic band gap. Cryogenic scanning electron microscopy and small-angle X-ray scattering were used to characterize the structural changes that occur on addition of the different solvents, while optical reflection measurements were used to determine the change in the photonic band gap. The work presented here highlights the necessary parameters for tuning the photonic band gap properties for block polymer materials using the combination of solvent quality (e.g., degree of polymer domain swelling) and changes in the refractive index.
4:06PM C50.00007: Can we design a reconfigurable photonic crystal in the visible light range?*  
ROSE CERSONSKY (Presenter), JULIA DSHEMUCHADSE, JAMES A ANTONAGLIA, GREG VAN ANDERS, SHARON GLOTZER, University of Michigan —  
Crystals with a complete photonic band gap are materials composed of mixed dielectric media which result in the reflection of all electromagnetic waves in a given range of wavelengths, commensurate to the length scale of the crystal, and pose an exciting avenue for novel materials. Diamond is a popular target for photonic crystals, which poses an opportunity for reconfigurable matter: can we create a colloidal crystal that switches reversibly to and from the diamond structure? Drawing inspiration from high-pressure phase transitions of diamond-forming atomic systems, we design a system of particles with polyhedral shapes that transitions from diamond to a tetragonal diamond derivative upon a small change in pressure and coincides with a noteworthy modulation of the photonic properties of the crystal. We propose that the transition provides a reversible reconfiguration process for a potential new colloidal material, and we draw parallels between this transition and the materials from which we take inspiration.  

*This work was done with support by the National Science Foundation, Division of Materials Research Award # DMR 1120923, the University of Michigan Rackham Merit Fellowship program, a Simons Investigator Award from the Simons Foundation, and NSF GRF Grant No. DGE 1256260.

4:18PM C50.00008: Photonic band gaps in self-assembled colloidal crystals  
DUANDUAN WAN (Presenter), SHARON GLOTZER, University of Michigan —  
Using computer simulations, we explore the effect of thermal disorder on the photonic band gap in a self-assembled photonic crystal. We find that photonic band gaps can exist over a large range of intermediate packing fractions and that the widest gap does not necessarily appear at the densest packing fraction. Further, we show that with judicious choices of particle shape, packing fraction, and particle internal structure, self-assembly can be a promising method to make photonic crystals with large band gaps despite the presence of disorder.

4:30PM C50.00009: The Importance of Being Inhomogeneous: Simulation Approaches for Liquid Crystal Optical Metasurfaces in the Visible*  
JAMES DOLAN (Presenter), Institute for Molecular Engineering, Argonne National Laboratory, HAOGANG CAI, Center for Nanoscale Materials, Argonne National Laboratory, LILY DELALANDE, XIAO LI, Institute for Molecular Engineering, University of Chicago, JUAN DE PABLO, Institute for Molecular Engineering, Argonne National Laboratory, DANIEL LOPEZ, Center for Nanoscale Materials, Argonne National Laboratory, PAUL F NEALEY, Institute for Molecular Engineering, Argonne National Laboratory —  
Optical metasurfaces—planar nanostructured devices which can arbitrarily tailor the wavefront of light—may be reconfigured by changing their dielectric environment. The application of external fields to liquid crystals is a particularly promising means by which to tune the optical properties of otherwise static metasurfaces. However, despite recent advances, there is still much progress to be made towards this goal. An outstanding issue is the behavior of liquid crystals adjacent to the nanoparticle “meta-atoms”. The optics of the device depend sensitively on this behavior, especially as the wavelength of operation approaches the visible and, therefore, the length scale of distortions in the liquid crystal director field. Here, we will demonstrate—through combined simulations and experiments—that it is not only the anisotropy of the liquid crystal which is important, but also its spatial inhomogeneity, if one wishes to accurately describe, and therefore predict, the optical properties of liquid crystal metasurfaces.  

*This work was supported by the Midwest Integrated Center for Computational Materials—and was performed, in part, at the Center for Nanoscale Materials—U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (5J-30161-0010A and DE-AC02-06CH11357).

4:42PM C50.00010: Liquid crystal based photonic topological insulators  
HAMED ABBASZADEH (Presenter), Lorentz Institute, Leiden University, MICHEL FRUCHART, VINCENZO VITELLI, The James Franck Institute and Department of Physics, University of Chicago, WIM VAN SAARLOOS, Lorentz Institute, Leiden University —  
Topological photonics harness the physics of topological insulators to control the behavior of light. An example of such control is to find modes of a photonic system that are robust against material imperfections. In this talk, we propose to use a soft-matter platform based on liquid crystals to implement some classes of photonic topological insulators. In such systems, the spatial orientation of the molecules introduces an extra geometric degree of freedom which in conjunction with suitably designed structural properties leads to the creation of topologically protected states of light. The use of soft building blocks potentially allows for reconfigurable systems that exploit the interplay between light and the soft responsive medium.
Electrically tunable structural colors of cholesterics with oblique helicoidal director

OLENA IADLOVSKA (Presenter), Advanced Materials and Liquid Crystal Institute / Department of Physics, Kent State University, Kent, OH 44242, USA, GRAHAM R MAXWELL, Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA, MATEUSZ MRUKIEWICZ, Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA; Institute of Applied Physics, Military University of Technology, 00-908 Warsaw, P, GRETA BABAKHANOVA, Chemical Physics Interdisciplinary Program, Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA, SERGIJ V SHIYANOVSKI, Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA, O D LAVRENTOVICH, Advanced Materials and Liquid Crystal Institute / Department of Physics, Kent State University, Kent, OH 44242, USA — A cholesteric liquid crystal was recently shown (Xiang, J. et al., Phys. Rev. Lett. 112, 217801 (2014); Xiang, J. et al., Adv. Mater. 27, 3014 (2015)) to exhibit a peculiar oblique helicoidal state (ChOH) when acted upon by an electric field. The period of ChOH structure depends strongly on the applied field, which enables electrically tunable structural colors in an extraordinary broad spectral range from ultraviolet to infrared. We present experimental and theoretical studies of light reflection from ChOH as a function of the electric field, surface anchoring, and incident angle. Unlike the case of conventional cholesterics, ChOH shows tunable reflection at periodicities that correspond to both pitch (for oblique incidence) and half-the-pitch. Reflection spectra are used for the first in-situ measurements of bend elastic constant of the chiral material.

*The work was supported by NSF grant DMR-1410378 and REU program CHE-1659571.

Switchable on-demand Pancharatnam-Berry phase modulation in polymer-stabilized cholesteric liquid crystals

BENJAMIN KOWALSKI (Presenter), TIMOTHY J WHITE, Chemical and Biological Engineering, University of Colorado at Boulder, MATTHEW S MILLS, Air Force Research Laboratory — Cholesteric liquid crystals (CLCs) self-assemble into chiral Bragg reflectors. It has recently been shown that by spatially patterning the reflector's helical phase, a geometric (Pancharatnam-Berry) phase modulation can be imparted on the reflected beam. Here we combine this approach with electrically driven reflection band tuning of polymer-stabilized liquid crystals. As a demonstration of this capacity, we show dynamically switchable, polychromatic generation of nondiffracting beam modes. We present a novel projection lithography system for reconfigurable helical phase landscape patterning, and analyze the fundamental limits on resolvable feature size in this landscape.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C51 DPOLY: Recent Developments in Nonequilibrium Dynamics and Rheology of Entangled Polymer Liquids

BCEC 253A - Shiqing Wang, Univ of Akron - Tag(s): Invited

Molecular Rheology of Entangled Polymeric Fluids: New Discoveries and Remaining Challenges

BAMIN KHOMAMI (Presenter), University of Tennessee — Quantitative understanding of the influence of environmental variables on the dynamic evolution of microstructure in polymeric fluids plays a central role in soft matter physics as well as the processing of a wide variety of soft materials. Atomistic simulation via non-equilibrium molecular dynamics (NEMD) offer a viable alternative to experiment wherein the dynamics of individual macromolecules can be tracked independently, thus allowing for relevant calculations of their single-chain configurational properties as well as bulk-average properties, which in turn allows detailed examination of the fundamental tenants of reputation/ tube based theories for flow of entangled polymeric fluids.

In this presentation, I will review the progress made in fundamental understanding of non-equilibrium dynamics of polymeric melts as well as the remaining challenges in development of a unified approach for predicting dynamics of this class of fluids in processing flows commonly used to produce structural and functional soft materials. Specifically, I will discuss: (1) Non-Equilibrium Molecular Dynamics Simulations (NEMD) results that depict existence of new phenomena that challenges the fundamental tenants of theories and models used to describe fast flow of entangled polymeric fluids, (2) the intricate connection between single chain dynamics and the macroscopic response of this class of fluids including the intriguing phenomena of shear banding and configurational microphase separation in elongational flow.

*Financial support was provided by the National Science Foundation under Grant No. CBET-1602890. Computational resources for this project were provided by allocation of advanced computational resources by the National Institute for Computational Sciences (NICS) and the Oak Ridge National Laboratory Joint Institute for Computational Sciences and the Extreme Science and Engineering Discovery Environment (XSEDE), ACI-1548562/TG-CTS150054..
3:06PM C51.00002: Rheological behavior of entangled polymer melts and solutions in fast extensional flow* [Invited]
QIAN HUANG (Presenter), Department of Chemical and Biochemical Engineering, Technical University of Denmark — Extensional rheology of polymer liquids is highly sensitive to molecular architecture. Accurate and reliable stress-strain measurements of extensional flow play a crucial role in understanding the nonlinear rheological properties of polymers. However, extensional flow is difficult to measure reliably.

In the first part of this presentation, we compare the stress-strain measurements of entangled polymer melts and solutions between two types of state-of-the-art extensional rheometers, namely the Sentmanat extensional rheometer (SER) and the filament stretching rheometer (FSR). While necking instabilities, which prevent steady flow, are observed in SER at some specific range of normalized stretch rate (Weissenberg number), kinematically steady extensional flow can be achieved in FSR with the help of an online control scheme [1]. At higher Weissenberg numbers, elastic fracture happens in both SER and FSR [1]. The significance of the observed necking, steady extensional flow, and elastic fracture will be discussed in the presentation.

In the second part, we show the results of extensional rheology measured in FSR for entangled polymer liquids with different molecular architectures, including linear, star, comb, and ring polymers. Some results are also compared with the ones measured in SER. Interpretation of the rheological results will be presented and compared with the results from ex-situ small angle neutron scattering (SANS). Furthermore, stress relaxation measurements following steady extensional flow for a linear polymer melt will be presented, together with the corresponding results of ex-situ SANS. We show that the chain stretch idea in the tube model can be critically tested through analyzing the SANS data at different time in stress relaxation process.


*Financial support from the Aage og Johanne Louis-Hansen Foundation is gratefully acknowledged.

3:42PM C51.00003: Forced-Based Microscopic Theories of the Equilibrium Dynamics and Nonlinear Rheology of Entangled Rod and Chain Polymer Liquids [Invited] KENNETH SCHWEIZER (Presenter), University of Illinois at Urbana-Champaign — Using ideas from microscopic glass physics, force-based statistical mechanical theories for the transverse tube confinement field of liquids of zero-excluded-volume rods (needles) and chains have been constructed based solely on dynamic uncrossability which is exactly enforced at the two body level. Coils are coarse grained to chains of self-consistently-determined primitive-path steps. Tube localization emerges above a universal critical degree of interpenetration, and the melt tube diameter scales with packing length. Importantly, the confinement field is anharmonic, softening for large transverse displacements, corresponding to a finite maximum entanglement force. The predicted form of the confinement field is in excellent agreement with f-actin solution experiments and chain melt simulations. The tube field softens with orientation, hardens for affinely stretched chains, and is potentially destroyed beyond a critical stress (microscopic yielding). Nonequilibrium theories and simple constitutive equations under continuous startup shear have been constructed. For chain melts, new physical aspects include a dynamic tension blob scaling construction of a grip force that is the microscopic origin of stretching, a force imbalance criterion for termination of affine deformation and onset of retraction, the influence of entanglement length heterogeneity, an emergent form of convective constraint release, and rate-accelerated retraction of strongly stretched chains. For fast deformations we predict novel fractional power law scalings with rate for the stress overshoot and undershoot, steady state total and orientational stress and contour length stretch, a universal master curve in the elastic-viscous crossover regime, and strong connections between the overshoot and steady state. No adjustable parameter numerical predictions are quantitatively compared with multiple experiments and simulations. This work was done in collaboration with Shi-Jie Xie and Daniel Sussman.
A central problem in polymer rheology is to understand how the intra- and interchain configurations are transformed by the macroscopic deformation. The rheo-small-angle-neutron-scattering (rheo-SANS) technique has long held the promise of offering a molecular perspective on this issue. However, despite decades of development, the full potential of this experimental technique is yet to be realized. By combining and extending several key concepts in the literature and drawing upon the so-called spherical harmonic expansion technique, here we describe a new framework (Phys. Rev. X 7, 031003 (2017); Phys. Rev. Lett. 121, 117801 (2018)) for connecting the SANS experiments and the molecular rheology of polymeric liquids. We show how several two-point spatial correlation functions, such as the anisotropic single-chain structure factor and pair distribution function, can serve as a bridge between rheo-SANS experiments on the one hand and theoretical studies on the other, providing a convenient platform for molecular rheology of polymers. To demonstrate the power of this idea, we will discuss in this talk our recent SANS experiments on deformed homopolymer melts as well as polymer blends.

*This research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT Battelle, LLC, for the U.S. Department of Energy.

Shear banding in semidilute polymeric solutions: Experiments and modeling* [Invited] NATALIE GERMANN (Presenter), Technical University of Munich — Shear banding is the formation of localized velocity bands with different shear rates, and is observed in semidilute polymer solutions and other soft materials. DNA solutions are convenient model systems owing to their characterization in standard rheometric geometries without edge fracture. Furthermore, their wall slip can be minimized by using glycerol as a solvent. In this talk, we focus on the investigation of shear banding of 13 mg/ml of 115 kbp double-stranded DNA (dsDNA) and 11 mg/ml of 50 kb single-stranded DNA (ssDNA) in glycerol/aqueous buffer solutions and compare the results with our recent works on polyacrylamide and polyethylene oxide. The frequency sweep of dsDNA corresponds to that of a soft gel with a small dependence at intermediate frequencies. On the other hand, the behavior of ssDNA is comparable to that of a dense micellar solution having a unique local minimum related to micellar breakage. Due to the much smaller persistence length, ssDNA is more flexible and easily creates small structural units most likely in association with glycerol. The strain sweep of dsDNA is strain thinning and the shear bands are mainly strain-dependent. Early strain stiffening with weak bands is observed for ssDNA followed by a terminal flow regime of the collapsed structure. To summarize our recent activities on shear banding, we will briefly discuss here our mesoscopic modeling and simulation efforts in mixed flows (e.g., 4:1 contraction, die extrusion).

References:

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Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C52 DPOLY DBIO: Polyelectrolyte Complexation II: Phase Behavior and Solutions Dynamics BCEC 253B - Samanvaya Srivastava, University of California, Los Angeles - Tag(s): Focus

2:30PM C52.00001: Polyelectrolyte solution confined between oppositely charged dielectric surfaces* DEBARSHEE BAGCHI (Presenter), TRUNG NGUYEN, MONICA OLVERA DE LA CRUZ, Materials Science, Northwestern University — We study a polyelectrolyte solution confined between two oppositely charged dielectric surfaces by a coarse-grained molecular dynamics simulations. Randomly charged beads as in sodium polystyrene sulfonate with varying degrees of sulfonation are modeled using implicit solvent with explicit ions. The charged electrodes that confine the polyelectrolyte solution are considered to be made of a low dielectric constant material such as graphene. We employ an efficient algorithm for computing the induced charges and investigate various properties of our system, such as the capacitance and its relation to the polymer conformation and charge density. We observe counter-intuitive phenomena such as charge amplification where a layer of ions adsorb close to a surface of same charge to allow more polymer adsorption.

*NSF DMR Award No. 1611076
Incorporating Molecular Structure into a Transfer Matrix Theory of Complex Coacervation

TYLER LYTLLE, CHARLES SING (Presenter), University of Illinois at Urbana-Champaign — Polymeric complex coacervation is a phase-separation process involving two oppositely-charged polyelectrolytes in an aqueous salt solution, where a polymer-dense phase is formed due to electrostatic interactions between the polyelectrolyte species. The resulting coacervate materials have seen widespread use in industry as viscosity modifiers and encapsulants, and are used in polymer research as an interaction motif for charge-driven self assembly. Despite this utility, a fundamental physical description of this process has remained elusive; a recent resurgence of interest in coacervation has led to a number of candidate theories. Here we present a transfer matrix theory that maps coacervate structure to a one-dimensional adsorption model, leading to a theory that can predict both coacervate phase behavior and local charge correlation features. We show that straightforward modifications to the theory can be used to account for a number of molecular features, including divalent ions, linear charge density, polymer stiffness, and polymer architecture. Comparison to simulation and experiment shows that we can capture qualitative trends that inform the molecular design of polymer complex coacervates.

Structure-Property Relationships for Oligonucleotide Polyelectrolyte Complex Micelles

JEFFREY VIEREGG (Presenter), MICHAEL LUECKHEIDE, ALEX MARRAS, MATTHEW TIRRELL, Institute for Molecular Engineering, University of Chicago — When a charged-neutral hydrophilic block copolymer is mixed with an oppositely-charged polyelectrolyte, micro-phase separation occurs, producing core-shell nanoparticles referred to as polyelectrolyte complex micelles by analogy to hydrophobically-driven micellization. PCMs have been proposed as a solution to the urgent problem of therapeutic delivery of (anionic) oligonucleotides into cells, as the dense polyelectrolyte core and neutral corona can shield the oligonucleotides from degradation and improve biodistribution. Several promising results have been reported, but until recently no structure-function relations existed to guide design of PCMs, and little data existed on the effect of chemical modifications to either polyelectrolyte. By combining small-angle X-ray scattering, multi-angle light scattering, and cryo-electron microscopy, we have characterized the morphology and internal structure of PCMs formed by oligonucleotides of varying size, structure, and chemical composition with poly(lysine)-poly(ethylene glycol) block copolymers. I will present results that illustrate the connections between molecular features and PCM morphology, as well as rules for producing oligonucleotide PCMs of desired size and shape with exceptionally low polydispersity.

Probing the size of coacervate core micelles

DEBRA AUDUS (Presenter), Materials Science and Engineering Division, National Institute of Standards and Technology, BRADY GARRINGER, Chemical Engineering, Boise State University, HAYLEY BOIGENZAHN, Chemical Engineering, University of Wisconsin-Madison — Coacervate core micelles, composed of diblock copolymers with oppositely charged blocks forming the core and neutral, hydrophilic blocks forming the corona, are of use for applications including drug delivery as the core can encapsulate hydrophilic, charged cargo. For such applications, it is essential to understand how the polymer architecture can be used to tune the size of these micelles. Using a model that captures the essential physics coupled with computational methods, we probe how the core size, corona size, and aggregation number.

Salt-concentration-dependent structure of Complex Coacervate Core Micelles

TAEYOUNG HEO (Presenter), SOOHYUNG CHOI, Department of chemical engineering, Hongik University — Complex coacervation is a liquid-liquid phase separation when two oppositely charged polyelectrolytes are mixed in an aqueous solution. Because of the nature of electrostatic interaction, the coacervates are highly responsive to solution condition such as ionic strength. In this study, complex coacervate core micelles (C3Ms) are formed by simple mixing of AB and A'B diblock copolyelectrolyte solutions in an aqueous solution where A and A' are oppositely charged blocks, and B is PEO block. Since the cores are coacervates, the C3Ms are also highly responsive to salt concentration. We investigate the salt-concentration-dependent structure of C3Ms with various molecular weight of charged block using dynamic light scattering (DLS) and small-angle X-ray/Neutron scattering (SAX/NS). As salt concentration increases, the aggregation number and core radii of C3M decrease. This reflects that the interfacial area per chain increases due to reduced interfacial tension between cores and solvent at higher salt concentration. In addition, salt resistance of C3Ms becomes stronger as the molecular weight is larger.
3:30PM C52.00006: Structural Evolution and Formation Kinetics of Polyelectrolyte Complex Micelles  HAO WU (Presenter), JEFFREY TING, MATTHEW TIRRELL, University of Chicago — Polyelectrolyte complex (PEC) micelles form when oppositely charged block polyelectrolytes are mixed together in aqueous media. The polyelectrolyte blocks, driven by electrostatic interaction, associate and phase separate, leading to a dense, polymer-rich PEC core stabilized by a neutral block corona. These nanoscale PEC micelles have various biomedical applications including RNA therapeutic delivery, tissue engineering, and diagnostics. The formation kinetics of PEC micelles, however, remains unknown. We employ time-resolved SAXS to investigate the formation kinetics of PEC micelles and the effects of various parameters on the growth rate. We focus on a model polyelectrolyte system that we have expertise in synthesis and has been extensively studied: poly(ethylene oxide)-block-poly(vinyl benzyl trimethyl ammonium chloride) (PEO-b-PVBTMA) complexed with either poly(ethylene oxide)-block-poly(styrene sulfonate sodium) (PEO-b-PSSNa) or poly(acrylic acid sodium) PAAc. Achieving a nanoscale description of the growth kinetics via TR-SAXS experiments will contribute towards enhancing our understanding of the complexation-driven assembly processes, and allow better design of polyelectrolyte complex based materials for biomedical applications.

3:42PM C52.00007: Dynamics of liquid coacervates formed by oppositely charged polyelectrolytes  CHRISTIAN APONTE-RIVERA (Presenter), MICHAEL RUBINSTEIN, Duke University — Mixtures of oppositely charged polyelectrolytes can undergo a phase separation to form a polymer rich phase, called a coacervate, and a polymer depleted phase. The polymer rich phase can be a soft, viscous liquid, or a solid complex. Both types have drawn much attention in the literature due to their technological applications as well as their role in biological systems. Models have been developed to predict thermodynamic properties of the coacervates. However, much less attention has been given to modeling coacervate dynamics. We develop a scaling theory to predict the dynamics of entangled and unentangled asymmetric liquid coacervates formed from oppositely charged polyelectrolytes. The theory predicts the scaling of properties such as the relaxation modulus and shear viscosity of the coacervate, and the diffusivity of the polyelectrolyte chains. The scaling theory highlights the different dynamic regimes of the system, and how the dynamic properties can be tuned by experimentally controllable parameters such as the degree of polymerization or the number density of charges along the polyelectrolyte backbone, providing a means with which to rationally design dynamic properties for technological applications.

3:54PM C52.00008: Polymer chemistry and effect on the linear viscoelasticity on polyelectrolyte complexes  YALIN LIU (Presenter), CRISTIAM F. SANTA CHALARCA, University of Massachusetts Amherst, REBECCA A. OLSON, RICHARD N. CARMEAN, Department of Chemistry, University of Florida, TODD EMRICK, University of Massachusetts Amherst, BRENT SUMERLIN, Department of Chemistry, University of Florida, SARAH PERRY, University of Massachusetts Amherst — Polyelectrolyte complexes are formed through the electrostatic interaction of oppositely charged polymers. Depending the identity of salt, polyelectrolyte complexes can result in both solid precipitates and/or a liquid-liquid phase separation known as complex coacervation. The material properties can also change based on variations in the polymer chemistry, and the complex interplay between electrostatic interactions and water structure, controlled by salt. We tested three different polymer systems over a range of polymer chain lengths and salt conditions to understand how variations in polymer chemistry affect the thermodynamic phase behavior and the resulting material dynamics. The linear viscoelasticity of each polymer system was investigated under different salt conditions to enable a time-salt superposition and facilitate a broader characterization of the stress relaxation behavior. We compare differences in the slope of the horizontal shift factors as a function of salt concentration, which can be related to the activation energy barrier for the rearrangement of ionic interactions between polymers. The goal of this systematic study is to establish a general understanding of how molecular-level parameters can be used to tune the phase behavior and viscoelastic properties.

4:06PM C52.00009: Ionic-group-dependent phase behavior of polyelectrolyte coacervates  SOJEONG KIM (Presenter), School of Chemical and Biological Engineering, Seoul National University, SOOHYUNG CHOI, Department of Chemical Engineering, Hongik University, WON BO LEE, School of Chemical and Biological Engineering, Seoul National University — Complex coacervates are polymer-rich phases of liquid-liquid phase separation when two oppositely charged polyelectrolytes are mixed in aqueous solutions. Previously, Voorn-Overbeek model (VO model), simple and intuitive combination of the entropy of mixing and electrostatic interaction, was proposed to capture the behavior of complex coacervates. Since the VO model doesn't account for the chain connectivity of polyelectrolytes and chemistry-specific details, advanced models have been suggested up to now. However, experimental data of model system is rare to compare with the theoretical description. In this study, 4 polyelectrolytes are prepared (e.g., strong/weak and polyanion/cation) and thus 4 pairs of polyelectrolyte complex coacervates are investigated to map out the phase diagrams as a function of the pair of the ionic group. It is found that the phase diagram shows distinctive features including (1) the salt resistance and the area of two-phase region are significantly dependent on the pairs of polyelectrolytes, and (2) the tie lines in the binodal curve show negative slope. We believe chemical-specific parameters play an important role to control phase behavior, and this observation shed a new light on the fascinating and biologically important topic of complex coacervation.
RONALD LARSON (Presenter), ALI SALEHI, Chemical Engineering, University of Michigan — We develop a modeling framework for phase behavior and transport of oppositely charged polyelectrolytes (PE) in coacervates and Layer-by-Layer (LbL) assemblies that accounts for diffusion of both oppositely charged chains and their complexation. The core of the phase behavior model is the development of a free energy model that includes free energies for ion pairing, counterion condensation, charge regulation, electrostatic free energy, as well as elastic energy of the network and Flory Huggins entropy and enthalpy. We quantify a very strong influence of ion pairing and counterion condensation on phase behavior, and on the distribution of salt and polyelectrolyte species between the coacervate and supernatant phases, and find consistency of predictions with experimental data. From this free energy model, and an extended Stefan-Maxwell flux law based on the Doi-Onuki Rayleighian approach, the transport of PE chains, salts, and waters through polyelectrolyte LbL films are modeled, including the effects of chemical and electrostatic potentials, as well as mechanic stresses. The result is a unified approach that connects phase behavior to transport in polyelectrolyte assemblies, and may eventually allow rates of Layer-by-Layer assembly to be inferred from measurements of phase behavior and rheology.

*The support of the National Science Foundation under grant DMR 1707640 is gratefully acknowledged.

4:54PM C52.00011: Teaching a New Dog Old Tricks: Phase Inversion in Polyelectrolytes  
DAVID DELGADO (Presenter), KAZI SADMAN, QIFENG WANG, KENNETH R SHULL, Northwestern University — While the design and synthesis of water filters required no activation; whereas for a low PAAm ionization level, the formed network was weak but consistent. Oscillatory shear deformation experiments revealed a strong dependence of the storage and loss moduli on the PAAm ionization degree of the system components, a strong network was formed but only after sonication, i.e. as a result of an activation; whereas for a low PAAm ionization level, the formed network was weak but required no activation.

5:06PM C52.00012: Stretchable Ionic Double Layer at the Interface Between Crosslinked Networks of Ionic Liquids  
HYEONG JUN KIM (Presenter), University of Massachusetts Amherst, BAOHONG CHEN, ZHIGANG SUO, Harvard University, RYAN HAYWARD, University of Massachusetts Amherst — Polymerized ionic liquids (PILs) are an emerging class of ion conducting materials wherein one of the ionic moieties in the ionic liquids is covalently attached to a polymer backbone. Crosslinked networks of ionic liquids (NILs) allows solid-state electrolyte that can selective conduct single ions. Herein, two oppositely charged NILs were prepared based on 1-ethyl-3-methyl imidazolium (3-sulfopropyl) acrylate ([ES]) and (1–(2–acyloxyethy)–3–buthyl–imidazolium bis(trifluoromethane) sulfonimides ([AT]). At the interface of [ES]/[AT], we show that an ‘ionic double layer’ (IDL) is formed. The mobile ions are diffused away from the interfacial region, resulting in a build-up of excess fixed charges with a capacitance of ~ 1 mF/cm². This IDL leads to asymmetric current flow when the polarity of the bias voltage is altered, analogous to the electrical rectification of a semiconductor diode. Moreover, the elastic properties of NILs allow a physical deformation which provides an electrical response that can be used for strain sensing or energy harvesting without the need for an external bias voltage. Our finding serves as a fundamentally new platform for a liquid-free, elastic and stretchable ionic diode that can harvest ambient mechanical energy such as human motion.

5:18PM C52.00013: Complexation and network formation in a suspension of oppositely charged cellulose nanocrystals and poly(allylamine)  
ARKADII ARINSTEIN (Presenter), PATRICK MARTIN, GLEB VASYLYEV, MOR BOAZ, GUANG CHU, EYAL ZUSSMAN, Nano-Engineering group, Department of Mechanical Engineering, Technion - Israel Institute of Technology — The structure formation, determined by tunable electrostatic interactions, in systems consisting of negatively charged cellulose nanocrystals (CNC) and a positively charged flexible weak polyelectrolyte, poly(allylamine) (PAAm), is discussed. Water dispersions, contained 3 wt.% CNC and 0.0364 wt.% PAAm of high molecular weight (65 kDa) that corresponds to the ionizable group stoichiometric ratio of system components, were examined. Variation in the dispersion pH allowed controlling the PAAm and CNC ionization level and hence the electrostatic interactions of the system constituents. For samples with high charge density, steady state viscosity measurements demonstrated cluster formation which consist of several CNC rods connected (due to ionic coupling) by PAAm tie macromolecules. Under certain conditions, these clusters (micro-gels) start to grow, merge and finally form a global network providing system elasticity. Oscillatory shear deformation experiments revealed a strong dependence of the storage and loss moduli on the PAAm ionization level. For high ionization degree of the system components, a strong network was formed but only after sonication, i.e. as a result of an activation; whereas for a low PAAm ionization level, the formed network was weak but required no activation.
Mechanophore activation in a crosslinked polymer matrix via instrumented indentation
CHELEA DAVIS (Presenter), MITCHELL L RENCHECK, Purdue University, JEREMIAH WOODCOCK, National Institute of Standards and Technology, MUZHO WANG, Northwestern University, RYAN BEAMS, STEPHAN STRANICK, AARON FORSTER, JEFREY GILMAN, National Institute of Standards and Technology — Scratches in transparent polymer coating and barrier layers can cause a host of problems, impacting optical (haze, light transmission, etc.) and mechanical properties (permeability, structural integrity, etc.) The primary focus of this project is to investigate the mechanical activation of a mechanophore (MP)-containing transparent polymer coating. Taking advantage of the amine functionality present in a polyetheramine/bisphenol A epoxy network, we have covalently attached a commercially available Rhodamine dye into a transparent, thermoset polymer. Utilizing the scratch profiles available on a typical nanoindenter, the load was varied so that a transition between ductile (plastic) to brittle deformation was observed within a single scratch. Subsequent fluorescence imaging of the MP-epoxy surfaces revealed the extent of fluorescence activation induced by the mechanical deformation. It has been shown that the Rhodamine-based mechanophore can be used to identify brittle fracture and local stress concentrations prior to macroscopic failure. Fluorescence lifetime and hyperspectral imaging of damage zones provide additional insight into the local deformation around each scratch.

Tryptophan based co-polymer as Fluorescence Turn-Off sensor for explosive detection
VISHAL KUMAR (Presenter), SOUMITRA SATAPATHI, Indian Institute of Technology Roorkee — The highly sensitive and reliable detection of explosives is of paramount importance for civilian and military security.1,2 Here, we report the synthesis and sensing applications of a highly emissive and electron-rich tryptophan based copolymer Poly[(N,N-dimethylacrylamide)-co-(Boc-Trp-EMA)] (RP)(Φf=35%) which exhibited high sensitivity and selectivity towards DNT, TNT and TNP with LOD 3.39, 2.55 and 0.7μM, respectively. In solution, PL signal from RP co-polymer gets quenched upon addition of aliquots of DNT, TNT and TNP caused by photo-induced electron-transfer i.e. quantified by plotting Stern–Volmer plot (KSV=7.6×10³,1.1×10⁴ and 3.3×10⁴ M⁻¹ for DNT, TNT and TNP). The quenching mechanism was further established by time-resolved PL and steady state absorption spectroscopy which was found to be predominantly dynamic in nature as lifetime of RP (2.1 ns) is reduced to 0.9, 0.8 and 1.3 ns for DNT, TNT and TNP. To explore the possibility of using the fluorescent co-polymer as sensor array, a prototype thin film polymer sensor was fabricated using drop-casted thin film of RP which was able to detect saturated nitroaromatic vapor in real time with high selectivity. The initial PL intensity of the 20 nm thin film of RP was quenched to 19% for DNT, 13% for TNT and 4% for TNP in just 2 min.

Tough and Photoluminescent Diblock Copolymer Elastomers via Lanthanide Coordination
FENG JIANG (Presenter), XIN ZHANG, DOUG HENDERSON, WONSEOK HWANG, ROBERT M BRIBER, HOWARD WANG, University of Maryland, College Park — Thermoplastic elastomers (TPEs) of poly(methyl methacrylate)-block-poly(n-butyl acrylate-co-vinyl imidazole) (PMMA-b-P(BA-co-VI)) diblock copolymers have been synthesized as a model system to demonstrate supramolecular photoluminescence (PL) TPEs via lanthanide coordination. Europium ion (Eu³⁺) with a red PL and terbium ion (Tb³⁺) with a green PL have been selected as the lanthanide ions to coordinate the imidazole groups of the soft block. Upon microphase separation, hard PMMA blocks form spherical domains in the continuous matrices of the soft P(BA-co-VI) phase. At a volume fraction of 0.29, PMMA hard sphere domains act as a physical network in the matrix. Upon incorporating lanthanide ions, the soft P(BA-co-VI) matrix is cross-linked through metal coordination to form a second physical network. Synergistic interaction and reinforcement of local segmental coordination network and global glassy particle percolation network greatly enhance both the tensile strength and toughness of TPEs without compromising the stretchability. Moreover, the PL spectrum of TPEs can be continuously tuned by varying the composition and molar ratio of Eu³⁺/Tb³⁺.
3:06PM C54.00004: Temperature and pH Dual-Responsive Shape-Transforming Block Copolymer Particles with Tunable Optical Property  JUNHYUK LEE (Presenter), BUMJOON KIM, chemical and biomolecular engineering, KAIST — We report a simple and robust strategy to prepare temperature/pH dual-responsive shape-switchable block copolymer (BCP) particles composed of polystyrene-b-poly(4-vinylpyridine) (PS-b-P4VP) and temperature/pH-responsive poly(N-(2-diethylamino)ethyl)acrylamide-r-N-isopropylacrylamide) (poly(DEAEAM-r-NIPAM)) surfactants. The polymer surfactants were carefully designed to produce a dramatic change in relative solubility in response to subtle temperature and pH change near physiological condition (i.e., human body temperature and neutral pH). The shape transition of BCP particles from lens to football shape was observed within very narrow temperature and pH range: no transition for pH 6.0, 40-50 °C for pH 6.5, and 25-35 °C for pH 7.0. Furthermore, the BCP particles showed reversible shape-transforming behavior in response to orthogonal temperature/pH changes. In addition, the incorporation of fluorescent dye-functionalized PS and P4VP into BCP particles allowed colorimetric monitoring of temperature and pH changes, which suggests a promising possibility of these particles in clinical and biomedical application.

3:18PM C54.00005: Effect of calcium ions on the interactions of end-tethered weak polyelectrolytes  RIKKERT NAP (Presenter), IGAL G SZLEIFER, Northwestern University — We use a molecular model, which combines theory with Monte Carlo and Molecular Dynamics simulations, to study the effect of divalent calcium ions on the interactions on the interactions between two planar surfaces end-tethered with poly(acrylic acid)(PAA). Polyelectrolyte-coated colloids and nanoparticles have nanotechnological and biomedical applications such as sensing and imaging. The addition of calcium ions to monovalent electrolyte solutions leads to a dramatic reduction in the size and range of effective interactions between the two polymer layers. This is caused by the formation of favorable calcium bridges that reduce the effective charge of the polymer layers and, at sufficiently high calcium ion concentrations, can cause the polymer layers to collapse. At physiological conditions and calcium ion concentrations above approximately 1mM, the repulsions between the opposing end-grafted surfaces disappear and attractions occur, accompanied by large structural changes of the opposing layers. These attractions are correlated with the occurrence of interlayer divalent calcium bridges and do not occur for PAA layers in contact with reservoir solutions containing only monovalent ions. Finally, the potential for microphase separation within the PAA layer is explored.

3:30PM C54.00006: In situ regeneration of oil absorbent via wettability switch of conjugated polymer surfaces  JIAN XU, Biomedical Engineering, Purdue University, WEI XIU, Brookhaven National Laboratory, YINLUN YUAN, GUOHAO GAO, EUI-HYEOK YANG (Presenter), Mechanical Engineering, Stevens Institute of Technology — Absorbent-based technology shows the possibility of full removal and reclaim of oils from water while bringing little adverse effects to the environment. In spite of their promises, the recycle and regeneration of saturated absorbents have been less-explored. Here, we demonstrate a light-weight high-efficient conjugated polymer foam as oil absorbent capable of in situ regenerating via wettability switch during electrochemical oxidation and reduction. We electopolymerize polypyrrole-dodecylbenzenesulfonate (PPy(DBS)) on the surfaces of commercially available carbon foam. The PPy(DBS) shows oleophilic property when oxidized, absorbing oils (i.e., oils stick to the polymer surface and trapped within the micro-pores of the foam). Under reduction, the surface switches to oleophobic, releasing the oils, while in situ regenerating the polymer surface. Using this approach, in situ absorption and release of various oils is demonstrated. We further demonstrate the wettability switch performance (characterizing the retention force when oxidized and switch time when reduced) of the absorbent during 250 redox cycles. Together, this novel adsorbent shows great promise towards high-efficient continuous oil/water separation applications.

3:42PM C54.00007: Design principle of multi-responsive smart copolymers  CARLOS M MARQUES (Presenter), Institute Charles Sadron, Strasbourg France, DEBASHISH MUKHERJI, Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver Canada, KURT KREMER, Max-Planck-Institute for Polymer Research, Mainz Germany — Design of multi-responsive smart, soft materials is at the onset of many developments in polymer physics, chemical physics, biophysics and biochemistry research. A system is known as smart responsive when a slight change in external stimuli can drastically alter its structure, function and stability. Furthermore, when the relevant energy scale is of the order of thermal energy, materials are classified as soft matter and are driven by large conformational/compositional fluctuations. At the same time it is very difficult to address these problems in both experimental and theoretical setups. In this work, combining molecular simulation and experiments, we propose design principles of a wide range of smart copolymer architectures in aqueous and mixed solvent environments. This provides an almost predictable conformational behavior and thus presents a highly tunable smart polymer design principle.

This work has been performed within a fruitful collaboration with several experimental colleagues, especially Mark Watson (Uni Kentucky), Manfred Wagner (MPIP Mainz) and Marc Schmutz (ICS Strasbourg).
3:54PM C54.00008: Controlling Swelling Behavior of Upper Critical Solution Temperature Micelle Containing Layer-by-Layer Films*  VICTORIA ALBRIGHT (Presenter), ALIAKSEI ALIAKSEYEU, VIKTOR SELIN, Materials Science & Engineering, Texas A&M University, JOHN F ANKNER, Spallation Neutron Source, Oak Ridge National Laboratory, SVETLANA A SUKHISHVILI, Materials Science & Engineering, Texas A&M University — We explore the role of binding partner strength on temperature-responsive swelling profiles of hydrogen-bonded layer-by-layer (LbL) films containing upper critical solution temperature micelles (UCSTM) composed of poly(acrylamide-co-acrylonitrile)-block-polyvinylpyrrolidone. LbL films were constructed at acidic pH, at temperatures below the UCST, using poly(methacrylic acid) (PMAA) and the PVPON corona of the UCSTM. By using isothermal microcalorimetry, the interaction between PMAA and PVPON in solution was found to be pH dependent and entropically driven at pH 4. The internal structure of UCSTM LbL films deposited at various pHs was monitored with neutron reflectometry using deuterated PMAA to highlight film stratification, while growth and temperature-responsive swelling profiles of multilayers were studied with spectroscopic ellipsometry. Films assembled at higher pH, featuring more ionized PMAA chains, were less well stratified and displayed larger amplitude temperature-triggered swelling changes than those assembled at lower pH. Using pH to control film stratification and functionality can potentially be used in other hydrogen-bonding polymer assemblies.

*Funding from Texas A&M University Graduate Merit Fellowship, Texas Engineering Experiment Station, and NSF DMR-1610725.

4:06PM C54.00009: Mobility and self-healing in star-polymer vitrimers  SIMONE CIARELLA, WOUTER ELLENBROEK (Presenter), Eindhoven University of Technology — Vitrimers are a rapidly developing class of polymeric materials that combine the strength and resilience of covalently crosslinked elastomers with the malleability of thermoplastics. They owe this remarkable feature to a chemical bond-swap mechanism that allows the polymer network to rearrange its architecture without ever being fully disconnected. We simulate this swap mechanism in molecular dynamics simulations of star polymer networks using a 3-body potential-based method we recently developed [1]. We find that the swapping allows the star polymers to diffuse through the material, even on timescales below the stress relaxation time. This provides a mechanism for self-adhesion and self-healing of fully annealed (non-freshly cut) vitrimer surfaces, highlighting their use as durable structural materials.


4:18PM C54.00010: Molecular Design of Precise Network Polymerized Ionic Liquids for Improved Understanding of Soft Actuators  CHRISTOPHER EVANS (Presenter), CHENGTIAN SHEN, QIUJIE ZHAO, University of Illinois at Urbana-Champaign — Crosslinked network polymerized ionic liquids (n-PILs), with tethered imidazolium cations and mobile bis(trifluoromethane sulfonimide) (TFSI) anions, were investigated as dopant-free (no water or free ionic liquid) soft actuators by sandwiching between flexible electrodes and applying 3V, either AC or DC. These networks are made via a modular synthetic route such that they have tunable polarity and modulus through the choice of either hydrocarbon (HC) or ethylene oxide (EO) monomers and crosslinking density. The $T_g$ is not substantially affected, and the role of conductivity, crosslinking, and modulus can be probed to understand how they systematically affect actuation. Under DC conditions, where conductivity is not a factor, the lower modulus ($E$) allows for greater bending strain with a non-linear $1/E$ relation. Under 0.1 Hz AC potentials, the conductivity is important and couples with modulus to affect beam displacement. The choice of EO monomers and low crosslinking density lead to the best performance due to high conductivity and low modulus. Because the n-PILs are hydrophobic (< 1 wt% water uptake under ambient conditions), they can be operated over a thousand cycles at 3 V with minimal degradation of performance, as leaching of ionic liquids or water splitting are not an issue.

4:30PM C54.00011: Chemically Actuated Liquid Crystal-Based Polymer Printer  YOUNG KI KIM (Presenter), Chemical and Biomolecular Engineering, Cornell University, DANIEL B. WRIGHT, Chemistry, Northwestern University, PRANATI MONDKAR, Chemical and Biological Engineering, University of Wisconsin-Madison, NATHAN C. GIANNESCHI, Chemistry, Northwestern University, NICHOLAS L. ABBOTT, Chemical and Biomolecular Engineering, Cornell University — Liquid crystals (LC) exhibit the mobility of liquids and long-range order of crystals, leading to anisotropic viscoelastic properties. These properties have been used to design responsive soft materials that can amplify a range of chemical/physical stimuli into macroscopic optical outputs. Recently, we have reported a new class of LC materials based on micrometer-sized aqueous droplets dispersed in thermotropic LCs that both optically report targeted stimuli and trigger release of microcargo initially sequestered within the LC. In this presentation, we will show that these LC materials can be programmed to print three-dimensional polymeric networks and assemblies with diverse sizes and morphologies (from nanometer to millimeter) via triggered polymerization. Specifically, we will demonstrate that it is possible to trigger the polymerization of hydrogels or amphiphilic polymers by hosting initiators within microcargo sequestered in LCs. This work illustrates how it is possible to exploit the elasticity of LCs in combination with polymerization processes to achieve multi-scale responses to molecular-level triggering events.
4:42PM C54.00012: THz Vibrations of Metal-Organic Frameworks: Thermal and Mechanical Stability  MATTHEW RYDER (Presenter), Neutron Scattering Division, Oak Ridge National Laboratory — Neutron scattering is a critical technique in understanding how materials behave at the molecular-level. High-resolution inelastic neutron scattering (INS) in conjunction with density functional theory (DFT) was used to study the lattice dynamics of framework materials and revealed a diversity of valuable information relating to the structural flexibility and was able to explain the origins of anomalous elastic phenomena. Intriguing vibrational motions identified the presence of gate-opening and breathing in zeolitic imidazolate frameworks (ZIFs), and ‘trampoline-like’ mechanisms and molecular rotors reminiscent of negative thermal expansion (NTE) in the MIL-140 series and HKUST-1. However, to fully understand how these promising next-generation materials behave in real-life conditions the thermal and pressure response must be carefully studied. The effect of external stimuli (pressure and temperature) can also reveal the nature and underlying mechanisms behind stimuli-induced phase changes and amorphization. Preliminary results obtained using the one-of-a-kind Spallation Neutron Source (SNS) facility at Oak Ridge National Laboratory (ORNL) indicate elevated levels of anisotropic thermal expansion present in a topical series of framework materials known as MOF 74-M.

4:54PM C54.00013: Smart and responsive flexible foams via 3D printing of polymer composites* [Invited] PEIRAN WEI, HOUMING LENG, QIYI CHEN, RIGOBERTO ADVINICULA, EMILY PENTZER (Presenter), Case Western Reserve University — We will report lightweight, highly-compressible, and piezoresistive polymer composite foam structure successfully prepared by 3D printing a thixotropic ink. The structures have exhibits tailorable mechanical strength, high compressibility and remarkable robustness. Inks are composed of nanoclay and carbon black particles in an organic solution polyurethane, and are processed using direct ink writing (DIW) into wearable strain sensor devices. Removal of the clay by chemical etching yields structures with high porosity and good elasticity, which have good compressibility and stable piezoresistive sensing signals at a strain of > 90%. We illustrate these structures can be used in pressure sensing, as well as the sensing of volatile organic solvents. The conductive structures can easily be reprocessed to different shapes and have great potential for lightweight, energy-saving, flexible, highly sensitive, and stable piezoresistive sensors.

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Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C55 DPOLY DCOMP DBIO GSNP: Advancing Polymer and Biopolymer Physics though Simulation and Theory I: Biopolymers BCEC 254B - Alexey Onufriev, Virginia Tech - Tag(s): Focus

2:30PM C55.00001: Chromosome organization by loop extrusion and phase separation* [Invited] LEONID MIRNY (Presenter), Massachusetts Institute of Technology — Inferring principles and mechanisms of 3D organization of chromosomes from Hi-C and imaging data is a challenging biophysical problem. Recently we proposed that an active process loop extrusion by SMC complexes is a universal mechanism responsible for formation of domains in interphase, and chromosome compaction and segregation in metaphase. I will review recent experimental studies that provide strong support to loop extrusion as a universal mechanism of chromosome folding.

These experiments have also showed that spatial segregation of euchromatin and heterochromatin is achieved by a different mechanism. To elucidate mechanisms of this spatial segregation, we examined Hi-C and microscopy for cells with inverted nuclei and conventional nuclear architecture. Polymer model base on these data show that attraction between heterochromatic regions drive the phase separation, while interactions with the lamina central for spatial positioning of phases in the nucleus.

Taken together our results demonstrate two major processes shape chromosome organization through the cell cycle: heterochromatin-driven phase segregation and SMC-driven loop extrusion.

3:06PM C55.00002: Modeling interphase chromosomes: Microrheology  ANDREA PAPALE (Presenter), ANGELO ROSA, International School for Advanced Studies — The nucleus of eukaryotic cells is one of the most investigated organelles, but its complete understanding is far from being reached. Recently considerable efforts have been devoted to experimentally analyze its viscoelastic properties, in particular through microrheology techniques.

We employ molecular dynamics computer simulations comparing experimental data with theoretical models. Mimicking experiments, we consider a polymeric model representing the crowding of interphase chromosomes [1] containing hundreds of brownian free particles as in [2]. We consider several sizes for particles from the tiny chromatin fiber to the mesh size of the chromatin solution. Tracking the motion of these fictitious nanoprobes we compute dynamical properties.

Then we investigate a simple variation of this polymeric model including a set of spring which modifies dramatically the viscoelastic properties. Interestingly, we observed the cage-and-escape dynamics peculiar for short times dynamics of nanoprobes seen in experiments.

We generalize also the model to the situation where active regulatory mechanics are present [3].


3:18PM C55.00003: Diffusion of nuclear proteins and its link to 3d chromatin organization*  ASSAF AMITAI (Presenter), Massachusetts Institute of Technology — The interaction of proteins with chromatin regulates many cellular functions. Most DNA-binding proteins interact both non-specifically and transiently with many chromatin sites, as well as specifically and more stably with cognate binding sites. These interactions and chromatin structure are important in governing protein dynamics. These questions can be addressed theoretically using diffusion models. I will show how that the dynamics of proteins is determined by the 3d organization of chromatin in the nucleus. The time to find a chromatin target depends on chromatin organization around it, which determines the local association and dissociation rates.

These ideas can be applied to study the dynamics of nuclear proteins and infer from single particle trajectories the geometry of the structures with which they interact.

*I acknowledge financial support from Massachusetts General Hospital (internal fund 214931).

3:30PM C55.00004: All-Atom Molecular Dynamics simulations of the interaction between viral capsid proteins and single-stranded RNA molecules.*  ZACHARY GVILDYS (Presenter), Chemistry & Biochemistry, University of California, Los Angeles, ROBIJN BRUINSMMA, Physics and Astronomy, University of California, Los Angeles — We carried out All-Atom Molecular Dynamics (MD) simulations of the interaction between the positively charged tails of viral capsid proteins and negatively charged homopolymeric polyU and polyA RNA molecules. Recent experiments showed that the encapsidation of homopolymeric RNA by viral capsids is sensitively dependent on the nature of the RNA nucleotide (C.Beren, L.Dreesens, K.Liu, C.Knobler and W.Gelbart, Biophys.J. 2017, 339). We found that the degree of base-stacking and helical ordering strongly influences the strength of the electrostatic component of the protein-RNA interaction, and hence the ability of the capsid proteins to package single-stranded RNA molecules. We compare the Potential of Mean Force measured by the MD simulations with the predictions of Poisson-Boltzmann theory for electrostatic interactions.

*We would like to thank the NSF-DMR for support under Grant 1610384.

3:42PM C55.00005: Pinning a protein (AQP1) structure by the interacting matrix elements  RAS PANDEY (Presenter), University of Southern Mississippi, PORNTHEP SOMPORNPSUT, Chemistry, Chulalongkorn University — The effect of temperature on a protein (AQP1) structure by a coarse-grained Monte Carlo simulation shows negative and positive responses in its native and denatured phases respectively. The same protein chain is then immersed in an interactive matrix with constitutive elements (i.e. effective solute particles with size comparable to residue) where an aquatic interactions between the residue and solute can be varied. Local and global physical quantities such as contact map, gyration radius, and structure factor are examined as a function of matrix interaction strength at a range of temperatures. The protein structures, from our preliminary studies, are found to be pinned by the solute, the radius of gyration becomes less sensitive to temperature, and structure factor shows a ramified structure with lower effective dimension than that without solute particles. In-depth analysis will be presented as the data will become available.
3:54PM C55.00006: Protein crystallizing assembly via free and grafted linkers*  YUBA DAHAL (Presenter), MONICA OLVERA DE LA CRUZ, Northwestern University — "Proteins have potential to form numerous lattices due to their highly anisotropic shape. However, the forces required to arrange proteins in a periodic fashion are not understood. In this study we introduce a coarse grained MD simulation approach to study the effects of length and geometry of linkers on the 3D crystalline assembly of ferritin protein. We find the optimal linker length dependence on the linker to protein ratio beyond which linkers fail to hold the proteins in a crystalline structure. We also study the effect of the length of the grafted linkers on the formation of the protein arrays. In the linker grafted case, we do not find an optimal length suggesting that the grafting of linkers on the protein surface is a better route to yield rich porosity crystalline structures. Our analysis suggests that the emergence of the optimal linker length is rooted at the expense of rotational freedom of the longer linker. The computationally inexpensive method that we present in this study could be useful as the guidelines to understand the assembly of complex molecules."

*Fairchild foundation

4:06PM C55.00007: Atomistic and Coarse-grained Simulations of Thermoresponsive Biopolymers*  PHILLIP TAYLOR (Presenter), PRHASHANNA AMMU, ARTHI JAYARAMAN, Chemical & Biomolecular Engineering, University of Delaware — This talk focuses on our multi-scale simulation studies on thermoresponsive biopolymers, specifically elastin-like peptides (ELP) and collagen-like peptides (CLP). ELPs are biopolymers that undergo a lower critical solution temperature (LCST)-like phase transition, which means ELPs are soluble below the transition temperature, $T_t$, and insoluble above $T_t$. The $T_t$ of ELPs can be tuned via conjugation to other thermoresponsive biomolecules such as CLPs. In our recent work, we used all-atom (AA) and coarse-grained (CG) simulations to elucidate how the guest residue impacts ELP stiffness, its secondary structure formation, and hydrophobicity and thus, the LCST-like transition of ELP and ELP-CLP conjugates. We used the structural data from AA simulations to modify our previous ELP CG model such that it captures the atomistically-informed stiffness while enabling simulations at experimentally relevant length scales. Our new ELP CG model also accounts for the hydrophobicity of the guest residue and its propensity to form compact, secondary structures. Through these modifications, our CG simulations are able to explain the experimental observations in $T_t$ of ELP and ELP-CLP conjugates with W and F as the guest residues.

*We thank NSF Grant 1703402 for financially supporting this work.

4:18PM C55.00008: Brownian Dynamics Simulation of Single Biomolecules: Contact Formation and Hydrodynamic Radius*  STEFFEN MÜHLE (Presenter), Third Physical Institute, Georg-August-University Goettingen, MAN ZHOU, Department of Biochemistry, University of Oxford, ARINDAM GHOSH, JÖRG ENDERLEIN, Third Physical Institute, Georg-August-University Goettingen — The conformational flexibility and dynamics of unfolded peptide chains is of major interest in the context of protein folding. The rate with which amino acids at different positions along the peptide chain meet sets an upper speed limit for protein folding. By using single-molecule photo-induced energy transfer (PET) spectroscopy, we have systematically measured end-to-end and end-to-internal site contact formation rates for several intrinsically disordered protein fragments (10 to 40 amino acids), and have also determined their hydrodynamic radius using dual-focus fluorescence correlation spectroscopy (2FCS). For interpreting the measured values, we have developed a Brownian dynamics model (a discretized elastic rod in a thermal bath including hydrodynamic interactions) which quantitatively reproduces all measured data surprisingly well while requiring only two fit parameters. The model provides a complete picture of the peptides' dynamics and allows us to translate the experimental rates and radii into molecular properties of the peptides: We find a persistence length of ~0.4 nm and a hydrodynamic radius of ~0.5 nm per amino acid.

*Funded by Deutsche Forschungsgemeinschaft (DFG) under SFB755's project A05.
Investigation into multivalently binding polymers

EMIKO ZUMBRO (Presenter), ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Biology frequently uses multivalent binding interactions to enhance weak, monovalent binding between molecules such as glycoligands and protein receptors. Synthetic glycopolymers have been shown to successfully bind to targets, such as viruses and toxic proteins. This binding indicates that the use of multivalent polymers can be a promising tool for inhibiting target attachment to and subsequent infection of cells. These polymers would act as decoys, suppressing virulence without killing their target and thus minimizing the development of resistance. Many studies have focused on creating multivalent binders with high affinity and high specificity to a single target. In contrast, we investigate how to design polymers that have broad-spectrum binding affinity, so that a single multivalent polymer could be used to inhibit multiple targets. We use a reactive-binding, Brownian dynamics simulation to examine how patterning of heterogeneous binding sites along a polymer chain control binding affinity of a polymer to multiple types of targets. Our results provide direction for designing polymeric inhibitors able to bind multiple targets simultaneously.

The authors were supported by the Department of Defense through the National Defense Science & Engineering Graduate Fellowship Program.

Disorder mediated oligomerization of chromosome translocation proteins of DISC1 gene.

DAVIT POTOYAN (Presenter), Iowa State University — Disrupted-in-Schizophrenia 1 (DISC1) gene is one of the highest risk factors for neural development including schizophrenia and other chronic mental illnesses. Depending on cellular context DISC1 gene expresses proteins of different length which have markedly different binding and oligomerization propensities. Due to highly disorder content the molecular level understanding of DISC1 protein assembly and oligomerization has been missing. We have carried out high throughput molecular dynamics simulations of all DISC1 expressed proteins at the coarse grained level to investigate conformational ensembles and oligomerization pathways of DISC proteins at the level of monomers dimers and various tetrameric combinations. Our findings reveal that disorder content present in DISC1 acts as a graded switch mediating non-additive binding and oligomerization preferences.

Characterizing the counterionic cloud of DNA-functionalized nanoparticles with molecular dynamics simulations

ALI EHLEN (Presenter), KURINJI KRISHNAMOORTHY, SUMIT KEWALRAMANI, MICHAEL J BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — DNA-functionalization of proteins allows for cell penetration and self-assembly of protein systems that have the potential for applications in therapeutics and other fields. However, the impacts of the resulting electrostatic interactions associated with the DNA shell and counterionic cloud are still being explored. Here, we use molecular dynamics simulations to examine the stability of a protein's DNA shell in the presence of DNase, as it relates to the composition of this counterionic cloud. We use molecular dynamics simulations and a simple thermodynamic model in tandem with SANS measurements to understand the composition of this cloud under varying salt conditions and protein shapes. This work builds on previous efforts to calculate this composition of this cloud using DFT calculations; detailed molecular dynamics simulations have been used to incorporate multiple species of ion as well as excluded volume effects and correlations.

Exploring the Structure and Dynamics of Carbohydrate Nanoparticles using Molecular Dynamics Simulations

ANDREW NAGEL (Presenter), MOHAMMAD HASSAN KHATAMI, HENDRICK W DE HAAN, University of Ontario Institute of Technology — PhytoSpherix is a carbohydrate-based nanoparticle composed of glucose units joined in a dendritic manner. These particles are of interest as they are a biodegradable and biocompatible nanomaterial. In this work, we present results from all-atom molecular dynamics simulations (GROMACS) of a PhytoSpherix-like particle. The particle is dynamically grown until it contains ~1100 glucose units. Analysis of structural features is conducted as the particle equilibrates to a relaxed state. The complex internal structure is characterized by hydrophobic interactions between chains and water-containing areas in contact with hydrophilic regions of the carbohydrate. Results concerning the dynamics inside of the particle are also examined. This characterization can assist the development of new applications for PhytoSpherix particles.

*OCE VIP II
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**5:18PM C55.00013: Investigating the Structure of Phytoglycogen using Coarse-Grained Simulations**

NICOLE DROSSIS (Presenter), HENDRICK W DE HAAN, Science, University of Ontario Institute of Technology — Phytoglycogen is a dendritic nanoparticle composed of repeatedly branching chains of glucose. Despite glucose being a common form of energy storage in plants, many questions still remain about the structure of this naturally occurring particle. In this work, pytoglycogen was modelled with a coarse-grained approach, simplifying each glucose unit to a single particle. A hydrophobic attraction between chains was observed in atomistic simulations and this was modelled in the coarse-grained simulations with a simple attraction between glucose particles. The strength of this attraction was used as a free parameter to investigate how changing it changes the structure of the particle. The simulated particles with radii similar to those seen in experiment were observed to have a hairy colloid shape, with a dense core and hairs extending out from the core.

*OCE VIP II
NSERC CRD

**Monday, March 4, 2019 2:30 PM - 5:18 PM**

**Session C56 GSNP: Networks of Oscillators** BCEC 255 - Daniel Lathrop, University of Maryland, College Park

**2:30PM C56.00001: Synchronous Clustering in Multilayered Networks**

LOUIS PECORA (Presenter), United States Naval Research Laboratory, KAREN BLAHA, Mechanical Engineering, University of New Mexico, KE HUANG, Electrical Engineering, University of New Mexico, FABIO DELLA ROSSA, Mechanical Engineering, University of New Mexico, MANI HOSSEIN-ZADEH, Electrical Engineering, University of New Mexico, ABU BAKAR SIDDIQUE, FRANCESCO SORRENTINO, Mechanical Engineering, University of New Mexico — The topic of cluster synchronization of oscillators in networks has an active history and has recently experienced renewed interest in the nonlinear dynamics community because of the use of such graph theory tools as symmetries and equitable partitions to predict what cluster structures are possible, calculate their dynamic stability, and characterize their bifurcations as they desynchronize. Another recent network structure that has caught the interest of the dynamics community is multilayered networks. We show how to extend the graph theory tools to multilayered networks. Certain multilayered networks have a structure that allows their dynamics to be simplified and fit into the existing structure of analysis of synchronous clusters. We also present a recent experiment on a simple 4-oscillator multilayer system. We show what can be discerned from experimental data including bifurcation plots and desynchronization patterns. This is the first experiment on cluster synchronization that we know of that uses totally analog oscillators with no computer-aided control of the oscillators. We also will discuss how some of the concepts can be generalized.

**2:42PM C56.00002: Spontaneous data clustering using collective synchronization in a network of phase oscillators**

TAKAYA MIYANO (Presenter), SHINYA TAKARAMOTO, Ritsumeikan University — We developed a method for spontaneous data clustering based on Kuramoto’s model for collective synchronization. A network of phase oscillators, to the natural frequencies of which multivariate data are input, achieves partial synchrony owing to short range interaction between neighboring phase oscillators. The common frequencies of the partial synchronous groups represent major feature patterns of the multivariate data. As a case study, we apply our method to actually observed time series of wind velocity and show major feature patterns of the wind data.

*This study was partly supported by JSPS KAKENHI Grant Number 15K00353.*
Interdependent and competitive dynamics in multilayer networks: synchronization and epidemics

MICHAEL DANZIGER (Presenter), Northeastern University, IVAN BONAMASSA, Department of Physics, Bar-Ilan University, STEFANO BOCCALETTI, CNR - Institute for Complex Systems, SHLOMO HAVLIN, Department of Physics, Bar-Ilan University — Since 2010, research on interdependent networks of networks, has demonstrated relevant new percolation phenomena including cascading failures and abrupt discontinuous transitions [1, 2]. However, this approach is limited to cases where connectivity can be taken as a proxy for functionality. Here, we present new research on interacting network dynamics exhibiting a wide range of new phenomena which are observed in the real-world but absent in previous models. By extending the concept of connectivity and dependency links to dynamical processes, we are able to shed light on real-world complex systems from social networks to the brain. We demonstrate our approach by implementing interdependent and competitive synchronization based on the Kuramoto model [3, 4] and SIS epidemics. This new framework provides a key missing link in the modeling of real-world multilayer networks. The talk is based on our recent manuscript [5].


Synchronization of chaotic oscillators using partial state space linear control*

KEYUR MISTRY (Presenter), Indian Institute of Technology Bombay, SUDESHNA DASH, National Institute of Technology, Tiruchirappalli, SIDDHARTH TALLUR, Indian Institute of Technology Bombay — The idea of synchronization of chaotic oscillators traces its origin to pioneering work by T. L. Carroll and L. M. Pecora in the late 1980s. Numerous implementations reported over the last three decades either require all state variables of a master oscillator to generate a locking signal to entrain the slave oscillators, or use a subset of the state variables, albeit with nonlinear transfer function. We present a novel methodology in which locking signal is generated as i) a linear combination of ii) a partial subset of state variables of the oscillators. The unused state variables can be exploited for applications in cryptography. A generalized algorithm for controller design is presented, and the efficacy of this algorithm is proved by analyzing the piece-wise oscillator as multi-mode linear system. Root-locus method is used to compute feedback gain. Simplicity of the control system makes it possible to reliably realize all-analog, all-digital, or mixed-signal implementations for electronic oscillators, with low power and cost overheads. The methodology is validated through numerical simulations and experiments using op-amp based electronic circuits.

*We acknowledge support from Wadhwani Electronics Laboratory, Department of Electrical Engineering, IIT Bombay.

Almost Perfect In-Phase and Anti-Phase Chaotic and Periodic Phase Synchronization in Large Arrays of Diode Lasers*

YEHUDA BRAIMAN (Presenter), NIKETH NAIR, Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, ERIK BOCHOVE, Directed Energy Directorate, Air Force Research Laboratory, Kirtland AFB, New Mexico, 87117 — We studied phase synchronization in large arrays of weakly coupled single mode semiconductor laser diodes [1,2]. We show that if the coupling topology is chosen appropriately, the laser array exhibits robust and almost perfect phase synchrony (including chaotic and non-chaotic phase synchrony). Furthermore, one can define coupling topologies that lead to chaotic anti-phase synchronization. When diodes are coupled via a decayed non-local coupling scheme, the leading spatial mode can be stable. This leads to an almost-perfect phase synchronous state where the phases are synchronized, even though the system is not being exactly on the synchronization manifold. This almost-perfect phase synchronous state is robust to noise and frequency and phase disorder and can be realized under periodic (fixed-intensity limit cycle) continuous-wave and chaotic behavior.

N. Nair, E. Bochove, and Y. Braiman, Optics Express 26, 20040 (2018).
N. Nair, E. Bochove, and Y. Braiman, Optics Communications 430, 104 (2019).

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Global Frequency Locking of Networks of Coherently Coupled Lasers  

JIAJIE DING (Presenter), MOHAMMAD-ALI MIRI, Queens College — Nonlinear dynamics of networks of coupled oscillators is a subject of great interest in various disciplines ranging from electrical circuits and chemical reactions to biological cells and social systems. A universal property of such networks is a self-organized oscillation at a common frequency, which is often referred to as synchronization. Here, we investigate the frequency locking of a network of coupled lasers. In this regard, we introduce a first-order nonlinear coupled-mode model for optical oscillators representing semiconductor lasers. We show that two coupled oscillators with different individual frequencies can be synchronized in frequency when the mutual coupling rate exceeds a critical level. The threshold coupling is calculated and explored in the parameter space of the system. Next, we investigate synchronization in one- and two-dimensional arrays of lasers with uniform nearest neighbor coupling and explore the synchronization threshold as a function of the size of the network. Finally, we discuss that a more complex network topology is required in order to enforce global synchronization in a large network of coupled lasers.

Optimal fluctuation pathways to desynchronization in coupled oscillator networks*  

JASON HINDES (Presenter), United States Naval Research Laboratory — There is great interest in understanding how topology, dynamics, and uncertainty conspire to produce rare and extreme events in networks. This is particularly the case for coupled oscillator networks since they appear at the core of many biological and physical systems where noise and uncertainty play a significant role. A primary example is desynchronization in power grids from input-power fluctuations. In this talk, we develop theory for the most-likely, or optimal, pathway of noise-induced desynchronization in phase-oscillator networks (with and without inertia) and in Stuart-Landau oscillator networks. We quantitatively characterize the scalings and patterns for the optimal path and the probability of desynchronization as a function of network topology and local dynamics, and compare the behavior for the various models. Lastly, we discuss the effects of non-Gaussian, “pulse” noise, and controls on the input power, on desynchronization. Such effects are especially relevant for power grids with renewable energy sources.

Control of a Multistable 3-ring Network of Chemical Oscillators*  

CHRISTOPHER SIMONETTI (Presenter), MICHAEL NORTON, MARIA ELENI MOUSTAKA, SETH FRADEN, Brandeis University — The Belousov-Zhabotinsky reaction is a limit cycle oscillator with dynamical attributes comparable to neurons. By fabricating microfluidic wells filled with the BZ chemistry, we create reaction-diffusion networks with rich dynamical patterns that can yield fundamental insights into dynamics of neural networks. A simple network of three inhibitor-coupled wells connected in a ring possesses two stable, dynamical steady states: clockwise and counterclockwise traveling waves. By photo-chemically perturbing the wells’ intrinsic frequencies we can force the system to switch states. In this work, we explore the steady states as a function of applied light gradient using the Kuramoto phase model and Vanaag-Epstein model for photosensitive BZ. Optimal control theory is then applied to determine the most efficient way to drive the system from one attractor to another.

Features of a rich attractor space in a system of repulsively coupled Kuramoto oscillators*  

SHADISADAT ESMAEILI (Presenter), Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech, DARKA LABAVIC, Universite de Lille, France, HILDEGARD MEYER-ORTMANNS, Jacobs University Bremen, Germany, MICHEL PLEIMLING, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — Rhythmic behaviors with a wide range of periods emerge from populations of coupled oscillators in many phenomena in nature. The Kuramoto model is one of the simplest models of coupled oscillators vastly used to explain many such phenomena. Choosing a repulsive coupling and a proper topology in this model leads to frustration and, as a result, versatile features of multistability. Also, by choosing non-homogeneous natural frequencies, in a large enough system orbits emerge with very long periods that are orders of magnitude longer than the natural frequencies. To understand the characteristics of the phase space we study the effects of tuning parameters like the coupling constant and the width of the frequency distribution.

*U.S. Naval Research Laboratory funding (N0001414WX00023) and the Office of Naval Research (N0001416WX00657) and (N0001416WX01643)

*The work by S. Esmaeili and M. Pleimling is supported by the US National Science Foundation through grant DMR-1606814.
4:18PM C56.00010: Overcoming oscillation quenching in coupled nonlinear oscillators*  NANNAN ZHAO (Presenter), ZHONGKUI SUN, Northwestern Polytechnical University — Rhythmic oscillation activity plays an important role in various natural and artificial systems. However, the appearance of oscillation quenching phenomena can lead to a loss or degradation of intrinsic function for many practical systems. In this work, we introduce a simple method based on the external positive feedback that can efficiently revoke these quenching states in different coupling schemes. Taking the limit cycle Stuart-Landau systems as example, we have illustrated numerically and analytically that tuning the feedback strength can shrink drastically the oscillation quenching regions in the parameter space. Our study will provide a new and general framework to retrieve the rhythmicity or the strengthen the robustness for dynamic activity of coupled nonlinear systems.

*This work was supported by the National Natural Science Foundation of China (Grants Nos. 11772254 and 11742013).

4:30PM C56.00011: Effects of variation of coupling offset \( \alpha \) in electronic oscillator experiments*  MACMILLAN WHEELER (Presenter), TAYLOR GURREITHUN, SHELBY STEGMAIER, DAVID MERTENS, Eckerd College — In biological systems that exhibit synchronization, oscillators within a single population vary in many aspects. To provide controlled experimental insight into how these variations affect synchronization, we have built an ensemble of highly configurable electronic oscillators. These oscillators have programmable speed, coupling strength, waveform shape, and coupling phase offset, known as \( \alpha \) in the Sakaguchi-Kuramoto model. Moreover, each oscillator can have a distinct coupling offset. We have examined how \( \alpha \) affects the degree of synchronization, and how variations in \( \alpha \) within a population alter the stability of the synchronous state. We will also compare our findings with those presented in the literature.

*Eckerd College NSSRP

4:42PM C56.00012: Relaxation oscillators, limit cycle oscillators, and somewhere in between: experimental exploration of waveform variation in synchronizing oscillators*  TAYLOR GURREITHUN (Presenter), MACMILLAN WHEELER, SHELBY STEGMAIER, DAVID MERTENS, Eckerd College — In biological systems that exhibit synchronization, oscillators within a single population vary not only in their natural rates, but in many other characteristics. To study such variations experimentally, we have built an ensemble of highly configurable electronic oscillators. These oscillators have programmable speed, coupling strength, coupling phase offset, and waveform. Each oscillator's waveform can be tuned from approximately sinusoidal to relaxational, effectively altering the interaction from a nearly sinusoidal one to a more complex form. To our knowledge, interactions between oscillators with different waveforms have not been examined. In this talk, we will present our findings on how variations in waveform in a single population affect the system's ability to synchronize.

*Eckerd College NSSRP

4:54PM C56.00013: Dynamics of the Kuramoto-Sakaguchi Oscillator Network with Asymmetric Order Parameter  JAN ENGELBRECHT (Presenter), Boston College, BOLUN CHEN, Brandeis University, RENATO MIROLLO, Boston College — Kuramoto oscillator networks are an important idealized class of oscillator models. We consider a generalized network in which the order parameter is the sum of the complex oscillator phases, but with non-identical coefficients. We analyze this model using a dimensional reduction from dynamics on an N-dimensional state space to a flow on the unit disk, where the natural hyperbolic metric facilitates the analysis. We give a fairly complete classification of the asymptotic dynamics with careful consideration of the subtleties of the flow near the disk's boundary, which includes both fully synchronized states and \((N-1,1)\) states where all but one of the oscillators are synchronized. The geometric connection also allows us to identify conditions for the flows to be gradient, or Hamiltonian or even simultaneously gradient and Hamiltonian. Examples of new behavior in the asymmetric model include, \((N-1,1)\) attractors with a basin of non-zero measure and homoclinic and heteroclinic non-periodic orbits to/from sync and \((N-1,1)\) states in the Hamiltonian case.

5:06PM C56.00014: Double-Period Breathers in a Driven-Damped Lattice  GOLAN BEL (Presenter), Environmental Physics, Ben-Gurion University of the Negev, BOIAN S ALEXANDROV, ALAN REGINALD BISHOP, KIM Ø RASMUSSEN, Theoretical Division, Los Alamos National Laboratory — Spatially localized and temporally oscillating solutions, known as discrete breathers, have been experimentally and theoretically discovered in many physical systems. We considered a lattice of coupled damped and driven Helmholtz-Duffing oscillators in which we found a spatial coexistence of oscillating solutions with different frequencies. Specifically, we demonstrated that stable period-doubled solutions coexist with solutions oscillating at the frequency of the driving force. Such solution represents period-doubled breathers resulting from a stability overlap between subharmonic and harmonic solutions and exist up to a certain strength of the lattice coupling. Our findings suggest that this phenomenon can occur in any driven lattice where the nonlinearity admits bistability (or multi-stability) of subharmonic and harmonic solutions.
2:30PM C57.00001: Characterization of fracture in topology-optimized bio-inspired networks*  CHANTAL NGUYEN (Presenter), Department of Physics, University of California, Santa Barbara, DARIN PEETZ, Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, AVIK MONDAL, Department of Physics, University of Michigan, AHMED ELBANNA, Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, JEAN CARLSON, Department of Physics, University of California, Santa Barbara — Trabecular bone is a flexible, lightweight bone tissue that exhibits an anisotropic microarchitecture resembling a web of interconnected struts (trabeculae). We simulate trabecular bone architectures with multi-objective topology optimization, effectively reverse-engineering trabecular structure by optimizing biologically-motivated objectives. Starting from an identical volume, we generate different topologies by varying the objective weights for compliance, surface area, and stability. We model these topologies as disordered, spatially-embedded networks where edges represent trabeculae and nodes represent branch points where trabeculae meet. We simulate mechanical loading on finite-element models where each edge is replaced by a beam, enabling direct comparison of mechanics and topology at multiple scales ranging from that of individual edges/beams to the network at large. We compare the mechanical response of the various topology-optimized networks and identify mechanisms of crack propagation. We characterize and predict crack pathways with community detection methods inspired by similar applications in the study of granular materials.

*NSF EAR-1345074 & CMMI-1435920, Institute for Collaborative Biotechnologies (ARO W911NF-09-D-0001), David and Lucile Packard Foundation

2:42PM C57.00002: Directed aging and memory: Teaching an old foam new tricks  NIDHI PASHINE (Presenter), DANIEL HEXNER, University of Chicago, ANDREA LIU, University of Pennsylvania, SIDNEY ROBERT NAGEL, University of Chicago — As a material ages, its physical properties change. Under an applied stress, it plastically deforms in order to relieve the internal stress in incremental steps. At each instant, it lowers the stress in the most effective way. Thus, over long times, the final state of the material depends on the external stresses it was exposed to during the aging process. A material thus has a memory of the stresses to which it was exposed during the aging process. We exploit this property and direct the aging process with specific protocols in such a way that our material reaches a distinct, final state with a prescribed and desired functionality. In order to demonstrate this behavior, we use sheets of foam that we cut with a laser cutter and place under stress in such a way that the material develops unusual elastic properties. To accelerate the aging process, we apply heat to the sample. We have been able to modify the Poisson's ratio of our system considerably; we can make a sample that was initially nearly incompressible and make it auxetic (negative Poisson's ratio). We can likewise take an auxetic sample and make it incompressible. We have also been able to train local behavior so that a sample responds with a prescribed local deformation in response to a global perturbation.

2:54PM C57.00003: Design and Control of Finite Conformational Changes in Mechanical Networks*  JASON KIM (Presenter), DANIELLE BASSETT, University of Pennsylvania — Conformational changes in physical networks play a crucial role in many systems, enabling error correction in DNA replication, cooperativity in hemoglobin, and mechanical capacities in metamaterials. Important work has begun to delineate the relationship between network structure and instantaneous conformational change. However, these efforts have failed to address finite conformations, which are critical for the successful function of most physical networks. Here we establish a simple framework for the design and control of mechanical spring networks in 2 and 3 dimensions. Specifically, for a set of nodes with arbitrarily specified initial and final positions, we characterize all bipartite networks with zero energy at these positions, demonstrate transitions between these positions, and design multi-stable networks for information storage. Finally, we use hysteresis and bi-stability to design networks demonstrating cooperativity.

*JZK acknowledges support from NIH T32-EB020087, PD: Felix W. Wehrli, and the NSF GRFP No. DGE-1321851. DSB acknowledges support from the John D. and Catherine T. MacArthur Foundation, the ISI Foundation, the Alfred P. Sloan Foundation, an NSF CAREER award PHY-1554488, and from the NSF through the University of Pennsylvania MRSEC DMR-1720530.
3:06PM C57.00004: Pattern Selection in Brine Shrimp Swarms  ANDREA WELSH (Presenter), FLAVIO FENTON, Georgia Institute of Technology — Swarming is a ubiquitous self-organization phenomenon which occurs in many biological systems such as flocks of bird and insect, schools of fish, and collections of bacteria. This sort of behavior emerges spontaneously, arising without any sort of centralized control or leadership. Many crustaceans such as brine shrimp produce swarms, in which individuals cluster together rather than spreading out uniformly in their environment. The size and distribution of these swarms are governed by local interactions between individuals. We will discuss the three-dimensional patterns that can be observed in brine shrimp swarms, specifically of the Great Salt Lake strain of *Artemia franciscana*, at high concentration. These patterns can be easily observed with simple tabletop experiments; however, the causes of these patterns are unknown. We experimentally test the effects of certain environmental conditions on the development of these swarms. We then develop a model an agent based model of shrimp which yields the same sort of spatial patterns as those that are observed. The model reproduces the basic length and times scales of the patterns, the type patterns selected, and the stability of those patterns.

3:18PM C57.00005: The effects of inhibitory neuron fraction on the dynamics of an avalanching neural network*  JACOB CARROLL (Presenter), ADA WARREN, UWE CLAUS TAUBER, Virginia Tech — The statistical analysis of the collective neural activity known as avalanches provides insight into the proper behavior of brains across many species. In this talk we present a neural network model based on the work of Lombardi, Herrmann, de Arcangelis et al. that captures the relevant dynamics of neural avalanches, and we show how the active neuron fraction can be used as a control mechanism to introduce exponential cut-offs in the distributions of avalanche strength and duration, transition the power spectral density of the network out of an epileptic regime, and drive the evolution of the network structure over time.

*Research was sponsored by the Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.

3:30PM C57.00006: A general geometric framework for knitted fabric elasticity  MICHAEL DIMITRIYEV (Presenter), KRISHMA SINGAL, ELISABETTA MATSUMOTO, Georgia Institute of Technology — Knitting is a process in which yarn, an essentially filament-like material, is shaped in space to form a fabric, an essentially sheet-like material, via stitching together a lattice of slip-knots. Due to fabric-level dependence on the stitch pattern, a single yarn can be used to create a large variety of fabric geometries and material responses. Moreover, the elasticity of knits remains poorly understood, as evidenced by the lackluster performance of spring-lattice models. We seek a continuum elastic model that predicts the three-dimensional shape of knitted fabric. This model should have the flexibility to be adapted to describe a wide range of stitch patterns and elasticity models. To this end, we have developed a geometric framework for relating the yarn path to the emergent surface geometry of the fabric. The generality of our approach allows for a systematic coarse-graining of yarn degrees of freedom, without *a priori* specification of a model of yarn elasticity. Thus, we are able to arrive at a stitch pattern-dependent, continuum elastic model of knits by assuming a simple phenomenological model of yarn, whilst allowing for the possibility of including more realistic yarn mechanics and experimental comparison.

3:42PM C57.00007: Model-dependent and model-independent control of biological network models*  JORGE GT ZANUDO (Presenter), Cancer Program, Broad Institute, GANG YANG, REKA Z ALBERT, Department of Physics, Pennsylvania State University — Network models of cell signaling and regulation are ubiquitous because of their ability to integrate the current knowledge of a biological process and test new findings and hypotheses. An often asked question is how to control a network model and drive it towards its dynamical attractors (which are often identifiable with phenotypes or stable patterns of activity of the modeled system), and which nodes and interventions are required to do so. In this talk, we introduce two recently developed network control methods - feedback vertex set control and stable motif control - that use the graph structure of a network model to identify nodes that drive the system towards an attractor of interest (i.e., nodes sufficient for attractor control). Feedback vertex set control makes predictions that apply to all network models with a given graph structure and stable motif control makes predictions for a specific model instance, and this allows us to compare the results of model-independent and model-dependent network control. We illustrate these methods with various examples and discuss the aspects of each method that makes its predictions dependent or independent of the model.

*Work supported by NSF Grants PHY 1205840 and 1545832. JGTZ is a recipient of an SU2C-TVF Convergence Scholar Award.

3:54PM C57.00008: TBD —
4:06PM C57.00009: Thouless and Relaxation Time Scales in Many-Body Quantum Systems*  MAURO SCHIULAZ (Presenter), Yeshiva University, E. JONATHAN TORRES-HERRERA, Benemerita Universidad Autonoma de Puebla, LEA SANTOS, Yeshiva University — We study the time scales involved in the relaxation process of isolated quantum many-body systems. Using experimental observables and a realistic many-body quantum model, we unveil three different time scales: a very short time that characterizes the early fast decay of the initial state, and two much longer times that increase exponentially with system size. These are the Thouless time, $t_{Th}$, and the relaxation time, $t_R$. The Thouless time refers to the point beyond which the dynamics acquire universal features, and relaxation happens when the evolution reaches a stationary state. We show that in chaotic systems, $t_{Th} < t_R$, while for systems approaching a many-body localized phase, $t_{Th}$ tends to $t_R$. We also compare these results with those for random matrices, and study how self-averaging properties depend on time scales.

*M.S. and L.F.S. are supported by the NSF Grant No.-DMR-1603418. E.J.T.-H. acknowledges funding from VIEP-BUAP, Mexico.

4:18PM C57.00010: Cyber-physical risks of hacked Internet-connected vehicles*  SKANDA VIVEK (Presenter), DAVID B YANNI, PETER YUNKER, JESSE L SILVERBERG, Georgia Institute of Technology — The interface of Internet-connectivity and automotive technology promises to dramatically improve transportation. However, with these known benefits come unknown risks, especially since Internet-connected vehicles have become targets for computer hacking. Vehicles, unlike sensitive data, can collide or physically interact when their systems become compromised, and there is a broad class of scenarios generically leading to Internet-connected vehicles being suddenly and simultaneously disabled. Here, we investigate how large-scale hacking affects traffic flow using agent-based simulations, and discover the critical relevance of percolation for predicting outcomes on a multi-lane road. Inspired by this discovery, we develop and validate an analytic percolation-based model to rapidly assess the effect of hacking. We then apply our analytic model to investigate the outcomes on the street network of Manhattan (NY, USA), revealing a latent risk. A small number of disabled vehicles can gridlock the city and substantially reduce access to emergency services. By discovering percolation as the phenomenological driver of city-wide disruption, we simultaneously uncover a strategy for risk-mitigation.

*GeorgiaTech Soft Matter Incubator
GeorgiaTech Institute for Robotics and Intelligent Machines

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C58 GSOFT: Self-Assembly III BCEC 257A - Alex Travesset, Iowa State University

2:30PM C58.00001: Droplets that decay, droplets that fährt: Restriction enzymes induce degradation, bubbling and propulsion in a DNA liquid phase*  OMAR SALEH (Presenter), University of California, Santa Barbara, TIM LIEDL, Department of Physics, Ludwig-Maximilians-Universitat, Munich — Multi-armed DNA particles (`nanostars') can be engineered to have weak inter-particle attractions, causing them to phase separate into liquid droplets. We are motivated to study this system both on the general grounds that bio-macromolecular liquids are interesting, and with the specific idea of using it to create a chromatin-inspired active matter system. To that end, we studied the interactions of proteins with DNA nanostar droplets, particularly measuring droplet degradation by DNA-cleaving restriction enzymes. Despite the droplet's small DNA volume fraction, enzyme degradation occurred primarily on surface of droplets, likely because enzyme transport was arrested by binding of the protein to the DNA. The degradation rate was surprisingly insensitive to variations in the number of restriction sites, but did vary with the strength of bonds between DNA particles. With certain tricks it was possible to force the enzyme inside the droplet, which caused the enzyme to carve out vacuoles that rose to the droplet surface and popped, driving droplet motion. I will discuss potential mechanisms behind this enzyme-induced motility.

*We thank the Alexander von Humboldt Foundation for support.
we are developing theoretical models to study the competition between flow force which induces clusters and electrostatic temperature to investigate whether adhesion also played a role in cluster formation. Comparing with experimental data, overcome electrostatic repulsion. Since particles deform and adhere when heated above Tg, we varied the ambient transition temperature (Tg) that could be robustly tuned from 0 °C to 80 °C. We find that fluid flow induced by evaporation evolution to be observed by light microscopy as a function of evaporation rates, salt concentrations and particle drying latex with initial volume fraction of 50% in a microfluidic channel, in a manner that allows the dynamic structure of the clusters is important to optimizing coating formulation. This talk reports a study of cluster formation induced by formation in colloidal suspensions is often observed during drying, and understanding the origins and physical properties of the clusters is important to optimizing coating formulation. This method is simple yet robust and easy to implement, and is straightforwardly scalable, involving a synergetic action of electric-field assembly, capillary and electrostatic interactions. Various aspects of our method, including the role of particle size and the voltages needed, are studied in detail.

Polymeric nanoparticles (NPs) are promising candidates for a wide range of applications such as colloidal self-assembly and targeted therapeutics. Flash Nanoprecipitation (FNP) is a scalable technique for fabricating monodisperse polymeric NPs through rapid micromixing of a polymer solution with a miscible poor solvent. In this simulation work, we are studying the fabrication of Janus NPs with one solvophilic and one solvophobic hemisphere, and their behavior at liquid-liquid interfaces. We performed coarse-grained molecular dynamics simulations of the FNP process using two types of solvophobic homopolymers and one type of amphiphilic blockcopolymers (BCPs). We investigated the influence of various process parameters on the resulting NPs morphology, namely, the composition and concentration of the BCPs. We determined the parameter space where amphiphilic Janus or core-shell NPs can be formed, and studied the conformation of BCPs at the NPs surface. Finally, we placed the fabricated NPs at the interface between two immiscible liquids. We observed a significant reduction of the interfacial tension when either core-shell or Janus NPs were placed at the interface compared to systems without NPs, demonstrating the potential of polymeric NPs as colloidal stabilizing agents.

Cluster formation in colloidal suspensions is often observed during drying, and understanding the origins and physical properties of the clusters is important to optimizing coating formulation. This method is simple yet robust and easy to implement, and is straightforwardly scalable, involving a synergetic action of electric-field assembly, capillary and electrostatic interactions. Various aspects of our method, including the role of particle size and the voltages needed, are studied in detail.

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Simulating Hepatitis B Virus antiviral agents* FARZANEH MOHAJERANI (Presenter), BOTOND TYUKODI, MICHAEL F HAGAN, Brandeis University — The infectivity of a virus depends on the complete assembly of a protein shell (capsid) around the viral nucleic acid. Molecules which block or alter assembly pathways have the potential to be used as antiviral agents. Recent in vitro experiments have identified a class of small molecules (assembly effectors) that accelerate assembly of Hepatitis B virus (HBV) capsids. In vivo experiments have shown that this acceleration of assembly in vitro correlates to antiviral activity in cells. However, the mechanism by which these molecules alter assembly pathways is unclear. In this talk I will describe a computational model which allows extremely efficient simulation of assembly dynamics of large protein shells. I will then show how application of this model to HBV assembly can elucidate the mechanism of action of assembly effectors. In particular, I will describe how the assembly effectors result in malformed capsid shapes, as seen in experiments.

*This work was supported by Award Number R01GM108021 from the National Institute Of General Medical Sciences and the Brandeis Center for Bioinspired Soft Materials, an NSF MRSEC, DMR-1420382.

Disorder Foreshadows Order in Colloidal Cubes* ABHISHEK SHARMA (Presenter), FERNANDO A ESCOBEDO, Robert Frederick Smith School of Chemical and Biomolecular Engineering, Cornell University — Prior molecular simulations have revealed that dense suspensions of hard nano-cubes are remarkable in that they form a mesophase near the ordering transition which is highly unusual when compared to typical crystals, plastic crystals, or liquid crystals. Monte Carlo simulations are used to study the disorder-to-order phase transition for a bulk system of colloidal hard cubes. It is observed that the ordered phase does not form via nucleation from the disordered phase, despite the prevalence in the latter of small locally ordered domains occurring transiently and sparsely. Instead, as the isotropic phase is brought to a marginally metastable concentration, such ordered domains increase in size and number, eventually reaching a critical point where they percolate the entire system and consolidate to form the mesophase. This process, quite different from nucleation observed for other particle shapes, arises presumably from a small interfacial tension. Simulations reveal that cubes infallibly form single-grain ‘crystals’ in the mesophase. This is traced to the abundant delocalized and transient vacancies and the high particle mobility in the mesophase which lead to formation of an active ‘recrystallization zone’ next to any grain boundary.

*NSF awards DMR-1609997 and CBET-1402117

Structure and dynamics of kinked line-slip defects in confined colloidal crystals NABILA TANJEEM (Presenter), VINOTHAN N MANOHARAN, Harvard University — Line-slip defects are found in crystals confined to the surface of a finite sized cylinder. These defects are identified by a line of particle pairs, each of which has one fewer contact than in bulk. They are known to appear in ground state of a cylindrical crystal when the cylinder cannot accommodate a perfect crystal. We study the structure and dynamics of these defects using an experimental system where submicron-sized colloidal spheres self-assemble into hexagonal lattices on a silica fiber with a diameter of a few micrometers. We find that most line-slip defects have kinks in them. A kink can be recognized from a discontinuity in the line-slip structure. The simplest kink in a line slip has four fewer bonds compared to a straight line-slip without any kink. We observe that the number of kinks in a line-slip defect does not change significantly over long time, but instead shows small fluctuations. We show that the average kink density is related to the average roughness of a 2D crystal grain. We find that by tuning the strength of interaction, we can tune the size of the crystal and the total length of the line-slip defects, allowing us to control the number of kinks in a line-slip defect and hence its shape.

Defect mediated coarsening of colloidal crystals on a cylinder* WILLIAM WILKIN (Presenter), NABILA TANJEEM, VINOTHAN N MANOHARAN, CHRISTOPHER RYCROFT, Harvard University — We perform Brownian dynamics simulations to investigate how geometrically stabilized defects in colloidal crystals on a cylindrical surface facilitate the approach to equilibrium. At intermediate times, a patchwork emerges of grains that generically exhibit vacancy-roughened helical line-slip defects, resulting in an ensemble of crystallites distinct from what is observed in the growth of crystals on planar surfaces. Interfaces between adjacent crystal grains typically exhibit a characteristic notch at the point of intersection with the line slip defect; this acts as a source for excitations of the line slip defect, coupling interfacial relaxation on opposite ends of each crystallite.

*This work was supported by the National Science Foundation through the Harvard Materials Research Science and Engineering Center (DMR-1420570)
4:18PM C58.00010: Directing Colloidal Assembly via Selective Depletion  MENA YOUSSEF (Presenter), STEFANO SACANNA, Chemistry, New York University — The ability to synthesize and assemble matter on the colloidal scale has recently been at the forefront of research in materials science and nanotechnology. In particular, the ability to direct the assembly of colloids in a directional manner presents a challenge, as many methods of assembly are inherently nonselective. In this work, colloids are synthesized via an emulsion-based method and depletants are made to selectively adsorb onto colloidal surfaces to direct assembly, thus allowing for depletion to only occur under certain conditions. We are able to achieve selective assembly by introducing polymers, changing the pH, and tuning the nature of the depletant. We demonstrate selective assembly by selectively forming single or mixed crystals from a bidispersed suspension of particles by modifying the environment that the colloids are suspended in. We further demonstrate degree of selectivity of the depletion interaction in our colloidal systems by directing the patch-to-patch assembly of Janus colloids into complex structures. Selective depletion offers a new tool to direct assembly in colloidal systems and has the potential to be used to direct the hierarchical assembly of building blocks such as patchy particles and Janus colloids towards desired complex structures.

4:30PM C58.00011: Stability and Free Energy of Nanocrystal Chains and Superlattices*  XUN ZHA (Presenter), ALEX TRAVESSET, Iowa State University — I present simulations of hydrocarbon-capped monodisperse nanocrystal superlattices. I compute the free energy for both bcc and fcc, including several ligand lengths, as well as the entropy and Gibbs free energy. We find that bcc superlattices with oriented or random nanocrystal cores have slightly different free energy and lattice constant. Consistent with experimental findings, we observe that nanocrystals capped with relatively long ligands form bundles. We also compared our calculated lattice constants to experimental values and predictions for the OTM (Orbifold Topological Model).

*NSF, DMR-CMMT 1606336 “CDS&E: Design Principles for Ordering Nanoparticles into Super-crystals”

4:42PM C58.00012: Multiscale Modeling of Precursor Molecule Alignment for Improving Pitch-Based Carbon Fiber Production*  YANMING WANG (Presenter), CUIYING JIAN, TAISHAN ZHU, NICOLA FERRALIS, JEFFREY C GROSSMAN, Massachusetts Institute of Technology — Carbon fiber (CF) is a versatile material widely applied in many fields, and one main method to produce CF is from pitch, a viscoelastic material composed of aromatic hydrocarbons. Though it is well known that the early stage alignment of precursor molecules has significant effects on the pitch-based fibers, a deeper understanding of its underlying microscopic mechanisms is lacking. Here we perform fully atomistic (FA) and coarse-grained (CG) simulations to study the alignment of pitch molecules. While the FA simulations generates accurate atomistic descriptions, the CG simulations provide a means to efficiently explore larger time and length scales. The ellipsoid algorithm is adopted to extract geometric features of these molecules from the FA trajectories, enabling a quantitative analysis of the intermolecular alignment as well as the construction of anisotropic CG particles. Our multiscale simulations identify the dependences of alignment on the molecule size, temperature and loading conditions. Further, the model suggests specific additives and operation conditions that can improve the molecule alignment. These calculations provide guidelines for optimizing the synthesis pathways for low cost and high-quality CF.

*The project is supported by DOE program DE-FOA-0001629.

4:54PM C58.00013: Controlled Self-Assembly of Peptide Nanotubes via Sequence Modification and Kinetic Control*  YU TIAN (Presenter), FRANK POLZER, University of Delaware, HUIXI ZHANG, JEFFERY G SAVEN, Department of Chemistry, University of Pennsylvania, KRISTI KIICK, DARRIN POCHAN, University of Delaware — Synthetic peptides with the high sequence- and shape-specificity can serve as the assembly building blocks for the construction of controllable and complex nanoarchitectures. Computational design was employed to design peptides that can form antiparallel, alpha-helical tetrameric coiled-coil bundles in solution that then further assemble into higher order structures with targeted organization. The bundles self-assemble into homogenous nanotubes at pH 4.5. As analyzed by cryo-TEM, SAXS and STEM, a mono-layer tilted-bundle model is proposed to explain the nanotube structure. The charged state and distribution of the peptide bundles associated with the acidic solution condition are believed to be the reason triggering the formation of nanotubes. Rational sequence modifications were applied to control the dimensions of the nanotubes or to disrupt the tube nanostructure or to add metal-binding functionality. Moreover, kinetic control was applied in the assembly process to produce a branched nanotube morphology. Further crosslinking treatment can be applied to the branched nanotube system for the development of stable hyper-branched materials with potential applications.

*This work is supported by NSF DMREF under DMR-1234161 and DMR-1235084, and partially funded by NSF CHE1213728.
RAVI KUMAR PUJALA (Presenter), School of Physics, University of Hyderabad — We propose an alternative method to tune the electrostatic interactions to obtain a transition from a repulsive to an attractive system of nanoplatelets by increasing the alcohol concentration, i.e. increasing the Bjerrum length. A phase diagram of Laponite® in alcohol solutions has been proposed, which clearly demarcates regions of stable sol, unstable sol, transparent gel, turbid gel, glass, and flocculation. A new class of soft materials, called nanoclay-organogels, was deeply explored using confocal and scanning electron microscopy that depicted spongy architecture and presence of nano and micron size pores inside the gel matrix indicating the hierarchical self-assembly of the nanoplatelets in the binary solvent. Universal power-law scaling of storage modulus and yield stress with alcohol concentration was observed. We have extensively examined the dispersion stability, aggregation and gelation behaviour of Laponite nanoplatelets in different alcohol -water binary solvents, thereby proposing a universal description of nanoclay dispersion in alcoholic solutions, which is poorly probed and marginally understood in the literature.

*RKP acknowledges receiving the Department of Science and Technology INSPIRE Faculty Award grant [DST/INSPIRE/04/2016/002370].

JIYEONG GU (Presenter), VICTOR DE LA CRUZ, Physics and Astronomy, California State University Long Beach — A monolayer of close-packed nanospheres can be used as a template or a mask to produce interesting magnetic nanostructures. Multi-step spin coating process was used to create the densely packed monolayer of nanospheres. Various parameters, such as, spin speed, spin acceleration, spin duration, nanosphere concentration, volume of the solution deposited on the substrate, the duration of each step, and the interval in between the steps, were adjusted to maximize uniform area of monolayer. After a systematic study, we found that the excess solution between the nanospheres should be removed quickly during the spin-coating process so the spheres move closer each other and form the close-packed monolayer. The spin coated nanospheres were examined using an optical microscope and a scanning electron microscope. Magnetic materials, such as Permalloy or cobalt, were sputter coated on top of monolayer nanospheres. Magnetic switching behavior of these curved magnetic thin films were investigated using an alternating gradient magnetometer, a vibrating sample magnetometer, and through the magneto-optical Kerr effect measurement. Nanocap layer showed a wider magnetic switching and distinctive magnetic anisotropy compared to the flat thin film samples.

**Monday, March 4, 2019 2:30 PM - 5:06 PM**

**Session C59 GSOFT GSNP: Rheology and Flow of Soft Matter I** BCEC 257B - Li-Chiun Cheng, Massachusetts Institute of Technology - Tag(s): Focus

**2:30PM C59.00001: Rheology of glassy and jammed emulsions**

CONG CAO (Presenter), ERIC WEEKS, Emory University — We study the rheology of monodisperse emulsions with various mean droplet sizes. Above a critical volume fraction, these systems will exhibit solid-like behaviors and possess a yield stress. Previous simulation work suggests that for small thermal particles, rheology will see a glass transition; for large athermal systems, rheology will see a jamming transition. However, at the crossover of thermal and athermal regimes, the glass and jamming transitions may be well separated and observed at different volume fractions for a fixed mean droplet size. We conduct an experiment by shearing different sizes of emulsion droplets (500 nm-5 μm diameter) with a rheometer. In this way, we measure rheological properties near the critical volume fraction. By varying the shear rate and particle size, our experiments cover a wide range of Péclet number (the ratio of shear and thermal motions), including the crossover regime.

*NSF(DMR-1609763)*
2:42PM C59.00002: Viscous fingering instabilities in carbon black gels* THIBAUT DIVOUX (Presenter), Civil and Environmental Engineering, CNRS / Massachusetts Institute of Technology, BADIS MARSIT, Mechanical Engineering, Massachusetts Institute of Technology, YACOUBA KALOGA, Civil and Environmental Engineering, CNRS / Massachusetts Institute of Technology, IRMGARD BISCHOFBERGER, Mechanical Engineering, Massachusetts Institute of Technology — Pattern formation in fluids occurs in numerous physical processes in which mechanical mixing, chemical reactions, evaporation and/or surface effects play a key role. When the pattern develops in a non-Newtonian fluid, the non-linear rheology interferes with the patterning process, which often generates a richer dynamics than that commonly observed for a Newtonian fluid. Here we focus on the viscous fingering instability in a time-dependent yield stress fluid. We study experimentally the flow of a carbon black gel sandwiched in a parallel plate geometry, for which the upper plate is being lifted up at constant velocity. We show the existence of a critical initial gap spacing and a critical lift velocity, above which the flow becomes unstable, leading to the growth of viscous finger originating from the Saffman-Taylor instability at the fluid-air interface. The resulting pattern in the gel consists in a tree-like branched structure, whose wavelength surprisingly follows the scaling established for Newtonian fluids. The signature of the fluid non-linear rheology lays in the spatial extent of the pattern, which is governed by the yield strain of the gel. Finally, we show that varying the shear history of the gel, one can produce patterns with a wealth of new morphologies.

*MISTI @MIT

2:54PM C59.00003: Microrheology of pH-Responsive Nanoparticle Monolayers at Fluid Interfaces SHIYI QIN (Presenter), XIN YONG, Binghamton University — The effect of shear on the structure and dynamics of polyelectrolyte-grafted nanoparticles (PGNP) straddling at a water–oil interface was investigated through mesoscale simulations. Using electrostatic dissipative particle dynamics, long-range electrostatic forces are solved in a triclinic simulation box, which allows us to apply continuous shear deformation to the monolayer. The monolayers with different particle coverages were examined under shear and degree of ionization of PGNPs were set to be high. While undisturbed, the particles arrange themselves on a hexagonal lattice due to the long-range electrostatic interactions. As the monolayer with low particle concentration is subjected to the shear flow, the free voids allow particles to move in the shear direction. However, strong inter-particle forces at high particle concentration result in the collective motion of domains to repair the adjacent defect. The in-plane structure of monolayer is analyzed by structure factor and Voronoi diagram. The dynamics of local domains are observed through snapshots and averaged velocity contours. The rheology measurements of the monolayer were also performed under small-amplitude oscillatory shear and the results were correlated with the detailed structure evolution.

3:06PM C59.00004: Microscopic Rearrangements in the Flow of Polydisperse Dense Emulsions* YONGLUN JIANG (Presenter), CARLOS S ORELLANA, ERIC WEEKS, Emory University — We study the flow of dense polydisperse quasi-two-dimensional emulsions. In particular, we are interested in highly polydisperse samples with the largest droplets as much as ten times the size of the smallest. The droplets are confined between two parallel glass plates and driven to flow by a syringe pump. We use video microscopy to examine how rearrangements differ for large and small droplets. In particular, we find the large droplets follow the mean flow, while the small droplets move more erratically. We try to quantify these results by looking at the nearest neighbor changes and nonaffine motions. We explore different means of defining affine motion, including definitions based on nearest neighbors and definitions based on regions of space. The former varies quite a bit depending on the size of droplets, whereas the latter is simpler but lacks a sensitivity to droplet size.

*NSF (CBET-1804186)
Rheological and Microstructural studies of semi-dense and dense suspensions in a Periodic Poiseuille Flow using Core-Modified Dissipative Particle Dynamics* ERIKA BARCELOS (Presenter), SHAGHAYEGH KHANI, Macromolecular Science and Engineering, Case Western Reserve University, ARMAN BOROMAND, Department of Mechanical Engineering and Materials Science, Yale University, MÔNICA NACCACHE, Department of Mechanical Engineering, Pontifícia Universidade Católica do Rio de Janeiro, JOAO MAIA, Macromolecular Science and Engineering, Case Western Reserve University — Shear-thickening is a nonlinear rheological behaviour often observed in semi-dense and dense suspensions at increasing shear rates and is commonly associated with microstructural changes in the material. Therefore, understanding the rheology-microstructure correlation has a fundamental importance in the development of many industrial and technological processes. Core-Modified Dissipative Particle Dynamics was employed as a computational method to capture the physics involved in the flow of semi-dense and dense suspensions subjected to a periodic Poiseuille flow at two confinement ratios. The interplay between hydrodynamic and frictional interactions in promoting shear-thickening was investigated as well as the microstructure evolution of those systems at increasing shear rates. Velocity profiles were found to increase with the Péclet number and the shear-thickening response was stronger and took place sooner for dense suspensions at narrower gap sizes. The microstructure followed the rheological trend, clusters of particles being bigger in size for denser and more confined systems.

*We acknowledge the financial support from CAPES (Brazilian Ministry of Education).

Active Microrheology in Emulsion Glass NESRIN SENBIL (Presenter), University of Fribourg, MARKUS GRUBER, University of Konstanz, CHI ZHANG, University of Fribourg, MATTHIAS FUCHS, University of Konstanz, FRANK SCHEFFOLD, University of Fribourg — Microscopic observations of probe particles under passive or force driven motion provides unique insights into the dynamics of colloidal dispersions. Here, we study experimentally the motion of polystyrene probe particles seeded in a micron scale oil-in-water emulsion system. We apply a well-defined constant force on the probe particles via a gradient intensity laser line trap and determine the displacements and probability distributions at various forces in the fluid and glass. Over the range studied, our emulsion droplets acts like hard spheres displaying a jamming and glass transition at 64% and 59% packing fractions, respectively. Both PS particles and emulsion droplets are sterically stabilized and identical in size. The crossover from localized to delocalized behavior happens at a threshold force which highly depends on the composition and corresponding cage strength (in the glass) and cage relaxation (in the fluid). Our experiments reveal intermittent dynamics and bimodal van Hove distribution functions around a depinning transition at a threshold force. For smaller forces, linear response connects the mean displacement and the quiescent mean squared displacement. We compare our observations to Mode coupling theory and find qualitative and semi-quantitative agreement.

Tuning friction and rheology at material-nanoparticle-liquid interfaces with an external electric field.* BIPLAV ACHARYA (Presenter), CAITLIN M SEED, DONALD W BRENNER, ALEX I SMIRNOV, JACQUELINE KRIM, North Carolina State University — Nanoparticles, both with and without polymeric surface coatings, dispersed in solutions are in common use as rheological and friction modifiers. The surface functionalization of the nanoparticles therefore provides a unique opportunity for active electro-tunable control of their flow in liquid. We report the use of electrophoretic forces to tune friction and rheology at material-nanoparticle-liquid interfaces with static or low frequency (0.6 – 50 mHz) electric fields. Negatively charged TiO2 or positively charged Al2O3 nanoparticles suspended in water were repositioned relative to a planar platinum surface of a quartz crystal microbalance, which was then used to monitor friction levels. Active electro-tunable control of friction was achieved, and investigated as a function of electric field frequency. Kinetic effects corresponding to nanoparticle repositioning at the solid interface were discovered to occur at glass-like time scales. The studies also reveal that nanoparticles manipulated by electric fields can act as “cantilever-free” atomic force probes capable of “tapping mode” exploration of interfacial properties and nanoscale interactions in geometries inaccessible to optical and micromechanical probes.

*National Science Foundation Award Number DMR1535082
3:54PM C59.00008: Understanding the effect of confinement on the viscosity of bacterial suspensions*  
ZHENG-YANG LIU (Presenter), KECHUN ZHANG, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota — Bacterial suspensions, a premier example of active fluids, show intriguing rheology different from their counterpart colloidal suspensions. When the confinement length scale is comparable or smaller than the intrinsic length scale of bacterial suspensions, we expect to see a qualitative change of their flow behaviors. Here, by using a microfluidic channel viscometer, we investigate the viscosity of *E. coli* suspensions under different degrees of confinement. For low concentration suspensions, we observe strong shear thickening at low flow rates. More importantly, a strong confinement effect is found when the confinement length is comparable to the running length of single bacterium. The viscosity of bacterial suspensions decreases by a factor of 2.5, when the confinement decreases from 50 down to 25 microns. In contrast, for high concentration suspensions, we observe strong shear thinning at low shear rates. The confinement leads to an increase rather than decrease of viscosity when the confinement length is comparable to the size of collective swarming of bacterial suspensions. Our study reveals the dynamics of bacterial suspensions under confinement and provides new insights into the transport of active fluids in confined geometries.

*NSF CBET-1702352, and DARPA YFA-D16AP00120

4:06PM C59.00009: Upstream vortex and elastic wave in the viscoelastic flow around a confined cylinder  
PAUL SALIPANTE (Presenter), National Institute of Standards and Technology, BOYANG QIN, Department of Mechanical Engineering & Applied Mechanics, University Of Pennsylvania, STEVEN HUDSON, Department of Mechanical Engineering & Applied Mechanics, University Of Pennsylvania — The flow of a viscoelastic fluid past a cylinder is a classic benchmark problem that is not completely understood. Using novel holographic particle velocimetry to measure 3D flow fields, we report two main discoveries of the elastic instability upstream of a single cylinder in confined microchannel flow. After the onset of corner vortices upstream of the cylinder, we find that the vortex becomes unsteady and switches between two distinct flow states, leading to symmetry breaking perpendicular to the cylinder axis that is highly three-dimensional in nature. Second, we show that the disturbance of the elastic instability propagates far upstream via an elastic wave and is weakly correlated with that in the cylinder wake. The wave speed and the extent of the instability increase with Weissenberg number, indicating an absolute instability in viscoelastic fluids.

4:18PM C59.00010: Glassy Dynamics in a Simulated Cell Monolayer with Division and Death*  
MICHAEL CZAJKOWSKI (Presenter), Department of Physics, Georgia Tech, DANIEL SUSSMAN, Soft and Living Matter Program, Dept of Physics, Syracuse University, M. CRISTINA MARCHETTI, Dept of Physics, UC Santa Barbara, M. LISA MANNING, Soft and Living Matter Program, Dept of Physics, Syracuse University — Recent experiments have indicated that quasi two-dimensional epithelial tissues undergo a transition to a rigid state which shares many characteristics with traditional particulate glass. At the same time, numerical work has suggested that the presence of cell division and death in dense particle-based models for tissues will always destroy signatures of glassy dynamics such as caging. Can then glassy behavior be recovered in real tissues where cells commonly divide and die? We address this question with a vertex-type model of motile tissue modified to include a balanced rate of cell division and death. The division and death rate competes with the motility-driven rate of cell rearrangement to control the tissue dynamics. We show that glassy dynamics is recovered for slow division and death rates. Further quantifying the displacements coming from a single division or death event, we are able to accurately predict the crossover between motility-dominated and division/death-dominated rheology.

*This work was partly supported by the Simons Foundation Targeted Grant in the Mathematical Modeling of Living Systems Number 342354 and Simons Foundation grants 446222 and 454947.

4:30PM C59.00011: Reversibility and diffusion in a meso-scale model for amorphous under cyclic shear.  
KAREEM ABDELSHAFY (Presenter), Northeastern University, BOTOND TYUKODI, brandeis University, DAMIEN VANDEMBROUQC, ESPCI Paris, CRAIG MALONEY, Northeastern University — We present results on a meso-scale model of amorphous plasticity subject to cyclic shear. We show that, after a transient, depending on the amplitude of cycling, the steady state behavior falls into one of three cases, in order of increasing strain amplitude: i) pure elastic behavior with cessation of all plastic activity, ii) reversible periodic plasticity with the period being an integer number of strain cycles (not necessarily a single cycle), and iii) irreversible plasticity with long-time diffusion. This behavior is consistent with what is seen in experiments on 2D amorphous particle rafts and confocal microscopy of emulsions and in athermal quasi-static particle-based simulations. We further show that, in the large amplitude regime, the steady state single-cycle plastic strain field is localized along line-like structures similar to the ones seen during avalanches during steady plastic shear, but there is little persistence in the localization from one cycle to the next.
4:42PM C59.00012: Front Microrheology of the non-Newtonian behaviour of blood  AURORA HERNANDEZ-MACHADO (Presenter), Fisica de la Materia Condensada, Universitat de Barcelona — We introduce a new framework to study the non-Newtonian behaviour of fluids at the microscale based on the analysis of front advancement. We apply this methodology to study the non-linear rheology of blood in microchannels. We carry out experiments in which the non-linear viscosity of blood samples is quantified at different haematocrits and ages. Under these conditions, blood exhibits a power-law dependence on the shear rate. In order to analyse our experimental data, we put forward a scaling theory which allows us to define an adhesion scaling number. By applying this scaling theory to samples of different ages, we are able to quantify how the characteristic adhesion energy varies as time progresses [1]. We also analyze numerically the rheology of dilute red blood cell suspensions in pressure driven flows at low Reynolds number in terms of the elasticity of the cells. We identify the relevant aspects of cell elasticity that contribute to the rheological response of blood [2]. We have related the viscosity of healthy, anemic and alpha-thalasemic blood samples with the bending rigidity of the erythrocyte membrane [3].


4:54PM C59.00013: Coarse-graining amorphous plasticity: shear-banding and rejuvenation  BOTOND TYUKODI, Brandeis University, ARMAND BARBOT, REINALDO GARCIA GARCIA, MATTHIAS LERBINGER, SYLVAIN PATINET, DAMIEN VANDEMBROUQ (Presenter), PMMH, CNRS/ESPCI Paris — The plastic behavior of glasses and disordered solids displays a rich and complex phenomenology, from scale free avalanches to localization of the strain field in shear bands. The recent years have seen an increasing effort of modeling of these phenomena at different length and time scales. In complement of numerous numerical simulations at atomistic scale of model or more realistic glasses, a new class of lattice models has emerged at mesoscopic scale that rely on the coupling between a local threshold dynamics and elastic interactions. The latter "Eshelby" interaction is associated to the internal stress induced by local rearrangements taking place in the surrounding elastic matrix and is characterized by a quadrupolar symmetry. While these lattice models reproduce most of the phenomenology observed in amorphous plasticity, a quantitative link remains to be done with atomistic simulations. Here we use a technique recently developed to characterize local yield stress in atomistic simulations to propose and study the quantitative connection between simulations operating at atomistic and mesoscopic scales.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C60 FED: Life, the Universe, and Everything: Teaching Biology to Physicists and Physics to Biologists BCEC 258A - Laurie McNeil, University of North Carolina at Chapel Hill - Tag(s): Education , Invited, Undergraduate

2:30PM C60.00001: Physics, biology and chemistry: teaching at the interface between the natural sciences [Invited] RHONDA DZAKPASU (Presenter), Georgetown University — The biological physics major at Georgetown University was created to attract premed students who might otherwise major in biology. Many of these students will have taken physics and calculus – frequently at the AP level – in high school and are often not aware that physics can be a viable path to medical school. This talk will discuss our philosophy in developing the major and the requirements to complete the major; I will focus on the two-semester sequence in biological physics and the independent research project. I will also present some of the benefits as well as the challenges that we have experienced as we work to refine the major as well as what types of paths our majors take after they graduate.

3:06PM C60.00002: ISC: An Integrated, Quantitative Introduction to the Natural Sciences at Princeton University [Invited] JOSHUA SHAEVITZ (Presenter), Princeton University — The Integrated Science Curriculum (ISC) at Princeton is an integrated, mathematically and computationally sophisticated introduction to physics and chemistry, drawing on examples from biological systems. This year long, four course sequence is a multi-disciplinary course taught across multiple departments and intended for students considering a career in science. Briefly, ISC teaches introductory Physics, Chemistry, Molecular Biology and Computer Science in an integrated setting through a combination of lectures, precepts, and laboratory exercises. The 2018-19 academic year represents our fifteenth year teaching the course and I will present a progress report on how the program has evolved over time.
**3:42PM C60.00003: Quantitative biology and the "hacker lab" : An interdisciplinary graduate program at UCSD**

[Invited] PHILBERT TSAI (Presenter), Physics, University of California, San Diego — The Quantitative Biology Program (Qbio) is a new integrative graduate specialization program that consists of a combination of theory classes, experimental labs, seminars, and critical reading courses. The program draws select graduate student from five different departments across three division at UCSD: physics, biology, chemistry, bioengineering, and biomedical sciences. In this talk, we will survey the program structure, but focus on two unique aspects of the program: the interactive critical reading program and the Qbio Hacker lab.

In brief, the Qbio Hacker lab serves as both classroom and shared resource. First, students enroll in a single-quarter “boot-camp” lab course. Though a combination of lectures and hands-on experimental modules, student work together in interdisciplinary pairs to achieve a basic proficiency in experimental skills ranging from 3D fabrication for instrumentation to computer-electronics-hardware interfacing to optical design for modern microscopy to fundamentals of microfluidics. The students then enroll in a second-quarter “project/rotation” quarter in which the students utilize their newly-developed experimental skills and resources to design and tackle a pilot research project under the guidance of individual Qbio faculty. Additionally, students work together in small groups through an interactive critical reading program, spending multiple weeks on an individual research paper to critically analyze its data, results, and theoretical claims. Through these multiple interdisciplinary interactions, students cement a foundation in reaching across fields to investigate biological phenomena with the full array of quantitative and technological tools available to them.

*We gratefully acknowledge funding from:
UCSD Quantitative Biology Initiative
NIH Training Grant in Quantitative Integrative Biology (T32GM127235).

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**4:18PM C60.00004: From Probability, Dynamics, and Modeling to Biology, Physics, and Instrumentation: Constructing an Upper-Division Course That Majors and Nonmajors Actually Take**

[Invited] PHILIP C NELSON (Presenter), Physics/Astronomy, University of Pennsylvania — Despite great progress in pedagogy, the actual content of upper-division Physics courses would in many cases be familiar to a time traveler from another century. I'll outline a strategy that I and others have used to create several new courses. Briefly, it involves: (1) Identifying an ongoing scientific revolution as a destination, then asking what classic frameworks are needed to go beyond mere description; (2) Identifying general-purpose skills that are needed for this and other current research; and (3) If necessary, asking what existing course could be remodeled to offer this new one within existing departmental constraints. For example, in a biological physics context the answers could involve (1) The current revolutions in optics; (2) Basic skills involving modeling, including probabilistic models; and (3) Revising the syllabus of "Modern Physics" or another such course. More broadly, I'll mention other case studies where this approach has worked, some rough metrics of success, and some new textbooks embodying these ideas.

*National Science Foundation PHY--1601894.
4:54PM C60.00005: Introductory Physics for Life Sciences: Design Principles, Resources, and Community*

CATHERINE CROUCH (Presenter), Swarthmore College — A national network of physics faculty have developed frameworks and extensive resources for teaching introductory physics to life science students in a way that highlights the value of physics in understanding biology, biochemistry, and medicine. These courses seek to give students practice in applying physics to analyze biologically significant phenomena. As more departments become interested in offering such courses, there is a need for curricular materials and support for faculty teaching such courses for the first time and adapting them to their local context.

The Living Physics Portal will provide a state-of-the-art online platform for sharing and developing such curricula. It will allow instructors to find materials through a searchable interface with extensive implementation metadata. More importantly, it will allow those who are new to such courses to learn from experienced instructors about the special features and challenges of such courses; and it will allow those who develop materials, whether novices or experienced, to share their materials for feedback at an early stage, or submit them for consideration for a “vetted collection” for materials that have been extensively used and refined.

This talk will present the motivation for and research supporting the introductory physics for life sciences approach, followed by an introduction to the capabilities of the Portal.


*The Living Physics Portal is funded by NSF (DUE #1624185); curriculum development and some research at Swarthmore funded by the Howard Hughes Medical Institute (Science Education Grant to Swarthmore College); other research funded by NSF (DUE #1122941, #1710875) and Swarthmore College.

Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C61 GSOFT DBIO GSNP: Active Matter I

2:30PM C61.00001: Bend instability and topological defects in 3D active nematics*

GUILLAUME DUCLOS (Presenter), Martin A. Fisher School of Physics, Brandeis University, DANIEL BELLER, Department of Physics, University of California, Merced, POOJA CHANDRAKAR, Department of Physics, University of California, Santa Barbara, MINU VARGHESE, Martin A. Fisher School of Physics, Brandeis University, DEBARGHYA BANERJEE, Max Planck Institute for Dynamics and Self-Organization, Göttingen, MATTHEW PETERSON, ARVIND BASKARAN, Martin A. Fisher School of Physics, Brandeis University, FEDERICO TOSCHI, Department of Applied Physics, Eindhoven University of Technology, VINCENZO VITELLI, James Franck Institute and Department of Physics, University of Chicago, SEBASTIAN STREICHAN, Department of Physics, University of California, Santa Barbara, ROBERT ALAN PELCOVITS, THOMAS POWERS, Department of Physics and School of Engineering, Brown University, APARNA BASKARAN, MICHAEL F HAGAN, Martin A. Fisher School of Physics, Brandeis University, ZVONIMIR DOGIC, Department of Physics, University of California, Santa Barbara — Active nematics describes a phase of matter where active particles that consume energy to produce mechanical work assemble at high density in a state with orientational order but no positional order. In this talk, I will show how the active nematic framework allows us to better understand aspects of the collective behaviors that emerge in bioinspired materials. In particular, I will present our recent efforts to describe the emergence of flows and topological defects in 3D active nematics composed of a passive colloidal liquid crystal doped with active microtubules and molecular motors. I will first describe the generic bend instability that emerges in a flow-aligned 3D active gel and show how the interplay between activity, nematic elasticity and confinement controls the wavelength of this activity driven instability. I will then present current work on the emergence of flows and topological defect in 3D.

*We acknowledge support from the Brandeis NSF MRSEC, Bioinspired Soft Materials, DMR-1420382 and the Human Frontier Science Program.
3:06PM C61.00002: Defect unbinding and a motile Kosterlitz-Thouless transition in active nematics*  
SURAJ SHANKAR (Presenter), Physics Department and Syracuse Soft and Living Matter Program, Syracuse University, SRIRAM RAMASWAMY, Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, M. CRISTINA MARCHETTI, Department of Physics, University of California, Santa Barbara, MARK BOWICK, Kavli Institute for Theoretical Physics — Active nematic liquid crystals formed by a collection of self-driven particles on a two-dimensional substrate exhibit complex spatio-temporal dynamics and spontaneous defect proliferation. An important consequence of the non-equilibrium drive is the spontaneous motility of strength +1/2 disclinations that drives flow in the system. Starting from the hydrodynamic equations of active nematics, we derive effective equations for the topological defects as interacting overdamped particles with pair forces and active torques. Using these equations we then show that activity lowers the defect-unbinding transition temperature driving a nonequilibrium variant of the Kosterlitz-Thouless transition into a state of defect chaos. Crucially, we find rotational noise stabilizes nematic order at low activity leading to a re-entrant transition. For large activity, orientational torques on the defects combined with many-body screening allows the spontaneous appearance of a polar defect ordered liquid, rationalizing previous work into a comprehensive phase diagram for two-dimensional active nematics.

*This work was supported by the NSF grants DMR-1609208, PHY-1748958 (KITP) and a J C Bose Fellowship of the Science & Engineering Research Board (India).

3:18PM C61.00003: Activity driven defect ordering in an active nematic on an anisotropic substrate*  
DANIEL PEARCE (Presenter), Dept. Of Physics, University of Geneva — We investigate the effect of an anisotropic substrate on the turbulent dynamics of a simulated two dimensional active nematic. This results in an effective anisotropic friction and viscosity, with the orientation of the anisotropy being defined by the substrate. In this system we observe the emergence of global nematic order of topological defects that is controlled by the degree of anisotropy in the viscosity and the magnitude of the active stress. No such alignment is seen in passive liquid crystals with anisotropic viscosity confirming that ordering is driven by the active stress. We then closely examine the active flow generated by a single defect to show that the kinetic energy of the flow is orientation dependent, resulting in a torque on the defect to align them with the anisotropy in the substrate.

*I acknowledge the support of SNSF/NCCR Chemical Biology.

3:30PM C61.00004: Self-organized dynamics of confined active nematics*  
ACHINI OPATHALAGE (Presenter), MICHAEL NORTON, MICHAEL P. N. JUNIPER, S.ALI AGHVAMI, BLAKE LANGESLAY, SETH FRADEN, Department of Physics, Brandeis University, ZVONIMIR DOGIC, Department of Physics, University of California at Santa Barbara — We study the role of boundary conditions on a simplified experimental model of biological active matter composed of extensile filamentous bundles of microtubules driven by clusters of kinesin motors, to elucidate the structure and dynamics of active nematic liquid crystals. These bundles form a quasi-2D active nematic liquid crystals when sedimented onto a surfactant-stabilized oil-water interface. We further confine this system onto circular boundary conditions, imposing a total topological charge of +1. For diameters of 400 micrometer and larger, multiple +/- ½ defects continuously nucleate and annihilate at the boundary as well as in the confinement core and generate flows of either handedness. As the diameter is reduced, defects periodically nucleate at the boundary with slow dynamics and migrate toward the confinement core rendering a fast pairwise procession, referred to as doubly-periodic dynamics. Existing continuum theories fail to predict this phenomenon and we hypothesize what additional physics needs to be included to reconcile experiment and theory.

*Experimental analysis was supported by DOE-BES through DE-SC0010432TDD. Developing microfluidic technology was supported by Brandeis MRSEC through NSF-MRSEC-1420382. Computational work was supported by NSF-DMR-1810077.
ANDREY SOKOLOV (Presenter), Argonne National Laboratory, RUI ZHANG, ALI MOZAFFARI, JUAN DE PABLO, University of Chicago, ALEXEY SNEZHKO, Argonne National Laboratory — Living liquid crystal (LLC), a synthetic material combining a lyotropic liquid crystal and swimming bacteria, demonstrates a number of out-of-equilibrium phenomena ranging from active turbulence to creation and annihilation of motile topological defects. In this talk, we report a spontaneous formation of undulation bands in circularly aligned LLC. The interplay between elasticity of liquid crystal and bacteria-induced hydrodynamic forces results in the emergence of a remarkable branched pattern of radially elongated bands of a highly curved director field. The average number of such branches is increasing with the distance from the center of the pattern and leads to the emergence of a radial fractal tree or a snowflake structure. Our experimental observations show that the shape of this structure, as well as a number of bands, is controlled by the activity of bacteria and elasticity of liquid crystal and suggest a new concept for a manipulation of active nematics at a microscale.

*This work was supported by the US DOE, Office of Basic Energy Sciences, Division of Materials Science And Engineering, under contract No. DE AC02-06CH11357

RUI ZHANG (Presenter), STEVEN REDFORD, University of Chicago, PAUL RUIJGROK, Stanford University, NITIN KUMAR, ALI MOZAFFARI, AARON DINNER, VINCENZO VITELLI, University of Chicago, ZEV BRYANT, Stanford University, MARGARET GARDEL, JUAN DE PABLO, University of Chicago — Active matter gives rise to intriguing spontaneous flows and motion whose collective behavior is difficult to steer and tailor, thereby placing limits on potential applications. Here, we present a new method to control the dynamics of an active liquid crystal. Theory shows that through the interplay of local active stresses it is possible to create anchoring effects that help confine activity-induced topological defects. This prediction is confirmed by hydrodynamic simulations of active nematics. Simulations further demonstrate that at moderate-to-high activity, local active stresses can be used to create defect pairs at will and direct the motion of +1/2 defects on demand; at low activity, such stresses can induce a spontaneous flow without strong elastic distortions of the nematic. Our calculations are compared to experiments of a flexible active liquid crystal.

ALI MOZAFFARI (Presenter), RUI ZHANG, Institute for Molecular Engineering, University of Chicago, ANDREY SOKOLOV, ALEXEY SNEZHKO, Materials Science Division, Argonne National Lab, JUAN DE PABLO, Institute for Molecular Engineering, University of Chicago — Active nematics represent a class of active systems, operating out of thermodynamic equilibrium that consists of self-driven units with long-range orientational ordering. Our numerical simulation was inspired by the experimental observation of the development of deformation patterns of branched, radially elongated elastic bands of the director field in living liquid crystals (suspension of self-propelled swimming bacteria in bio-compatible lyotropic liquid crystal).

As a model system, we chose a suspension of elongated rods which exerts extensile active stresses and we employed the theory of active nematodynamics to study the spatiotemporal dynamics of this system. The interplay of activity induced spontaneous flow which drives the system away from the minimum of the free energy, and the orientational ordering of the liquid crystal give rise to rich dynamical behavior over length scales much larger than the size of each individual active entity. Continuum simulations of the active nematic explain how activity fueled instabilities result in appreciable spatial inhomogeneities of the nematic ordering, giving rise to the formation of alternating bands of opposite curvature. Our study examines regimes beyond experimental limits providing important insights into the origin of the observed pattern.
4:18PM C61.00008: “Catapulting” of topological defects through elasticity bands in active nematics  NITIN KUMAR, James Franck Institute, University of Chicago, RUI ZHANG (Presenter), Institute for Molecular Engineering, University of Chicago, STEVEN REDFORD, James Franck Institute, University of Chicago, JUAN DE PABLO, Institute for Molecular Engineering, University of Chicago, MARGARET GARDEL, James Franck Institute, University of Chicago — Local injection of energy in active liquid crystals (LC) results in spontaneous defect generation and emerging complex flows. Elucidating the role of competition between activity and nematic elasticity is crucial to understanding this phenomenon. Here, we present our experimental results on nematic LCs composed of short actin filaments, driven by myosin motors where the elasticity is tuned by varying the filament length, \( l \). We find that for \( l = 2 \) µm where the elasticity is high compared to an LC with \( l = 1 \) µm, elongated regions of uniform bend distortions form, which we define as elasticity bands. The bands are evocative of domain walls observed in hydrodynamic simulations of active nematics. The emergence of a shoulder in the elastic energy distribution provides an explanation – a nematic LC with high elasticity tends to minimize the total elastic deformation by localizing it to narrow regions in space. Moreover, we find that as the activity decays, the LC dissipates excess elastic energy by eliminating these bands resulting in “catapulting” of +1/2 defects at a very high speed which scales inversely with the width of the band. Our results are fully supported by hydrodynamic simulations of active nematics and advance our understanding of complex flows in active liquid crystals.

4:30PM C61.00009: Emergent lengthscales in confined 3D Active Incipient Nematics*  MINU VARGHESE (Presenter), Physics Department, Brandeis University, YI FAN, Department of Engineering, Brown University, ARVIND BASKARAN, Physics Department, Brandeis University, KUN-TA WU, Physics Department, Worcester Polytechnic Institute, ZVONIMIR DOGIC, Physics Department, University of California, Santa Barbara, SETH FRADEN, MICHAEL F HAGAN, Physics Department, Brandeis University, KENNY BREUER, Department of Engineering, Brown University, APARNA BASKARAN, Physics Department, Brandeis University — An incipient nematic is a system whose density is smaller than the critical density for isotropic-nematic transition. The stationary isotropic state, which is the stable equilibrium of a passive incipient nematic, can be destabilized by the effects of extensile activity combined with flow alignment. We study the properties of flows that arise from this instability in confined 3D systems. Calculations from hydrodynamic theory, and experimental measurements on a microtubule-based system show long-range velocity correlations, in the absence of such correlations in nematic order. Further, we show that there exists a confinement-independent lengthscale intrinsic to flows in an active incipient nematic that determines its bulk behavior.

*This work was supported by the Brandeis University MRSEC, and high performance computing resources from Texas Advanced Computing Center

4:42PM C61.00010: Avalanches and Clogging in Active Matter Systems  CYNTHIA REICHHARDT (Presenter), CHARLES REICHHARDT, Los Alamos National Laboratory — Jamming and clogging have been extensively studied in passive soft matter systems such as granular matter or colloids moving through disordered environments such as obstacle arrays. Here we consider a system of disks moving through a random obstacle array and examine the transition to a clogged state as function of obstacle density as we go from the passive particle limit to an active matter limit. In the passive case, for a fixed disk density there is a well defined obstacle density above which the system reaches a clogged state. As the activity is increased, the disks can become mobile again when the activity breaks up the clogs; however, for large activity, which corresponds to long run times in a run-or-tumble system, the disks undergo intermittent clogging and we find that above a certain activity level, the unclogging events exhibit a power law distribution. We argue that the activity induced clustering brings the system into a critical state associated with local regions that have reached the jamming density known as point \( J \). For infinite run times or the ballistic active matter limit, the system can reach a completely clogged state with no avalanches for disk densities that are much lower than those at which clogging is observed for passive particles.
Controlling collective patterns has attracted interest due to their potential in exploiting their hidden ordered phase of active bacterial suspension. Here, by imposing a geometric boundary condition, we study controlled collective motion of *Escherichia coli* bacteria inside designed microwells. In a doublet circles, two vortices emerge but their spinning directions show two distinct phases of either parallel pattern (ferromagnetic vortices, FMV) or anti-parallel one (anti-ferromagnetic vortices, AFMV). The transition from FMV to AFMV occurs when the ratio of vortex size to vortex distance is $\sqrt{2}$. Analytical solution with mean-field approximation accounts for this geometric rule [1]. By using this relation, we can control quadruplet pairing of bacterial vortices. Moreover, in a triplet circles, coexistence of FMV and AFMV pairings is emerged despite frustration, and the transition point from FMV pattern to coexisted phase is shifted because frustration stabilizes FMV pattern. Our result proposes simple design of boundary as promising mean in order to understand collective ordering of bacterial vortices.

Reference


*Grant-in-Aid for Scientific Research on Innovative Areas “Molecular Engines” 18H05427*

Microswimmers such as bacteria exhibit collective behavior that can be controlled when placed in a nematic liquid crystal (NLC) with long-range orientational order [1]. We explore the collective motion of motile *Bacillus subtilis* dispersed in an aqueous solution of DSCG, a lyotropic chromonic NLC. The director field, imposed through photoalignment, contains defects of topological charge +1 which serve as attractors for bacteria. We vary the azimuthal angle of the director from 0 to 90 degrees to have predominant director distortions of either splay, bend, or a mixture of the two. The bacteria exhibit collective circular motion around +1 defects, with the radius of maximum concentration and velocity increasing as bend distortion dominates over splay. The experiment presents an example of how microswimmers interact with attractor type singular defects with different degrees of splay or bend deformation. The ability to control the collective motion of microswimmers can be used as a source of energy to power microscopic mechanical systems.

Reference


*This work is supported by NSF DMREF grant DMS-1729509.*

Magnetotactic bacteria are inherently magnetic motile micro-organisms. Hence, their swimming orientations are readily controlled by external magnetic fields making them a valuable model active matter system. When oriented perpendicular to a surface, they experience attractive hydrodynamic interactions that result in spontaneous self-organization (clustering). By tuning the cell density and magnetic field strength, this ordering may be systematically removed and restored, permitting construction of a phase boundary defining the onset of ordering and experimental exploration of cluster kinetics. The self-organization process is quantified using an order-parameter independent approach based on lossless compression algorithms (Lempel-Ziv), as well as a more conventional method employing the radial distribution function. These analyses reveal that the clusters scale logarithmically in time, representing a non-equilibrium analog of the “self-focusing” regime of charged colloids, and implying that the interplay between hydrodynamic attraction and magnetic repulsion control the kinetics. Furthermore connections between experimentally determined pair-wise interactions and the many-body dynamics, as well as the role viscous dissipation plays in stabilizing the structures will be discussed.
In recent years, enormous data sets have begun to appear in real-space visualizations (scanning probes) and reciprocal-space visualizations (scattering probes) of electronic quantum matter. Increasing volume and variety of such data present new challenges and opportunities that are ripe for a new approach: machine learning. However, the scientific questions in the field of electronic quantum matter require fundamentally new approaches to data science for two reasons: (1) quantum mechanical imaging of electronic behavior is probabilistic, (2) inference from data should be subject to fundamental laws governing microscopic interactions. In this talk, I will review the aspects of machine learning that are appealing for dealing with quantum complexity and present how we implemented a machine learning approach to the analysis of scanning tunneling spectroscopy data and X-ray scattering data.

*Theoretical studies are supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-SC0018946.

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**2:30PM C62.00001: Learning Quantum Emergence with AI.**

**EUN-AH KIM (Presenter), Cornell University —**

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**3:06PM C62.00002: Electron Microscopy of Quantum Materials: From Learning Physics to Atomic Manipulation**

**SERGEI KALININ (Presenter), ANDREW LUPINI, STEPHEN JESSE, RAMA K VASUDEVAN, MAXIM ZIATDINOV, Oak Ridge National Laboratory —**

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**3:42PM C62.00003: Bridging simulations and theories of correlated electron materials using ideas from machine learning**

**LUCAS WAGNER (Presenter), University of Illinois at Urbana-Champaign —**

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*Research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

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*This work was partially supported by the Simons Collaboration on the Many-Electron Problem. Results were obtained using the Blue Waters supercomputer.
4:18PM C62.00004: Autonomous Quantum Materials Research: Phase Mapping [Invited]  A. GILAD KUSNE (Presenter), Materials Measurement & Science Division, National Institute of Standards & Technology, TIEREN GAO, Materials Science & Engineering Dept, University of Maryland, BRIAN DECOST, JASON HATTRICK-SIMPERS, Materials Measurement & Science Division, National Institute of Standards & Technology, APURVA MEHTA, SLAC, ICHIRO TAKEUCHI, Materials Science & Engineering Dept, University of Maryland — The last few decades have seen significant advancements in materials research tools, allowing researchers to rapidly synthesize and characterize large numbers of samples - a major step toward high-throughput materials discovery. Machine learning has been tasked to aid in converting the collected materials property data into actionable knowledge, and more recently it has been used to assist in experiment design. In this talk we present the next step in machine learning for materials research - autonomous materials research systems. We first demonstrate autonomous measurement systems for phase mapping, followed by a discussion of ongoing work in building fully autonomous systems. For the autonomous measurement systems, machine learning controls X-ray diffraction measurement equipment both in the lab and at the beamline to identify phase maps from composition spreads with a minimum number of measurements. The algorithm also capitalizes on prior knowledge in the form of physics theory and external databases, both theory-based and experiment-based, to more rapidly hone in on the optimal results.

4:54PM C62.00005: Machine learning modeling of superconducting critical temperature* [Invited] VALENTIN STANEV (Presenter), University of Maryland, College Park — Machine learning has emerged as a powerful new research tool that can be used to answer many scientific questions in unconventional ways. In this talk I will discuss how it can help us address one of the most challenging problems in the study of quantum matter – finding connection between superconductivity – in particular critical temperature $T_c$ – and chemical/structural properties of materials. I will present several recently developed machine learning methods for modeling $T_c$ of the 12,000+ known superconductors available via the SuperCon database. These models use coarse-grained predictors based only on the chemical composition of the materials. They demonstrate good performance and strong predictive power, with learned predictors offering insights into the mechanisms behind superconductivity in different families. The models can be combined into a single pipeline and employed to search for potential new superconductors. Searching the entire Inorganic Crystallographic Structure Database led to the identification of 35 compounds as candidate high-$T_c$ materials. I will also discuss how machine learning can be used to guide and accelerate the experimental process.

*This research is supported by ONR N000141512222, ONR N00014-13-1-0635, and AFOSR No. FA 9550-14-10332.

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C63 DBIO: Quantum Phenomena, Instrumentation, and Techniques in Biology

BCEC 259A - Jason Hafner, Rice University

2:30PM C63.00001: Ab-initio Electronic Structure Calculations of Entire Metalloproteins* CARLOS ROMERO-MUÑIZ (Presenter), MARÍA ORTEGA, Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, JOSÉ G. VILHEN, Basel University, ISMAEL DÍEZ-PÉREZ, Material Science and Physical Chemistry, Universidad de Barcelona, JUAN CARLOS CUEVAS, RUBEN PEREZ, LINDA ANGELA ZOTTI, Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid — In this work we present a theoretical approach to deal with entire metalloproteins at quantum level. In particular we focus on single-Cu azurins and cytochrome c, which contains a heme group with its typical Fe-center. In this approach we consider the complete structure of these proteins as a whole rather than limiting our analysis to relevant fragments of coordination complexes. This is accomplished by combining fully ab-initio calculations based on density functional theory with atomic-scale molecular dynamics simulations. Beyond the main features arising from the metallic ions, our study reveals that the role played by the peripheral parts of the proteins could be of remarkable importance. More precisely, we find that oxygen atoms belonging to carboxyl groups of acidic amino acids, distributed all over the protein contribute to electronic states near the HOMO in the case of azurins. The contribution of the outer regions to the electronic structure of metalloproteins had so far been overlooked. Our results stress the need to investigate them thoroughly; this is especially important in prospect of understanding complex processes like the electronic transport through metal-metalloprotein junctions.

Quantum Mechanics of Proteins in Water: The role of Plasmon-like Solute-Solvent Interactions

MARTIN STOEHR (Presenter), ALEXANDRE TKATCHENKO, University of Luxembourg — van der Waals dispersion interactions form a major component of both intra-protein and protein-water interactions. As such, they play an essential role for the spontaneous folding of proteins in water. van der Waals forces arise from long-range electron correlation and are thus inherently quantum-mechanical and many-body in nature. Nevertheless, they are typically only treated in a phenomenological manner via pairwise potentials. Here, we employ an explicit quantum-mechanical framework based on the many-body dispersion formalism, which allows us to highlight the importance of the many-body character of dispersion interactions for protein energetics and protein-water interactions. As such, our study provides insights into the fundamental quantum-mechanics of proteins in water. Contrary to commonly used pairwise approaches, many-body quantum effects significantly affect relative stabilities during protein folding in the gas-phase. Embedding in an aqueous environment leads to a quenching of such effects and stabilizes native conformations. Remarkably, this arises from a high degree of delocalization and collectivity of protein-water dispersion interactions. Our findings are exemplified on several prototypical proteins, emphasizing their broad validity in the biomolecular context.

Discrimination of bosonic loss: Applications to biological samples and photo-degradable materials

GAETANA SPEDALIERI (Presenter), STEFANO PIRANDOLA, SAMUEL LEON BRAUNSTEIN, University of York — We consider quantum discrimination of bosonic loss based on both symmetric and asymmetric hypothesis testing. In both approaches, an entangled resource is able to outperform any classical strategy based on coherent-state transmitters in the regime of low photon numbers. In the symmetric case, we then consider the low energy detection of bacterial growth in culture media. Assuming an exponential growth law for the bacterial concentration and the Beer-Lambert law for the optical transmissivity of the sample, we find that the use of entanglement allows one to achieve a much faster detection of growth with respect to the use of coherent states. This performance is also studied by assuming an exponential photo-degradable model, where the concentration is reduced by increasing the number of photons irradiated over the sample. This investigation is then extended to the readout of classical information from suitably-designed photo-degradable optical memories (quantum reading).

Surface-Enhanced Raman Scattering as a Tool for Biomembrane Structure

JASON HAFNER (Presenter), Physics & Astronomy, Rice University — Gold nanostructures focus light to the molecular length scale at their surface. The large optical intensity leads to surface-enhanced Raman scattering (SERS) from nearby molecules. SERS spectra contain information on molecular position and orientation relative to the surface but are difficult to interpret quantitatively. Here we describe a ratiometric analysis method that combines SERS and unenhanced Raman spectra with theoretical calculations of the optical field and molecular polarizability. The analysis was also applied to fluid phase phospholipid bilayers that contain tryptophan on the surface of gold nanorods. The lipid double bond was found to be oriented normal to the bilayer and 13 Å from the nitrogen atom. Tryptophan was found to sit near the glycerol headgroup region with its indole ring 43° from the bilayer normal. The potentiometric membrane probe di-4-ANEPPS has also been detected and its orientation characterized in the lipid bilayer. This new method can determine specific interfacial structure under ambient conditions, with microscopic quantities of material, and without molecular labels.

The authors acknowledge funds from the Robert A. Welch Foundation under grant C-1761, as well as the National Science Foundation under project 1709084.
Previous studies have indicated selective biological cell damage due to local rapid thermalization [1] effects induced by laser irradiation. We have studied the effects of intense pulsed laser radiation on the prokaryote S. cerevisiae and eukaryote E. coli. These species are comparable to either cells found in the human body or pathogenic cells, respectively. We obtained the optical absorption spectra for the cells, and found frequency bands in the far-infrared (FIR/THz) range where notable spectral differences emerge. We report results of strong laser illumination at these selected bands.


*This work was supported by the National Science Foundation, grant No. PHY1725118.

The dynamics of concentrated suspensions of the crystallin eye-lens protein alpha crystallin was measured using x-ray photon correlation spectroscopy. For pure alpha crystallin suspensions the diffusive dynamics near the peak in the hard sphere structure are well described by a polydisperse hard sphere model. The intermediate scattering factor can be described by a stretched exponential function, and the concentration dependence of the relaxation time agrees with predictions from Langevin dynamics simulations.

*Research was supported by the National Eye Institute of the National Institutes of Health under Award Number R15EY018249. Work at the APS was supported by DOE Contract No. DE-AC02-06CH11357. UFXC32k detector development was supported by the national center for Research and Development, Poland PBS1/A3/12/2012

We report a novel method, dual color axial nanometric localization by Metal Induced Energy Transfer (dcMIET), and combine it with Förster Resonant Energy Transfer (FRET) for resolving structural details in cells on the molecular level. We demonstrate the capability of this method on cytoskeletal elements and adhesions in human mesenchymal stem cells (hMSCs). Our approach is based on Fluorescence-Lifetime-Imaging Microscopy (FLIM), and allows for precise determination of the 3D architecture of intracellular structures, here in particular, stress fibers anchoring at focal adhesions, thus yielding crucial information to understand cell-matrix mechanics. In addition to resolving nanometric structural details along the z-axis, we use FRET to gain precise information on the distance between actin and vinculin at focal adhesions. Here, we will present data where we use our method to follow the maturation of focal adhesions and acto-myosin fibers in hMSCs over time and show that actin fibers are nearly parallel to the substrate yielding an inclination angle of only 0.2°.

*Deutsche Forschungsgemeinschaft (DFG) via CNMPB, SFB 937(A13, A14), SFB 755 (B8), and the Niedersachsen-Israel framework (MWK-VWZN2722).
3:54PM C63.00008: Separation of Protein and Water Dynamical Transitions Using Terahertz Spectroscopy*

AKANSHA SHARMA (Presenter), DEEPU GEORGE, ANDREA MARKEZ, University at Buffalo, The State University of New York — Terahertz Time Domain spectroscopy (THz TDS) has been used to characterize the protein dynamical transition [1, 2]. The dynamical transition has been considered a manifestation of the slaving of protein motions to thermally activated motions of the solvent, however recently is has been reported that sharp temperature increases in protein dynamics occur independent of the solvent [3]. Potentially terahertz spectroscopy can resolve both the protein and water dynamical transitions using the ~ 5 THz intermolecular water vibrational line and the broad ~ 1.0 THz absorption arising from the protein intramolecular motions. Here we use a combination of THz TDS and FTIR to examine this possibility and resolve the protein and water contributions using a combination of spectral decomposition and concentration dependent measurements. Concentration dependent measurements using hen egg white lysozyme (HEWL) confirm that the transition measured at 1 THz is dominated by the protein dynamics.


*Work supported by NSF grants DBI 1556359 and MCB 1616529.

4:06PM C63.00009: Non-destructive prediction of transcriptomic profiles by Raman microscopy

KOSEKI KOBAYASHI-KIRSCHVINK (Presenter), YUICHI WAKAMOTO, Department of Basic Science, Graduate School of Arts and Sciences, University of Tokyo — Raman microscopy can report on whole single-cell molecular compositions in both comprehensive and non-destructive manners. However, molecular compositions of cells are diverse and compounds such as proteins have severe spectral overlaps, making them nearly intractable to interpret. Instead of pursuing the spectral decomposition, we show that transcriptomic profiles of Schizosaccharomyces pombe and Escherichia coli can be computationally linked and be predicted from their single-cell Raman spectra. Our method employs the low-dimensional structure of transcriptomes, and learns a non-linear linkage between the transcriptomes and Raman spectra. Permutation tests show that the probability of accidentally finding the same prediction precision level is extremely low (p-value<0.0001), suggesting that the prediction is real. These results demonstrate that whole-cell Raman spectra could unravel cellular omics information in non-destructive manners, opening the possibility of conducting living-cell genomic analyses.

*Japan Society for the Promotion of Science KAKENHI (grant number 15KT0075 and 15H05746)

4:18PM C63.00010: Probing Mechanical Properties of Biomolecules using Nanopores

PRASAD BANDARKAR (Presenter), ROBERT HENLEY, HUAN YANG, MENI WANUNU, PAUL WHITFORD, Physics, Northeastern University — Nanopore translocation is a promising label-free single molecule technique to distinguish between bio-molecules. The confined nature of the nanopore restricts the allowed conformations of the molecules or necessitates a conformational change. These effects are reflected in the observed current traces and thus help us in measuring the flexibility of these biomolecules. Recently, we applied molecular dynamics simulations using a structure-based model to observe a correlation between the maximum RMSF of the protein and the width of the experimental current blockade distribution. This suggests that protein translocation can be utilized as a high-throughput method to distinguish between functional conformers in proteins. Applying this technique to translocation of tRNA offers an interesting challenge since the tRNA is expected to undergo a conformational change due to the constricted size of the nanopore. Using the same energy landscape techniques, we have calculated the mean first passage time (MFPT) for crossing the rate-limiting free-energy barrier for multiple tRNA species. We find agreement between the MFPT values and the experimental translocation times. Further, these calculations suggest that the experiments specifically observe transient partial unfolding of tRNA.
4:30PM C63.00011: Interferometric scattering for label-free electrokinetic trapping of single nanoparticles*
ABHIJIT A LAVANIA (Presenter), ALLISON H. SQUIRES, PETER D. DAHLBERG, W E MOERNER, Stanford University — Anti-Brownian ELectrokinetic (ABEL) trapping is a technique to trap single particles in solution, enabling extended characterization of their properties. It utilizes photon-by-photon fluorescence to estimate a particle's position, and fast electrophoretic and electroosmotic feedback forces to counteract Brownian motion and confine a particle to the center of a nanofluidic chamber. This enables the observation of photophysical properties, diffusion constants, and electrokinetic mobility. However, trapping is limited to particles that are either tagged with a fluorescent label, or have bright native fluorescence. Here we present the Interferometric Scattering Anti-Brownian ELectrokinetic trap (ISABEL trap), which uses interferometric scattering to enable fast detection and trapping of non-fluorescent particles. The weak scattered light from a nanoparticle is enhanced by interference with a strong reflection from a nearby interface. This enables direct and extended-duration study of single particles that do not fluoresce, or which exhibit intermittent fluorescence or photobleaching.

*This work is supported by the DOE Office of Basic Energy Sciences, Award DE-FG02-07ER15892, and the Albion Walter Hewlett Stanford Graduate Fellowship.

4:42PM C63.00012: Study of interaction of Bovine Serum Albumin with Gold Nanoparticles
KAVINDYA SENANAYAKE (Presenter), ASHIS MUKHOPADHYAY, Wayne State University — The protein-nanoparticle conjugates have potential applications in the fields of colloidal science and biophysics. We study the pH-dependent thickness of bovine serum albumin (BSA) layer on gold nanoparticles (AuNPs). pH-dependent conformations of BSA were determined between pH values 4 and 8. Comparison of pH-dependent hydrodynamic radii results of BSA-AuNp conjugates with Langmuir binding isotherm will be presented.

4:54PM C63.00013: Spatiotemporal dynamics of Pma1 in Saccharomyces cerevisiae using a reversibly interacting tag-probe system*
SUSAN PRATT (Presenter), Physics, Yale University, MICHAEL HINRICHSEN, Molecular Biophysics and Biochemistry, Yale University, LYNNE REGAN, School of Biological Sciences, University of Edinburgh, YONGDENG ZHANG, JOERG BEWERSDORF, Cell Biology, Yale University, BENJAMIN P BRATTON, JOSHUA SHAEVITZ, Physics, Princeton University, SIMON G MOCHRIE, Physics, Yale University — When fluorescent proteins (FPs) are directly fused to a protein of interest, they can interfere with wild-type protein functionality. For example, when plasma membrane (PM) protein Pma1, in *Saccharomyces cerevisiae*, is directly fused to an FP, it is mislocalized to the cells' vacuoles. To circumvent such problems, we are developing a versatile live-cell imaging strategy in which a fluorescently-labeled tetratricopeptide repeat affinity protein (TRAP) probe can reversibly bind to a conjugate 5 amino-acid peptide tag, which is bound to the target protein's C-terminus. We demonstrate the utility of this reversibly binding tag-probe system, showing that it properly localizes Pma1 to the PM. To further characterize the behavior of Pma1, we present the results of fluorescence recovery after photobleaching (FRAP), and single-particle tracking photoactivated localization microscopy (sptPALM) measurements under total internal reflection fluorescence (TIRF) illumination. Remarkably, we find significant differences in the diffusional dynamics of Pma1 imaged using our novel labeling methodology, and Pma1 directly fused to FP.

*We acknowledge support of the NIGMS via AWDA10958.

5:06PM C63.00014: Real-time Electrophysiological Monitoring of Anti-histamine Drug Effects on Live Cells via Reusable Carbon Nanotube Sensor
JIN-YOUNG JEONG (Presenter), VIET ANH PHAM BA, DONG-GUK CHO, HANEUL YOO, Department of Physics and Astronomy, Seoul National University, Korea, VAN-THAO TA, Department of Chemistry, Hanoi National University of Education, Vietnam, SEUNGHUN HONG, Department of Physics and Astronomy, Seoul National University, Korea — Here, we developed a real-time electrophysiological method for monitoring the effects of drugs on live cells via a reusable carbon nanotube field-effect transistor (CNT-FET) sensor. The real-time electrophysiological responses of an individual HeLa cell could be measured repeatedly with the system. The sensor measured the electrical signal induced by the activity of histamine type 1 receptors on a HeLa cell regulated by histamine. Furthermore, the effects of drugs such as cetirizine and chlorphenamine on the HeLa cell were assessed. Remarkably, we exploited only a single sensor to record the activity of numerous HeLa cells to reduce the errors caused by device-to-device variations. Our method provides reliable and statistically-meaningful data to study the activity of live cells. We could expect our method using the reusable CNT-FET sensors to contribute to the pharmaceutical and biological research.

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C64 DBIO: Biopolymers II (DNA, RNA, Biocompatible, Gels) BCEC 259B - Caroline Werlang,
Massachusetts Institute of Technology - Tag(s): Focus
2:30PM C64.00001: The Mechanism of DNA Junction Melting
ABRAHAM KIPNIS (Presenter), ISHITA MUKERJI, FRANCIS STARR, Physics Department, Wesleyan University, Middletown, CT — Four-way Holliday junctions play vital roles in genetic recombination, DNA damage repair, and other mechanisms of chromosomal rearrangement. Here we examine the melting of Holliday junctions through a combination of FRET experiments and MD simulations. We show that melting of this junction initiates at specific locations. At physiological salt concentrations, the junction “folds” into a stacked conformation consisting of two crossing pseudo-duplexes, and our results indicate that melting proceeds as a quasi-independent process along these pseudo-duplexes, rather than as a uniform process throughout the junction. We interrogate the melting locally by measuring FRET from fluorescent nucleotide analogs strategically placed at several locations in the junction. To help interpret the FRET data, we use the coarse-grained 3SPN.2 model to simulate the junction melting. By analyzing an ensemble of simulations, we describe approaches to characterize junction conformation and the dynamics of melting. Our results demonstrate the ability of the 3SPN.2 model to predict structural and dynamic aspects of Holliday junctions and offer a two-step mechanism for junction melting.

2:42PM C64.00002: Dynamic conversion of RNA in crowded environments: implication of significance of micro-viscosity against molecular confinement
JOON HO ROH (Presenter), University of Maryland, College Park, MADHUSUDAN TYAGI, Center for Neutron Research, National Institute of Standards and Technology, SARAH A WOODSON, Biophysics, Johns Hopkins University, JOSEPH CURTIS, Center for Neutron Research, National Institute of Standards and Technology, ROBERT M BRIBER, University of Maryland, College Park — The conformational behavior of RNA in densely packed intracellular conditions is a long-standing area of interest and is critical for understanding biologically important dynamics in a living cell. The effect of viscosity at the solvent-accessible surface area on the concerted conformational motions of tRNA in crowded conditions must be considered. We have examined the effect of PEG-induced crowding on the internal dynamics of unfolded and folded tRNA using ps ~ ns Quasi-Elastic Neutron Scattering spectroscopy (QENS) to probe the role of the local micro-viscosity as a function of the molecular confinement effects from crowding. At temperatures lower than water crystallization (Tc) and higher than dynamic glass transition temperature (Td) of tRNA, the conformational flexibility becomes larger with more confinement, and it is suppressed more strongly at higher temperatures. The dynamic conversion across Tc indicates the significance of the micro-viscosity versus molecular confinement, both of which can orthogonally vary with crowding conditions. Comparison of dynamics from QENS with the aid of molecular dynamics simulations provides insight into the physical origin of this dynamic conversion and its coupling with the local structure of water at the macromolecular surface.

2:54PM C64.00003: Diffusion and Conformational Dynamics of Linear and Circular DNA in Crosslinked Cytoskeleton Composites*
KATHRYN REGAN (Presenter), DEVYNN WULSTEIN, SHEA RICKETTS, RYAN J. MCGORTY, RAE ROBERTSON-ANDERSON, University of San Diego — In order to carry out key cellular processes, DNA molecules must diffuse through the crowded cytoskeletal network, comprised of thin semiflexible actin filaments and thick rigid microtubules. Each of these cytoskeletal filaments can also be crosslinked to varying degrees, altering the network structure and dynamics and hence the impact on DNA diffusion and conformational dynamics. Here, we use single-molecule conformational tracking to investigate the effect of cytoskeleton crosslinking on the transport properties and time-varying conformations of diffusing DNA molecules. Specifically, we track the center-of-mass, size, and shape of single linear and circular DNA molecules diffusing in crosslinked composites of actin and microtubules. We quantify transport coefficients, anomalous diffusion scaling exponents, lengths and timescales of intramolecular fluctuations, and shape and size dynamics of DNA. We determine the role of DNA topology (circular vs linear) as well as cytoskeleton crosslinking motif on DNA dynamics and conformations. Our results shed light on how macromolecular topology and network structure impact macromolecular mobility in crowded cell-like environments.

*This work was funded by NIH NNIGMS Grant No. R15GM123420, AFOSR Grant No.FA9550-17-1-0249, and NSF-CBET-1603925
3:06PM C64.00004: Binding of oligos to DNA secondary structures*  OLIVIA ZOU (Presenter), SHIRA ROSENBERG, WILLIAM B ROGERS, Brandeis University — RNAs are molecules that rely on their 3D structure to regulate cell processes, such as delivering molecules or making proteins. Therefore, disrupting the structure of RNA could help us better understand or even modulate these functions. In principle, one way to do this is to bind DNA oligonucleotides to the RNA to change its conformation so that it no longer works. In practice, this is a difficult task as the complex secondary and tertiary structures of RNA often prevent DNA from binding stably. We aim to understand the kinetic and thermodynamic reasons why oligonucleotides fail to bind to secondary structures. In this talk, I will describe a series of experiments investigating the binding of short DNA oligonucleotides to nucleic acids with prescribed secondary structures. We design a set of hairpins, bulge loops, and internal loops with various loop and toehold lengths, which should result in different opening rates when the oligo binds. A fluorescent probe binds to all these structures, allowing us to make measurements of the amount of unfolded molecules. Preliminary results show that opening rates of different secondary structures vary by orders of magnitude, with hairpins being fastest, and internal loops being slowest.

*We acknowledge support from the Smith Family Foundation.

3:18PM C64.00005: Molecular Dynamics Simulation of Supercoiled DNA with Mismatched Base Pair-Probing the Role of Structural Defect on Plectoneme Pinning  PARTH RAKESH DESAI (Presenter), SIDDHARTHA DAS, Department of Mechanical Engineering, University of Maryland, College Park, KEIR C NEUMAN, NHLBI, National Institute of Health — Mismatch repair (MMR) proteins correct mismatches in DNA. The exact mechanism by which MMR proteins recognize mismatch is still not well understood, but it is believed that the process involves introducing a sharp bend in the DNA and flipping out the mismatched base. Recent, single-molecule magnetic tweezers-based DNA supercoiling studies, conducted at salt concentrations of 0.5 M NaCl and higher, have shown that the mismatched base pair will always localizes at the end of the plectoneme loop and this may facilitate mismatch detection. Theoretical studies have found that the localization of mismatched base pair in the plectoneme end loop, at 0.2 M NaCl, becomes probabilistic. However, these studies were limited to positively supercoiled DNA. Here, we carry out molecular dynamics simulation to study supercoiling of DNA in presence of mismatched base pairs. We study both positively and negatively supercoiled DNA at salt concentration of 0.2 M NaCl using the oxDNA model. We simulate a DNA molecule with 0, 2, 4 and 6 consecutive G:T type mismatches. We find that the plectoneme localization at the mismatched base pair becomes probabilistic. We will present the details of the relationship between the number of mismatched base pairs and the probability of plectoneme localization.

3:30PM C64.00006: Mechanical Properties of DNA Replication  STUART SEVIER (Presenter), MIT — Successful DNA replication requires significant mathematical and physical constraints to be met. The helical structure of DNA results in interwound replicated strands of DNA causing over twisting in the unreplicated portion of DNA presenting a significant topological barrier to cellular division. Though the basic conceptual elements of this process have long been known the necessary physics has just recently been developed. In this work, we outline the basic mathematical and physical properties of an idealized DNA replication process. The resulting framework makes predictions on the relative concatenation of replicated DNA and supercoiled unreplicated DNA generated during replication. These elements are central in understanding the mechanical nature of the replication machinery as well as in transcription replication conflicts.

3:42PM C64.00007: Quantifying free energy pathways of competitive DNA-ligand interactions  ALI ALMAQWASHI (Presenter), King Abdulaziz University — DNA intercalators are considered for potential DNA targeted therapeutics. The kinetics of simple DNA intercalators are well-modeled and characterized in single molecules studies. However, DNA-ligand that have multi-binding modes including intercalation are often studied in equilibrium approach, which does not address the governing free energy pathways. It is crucial to map the transition pathways, in particular, for competitive DNA-ligand interactions that alter DNA extension, which provides insights for rational drug design. While intercalation elongates DNA, other binding modes can be distinguished by distinct rates of increase or decrease of DNA extension. For practical experimental conditions, a frame work is proposed here to analyze the kinetics of DNA-ligand multi-binding modes probed by time-dependent and force-dependent DNA extension. This enables characterizing and quantifying the free energy pathways in order to identify and further optimize the molecular binding mechanism.
In my talk, I present the Looping and Clustering model [1], a simple statistical physics approach to describe how proteins assemble into a protein-DNA cluster with multiple loops. Our analytic model predicts binding profiles of ParB proteins in good agreement with data from high precision ChiP-sequencing – a biochemical technique to analyze the interaction between DNA and proteins at the level of the genome. The Looping and Clustering framework provides a quantitative tool that could be exploited to interpret further experimental results of ParB-like protein complexes and gain some new insights into the organization of DNA.


**4:06PM C64.00009: Coarse-grained molecular simulation studies of effect of solvent quality on melting thermodynamics of oligonucleic acids (ONA) and ONA-polymer conjugates**

PRHASHANNA AMMU (Presenter), ARTHI JAYARAMAN, Chemical & Biomolecular Engineering, University of Delaware — Hybridization or melting thermodynamics of oligomers of nucleic acids (e.g., DNA, RNA, PNA) duplexes is dependent on oligonucleic acid (ONA) backbone chemistry, length, base sequence and composition, and solvent chemistry. Understanding how solvent quality affects ONA stability, in free state and when conjugated to polymers is important for use of ONA in nucleotide-based bio- and nano-technologies. In this talk, I will present our recent molecular simulation work using a coarse-grained model capable of capturing the specific and directional H-bonds between complementary bases in ONA, in implicit solvents. We found that, as the solvent quality worsens for the polymers conjugated to neutral and flexible ONAs (such as PNA), the ONA melting temperature increases for all the ONA sequences, G-C content and polymer length studied. For negatively charged and semi-flexible ONAs (DNA-like), the conjugation of longer solvophobic polymer (as compared to ONA length) decreases the ONA melting temperatures while conjugation of relatively shorter solvophobic polymer, similar to ONA length, does not affect melting temperatures for all the ONA sequences and G-C content studied.

*The authors thank National Science Foundation grant NSF-DMR1420736 for financial support.

**4:18PM C64.00010: Terahertz Spectroscopic Study on Protein Myoglobin: Polymer-Like Behavior of Vibrational Density of States**

LEONA MOTOJI (Presenter), TATSUYA MORI, Division of Materials Science, University of Tsukuba, YASUHIRO FUJI, AKITOSHI KOREEDA, Department of Physical Sciences, Ritsumeikan University, YUE JIANG, KENTARO SHIRAKI, YOHEI YAMAMOTO, SEIJI KOJIMA, Division of Materials Science, University of Tsukuba — We performed terahertz time-domain spectroscopy on protein myoglobin to investigate the boson peak dynamics which universally appears in glassy materials and fraction which is expected to universally appear in polymer glasses. The obtained spectral shape of log ε“ vs log frequency [ε“: the imaginary part of complex dielectric constants] indicates that the fracton region appears above the boson peak frequency. The fractal and fracton dimensions were evaluated from the obtained spectra.

*This work was partially supported by JSPS KAKENHI Grants No. 17K14318, No. 18H04476 and No. 26287067, and the Asahi Glass Foundation.

**4:30PM C64.00011: Dynamics of supercoiled knotted DNA: largescale rearrangements and persistent multistrand interlocking**

LUCIA CORONEL (Presenter), International School for Advanced Studies, ANTONIO SUMA, Temple University, CRISTIAN MICHELETTI, International School for Advanced Studies — Catalytic processes in bacterial plasmid introduce knots and supercoiling. The effect of the latter has been separately and extensively studied, however much less is known about their concurrent action. Thus, to study the kinetic and metric changes introduced by complex knots and supercoiling in 2kbp-long DNA rings, we use molecular dynamics simulation and oxDNA, a mesoscopic DNA model, finding several unexpected results. First, two distinct states dominate the conformational ensemble, they differ in branchedness and knot size; secondly, fluctuations between these states are as fast as the metric relaxation of unknotted rings. Nevertheless, certain boundaries of knotted and plectonemically wound regions can persist over much longer timescales. These regions involve multiple strands that are interlocked by the cooperative action of topological and supercoiling constraints. Their long liver character may be relevant for the simplifying action of topoisomerases.
4:42PM C64.00012: Fast combinatorial nanofluidic device for the dynamic study of biomolecular interactions* SAROJ DANGI (Presenter), PARMINDER KAUR, HAI PAN, HONG WANG, ROBERT RIEHN, North Carolina State University — We present a nanofluidic device for fast combinatorial exposure of stretched and localized DNA molecules to reagents, such as DNA binding proteins, salts, and restriction enzymes. Nanofluidic devices with channel sizes close to the persistence length of DNA have long been used to stretch, visualize, and study biomolecular interactions that modify the configuration of DNA. However, there is a temporal limitation on how long you can study the interaction dynamics before the probing light photocleaves DNA and fluorescence dyes. In addition, study of the interactions among DNA and multiple reagents in different sequences needs the rapid exchange of buffers. Such studies in the nanochannels with traditional passive exchange of buffers via diffusion process is not feasible. Our device allows the simultaneous or the sequential exposure of multiple reagents with active flow of buffers. The buffers could be exchanged under 20 sec while DNA molecule still confined in the field of view. To illustrate the concept of the device, we will show the conformational change of DNA in the varying ionic concentration, restriction enzymes and DNA binding proteins.

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4:54PM C64.00013: Multiscale Modeling of DNA Translocation through Multiple Nanopores TOWFIQ AHMED (Presenter), Los Alamos National Laboratory, ANIKET BHATTACHARYA, Physics Department, University of Central Florida — We report preliminary results for a multiscale modeling scheme to decipher signals recorded for a translocating DNA through a series of nanopores. We propose to relate the time series of the cross-correlation current from different pores calculated from ab initio studies [1] to the velocity correlation obtained by carrying out Brownian dynamics simulation on a coarse-grained (CG) model of a DNA as well as the nano-pores [2]. By suitable choices of different pore-polymer interactions we propose to relate the results obtained from a simple CG model to more refined but computationaly expensive models.


5:06PM C64.00014: DNA-based molecular force sensors in reconstituted actin networks* CHRISTINA JAYACHANDRAN (Presenter), Third Institute of Physics - Biophysics, University of Göttingen, 37077 Göttingen, Germany, MAX WARDETZKY, Institute of Numerical and Applied Mathematics, University of Göttingen, 37077 Göttingen, Germany, FLORIAN REHFELDT, Third Institute of Physics - Biophysics, University of Göttingen, 37077 Göttingen, Germany, CHRISTOPH F. SCHMIDT, Third Institute of Physics - Biophysics, University of Göttingen, 37077 Göttingen, Germany, Department of Physics,Duke University, Durham, NC 27708, USA — Actin, a major cytoskeletal biopolymer of eukaryotic cells self-assembles into networks of crosslinked filaments and bundles and is largely responsible for cellular shape and mechanical stability. Actin assemblies are also responsible for active cellular processes ranging from migration, division and intracellular transport to morphogenesis. Crucial for such processes is the spatial and temporal regulation of the structure and dynamics of the networks and the generation of force, mostly by myosin motors. To measure forces in cytoskeletal networks, we have developed a FRET based molecular force sensor consisting of a DNA hairpin loop, which can be cross-linked into actin networks. We characterized the force sensor via fluorescence lifetime imaging.

*SFB 755 A3

Monday, March 4, 2019 2:30 PM - 5:18 PM

Session C65 DBIO: Biomaterials: Structure, Function, Design I BCEC 260 - Suzanne Kane, Haverford College -
Tag(s): Focus
Hierarchical biological materials – structure, design and synthesis

MARKUS BUEHLER (Presenter), Massachusetts Institute of Technology — What if we could design materials that integrate powerful concepts of living organisms - self-organization, the ability to self-heal, tunability, and an amazing flexibility to create astounding material properties from abundant and inexpensive raw materials? This talk will present a review of bottom-up analysis and design of materials for various purposes - as structural materials such as bone in our body or for lightweight composites, for applications as coatings, and as multifunctional sensors to measure small changes in humidity, temperature or stress. These new materials are designed from the bottom up and through a close coupling of experiment and powerful computation as we assemble structures, atom by atom. We review case studies of joint experimental-computational work of biomimetic materials design, manufacturing and testing for the development of strong, tough and smart mutable materials for applications as protective coatings, cables and structural materials. The use of a new paradigm to design materials from the bottom up plays a critical role in advanced manufacturing, providing flexibility, tailorability and efficiency.

The hidden structure of mouse and human enamel

PUPA GILBERT (Presenter), University of Wisconsin - Madison — Enamel is the hardest and most resilient tissue in the human body. The morphology of human and mouse enamel is well established: it consists of space-filling, aligned, parallel, ~100 nm wide, microns-long nanocrystals, bundled into 5-micron-wide rods. The orientation and arrangement of enamel crystals, however, are poorly understood yet they confer outstanding materials properties. We show with polarization-dependent imaging contrast (PIC) mapping that in mouse enamel, within a rod, crystals are co-oriented with one another but not with the long axis of the rod in human enamel they are not co-oriented with either: the c-axes of adjacent crystals are most frequently mis-oriented by 1°-30°, and their orientation gradually changes up to 30°-90° within a rod. Molecular dynamics simulations demonstrate that the mis-orientations of adjacent crystals observed in human enamel induce crack deflection. This toughening mechanism, therefore, contributes to make our enamel last a lifetime.

Does the crystal structure of shark teeth make them stronger?

CAYLA STIFLER (Presenter), AMBER LIM, BENJAMIN HARPT, CHANG-YU SUN, PUPA GILBERT, University of Wisconsin - Madison — C. megalodon, a huge ancient shark, was capable of producing bite forces as large as 110,000-180,000 N. In comparison, great white sharks, a much smaller modern analogue, can only exert a force of 7,400 N when biting. In both cases, the mechanical stress that the teeth undergo suggests that there might be mesoscale structural features in the fluorapatite crystals in enameloid, which contribute to the superior mechanical properties. Previously, we used PIC (Polarization-dependent Imaging Contrast) mapping to reveal an intricate woven structure in the fluorapatite crystals in parrotfish enameloid, and hypothesized that this structure contributes to enameloid's impressive stiffness. PIC maps from megalodon and great white shark reveal the mesoscale c-axis orientations of enameloid crystals, which contribute to understanding the structure that allows shark teeth to withstand the large bite forces.
3:30PM C65.00004: Bound-state mobility within the nuclear pore complex  LAURA MAGUIRE (Presenter), Physics and BioFrontiers, University of Colorado Boulder, MICHAEL W STEFFERSON, M. BETTERTON, Physics, University of Colorado Boulder, LOREN HOUGH, Physics and BioFrontiers, University of Colorado Boulder — Biopolymeric filters are essential to life. Nuclear transport in particular is an unusual form of filtering in which the flux of select large particles is greatly enhanced over that of smaller nonspecific molecules. The nuclear pore complex, a channel lined with intrinsically disordered FG nucleoporins, facilitates all transport between the nucleus and cytoplasm. It prevents most macromolecules from crossing the nuclear envelope while allowing the passage of transport factors and their cargo. While the basic biochemical interactions leading to transport are well-understood, the detailed mechanism remains a topic of significant debate. We have developed a model of nuclear transport which predicts that nuclear pore selectivity is largely determined by the mobility of FG nucleoporin–transport factor complexes within the pore. We test this prediction by measuring bound-state diffusion of transport factors in tunable nuclear pore mimics which consist of hydrogels filled with FG nucleoporins. Bound-state diffusion is determined for several conditions, including FG nucleoporins of varying length. Bound-state mobility occurs in many biological systems in addition to the nuclear pore complex and could help explain the selectivity of other biopolymeric filters.

3:42PM C65.00005: Emergence of helical growth in fungal cells from a self-organizing cell wall*  FRANCK VERNEREY (Presenter), SHANKAR LALITHA SRIDHAR, REVATHI PRIYANKA MOHAN, Mechanical Engineering, University of Colorado, Boulder, JOSEPH ORTEGA, Mechanical Engineering, University of Colorado Denver — Walled cells such as plants, algae and fungi achieve expansive growth using turgor pressure that helps mediate irreversible wall deformation and regulates their shape and volume. The architecture of the cell wall plays a crucial role in this process where a network of microfibrils and tethers (complex polysaccharides and proteins) dynamically mediate the network topology via continuous detachment and reattachment events. A direct consequence of wall architecture, through microfibril re-orientation, is the helical growth of the fungal cells of Phycomyces Blakesleeanus. Powered by turgor pressure and the biochemistry to regulate molecular processes that induce network organization, these cells can control the growth rate and direction of the helix. The relationship between local molecular mechanisms and global emerging behaviors of these cells is still poorly understood. We present a novel approach based in statistical mechanics to model the organization of microfibrils and tethers in the cell wall. The model is then used to predict (a) the longitudinal elongation and rotation rates along the growth zone and (b) the inversion in rotation direction during growth stages in wild-type sporangiophores, and for radial expansion in piloboloid mutants.

*NSF Career Award 1350090

3:54PM C65.00006: Harnessing Design Principles from Glass Sponges for Structurally Robust Lattices  MATHEUS FERNANDES (Presenter), School of Engineering and Applied Sciences, Harvard University, JAMES C WEAVER, Wyss Institute, Harvard University, KATIA BERTOLDI, School of Engineering and Applied Sciences, Harvard University — The glass sponge Euplectella Sp. are predominately deep sea sponges that live in ocean depths of 100-2000m. Beyond their fracture propagation inhibiting material composition, these sponges are perceived to exhibit large structural rigidity and strength against buckling. Since these sponges are primarily made of ‘brittle silica’, buckling strength may be a crucial property in making them resistant to impact and environmentally applied stresses. Structurally, they exhibit a base square-grid architecture and regular ordering of vertical and horizontal struts that form the skeletal system. Furthermore, their base structure is overlaid with double diagonal reinforcement struts, which create a checkerboard-like pattern of open-closed cell structure. Based on its similarity to square lattices found in structural engineering, we explore the following research question: Can we generate design principles for diagonal reinforcements of square beam lattices that are optimally designed to avoid global structural buckling? Here, we present a numerical analysis of the structure deformation under various loading conditions as well as survey different arrangements within similar design space of the sponge. Furthermore, we present experimental evidence that supports our numerical analysis.
4:06 PM C65.00007: TOPOLOGICAL PHONONS IN MICROTUBULES: THE LINK BETWEEN LOCAL STRUCTURE AND DYNAMICS OF MICROTUBULES
SSU-YING CHEN (Presenter), AROOJ ASLAM, CAMELIA PRODAN, physics, New Jersey Institute of Tech, EMIL PRODAN, physics, Yeshiva University — We have developed a model for analyzing thermal energy propagation through a microtubule by tracking its movement over time, and extracting a phonon spectrum of energy states and the speed of energy propagation through a microtubule. The microtubule is a self-assembling protein structure, and it has been reported that changes in the tubulin proteins that make up the bulk structure of the microtubule can alter its dynamic properties, in particular the polymerization and depolymerization rates. The pathways that dictate how local structure affects system wide dynamics has yet to be elucidated by current measurement techniques. This is because previous methods of defining structural properties of the microtubule hinge on static parameters, such as persistence length and Young's modulus, which neglect the dynamic properties of the microtubule and the anisotropic behavior of these local changes. Our methods look at the vibrational energy propagation through microtubules as an energy source for the energy intensive dynamics of the microtubule. In our methodology, the increased spatial resolution accommodates anisotropy along the length of the microtubule and paves the way for developing a dynamic measurement of microtubule mechanics.

4:18 PM C65.00008: Characterization of fracture in topology-optimized bio-inspired networks*
CHANTAL NGUYEN (Presenter), Department of Physics, University of California, Santa Barbara, DARIN PEETZ, Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, AVIK MONDAL, Department of Physics, University of Michigan, AHMED ELBANNA, Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, JEAN CARLSON, Department of Physics, University of California, Santa Barbara — Trabecular bone is a flexible, lightweight bone tissue that exhibits an anisotropic microarchitecture resembling a web of interconnected struts (trabeculae). We simulate trabecular bone architectures with multi-objective topology optimization, effectively reverse-engineering trabecular structure by optimizing biologically-motivated objectives. Starting from an identical volume, we generate different topologies by varying the objective weights for compliance, surface area, and stability. We model these topologies as disordered, spatially-embedded networks where edges represent trabeculae and nodes represent branch points where trabeculae meet. We simulate mechanical loading on finite-element models where each edge is replaced by a beam, enabling direct comparison of mechanics and topology at multiple scales ranging from that of individual edges/beams to the network at large. We compare the mechanical response of the various topology-optimized networks and identify mechanisms of crack propagation. We characterize and predict crack pathways with community detection methods inspired by similar applications in the study of granular materials.

*NSF EAR-1345074 & CMMI-1435920, Institute for Collaborative Biotechnologies (ARO W911NF-09-D-0001), David and Lucile Packard Foundation
Spherulites in coral skeletons are composed of acicular aragonite crystals radiating from common centers and exhibiting a 0°–35° misorientation of crystallographic c-axes across grain boundaries, previously misattributed entirely to a mechanism called non-crystallographic branching [1,2]. Here, we examine skeletons from 9 diverse species with quantitative nanoscale crystal orientation analyses using Polarization-dependent Imaging Contrast (PIC) mapping [3]. We discovered that, in addition to spherulites, 4 of the species also form tiny (0.2–2 µm), randomly oriented, equant crystals, termed sprinkles. Supported by theoretical phase field simulations, we propose that all initially nucleated crystals are randomly oriented sprinkles, and that these later coarsen, with radially oriented crystals growing at the expense of smaller, randomly oriented sprinkles. This mechanism is analogous to solidification or annealing in metals, both of which are high-temperature phenomena, whereas in coral skeletons coarsening occurs at ambient conditions.

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Optical characterization of nacre using hyperspectral imaging* [Invited] MIKHAIL A. KATS (Presenter), Electrical and Computer Engineering, University of Wisconsin - Madison — Nacre is an organic-inorganic biomineral that lines the inside of shells of various species of mollusks, and comprises layers of aragonite tablets with thicknesses on the order of hundreds of nanometers, bound by an organic protein. The iridescent appearance of nacre results from thin-film interference effects within this layered structure, even though the layers are quite inhomogeneous due to surface roughness, shell curvature, and the disordered nature of the tablets comprising the aragonite layers.

The average thickness (and variance) of the nacre layers can encode information, for example the ocean temperature at the time of formation. However, obtaining information about the layer thickness typically requires destructive methods involving preparing and imaging cross-sections, and can require many cross-sections to map an entire sample.

Here, we present a method that combines polarized hyperspectral imaging with thin-film modeling, that is capable of nondestructively mapping the thickness of nacre layers across an entire specimen.

This work was performed together with Jad Salman, Alireza Shahsafi, Chang-Yu Sun, Steve Weibel, Chris Draves, Michel Frising, Brad Gundlach, Yuzhe Xiao, Gabor Kemeny, and Pupa Gilbert.

*MK acknowledges funding through the Air Force Office of Scientific Research.
2:30PM C66.00001: Mechanical feedback maintains polarization in budding yeast mating projection growth
SAMHITA BANAVAR (Presenter), University of California, Santa Barbara, MICHAEL TROGDON, Salk Institute, BRIAN DRAWERT, University of North Carolina, Asheville, LINDA R PETZOLD, OTGER CAMPAS, University of California, Santa Barbara — Cell polarization is one of the commonly studied cases of spontaneous symmetry breaking in cells and controls many cellular processes, including morphogenesis, in budding yeast. However, the mechanisms that coordinate continued polarization to the growth region during mating projection formation, and the subsequent change in geometry from a spherical cell, remain unknown. We theoretically show that a genetically-encoded mechanical feedback relaying information about cell's geometry is sufficient to maintain key polarity molecules and growth machinery remain localized to the site of growth. We have demonstrated that this same feedback mechanism also results in cell wall stability.

2:42PM C66.00002: Active mechanics in the growth of a bacterial cell wall JORDAN PRICE (Presenter), GIACOMO PO, ALEXANDER JACOB LEVINE, JEFF ELDREDGE, University of California, Los Angeles — It is well known that rod-shaped bacterial cell walls—a thin shell made of a disordered peptidoglycan network—grow rapidly in length. This speed allows cells to divide several times per hour. However, fast growth requires the cell to rapidly add material to a highly pressurized (osmotically) shell without bursting. The basic mechanism for growth is actively driven dislocations plowing through the shell in the circumferential direction. These motor-driven defects introduce new material (MreB filaments) into the shell but generate stress concentrations surrounding the moving defects. Motivated by the large deformations inherent in bacterial growth, we develop a nonlinear continuum mechanics model with actively driven dislocations to describe the growth of the cell wall. Using numerical simulations, we study the interaction of stress fields that arise as these filaments are added to the existing peptidoglycan mesh. Furthermore, we investigate how the growth mechanics are affected by fluctuations in turgor pressure, and the presence of heterogeneities and defects in the cell wall that can form during an osmotic shock or antibiotic treatment.

2:54PM C66.00003: Limitations on Tissue Shape Control by Mechanical Feedback* ALEXANDER GOLDEN (Presenter), Physics, Boston University, DAVID K LUBENSKY, University of Michigan — How size and shape of living tissues are controlled is a fundamental question of developmental biology. What are the mechanisms that can produce correct sizes? How does size control relate to shape control? We investigate how size and shape control interact in a model of growth control in the *Drosophila* wing disc epithelium, which appears to achieve a robust final size. In particular, we study the capacity of mechanical feedback models to control not only tissue size, but tissue shape. We develop an analytic model capable of integrating mechanical feedback on tissue growth into an elastic theory. This allows us to make precise claims about the limitations of shape control by mechanical feedback, and demonstrate how these limitations derive from underlying elastic principles.

*NSF DMR-1056456

3:06PM C66.00004: Inflationary Embryology and the Statistical Physics of Noisy Tissue Growth* OJAN KHATIB DAMAVANDI (Presenter), DAVID K LUBENSKY, University of Michigan — Tissue growth is fundamental to biology and is noisy. Noise has important implications for morphogenesis and tissue integrity, yet a basic theoretical description of noisy tissue growth has been lacking. Growth nonuniformity leads to a build-up of mechanical stresses, and many tissues respond to stress by modulating their growth. Then, how does the interplay between noise and stress feedback affect tissue growth, and what can we predict about the statistical properties of experimentally accessible quantities? We model the tissue as a continuum, elastic sheet undergoing exponential growth with mechanical feedback and find that the density-density correlations show power-law scaling in space. In anisotropic growth, the standard deviation in clone sizes is comparable to the mean, in contrast to the isotropic case where relative variations in clone size vanish at long times. The high variability in clone statistics observed in anisotropic growth is due to the presence of two soft growth modes, which generate no stress. Our work analyzes the simplest model of noisy growth of elastic tissues. It thus both introduces a new class of nonequilibrium growth models and represents a first step towards understanding specific biological contexts.

*NSF DMR-1056456; NSF GRFP DGE-1256260.

3:18PM C66.00005: Biophysically Inspired Morphometrics SALEM AL MOSLEH (Presenter), GARY P. T. CHOI, MAHADEVAN, John A. Paulson School Of Engineering And Applied Sciences, Harvard University — Motivated by the quest to understand shape changes in biology, both in a developing organism and over evolutionary time scales, we develop a computational framework for analyzing geometric shape changes between surfaces embedded in three dimensions. Our approach allows us to simultaneously solve the problem of registration and the morphing of shapes onto each other using biophysically inspired distance functions. We then discuss how this framework can be used to analyze shape changes in such instances as planar wings and human faces.
3:30PM C66.00006: Dynamic Morphoskeleton  MATTIA SERRA (Presenter), Harvard University, SEBASTIAN STREICHAN, UCSB, L MAHADEVAN, Harvard University — During embryonic development, cells undergo large-scale motion generating tissues rearrangement, which ultimately defines the final shape of the embryo. While developmental biology has identified several genes driving local cellular processes, the interplay between cell-intrinsic and external stresses is fairly less understood because several local mechanisms are still unknown or hard to measure. By contrast, with the significant advances in live imaging techniques, it is now possible to fully track cell trajectories. Using ideas from nonlinear dynamics, we propose a rigorous objective kinematic framework for analyzing cell motion, which uncovers the underlying dynamic morphoskeleton, i.e. the centerpieces of cell trajectory patterns in space and time. The dynamic morphoskeleton provides a quantitative tool for comparing different morphogenetic phenotypes, quantifying the impact of genetic and physical manipulations, studying cell fate, and overall bridging the gap between bottom-up and top-down modeling approaches. We illustrate our results on a Drosophila gastrulation dataset obtained by in toto light-sheet microscopy.

3:42PM C66.00007: Morphology analysis based on information theory  VASYL ALBA (Presenter), MADHAV MANI, RICHARD CARTHEW, Northwestern University, JAMES CARTHEW, The University of British Columbia — We used machine vision and information theory approach to address a question of quantitative description of the morphological traits in biological systems. We used a population of fruit flies that was under developmental pressure to demonstrate the potential of the newly developed method. In particular, we changed diet and temperature to increase morphological variation.

3:54PM C66.00008: Activity driven buckling in early steps of organogenesis*  FRANCESCO SERAFIN (Presenter), SURAJ SHANKAR, BENJAMIN LOEWE, Syracuse University, BORIS I SHRAIMAN, MARK BOWICK, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, M. CRISTINA MARCHETTI, Physics Department, University of California Santa Barbara — Morphogenesis, the complex process by which the shape of organs and organisms emerges from cell organization, intertwines chemical and physical processes. In many situations, 3D biological structures are achieved through targeted active folding processes of 2D tissue layers. An example is the process of lumen formation – the buckling, folding and invagination of a planar cell sheet that leads to the formation of a hollow cavity enwrapped by a polarized epithelium. In this talk, starting with an active elastic continuum description of a cellular tissue layer of finite thickness, we derive an effective 2D model that includes contractility and cell division. We show that the model can account for the buckling instability at the onset of lumen formation. We find that traction localizes contractile stresses at the boundary of the tissue, while cell division induces an in-plane outward pressure. These two competing effects destabilize the initial planar state forcing the tissue to buckle.

*This work was supported by the NSF grants DMR-1609208, DMR 1720256 (iSuperSeed) and PHY-1748958 (KITP) and by the Simons Foundation Targeted Grant in the Mathematical Modeling of Living Systems Number 342354.

4:06PM C66.00009: Active junctions as a pathway to stress generation in morphogenesis*  SILKE HENKES (Presenter), ILYAS DJAFER-CHERIF, Mathematics, University of Bristol, LUKE COBURN, ICSMB, University of Aberdeen, GUILLERMO SERRANO-NAJERA, KEES WEIJER, RASTKO SKNEPNEL, SLS, University of Dundee — During gastrulation, and other development stages like germ band extension, epithelial cell sheets spontaneously organise to exert contractile mechanical forces, resulting in convergence-extension flow. Current models assume different types of chemical signalling based pre-patterning of the junctions, leading to both tension and flow. Here we present a model of self-amplifying contractile cell sheets that posits a myosin-dependent junction contractility with a tension-dependent feedback loop. This active mechanics model leads to the spontaneous formation of tension chains with both isotropic characteristics and directionality in the presence of an applied stress. We discuss the necessary and sufficient ingredients for the local mechanics to generate chains, and then focus on the flow that results from the activated junctions. We find that disordered flow arises spontaneously, and characterize the conditions for convergence-extension flow using small active cell groups embedded in a passive matrix.

*We acknowledge funding from the UK BBSRC through grants BB/N009150/1, BB/N009150/2 (SH,LC,IDC) and BB/N009789/1 (RS,CJW).
4:18PM C66.00013: Coordination of epithelial cells during morphogenesis. MATTHIAS HÄRING (Presenter), Max Planck Institute for Dynamics and Self-Organization, PRACHI RICHA, JÖRG GROSSHANS, Universitätsmedizin Göttingen, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — Despite a long-standing effort to uncover the physical principles governing animal morphogenesis, the knowledge of embryonic tissue mechanics remains elusive. We address the physical aspects of embryonic tissue mechanics using fruit fly gastrulation as a model. During this process, a subset of cells in the ventral part of the embryo constrict on one side and subsequently invaginate into the interior of the embryo, thereby causing the embryonic surface to form a furrow. To determine the mechanism of tissue shape change during gastrulation, we have developed a toolbox of biophysical methods that allow accurate quantification of material tissue properties in live fruit fly embryos. Specifically, we have developed magnetic tweezeers exploiting either fluorescent magnetic microspheres or ferrofluid droplets, as well as flexible cantilevers microfabricated from PDMS, allowing highly quantitative measurements of the rheological properties in the early fly embryo. Our measurements directly translate into a predictive theory that explains key aspects of tissue dynamics during fruit fly gastrulation. Specifically, our model explains the marked anisotropy of tissue constriction in the initial phase of gastrulation as well as the mechanism of tissue invagination during the subsequent phase.

4:30PM C66.00010: Physical Aspects of Drosophila gastrulation. KONSTANTIN DOUBROVINSKI (Presenter), Biophysics, MPI-KS, AKANKSHA JAIN, PAVEL TOMANČAK, Tomancak, MPI-CBG, STEPHAN W GRILL, Biophysics, TU Dresden — Gastrulation is a critical step during the development of multicellular organisms in which a single-layered tissue folds into a multi-layered germ band. This shape change is characterized by tissue folding and large-scale tissue flow. The myosin-dependent forces that underlie this process have been increasingly investigated; however, thus far, the possible interaction between the moving tissue and the rigid shell surrounding the embryo has been neglected. Here, we present our quantitative findings on the physical mechanisms governing gastrulation in the red flour beetle, Tribolium castaneum. We investigated the forces expected within the tissue given the myosin distribution observed by multi-view light-sheet microscopy and discovered that an additional external force must be counteracting this tissue-intrinsic contractility. We then identified that a specific part of the tissue tightly adheres to the outer rigid shell. This attachment is mediated by a specific integrin whose knock-down leads to a complete loss of the counter-force. Moreover, in the fruit fly Drosophila melanogaster, knock-down of another integrin leads to a severe twist of the germ band, suggesting that the integrin-mediated interaction between tissue and vitelline envelope may be conserved in insects.

4:30PM C66.00011: External forces generated by the attachment between blastoderm and vitelline envelope impact gastrulation in insects. STEFAN MÜNESTER (Presenter), Biophysics, TU Dresden, ALEXANDER MIETKE, Biophysics, MPI-KS, AKANKSHA JAIN, PAVEL TOMANČAK, Tomancak, MPI-CBG, STEPHAN W GRILL, Biophysics, TU Dresden — Gastrulation is a critical step during the development of multicellular organisms in which a single-layered tissue folds into a multi-layered germ band. This shape change is characterized by tissue folding and large-scale tissue flow. The myosin-dependent forces that underlie this process have been increasingly investigated; however, thus far, the possible interaction between the moving tissue and the rigid shell surrounding the embryo has been neglected. Here, we present our quantitative findings on the physical mechanisms governing gastrulation in the red flour beetle, Tribolium castaneum. We investigated the forces expected within the tissue given the myosin distribution observed by multi-view light-sheet microscopy and discovered that an additional external force must be counteracting this tissue-intrinsic contractility. We then identified that a specific part of the tissue tightly adheres to the outer rigid shell. This attachment is mediated by a specific integrin whose knock-down leads to a complete loss of the counter-force. Moreover, in the fruit fly Drosophila melanogaster, knock-down of another integrin leads to a severe twist of the germ band, suggesting that the integrin-mediated interaction between tissue and vitelline envelope may be conserved in insects.

4:42PM C66.00012: Optogenetic control of contractile tissue forces during Drosophila morphogenesis. MARISOL HERRERA PEREZ (Presenter), KAREN E. KASZA, Columbia University — Epithelial tissues undergo dramatic changes in shape during development. These changes are driven in large part by contractile forces generated by the actomyosin cytoskeleton of cells. In addition to physically shaping cells and tissues, mechanical forces can act as cues to influence cell behavior and could help coordinate cell behaviors across multicellular tissues. A major obstacle to dissecting the mechanisms of how mechanical forces shape tissues has been the lack of tools for precise manipulation of forces in vivo. To address this, we have developed a collection of optogenetic tools to locally and systematically modulate actomyosin contractility in the Drosophila embryo. With these tools, we have demonstrated local, light-gated myosin recruitment, and changes in myosin localization patterns across tissues. Using these tools in combination with live confocal imaging and quantitative images analysis, we find that inducing contractile forces in small groups of cells in an epithelial tissue can deform and influence cell behaviors across the tissue in the developing embryo. These studies are shedding light on the roles of mechanical cues in coordinating cell behaviors in multicellular tissues during development.

4:42PM C66.00013: Coordination of epithelial cells during morphogenesis. MATTHIAS HÄRING (Presenter), Max Planck Institute for Dynamics and Self-Organization, PRACHI RICHA, JÖRG GROSSHANS, Universitätsmedizin Göttingen, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — Epithelial cells are capable of sensing and reacting to the forces and movements of their neighbours. We fully quantify the dynamics of epithelial tissue using a novel high-throughput image analysis pipeline based on deep neural networks. Inspired by graph theory, we decompose cell-cell interactions into three distinct coupling types. With this approach, the epithelium can be represented by a planar graph of cell couplings whereby cells are interpreted as vertices and junctions between cells as edges. Utilizing graph-theoretic measures, we compare wild type tissue and mutants with impaired signal transduction capabilities revealing significant differences in e.g. composition of coupling types and spatial distributions. In contrast to the wild type, tension in those mutants is anisotropically distributed, indicating that local cell-cell coordination through mechano-sensing is essential for the function of an epithelium as force-generating tissue.
5:06PM C66.00014: Cell-cell adhesion in tissue mechanics and morphogenesis  XUN WANG, KAREN KASZA (Presenter), Mechanical Engineering, Columbia University — During development, simple epithelia reorganize into tissues with complex form and structure. Tissue reorganization during morphogenesis can be rapid. In Drosophila, cell rearrangements in the embryonic epithelium double the length of the body axis in 30 minutes. Adhesion at cell-cell contacts, mediated by junctional proteins, and contractile tension, generated by actomyosin, are thought to be key machineries controlling epithelial tissues. However, it remains unclear how the balance between adhesion and tension determines epithelial structure and mechanics. To gain insight, we are systematically modulating the balance between adhesion and tension in vivo. E-cadherin is a primary component of cell-cell adhesions. Using multiple approaches, we increase or decrease E-cadherin levels relative to wild type and use confocal imaging to study the effects on cell shapes and movements. We find that modulating adhesion influences cell shapes prior to the onset of axis elongation as well as cell rearrangement rates during elongation. We will discuss how our results compare to vertex model predictions. These systematic, quantitative experimental studies of tissue mechanics in vivo are an essential step in building models of morphogenesis.

5:18PM C66.00015: Superstretching epithelial sheets  ERNEST LATORRE-IBARS, Institute for Bioengineering of Catalonia (IBEC), SOHAN KALE, Polytechnic University of Catalonia, XAVIER TREPAT, Institute for Bioengineering of Catalonia (IBEC), MARINO ARROYO (Presenter), Polytechnic University of Catalonia — During morphogenesis, cell monolayers need to change their shape in various ways. For instance, cell monolayers undergo very large stretching during blastocyst hatching in mammalian embryos. In this talk, I will discuss a mechanism by which epithelial tissues can withstand extreme stretches without significantly increasing tissue tension, which would otherwise compromise tissue integrity [1]. I will describe how, under applied tension, epithelial cells can adopt two “metastable” states, one in a barely stretched state, and one in a superstretched state. This phase coexistence allows tissues to further stretch at constant tension by switching cells into the super-stretched phase, in close analogy with the phenomenology of superelasticity exhibited by NiTi alloys or by intermediate filaments. In epithelial monolayers, this phenomenology has an active origin that depends on cytoskeletal dynamics. I will present experimental evidence of epithelial active superelasticity, a theoretical model explaining it and bridging from cytoskeletal dynamics to emergent material behavior, and will discuss the implications during morphogenesis.


Monday, March 4, 2019 2:30 PM - 5:30 PM

Session C67 APS/SPS: Undergraduate Research III  BCEC 050 - Brad Conrad, American Institute of Physics - Tag(s): Undergraduate

2:30PM C67.00001: Neuronal dynamics on patterned substrates measured by fluorescence microscopy*  JOAO MARCOS VENSI BASSO (Presenter), CRISTIAN STAII, Physics and Astronomy, Tufts University — Geometrical features are known to be very important in neuronal growth and the formation of neuronal networks. We present experimental and theoretical investigations of axonal growth and dynamics for neurons cultured on patterned surfaces. We utilize fluorescence microscopy to image the axonal dynamics and show that these substrates impart a strong directional bias to neuronal growth. We model axonal dynamics using a general stochastic model and use this framework to extract key dynamical parameters. These results provide novel insight into how geometrical cues influence neuronal growth and represent important advances toward bioengineering neuronal growth platforms.

*Tufts Faculty Research Award
ANDREA CAPA SALINAS (Presenter), JESUS VELASQUEZ, PEI-CHUN HO, Physics, California State University, Fresno — When a temperature gradient is imposed at the ends of a conducting material, a voltage will be generated on this material. This phenomenon is known as the Seebeck effect and is characterized by the Seebeck coefficient. Thermopower, or Seebeck coefficient measurements, can provide a deeper understanding of the properties of a sample, its normal state behavior, and help progress on applications, such as thermoelectric generators, cooling systems, and temperature measurement devices. The samples of interest for thermopower measurements in our lab are filled-skutterudite compounds, for they exhibit thermoelectric effects. For this purpose, a thermopower measurement probe was designed and its resolution tested using Nickel 201 alloy and platinum samples. It was concluded that the device provides measurements within 3% error in the 100K-300K range. However, measurements below 100K must be improved, since current data indicates measurements are limited by the operating range of the type-T thermocouple used. Thus, future improvement will consist of adding a Cernox thermometer on the hot platform to account for a more accurate temperature difference at low temperatures.

*Research at CSU-Fresno is supported by NSF DMR-1506677.

Andrea Capa Salinas is also supported by a URG at Fresno State.

GREGORY PRICE (Presenter), Chemistry and Physics, Augusta University, UMESH KUMAR, Physics and Astronomy, University of Tennessee, KENNETH C STIWINTER, Chemistry and Physics, Augusta University, STEVEN JOHNSTON, Physics and Astronomy, University of Tennessee, TRINANJAN DATTA, Chemistry and Physics, Augusta University — Resonant inelastic x-ray scattering (RIXS) is a novel spectroscopic method for probing charge and spin excitations in quantum magnets. In one dimension, where quantum fluctuations are most prominent, a system of interacting electrons can support fractionalized spinless charge excitations (holons) and chargeless spin excitation (spinons). Currently, X-ray spectroscopic techniques such as RIXS can excite the O K-edge core electrons of correlated quantum magnets to probe the physical nature of the above mentioned spin-charge separated state. Using exact diagonalization we investigate the O K-edge RIXS response of the one dimensional antiferromagnetic spin chain compound with nearest and next-nearest neighbor hoppings. We also study the spin-anisotropic version of the same model. Interaction of the core electrons with the X-rays generate multi-spinon excitations in the RIXS spectrum, for example in strontium copper oxide. We find that the RIXS spectrum of the $t_1-t_2-J$ model with spin anisotropy presents a rich source of physical information, including allowing us to identify microscopic pathways for how the quantum spin fluctuations control the appearance of the four spinon excitations observed in the isotropic O K-edge spectrum.

EMILY SUTHERLAND (Presenter), QUE HUONG NGUYEN, Physics, Marshall University — We report a theoretical research on Wannier-Frenkel hybrid exciton in a semiconductor nanorod coated by an organic shell.

There are two kinds of excitons in solids: the Frenkel exciton in molecular and organic materials and the Wannier-Mott exciton in semiconductors. The two kinds of excitons have very different and complementary properties. In heterostructure combining of semiconductors and organic materials with exciton energies close to each other, the coupling between them will form a hybridization state having complimentary properties of both kinds of excitons.

Our model considers a system consisting of a semiconductor nanorod coated by a thin shell of an organic material. At the surface of the nanorod, due to a dipole-dipole interaction a hybridization exciton state will be formed. The electronic structures, the energies, wave function as well as dispersion relations of the new hybrid exciton state will be obtained, depending on the size and the parameters of the rod and the materials. We also investigate the effect of applying an external electric field on the hybrid excitons.

ALEXANDER GLICKFIELD (Presenter), GONZALO ORDONEZ, Butler University — The Friedrichs model consists of an interaction between the discrete states of a quantum system (say, a set of atoms) and a set of continuous states. The interaction produces a resonance, resulting in complex eigenenergies. The resonance appears as a pole of the analytic continuation of the reduced resolvent corresponding to the interacting Hamiltonian. As the imaginary component approaches 0, the eigenstate's lifetime becomes infinite, forming a bound state in the continuum. We solve for a set of parameters that generates multiple resonances with infinite lifetime within the model.
3:30PM C67.00006: Static and dynamic properties of a one-dimensional spin-1/2 system*  
AVIVA SHOOMAN (Presenter), LEA SANTOS, Yeshiva University — We study the static properties and the dynamics of a quantum system described by a one-dimensional spin-1/2 model with nearest neighbor couplings. We analyze the eigenvalues and the eigenstates of this model with different chain sizes and different boundary conditions. From this analysis, we are able to anticipate how fast the excitations should spread over the chain. The more delocalized the eigenstates are, the faster the excitations should move along this chain. Next, we study the evolution of the system numerically and confirm our predictions. All our Mathematica codes are available upon request.

*NSF Grant No. DMR-1603418

3:42PM C67.00007: Charge Density Wave States in CeTe2  
BURHAN AHMED (Presenter), BISHNU SHARMA, MANOJ SINGH, BONING YU, Clark University, PHILIP WALMSLEY, IAN R FISHER, Stanford University, MICHAEL C BOYER, Clark University — Charge density wave (CDW) states are formed in some, typically low-dimensional, materials below a transition temperature, T_{CDW}. The transition of a material into a CDW state leads to the formation of a periodic charge modulation, a periodic lattice modulation, and the opening of an energy gap. While CDW states exist in many condensed matter systems, there is much to be known about the driving-mechanisms for these states as well as how these states coexist with other phases such as superconductivity. Here we present our work using scanning tunneling microscopy (STM) to study CDW states in CeTe2, a rare-earth ditelluride with a CDW transition well over room temperature. In particular, we will present our work on quantifying nanoscale strain in CeTe2 in an effort to better understand the local properties of the CDW states we observe.

3:54PM C67.00008: Development and characterization of an improved wireless centrifuge force microscope using acrylate microspheres and silicon nitride membranes*  
LOGAN FAIRGRIEVE-PARK (Presenter), TRISTAN STARK, DAVID FORTIN, Department of Physics, University of Alberta, AMY AU, Ross Sheppard High School, MICHAEL WOODSIDE, NOEL Q HOFFER, MARK FREEMAN, Department of Physics, University of Alberta — Centrifuge force microscopy allows for multiple concurrent single molecule measurements which cannot be achieved using more traditional experimental platforms. By altering the design of a wireless centrifuge force microscope (CFM) created at the University of Albany [1], we have developed an improved model. By upgrading the integrated single board computer to a Rock64 (Pine Microsystems Inc.) with a USB 3 connector we can achieve higher image transfer rate. Additionally, we describe a novel technique for CFM calibration. By adhering acrylate microspheres of multiple sizes to a silicon nitride membrane (Norcada) [2], we are able to quantify membrane displacement as a function of centripetal force. This technique could be extended to other CFMs as a method for calibration of the centrifuge and optics. Upon completion of the experimental use of the CFM, it will be integrated into a senior undergraduate physics lab course at the University of Alberta.


*We gratefully acknowledge funding from the University of Alberta Teaching and Learning Enhancement Fund, the Faculty of Science, and the Canada Foundation for Innovation.
4:06PM C67.00009: Surface Species in Graphene Liquid Cells for Transmission Electron Microscopy* NATHAN ROSEN Mann (Presenter), LOPA BHATT, ARUNACHALA NUTALAPATI, SOOMIN PARK, JAKE R JOKISAARI, MARK SCHLOSSMAN, ROBERT KLIE, Physics, University of Illinois at Chicago — The behavior of nanoparticles in liquid is important to a wide variety of fields, from medical to environmental. The aggregation of such particles is an important factor for nanoparticle removal during processes such as water purification. However, due to their size, nanoparticles in solution are difficult to characterize directly by optical or x-ray based methods. An effective method to observe nanoparticles in liquid is using the scanning transmission electron microscope(STEM) combined with graphene-based liquid cells(GLC).

The preparation of GLC’s usually requires wet chemical etching steps which often leave surface species on the etched graphene. This may change the properties of the water-graphene interface depending on the chemicals used for the etching process, and the surface species produced from the reactions. In this contribution we examine the presence of such species using a combination of STEM, energy dispersive x-ray analysis(EDX), and Raman spectroscopy to analyze the molecular species present at the graphene interface in the GLC’s and how certain surface species affect liquid cells containing gold nanoparticles.

*Supported by the Chancellor’s Undergraduate Research Award. Made use of instruments in the Electron Microscopy Service at Research Resources Center, UIC.

4:18PM C67.00010: Using the "EasySpin" toolbox in MATLAB to model the magnetism of clusters and chains* ORLANDO TREJO (Presenter), MARK MEISEL, Dept. of Physics and NHMFL, University of Florida, ERIK CIZMAR, Dept. of Condensed matter, Institute of Physics, P.J. Šafárik University — The “EasySpin” toolbox [1], which runs within MATLAB software, was designed as an analysis tool of EPR spectra. Yet, the 4.5 version of the toolbox was used to generate algorithms that allowed the isothermal magnetization and temperature-dependent magnetic susceptibility of clusters to be modelled [2,3]. Now, the 5.2 version contains library functions that allow these magnetic properties to be calculated. The first step was to compare the results of the new version with the published work [2,3]. Next, the magnetic response of [Mn₃O(O₂PPh₂)₃(mpko₃)] [4] was simulated with “EasySpin”, and these results will be discussed. Ultimately, the goal is to simulate the low-field, temperature-dependent, magnetic susceptibility reported for an S = 1, one-dimensional spin chain, [Ni(HF₂)(3-Clpy)₄]BF₄ [5] with nearest-neighbor interactions, J, and single-ion anisotropy, D. These results will be presented for chain lengths of at least 7 spins.


*NSF via DMR-1708410 (MWM) and DMR-1644779 (NHMFL).

4:30PM C67.00011: Switching of biaxial synthetic antiferromagnets: a micromagnetic study* MICHAEL ACKERMANN (Presenter), SATORU EMORI, Department of Science, Virginia Tech — We simulate the switching behavior of nanoscale synthetic antiferromagnets, inspired by recent experimental progress in spin-orbit-torque switching of crystal antiferromagnets. The synthetic antiferromagnet consists of two ferromagnetic thin films with in-plane biaxial anisotropy and interlayer exchange coupling, which leads to enhanced stability against external field perturbations compared to single-layer ferromagnets. Switching between the orthogonal easy axes is enabled by current-induced Rashba spin-orbit fields from the opposite surfaces of the synthetic antiferromagnet. The use of the field-like spin-orbit torque allows for faster switching with increased Gilbert damping, without a significant detrimental increase of the threshold switching current density. Our results point to the potential of these model systems, based on simple ferromagnetic metals, to mimic antiferromagnetic device physics.

*This work was supported in part by the Luther and Alice Hamlett Undergraduate Research Support Program in the Academy of Integrated Science at Virginia Tech.
Implementation of a microwave readout for scanning superconducting quantum interference devices (SQUIDs)*

RACHEL RESNICK (Presenter), JUSTIN OH, Cornell University, FARSHAD FOROUGHI, JAN-MICHAEL MOL, RWTH Aachen University, ALEXANDER B JARJOUR, DAVID LOW, Cornell University, JOHN ROBERT KIRTLEY, Stanford University, HENDRIK BLUHM, RWTH Aachen University, KATJA NOWACK, Cornell University — In scanning superconducting quantum interference device (SQUID) microscopy a SQUID is rastered close to the surface of a sample to obtain images of the sample's magnetic properties. In this talk we will discuss a microwave readout for scanning SQUIDs that incorporate an on-chip capacitor as reported in [1]. In this case, the SQUID acts as a flux-dependent inductor, that forms an LC resonant circuit with the on-chip capacitor. The phase and amplitude of microwaves reflected by this circuit encode changes in magnetic flux. We will present our progress towards implementing this microwave readout and characterizing the SQUID noise performance at mK temperatures. The microwave readout holds the promise to both increase our flux sensitivity to below 100nPhi_0/sqrt(Hz) and our measurement bandwidth to several hundreds of MHz [1].


*This work was supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875). The SQUIDs used in this study were developed under an NSF IMR-MIP contract, Award No. 0957616.

Optimizing a cryogen-free measurement system for measurement of single electron devices

LETICIA DAMIAN (Presenter), JUSTIN K PERRON, California State University San Marcos, San Marcos, Ca 92069 — Single electron devices (SEDs) are electronic devices capable of isolating individual electrons along a conducting path. This ability has many proposed applications including their use in metrology, and quantum information science. Recently our lab has installed a cryogen-free dilution refrigeration system for the purpose of investigating SEDs and their use in these applications. In this talk I will describe our efforts in optimizing the electrical measurement setup of this system. Our primary metric for optimization is electron temperature, a limiting factor in measurements of this type.

Kinetic Separation of Hydrogen Isotopes in Metal-Organic Frameworks*

KATHARINE RIGDON (Presenter), NAIYUAN (JAMES) ZHANG, STEPHEN FITZGERALD, Oberlin College — Deuterium is a valuable hydrogen isotope with applications in NMR, nuclear power, and as a medical tracer. It constitutes less than 0.02% of naturally occurring hydrogen and is challenging to isolate. Current industrial separation techniques, which rely on tiny differences in the isotopes' chemical behavior, are expensive and energy intensive. Recently a new approach based on difference in the confined isotopes' zero-point energy has emerged. While these "quantum sieving" methods exhibit higher selectivity, many practical obstacles remain for them to replace the standard chemical approach. I will present data on a kinetics based separation within highly porous pellets of metal-organic frameworks (MOF). Mass spectroscopy with isotope mixtures shows breakthrough times that differ by more than three minutes. While these results are obtained at liquid nitrogen temperature, it is expected that planned experiments with the MOF known as Cu-MFU-4l should produce similar time differences at room temperature.

*NSF grant # CHE-1565961

Quantitative Imaging of Cytoskeletal Filaments of C17.2 Cells

JAY MAGERS (Presenter), JULIA HUTSKO, Physics, Susquehanna University, SABRINA JEDLICKA, SWETHA CHANDRASEKAR, Material Science, Lehigh University, SLAVA V. ROTKIN, Material Research Institute, Penn State, MASSOOMA PIRBHAI, Physics, Susquehanna University, LISA SCHNEIDER, Math and Computer Science, Salisbury University — The ability of cells to resist deformation, to transport intercellular cargo and to change shape during movement depends on the cytoskeletal filaments. Recent work has demonstrated that internal and external stimuli can affect these filaments and thus cellular behavior. Therefore, it is important to understand how to quantitatively extract data about the network of filaments and their changes. This research focuses on the modeling of the cytoskeletal networks to create a catalogue of them. While many cell analysis programs already exist, most are complex to use and are designed to analyze multiple types of cells and situations with limited customization in the program's analysis. Therefore, in order to obtain a more specialized analysis, different programming languages were explored in order to develop a custom analysis method. Several custom program were developed primarily utilizing the Python image analysis library OpenCV and MATLAB. This talk will explore the actin structures in C17.2 neural stem cells and compare the different programs' methods and capability to segment individual cells then calculate their fluorescent density.

Monday, March 4, 2019 2:30 PM - 4:54 PM

2:30PM C69.00001: The Universe as a Quantum Computer* [Invited] SETH LLOYD (Presenter), Massachusetts Institute of Technology — Every elementary particle carries with it bits of information that describe its type, charge, mass, position, and velocity. Every time two or more particles interact, that information is transformed and processed. The universe computes; and it computes in a way that is governed by the laws of quantum mechanics. The computational nature of the universe has nontrivial implications for its history, including how complex structures are generated, and the future of these structures. This talk discusses the implications of quantum information processing for the history and future of the universe.

*This work was funded by NSF

3:06PM C69.00002: Does This Ontological Commitment Make Me Look Fat? A Defense of Many-Worlds [Invited] SEAN CARROLL (Presenter), Caltech — The Everettian or Many-Worlds formulation of quantum mechanics features the simplest and most straightforward set of concepts and equations, but comes at the cost of the non-uniqueness of our observed part of reality. I will give a brief introduction to this approach, and discuss both a set of misguided objections and some true challenges. Among the true challenges are the issue of structure (how do complicated aspects of observed reality emerge from an austere vector in Hilbert space?) and probability (why are probabilities given by amplitudes squared if every outcome happens on some branch of the wave function?).

3:42PM C69.00003: The Relational Interpretation of Quantum Mechanics [Invited] CARLO ROVELLI (Presenter), Aix-Marseille University — The Relation Interpretation of Quantum Mechanics is a refinement of textbook “Copenhagen” quantum mechanics, which is receiving increasing attention. It does not assume an absolute split of the world into “quantum system” and “classical observer”; it rather assumes that any physical system can play either role. It avoids the “many worlds” of some Everettian interpretations, the un-observable entities of Bohmian interpretations, as well as the un-observed dynamical collapse of physical-collapse theories. The prices to pay is to accept that all physical quantities are relational, in the sense in which velocity is relational in classical mechanics: it expresses a relation between a system another system. I shall illustrate this understanding of quantum theory in detail and compare it with different and similar ways of viewing quantum mechanics.

4:18PM C69.00004: Quantum theory of the classical: quantum jumps, Born’s Rule and objective classical reality via quantum Darwinism [Invited] WOJCIECH ZUREK (Presenter), Los Alamos National Laboratory — The emergence of the classical from the quantum substrate is a long-standing conundrum. I will describe three insights into the transition from quantum to classical based on recognition of the role of the environment [1]. I will first derive preferred sets of states that define what exists -- our everyday classical reality. They arise as a result of breaking of the unitary symmetry of the Hilbert space resulting from the conflict between linearity of quantum evolutions and nonlinearities inherent in the process of amplification -- of replicating information. This accounts for quantum jumps and the emergence of the preferred pointer states consistent with those obtained via environment-induced superselection, (einselection), but is accomplished without the usual tools of decoherence. Pointer states determine what can happen -- define events -- without appealing to probabilities. Therefore, Born’s Rule can now be deduced from entanglement-assisted invariance, or envariance -- a symmetry of entangled quantum states. Envariance also provides new basis for statistical physics, allowing one to deduce thermodynamics from symmetries of entanglement -- that is, without the need for ensembles [2]. Information flows accompanying decoherence explain how the perception of objective classical reality arises from the quantum substrate: the effective amplification they represent accounts for the objective existence of the einselected states of macroscopic quantum systems through redundancy of their records in the environment -- through quantum Darwinism [1].


Monday, March 4, 2019 5:45 PM - 6:45 PM

Session D43 APS: APS Prizes & Awards Ceremony BCEC 210B

5:45PM D43.00001: APS Prizes & Awards Ceremony — Prizes and awards will be bestowed on several individuals for outstanding contributions to physics. Please join us in honoring these individuals.

Monday, March 4, 2019 6:00 PM - 7:00 PM
Session D70 APS/SPS: Building Your Undergraduate Physics Career BCEC Exhibit Hall A - Tag(s): Careers, Undergraduate

6:00PM D70.00001: Building Your Undergraduate Physics Career — Building Your Undergraduate Physics Career

Monday, March 4, 2019 6:45 PM - 8:15 PM

Session D71 APS: Welcome Reception BCEC Exhibit Hall A - Tag(s): Undergraduate

6:45PM D71.00001: Welcome Reception — Welcome Reception

Monday, March 4, 2019 7:30 PM - 9:40 PM

Session D51 DCMP DMP: Enabling Quantum Leap: National Quantum Initiative Special Outreach Session BCEC 253A - Tomasz Durakiewicz, National Science Foundation - Tag(s): Invited, Undergraduate

7:30PM D51.00001: Expanding American Leadership in Quantum Information Science [Invited] JACOB TAYLOR (Presenter), NIST — TBD

7:50PM D51.00002: Developing our Quantum Future [Invited] KRYSTA M SVORE (Presenter), Microsoft — TBD

8:10PM D51.00003: Physics community input to federal QIS legislation [Invited] FRANCIS SLAKEY (Presenter), American Physical Society — TBD

8:30PM D51.00004: Enabling Quantum Leap [Invited] LINDA SAPOCHAK (Presenter), National Science Foundation — TBD

8:50PM D51.00005: Opportunities at the entanglement frontier [Invited] JOHN PRESKILL (Presenter), Caltech — TBD

9:10PM D51.00006: Round Table Discussion [Invited] —

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E01 DCMP: Electronic Structures of Weyl Semimetals and Topological Insulators BCEC 106 - Andrew Weber, Donostia International Physics Center

8:00AM E01.00001: Evolution of the Electronic Structure of MoTe2 under Pressure YAJIAN HU (Presenter), YUK TAI CHAN, KWING TO LAI, KIN ON HO, XIAOYU GUO, KING YAU YIP, SWEE KUAN GOH, Physics, The Chinese University of Hong Kong, YUJI AOKI, TATSUMA D. MATSUDA, Department of Physics, Tokyo Metropolitan University — Transition metal dichalcogenides have recently been heavily studied owing to their intriguing physical properties such as extremely large magnetoresistance (MR) in WTe2 and MoTe2. Further interests are attracted when they are predicted as candidates of type-II Weyl semimetals. Moreover, as both WTe2 and MoTe2 host superconductivity, this opens up the possibility of topological superconductivity.

In this work, we present the magneto-electronic transport study of MoTe2 under pressure. We did the magneto-resistance measurement with magnetic field up to 14 T and temperature down to 30 mK. The large MR and the Hall coefficient decrease rapidly with increasing pressure. Beyond 10 kbar, where the $T_d$ phase is completely suppressed and the superconducting transition temperature $T_c$ is significantly enhanced, the Hall coefficient becomes very small and saturated. We will discuss the evolution of Fermi surface across the temperature-pressure phase diagram. The electronic structure study would help us investigate the ground state and superconductivity of MoTe2.
**8:12AM E01.00002:** Crystal structure and electronic structure of non-centrosymmetrical trigonal PtBi₂*

WENXIANG JIANG (Presenter), FENGFENG ZHU, PING LI, HAIYANG MA, HAOHUA SUN, ZHONGQIANG YANG, CANHUA LIU, DANDAN GUAN, JINFENG JIA, WEIDONG LUO, DONG QIAN, Department of Physics and Astronomy, Shanghai Jiao Tong University — Electronic structure of single crystalline y-PtBi2 is studied by angle-resolved photoemission spectroscopy (ARPES). It is proposed by theoretical calculation that the stable structure of y-PtBi2 should be non-centrosymmetric. ARPES measurement gives powerful evidences in this paper that different band structures between two types of cleaved surface are clearly observed. Bulk and surface bands are characterized through systematically photon dependent measurement. The bulk band dispersions agree well with the first-principle calculation except Rashba shaped surface states. The topography studied by STM also confirms the existence of two different cleaved surfaces. Besides, some efforts has been made to demonstrate the existence of triply degenerate point fermions.

*This work is supported by National Basic Research Program of China (Grants No.2012CB927401, No.2013CB921902), National Natural Science Foundation of China (Grants No. 11574201, No11521404, No 11134008, No. 11174199, No.11374206, No. 11274228., No 11227404, No. 91421312, and No. 91221302), Shanghai Committee of Science and Technology (No. 12JC140530). D.Q. acknowledges support from the Changjiang Scholars Program and the Program for Professor of Special Appointment (East Scholar).*

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**8:24AM E01.00003:** Spin-Resolved Electronic Response to the Phase Transition in MoTe₂*

ANDREW WEBER (Presenter), Donostia International Physics Center, PHILIPP RÜSSMANN, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, NANN XU, Swiss Light Source, Paul Scherrer Institute, STEFAN MUFF, MAURO FANCIULLI, ARNAUD MAGREZ, PHILIPPE BUGNON, HELMUTH BERGER, Institute of Physics, École Polytechnique Fédérale de Lausanne, NICHOLAS C PLUMB, MING SHI, Swiss Light Source, Paul Scherrer Institute, STEFAN BLUEGEL, PHIVOS MAVROPOULOS, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, J. HUGO DIL, Institute of Physics, École Polytechnique Fédérale de Lausanne — The Weyl semimetal MoTe₂ is studied by spin- and angle-resolved photoemission spectroscopy across the centrosymmetry-breaking structural transition temperature of the bulk. A three-dimensional spin-texture is observed in the bulk Fermi surface in the low temperature, noncentrosymmetric phase that is consistent with first-principles calculations. The spin texture and two types of surface Fermi arc are not completely suppressed above the bulk transition temperature. The lifetimes of quasiparticles forming the Fermi arcs depend on thermal history and lengthen considerably upon cooling toward the bulk structural transition. The results indicate that a new form of polar instability exists near the surface when the bulk is largely in a centrosymmetric phase.

*This work was supported by the Swiss National Science Foundation Project No. PP00P2_144742, No. 200021-137783, No. PP00P2_170591, NCCR-MARVEL, the Sino-Swiss Science and Technology Cooperation (Grant No. IZLCZ2-170075), DFG (SPP-1666, Project No. MA 4637/3-1) and the VITI project of the Helmholtz Association.*

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**8:36AM E01.00004:** Investigation of the magnetic Weyl semimetal candidate Co₃Sn₂S₂ by ARPES.*

ILYA BELOPOLSKI (Presenter), TYLER COCHRAN, Princeton University, ENKE LIU, YU-HSIN SU, Max Planck Institute for the Chemical Physics of Solids, JIAJIN YIN, GUOQING CHANG, SONGTIAN SONIA ZHANG, Princeton University, ZURAB GUGUCHIA, Paul Scherrer Institut, CLAUDIA FELSER, Max Planck Institute for the Chemical Physics of Solids, ZAHID HASAN, Princeton University — Topological phases in magnetic materials are a topic of current interest in the community. Recently, the kagome-lattice ferromagnet Co₃Sn₂S₂ was predicted to be a Weyl semimetal, while transport showed an exceptionally large anomalous Hall angle. Motivated by these exciting results, we use synchrotron ARPES to study single crystal Co₃Sn₂S₂. We observe a strong photon energy dependence consistent with out-of-plane $k_z$ dispersion, even at moderate VUV photon energies. We compare our ARPES results with DFT and find a general match, with typical disagreement of ~ 0.1 eV. To address this disagreement, we perform muon/neutron scattering on Co₃Sn₂S₂ to better understand the magnetic state experimentally. We comment on progress using our muon/neutron results to match DFT to ARPES and evaluating possible changes in the predicted Weyl phase and other topological indices. Our results suggest that the search for topological magnets might benefit from an iterative approach building on muon/neutron measurements of the magnetic state, DFT and ARPES.

*Work at Princeton was supported by the US DOE under the Basic Energy Sciences programme (Grant #: DOE/BES DE-FG-02-05ER46200) and the Gordon and Betty Moore Foundation (GBMF4547/Hasan).*
8:48AM E01.00005: Surface resonances of topological origin in bcc iron*  OLEG YAZYEV (Presenter), DANIEL GOSÁLBEZ MARTÍNEZ, GABRIEL AUTÉS, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland — Chiral band degeneracies are ubiquitous in the band structures of systems with broken inversion or time-reversal symmetries. While in Weyl semimetals such degeneracies are isolated near the Fermi level, the broadly defined notion of topological metal implies the presence of disconnected Fermi surface sheets characterized by non-zero Chern numbers. Bcc iron is an archetypal example of ferromagnetic metal with two non-trivial Fermi surface electron pockets along the direction parallel to the magnetization [1]. In this work, we investigate the surface-state signatures of the topological nature of these Fermi surface pockets. We find that the (110) surface presents arc-like resonances attached to the non-trivial electron pockets. These Fermi arc resonances are due to two chiral degeneracies, a type-I elementary Weyl point and a type-II composite (Chern number ±2) Weyl point, located at slightly different energies. We further show that such surface resonances can be controlled by the orientation of magnetization, and can eventually be eliminated following a topological phase transition.


*We acknowledge support by the NCCR Marvel.

9:00AM E01.00006: Sharp Orientation-dependent Quantum Oscillations in HoPtBi  CONNOR RONCAIOLI (Presenter), PRATHUM SARAF, YUN SUK EO, HYUNSOO KIM, JOHNPIERRE PAGLIONE, University of Maryland, College Park — Rare-earth platinum and palladium-bismuthides have been host to rich phenomenon in the search for topological states and Weyl semimetals. YPtBi in particular is host to a spin-split fermi surface which hosts a spin-3/2 superconducting state. In this study we expand this investigation to HoPtBi, a magnetic analog to YPtBi with an AFM ground state and a paramagnetic state above 1.2K. We present orientation-dependent measurements of quantum oscillations in HoPtBi and find a strong orientation dependence near the crystallographic [110] direction very similar to, but phenomenologically distinct from the behavior of YPtBi.

9:12AM E01.00007: Observation of surface Dirac dispersion in transition metal dipnictides*  GYANENDRA DHAKAL (Presenter), MD MOFAZZEL HOSEN, University of Central Florida, WEI-CHI CHIU, BAHADUR SINGH, Department of Physics, Northeastern University, KLAUSS DIMITRI, University of Central Florida, BAOKAI WANG, Department of Physics, Northeastern University, FIROZA KABIR, CHRISTOPHER SIMS, SABIN REGMI, University of Central Florida, HSIN LIN, Institute of Physics, Academia Sinica, DARIUSZ KACZOROWSKI, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ARUN BANSIL, Department of Physics, Northeastern University, MADHAB NEUPANE, University of Central Florida — The experimental discovery of Dirac and Weyl Fermions, quasi-particles existing in low energy excitation in condensed matter physics, has paved a new avenue of research interests in condensed matter physics. Recently, the Lorentz-invariance breaking Weyl semimetallic state has been reported in MoP2 and WP2. Arsenic counterparts of these compounds, which also harbor high magnetoresistance, demand the detailed study to investigate the possible semimetallic state possessed by them. Here, we discuss our angle-resolved photoemission spectroscopy (ARPES) and first-principles calculations results on the electronic structures of MoAs2 and WAs2, which reveal the presence of a surface Dirac cone. Our systematic electronic structures analysis reveals the termination dependent electronic structure in these compounds. Our study offers the opportunity to study the various quantum phase transitions within this family.

*This work is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415 and the startup fund from UCF (M.N.).

9:24AM E01.00008: ARPES measurements on Dirac nodal-line semimetal candidate TiRhAs  HANG LI (Presenter), DAYU YAN, CONGCONG LE, BINBIN FU, YOUGUO SHI, HONG DING, TIAN QIAN, Chinese Academy of Sciences — In the family of topological materials, a new Dirac nodal-line (DNL) semimetal TiRhAs was recently predicted by first-principles calculations. Unlike most of DNL semimetals, TiRhAs has a single nodal ring residing near the Fermi level with no interference from other bands, which makes that the carriers in TiRhAs are entirely contributed by nodal-line fermions. Moreover, the calculations show that the hybridization gap induced by SOC is negligible in TiRhAs. Therefore, TiRhAs can be regarded as a hydrogen-atom-like DNL semimetal. By the soft X-ray ARPES, we systemetically studied the band structure of TiRhAs and observed a single nodal ring at kx=0 plane in BZ.
9:36AM E01.00009: Observation of Yamaji Magic Angles in Bismuth Nanowires*  TITO HUBER (Presenter), Chemistry, Howard University, Washington DC 20059, ALBINA NIKOLAEVA, LEONID KONOPKO, Academy of Sciences, Chisinau, Moldova, MD-2028 — Experimental studies that probe the surface of bulk bismuth as a composite of topological insulator edges and hinges on the surface of bulk Bi are lacking. We present angle-dependent transverse magnetoresistance (TMR) oscillation measurements of small diameter (50 nm) bismuth nanowires where electronic transport is dominated by the surface, rather than the bulk in the core of the nanowire, because of quantum confinement. We find that the TMR of the surface states in our nanowires exhibits peaks for a sequence of nanowire rotation angles that strongly suggest an interpretation in terms of Yamaji magic angles. Magic angles are observed in layered and other low-dimensional conductors with weak interplanar coupling that are amenable to be described by an open, corrugated, Fermi surface. In contrast to surface states, bulk bismuth does not display magic angles since the Fermi surface is closed. We will discuss our interpretation of surface states of bismuth and the main Fermi surface parameters that we observe: orientation of the Fermi surface, Fermi wavevector, and coupling strength.

*We acknowledge support by NSF-CIQM 1231319 and by The Keck Foundation.

9:48AM E01.00010: Topological Line-Like Bound States in the Continuum* MANABU TAKEICHI (Presenter), SHUICHI MURAKAMI, Tokyo Institute of Technology — Bound states in the continuum (BIC) have been studied mainly in optics. Recently, electronic BIC have been proposed. They appear as points in the momentum space and are protected topologically by the Chern number. In this study, we propose a new type of BIC protected by the winding number, which is one of the topological invariants. These BIC appear as lines in the momentum space, and are realized in a multilayer model consisting of honeycomb-lattice layers. We show band structure and spatial localization of the BIC in this model. The wavenumbers at which the BIC appear can be explained in terms of topology in the momentum space.

*This work is supported by Grant-in-Aid for Scientific Research from MEXT (Grant No. 18H03678), and CREST, JST (No. JP-MJCR14F1).

10:00AM E01.00011: Scanning tunneling spectroscopy studies of the topological states in the Dirac metal Hf$_2$Te$_2$P TIMOTHY BOYLE (Presenter), ANTONIO ROSSI, PETER CARLSON, MOIRA K MILLER, JINGTAI ZHAO, MORGAN WALKER, VALENTIN TAUFOUR, INNA VISHIK, EDUARDO H DA SILVA NETO, University of California, Davis — Recent angle-resolved photoemission spectroscopy experiments and theoretical calculations indicate the existence of multiple Dirac states in the topological material Hf$_2$Te$_2$P [1]. In this study we use scanning tunneling spectroscopy (STS) to measure the electronic band structure of the material. Using STS as a direct probe of the real-space local density of states, we identify quasiparticle interference patterns that allow us to measure the topological surface states. The results will be discussed in the context of density functional theory calculations that predict multiple topological states below and above the Fermi energy.

Since the establishment of topological insulators, a lot of interest has turned to finding systems that combine topology with strong electron correlations. This led Dzero et al. to propose that Kondo insulators, materials that open a band gap by mixing local and itinerant states of opposite parity, should fall into this category [1]. The effort spurred by this proposal has advanced the state of knowledge on SmB6, the leading candidate for a topological Kondo insulator [2]. The question of its topology, however, remains unanswered.

The apparently contradictory results from different experimental techniques form major obstacle to resolving this issue. In this paper we tackle one of these apparent contradictions: Researchers using scanning tunneling microscopy [3,4] have reached different conclusions on the surface terminations than those using photoemission spectroscopy [5]. By combining both techniques we find the results from these methods can be reconciled, a conclusion that will help settle this topical issue.


In this work, we explore surface states of nonsymmorphic semimetals with lifted band degeneracy at the symmetry points. HfSiS, a typical Dirac nodal-line semimetal with the nonsymmorphic symmetry exhibits a Rashba-type spin-split surface state. In this regard, we explore the Rashaba surface states which draw an analogy to the topological materials, where the spin and orbital entanglement takes place. We have performed spin- and angle-resolved photoemission spectroscopy experiment on HfSiS and ZrSiS single crystals with \( p \)-polarized and \( s \)-polarized light. The observed variation in the intensity distribution upon changing the light polarization tells us that the surface states along the M-X-M line are mainly composed of \( d_{z^2} \) orbitals, and change into \( d_{xy} \) along the G-X-G line. Combining the observed spin polarizations with the result of the slab calculation, we have concluded that the surface bands surrounding the X point exhibit a quite anisotropic spin and orbital texture. Our findings provide a new way of light manipulation by controlling the spin structure in materials which is important for future applications.
10:48AM E01.00015: Interaction of coherent phonons with spin-orbit coupled surface states*  JONATHAN SOBOTA (Presenter), SLAC National Accelerator Laboratory, HADAS SOIFER, Stanford University, PATRICK S KIRCHMANN, SLAC National Accelerator Laboratory, ZHIXUN SHEN, Stanford University — Spin-polarized electronic states form at the surface of materials due to the combination of spin-orbit coupling and broken inversion symmetry. This phenomenon was first established for Shockley states at the surface of noble metals such as gold, and more recently, has been recognized as a central mechanism responsible for the formation of topologically non-trivial states. Given the fundamental significance of these states, as well as their potential role in spintronics applications, it is important to understand their interaction with collective excitations of the crystal lattice.

Here we use time- and angle-resolved photoemission spectroscopy (trARPES) to investigate electron-phonon coupling in a model system: the Rashba-split surface state of the semimetal Antimony (Sb). The simplicity of the structure permits us to coherently excite all zero-momentum optical modes of the crystal, and study their coupling to both bulk and surface electronic states. In addition, this material provides an ideal platform for testing coherent control schemes, as well as exploring excitation mechanisms for finite-momentum phonon modes. We will discuss our results in the context of similar measurements on topological insulators.

*Supported by the U.S. Department of Energy, Office of Science.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E02 DMP DCOMP: Dielectric & Ferroic Oxides -- Optically Induced Properties and Optical Measurements 8CEC 107A - Dennis Meier

8:00AM E02.00001: Ultrafast photoinduced transient strain in BiFeO3 thin film probed by x-ray free electron laser diffraction  HYEONJUN LEE (Presenter), YOUNGJUN AHN, SAMUEL MARKS, Department of Materials Science and Engineering, University of Wisconsin-Madison, ERIC C LANDAHL, Department of Physics, DePaul University, JOONYOUNG LEE, TAYEON KIM, SANJITH UNITHRATTIL, JI YOUNG JO, School of Materials Science and Engineering, Gwangju Institute of Science and Technology, SEHWAN CHEON, SUNAM KIM, Pohang Accelerator Laboratory,, Pohang Accelerator Laboratory,, CAROLINA ADAMO, Department of Applied Physics, Stanford University, DARRELL G. SCHLOM, Department of Materials Science and Engineering, Cornell University, HAIDAN WEN, X-ray Science Division,, Argonne National Laboratory, PAUL G EVANS, Department of Materials Science and Engineering, University of Wisconsin-Madison — Photoinduced structural effects provide an emerging method for manipulating the crystal structure of polar perovskites and for eventual ultrafast control of phenomena such as ferroelectricity and magnetism. Studies of the dynamics of the strain generation and relaxation after photoexcitation can provide fundamental insight into the origin of these photoinduced phenomena. Experiments probing a 35 nm thick BiFeO3 thin film using an x-ray free electron laser (XFEL) providing 100 fs time resolution show that a transient lattice expansion can be produced by intense ultrafast optical excitation. The diffraction employed an x-ray fluence below the BiFeO3 damage threshold. Optical excitation induced a shift of the BiFeO3 002 reflection to lower wavevector by up to 0.8% within 9 ps. Temporal oscillations of the scattered intensity were observed over a wide range of wavevectors, equivalent to several thickness fringes. The diffraction matched the longitudinal acoustic (LA) sound velocity indicates that an impulse propagated into the film in a manner consistent with kinematical calculations. The predicted intensity at 5 ps is not predicted accurately, which may indicate that there is a more complex distribution of the initial stress than is expected from the optical absorption profile.

8:12AM E02.00002: Ultrafast optical control of ferroelectric polarization via resonant magnon excitation*  HARICHARAN PADMANABHAN (Presenter), YAKUN YUAN, Pennsylvania State University, ALEXANDER MELVILLE, Massachusetts Institute of Technology, DARRELL G. SCHLOM, Cornell University, VENKATRAMAN GOPALAN, Pennsylvania State University — Optical control of order parameters in condensed matter is of great interest in fundamental as well as applied science. In the context of ferroic materials, controlling ferroic degrees of freedom using ultrafast optical pulses could pave the way towards ultrafast switches and devices that work on femtosecond timescales. Attempts to achieve this by direct excitation of ferroic modes have not been completely successful, necessitating other novel strategies.

In this work, we demonstrate a transient suppression of the ferroelectric polarization in the prototypical multiferroic BiFeO3 by resonant excitation of a magnon coupled to the ferroelectric mode. Ultrafast pump-probe measurements using a second harmonic generation probe reveal that the suppression and recovery of the polarization occur at a femtosecond timescale. Furthermore, we observe that the zero polarization transient state can be stabilized by tuning the domain structure of the lattice, increasing its lifetime by one order of magnitude.

*DOE Grant No. DE-SC0012375
8:24AM E02.00003: Reversible optical control of multiferroicity in BiFeO$_3$ thin films  YI-DE LIOU, National Cheng Kung University, Tainan 70101, Taiwan, YEN-LIN HUANG, National Chiao Tung University, Hsinchu 30010, Taiwan, RYAN THOMAS HART, University of Texas at Arlington, Arlington, TX 76019, USA, YUAN-CHIH WU, National Cheng Kung University, Tainan 70101, Taiwan, RAJESH V CHOPDEKAR, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, VALANOOR NAGARAJAN, University of New South Wales, Sydney, 2052, Australia, YING-HAO CHU, National Chiao Tung University, Hsinchu 30010, Taiwan, YI-CHUN CHEN, National Cheng Kung University, Tainan 70101, Taiwan, YE CAO, University of Texas at Arlington, Arlington, TX 76019, USA, JAN-CHI YANG (Presenter), National Cheng Kung University, Tainan 70101, Taiwan — Nowadays, increasing technology interest has focused on the optical control of non-volatile functional units. In this work, we present the deterministic switching/modulation of the ferroelectric and (anti)ferromagnetic orders at ambient temperature through laser illumination.

With well-tuned laser illumination, the local temperature of illuminated region increases, resulting in a significant flexoelectric field at the boundaries of illuminate and non-illuminated region. The induced flexoelectric field is then adopted to modulate the local ferroelectricity of BiFeO$_3$ thin film, generating a wide spectrum of tunable domain structures. To verify the role of flexoelectric effect, phase field simulation is processed to simulate the correlation between the as-grown and light induced domain architecture. Due to the fact that BiFeO$_3$ thin film has its ferroelectricity coupled strongly with inherent antiferromagnetism/ferromagnetism, the optical modulation of ferroelectric order gives rise to corresponding alteration of the antiferromagnetism/ferromagnetism as well. Furthermore, we show that the domain conductivity and piezoresponse enhancement could also be turned on and off via laser illumination.

8:36AM E02.00004: Prediction of photo-induced phase transitions and coherent optical phonon generation in BaTiO$_3$*  FANGYUAN GU (Presenter), Department of Materials, Imperial College London, ÉAMONN MURRAY, PAUL TANGNEY, Department of Physics and Department of Materials, Imperial College London — We investigate the effects of above band gap ultrafast laser pulses on the lattice dynamics and structural properties of the prototypical perovskite, BaTiO$_3$, using electronic structure methods and atomistic simulations. We use a constrained density functional method to study the local changes induced by ultrafast laser excitation. Our work shows a reduction in the ionicity due to electrons being returned by O anions to Ti cations. We calculate the dependences of phonon frequencies and equilibrium structures on excited carrier density and find that moderate levels of photo-excitation reduces the polarization, coherently excites and softens optical phonons of A1 symmetry, and lowers the local barriers to ferroelectric domain reversal. We use our first-principles calculations to fit atomistic potentials and study structural changes on significantly longer time-scales. Our results suggest that pump-probe spectroscopy could be used to induce a purely-displacive transition to higher symmetry phase at low temperature and to study the decay of coherent optical phonons. Our findings may also provide guidance to the design of optically controlled devices.

*Supported by EPSRC grants EP/L015579/1, EP/P020194/1.

8:48AM E02.00005: Optically Induced Nanoscale Domain Transformation in Low-Strain BaTiO$_3$ Thin Films YOUNGJUN AHN (Presenter), ANASTASIOS PATERAS, HYEON JUN LEE, JOONKYU PARK, Department of Materials Science & Engineering, University of Wisconsin - Madison, Madison, Wisconsin 53706, USA, SILVIA DAMERIO, ARNOUD EVHERHARDT, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands, ANTHONY DICIARA, HAIDAN WEN, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, BEATRIZ NOHEDA, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands, PAUL G EVANS, Department of Materials Science & Engineering, University of Wisconsin - Madison, Madison, Wisconsin 53706, USA — Above-bandgap ultrafast optical excitation provides the means to extend the current state of understanding of polarization domain phenomena and the relationship between electronic dynamics and mesoscale transformation. We report a time-resolved synchrotron x-ray diffraction study of a BaTiO$_3$ film grown on a NdScO$_3$ substrate in which an optically induced domain transformation is observed. The key experimental feature is an optically induced change in the intensities and reciprocal space positions of the diffuse scattering patterns arising from aa*/ca* and ca$_1$/ca$_2$ domain configurations. Following above-bandgap optical excitation, the diffuse scattering intensity of the aa*/ca* domains increases within 1 ns while that of the ca$_1$/ca$_2$ domains decreases. The change in intensities indicates a transformation from the ca$_1$/ca$_2$ to the aa*/ca* domain configuration. The transformation is accompanied by polarization rotation toward the out-of-plane direction, which has the same time dependence as the intensity variation. The degree of the polarization rotation varies depending on the optical fluence and is different for the two domain configurations. The results show that the mechanism of the domain transformation is associated with the polarization rotation induced by the optical excitation.
9:00AM E02.00006: Photostrictive characteristics in Perovskite Strontium Iridate Thin Films  YI-DE LIOU (Presenter), Physics, National Cheng Kung University, WEN-YEN TZENG, Electrophysics, National Chiao Tung University, HENG-JUI LIU, Materials Science and Engineering, National Chung Hsing University, CHIH WEI LUO, Electrophysics, National Chiao Tung University, YI-CHUN CHEN, Physics, National Cheng Kung University, YING-HAO CHU, Materials Science and Engineering, National Chiao Tung University, JAN-CHI YANG, Physics, National Cheng Kung University — Photostrictive effect depicts a direct light-matter interaction that exhibits a reversible mechanical deformation in a material under light illumination. In this work, we investigate the giant visible-light-induced deformation of orthorhombic perovskite SrIrO$_3$ (SIO), taking advantages of its sizable crystal field and high absorption across the visible spectrum at room temperature. By using highly structural sensitive in-situ Raman spectroscopy, the red-shift behaviors of all the optical phonons of SIO were observed as the increase of light intensities. The corresponding local strain states were analyzed by means of the phonon deformation potential theory, which unveils the giant photostrictive behavior in SIO thin films. The fast response time is also discovered by ultra-fast pump probe spectroscopy. We found that SIO shows significant photostriction properties compared to conventional semiconductors, polymers and perovskite oxides. The strong photostrictive effect, fast response time and superior stability of SIO at room temperature pave a promising route towards new applications and multifunctionalities of photon-driven devices.

9:12AM E02.00007: Coherent Phonons and Magnons in Hetero-Epitaxial BTO-BFO Films and Nano-rods*  BRENDEN A MAGILL (Presenter), RATHSARA R HERATH MUDIYANSELAGE, GITY KHODAPARAST, JOSEPH A SPENCER, JOHN BURTON, KIARA MCMILLAN, MIN GYU KANG, HAN-BYUL KANG, Virginia Tech, SHASHANK PRIYA, Virginia Tech/Penn State, JADE HOLLEMAN, STEPHEN A MCCGILL, Florida State/NHMFL — The desire to create monolithic multifunctional devices has driven significant research toward exploring multiferroics, where the coupling between electric, magnetic, optical, and structural order parameters can provide added functionality. In this study, we utilize time resolved responses of (1-x)BaTiO$_3$(x)BiFeO$_3$, x = 0.725 epitaxial films grown on LSMO with STO substrate and the BTO-BFO nanorods grown on Pt with Si as the substrate to reveal several coherent dynamics. We probed the dynamics of photo-excited carriers in several films and nanorods to obtain information on the time scale of different relaxation process, including coherent phonon and magnon dynamics. The ability to generate and manipulate the time resolved, phononic, and magnonic degrees of freedom in materials with external optical, electric, and magnetic fields promises to usher in a new era of revolutionary.

*Sponsored by the Air Force Office of Scientific Research under award number FA9550-17-1-0341, and DURIP funding (FA9550-16-1-0358). D. M. would like to acknowledge the financial support through National Science Foundation (1832865). S. Priya acknowledges the support through Office of Naval Research (N00014-16-1-3043) and S. McGill acknowledges the support from NSF DMR-1644779.

9:24AM E02.00008: Terahertz optical diode effect in multiferroics FeZnMo$_3$O$_8$ and BaCoSiO$_4$*  SHUKAI YU (Presenter), Tulane University, BIN GAO, JAE WOOK KIM, ALEMAYEHU S. ADMASU, XIANGHAN XU, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, XING ZHU, MICHAEL K. L. MAN, JULIEN MADÉO, KESHAV M DANI, Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology Graduate University, DIYAR TALBAYEV, Tulane University — We present a terahertz (THz) spectroscopic study of multiferroic FeZnMo$_3$O$_8$ and BaCoSiO$_4$. THz optical diode effect (ODE) is observed in both compounds. Two mechanisms for the ODE will be discussed in terms of symmetry. The ODE in FeZnMo$_3$O$_8$ is due to the toroidal moment which is the vector of cross product of polarization and magnetization. When the light is travelling along toroidal moment, the propagation of light is nonreciprocal if we flip the propagation direction. While the propagation of light in BaCoSiO$_4$ which has magneto-chiral structure is also nonreciprocal. For both of materials, the magnetic excitation plays a key to ODE. Magnetic dipole active magnetic excitation which is from electron spin resonance between the eigenstates of single-ion anisotropy Hamiltonian produces giant ODE in paramagnetic FeZnMo$_3$O$_8$ where the material doesn't have long range magnetic ordering. However, the magnetic excitation in BaCoSiO$_4$ generates weaker ODE in ferrimagnetic phase. We will discuss the resonant enhancement of the THz optical diode effect in both materials due to terahertz-frequency spin excitations.

*Rutgers University: No. DOE: DE-FG02-07ER46382. Tulane University: No. DMR-1554866 and by the Carol Lavin Bernick Faculty Grant Program.
9:36AM E02.00009: Acoustic study of ferroelectric phase transitions, from bulk materials to thin films.* ROBERT MECH (Presenter), BETZAI DA BERRIOS, OLEKSIY SVITELSKI, Gordon College, GARY PENNINGTON, RAJESWARI M KOLAGANI, GRACE YONG, Towson University, LYNN A BOATNER, Oak Ridge National Lab — The purpose of this project is to investigate how elastic properties of ferroelectric materials change when dimensionality of the specimen is reduced. Measurements done using ultrasound phase-sensitive pulse-echo technique. Ultrasound frequency ~50 MHz, length of pulses ~1us, pulse frequency ~ 10 kHz. We start investigation with bulk ferroelectric KTa0.92Nb0.08O3 crystal, exploring propagation of ultrasound waves as the crystal undergoes ferroelectric transitions spontaneously and in the presence of electric field with strength from 100 V/cm up to 2 kV/cm. The speed and attenuation of sound are both sensitive to the changes in the crystal. The observed behavior can be understood in terms of a mixed model that includes elements of soft-mode and disorder to order mechanisms of the transitions. The obtained data will be applied for understanding behavior of ferroelectric films.

*This work was partially supported by NSF DMR awards # 1709282 and 1709781.

9:48AM E02.00010: Controlling Distinguishable Ferroelectric States with Pulsed Electric Fields FRED FLORIO (Presenter), RAVISHANKAR SUNDARARAMAN, JIAN SHI, YANG HU, Rensselaer Polytechnic Institute — Ferroelectric materials are of increasing interest for novel computing paradigms such as neuromorphic computing, which require a large number of distinguishable states that can be set and read out in a controllable way. Achieving this necessitates a deeper understanding of polarization dynamics and their interplay with material grains and boundaries, down to the nanoscale. Using large ensembles of phase field simulations, we investigate domain switching dynamics under different field conditions for realistic device and grain size distributions. With statistical analyses and machine-learning approaches on these simulation results, we identify relationships between electric field pulse patterns and polarization states as a function of grain distributions, and quantify the capacity for realistic ferroelectric materials to be poled into a multitude of distinguishable states.

10:00AM E02.00011: Subtle structural distortions in LiOsO3 observed using optical second harmonic generation JUN-YI SHAN (Presenter), ALBERTO DE LA TORRE, NICHOLAS LAURITA, Department of Physics, California Institute of Technology, LIUYAN ZHAO, Department of Physics, University of Michigan, CAMERON DASHWOOD, Department of Physics, California Institute of Technology, DANIL0 PUGGIONI, Department of Materials Science and Engineering, Northwestern University, KAZUNARI YAMAURA, Research Center for Functional Materials, National Institute for Materials Science, YOUGUO SHI, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, JAMES M RONDINELLI, Department of Materials Science and Engineering, Northwestern University, DAVID HSIEH, Department of Physics, California Institute of Technology — LiOsO3 is a metal that undergoes a non-polar to polar structural phase transition upon cooling below a critical temperature Tc ~ 140 K, which is unusual because the presence of itinerant carriers is usually incompatible with ferroelectric-like structural distortions. To explore the microscopic mechanism of this phase transition, we performed angle-of-incidence dependent optical second harmonic rotational anisotropy measurements on LiOsO3 single crystals. We observe subtle distortions in the paraelectric phase above Tc and I will discuss their implications for an order-disorder versus a displacive picture of the polar phase transition.

10:12AM E02.00012: Optical nonlinearity and the anharmonicity of oxides ALI HAMZE (Presenter), ALEXANDER DEMKOV, University of Texas at Austin — Integration of crystalline oxides on silicon is one of the most promising ways to continue enhancing the performance and functionality of silicon-based technology. Oxide integration offers access to new physical phenomena not present in current semiconductor platforms to make use of in devices. In this work, we discuss one such phenomenon, the Pockels effect (also known as the linear electro-optical effect), and its connection with crystal anharmonicity. The Pockels effect describes the linear change in a material’s index of refraction in response to an applied electric field, and as such, is only present in non-centrosymmetric crystals. Anharmonic crystals with soft phonon modes can have enormous Pockels responses, and anharmonicity often manifests itself via large thermal expansion. However, one does not imply the other. Highly anharmonic crystals like BaTiO3 (and, under strain, SrTiO3) do exhibit large Pockels effect, while the even more anharmonic LiB3O5 does not. We will discuss the relationship between the thermal expansion, anharmonicity and the electro-optical effect.
10:24AM E02.00013: Raman scattering study of lattice and electronic excitations in Ce₂O₃**

ASTHA SETHI (Presenter), JOHN SLIMAK, University of Illinois at Urbana-Champaign, TARAS KOLODIAZHNYI, National Institute of Materials Science, S. LANCE COOPER, University of Illinois at Urbana-Champaign — The giant magnetodielectric effect exhibited by Ce₂O₃ near Tₙ suggests the presence of strong electron-lattice coupling effects. To clarify the microscopic details of these effects, we present a temperature and magnetic field dependent Raman scattering study of the lattice and electronic excitations in Ce₂O₃. Two crystal field excitations (CFEs) are observed at low temperatures, corresponding to transitions within the crystal-field-split J=5/2 manifold. We provide evidence that electron-phonon coupling is significantly enhanced at low temperatures, leading to a mixing of electronic and phononic states. The magnetic field-dependence of these coupled excitations provide insight into the microscopic mechanism associated with magnetodielectric behavior in Ce₂O₃.

**Research was supported by the National Science Foundation under Grant NSF DMR 1800982.

10:36AM E02.00014: Raman Study of Crystal Field Excitations and Soft Modes in Pr₂O₃*

JOHN SLIMAK (Presenter), ASTHA SETHI, University of Illinois at Urbana-Champaign, TARAS KOLODIAZHNYI, National Institute for Materials Science, Japan, S. LANCE COOPER, University of Illinois at Urbana-Champaign — The rare earth sesquioxides constitute an interesting class of materials because of the diverse ways in which lattice degrees of freedom interact with f-electrons. Several members of this class of materials exhibit unit cell doubling, as is the case with La₂O₃ at high pressures, or magnetodielectric effects, such as Ce₂O₃ at low temperatures, however Pr₂O₃ has only been only minimally investigated under high pressures or high fields. We report a preliminary Raman scattering study of the phonon and crystal field excitations Pr₂O₃ as functions of temperature and magnetic field. We observe significant softening of an A1g phonon that may be indicative of an incipient structural distortion that cannot be accessed at ambient pressures. Two crystal field excitations (CFEs) are also observed at low temperatures, and we observe splitting and evidence of electron-phonon coupling effects associated with the lowest CFE under an applied magnetic field. We discuss the relevance of these results to the possibility of a pressure-dependent structural change for Pr₂O₃.

*Research was supported by the National Science Foundation under Grants NSF DMR 1800982 and NSF DMR 1464090.

10:48AM E02.00015: Direct Measurements of the Atomic Displacements Related to the Ferroelectric Transition in Sn₂P₂S₆*

SIZHAN LIU (Presenter), HAN ZHANG, New Jersey Institute of Technology, SANJIT GHOSE, Brookhaven National Laboratory, SUYIN GRASS WANG, YU-SHENG CHEN, Argonne National Laboratory, DEAN R EVANS, Air Force Research Lab - WPAFB, TREVOR TYSON, New Jersey Institute of Technology — The Sn₂P₂S₆ is known to be ferroelectric and is one of the few Sn based ferroelectric (FE) systems which have been discovered. The true nature of the onset of the electric polarization has not been previously correlated with the changes in atomic structure. We have conducted structural measurements on multiple length scales as a function of temperature. In addition the structural results are compared to the low frequency phonons obtained from Raman scattering measurements. A complete model of the polar state of this system is developed.

*This work is supported by the U.S. Air Force under Grant FA8650-16-D-54.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E03 DCMP: Novel Transport in Topological Systems

8:00AM E03.00001: Ultrafast Photocurrents in the Weyl Semimetal TaAs

NICHOLAS SIRICA (Presenter), RA’ANAN TOBEY, Los Alamos National Laboratory, LINGXIAO ZHAO, GENFU CHEN, BING XU, RUN YANG, institute of physics chinese academy of sciences, BING SHEN, Physics and Astronomy, university of california los angeles, DZMITRY A. YAROTSKI, PAMELA BOWLAN, STUART TRUGMAN, JIAN-XIN ZHU, Los Alamos National Laboratory, YAOMIN DAI, School of Physics, Nanjing University, ABUL K AZAD, Los Alamos National Laboratory, ANTOINETTE TAYLOR, ROHIT P PRASANKUMAR, Los Alamos National Laboratory — We investigate polarization-dependent, ultrafast photocurrents in the Weyl semimetal TaAs using terahertz (THz) emission spectroscopy. Our results reveal that highly directional, transient photocurrents are generated along the non-centrosymmetric c-axis regardless of incident light polarization, while helicity-dependent photocurrents are excited within the ab-plane. This is consistent with both the bulk photovoltaic effect and the circular photogalvanic effect observed in direct photocurrent experiments, and provides additional insight into their microscopic origin by way of the dynamical information gained from the emitted THz waveform.
8:12AM E03.00002: Elastic gauge fields and zero-field 3D quantum Hall effect in hyperhoneycomb lattices* SANG WOOK KIM (Presenter), BRUNO UCHOA, University of Oklahoma — We derive the elastic gauge fields that emerge from lattice deformations in the hyperhoneycomb lattice, a three-dimensional structure with trigonally connected sites. In its semimetallic form, this lattice is a nodal-line semimetal with a closed loop of Dirac nodes. Using strain engineering, we find the strain fields that create nearly uniform 3D Landau level quantization. In the 3D quantum anomalous Hall phase, we show that the elastic Hall viscosity is \( \eta_H = \frac{\beta^2 \sqrt{3}}{16\pi a^3} \), where \( a \) is the lattice constant.

*S.W.K. and B.U. acknowledge NSF CAREER Grant No. DMR-1352604 for support.

8:24AM E03.00003: Proximal Anomalous Hall Effect in Ferromagnetic Insulator/Bulk-insulating BiSbTeSe2 Heterostructures* SHIHUA ZHAO (Presenter), HAIMING DENG, City College of New York, DANIEL RHODES, JAMES HONE, Columbia University, MARCIN KONCZYKOWSKI, Ecole Polytechnique, AGNIESZKA WOLOS, University of Warsaw, LIA KRUSIN-ELBAUM, City College of New York — Realization of Quantized Anomalous Hall Effect in topological insulators (TIs) thus far has been limited to ultra-thin MBE films of Cr- or V-doped (Bi,Sb)2Te3. In this system the disorder of the dopant landscape may limit the quantization temperature range in which the chiral channels can be observed. The alternative is to obtain proximal ferromagnetism in a 3D TI by creating a trilayer sandwich comprising ferromagnetic insulator (FMI) on the top and bottom surfaces of a TI. Here we report on the trilayer structure comprising bulk-insulating TI BiSbTeSe2 (BSTS) sandwiched between a two-dimensional van der Waals ferromagnetic insulator Cr2Ge2Te6 (CGT) grown using Bridgeman method. The structure was assembled in the inert-gas glovebox to prevent oxidation and contamination of the interface. h-BN capping was used to protect CGT against degradation in air. The out-of-plane magnetization of CGT down to thicknesses of 18 nm was confirmed by exfoliating it directly atop our custom-designed Hall microsensor chips. The enhancement of proximal magnetism obtained by (1) the optimal thickness of BSTS, (2) using pressure to obtain a better interfacial coupling, and (3) by electrostatic gating to the Dirac gap will be discussed.

*NSF DMR-1312483-MWN, NSF DMR-1420634, NSF HRD-1547830

8:36AM E03.00004: Nodal Arc in Disordered Dirac Fermions: Connection to Non-Hermitian Band Theory* MICHAL PAPAJ (Presenter), HIROKI ISOBE, LIANG FU, Massachusetts Institute of Technology — We show that Dirac fermion systems in two dimensions generally exhibit disorder-induced nodal arc replacing the nodal point and tilted Dirac cone, provided that the two components of the Dirac fermion correspond to two distinct orbitals unrelated by symmetry. This result is explicitly demonstrated using renormalization group analysis in a disordered Dirac model that we introduce, where the disorder potential acts differently on the two orbitals. As we show by numerical simulations and self-consistent Born approximation calculation, this drives the system into a new strongly disordered phase.

*This work was supported by the David and Lucile Packard Foundation.

8:48AM E03.00005: Interacting Dirac Semimetals* RUI-XING ZHANG (Presenter), Department of Physics, University of Maryland, SHENG-JIE HUANG, Department of Physics, University of Colorado, Boulder, JIABIN YU, Department of Physics, The Pennsylvania State University — The experimental discovery of three dimensional (3d) Dirac semimetals has opened up a new world of symmetry protected gapless state with non-trivial topological properties. While most existing studies have focused on the free fermion descriptions, we will show that interaction effects will significantly change the topological classification of Dirac semimetals. With the help of the dimensional reduction technique, we explicitly show that 3d Dirac semimetals protected by C_n rotation symmetries, such as Cd3As2 and Na3Bi, can be adiabatically connected to a gapped 3d axion insulator and gapless 1d axion strings in a symmetric way. This construction demonstrates that the anomaly nature of 3d Dirac semimetals is one dimensional. We further show that the non-interacting classification of a 3d Dirac semimetal generally reduces from Z to its Z_n subgroup in the presence of strong interactions. Our work lays the theoretical foundation for strongly interacting topological semimetals and paves the way for their future material realizations.

*RXZ acknowledges the JQI Postdoc Fellowship of University of Maryland. SJH acknowledges support from the U.S. Department of Energy, Office of Science, Basic Energy Sciences (BES) under Award number DE-SC0014415.
9:00AM E03.00006: Influence of Landau levels in the phonon dispersion of Weyl semimetals* PIERRE RINKEL, Universite de Sherbrooke, PEDRO LOPES, Physics, University of British Columbia, ION GARATE (Presenter), Universite de Sherbrooke — Discovered in high-energy physics, the chiral anomaly has recently made way to materials science by virtue of Weyl semimetals (WSM). Thus far, the main efforts to probe the chiral anomaly in WSM have concentrated on electronic phenomena. Nevertheless, recent theoretical works [1,2] have studied signatures of the chiral anomaly in the dynamics of lattice vibrations, to first order in the external magnetic field. In this work, we generalize those earlier results to magnetic fields of arbitrary strength by incorporating the influence of Landau levels in the phonon spectra. We predict a hybridization between plasmons and optical phonons that becomes potentially observable at high magnetic fields, and we identify fingerprints of chiral Landau levels in the sound velocity.


*This research has been funded by the Natural Sciences and Engineering Research Council of Canada, the Fonds de Recherche du Québec - Nature et Technologies, and Canada's First Research Excellence Fund.

9:12AM E03.00007: Anomalous off-diagonal thermal response in Mn$_3$Ge LIANGCAI XU, XIAOKANG LI, XIUFANG LU, Wuhan National High Magnetic Field Center and School of Physics, Huazhong University of Science and Technology, CLEMENT COLLIGNON, Laboratoire de Physique Et Etude des Matériaux, ESPCI Paris, ALASKA SUBEDI, Centre de Physique Theorique, Ecole Polytechnique, BENOIT FAUQUE, Laboratoire de Physique Et Etude des Matériaux, ESPCI Paris, ZENGWEI ZHU (Presenter), Wuhan National High Magnetic Field Center and School of Physics, Huazhong University of Science and Technology, KAMRAN BEHNIA, Laboratoire de Physique Et Etude des Matériaux, ESPCI Paris — We present a study of anomalous transverse response in non-collinear antiferromagnet Mn$_3$Ge down to sub-Kelvin temperature. Special attention is paid to the amplitude and temperature dependence of the anomalous Lorenz ratio $L^A_{ij} = \kappa^A_{ij} / T \sigma^A_{ij}$ relative to the Sommerfeld value. The contrast with Mn$_3$Sn [1] provides crucial information in the ongoing effort to identify the k-space location of the Weyl points. We also present measurements of the anomalous Ettingshausen and the anomalous Nernst effects in order to verify the Bridgman relation, a consequence of Onsager reciprocity.


9:24AM E03.00008: Localized Plasmons in One Dimensional Topological Systems ZHIHAO JIANG (Presenter), ROELOF E GROENEWALD, MALTE ROESNER, STEPHAN WOLFGANG HAAS, University of Southern California — One dimensional topological systems (the Schrieffer-Su-Hegger model and the generalized Aubry-André-Harper model) support strongly localized electronic states in the topologically nontrivial phases. In this work, we study plasmon modes in these systems by calculating the real space dielectric function within the random phase approximation. We observe localized plasmon modes in the electron energy loss spectra. In the topologically nontrivial sectors, these localized plasmon modes are shown to originate from the localized electronic edge states by separating the full polarization into contributions from pure bulk transitions without localized electronic states and edge-bulk transitions involving localized electronic states. We also show that the Coulomb interaction plays a role of delocalizing plasmons due to its long-range property. Therefore, the localization of plasmon modes is less strong than the localized electronic states obtained from non-interacting tight binding models.

9:36AM E03.00009: μ-ARPES studies of few-layer WTe2* ANTONIO ROSSI (Presenter), University of California, Davis, CHRIS JOZWIAK, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, Lawrence Berkeley National Lab, SENG HUAT LEE, RONALD DEAN REDWING, KEVIN DRESSLER, The Pennsylvania State University, INNA VISHIK, University of California, Davis — WTe2 exhibits a wide variety of physics in its bulk and monolayer regimes including two different topological phases, non-saturating magnetoresistance, and superconductivity under pressure or gating. We will present micro-ARPES studies on bulk and few-layer WTe2, which connect microscopic electronic structure to observations from transport experiments. Doping-dependence, spatial inhomogeneity, and layer-dependence of electronic structure and interactions will be discussed.

*This research used resources of the Advanced Light Source, which is a US Department of Energy Office of Science User Facility under contract no. DE-AC02-05CH11231. A portion of the work was supported by NSF cooperative agreement DMR-1539916.
9:48AM E03.00010: “Glide-resolved selection rules for scanning-tunneling microscopy; application to Black Phosphorus and Zirconium(III) Chloride” JUNG PYO HONG (Presenter), BENJAMIN WIEDER, ZHIJUN WANG, Physics, Princeton University, MICHAEL ZALETEL, Physics, University of California at Berkeley, ANDREI B BERNEVIG, Physics, Princeton University — Recently Queiroz et al. predicted that the Bloch bands of nonsymmorphic crystals can exhibit novel selection rules in their quasiparticle interference (QPI) pattern, characterized by a quasi-Brillouin Zone (BZ) periodicity of extinction patterns in the momentum transfer channel. Here, we focus on glide reflection symmetry—i.e. the combined operation of mirror reflection and in-plane half-integer lattice translation—to quantitatively realize ‘glide-resolved QPI (gQPI) selection rules’ on 2D minimal tight-binding models respecting the symmetries of layer group pma2 (LG 24), considering the limits of both strong and negligible spin-orbit coupling (SOC). We numerically compute the lattice- and energy-resolved local density of states (LDOS) in the presence of a local impurity and demonstrate the existence of quasi-BZ periodicity in the momentum-space LDOS. We propose Zirconium(III) Chloride and Black Phosphorus, whose monolayers respect pma2, as material candidates for the observation of gQPI in the presence and absence of SOC, respectively. By utilizing Topological Quantum Chemistry and density functional theory to construct tight-binding models, we find numerical evidence for gQPI in these materials, which can potentially be detectable through scanning-tunneling microscopy (STM).

10:00AM E03.00011: Purely Rotational Symmetry-Protected Topological Crystalline Insulator α-Bi₄Br₄ CHUANG-HAN HSU (Presenter), Department of Physics, National University of Singapore, TAY-RONG CHANG, XIAOTING ZHOU, Department of Physics, National Cheng Kung University, QIONG MA, NUH GEDIK, Department of Physics, Massachusetts Institute of Technology, ARUN BANSIL, Department of Physics, Northeastern University, VITOR PEREIRA, Department of Physics, National University of Singapore, LIANG FU, SUYANG XU, Department of Physics, Massachusetts Institute of Technology, HSIN LIN, Institute of Physics, Academia Sinica — Recent theoretical advances have proposed a new class of topological crystalline insulator (TCI) phases protected by rotational symmetries. Distinct from topological insulators (TIs), rotational symmetry-protected TCIs are expected to show unique topologically protected boundary modes: First, the surface normal to the rotational axis features "unpinned" Dirac surface states whose Dirac points are located at generic \( k \) points. Second, due to the "higher-order" bulk boundary correspondence, a 3D TCI also supports 1D helical edge states. Despite the unique topological electronic properties, to date, purely rotational symmetry-protected TCIs remain elusive in real materials. Using first-principles band calculations and theoretical modeling, we identify the van der Waals material α-Bi₄Br₄ as a TCI purely protected by rotation symmetry. We show that the α-Bi₄Br₄'s (010) surface exhibits a pair of unpinned topological Dirac fermions protected by the two-fold rotational axis. These unpinned Dirac fermions show an exotic spin texture highly favorable for spin transport and a band structure consisting of van Hove singularities due to Lifshitz transition.

10:12AM E03.00012: Modeling Image Potential States on Topological Semimetal Antimony Surface* HAIMEI ZHANG (Presenter), Wellesley College, JIANFENG GE, YANG HE, Harvard University, YAU CHUEN YAM, University of British Columbia, PENGCHENG CHEN, Princeton University, JENNIFER HOFFMAN, Harvard University — Topological materials host protected surface states with locked spin and momentum degrees of freedom that are predicted to give rise to exotic excitations such as Majorana fermions and magnetic monopoles. The topological semimetal antimony (Sb) offers a pristine platform in which to search for these excitations. Here we present scanning tunneling spectroscopy (STS) studies of Sb at high energy where quantized image potential states form due to the binding between the tunneling electron and the polarized surface. We fit the energies of these quantized states using a one-dimensional model based on the image potential on metal surfaces, the electric field applied between tip and sample, and the work functions of both tip and sample materials. The model fits well with the experimental data as a function of tip-sample voltage and distance. The study of these image potential states allows exploration of the image charge geometry necessary to realize a magnetic monopole.

*Experiments were supported by National Science Foundation DMR-1410480, and data analysis was supported by the Science and Technology Center for Integrated Quantum Materials under NSF DMR-1231319.
10:24AM E03.00013: pnictide square net materials with reduced symmetry, the rare earth diantimonides: electronic structure and topology  MATTEO MICHIARDI (Presenter), Quantum Matter Institute, University of British Columbia, FABIAN ARNOLD, Physics and Astronomy, Aarhus University, ELIA RAZZOLI, Quantum Matter Institute, University of British Columbia, KARL F. FISHER, Department of chemistry, Aarhus University, VAITHHEESWARAN GANAPATHY, Andvanced Center for Research in high energy materials, Hyderabad University, GIORGIO LEVY, FABIO BOSCHINI, ILYA ELFIMOV, Quantum Matter Institute, University of British Columbia, BO B IVERSEN, Department of chemistry, Aarhus University, PHILIP HOFMANN, Physics and Astronomy, Aarhus University, ANDREA DAMASCELLI, Quantum Matter Institute, University of British Columbia — With the discovery of Dirac fermions, much research effort has been put into finding the structural elements that can generate Dirac-like degeneracies in the electronic band structures [1]. It was discovered that some layered materials can host planar square nets of group IV-V elements within their lattice. Analogously to graphene, these square nets possess a 2-atom basis and feature wide Dirac bands. Most of the known layered compounds that retain the electronic properties of the net, such as (Sr,Ca)MnBi2 and ZrSiS, crystallize in a tetragonal structure, and exhibit a Dirac semimetal or nodal line phase that can host a rich plethora of electronic and magnetic quantum properties [2]. In this talk we will show a new variety of square net semimetals whose structure breaks the 4-fold symmetry, the rare earth di-antimonides. These materials crystallize in the orthorhombic group Cmca reducing the overall symmetry of the system. We employed ARPES and DFT calculations on the series precursor, LaSb2, to study its electronic structure. We will discuss the effect that the symmetry reduction has on the electronic properties, on the Dirac states, as well as its interplay with spin-orbit coupling.


10:36AM E03.00014: de Haas-van Alphen effect of correlated Dirac states in kagome metal Fe3Sn2*  LINDA YE (Presenter), Massachusetts Institute of Technology, MUN KEAT CHAN, ROSS MCDONALD, National High Magnetic Field Laboratory, LANL, DAVID E GRAF, National High Magnetic Field Laboratory, Florida State University, MIN GU KANG, Massachusetts Institute of Technology, JUNWEI LIU, Hong Kong University of Science and Technology, TAKEHITO SUZUKI, RICCARDO COMIN, LIANG FU, JOSEPH CHECKELSKY, Massachusetts Institute of Technology — We report the study of the de Haas-van Alphen effect in the ferromagnetic kagome metal Fe3Sn2, where massive Dirac electronic states have been identified by spectroscopic means [1,2]. Through magneto-quantum oscillations we observe two quasi-2D Fermi surfaces that are consistent with the quasi-2D double Dirac cone structures. Moreover, these Fermi surfaces appear to change following the rotation of the soft ferromagnetic moment, implying a strong coupling of the Dirac states with the ferromagnetic order through spin-orbit coupling. Finally, these observations establish the bulk nature of the Dirac bands and offer unique insight into lattice-borne topological electronic states. These results are summarized in arxiv/1809.11159 [3].

[3] L. Ye et al., arxiv/1809.11159

*We acknowledge support by support by the STC Center for Integrated Quantum Materials, NSF grant number DMR-1231319 and the Tsinghua Education Foundation. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation Cooperative Agreement No.DMR-1157490 and DMR-1644779, the State of Florida and the U.S. Department of Energy.

10:48AM E03.00015: Topological insulator materials for advanced nonlinear in-chip plasmonic devices  YINXIAO XIANG (Presenter), CHENHUI YAN, LIAN LI, CHENG CEN, Physics and Astronomy, West Virginia University — Topological insulator (TIs) has fascinating nonlinear optical properties that are inaccessible in classical materials. We report extraordinarily large third harmonic generation (THG) signal from telecom wavelength incidences in Bi2Se3 and Sb2Te3 grown by molecular beam epitaxy (MBE). Nonlinear optical measurements performed in samples with different thicknesses and stoichiometries are combined with angle-resolved photoemission spectroscopy (ARPES) characterizations to elucidate the nature of the giant THG signals. Moreover, by integrating with nanoscaled plasmonic devices on top of TIs, the strong plasmonic field enhancement further enables us to produce controllable nonlinear optical functionalities with very low input energy threshold. Our findings demonstrate a great potential for a new class of topological materials based on-chip nonlinear photonic devices.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM
Session E04 DMP: Dirac/Weyl Semimetals -- Materials Prediction I  BCEC 107C - Arun Bansil - Tag(s): Focus
8:00AM E04.00001: Weyl Points Enabled by Three-dimensional Flat Band*  YINONG ZHOU (Presenter), KYUNG-HWAN JIN, HUAQING HUANG, Department of Materials Science and Engineering, University of Utah, ZHENGFEI WANG, University of Science and Technology of China, FENG LIU, Department of Materials Science and Engineering, University of Utah — Topological flat band (FB) has attracted much interest because it exhibits a range of exotic quantum phases. Here, we discover yet another novel physical manifestation arising from three-dimensional (3D) FB but absent for 2D FB. We show that in the presence of spin-orbit coupling, magnetization of 3D FBs induces a transition from a 3D topological insulator (TI) into a Weyl semimetal, while for a 2D FB a transition from a 2D TI into a Chern insulator is known previously. The Weyl semimetal so formed may contain only a minimum of two Weyl points. The formation of Weyl points by symmetry breaking of highly degenerate 3D FBs is distinctively different from the conventional mechanism by symmetry breaking of a Dirac point. We demonstrate this unusual 3D-FB-enabled Weyl state first in a pyrochlore lattice model using tight-binding method and then in a real material Sn2Nb2O7 using first-principles calculations. The main features of the resulting Weyl points are analyzed with respect to symmetry, topological invariant and surface state. The Weyl fermions associated with FB may open new frontiers in the research of topological physics and materials.

*DOE-BES (Grant No. DE-FG02-04ER46148). CHPC. DOE-NERSC.

8:12AM E04.00002: Probing Hydrodynamic Materials from First Principles*  JENNIFER COULTER (Presenter), PRINEHA NARANG, Harvard University — In the hydrodynamic regime of transport, momentum-conserving scattering dominates momentum-relaxing processes such as Umklapp, defect, and boundary scattering so that momentum is quasi-conserved and electron flow obeys the formalism of hydrodynamics. In light of recent experimental evidence of hydrodynamic transport in PdCoO2, WP2, and PtSn4, understanding the specifics of microscopic scattering processes in these materials is of fundamental interest. In order to provide a more comprehensive perspective of experimentally observed hydrodynamic phenomena, we use first-principles methods including calculations of electron-phonon coupling to evaluate a number of different scattering lifetimes, the electrical and thermal conductivities, and optical properties of these materials. Through our ab initio framework, we aim to to probe the microscopic properties of the recently experimentally observed hydrodynamic solids and study the interplay between topological physics and ultrafast dynamics in these materials.

*JC acknowledges the DOE Computational Science Graduate Fellowship (CSGF) (DE-FG02-97ER25308) and that this work was supported by the DOE Photonics at Thermodynamic Limits Energy Frontier Research Center (EFRC) under grant #DE-SC0019140.

8:24AM E04.00003: Catalogue of Topological Electronic Materials  TIANTIAN ZHANG (Presenter), YI JIANG, ZHIDA SONG, Institute of physics, Chinese Academy of Sciences, HE HUANG, YUQING HE, Computer Network Information Center, Chinese Academy of Sciences, ZHONG FANG, HONGMING WENG, CHEN FANG, Institute of physics, Chinese Academy of Sciences — Topological electronic materials are new quantum states of matter hosting novel linear responses in the bulk and anomalous gapless states at the boundary, and are for scientific and applied reasons under intensive research in physics and in materials sciences. Here we introduce an effective, efficient and fully automated algorithm in obtaining the topological invariants for all non-magnetic materials that are known to human, based on recently developed principles that allow for exhaustive mappings between the symmetry representation of occupied bands and the topological invariants. Equipped with this method we have scanned through a total of 39519 materials available in structural databases, and found that as many as 8056 of them are actually topological (8889 if spin-orbital coupling is neglected). These are further catalogued into classes of 5005 topological semimetals, 1814 topological insulators and 1237 topological crystalline insulators, most of which are new to human knowledge. All the results are available and searchable at http://materiae.iphy.ac.cn/; and for each topological material, we have plotted the band structure as well as the local density of states, shown on the same website.

8:36AM E04.00004: Topological crossings in magnetic space groups  DARSHAN G. JOSHI (Presenter), Max-Planck-Institute for Solid State Research, Stuttgart, Germany, YANG-HA0 CHAN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan, ANDREAS P SCHNYDER, Max-Planck-Institute for Solid State Research, Stuttgart, Germany — Non-symmorphic symmetry is known to enforce topological crossings in crystals. Using the elementary band irreducible representations non-trivial crossings in the form of hour-glass or accordian spectrum have been discovered in certain space groups. Here we extend such an analysis to a wider domain of magnetic space groups (MSGs). We show that the magnetic co-representations (coreps), which are derived from the non-magnetic irreducible representations, can be used to detect non-symmetric symmetry enforced topological crossings in MSGs. We demonstrate this with two examples, where we find magnetic Weyl points and hour-glass dispersions. DFT band-structure calculation of corresponding magnetic materials confirms our findings. Furthermore, we compute the surface states and discuss other experimental consequences of the hourglass dispersion in magnetic materials.
8:48AM E04.00005: Chemical Principles of Topological Semimetals* [Invited] LESLIE SCHOOP (Presenter), Chemistry, Princeton University — Chemical principles can be a powerful tool for predicting, understanding and synthesizing new topological materials. In this talk I will introduce these concepts. A common practice in solid state chemistry is to connect structural motifs with properties. In this spirit, I will focus on a common structural motif, a square-net arrangement of atoms. I will explain how simple chemical rules, for example electron counting or geometrical considerations, such as atomic distances, can be used for identifying topological semimetals in such compounds. By connecting the crystal structure to the electronic properties, we can define a tolerance factor, solely based on atomic distances, which separates square-net-based nodal line semimetals from other trivial compounds. The talk is largely based on these two references [1,2].


*This research was partially supported by NSF through the Princeton Center for Complex Materials, a Materials Research Science and Engineering Center DMR-1420541, and by a MURI grant on Topological Insulators from the Army Research Office, grant number ARO W911NF-12-1-0461.

9:24AM E04.00006: Comparative first-principles study of a prototypical Dirac semimetal by GGA and SCAN meta-GGA energy functionals WEI-CHI CHIU (Presenter), Department of Physics, Northeastern University, BAHADUR SINGH, SZU-NUS Collaborative Center and International Collaborative Laboratory of 2D Materials for Optoelectronic Science \& Technology, Engineering Technology Research Center for 2, JOHANNES NOKELAINEN, Department of Physics, Lappeenranta University of Technology, CHENLIANG SU, SZU-NUS Collaborative Center and International Collaborative Laboratory of 2D Materials for Optoelectronic Science \& Technology, Engineering Technology Research Center for 2, HSIN LIN, Institute of Physics, Academia Sinica, BERNARDO BARBIELLINI, Department of Physics, School of Engineering Science, Lappeenranta University of Technology, ARUN BANSIL, Department of Physics, Northeastern University — Density functional theory is widely used to study topological properties of materials, limitations of the underlying exchange-correlation functionals notwithstanding. In this connection, the recently constructed strongly-constrained-and-appropriately-normed (SCAN) meta-GGA exchange-correlation functional has shown significant improvements in many classes of materials. Here we discuss SCAN-based electronic properties of the prototypical Dirac semimetal Na\(_3\)Bi and compare our results with those based on the commonly used generalized gradient approximation (GGA). In particular, SCAN yields a spin-orbit coupling driven topological phase transition from the normal insulator to Dirac semimetal state in contrast with the GGA results. SCAN produces Dirac-node locations, Fermi velocities and s-band shift around the \(\Gamma\) point that are in better accord than the GGA predictions with the corresponding experimental results.

9:36AM E04.00007: A Monopole Mining Method for High Throughput Screening Weyl Semimetals VSEVOLOD IVANOV (Presenter), SERGEY SAVRASOV, University of California, Davis — Although topological invariants have been introduced to classify the appearance of protected electronic states at surfaces of insulators, there are no corresponding indexes for Weyl semimetals whose nodal points may appear randomly in the bulk Brillouin Zone (BZ). Here we use a well–known result that every Weyl point acts as a Dirac monopole and generates integer Berry flux to search for the monopoles on rectangular BZ grids that are commonly employed in self–consistent electronic structure calculations. The method resembles data mining technology of computer science and is demonstrated on locating the Weyl points in known Weyl semimetals. It is subsequently used in high throughput screening several hundreds of compounds and predicting a dozen new materials hosting nodal Weyl points and/or lines.
Chiral crystals are materials whose lattice structure with a well-defined handedness due to the lack of inversion, mirror, or other roto-inversion symmetries, which represent a broad, important class of quantum materials. Yet, the topological properties of chiral crystals have still remained largely uncharacterized. Here, we show that Kramers-Weyl fermions are a universal topological electronic property of chiral crystals with spin-orbit coupling (SOC). Unlike conventional Weyl fermions, they appear at time-reversal-invariant momenta. By combining our analysis with the results of previous works, we further determine that all point-like nodal degeneracies in nonmagnetic chiral crystals with relevant SOC carry nontrivial Chern numbers. Using this theory, we identify representative chiral materials in 33 of the 65 chiral space groups in which topological chiral fermions are relevant to low-energy physics. Among all the materials, RhSi family exhibit the ideal topological band structures with longest Fermi arcs and nontrivial energy windows.

[1] Nat. Mater. 17, 978–985

Work at Princeton was supported by the US DOE under Basic Energy Sciences (grant no. DOE/BES DE-FG-02-05ER46200) and the Gordon and Betty Moore Foundation (GBMF4547/Hasan).

Fermi arcs in topological chiral crystals

The telltale trademarks of a Weyl semimetal are the topologically protected Fermi arc surface states. While these surface states have been demonstrated in conventional Weyl semimetals (for instance, the TaAs family), they should also be present in the recently proposed unconventional Weyl semimetals. However, there is still a lack of candidate materials for experimental exploration. In this talk, we comment on a number of chiral crystals in space group No. 198, as platforms for expanding the list of Fermi arc materials. Notably, RhSi, CoSi, CoGe, RhGe, AlPd, AlPt, BaPtP, and BaPtAs constitute promising candidate materials. Indeed, these compounds should exhibit the longest possible Fermi arcs, spanning across the entire surface Brillouin zone. These predictions are closely tied to the maximally separated 4-fold and 6-fold unconventional chiral fermions that have recently been predicted in this class of compounds. We further comment on experimental progress and the current challenges in using ARPES to observe a chiral Weyl semimetal phase with Fermi arcs in these materials.

Work at Princeton was supported by the US DOE under Basic Energy Sciences programme (grant number DOE/BES DE-FG-02-05ER46200) and the Gordon and Betty Moore Foundation (GBMF4547/Hasan).

Pr$_2$Ir$_2$O$_7$: when Luttinger semimetal meets Melko-Hertog-Gingras spin ice state

In quantum materials with multiple flavors of degrees of freedom (DOF), the interplay between them leads to intriguing phenomena and allows the mutual control. Here we study band topology and engineering from the interplay between local moments and itinerant electrons in pyrochlore iridates. For metallic Pr$_2$Ir$_2$O$_7$, the Ir 5d conduction electrons interact with the Pr 4f local moments via the f-d exchange. While the Ir electrons form a Luttinger semimetal, the Pr moments can be tuned into an ordered spin ice with a finite ordering wavevector, dubbed Melko-Hertog-Gingras (MHG) state, by varying Ir and O contents. We point out that the Pr Ising order generates an internal field that reconstructs the Ir bands. Besides the broad existence of Weyl nodes, we predict that the magnetic translation of the Pr MHG state protects the Dirac band touching at certain time reversal invariant momenta for the Ir bands. We propose the magnetic fields to control the Pr magnetism and indirectly influence the Ir electrons. Our prediction can be immediately tested in ordered Pr$_2$Ir$_2$O$_7$ samples. Our theory constitutes a nontrivial and realistic example for the interplay between itinerant electrons and local moment in three dimensions, and shed lights on hybrid quantum materials with multiple flavors of DOF.
Optically-Controlled Orbitronics on a Triangular Lattice

VO TIEN PHONG (Presenter), ZACHARIAH ADDISON, University of Pennsylvania, SEONGJIN AHN, HONGKI MIN, Physics and Astronomy, Seoul National University, RITESH AGARWAL, EUGENE JOHN MELE, University of Pennsylvania

Orbital polarization of a Bloch state in a crystal can endow a band structure with nontrivial geometry and manifest itself in unique responses to applied fields. We study this for an on-site orbital multiplet on a 2D primitive triangular lattice where orbital degeneracies are lifted by propagation on a Bravais lattice. The model contains fully orbitally-derived band structure degeneracies including a line-node required by the perpendicular mirror symmetry and two types of point degeneracies protected by PT symmetry.

Crucially, and in contrast to the well-studied analogous problem on the honeycomb lattice, here point degeneracies with opposite winding numbers are generically offset in energy which enables the activation of anomalous transport responses using readily-implemented spatially-uniform local potentials. We demonstrate this by calculation of an anomalous charge Hall effect activated by coherently coupling to a circularly polarized optical field and an orbital Hall effect describing an orbital angular momentum current directed perpendicular to an applied in plane electric field.

Chiral Vortical and Gyrotropic Effects in Weyl Semimetals

ZHAO HUANG (Presenter), PAVAN HOSUR, University of Houston

The chiral anomaly is the source of various interesting phenomena for chiral fermions, and especially in Weyl semimetals which contain chiral fermions as low energy excitations. For example, a magnetic field leads to a longitudinal current flow in the absence of electric fields, well known as the chiral magnetic effect. Since the Coriolis force behaves like a Lorentz force in many ways, one expects an axial current induced by rotation for chiral fermions. This is known as the chiral vortical effect. This effect has attracted a lot of attention in nuclear physics for its possible consequences for heavy ion collisions [1]. In this work, we theoretically explore the possibility of the chiral vortical effect in Weyl semimetals. In particular, we argue that naively rotating a Weyl semimetal is not the correct way to induce the chiral vortical effect. Instead, one must rotate the chiral fluid of electrons relative to the background lattice. The latter can be achieved via an electric field with a non-zero curl, and is otherwise known as the gyrotropic effect.

Reference:

Prediction of Weyl semimetal, AFM topological insulator, nodal line semimetal, and Chern insulator phases in Bi$_2$MnSe$_4$

SUGATA CHOWDHURY (Presenter), KEVIN GARRITY, FRANCESCA TAVAZZA, Materials Measurement Laboratory, National Institute of Standards and Technology

Three dimensional materials with strong spin-orbit coupling and magnetic interactions represent an opportunity to realize a variety of rare and potentially useful topological phases. In this work, we use first principles calculations to show that the recently synthesized material Bi$_2$MnSe$_4$ displays a combination of band inversion and magnetic interactions, leading to several topological phases. In bulk form, the ferromagnetic phase of Bi$_2$MnSe$_4$ is either a nodal line or Weyl semimetal, depending on the direction of the spins. When the spins are arranged in a layered antiferromagnetic configuration, the combination of time reversal plus a partial translation is a new symmetry, and the material instead becomes an antiferromagnetic topological insulator. However, the intrinsic TRS breaking at the surface of Bi$_2$MnSe$_4$ removes the typical Dirac cone feature, allowing the observation of the half-integer quantum anomalous Hall effect (AHC). Furthermore, we show that in thin film form, for some thicknesses, Bi$_2$MnSe$_4$ becomes a Chern insulator with a band gap of up to 58 meV. This combination of properties in a stoichiometric magnetic material makes Bi$_2$MnSe$_4$ an excellent candidate for displaying robust topological behavior.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E05 DMP: Topological Superconductivity: TMD, Quantum Wells

BCEC 108 - Vidya Madhavan, Univ of Illinois - Urbana - Tag(s): Focus
Quantum spin Hall state in monolayer 1T'-TMDCs*  

SHUJIE TANG (Presenter), SIMES, Stanford University — Quantum spin Hall (QSH) insulator, also known as 2D topological insulator (TI), hosts quantized helical edge state, which is a superior candidate to construct artificial 1D superconductor utilizing the superconductivity proximity effect. Among the rapidly developing 2D TI family, group VI transition metal dichalcogenides (TMDCs) in 1T' structural phases are unique in their van der Waals layered structure, which can be easily integrated into vertical heterostructures. Bottom-up synthesis of monolayer 1T'-TMDCs (WTe2, WSe2 and MoTe2) on graphitized SiC substrate were achieved using molecular beam epitaxy. Together with theoretical calculation and ARPES measurement, the characteristic signatures of QSH states such as band inversion and bulk gap opening have been confirmed in 1T'-WTe2 and WSe2 [1, 2]. Scanning tunneling spectroscopy (STS) measurements further provide evidence for the robust edge states reside in the bulk gap. It is also found that, although conduction and valence band degeneracy is lifted in 1T'-MoTe2, the spin-orbital coupling is not strong enough to further separate them, leaving 1T'-MoTe2 a semimetal [3].


*United States Department of Energy (DOE)
9:00AM E05.00004: Observation of Superconductivity in Few-layers WTe₂ Induced by Normal Contacts**

ARTEM KONONOV (Presenter), GULIBUSITAN ABULIZI, ANDREAS BAUMGARTNER, Department of Physics, University of Basel, KEJIAN QU, JIAQIANG YAN, DAVID GEORGE MANDRUS, Materials Science and Engineering, The University of Tennessee, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, CHRISTIAN SCHONENBERGER, Department of Physics, University of Basel — WTe₂ is a material possessing topological properties both as a bulk crystal and single layer. In the former case, it is a type-II Weyl semimetal and in the latter a quantum spin Hall state. Recent reports showing the possibility to induce superconductivity in WTe₂ by proximity to a bulk superconductor or by electrostatic gating make it a promising platform for topological superconductivity and quantum computation. Here we report on a novel mechanism of inducing superconductivity within few-layers of WTe₂ by normal metal contacts. In transport measurements we find that the induced superconductivity is highly anisotropic in magnetic field and survives up to 7 Tesla in in-plane field. Superconducting transport persists over μm distances at temperatures up to 1 Kelvin. Our results could provide insight to the superconducting state in WTe₂ and its topological nature.

**Supported by the Georg H. Endress foundation and the European Research Council project Top-Supra (787414)

9:12AM E05.00005: Proximity-induced superconductivity with sub-gap anomaly in type-II Weyl semimetal WTe₂

QIAO LI (Presenter), School of Physics, Nanjing University — Tungsten ditelluride (WTe₂) is one of the material candidates in the family of type-II Weyl semimetals, exhibiting many exotic properties, such as anisotropic chiral anomaly. Due to the intrinsic topological band structure and tilted Weyl cone in WTe₂, it has been predicted that unconventional superconducting properties will emerge when WTe₂ enters to superconducting phase. In this work, we report the observation of superconductivity in the type-II Weyl semimetal WTe₂ based on WTe₂/NbSe₂ heterostructure induced by proximity effect. We find a long coherence length along c axis of WTe₂. Furthermore, we observe anomalous oscillations of the differential resistance spectrum during the transition from superconducting to normal state. Theoretical calculations indicate that the stage change in the differential resistance spectrum can be associated with anomalous density of states in superconducting state and reveals that such a sub-gap anomaly is the intrinsic property of WTe₂ in superconducting state induced by the proximity effect. Our findings can enrich the understanding of superconductivity mechanism in type-II Weyl semimetal and pave the way for their future applications in topological quantum computing.

9:24AM E05.00006: Quantum transport in MoTe₂ and WTe₂ topological monolayers

XIRUI WANG (Presenter), KENJI YASUDA, YAFANG YANG, SANFENG WU, TAKEHITO SUZUKI, LIN ZHOU, JING KONG, JOSEPH CHECKELSKY, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — There has been growing interest in the study of 2D topological quantum states. Recent experiments established monolayer WTe₂ as a 2D topological insulator, which also becomes a superconductor via gating. This has triggered a lot of excitement in studying a wide range of topological properties of monolayer WTe₂ and its cousins, such as MoTe₂. We will report our investigations on the quantum transport behavior of monolayer WTe₂ and MoTe₂ in nano-fabricated devices, in the direction of searching for topological superconductivity.

9:36AM E05.00007: Procedural Determination of Novel Stoichiometric Topological Superconductors through Surface and Pressure Effects

ABHISHEK ALLAMSETTY (Presenter), Thomas Jefferson High School for Science and Technology — Topological superconductors have attracted great interest as a groundbreaking platform to allow for fault-tolerant quantum computing and overcome the limitations of classical processors defined by Moore’s law. In this paper, we discover eight novel topological superconductors, ABX₂ (A=Bi, In; B=Nb, Ta; X=Se, S) and propose a new systematic method to realize topological superconductors by combining of transition metal dichalcogenides with spin-orbit post-transitional elements. These eight compounds are bulk superconductors with intrinsic topological surface states and can be realized without any tampering, a coveted quality for topological superconductors. Utilizing density functional theoretical calculations, we determined topological surface states and bulk superconductivity from the electronic band structures of our compounds. In addition, we demonstrated the robust nature of our materials under high-pressure conditions, as their non-trivial topology and superconductivity were maintained. Our eight novel compounds hold great promise towards the practical realization of fault-tolerant quantum computers through their ability to eliminate the longstanding problem of quantum decoherence within quantum computational systems.
9:48AM E05.00008: Enhancing Superconductivity in Indium Arsenide Quantum Well Heterostructures* ANDREW SAYDJARI (Presenter), MICHAEL KOSOWSKY, ANDREW T PIERCE, Physics, Harvard University, JOSEPH YUAN, KAUSHINI WICKRAMASINGHE, Physics, New York University, JAVAD SHABANI, AMIR YACOBY, Physics, Harvard University — Hybrid superconductor-semiconductor heterostructures containing indium arsenide quantum wells combine strong spin-orbit effects, s-wave superconductivity, and arbitrary lithographic confinement. This platform facilitates both study of induced superconductivity in the quantum well and topological states in quasi-one-dimensional systems. While epitaxial aluminum provides transparent contact to the quantum well, aluminum cannot sustain large magnetic fields (>1 T) required to explore many topological effects. Further, the small (150 µeV) superconducting gap of aluminum can complicate detection and inhibit manipulation of states required for applications to topological quantum computing. In this work, we present a method of coupling niobium-based superconductors to indium arsenide quantum wells to supplement the critical magnetic field and superconducting gap in this platform. Experimental progress on fabrication of superconductor-semiconductor-superconductor (SNS) junctions and quantum point contacts will be presented.

*This work was supported by the Center for Integrated Quantum Materials (DMR-1231319) and National Science Foundation (DMR-1708688 and DMR-1836687).

10:00AM E05.00009: Multi-terminal Josephson effect in epitaxial InAs/Al superconductor/semiconductor devices I: current-biased measurements HANHO LEE (Presenter), NATALIA PANKRATOVA, ROMAN KUZMIN, KAUSHINI WICKRAMASINGHE, University of Maryland, College Park, ALEX LEVCHENKO, MAXIM VAVILOV, University of Wisconsin-Madison, JAVAD SHABANI, New York University, VLADIMIR MANUCHARYAN, University of Maryland, College Park — Junctions of more than two topological superconductors are typically required for implementing braiding operations on Majorana fermions [1]. Here we report the first realization of 3- and 4-terminal Josephson junctions fabricated from a Majorana-compatible hybrid InAs/Al epitaxially-grown heterostructure [2]. We observed several novel phenomena: interaction of intersecting supercurrents, multi-terminal Fraunhofer effect in a magnetic field, and out-of-equilibrium multiple Andreev reflections (MAR) at bias voltages far exceeding the gap of Al. The data in a large number of channels regime can be modeled using random matrix circuit theory of superconducting transport. Progress towards realizing the phase-control of zero-energy quasiparticle states, predicted in such structures in the absence of Zeeman fields [3,4,5], will be discussed.


10:12AM E05.00010: Multi-terminal Josephson effect in epitaxial InAs/Al superconductor/semiconductor devices II: phase-biased measurements NATALIA PANKRATOVA (Presenter), HANHO LEE, ROMAN KUZMIN, KAUSHINI WICKRAMASINGHE, University of Maryland, College Park, ALEX LEVCHENKO, MAXIM VAVILOV, University of Wisconsin-Madison, JAVAD SHABANI, New York University, VLADIMIR MANUCHARYAN, University of Maryland, College Park — Junctions of more than two topological superconductors are typically required for implementing braiding operations on Majorana fermions [1]. Here we report the first realization of 3- and 4-terminal Josephson junctions fabricated from a Majorana-compatible hybrid InAs/Al epitaxially-grown heterostructure [2]. We observed several novel phenomena: interaction of intersecting supercurrents, multi-terminal Fraunhofer effect in a magnetic field, and out-of-equilibrium multiple Andreev reflections (MAR) at bias voltages far exceeding the gap of Al. The data in a large number of channels regime can be modeled using random matrix circuit theory of superconducting transport. Progress towards realizing the phase-control of zero-energy quasiparticle states, predicted in such structures in the absence of Zeeman fields [3,4,5], will be discussed.

10:24AM E05.00011: Probing Spin-Orbit Coupling in InAs/Al SQUIDs* WILLIAM ANDREW MAYER (Presenter), SICHAO YU, Physics, New York University, KAUSHINI WICKRAMASINGHE, Physics, University of Maryland, College Park, JOSEPH YUAN, Physics, New York University, NARAYAN MOHANTA, ALEX MATOS ABIAGUE, Physics, Wayne State University, IGOR ZUTIC, Physics, University at Buffalo, The State University of New York, JAVAD SHABANI, Physics, New York University — InAs/Al epitaxial heterostructures allow for transparent semiconductor/superconductor interfaces to study superconducting proximity effect, particularly in Josephson junctions. A superconducting quantum interference device (SQUID) constructed from such junctions opens the possibility of studying current-phase relations in these materials systems. One distinct property of this system is the gate-tunability where each junction can be depleted, effectively turning off the current in that junction. This allows for detailed analysis of the supercurrent properties not previously possible in a single device. The second important feature of this system is the presence of spin-orbit coupling in InAs, whose strength is gate-tunable. We study the SQUID signal as we tune the spin-orbit coupling in each arm using independent gate voltages. The comparison between experimental data and theoretical simulation suggests that spin-orbit coupling can be detected in SQUID signal. This direct probe of spin-orbit coupling in proximitized systems represents an important tool to study systems which potentially host Majorana fermions.

*We acknowledge support from DARPA TEE

10:36AM E05.00012: Induced superconductivity in InSb 2DEGs CHUNG-TING KE (Presenter), CHRISTIAN M. MÖHLE, FOLKERT DE VRIES, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands, CANDICE THOMAS, SARA METTI, CHARLES R GUINN, Department of Physics and Astronomy and Station Q Purdue, Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, USA, RAY KALLAHER, GEOFFREY C. GARDNER, Microsoft Quantum at Station Q Purdue, Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, USA, MICHAEL MANFRA, Department of Physics and Astronomy and Station Q Purdue, Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, USA, SRIJIT GOSWAMI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands — Superconductor-semiconductor hybrid systems are promising candidates to create Majorana zero modes (MZMs). Using a semiconductor two-dimensional electron gas (2DEG) could allow one to create complex networks required for Majorana qubit schemes. In this regard, InSb 2DEGs stand out due to their large g-factor, strong spin-orbit coupling, and low disorder. We integrate such high-quality 2DEGs with NbTiN to create Josephson junctions (JJs), thus providing the first demonstration of induced superconductivity in InSb 2DEGs. Remarkably, the supercurrent persists over several microns and shows distinct signatures of ballistic transport. Applying an in-plane magnetic field produces a revival of the supercurrent due to a Zeeman induced 0-π transition, where the transition field scales linearly with the junction length. Moreover, we show that this transition can be tuned in-situ using gate voltages, which allows us to map out the free energy landscape of the JJ as a function of density and magnetic field. Our experiments are consistent with the expected behavior of 0-π transitions in ballistic JJs and are an important step toward creating robust MZMs in 2DEG-based π-junctions.

10:48AM E05.00013: Transport phenomena in epitaxial Al / InAs heterostructures with strong spin-orbit coupling in the presence of in-plane magnetic fields* MICHAEL KOSOWSKY (Presenter), ANDREW SAYDJARI, ANDREW T PIERCE, Physics, Harvard University, HECHEN REN, Physics, California Institute of Technology, KAUSHINI WICKRAMASINGHE, JOSEPH YUAN, JAVAD SHABANI, Physics, New York University, AMIR YACOBY, Physics, Harvard University — Two-dimensional electron gas (2DEG) systems with strong spin-orbit coupling (SOC) and induced s-wave superconductivity are predicted to realize topological superconductivity when in the presence of in-plane magnetic fields. A major obstacle in studying these systems arises due to the tendency of magnetic fields to suppress superconductivity. By growing epitaxial aluminum on top of an InAs quantum well heterostructure, it is possible to create a high-transparency interface between the superconductor and the 2DEG. This interface results in induced superconductivity that is comparable with the true aluminum superconducting gap, thereby sustaining larger in-plane fields than achieved by ex situ aluminum deposition. Here, we discuss the devices that we have fabricated to explore this exciting system, as well as present initial millikelvin measurements studying Josephson phenomena in the presence of varying in-plane and perpendicular magnetic fields.

*The device fabrication and measurements are supported by the NSF DMR-1708688 and by the STC Center for Integrated Quantum Materials under NSF DMR-1231319. The material growth was supported by NSF-DMR-1836687.

Tuesday, March 5, 2019 8:00 AM - 10:48 AM

Session E06 DCMP: Electronic States in Se Chalcogenides: Including Excitonic Behavior
BCEC 109A - Johnpierre Paglione, University of Maryland, College Park
8:00AM E06.00001: Response of FeSe to in-plane anisotropic strain* CLIFFORD HICKS (Presenter), JACK BARTLETT, ALEXANDER STEPPKE, Max Planck Institute for Chemical Physics of Solids, SUGURU HOSOI, Osaka University, TAKASADA SHIBAUCHI, Tokyo University, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids — By affixing thin single crystals of FeSe to rigid sample carriers and then applying uniaxial stress to the carrier, we apply in-plane uniaxial strains of up to ~0.7% to FeSe. Above the structural transition temperature $T_s$, anisotropic strain drives partial polarization of the nematic order, and a corresponding strong resistive anisotropy [1, 2]. However the resistive anisotropy saturates rapidly as strain is applied, and the resistivity then varies nonmonotonically for compressions above ~0.3%. Below $T_s$, the extrinsic contribution to the resistance from twin boundaries can be identified. The twin boundaries are weakly pinned and can be partially annealed, allowing the intrinsic elastoresistivity below $T_s$ to be resolved.


*Max Planck Society

8:12AM E06.00002: Nonequilibrium dynamics of local lattice distortions in FeSe TATIANA Konstantinova (Presenter), Lijun Wu, Milinda Abeykoon, Cedomir Petrovic, CMPMSD, Brookhaven National Laboratory, Xijie Wang, SLAC, Yimei Zhu, Aifeng Wang, CMPMSD, Brookhaven National Laboratory — The role of the lattice in unique properties of iron-based superconductors, such as electronic nematicity, is still unclear. This rises an interest in investigating the local structure modifications during the phase transitions in these materials. We report the study of the local crystal structure of FeSe and its connection to electronic nematicity using ultrafast electron diffraction, x-ray diffraction, and transmission electron microscopy. The study reveals the local distortions in form of iron dimers, ordered within nanometer-sized domains. The observed nonequilibrium lattice dynamics implies sensitivity of the lattice distortions to the nematic order parameter.

8:24AM E06.00003: Character of excitonic insulator phase in a transition metal dichalcogenide 1T-TiSe$_2$. JIN MO BOK (Presenter), HAN-YONG CHOI, Sungkyunkwan University — We revisit the question of the transition metal dichalcogenide 1T-TiSe$_2$ charge density wave (CDW) state being an excitonic insulator. The BCS-like CDW gap equation with statically screened Coulomb interaction was employed to calculate the transition temperature ($T_c$) as a function of the energy gap. Realistic dispersions for one hole band centered at $\Gamma$ and three electron bands at M points in two-dimensional periodic hexagonal lattice were considered to model the TiSe$_2$. The obtained $T_c$ (~240K) is comparable to measured one for monolayer (~232K), and $T_c$ suppression as a function of doping concentration and pressure are reproduced by controlling chemical potential and energy gap. We discuss possibility of the 1T-TiSe$_2$ CDW state originating from exciton condensation through the calculated $T_c$, ARPES intensity and density of states.

8:36AM E06.00004: Intrinsic Insulating Ground State in Transition Metal Dichalcogenide TiSe$_2$. DANIEL CAMPBELL (Presenter), CHRIS ECKBERG, PETER ZAVALIJ, JOHNPIERRE PAGLIONE, University of Maryland, College Park — TiSe$_2$ has received significant research attention over the past four decades, in large part due to the uniqueness of its charge-ordered state. Different techniques can suppress the charge density wave transition, vary low temperature resistivity by orders of magnitude, and stabilize magnetic or superconducting states. This talk will present the results of a new synthesis method whereby samples were grown in an argon gas environment at elevated pressures up to 180 bar. Above 100 K, properties (including those of the 200 K CDW) are unchanged from prior reports. However, a hysteretic resistance region beginning around 80 K, accompanied by insulating low temperature behavior, is distinct from anything previously observed. This new feature suggests that pressure growth may allow access to a nonmetallic ground state in a material long speculated to be an excitonic insulator.
Folded superstructure and degeneracy-enhanced band gap in the weak-coupling charge density wave system 2H–TaSe₂

YIWEI LI (Presenter), Department of Physics, University of Oxford, United Kingdom, JUAN JIANG, School of Engineering & Applied Science, Yale University, USA, HAIFENG YANG, School of Physical Science and Technology, ShanghaiTech University, People's Republic of China, DHARMALINGAM PRABHAKARAN, Department of Physics, University of Oxford, United Kingdom, ZHONGKAI LIU, School of Physical Science and Technology, ShanghaiTech University, People's Republic of China, LEXIAN YANG, Department of Physics and Collaborative Innovation Center of Quantum Matter, Tsinghua University, People's Republic of China, YULIN CHEN, Department of Physics, University of Oxford, United Kingdom — Using high-resolution angle-resolved photoemission spectroscopy (ARPES), we have mapped out the reconstructed electronic structure in the commensurate charge-density-wave (CDW) state of quasi-two-dimensional transition metal dichalcogenide 2H–TaSe₂. The observation of the fine structure near Brillouin zone (BZ) center supplements the picture of Fermi surface folding in the 3×3 CDW state. In addition to the anisotropic CDW band gaps that energetically stabilize the system at the Fermi level in the first-order lock-in transition, we found band reconstruction at high binding energy, which can be well explained by the hybridization between main bands (MBs) and folded bands (FBs). Furthermore, in contrast to the perfectly nested quasi-one-dimensional system, triple-nesting-vector-induced CDW FBs increase the degeneracy of the band crossing and thus further enlarge the magnitude of band gap at certain momentum-energy positions. The visualization and modeling of CDW gaps in momentum-energy space reconcile the long-lasting controversy on the gap magnitude and suggests a weak-coupling Peierls physics in this system.

Observation of anomalous electron relaxation in optically excited 1T-TaSe₂

YINGCHAO ZHANG (Presenter), XUN SHI, WENJING YOU, ZHENSHENG TAO, Department of Physics and JILA, University of Colorado, Boulder, KAI ROSSNAGEL, MICHAEL BAUER, Institute of Experimental and Applied Physics, Kiel University, HENRY C KAPTEYN, MARGARET MARY MURNANE, Department of Physics and JILA, University of Colorado, Boulder — Ultrafast light pulses can drive materials far from their equilibrium states and is a powerful approach for manipulating their states. In this work, we present a series of anomalous behaviors observed in the electron relaxation in the charge density wave (CDW) material 1T-TaSe₂. After exciting the material with a femtosecond laser pulse, we measure the temporal evolution of the band structure and electron temperature. We observe a band oscillation that is coherently coupled to the CDW amplitude mode. Meanwhile, the hot electron temperature relaxes anomalously fast, and very different from that predicted by the widely-used N-temperature model. Moreover, this anomaly shows a critical change at the laser fluence corresponding to the ultrafast phase transformation to a new long-lived metastable state. These results offer a rare opportunity for better understanding of the coherent electron-phonon coupling.

Spinon Fermi Surface in a Cluster Mott Insulator Model on a Triangular Lattice and Possible Application to 1T-TaS₂

WENYU HE (Presenter), XIAO YAN XU, Hong Kong University of Science and Technology, GANG CHEN, Department of Physics, Fudan University, KAM TUEN LAW, Hong Kong University of Science and Technology, PATRICK LEE, Department of Physics, Massachusetts Institute of Technology — 1T-TaS₂ is a cluster Mott insulator on the triangular lattice with 13 Ta atoms forming a star of David cluster as the unit cell. We derive a two-dimensional XXZ spin-1/2 model with a four-spin ring exchange term to describe the effective low energy physics of a monolayer 1T-TaS₂, where the effective spin-1/2 degrees of freedom arises from the Kramers degenerate spin-orbital states on each star of David. A large scale density matrix renormalization group simulation is further performed on this effective model and we find a gapless spin liquid phase with a spinon Fermi surface at a moderate to large strength region of the four-spin ring exchange term. All peaks in the static spin structure factor are found to be located on the“2kF” surface of a half-filled spinon on the triangular lattice. Experiments to detect the spinon Fermi surface phase in 1T-TaS₂ are discussed.
distortion associated with the formation of the EI state allows bidirectional electronic dynamics in quantum solid material. In this talk, we will present the electronic evidence of quenching the bandgap, TNS is believed to realize the pure excitonic insulator state, free from the complications of coexisting density-many-body gap, as well as a coherent amplitude-like response observed in optical pump-probe data. Due to its direct optical band gap $E_g = 160$ meV. At the same time, the gap gradually fills from the high-frequency side with significant spectral weight from above-gap states. This transfer of spectral weight can be interpreted as predominant incoherent hopping of charge carriers along the Ta-Ni chains in the orthorhombic phase and as evidence for near-zero-gap behavior at high temperature. A phonon centered at 4.71 meV in both the $a$- and $c$-axis response suggests that the monoclinic distortion associated with the formation of the EI state allows bidirectional $a$-plane activity of the $B_{1u}/B_{3u}$ modes.

9:36AM E06.00009: Terahertz spectroscopy of excitonic insulator candidate Ta$_2$NiSe$_5$  
ROBERT DAWSON (Presenter), TIMOFEI LARKIN, MARC HOEFFNER, TOMOHIRO TAKAYAMA, MASAKI YAMAMOTO, HIDENORI TAKAGI, BERNHARD KEIMER, ALEXANDER BORIS, Max Planck Institute for Solid State Research — An excitonic insulator (EI) is a correlated-electron state in which excitons condense into an insulating ground state in analogy with the condensation of Cooper pairs in a superconductor. A handful of EI candidates have been proposed, but to date experimental verification of such a state has not been conclusively found. Recent transport and specific heat measurements have placed Ta$_2$NiSe$_5$ as the leading EI candidate with $T_c = 326$ K. Here we present measurements of the terahertz and far-infrared optical conductivity of Ta$_2$NiSe$_5$, which show that at temperatures far below $T_c$ a thermally-activated Drude peak gradually develops inside the optical band gap $E_g^{op} = 160$ meV. At the same time, the gap gradually fills from the high-frequency side with significant spectral weight from above-gap states. This transfer of spectral weight can be interpreted as predominant incoherent hopping of charge carriers along the Ta-Ni chains in the orthorhombic phase and as evidence for near-zero-gap behavior at high temperature. A phonon centered at 4.71 meV in both the $a$- and $c$-axis response suggests that the monoclinic distortion associated with the formation of the EI state allows bidirectional $a$-plane activity of the $B_{1u}/B_{3u}$ modes.

9:48AM E06.00010: Cooperative Exciton-Phonon Bose-Einstein Condensation in an Excitonic Insulator*  
EDOARDO BOLDINI (Presenter), Department of Physics, Massachusetts Institute of Technology, YAO WANG, Department of Physics, Harvard University, ALFRED ZONG, CHANGMIN LEE, DEBANJAN CHOWDHURY, Department of Physics, Massachusetts Institute of Technology, YANGFAN LU, Department of Physics, University of Tokyo, TOMOHIRO TAKAYAMA, HIDENORI TAKAGI, Max Planck Institute for Solid State Research, EUGÈNE DEMLER, Department of Physics, Harvard University, NÜH GEDIK, Department of Physics, Massachusetts Institute of Technology — The excitonic insulator is an exotic phase of matter in which excitons spontaneously form and collectively undergo Bose-Einstein condensation. Recently, increasing evidence has shown that this ground state is stabilized in the layered transition metal chalcogenide Ta$_2$NiSe$_5$ (TNS). Distinctive signature of exciton condensation is the pronounced flattening of the valence band top with decreasing temperature, signaling the opening of an additional many-body gap, as well as a coherent amplitude-like response observed in optical pump-probe data. Due to its direct bandgap, TNS is believed to realize the pure excitonic insulator state, free from the complications of coexisting density-wave orders or strong coupling to other degrees of freedom. Here, we reveal that a cooperative exciton-phonon mechanism lies instead at the origin of the condensate in TNS. Specifically, we use time- and angle-resolved photoemission spectroscopy to show that the vibrational degrees of freedom play a crucial role in the photoinduced melting of the exciton Bose-Einstein condensate. Our results open new routes towards the selective manipulation of the excitonic insulating state via specific modes of the crystal lattice.

*US Department of Energy and Swiss National Science Foundation

10:00AM E06.00011: Time- and Angle-Resolved Photoemission Study on the Excitonic Insulator Candidate Ta2NiSe5  
WENTAO ZHANG (Presenter), School of Physics and Astronomy, Shanghai jiao Tong University — Ultra-high resolution laser-based time- and angle-resolved photoemission is a unique technique in probing the momentum resolved ultrafast electronic dynamics in quantum solid material. In this talk, we will present the electronic evidence of quenching the excitonic insulating state and a hidden semimetallic state upon excited by a strong infrared laser pulse in the excitonic insulator candidate Ta2NiSe5.
10:12AM E06.00012: Exciton Mott transition revisited*  
DANIELE GUERCI (Presenter), MASSIMO CAPONE, MICHELE FABRIZIO, International School for Advanced Studies — The dissociation of excitons into holes and electrons in photoexcited semiconductors, despite being one of the first recognized examples of a Mott transition, still defies a complete understanding, especially regarding the character of the transition, which is first order in some cases and second order in others. We tackle this issue by a recently proposed and very powerful variational technique, which extends the conventional Gutzwiller variational wavefunction and has been named ghost Gutzwiller wavefunction (g-GA). The results that we present [1] are in accordance with experiments and allow identifying the key parameter that controls the nature of the transition: the magnitude of the exciton binding energy.


*This work has been supported by the European Union under H2020 Framework Programs, ERC Advanced Grant No. 692670 “FIRSTORM”.

10:24AM E06.00013: A Description of Phases with Induced Hybridisation at Finite Temperatures*  
DENIS GOLOSOV  
(Presenter), Department of Physics and the Resnick Institute, Bar-Ilan University, Ramat-Gan 52900, Israel — In an extended Falicov-Kimball model, an excitonic insulator phase can be stabilised at zero temperature. With increasing temperature, the excitonic order parameter (interaction-induced hybridisation on-site, characterised by the absolute value and phase) eventually becomes disordered, which involves fluctuations of both its phase and (at higher T) its absolute value. In order to build an adequate mean field description, it is important to clarify the nature of degrees of freedom associated with the phase and absolute value of the induced hybridisation, and the corresponding phase space volume. We show that a possible description (including the phase space integration measure) is provided by the on-site density matrix parametrisation. In principle, this allows to describe both the lower-temperature regime where phase fluctuations destroy the long-range order, and the higher temperature crossover corresponding to a decrease of absolute value of the hybridisation relative to the fluctuations level. This picture is also expected to be relevant in other contexts, including the Kondo lattice model.

*This work was supported by the Israeli Absorption Ministry.

10:36AM E06.00014: Gutzwiller Molecular Dynamics Simulation using Second-Moment Approximation  
PEDROM ZADEH (Presenter), GIA-WEI CHERN, University of Virginia — Molecular dynamics (MD) simulations are crucial to modern computational physics, chemistry, and material science, especially when combined with potentials derived from density-functional theory. However, even in state of the art MD codes, the on-site Coulomb repulsion is only treated at the self-consistent Hartree-Fock level. This standard approximation may miss important effects due to electron correlations. The recently developed Gutzwiller molecular dynamics (GMD) method provides a feasible approach for realistic correlated materials [1]. The Gutzwiller variational method captures the essential physics of correlated electron systems, and is much faster than, for example, the dynamical-mean field theory approach. In its current implementation, however, the GMD method is limited to small system sizes mainly due to the heavy computational cost of solving the renormalized electron Hamiltonian at every time-step. Here we demonstrate significant improvement of the GMD efficiency using the second-moment approximation. Importantly, we show that this approximation still captures the main features of the correlation-induced metal-insulator transition.


Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E07 DCMP: Correlated Chains and Ladders  
BCEC 109B - Satya Kushwaha, Los Alamos National Laboratory
Here we explore the non-equilibrium steady-state of an XY spin chain in a transverse magnetic field coupled at its ends to magnetic thermal reservoirs. We generalize the phase diagram to non-equilibrium conditions obtained by applying a magnetization bias to the reservoirs.

Upon increasing the bias we observe a discontinuous jump of the magnetic order parameter that coincides with a divergent correlation length. While the first observation is a signature of a first-order transition, in equilibrium, the second arises only for continuous transitions. Thus, our findings show that out-of-equilibrium conditions allow for novel critical phenomena not possible at equilibrium. Moreover, for steady-states with a non-vanishing conductance, the entanglement entropy at the zero temperature was found to have logarithmic corrections that differ from the well-known equilibrium case.

*The authors acknowledge support by NSFC China, FCT Portugal, and National Key R&D Program of the MOST of China.

8:12AM E07.00002: Estimates of the Quantum Fisher Information in the $S = 1$ Anti-Ferromagnetic Heisenberg Spin Chain with Uniaxial Anisotropy* 

JAMES LAMBERT (Presenter), ERIK SORENSEN, McMaster University — The quantum Fisher information has relevance to quantum metrology and as an entanglement measure. We focus on the $S = 1$ anti-ferromagnetic Heisenberg model with uniaxial anisotropy. Quantum Monte Carlo techniques are used to determine low temperature correlations from which the quantum Fisher information can be estimated within the single mode approximation. The quantum Fisher information is compared to the quantum variance for the staggered magnetization operators in the transverse direction and inequalities between the quantum Fisher information, the quantum variance and the full variance are discussed.

Both the quantum and full variance as well as the quantum Fisher information are examined at finite temperatures above the isotropic point and at the quantum critical point for the Haldane-Néel transition. A finite size scaling study of the quantum Fisher information is performed at the quantum critical point and used to confirm the Ising nature of the Haldane-Néel transition.

*This research was supported by NSERC and enabled in part by support provided by (SHARCNET) (www.sharcnet.ca) and Compute/Calcul Canada (www.computecanada.ca).

8:24AM E07.00003: Reduced density operators of finite-sized Heisenberg XXZ chains* 

BOHAN LU (Presenter), ALEXANDER SEIDEL, Physics, Washington University — In quantum many-body physics, reduced density operators play a central role in revealing the properties of a given system. We elaborate on this by studying finite size Heisenberg XXZ chains in the presence of periodic boundary conditions. As pointed out by F. Verstraete and J. Cirac, the admissible (2-site) local density matrices form a convex set determined by compatibility with translational invariance. The density matrices of ground states of translationally invariant nearest-neighbor Hamiltonians will define the boundary of this set. It is hard to determine this boundary without actually solving for many-body ground states, as knowledge of it would give immediate access to ground state energies of a rich class of models. Here we present studies on the size dependence of this mysterious boundary manifold. We also discuss non-analyticities of the boundary characterizing quantum phase transitions in the thermodynamic limit.

*I am grateful for the financial support made possible by the Greg Delos Summer Fellowship.
8:36AM E07.00004: Localization in a t − J type ladder with translational symmetry  RONGYANG SUN (Presenter), Institute for Advanced Study, Tsinghua University, ZHENG ZHU, Department of Physics, Massachusetts Institute of Technology, ZHENG-YU WENG, Institute for Advanced Study, Tsinghua University — An explicit spatial localization of a hole is shown in a two-leg t-J ladder in the presence of a staggered chemical potential, which still retains translational symmetry, by density matrix renormalization group method. Delocalization can be recovered in following cases, in which either the hidden phase string effect is turned off or a finite next-neighbor hopping $t'$ is added to sufficiently weaken the phase string effect. In particular, two holes are always delocalized by forming a mobile bound pair in contrast to the localized single holes, pointing to a novel pairing mechanism of strong correlation nature.

8:48AM E07.00005: Flexible magnetism in flexible crystals*  ELISE KENNY (Presenter), ANTHONY C JACKO, BEN J POWELL, School of Mathematics and Physics, The University of Queensland — We predict that the elastically flexible crystal, $[\text{Cu(acac)}_2]$ [1], contains quasi-one-dimensional magnetic interactions that change dramatically when the crystal is bent. In the unbent crystal, all interchain interactions are doubly frustrated – geometrically and by the equipoise of antiferromagnetic and ferromagnetic interactions in the two planes perpendicular to the chains. We parametrize a Heisenberg model for the unbent and bent crystal from broken-symmetry density functional theory [2], revealing that the intrachain exchange interaction is an order of magnitude larger than the interchain exchange interactions. We calculate the three dimensional Néel temperature, $T_N$, from the chain random phase approximation (CRPA) [3], which reveals that $[\text{Cu(acac)}_2]$ is an almost perfect Tomonaga-Luttinger liquid (TLL) with a $T_N$ that increases by approximately 175 orders of magnitude when the material is bent. This is a proof of principle demonstration that magnetic properties can be significantly altered by bending flexible crystals.


*This work was supported by the Australian Research Council through Grants No. FT130100161 and DP160100060.

9:00AM E07.00006: Ladder-like optical conductivity in the spin-fermion model*  LAURA CLASSEN (Presenter), CMPMSD, Brookhaven National Laboratory, NEIL ROBINSON, Institute for Theoretical Physics, University of Amsterdam, ALEXEI TSVELIK, CMPMSD, Brookhaven National Laboratory — In the nested limit of the spin-fermion model for the cuprates, 1D-type physics in the form of half-filled two-leg ladders emerges. We show that the RG flow of the corresponding ladder is towards the dMott phase, a gapped spin-liquid with short-ranged d-wave pairing correlations, and reveals an intermediate SO(5)xSO(3) symmetry. We use the results of the RG in combination with a memory-function approach to calculate the optical conductivity of the spin-fermion model in the high-frequency regime, where processes within the hotspot region dominate the transport. For finite temperature, we determine the resistivity in the zero-frequency limit. We argue that Umklapp processes play a major role. Our results show an approximate linear temperature dependence of the resistivity and a conductivity that follows a non-universal power law, qualitatively consistent with experiment.

*This project has received funding from the Alexander-von-Humboldt foundation (L.C.), the European Union's Horizon 2020 research and innovation program under grant agreement No 745944 (N.J.R) and the U.S. Department of Energy, Office of Basic Energy Sciences, Contract No. DE-SC0012704 (A.M.T., LC).

9:12AM E07.00007: Spectrum of Dissipative Ising Chain  JIAN WANG (Presenter), SUDIP CHAKRAVARTY, physics and astronomy, University of California, Los Angeles — This paper extends the (0+1)D spin-boson problem to its (1+1)D version, a dissipative Ising Chain. Monte Carlo simulation and analytic continuation methods are used to explore its phase and dynamics. We find that, the quasi-particle excitation picture is destroyed, when the dissipation strength is greater than a critical value.

9:24AM E07.00008: Single-component fermion chain: emergent mode and liquids of bound states  YUCHI HE (Presenter), Physics, Carnegie Mellon University, BINBIN TIAN, DAVID PEKKER, ROGER MONG, Physics and Astronomy, University of Pittsburgh — We study the formation of bound states in a single-component Fermi chain with attractive interactions. The phase diagram, computed from DMRG (density matrix renormalization group), shows not only a superfluid of paired fermions (pair phase) and a liquid of fermion triplets (trion phase), but also a phase (2M phase) with two gapless modes. We argue based on our numerical data, that the single, pair, and trion phases are descendants of the 2M phase with a 2-component (“emergent”) Tomonaga-Luttinger liquid theory description.
We thus introduce and study interacting Majorana chains with $N = 1$ SUSY [3]. The Hamiltonian is defined by the square of a supercharge with a parameter, which is constructed solely by Majorana fermions. In the parameter space of the model, we find a particular point at which SUSY is unbroken and the ground states can be obtained analytically. We also find that SUSY is restored in the thermodynamic limit for modest values of the parameter. We prove, for large enough parameter values, that the system exhibits spontaneous SUSY breaking. We also prove the existence of NG fermions associated with this SUSY breaking, the dispersion of which is found to be cubic in momentum.


9:48AM E07.00010: Majorana-Hubbard Ladders  ARMIN RAHMANI (Presenter), Western Washington University, DMITRY PIKULIN, Microsoft Station Q, IAN AFFLECK, The University of British Columbia — Models of interacting Majorana modes may be realized in vortex lattices in superconducting films in contact with topological insulators and may be tuned to the strong interaction regime by adjusting the chemical potential. Extending the results on one- and two-dimensional Majorana-Hubbard models, here we study two- and four-leg ladders using both field theory and the (density-matrix renormalization group (DMRG)) methods, finding a phase diagram largely consistent with that proposed for the two-dimensional model on the square lattice.

10:00AM E07.00011: Ising ferromagnet to valence bond solid transition in a one-dimensional spin chain-analogies to deconfined quantum critical points*  SHENGHAN JIANG (Presenter), OLEXEI I MOTRUNICH, Caltech — We study a 1D system that shows many analogies to proposed 2D deconfined quantum critical points. Our system is a translationally invariant spin-1/2 chain with on-site $Z_2 \times Z_2$ symmetry and time reversal symmetry. It undergoes a direct continuous transition from a ferromagnet (FM), where one of the $Z_2$ symmetries and the time reversal are broken, to a valence bond solid (VBS), where all on-site symmetries are restored while the translation symmetry is broken. The other $Z_2$ symmetry remains unbroken throughout, but its presence is crucial for both the direct transition and the characterization of the VBS phase. The transition has a description in terms of either two domain wall species that "fractionalize" the VBS order parameter or in terms of partons that "fractionalize" the FM order parameter. The two descriptions are dual to each other. We also find an exact reformulation of the transition that leads to a simple field theory description that explicitly unifies the two order parameters, which can be interpreted as a new parton approach that encodes the two order parameters in instantons.

*This work was supported by IQIM Caltech, an NSF Physics Frontiers Center, with support of the Gordon and Betty Moore Foundation, and also by NSF through grant DMR-1619696.
DONGHWAN KIM (Presenter), Department of Physics, Pohang University of Science and Technology, KYUNG-TAE KO, Max Planck POSTECH center for Complex Phase Materials, YOUNGHAK KIM, Department of Physics, Pohang University of Science and Technology, YOON SEOK OH, Department of Physics, Ulsan National Institute of Science and Technology, JAE-HOON PARK, Max Planck POSTECH center for Complex Phase Materials — A minor canted component of antiferromagnetic order below $T_N \sim 30.5$ K of NiTe$_2$O$_5$ was investigated by the soft x-ray resonant scattering on Ni $L_3$ edge. It is a $S=1$ (Ni$^{2+}$) magnetic insulator composed of edge shared NiO$_6$ one dimensional chains along b axis with four Ni atoms per period. The nearly 90° superexchange path between two adjacent Ni stabilizes intra-chain ferromagnetic order along b axis, which is ordered antiferromagnetically between adjacent chains. A detailed analysis on the azimuthal and polarization dependence of the (010) structural forbidden peak reveals that the resonant peak is a result of interference between the anisotropic tensor susceptibility and the magnetic resonant scattering amplitude from ‘up-down-down-up’ minor canted moment in ac plane. The non-collinear spin structure is related to the distortion of Ni-O-Ni bonding to induce non-zero Dzyaloshinskii-Moriya interaction, and rather large spin-orbit coupling of Ni 3d orbital.

This work was supported by Max Planck POSTECH/Korea Research Initiative, Study for Nano Scale Optomaterials and Complex Phase Materials (2016K1A4A4A01922028), through National Research Foundation (NRF) funded by MSIP of Korea.

SAMUEL DETMER (Presenter), ANJAN SOUMYANARAYANAN, MICHAEL YEE, YANG HE, Harvard University, MARTHA GREENBLATT, Chemistry and Chemical Biology, Rutgers University, NIGEL HUSSEY, Physics, University of Bristol, JENNIFER HOFFMAN, Harvard University — The marked deviation from Fermi liquid behavior for the quasi-one-dimensional (1D) purple bronze Li$_{0.9}$Mo$_6$O$_{17}$ (LMO) has been observed both by bulk transport and by surface-sensitive spectroscopic probes, and has generated much theoretical interest. Here we present spectroscopic scanning tunneling microscope (STM) images of 1D ‘chains’ on the surface of LMO. We find that the Coulomb suppression of tunneling around the Fermi energy is inhomogenous on the nanometer length scale, which necessitates a revision of the existing model of Luttinger-liquid-like behavior that was based on spatially-averaged spectroscopic techniques. We further report that chains of varying length exhibit resonances at varying energies, and we discuss the implications of this phenomenon for modeling the surface structure of LMO as a 1D quantum system.

KHAGENDRA ADHIKARI (Presenter), KEVIN BEACH, University of Mississippi — The dynamical behavior of many-particle systems is characterized by the lifetime of quasi-particles or excitations. Observables of any non-conserved quantity decay exponentially, but those of a conserved quantity relax to equilibrium with a power law ($t \sim 1/\Delta - L^z$). Such decay processes are associated with a dynamical exponent (e.g., $z = 1$ for the ballistic spread of quasi-particles and $z = 2$ for diffusion) that relates the spread of correlations in space and time. We present numerical results for the Fredkin model—a quantum spin chain with an unusual three-body interaction term—which exhibits a dynamical exponent $z \approx 3$. We discuss our efforts to make a reliable, quantitative estimate of $z$ and to explain the very slow dynamics in terms of a random walk executed by the excitation in Monte Carlo time.

SHINTARO TAKAYOSHI (Presenter), Max Planck Institute for the Physics of Complex Systems, THIERRY GIAMARCHI, Department of Quantum Matter Physics, University of Geneva — Localization caused by disorder has a long history of study since the pioneering work of Anderson. Recently many-body localization (MBL) has been intensively studied in the field of both condensed-matter and statistical physics. Considering the detection of MBL in experiments, it is an important task to investigate on the behavior of physical quantities, especially dynamical ones, in interacting disordered systems. We study the dynamical spin conductivity in XXZ antiferromagnets with random magnetic field. We start from the XX models, which is equivalent to the free fermion system, and then include an Ising interaction. The ground state of easy-plane XXZ chains is gapless Luttinger liquid, and the system is localized by disorder when the Luttinger parameter satisfies $K<3/2$. We calculate dynamical spin conductivity numerically using the technique of Chebyshev matrix product states. We investigate this quantity in the low and high frequency region, and the behavior is power law in both regions. The power depends on the strength of Ising interaction in the high frequency region.

*This work is partly supported by the Swiss National Science Foundation under Division II and ImPact project (No. 2015-PM12-05-01) from the Japan Science and Technology Agency.
8:00AM E08.00001: Nanocalorimetric Evidence for Nematic Superconductivity in Sr0.1Bi2Se3*  KRISTIN WILLA, ROLAND WILLA, KOK WEE SONG, Materials Science Division, Argonne National Laboratory, GENDA GU, RUIDAN ZHONG, JOHN A. SCHNEELOCH, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, ALEXEI E KOSHELEV, WAI-KWONG KWOK, ULRICH WELP (Presenter), Materials Science Division, Argonne National Laboratory — Spontaneous rotational-symmetry breaking in the superconducting state of doped Bi2Se3 has attracted significant attention as an indicator for topological superconductivity. High-resolution calorimetry of single-crystal Sr0.1Bi2Se3 provides unequivocal evidence of a twofold rotational symmetry in the superconducting gap by a bulk thermodynamic probe, a fingerprint of nematic superconductivity. The extremely small specific heat anomaly resolved with our high-sensitivity technique is consistent with the material’s low carrier concentration proving bulk superconductivity. The large basal-plane anisotropy of Hc2 is attributed to a nematic phase of a two-component topological gap structure η = (η1, η2) and caused by a symmetry-breaking energy term δ(|η1|² - (|η2|²)Tc. A quantitative analysis of our data excludes more conventional sources of this two-fold anisotropy and provides the first estimate for the symmetry-breaking strength δ ~ 0.1.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. K. W. and R. W. acknowledge support from the Swiss National Science Foundation through the Postdoc Mobility program.

8:12AM E08.00002: μSR and Magnetometry Study of the Type I Superconductor BeAu*  JAMES BEARE (Presenter), MATTHEW NUGENT, MURRAY N WILSON, McMaster University, ETERI SVANIDZE, Max Planck Institute for Chemical Physics of Solids, YIPENG CAI, McMaster University, ALFRED AMON, ANDREAS LEITHE-JASPER, Max Planck Institute for Chemical Physics of Solids, ZIZHOU GONG, ZURAB GUGUCHIA, Columbia University, YURI GRIN, Max Planck Institute for Chemical Physics of Solids, YASUTOMO J UEMURA, Columbia University, GRAEME LUKE, McMaster University — We present Muon Spin Rotation and Relaxation (μSR) measurements as well as demagnetisation corrected magnetometry measurements on polycrystalline samples of the noncentrosymmetric superconductor BeAu. From μSR measurements in a transverse field we find that BeAu is a rare Type I superconducting alloy. To account for demagnetising effects in magnetometry measurements we produced an ellipsoidal sample for which we could calculate the demagnetising factor and found results comparable with our μSR measurements. From both sets of measurements we have constructed a phase diagram from 30 mK to Tc ≈ 3.25K. We also studied the effect of hydrostatic pressure and find that 450 MPa decreases Tc by 44 mK, comparable to the change seen in several elemental type I superconductors.

*We would like to acknowledge funding from the Natural Sciences and Engineering Research Council of Canada as well as the Canadian Institute for Advanced Research

8:24AM E08.00003: Direct evidence of multi-band superconductivity in Mo8Ga41*  ANSHU SIROHI (Presenter), Indian Institute of Science Education and Research, Mohali, SURABHI SAHA, Indian Institute of Science, Bangalore, PRAKRITI NEHA, Jawaharlal Nehru University, New Delhi, SHEKHAR DAS, Indian Institute of Science Education and Research, Mohali, SATYABRATA PATNAIK, Jawaharlal Nehru University, New Delhi, TANMOY DAS, Indian Institute of Science, Bangalore, GOUTAM SHEET, Indian Institute of Science Education and Research, Mohali — Mo8Ga41, a member of the family of endohedral gallide cluster compounds shows superconductivity with relatively large Tc of 9.8 K as compare to the other members in this family. In order to study the superconducting phase of Mo8Ga41 a number of experiments have been employed and it was shown that this compound manifests unusually high electron-phonon coupling leading to a large ∆/kBTc ratio and an indication of multi-gap superconductivity was also found. In this talk, from the direct measurement of the superconducting energy gap measured by Scanning Tunneling Spectroscopy (STS), I will show that Mo8Ga41 is a two-gap superconductor like MgB2 with the superconducting energy gaps of magnitude 0.85 meV and 1.6 meV respectively. Evolution of superconducting energy gaps with temperature and magnetic field demonstrates the conventional nature of both of the gaps as per the BCS prediction. In addition, through the band structure calculations, we have also identified the bands responsible for the two respective gaps and also shows that only two specific Mo sites in an unit cell contribute to superconductivity. Magnetic field dependent STS experiments further suggest that the interband coupling is weak in Mo8Ga41, as in case of MgB2.

*Department of Science and Technology, India
8:36AM E08.00004: Evidence of a structural quantum critical point in \((\text{Ca}_{x}\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}\) from a lattice dynamics study* YIU WING CHEUNG (Presenter), YAJIAN HU, Department of Physics, The Chinese University of Hong Kong, MASAKI IMAI, YASUAKI TANIOKU, HIBIKI KANAGAWA, JOICHI MURAKAWA, KODAI MORIYAMA, Department of Chemistry, Kyoto University, WEI ZHANG, KWING TO LAI, Department of Physics, The Chinese University of Hong Kong, KAZUYOSHI YOSHIMURA, Department of Chemistry, Kyoto University, MALTE GROSCH, Cavendish Laboratory, University of Cambridge, KOJI KANEKO, Materials Sciences Research Center, Japan Atomic Energy Agency, SATOSHI TSUTSUI, Japan Synchrotron Radiation Research Institute, SWEE KUAN GOH, Department of Physics, The Chinese University of Hong Kong — The nonmagnetic quasiskutterudite \((\text{Ca}_{x}\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}\) represents a precious system to explore the interplay between structural instabilities and superconductivity by tuning the Ca concentration \(x\) [1-3]. We performed inelastic x-ray scattering to probe the phonon spectrum of \((\text{Ca}_{x}\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}\) for various calcium contents. We detected a complete phonon softening at the \(M\) point when approaching the structural transition temperature from above. Intriguingly, at \(x = 0.85\), the energy squared of the soft mode at \(M\) extrapolates to zero at \((-5.7 \pm 7.7)\) K, providing the first compelling microscopic evidence of a structural quantum critical point (QCP) in \((\text{Ca}_{x}\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}\). The observed phonon softening around the \(M\) point provides the essential ingredient for realizing strong-coupling superconductivity near the structural QCP [4].


8:48AM E08.00005: Singlet superconductivity in single-crystal NiBi\(_3\) superconductor* GEJIAN ZHAO, Southern University of Science and Technology, Institute for Quantum Science and Engineering and Department of physics, XINXIN GONG, PENGCHAO XU, Department of Physics, Fudan University, BOCHAO LI, ZHIYU HUANG, Arizona State University, XIAOFENG JIN, Department of Physics, Fudan University, XIANG-DE ZHU, High Magnetic Laboratory, Chinese Academy of Sciences, TINGYONG CHEN (Presenter), Arizona State University — Verification of triplet superconductors (SCs), especially those that can carry spin angular momentum, is essential for understanding fundamental mechanism of unconventional superconductivity as well as important applications in quantum computing and spintronics. But singlet and triplet SCs have similar macroscopic properties, an ideal experiment would be to directly measure the spin states of Cooper pairs. In this work, Andreev reflection spectroscopy with unpolarized and highly spin-polarized currents has been utilized to study an intermetallic single-crystal SC NiBi\(_3\). Magnetoresistance at zero bias voltage of point contacts shows the occurrence and suppression of Andreev reflection by unpolarized and polarized current, respectively. The gap value, its symmetry and temperature dependence have been determined using an unpolarized current. The spin state in the NiBi\(_3\) sample is determined to be antiparallel using a highly spin-polarized current. The gap value \(2D/k_B T\), gap symmetry and its temperature dependence, combined with the antiparallel spin state show that the bulk NiBi\(_3\) is a singlet \(s\)-wave superconductor.

*The work was supported as part of SHINES, an EFRC center funded by the U. S. Department of Energy, Office of Science, Basic Energy Science, under award SC0012670.

9:00AM E08.00006: Magnesium Diboride Thin Film Cavity Fabricated by Hybrid Physical Chemical Vapor Deposition XIN GUO (Presenter), WENURA K WITHANAGE, JAY R. PAUDEL, Department of Physics, Temple University, ALIREZA NASSIRI, Argonne National Laboratory, XIAOXING XI, Department of Physics, Temple University — Magnesium diboride (MgB\(_2\)) is considered as a potential material for superconducting radio frequency cavities. MgB\(_2\) thin film fabricated on an inner surface of the Cu cavity will allow for a higher operational temperature because of the higher transition temperature of MgB\(_2\) and the high thermal conductivity of Cu. Using the hybrid physical chemical vapor deposition (HPCVD) technique, a uniform MgB\(_2\) coatings were achieved on the inner wall of the 3 GHz Cu cavity. The quality of the films were characterized on small Cu samples which were mounted at different selected locations of the cavity. Preliminary RF result for the MgB\(_2\) thin film cavity will be presented.
9:12AM E08.00007: The extraordinary superconductivity of commercial niobium-titanium wire at extreme pressures  
LILING SUN (Presenter), JING GUO, GONGCHANG LIN, SHU CAI, Institute of Physics, CAS, CHUANYING XI, CHANGJIN ZHANG, High Magnetic Field Laboratory, CAS, WANSHUO SUN, QIULIANG WANG, Institute of Electrical Engineering, CAS, QI WU, Institute of Physics, CAS, YUHENG ZHANG, High Magnetic Field Laboratory, CAS, TAO XIANG, Institute of Physics, CAS, ROBERT CAVA, Princeton University — We report the observation of extraordinary superconductivity in a pressurized commercial niobium-titanium alloy wire. We demonstrate that its zero-resistance superconductivity persists from ambient pressure to pressures as high as 261.7 GPa, a pressure that falls within that of the outer core of the earth, establishing the record where a superconducting state continuously survives. At such high pressures the superconducting transition temperature (Tc) has increased from ~9.6 K to ~19.1 K and the critical magnetic field (Hc2) at 1.8 K from 15.4 T to 19 T, setting new records for both Tc and Hc2 among all the known transition element alloy superconductors, all, remarkably, in spite of a 45% volume shrinkage. The behavior is quite different from what is seen in copper oxide and iron pnictide superconductors, whose superconducting transition temperatures are quite sensitive to subtle changes in the lattice structure. Our results therefore not only provide fresh information on the remarkable properties of this commercial superconductor, but also pose a substantial challenge for models of a phenomenon as “well understood” as conventional electron-phonon coupled superconductivity.

9:24AM E08.00008: Field-induced large resistance peak in superconducting niobium thin films deposited on surface reconstructed SrTiO3 substrate  
AKHILESH SINGH (Presenter), TSUNG-CHI WU, UDDIPTA KAR, Institute of Physics, Academia Sinica, Nankang, Taipei, 11529, Taiwan, WEI-CHENG LEE, Department of Physics, Applied Physics and Astronomy, Binghamton University, Binghamton, New York 13902, USA, WEI-LI LEE, Institute of Physics, Academia Sinica, Nankang, Taipei, 11529, Taiwan — It is known that oxygen vacancies in SrTiO3(STO) can result in surface reconstructions (SR), giving rise to a metallic surface and unusual surface phonon modes. Few earlier works have demonstrated intriguing phenomena of a huge superconducting transition temperature enhancement in a monolayer FeSe on SR-STO substrate, where its intrinsic mechanism remains debatable. In this work, we constructed a phase diagram of SR-STO with surface structures of, where SR-STO samples were prepared via thermal annealing in ultra-high vacuum followed by low energy electron diffraction analysis. Thin Nb films with different thicknesses (t) were deposited on the SR-STO. The detail studies on the magnetotransport and superconducting properties of the Nb(t)/SR-STO films revealed a large positive magnetoresistance, and a pronounced resistance peak occurred near the onset of the resistive superconducting transition in the presence of a large magnetic field. Remarkably, amplitude of the resistance peaks increases with increasing fields, reaching a value of nearly 340 % of the normal state resistance at 12 T. Such resistance peaks were not observed for the control samples of Nb(t)/STO and Nb(t)/SiO2. Possible mechanisms of the large field-induced resistance peak will be discussed.

9:36AM E08.00009: Effects of dimensionality and magnetic correlations on superconducting properties of MoCo thin films  
TOMAS POLAKOVIC (Presenter), Physics Division, Argonne National Laboratory, TERENCE BRETZ-SULLIVAN, JOHN E. PEARSON, J SAMUEL JIANG, ANAND BHATTACHARYA, AXEL F HOFFMANN, Materials Science Division, Argonne National Laboratory, GORAN KARAPETROV, Department of Physics, Drexel University, VALENTYN NOVOSAD, Materials Science Division & Physics Division, Argonne National Laboratory — The ability to precisely control superconducting transition within a narrow range of temperatures is crucial for many applications in cryogenic detectors. One way of achieving this is by utilizing magnetic impurities in superconductors. We present a systematic study of the effect of Co dopant on superconducting Molybdenum thin films prepared by sputtering from alloyed targets over a broad range of impurity concentrations and film thicknesses. Electric and magnetic measurements show strong dependence of the critical temperature on Co concentration, as well as presence of Kondo effect that vanishes as the film thickness is reduced. In addition to the pair-breaking effect due to magnetic impurities, we also explore the trend of Tc reduction with decreasing film thickness, generally attributed to the reduction of the superconducting order parameter on the surfaces.

*This work was supported by the U. S. Department of Energy (DOE), Office of Science, Offices of Nuclear Physics, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-06CH11357.
Kenichi Kaminaga (Presenter), WPI-AIMR, Tohoku Univ., Daichi Oka, Graduate School of Science, Tohoku Univ., Tetsuya Hasegawa, Graduate School of Science, University of Tokyo, Tomoteru Fukumura, WPI-AIMR, Tohoku Univ. — We report effects of carrier density and epitaxial strain on superconductivity in rock-salt lanthanum monoxide (LaO) epitaxial thin film [1]. Electron carrier doping via introducing oxygen vacancies resulted in a dome-shaped $T_c$ as a function of carrier density. In addition, epitaxial strain influenced significantly the $T_c$ despite its highly symmetric rock-salt structure. $T_c$ was raised up to 5.2 K in tensilely strained thin film on LaAlO$_3$ substrate, in contrast with $T_c$ of at most 4.5 K in compressive strained film on YAIO$_3$ substrate. [1] K. Kaminaga et al., J. Am. Chem. Soc. 140, 6754 (2018).

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Chi-Tie Liang (Presenter), Guan-Ming Su, Ankit Kumar, Chau-Shing Chang, Ching-Chen Yeh, Bi-Yi Wu, Dinesh Patel, Physics, National Taiwan University, Yen-Ting Fan, Sheng-Di Lin, Electronics Engineering, National Chiao Tung University, Lee Chow, Physics, University of Central Florida — In this work, we present experimental evidence for the Berezinskii–Kosterlitz–Thouless (BKT) transition in an atomic-scale aluminum nanofilm grown on a GaAs substrate by molecular beam epitaxy (MBE). Such a MBE-grown Al film has a higher superconducting critical temperature and a larger critical magnetic field compared to those of bulk Al. In a 4-nm-thick Al film, our results show that $V/I^2$ can occur in both the low-voltage (the BKT transition temperature $T_{BKT} = 1.97$ K) and high-voltage ($T_{BKT} = 2.17$ K) regions where $V$ and $I$ correspond to the voltage across the device and the driving current, respectively. By fitting our data to the vortex/anti-vortex model and a model based on dynamical scaling, we unequivocally determine that $T_{BKT} = 2.17$ K in our nanofilm. Our new experimental results suggest that when one uses the temperature for which $V/I^2$ to determine $T_{BKT}$, great care has to be taken as one also needs to fit one's data to both dynamical scaling and vortex/anti-vortex models.

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Catalin Martin (Presenter), Eng. Physics, Ramapo College of NJ, Ali S. M. Radmanesh, Advanced Materials Research Institute and Department of Physics, University of New Orleans, Yanglin Zhu, Zhiqiang Mao, Physics and Engineering Physics, Tulane University, Leonard Spinu, Advanced Materials Research Institute and Department of Physics, University of New Orleans — Using the combination of a tunnel diode oscillator (TDO) and a commercial dilution refrigerator, we measured temperature dependent magnetic penetration depth $\lambda(T)$ in single crystals of YPdBi and TbPdBi, down to temperatures as low as 0.1 K. We found that penetration depths of both compounds do not show exponential temperature dependence and saturation at low temperatures, as expected for conventional BCS superconductors. Instead, in both materials, the penetration depth can be described by a power law $\lambda(T) = A \times T^n$. The coefficient A was found to be about 50% smaller in TbPdBi, but the exponents are very similar, $n = 2.76 \pm 0.04$ in YPdBi and $n = 2.6 \pm 0.3$ in TbPdBi, respectively. Our results suggest unconventional superconductivity in both YPdBi and TbPdBi.

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National Science Foundation, the Independent Research/Development (IR/D) Program.
**10:24AM E08.00013: Effect of magnetic field on short-range antiferromagnetic correlations in the filled skutterudite Pr$_{1-x}$Eu$_x$Pt$_4$Ge$_{12}$**

RAM ADHIKARI (Presenter), PENGTAO SHEN, DOM LAL KUNWAR, Kent State University, INHO JEON, M BRIAN MAPLE, Physics, University of California, SanDiego, MAXIM DZERO, CARMEN CRISTINA ALMASAN, Kent State University — We have investigated the effects of Eu substitution through thermodynamic measurements on the superconducting filled skutterudite Pr$_{1-x}$Eu$_x$Pt$_4$Ge$_{12}$ in an applied magnetic field H. A heat capacity Schottky anomaly is present over the whole doping range. For the samples with x > 0.5, these peaks shift to lower temperature with increasing applied magnetic field H, hence they reveal the antiferromagnetic (AFM) ordering of the Eu moments, as the AFM transition is suppressed by H. The heat capacity peaks in the samples with x ≤ 0.5 shift to higher temperatures with increasing magnetic field. These latter Schottky peaks are a result of Zeeman splitting by internal magnetic field due to short-range AFM correlations of random magnetic moments of nearing Eu sites, thus increases with Eu concentration x. In low H, the Schottky gaps show a non-linear relationship with H as the magnetic moments become weakly magnetized. In the case of a high applied H, the magnetic moments of Eu sites become completely aligned along H. Thus, Increasing H will not increase further the magnetization, hence the Schottky gaps are a linear function of the external field H.

*This work was supported by the Grants No. NSF-DMR-1505826, DMR-1506547, DE-SC0016481 at KSU and Grant No. DE-FG02-04ER46105 at UCSD.

**10:36AM E08.00014: Increase in Birr and reduction of anisotropy of MgB2 with Dy2O3/C co-doping**

MIKE SUMPTION (Presenter), Ohio State University — In this study a series of Dy$_2$O$_3$/C co-doped MgB$_2$ bulks and strands were fabricated. The C – doping level was fixed at 2.0 mol% for all the MgB$_2$ strands. The transport and magnetic properties of MgB$_2$ strands was systematically investigated in terms of Dy$_2$O$_3$ doping level over a wide temperature range. Compared to C-doped-only MgB$_2$ strand, the Dy$_2$O$_3$/C co-doped MgB$_2$ strands have higher transport $J_{ct}$ at 4.2 K. The improved transport $J_{ct}$ – $B$ performance results from the fact that Dy$_2$O$_3$ doping can further improve the anisotropy and flux pinning strength of C-doped MgB$_2$ strand. TEM results of REO doped sample showed nano-size inclusions (20 – 100 nm) present both inside MgB$_2$ grains and on grain boundaries. In-field resistivity measurement (up to 28 T) was performed from 4-40 K. The Bc2 values extracted from both resistivity and magnetic measurements were unchanged by Dy2O3 additives. However, the irreversibility field Bk was increased in response to Dy2O3 doping suggesting a decrease in the anisotropy. The Bk increase, about 1 T between 4-35 K, is of particular interest at higher temperatures (20-30 K).

**10:48AM E08.00015: Superconductivity and phase diagram in a transition metal doped Zr$_5$Ge$_3$ compound**

XIAOYUAN LIU (Presenter), SHENG LI, VARUN ANAND, BING LV, University of Texas at Dallas — Systematic doping studies have been carried out to search for superconductivity in the transition metal doped Zr$_5$Ge$_3$ system at different sites. Superconductivity is only discovered with Pt doping at Ge site with $T_c$~2.8K and remain absent with other transition metal doping such as Y, Cr, Ir, and Pd at other different sites. Coincidental with our previous findings in the Zr$_5$Ge$_3$-$x$Ru$_x$ system, it appears that the induced superconductivity is not only site-selective (only at Ge site) but also dopant selective (only with Pt and Ru dopants). The bulk superconductivity in Zr$_5$Ge$_{3-x}$Pt$_x$ has been investigated through resistivity, magnetization, and heat capacity measurements. The superconducting phase diagram of Pt doped Zr$_5$Ge$_{3-x}$Pt$_x$ is also proposed.

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**Tuesday, March 5, 2019 8:00 AM - 10:48 AM**

**Session E09 DCMP DMP: Novel and Less-common Superconductors**

BCEC 151A - Chunjing Jia, SLAC

National Accelerator Laboratory
8:00AM E09.00001: Superconductivity in Chevrel phases  GIANNI PROFETA (Presenter), GIOVANNI MARINI, Physical and Chemical Sciences, University of L'Aquila, ANTONIO SANNA, Max Planck Institute — Chevrel phases is a class of interesting materials discovered more than 40 years ago including more than 100 examples. They are ternary compounds of general stoichiometry M_xMo_6X_8 (X = chalcogen and M=metal) and many of them show interesting superconducting properties with critical temperatures as high as 15K and high critical magnetic fields (around 50 Tesla).

We present the results of the prediction of the superconducting phase in Chevrel compound, PbMo_6S_8, within the SuperConducting Density Functional Theory (SCDFT), a first-principles theory of the superconducting phase which does not rely on any semi-empirical parameter.

We successfully predict the critical temperature of PbMo_6S_8 at ambient conditions highlighting the role of phase instability, electron-phonon coupling with different intra-molecular and inter-molecular phonon modes and the fundamental role of repulsive electron-electron interaction, treated from first-principles. The evolution of the superconducting critical temperature as a function of the external pressure results in excellent agreement with available experiments.

Despite the interesting physical and chemical properties of Chevrel phases their fundamental explanation was still lacking: SCDFT opens way to systematic investigation of this large class of compounds.

8:12AM E09.00002: New magnetic phases and the absence of superconductivity in doped Hematophanite, Pb_4Fe_3O_8Cl*  ALEX HOJEM (Presenter), JAMES WAMPLER, IVAN SCHULLER, Department of Physics and Center for Advanced Nanoscience, University of California, San Diego — We searched for new magnetic and superconductivity phases in the hematophanite system [1], Pb_4Fe_3O_8Cl, which has structural similarities to some cuprates [2]. To enhance the potential number of subphases we synthesized inhomogeneous samples via powder metallurgy and explored electron and hole doping of both Pb, with Ga and Bi, and Fe, with Mn and Co. We used magnetic field modulated microwave spectroscopy [3], as well as vibrating sample magnetometry, to identify magnetic phase transitions as a function of temperature. Crystallographic phase information is obtained via x-ray diffraction and Rietveld refinement. We observe that in both the Ga and Co doped systems we induce multiple magnetic phase transitions that correspond to various subphases present in our samples. Although many magnetic phases were created in these samples there is no indication of the presence of a new superconducting phase above 4 K.


*Supported by AFOSR: FA9550-14-1-0202

8:24AM E09.00003: Discovery of a new strong-coupling superconductor Y_7Ru_4InGe_12 by indium flux*  JINKE BAO (Presenter), DANIEL BUGARIS, KRISTIN WILLA, ULRICH WELP, DUCK YOUNG CHUNG, MERCOURI KANATZIDIS, Materials Science Division, Argonne National Laboratory — Compounds containing rare earth, transition metal and germanium elements can exhibit interesting phenomena such as charge density wave, complex magnetism and superconductivity. Using indium flux makes it possible to synthesis new compounds under a relative low temperature. Here we discovered a new superconductor Y_7Ru_4InGe_12 with T_c ~ 5.8 K grown from the indium flux, which is confirmed by resistivity, magnetization and specific heat measurements. It is a type-II superconductor and its upper critical fields are estimated to be 5.4 and 2.7 T along and perpendicular to the c axis, respectively. The estimated mean free path along the c axis is ~ 29 Å, much smaller than the superconducting coherence length ~ 172 Å, putting it in a dirty limit regime. The specific heat jump of this superconductor ΔC/γeT_c = 2.4 is much larger than the BCS theoretical value 1.43, pointing to a strong-coupling scenario. A new polymorphism of LuRuGe and several trials to synthesize isostructural compounds of Y_7Ru_4InGe_12 by replacing the rare earth elements will also be presented in this talk.

*Work at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Basic Energy Science, Materials Sciences and Engineering Division.
8:36AM E09.00004: Superconducting SrSnP with Strong Sn-P Antibonding Interaction: Is the Sn Atom Single or Mixed Valent? XIN GUI (Presenter), Department of Chemistry, Louisiana State University, ZUZANNA SOBCZAK, Department of Solid State Physics, Gdansk University of Technology, TAY-RONG CHANG, Department of Physics, National Cheng Kung University, XITONG XU, SHUANG JIA, International Center for Quantum Materials, Peking University, TOMASZ KLIMCZUK, Department of Solid State Physics, Gdansk University of Technology, WEIWEI XIE, Department of Chemistry, Louisiana State University — The large single crystals of SrSnP were prepared using Sn self-flux method. SrSnP crystallizes in the CaGaN structure type with space group $P4/nmm$ (S.G.129, Pearson symbol tP6). A combination of magnetic susceptibility, resistivity, and heat capacity measurements confirms the bulk superconductivity with $T_c = 2.3(1)$ K in SrSnP. According to the X-ray photoelectron spectroscopy (XPS) measurement, the assignments of Sr$^{2+}$ and P$^{3-}$ are consistent with the chemical valence electron balance principles. Moreover, it is highly likely that Sn atom has only one unusual oxidation state. First-principles calculations indicate the bands around Fermi level are hybridized among Sr-$d$, Sn-$p$, and P-$p$ orbitals. The strong Sn-P and Sr-P interactions pose as keys to stabilize the crystallographic structure and induce the superconductivity, respectively. The physics-based electronic and phononic calculations are consistent with the molecular viewpoint. After including the spin-orbit coupling (SOC) into the calculation, the band degeneracies at G-point in the first Brillouin zone (BZ) split into two bands, which yield to the van Hove singularities around Fermi level.

8:48AM E09.00005: Superconductivity and Sn-Mössbauer spectra of the antiperovskite oxide $\text{Sr}_{3-x}\text{SnO}$* ATSUTOSHI IKEDA (Presenter), Department of Physics, Kyoto University, Japan, SHINJI KITAO, Institute for Integrated Radiation and Nuclear Science, Kyoto University, Japan, SHUN KOIBUCHI, MOHAMED OUDAH, Department of Physics, Kyoto University, Japan, IGOR MARKOVIC, School of Physics and Astronomy, University of St Andrews, UK, JAN NIKLAS HAUSMANN, SHINGO YONEZAWA, Department of Physics, Kyoto University, Japan, MAKOTO SETO, Institute for Integrated Radiation and Nuclear Science, Kyoto University, Japan, YOSHITERU MAENO, Department of Physics, Kyoto University, Japan — We recently reported bulk superconductivity in the antiperovskite oxide $\text{Sr}_{3-x}\text{SnO}$, with a possibility of topological nature. We investigate the evolution of superconducting properties with the nominal Sr deficiency $x$. In all superconducting samples, two superconducting phases with $T_c \approx 5$ K and 1 K appear concurrently that originate from $\text{Sr}_{3-x}\text{SnO}$. Mössbauer spectroscopy reveals an unusual Sn$^{4+}$ ionic state in both stoichiometric and superconductive samples. In addition to the main absorption peak, we observe a satellite peak attributable to the Sn sites with nearest-neighbor Sr deficiencies. The intensities of these two peaks exhibit a rather different temperature dependence, possibly reflecting different environment of the lattice vibrations. These results clarifying the Sr deficiency dependence of the normal and superconducting properties of the antiperovskite oxide $\text{Sr}_{3-x}\text{SnO}$ will promote future work on this class of materials.

*This work was supported by the JSPS KAKENHI Nos. JP15H05851, JP15K21717, JP17J07577, and JP17H04848, by the JSPS Core-to-Core Program, and by Izumi Science and Technology Foundation (Grant No. H28-J-146). AI is supported by Japan Society for the Promotion of Science as JSPS Research Fellow.

9:00AM E09.00006: Palladium Dependent Superconductivity in the $\text{Nb}_2\text{Pd}_x\text{Se}_5$ System* JENNIFER NEU (Presenter), YOU LAI, DAVID E GRAF, National High Magnetic Field Laboratory, DAVID SINGH, University of Missouri, RYAN BAUMBACH, THEO SIEGRIST, National High Magnetic Field Laboratory — Single crystals of $\text{Nb}_2\text{Pd}_x\text{Se}_5$ across the range $0.68<x<0.95$ were grown with the objective of studying the superconducting properties as a function of Pd stoichiometry. Electrical conductivity measurements down to 0.4K indicate a Pd-concentration dependent dome of superconductivity in this system. Here we discuss the crystal growth method, structural characterization, and the evolution of the superconducting properties within the accessible range of Pd stoichiometries.

*NSF DMR-1606952, NHMFL NSF DMR 1677449, DOE DE-SC0019114 and the State of Florida
9:12AM E09.00007: Highly reproducible superconductivity in K-doped triphenylbismuthine and tris(2/4-methylphenyl)bismuthine*  ZHONGBING HUANG (Presenter), Physics, Hubei University, REN-SHU WANG, JIA CHENG, Materials Science, Hubei University, XIAO-LIN WU, HUI YANG, Physics, Hubei University, YUN GAO, Materials Science, Hubei University, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research, Shanghai — To search for new organic superconductors, we perform a systematic study on the magnetic and electrical properties of K-doped triphenylbismuthine and tris(2/4-methylphenyl)bismuthine, which are successfully synthesized by a two-step method - ultrasound treatment and low temperature annealing. The combination of dc and ac magnetic measurements show that one hundred percent of synthesized samples exhibit superconductivity at 3.5 K and/or 7.2 K for triphenylbismuthine, and at 3.6 K for tris(2/4-methylphenyl)bismuthine. The observed superconductivity is strongly supported by the resistivity measurements. Both calculated electronic structures and measured Raman spectra indicate that superconductivity is realized by transferring electron from potassium to carbon atom. Our study opens an encouraging window for the search of organic superconductors in organometallic molecules.

*We acknowledge financial support from the National Natural Science Foundation of China under Grants Nos. 11574076, 11674087, and 91221103.

9:24AM E09.00008: Structures and charge transfer in metal-doped aromatic hydrocarbons  GUO-HUA ZHONG (Presenter), Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research, HAI-QING LIN, Beijing Computational Science Research Center — Organic based compounds were suggested as candidates for high temperature or room temperature superconductors since the electrons can interact with much higher excitation energy than the phonon energy in these materials. Recently, the discovery of superconductivity in aromatic hydrocarbons seemingly supports the above idea suggested by Little and Ginzburg. Chen et al reported that the Tc exceeds 120 K in K-doped p-terphenyl. This result clearly shows that organic compounds are potential room-temperature superconductors. However, the structural characteristics of metal-doped aromatic hydrocarbons and the charge transfer from metal to organic molecule have always been puzzled. Here we report these research results by employing the first-principles calculations. In this work, we will present the atomic positions in metal (K, Al, Ga, and In)-doped aromatic hydrocarbons and the distribution and the number of transferred charge, as well analyze the relation between them and electronic structures. The results is meaningful to understand this superconductivity in this kind of materials.

9:36AM E09.00009: Signatures of two-gap superconductivity in epitaxial La(Pt_xSi_1-x)_2 films*  JIAN LIAO (Presenter), Department of Physics, University of Texas at Dallas, Richardson, TX, 75080, YUNBO OU, Plasma Science and Fusion Center and Francis Bitter Magnet Laboratory, MIT, Cambridge, MA, 02139, JAGADEESH MOODERA, Department of Physics, MIT, Cambridge, MA, 02139, XIAOYAN SHI, Department of Physics, University of Texas at Dallas, Richardson, TX, 75080 — Symmetry plays an important role in superconductivity. In noncentrosymmetric superconductors, the pairing state might become a mixture of spin-singlet and spin-triplet components due to the anti-symmetric spin-orbit coupling (ASOC), which is “protected” by the lack of an inversion center. This mixing can further lead to two-gap physics. We investigated the transport properties of various La(Pt_xSi_1-x)_2 thin films grown by molecular beam epitaxy (MBE), where the inversion symmetry and spin-orbit coupling strength are tunable by varying the Pt concentration x. For certain x, magnetoresistance shows a two-step transition at finite temperatures below Tc, and the upper critical field is well described by a two-band model. Furthermore, the current-voltage characteristics, along with the differential resistance measurements, reveal a two-gap structure in magnetic fields up to 1 T. These observations indicate the multi-gap superconductivity in La(Pt_xSi_1-x)_2 films.

*This work was supported by UT Dallas research enhancement funds, National Science Foundation (NSF-DMR 1700137), Office of Naval Research (N00014-16-1-2657), and Center for Integrated Quantum Materials (DMR-1231319).
Phase separation at the dimer-superconductor transition in Ir$_{1-x}$Rh$_x$Te$_2$* RUNZE YU, SOHAM BANERJEE, HECHANG LEI, MILINDA ABEYKOON, CEDOMIR PETROVIC, ZURAB GUGUCHIA, EMIL BOZIN (Presenter), Brookhaven National Laboratory — The detailed evolution of the local atomic structure across the (x, T) phase diagram of Ir$_{1-x}$Rh$_x$Te$_2$ superconductor (0≤x≤0.3, 10K≤T≤300K) is obtained from high-quality x-ray total scattering data using the atomic pair distribution function method. The observed hysteretic thermal structural phase transition from a trigonal to a triclinic dimer phase for low Rh content emphasizes the intimate connection between the lattice and electronic properties. For superconducting samples away from the dimer/superconductor boundary, structural transition is absent and the local structure remains trigonal down to 10 K. In the narrow range of compositions close to the boundary structural phase separation is observed, suggestive of weak first-order character of the Rh-doping induced dimer-superconductor quantum phase transition. Samples from this narrow range show weak anomalies in electronic transport and magnetization, hallmarks of the dimer phase, as well as superconductivity albeit with incomplete diamagnetic screening. The results imply competition of the dimer and superconducting orders.


*Work at Brookhaven National Laboratory was supported by US DOE-BES under Contract No. DE-SC0012704.

Angle-Resolved Photoemission Spectroscopy Study of Planar Nickelate Pr$_4$Ni$_3$O$_8$ HAOXIANG LI (Presenter), XIAOQING ZHOU, KYLE GORDON, University of Colorado, Boulder, HONG ZHENG, JUNJIE ZHANG, JOHN MITCHELL, Material Science Division, Argonne National Lab, DANIEL DESSAU, University of Colorado, Boulder — Planar nickelates share the similar crystal structure and 3d electron configuration with high $T_c$ cuprate materials, and thus can be considered as a potential proxy for cuprate physics as well as a possible candidate for hosting high-temperature superconductivity. A previous study has shown that Pr$_4$Ni$_3$O$_8$, a metallic material in the planar nickelate family, has a pronounced orbital character of $dx^2-y^2$ near the Fermi energy [1], which is a signature of the cuprate electronic structure. Here we present the first angle-resolved photoemission spectroscopy study of Pr$_4$Ni$_3$O$_8$. Consistent with the electron counting, planar nickelate Pr$_4$Ni$_3$O$_8$ shows a non-gapped Fermi surface that resembles the one in the heavily over-doped cuprate. A detailed comparison of the ARPES result shows more similarity in the electronic structure. Our observations demonstrate that planar nickelate Pr$_4$Ni$_3$O$_8$ material can be a potential test ground for the study of cuprate physics.


Isotope effect in the layered bismuth chalcogenide (BiCh$_2$-based) superconductor* KAZUHISA HOSHI (Presenter), YOSHIKAZU MIZUGUCHI, YOSUKE GOTO, Physics, Tokyo Metropolitan University — We have investigated the selenium isotope effect on $T_c$ in the layered bismuth chalcogenide (BiCh$_2$-based) superconductor LaO$_{0.6}$F$_{0.4}$Bi(S,Se)$_2$ using $^{76}$Se and $^{80}$Se. For all examined samples, the Se concentration, which is linked to the superconducting properties, is successfully controlled within x = 1.09–1.14 in LaO$_{0.6}$F$_{0.4}$BiS$_2–x$Se$_x$. From the transition temperature estimated from the magnetization and electrical resistivity measurements, we found that the changes in $T_c$ between $^{76}$Se and $^{80}$Se were apparently smaller than that expected from phonon-mediated pairing mechanism. The estimated isotope effect exponent $\alpha_{Se}$ is close to zero (-0.04 $\leq \alpha_{Se}$ $\leq$ +0.04) [1]. Our results may indicate that the pairing in LaO$_{0.6}$F$_{0.4}$Bi(S,Se)$_2$ is not mediated by phonons, which is consistent with recent theoretical and experimental studies suggesting that unconventional pairing mechanisms are essential for the BiCh$_2$-based superconductor. We will show the recent results on sulfur isotope effect on the BiS$_2$-based superconductors.


*We thank O. Miura and R. Higashinaka for their experimental support and K. Kuroki for his fruitful discussion.
MENDELEEV'S PERIODIC TABLE and SUPERCONDUCTIVITY: Here it is pointed out that, like chemical properties, elemental metals in the same column of the table and in one headed by a nonmagnetic metal typically have similar Tc's. GORDON RIBLET (Presenter), Microwave Development Laboratories — In the first and second columns of the periodic table, headed by lithium and beryllium, none of the 5 alkali metals or 5 alkaline earth metals is a superconductor (see the table on p. 356 of the 5th edition of Kittel). Of the many rare earth metals in the third column only lanthanum is a superconductor. In the fourth and fifth columns, headed by titanium and vanadium, all three metals in each column is a superconductor. In the fourth column Tc's vary between .37 K and .56 K. In the fifth column Tc's are an order of magnitude higher with niobium having the highest at 9.2 K. Skipping over the next few columns headed by magnetic metals we arrive at the column of the precious metals. None of the these is a superconductor. Once again in the next column headed by zinc all three elemental metals are superconductors. Mercury's Tc of 4.2 K is higher than Zn(.8 K) and Cd(.6 K) perhaps due to it's low melting point(-40 C). This brings us to the last column headed by a metal in this case aluminum. All 4 elemental metals are superconductors. Ga(1.1 K) has the lowest Tc while In(3.4 K) has the highest. Of the 5 light elemental metals in the top two rows of the periodic table only aluminum is superconducting! Why? In time will it become possible to calculate its Tc accurately from first principles?

Signature of Nematic Superconductivity in Cu4Bi2Se3: Ginzburg-Landau Theory with External Stress* PYE TON HOW (Presenter), SUNGKIT YIP, Institute of Physics, Academia Sinica — Cu4Bi2Se3 displays superconductivity[1]. It garners considerable interest because Bi2Se3 is a topological insulator. Evidence of two-fold anisotropy suggests that the superconducting phase may be nematic[2, 3]. However, the upper critical field Hc2 also appears two-fold anisotropic[3], and this actually contradicts the nematic hypothesis[4]. A pre-existing "pinning field" could break the symmetry explicitly[4], but then this casts in doubt the interpretation of any two-fold anisotropy. We study the Ginzburg-Landau theory of a nematic order parameter coupled to external stress as a pinning field. We classify possible phase diagrams, and indicate experimental signatures that might distinguish, in a pre-existing pinning field, a true nematic phase from an isotropic phase.

1. Hor et. al. PRL 104, 057001
2. Matano et. al. Nat. Phys. 12, 852
3. Yonezawa et. al. Nat. Phys 13, 123
4. Venderbos et. al. PRB 94, 094522

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Tuesday, March 5, 2019 8:00 AM - 10:24 AM

Session E10 DMP DCOMP: Fe-based Superconductors -- Bulk FeSe

Laser ARPES on Orbital Origin of Extremely Anisotropic Superconducting Gap in FeSe Superconductor* CONG LI (Presenter), DEFA LIU, JIANWEI HUANG, Institute of Physics, Chinese Academy of Sciences, BIN LEI, Department of physics, University of Science and Technology of China, LE WANG, XIANXIN WU, QIANG GAO, YUXIAO ZHANG, XU LIU, YONG HU, LIN ZHAO, SHAOULONG HE, GUODONG LIU, XIAOLI DONG, XIAOWEN JIA, YOUGUO SHI, JIANGPING HU, TAO XIANG, Institute of Physics, Chinese Academy of Sciences, XIANHUI CHEN, Department of physics, University of Science and Technology of China, ZUYAN XU, CHUANGTIAN CHEN, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, XINGJANG ZHOU, Institute of Physics, Chinese Academy of Sciences — We have carried out high resolution laser-based angle-resolved photoemission (ARPES) measurements on bulk FeSe superconductor (Tc=8~9K). We will report direct observation of highly anisotropic Fermi surface and extremely anisotropic superconducting gap in the nematic state of the FeSe superconductor. We find that the low-energy excitations of the entire hole pocket at the Brillouin zone center are dominated by the single dzx orbital. The superconducting gap exhibits an anticorrelation relation with the dzx spectral weight near the Fermi level. These observations provide new insights in understanding the orbital origin of the extremely anisotropic superconducting gap in the FeSe superconductor and the relation between nematicity and superconductivity in the iron-based superconductors.

*This work is supported by the National Key Research and Development Program of China (Grants No. 2016YFA0300300 and No. 2017YFA0302900), the National Natural Science Foundation of China (Grants No. 11334010 and No. 11534007), the National Basic Research Program of China (Grants No. 2015CB921000 and No. 2015CB921300), and the Strategic Priority Research Program (B) of the Chinese Academy of Sciences (Grants No. XDB07020300 and No. XDPB01).
STM studies of Iron-based Superconductor FeSe$_{0.5}$Te$_{0.5}$

ZHENDA GU, CIDAYA MADHAVAN, Department of Physics, University of Illinois Urbana Champaign — Recent studies on the iron-based superconductor, FeSe$_{0.5}$Te$_{0.5}$ have suggested that it is in a topologically non-trivial phase and harbors topological surface states. When these states are gapped by proximity effect, Majorana bound states are expected in the vortex cores, which have been confirmed by STM. In this work we present STM studies of both the vortex core states as well as boundary states in FeSe$_{0.5}$Te$_{0.5}$. Our data provide supporting evidence for the existence of Majorana modes in this system.

*The work was supported by the National Science Foundation and the Department of Energy. The STM component was made possible through the NSF Award DMR-1610143 while the data analysis was funded by the DOE Scanned Probe Division under the Award Number DE-SC0014335.

Itinerant approach to magnetic neutron scattering of FeSe: effect of orbital selectivity

ANDREAS KREISEL (Presenter), Faculty of Physics and Earth Sciences, Universität Leipzig, BRIAN M. ANDERSEN, Niels Bohr Institute, University of Copenhagen, PETER HIRSCHFELD, Univ of Florida - Gainesville — Recent STM experiments and theoretical considerations have highlighted the role of interaction-driven orbital selectivity in FeSe, and its role in generating the extremely anisotropic superconducting gap structure in this material. We study the magnetic excitation spectrum resulting from the coherent quasiparticles within the same renormalized random phase approximation approach used to explain the STM experiments, and show that it agrees well with the low-energy momentum and energy dependent resonance measured by inelastic neutron scattering experiments. We find a correlation-induced suppression of (π,π) scattering due to a small quasiparticle weight of states of d$_{xy}$ character [1]. We compare predictions for twinned and untwinned crystals, and predict in particular a strongly (π,0)-dominated susceptibility at low energies in untwinned systems. These results will be discussed in comparison to recent inelastic neutron scattering on detwinned FeSe.

The same description of the coherent quasiparticles is used to make further predictions of physical observables in FeSe such as the magnetic penetration depth which has recently been examined in detail by μSR experiments [2].


Pressure-induced tetragonal magnetic order in FeSe

ANDREAS KREYSSIG (Presenter), Ames Laboratory, Iowa State University, Dept. of Physics and Astronomy, Ames; ANNA E. BÖHMER, Ames Laboratory, Iowa State University, Ames; Karlsruhe Institute of Technology, Karlsruhe, KARUNAKAR KOTHAPALLI, Ames Laboratory, Iowa State University, Ames; King University, Bristol, WAGEEFA T JAYASEKARA, JOHN M. WILDE, BING LI, Ames Laboratory, Iowa State University, Dept. of Physics and Astronomy, Ames, AASHISH SAPKOTA, Ames Laboratory, Iowa State University, Ames; Brookhaven National Laboratory, Brookhaven, BENJAMIN G. UELAND, Ames Laboratory, Iowa State University, Dept. of Physics and Astronomy, Ames, PINAKI DAS, Ames Laboratory, Iowa State University, Ames; Argonne National Laboratory, Argonne, YUMING XIAO, WENLI BI, JIYONG ZHAO, ESEN ALP, Advanced Photon Source, Argonne National Laboratory, Argonne, SERGEY L. BUD’KO, PAUL C. CANFIELD, ROBERT J. MCQUEEN, ALAN I. GOLDMAN, Ames Laboratory, Iowa State University, Dept. of Physics and Astronomy, Ames — We present a microscopic study of magnetism and lattice distortion on FeSe single crystals by high-energy x-ray diffraction and time-domain Mössbauer spectroscopy over wide temperature and pressure ranges. The magneto-structural ground state can be tuned by pressure from a paramagnetic state with an orthorhombic lattice distortion through a strongly coupled magnetically ordered and orthorhombic state to a magnetically ordered state without an orthorhombic lattice distortion. Close to the reported maximum of the superconducting critical temperature, the orthorhombic distortion suddenly disappears and FeSe remains tetragonal down to the lowest temperature measured. Analysis of the structural and magnetic order parameters suggests an independent origin of the structural and magnetic ordering phenomena, and their cooperative coupling leads to the similarity with the canonical phase diagram of iron pnictides.

*Work at the Ames Laboratory was supported by the U. S. Department of Energy (DOE), BES, Division of Materials Sciences and Engineering, under Contract No. DEAC02-07CH11358. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.
8:48AM E10.00005: Relationship between Superconductivity and Antiferromagnetic Fluctuations in FeSe$_{0.9}$S$_{0.1}$ under Pressure Studied by $^{77}$Se NMR

Khusboo Rana (Presenter), Ames Lab & Dept of Physics and Astronomy, Iowa State University, Paul Wiecki, Anna Boehmer, Institut für Festkörperphysik, Karlsruhe Institute of Technology, Sergey Budko, Paul Canfield, Yuji Furukawa, Ames Lab & Dept of Physics and Astronomy, Iowa State University — Magnetic fluctuations and/or nematic fluctuations are considered to be candidates for the pairing mechanism in unconventional superconductors such as iron pnictide superconductors. Quite recently nuclear magnetic resonance (NMR) measurements revealed strong correlation between superconductivity and antiferromagnetic (AFM) fluctuations despite being near a nematic quantum critical point in FeSe$_{1-x}$S$_x$ [1]. To understand the quantitative relationship between superconductivity and magnetic fluctuations, we carried out $^{77}$Se NMR on the optimally doped FeSe$_{0.9}$S$_{0.1}$ under pressure. In this presentation, we will report the NMR results, especially temperature dependence of nuclear spin lattice relaxation rate under different pressures. Upon analyzing the new together with the previous data [1, 2] we will discuss the relationship between AFM fluctuations and superconductivity in the system.


*This work is supported by the USDOE, Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-07CH11358

9:00AM E10.00006: Evidence for time-reversal symmetry breaking in the superconducting state of FeSe

Kohei Matsura (Presenter), Takaaki Takenaka, Yuichi Sugimura, Takasada Shibauchi, University of Tokyo, Kohtaro Yamakawa, Qi Sheng, Zurab Guguchia, Yasutomo J Uemura, Columbia University, Yipeng Cai, Graeme Luke, McMaster University, Shengli Guo, Licheng Fu, Zhenlong NING, Zhejiang University, Guoqiang Zhao, Guangyang Dai, Chaoqing Jin, Institute of Physics, Chinese Academy of Sciences — The iron-based superconductor FeSe has attracted special attention because it uniquely has a pure nematic phase without a magnetic ordering. It is considered as a key material for investigating the influence of nematicity on superconductivity. The superconducting state inside the nematic phase also has unique properties, and it has been recently proposed that the superconducting order parameter breaks the time-reversal symmetry near the nematic twin boundaries. The lifting of superconducting gap nodes due to twin boundaries has been observed in scanning tunneling spectroscopy and angle-resolved photoemission spectroscopy, which is consistent with the induced imaginary component. However, these measurements of the gap structure provide only indirect evidence for time-reversal symmetry breaking (TRSB), and thus the observation of spontaneous internal magnetic field generated by TRSB is indispensable. Here we report on the zero-field muon spin rotation ($\mu$SR) measurement, which is one of the most sensitive magnetic probes, in high-quality single crystals of FeSe. We find that the relaxation rate starts to grow just below $T_c$ (=9 K). This indicates that weak but finite internal magnetic field is induced in the superconducting state, providing strong evidence for TRSB state in FeSe.

9:12AM E10.00007: Superconductivity and magnetism of S-doped FeSe with a high $T_c$ (≈25-30K) studied via $^{77}$Se-NMR measurements under pressure

Naoki Fujiwara (Presenter), Takanori Kuwayama, Kyoto University, Kohei Matsura, Yuta Mizukami, University of Tokyo, Shigeru Kasahara, Yuji Matsuda, Kyoto University, Takasada Shibauchi, Yoshiya Uwatoko, University of Tokyo — 12%-S doped FeSe system has a high $T_c$ of 25-30 K class under a pressure of 3.0 GPa. We have succeeded in investigating its microscopic properties for the first time via $^{77}$Se-NMR measurements under pressure. We measured the relaxation time ($T_1$), the Knight shift, and the AC susceptibility under pressures up to 3.0 GPa. Unexpectedly, the antiferromagnetic (AFM) fluctuation measured from $1/T_1 T$ at the optimal pressure was strongly suppressed compared to the AFM fluctuation at ambient pressure, despite that the optimal pressure is close to the phase boundary of the AFM phase induced at a high pressure region. In addition, we revealed that the SC phase at an applied field of 6 T exhibited a remarkable double-dome structure in the pressure-temperature phase diagram, unlike the SC phase at zero field. These phenomena are explained by a pressure-induced Lifshitz transition, a topological changes in Fermi surfaces under pressure. The strong AFM fluctuation at ambient pressure is attributable to a hidden AFM quantum critical point.

*The NMR work is supported by JSPS KAKENHI Grant Number JP18H01181 and a grant from Mitsubishi Foundation.
Scaling of the superconducting gap with orbital character in FeSe

LUKE RHODES (Presenter), Department of Physics, Royal Holloway University of London, MATTHEW WATSON, School of Physics and Astronomy, University of St. Andrews, AMIR HAGHIGHIRAD, Institute for Solid State Physics, Karlsruhe Institute of Technology, DANIIIL EVTUSHINSKY, Institute of Physics, Ecole Polytechnique Federale Lausanne, MATTHIAS ESCHRIG, Department of Physics, Royal Holloway University of London, TIMUR KIM, Diamond Light Source — It is often hypothesized that superconductivity in the iron-based superconductors is mediated by a spin-fluctuation pairing mechanism, however direct evidence of this pairing is challenging to obtain. Here we present a high-resolution angle-resolved photoemission spectroscopy (ARPES) study on the three-dimensional superconducting gap of FeSe. We observe a direct scaling between the $d_{xz}$ orbital weight at the Fermi level and the size of the superconducting gap at both the hole and electron pockets. Suggesting that superconducting pairing is mediated by strong, local Coulomb interactions.

We then present an ARPES-derived tight binding model which quantitatively takes into account all the features present in the nematic phase of FeSe; including spin-orbital coupling, nematic ordering, and most crucially the incoherence of an electron pocket. Using this model, we show that the calculated momentum dependence of the superconducting gap, assuming spin-fluctuation mediated superconductivity, directly reproduces the experimental results.

These findings provide both experimental and theoretical support for spin-fluctuation mediated superconductivity in FeSe.


Ultra-long quasiparticle relaxation times in the superconducting state of FeSe

GRAHAM BAKER (Presenter), JAMES DAY, SHUN CHI, RYAN P DAY, RUIXING LIANG, WALTER HARDY, DOUGLAS BONN, University of British Columbia — We report on measurements of the in-plane microwave conductivity of FeSe in the superconducting state. Our measurements were performed from 0.5 to 20 GHz and from 1.2 to 10 K by means of bolometric broadband microwave spectroscopy. In this frequency range, we are sensitive to the charge dynamics of thermally excited quasiparticles. We observe a dramatic narrowing in the conductivity spectra below $T_c$, corresponding to a rapid suppression of quasiparticle scattering. Using a phenomenological model, we extract a temperature-dependent quasiparticle relaxation rate $\Gamma$ from the conductivity, which can be understood as the sum of two contributions. The contribution to $\Gamma$ from inelastic scattering has an exponential temperature dependence. This implies that the excitation spectrum responsible for the inelastic scattering of quasiparticles is electronic in origin and gapped below $T_c$. The contribution to $\Gamma$ from elastic scattering is consistent with Born-limit scattering from a dilute concentration of impurities. At 1.2 K, the quasiparticle relaxation rate reaches a value corresponding to a mean free path greater than 100 $\mu$m.

Anisotropic Vortex Pinning in Single Crystal FeSe

IRENE ZHANG (Presenter), LOGAN BISHOP-VAN HORN, JOHANNA PALMSTROM, JOHN ROBERT KIRTLEY, YUSUKE IGUCHI, IAN R FISHER, KATHRYN ANN MOLER, Stanford University — Iron-based superconductors are known for their complex interplay between magnetic, nematic, and superconducting order. FeSe is an iron-based superconductor with a structural transition at 90 K without the appearance of magnetic ordering. The lack of magnetic order allows us to probe the superconducting transition of an iron-based superconductor from a purely nematic phase. We study single crystal FeSe using a scanning SQUID microscope that has both a field coil to apply a local magnetic field and a pickup loop to measure the vortex response. We model the effect of the SQUID geometry on vortex motion in an anisotropic pinning potential and find that SQUID orientation has a significant effect. Our initial findings suggest that the pinning potential anisotropy aligns with twin domain boundaries produced by the structural transition. We also check for correlation between spatial variation in diamagnetic response and anisotropy. These studies will help elucidate whether the relationship between nematic and superconducting order in these materials is competing or enhancing.

*This work was supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-76SF00515.
10:00AM E10.00011: Quantum vortex core and missing pseudogap in the multi-band BCS-BEC-crossover superconductor FeSe

TETSUO HANAGURI (Presenter), RIKEN CEMS, SHIGERU KASAHARA, Dept of Physics, Kyoto Univ., JAKOB BOKER, ILYA EREMIN, Theoretische Physik III, Ruhr-Univ. Bochum, TAKASADA SHIBAUCHI, Dept. Adv. Mat. Sci., Univ. Tokyo, YUJI MATSUDA, Dept of Physics, Kyoto Univ. — The iron-based superconductor FeSe is considered to be in the BCS-BEC crossover regime where the superconducting gap is comparable to the Fermi energy. We performed spectroscopic-imaging scanning tunneling microscopy to search for spectroscopic signatures of the BCS-BEC crossover. The large superconducting-gap to Fermi-energy ratio may yield well separated discrete bound states in the vortex core, as well as a pseudogap above the superconducting transition temperature due to preformed Cooper pairs. We found a signature of the discrete vortex bound states but could not detect the pseudogap. We argue that these conflicting observations can be resolved if multi-band nature is taken into account.

*This work was supported by KAKENHI (Grant Nos. 15H02106, 15H05852, 16H04024, 18H01177, and 18H05227) and by the joint DFG-ANR Project (No.ER463/8-1) and DAAD PPP USA Grant No.N57316180.

10:12AM E10.00012: Superconductivity fluctuation in FeSe investigated by magnetic torque measurement using optical interference

HIDEYUKI TAKAHASHI, Kobe University, FUYUKI NABESHIMA, RYO OGAWA, Department of Pure and Applied Sciences, University of Tokyo, EIJJI OHMICHI, HITOSHI OHTA, Kobe University, ATSUTAKA MAEDA (Presenter), Department of Pure and Applied Sciences, University of Tokyo — We investigated the superconducting fluctuation (SCF) in FeSe by a magnetic torque measurement. This material has a large ratio of the superconducting gap to Fermi Energy, and is proposed to be located in BCS-BEC crossover regime [1]. In our method, the absolute value of the cantilever displacement can be measured with high resolution by detecting the interference intensity of the Fabry-Perot type cavity formed between the cantilever and the optical fiber. We observed SCF signal originating from the surviving vortex liquid state, whose onset temperature increases up to above 1.5 Tc in high magnetic field. Its contribution to the magnetic torque is about 0.5 % of that of the total sample magnetization at 10 K and 10 T. These features are totally different, both qualitatively and quantitatively, from those of the signal observed in the previous torque magnetometry study using a piezoresistive cantilever[1], while similar to what reported in cuprate superconductors [2]. Therefore, we conclude that SCF in FeSe is not anomalous and it can be understood in the same framework as other superconductors using Ginzburg number.


Tuesday, March 5, 2019 8:00 AM - 10:24 AM

Session E11 DMP DCOMP FIAP: Defects in Semiconductors -- Oxides BCEC 152 - Leonard Brillson, Ohio State University - Tag(s): Focus

8:00AM E11.00001: Electronic states in electron-doped rare-earth nickelates from first principles*[Invited] MICHELE KOTIUGA (Presenter), Rutgers University, New Brunswick — Correlation effects in transition metal based materials give rise to many interesting and exotic properties. The rare-earth nickelates, with a rich composition-phase diagram, are no exception. Doping rare-earth nickelates can lead to electron localization, introducing defect states that are unlike typical shallow or deep donor states familiar in conventional semiconductors. We present first-principles density-functional-theory-based calculations of rare-earth nickelates, with a focus on lanthanum nickelate and samarium nickelate, in which we add electrons to the material. Here, we investigate doping concentrations on the order of one electron per formula unit with the goal of changing the orbital occupation and triggering a phase transition, akin to the phase control seen with strain modulation. We carry out calculations where a uniform compensating background charge (jellium*) has been added to maintain charge neutrality when electrons are added, as well as supercell configurations with defects that electron dope the system, and superlattices where an electron is transferred at interfacial layers. In particular, we explore the effects of intercalated hydrogen and lithium as well as oxygen vacancies in samarium nickelate as well as lanthanum nickelate/strontium iridate superlattices. In comparing these calculations, we find the jellium-background calculations capture the changes to the electronic structure seen with the explicit inclusion of defects and interfaces. The resulting changes to the electronic structure, intimately linked to structural changes, cannot be understood with a rigid shift of the states: the bands are reorganized and the character of the gap is fundamentally altered. This class of doping effects introduces a new knob to turn in the field of materials design.

*We acknowledge financial support from Office of Naval Research Grant N00014-17-1-2770
8:36AM E11.00002: Energy Band Gap Tuning based on Ag doped LaFeO3 Nano-porous*  WAFAA AZOUZI (Presenter), Physics Department, Mohammed V University -Rabat, HICHAM LABRIM, DERS, Centre National de l’Energie, des Sciences et des Techniques Nucléaires / Rabat, MOHAMMED BENAÏSSA, Physics Department, Mohammed V University -Rabat — porous lanthanum ferrite LaFeO3 has been elaborated with wet chemical method. We have employed both DFT simulation and Rietveld refinement to understand deeply the complex optical behavior accurate in synthesized Nano-powders [1], with different amount of silver as dopant, and also evaluate the stoichiometry-optical properties relationship in this insulator oxide. It found that all samples, with different gap value depending on the silver concentration, exhibit a p-type semiconductor with a direct gap in the visible light spectrum. The results showed that lanthanum defects present in the synthesized samples improve optical absorption [2] in the visible range comparing with bulk calculated spectrum making it potentially useful in solar photovoltaic application.


*We thank :  
The University Mohammed V -Morocco  
Centre National pour la Recherche Scientifique et Technique / Rabat (CNRST) -Morocco  
Centre National de l’Energie, des Sciences et des Techniques Nucléaires / Rabat (CNESTEN) -Morocco

8:48AM E11.00003: The role of hydrogen in the persistent photoconductivity of SrTiO3*  ZHIQIANG ZHANG (Presenter), Physics and Astronomy, University of Delaware, ANDERSON JANOTTI, Department of Materials Science & Engineering, University of Delaware — Strontium titanate (STO) is a perovskite oxide with an indirect bandgap of 3.25 eV at room temperature. It has been often used as substrate to grow other materials, and it is the basis of widely reported perovskite heterostructures that show high-density two-dimensional electron gas. Recently, an extremely long persistent photoconductivity (PPC) at room temperature has been observed in annealed strontium titanate single crystals upon illumination with sub-gap light [M. C. Tarun, F. A. Selim, and M. D. McCluskey, Phys. Rev. Letters, 111, 187403 (2013)]. Annealed studies indicate the importance of hydrogen impurities as well as oxygen vacancies to induce PPC. We use electronic structure calculations based on density functional theory (DFT) to investigate possible mechanisms behind the PPC effect. We present results of defect formation energies, defect-related absorption, and defect migration barriers, in an attempt to identify the defect associated with the observed PPC in STO. The results are combined to explain the experimental observations, and we further generalize the model to predict similar effects in other oxide like TiO2 and BaTiO3.

*This work was supported by the National Science Foundation Faculty Early Career Development Program DMR-1652994.

9:00AM E11.00004: Characterization and modulation of oxygen vacancy defects in metal/SrTiO3-δ Schottky heterojunctions  HAOMING JIN (Presenter), XIAOCHEN ZHU, ARTHUR F HEBARD, University of Florida — Strontium titanate, SrTiO3-δ (STO), can be made semiconducting and even metallic using high temperature anneals by introducing oxygen vacancy defects (δ > 0). Controlled thermal anneals with various temperatures and durations are employed to create specific defect profiles near the STO surfaces. Thermal sublimation or e-beam evaporation technique is then used to apply gold (Au) contact electrodes to the thermally treated STO substrates and create Schottky junctions. The presence of the oxygen vacancy defects strongly alters the electrical properties of these junctions as measured by transport, capacitance and low frequency noise. Our comparative study of these Schottky Au/STO junctions reveals that (i) the concentration of oxygen vacancy defects increases at the higher annealing temperature (ii) an improved spatial distribution/uniformity of defects is obtained by either lengthening the annealing duration or raising the annealing temperature. We show that the electrical characterizations of Schottky junction discussed here can serve as a useful tool to probe defects near the interfaces of novel materials and unravel information that is not easily accessed by other approaches.
9:12AM E11.00005: Doping in perovskite stannates* SANTOSH KC (Presenter), University of California, Santa Barbara, CA 93106, USA, LEIGH WESTON, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, CHRIS VAN DE WALLE, University of California, Santa Barbara, CA 93106, USA — The perovskite stannates (A\text{SnO}_3; A = Ba, Sr, Ca) are being actively explored for potential applications as transparent conducting oxides (TCOs) and in oxide electronics. To realize this potential, doping needs to be controlled. Using first-principles hybrid density functional calculations, we have performed comprehensive investigations of La donors as well as various types of defects. We examine the impact on doping as a function of growth conditions and impurity concentrations. For native defects, we investigate not only vacancies but also antisites. Trends among the various materials in the family (BaSnO3, SrSnO3, and CaSnO3) are analyzed. Our results identify optimum growth conditions for high n-type doping and identify defects that are most likely to impact device properties.

*Work supported by ONR.

9:24AM E11.00006: The Effects of Excess Charge Carriers in BiVO4* IFLAH LARAIB (Presenter), MARCIANO ALVES CARNEIRO, ANDERSON JANOTTI, Materials Science and Engineering, University of Delaware — Research on photoelectrochemical (PEC) performance of BiVO4 has gained momentum in the past few decades due to the potentially low cost solar-to-hydrogen conversion pathway provided by using this material as a PEC cell anode. While this material exists in four different phases, it is only its monoclinic phase doped with n-type carriers that exhibits significant PEC activity. These carriers typically involve hydrogenation, which supposedly introduces hydrogen interstitial and oxygen vacancy defects in the lattice. In this work, we use density functional theory calculations to explore the effects of excess n-type carriers on the structure and electronic properties of BiVO4, focusing on the most prominent tetragonal and monoclinic phases, and link it to its enhanced photo activity and possible carrier localization through electron small-polaron formation. The obtained results are compared to previous calculations and available experimental findings.

*This work was supported by the National Science Foundation Faculty Early Career Development Program DMR-1652994.

9:36AM E11.00007: Role of Point Defects in Enhancing the Conductivity of BiVO4 HOSUNG SEO, Department of Physics and Department of Energy Systems Research, Ajou University, YUAN PING (Presenter), Department of Chemistry and Biochemistry, University of California Santa Cruz, GIULIA GALLI, The Institute for Molecular Engineering, University of Chicago — Bismuth vanadate (BiVO4) is a promising photoanode for solar-to-fuel photocatalytic applications, and it has been extensively studied in recent years. However, the microscopic mechanism underlying the observed changes in electronic conductivity due to oxygen vacancies and nitrogen dopants remains unclear. Here, we combine electronic structure calculations at the hybrid density functional theory (DFT) level with constrained DFT, and we elucidate the role of defects in enhancing the transport properties of the material [1]. We show that at low temperature, oxygen vacancies give rise to deep levels within the fundamental gap of BiVO4; however even as deep levels, oxygen vacancies can act as effective n-dopants and polaronic charge carriers, due to their favorable position in energy relative to polarons in the pristine bulk. In addition, we show that N atoms can be easily introduced in n-doped BiVO4 and that the presence of substitutional nitrogen affects the formation energy of polarons, effectively contributing to an increase of the carrier mobility in the material. Our results reconcile apparently conflicting experiments and they may provide a foundation for polaronic defect engineering for photoanodes oxides. [1] H. Seo et al, Chem. Mater.

DOI: 10.1021/acsmatter.8b03201
Computational Study of LiGaO₂ Electron Paramagnetic Resonance Spectra of Li and Ga Vacancies

DMITRY SKACHKOV (Presenter), WALTER R L LAMBRrecht, Case Western Reserve University — LiGaO₂ is an ultra-wide-band-gap material with a wurtzite-like crystal structure and band gap of 5.3 eV. Electron paramagnetic resonance (EPR) experiments on irradiated samples of this material were recently published by Lenyk et al. (J. Appl. Phys. 124, 135702, 2018). In the present work, density functional theory (DFT) calculations are carried out of the Ga and Li vacancies using the DFT+U approach in the charge states which carry an unpaired spin. In both vacancies the p-hole is located on one oxygen atom adjacent to the vacancy. Apical O and basal plane O are considered. The magnetic resonance parameters of the defects are determined using the Gauge Including Projector Augmented Wave (GIPAW) method. The EPR spectra of VGa²⁻ is characterized by a quasi-isotropic superhyperfine interaction with one Ga nucleus and for the apical O spin gives a g-tensor with maximum oriented along b axis. For VLi⁰ there is a quasi-isotropic superhyperfine interaction with two Ga nuclei and the g-tensor maximum is along c for the basal plane O spin. Both of these are in agreement with experiment but we predict also the g-tensors for the other possible localization of the spins. The energy ordering and transition levels for the different models will be discussed.

Towards bipolar tin monoxide: revealing unexplored dopants

JOSE FLORES LIVAS (Presenter), MIGLE GRAUZINYTE, STEFAN A C GOEDECKER, University of Basel — The advancement of transparent electronics, one of the most anticipated technological developments for the future, is currently inhibited by a shortage of high performance p-type semiconductors. Recent demonstration of tin monoxide as a successful transparent p-type thin film transistor and the discovery of its potential for ambipolar doping, suggests that tin monoxide -- an environmentally friendly earth-abundant material -- could offer a solution to this challenge. With the aim of enhancing the electronic properties, an extensive search for useful dopant elements was performed. Substitutional doping with the family of alkali metals was identified as a successful route to increase the concentration of acceptors in SnO and over ten shallow donors, that to the best of our knowledge have not been previously contemplated, were discovered. During this talk I will present a detailed analysis of the most promising n-/p-type dopants -- offering new insights into the design of an ambipolar SnO. If synthesized successfully, such a doped ambipolar oxide could open new avenues for many transparent technologies.

Experimental and computational evidence of defect centres in amorphous titanium dioxide and their confluence in resistive switching

DIP DAS (Presenter), ARABINDA BARMAN, Department of Physics, Shiv Nadar University, ANIL KUMAR SINHA, AD-XRD Lab, Indus-2 Synchrotron Utilization Division, Raja Ramanna Center for Advanced Technology (RRCAT), MUKUL GUPTA, SIMS Lab, UGC-DAE Consortium for Scientific Research, D. M. PHASE, Beamline Lab, UGC-DAE Consortium for Scientific Research, RAHUL SINGHAL, Department of Physics, Malaviya National Institute of Technology, SERGEI ZVYAGIN, High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), PRIYA JOHARI, ALOKE KANJILAL, Department of Physics, Shiv Nadar University — This work identifies dominant defect centres in amorphous titanium dioxide (a-TiO₂) films and their role in resistive random access memories with the help of combined experimental and theoretical studies. X-ray absorption spectroscopy reveals a significant decrease in peak splitting between t₂g and e₈ sub-bands at the Ti-L edge, which is attributed to lower valence of Ti-ions. Deconvolution of the Ti-2p X-ray photoelectron spectrum also suggests the existence of Ti³⁺ state along with oxygen vacancies in a-TiO₂. Further, the role of oxygen vacancies as intrinsic electron trapping centres in such system is recognized by low-temperature electron paramagnetic resonance measurements. The same has been verified using ab-initio density functional theory based simulations for a-TiO₂ phase, generated using ab-initio molecular dynamics simulations. The partial charge density and Bader charge analysis were done, in particular, to manifest the localized character of the excess electrons ejected during the creation of oxygen vacancies. Such electronic localisations facilitate local high conducting regions in the amorphous matrix, which in turn leads to forming free resistive switching behaviour in Pt/a-TiO₂/Pt devices.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E12 DMP: Devices from 2D Materials -- Sensors
8:00AM E12.00001: Graphene and Black Phosphorus Infrared Photodetectors* [Invited]  FENGNIAN XIA (Presenter), QIUSHI GUO, BINGCHEN DENG, XIAOLONG CHEN, Yale Univ — In this talk, we will discuss latest development on infrared photodetectors based on graphene and black phosphorus. We will first cover graphene plasmon-enhanced mid-infrared photodetectors in which the detection leverages the bolometric effect in graphene nanoribbons. Then we will review the infrared detection properties of black phosphorus. Gated tunable black phosphorus photodetectors will also be presented, in which the bandgap of black phosphorus is tuned for the light detection up to the wavelength of around 8 μm. Finally we will compare the performance of infrared photodetectors based on graphene and black phosphorus and discuss their possible applications.

*National Science Foundation, Office of Naval Research and Air Force Office of Scientific Research

8:36AM E12.00002: A fast, sensitive, room-temperature graphene nanomechanical bolometer*  ANDREW BLAIKIE (Presenter), DAVID MILLER, BENJAMIN J ALEMAN, University of Oregon — Bolometers are a powerful and vital means of detecting light in the IR to THz frequencies, and have been adopted for applications ranging from astronomy to thermal imaging. As uses diversify there is an increasing demand for faster, more sensitive room-temperature bolometers. To this end, graphene has generated interest because of its vanishingly small heat capacity and its intrinsic ultra-broadband absorption, properties that would allow it quickly detect low levels of light of nearly any color. Yet, it is challenging to operate a traditional electrical graphene bolometer at room temperature due to its weakly temperature-dependent resistivity and high thermal conductivity. Our method overcomes these challenges with a simple approach that employs suspended graphene as a nanomechanical bolometer, where absorbed light is detected as shift in its mechanical resonance frequency. We report on the measured sensitivity and response bandwidth of these graphene nanomechanical bolometers, which compare favorably to the state-of-the-art. Furthermore, we model the response of these devices and discuss a path to reach femtowatt sensitivity at room temperature.

*This work was supported by the University of Oregon and the National Science Foundation under grant No. DMR-1532225.

8:48AM E12.00003: Transient and Flexible Photodetectors  SHIH-YAO LIN, GOLAM HAIDER, YU-MING LIAO, CHEN-YOU SU (Presenter), YANG-FANG CHEN, Physics, National Taiwan University — With the rapid development of technology, electronic devices have become omnipresent in our daily life as they have brought much convenience in human activity. Side-by-side, electronic waste has become a global environmental burden creating an ever-growing ecological problem. The transient device technology in which the devices can physically disappear completely in different environmental conditions has attracted widespread attention in recent years owing to its emerging application potential spanning from biomedical to military use. In this work, we demonstrated the first attempt for a dissolvable ecofriendly flexible photodetector using a hybrid of graphene and chlorophyll on a PVA substrate. The whole device can physically disappear in aqueous solutions in a time span of ~30 min, while it shows a photoresponsivity of ~200 A W−1 under ambient conditions. The high carrier mobility of graphene and strong absorption strength of a green photon harvesting layer, chlorophyll, result in the photocurrent gain of the device as high as 103 with subsecond response time under the illumination of red light. The newly designed photodetector shown here yields zero waste with a minimum impact on the environment, which is very useful for the development of the sustainability of our planet.

9:00AM E12.00004: Electromechanical resonators based on h-BN graphene heterostructures  ROHIT KUMAR (Presenter), DERIC W SESSION, HARRISON PAAS, RYUICHI TSUCHIKAWA, VIKRAM DESHPANDE, University of Utah — The exceptional robustness, stability, ultra-low weight, and high tunability are some of the most intriguing attributes of 2D atomically thin crystals like graphene, MoS2 to name a few. These remarkable properties make them promising candidates for a new generation of nanoelectromechanical systems (NEMS). Many microelectromechanical (MEMS) sensors used today employ two or more layers of different materials; however, the area of 2D heterostructure based NEMS has not been explored much. In this study, we discuss the fabrication and characterization of circular heterostructure resonators based on hexagonal boron nitride (h-BN) and graphene stacks. The stacks are electrically actuated and measured using the vector network analyzer (VNA) from room temperature down to cryogenic temperatures. h-BN graphene provides a flat and clean interface and resonators are tunable with gate voltage. The temperature dependence of strain induced in resonators of different thicknesses will be discussed.
Graphene-enabled and directed nanomaterial placement from solution for large-scale device integration*

MICHAEL ENGEL, IBM Research - Brazil, DAMON FARMER, IBM Research - USA, JAIONE TIRAPU AZPIROZ, IBM Research - Brazil, JUNG-WOO T. SEO, JOOHOOON KANG, Department of Materials Science and Engineering and Department of Chemistry, Northwestern University, PHAEDON AVOURIS, IBM Research - USA, MARK HERSAM, Department of Materials Science and Engineering and Department of Chemistry, Northwestern University, RALPH KRUPKE, Institute of Nanotechnology, Karlsruhe Institute of Technology, MATHIAS B STEINER (Presenter), IBM Research - Brazil — In this presentation we report on a process for electric-field assisted placement of nanomaterials from solution using large-scale graphene layers having patterned nanoscale deposition sites. The patterned graphene layers are prepared via either transfer or synthesis on standard substrates, then are removed once nanomaterial deposition is completed, resulting in material assemblies with nanoscale resolution that cover surface areas larger than 1mm². In order to demonstrate the universality of this approach, we have assembled representative zero-, one-, and two-dimensional semiconductors at predefined substrate locations and integrated them into nanoelectronic devices. Finally, we explore the scaling behavior of this approach for integration of high performance nanoelectronic devices.

*W.T.S. and M.C.H acknowledge support from the National Science Foundation (DMR-1505849)

Chemical Vapor Sensing with Transition Metal Dichalcogenides via Photoluminescence Modulation

AUBREY HANBICKI (Presenter), PAUL MICHAEL CAMPBELL, United States Naval Research Laboratory, SAUJAN SIVARAM, NRC Postdoc at Naval Research Laboratory, ANDREW KUSTERBECK, Nova Research Inc., VIET NGUYEN, R. ANDREW MCGILL, KATHLEEN MCCREARY, BEREND JONKER, ENRIQUE COBAS, F. KEITH PERKINS, United States Naval Research Laboratory, ADAM FRIEDMAN, Laboratory for Physical Sciences — Two-dimensional transition metal dichalcogenides (TMDs) such as MoS₂ and MoSe₂ are promising materials for chemical vapor sensing applications. Their potential includes straightforward fabrication, readily available materials, and good selectivity, sensitivity, and speed of response. Another attractive aspect is that they have been shown to detect chemical vapors and gases in several ways. More commonly, sensors have been fabricated based on the chemiresistive device properties. Here, however we will discuss our recent studies implementing TMD sensors using the optical properties, in particular the photoluminescence (PL) as the core element of the sensor. We examine the PL of MoSe₂ while it is exposed to strong electron donor gases such as triethylamine. There is a fast and significant decrease in the PL upon exposure with PL reduction by as much as 75% during exposure. When the vapor is turned off, the PL quickly recovers indicating fast adsorption/desorption of the analyte. We compare the temporal response and sensitivity of the PL with that of the electrical change in conductivity and analyze the data in terms of possible applications to chemical vapor sensing of chemicals relevant to nerve gas and explosive sensing. This work was supported by core programs at NRL.

Raman enhancement of blood constituent proteins using graphene

SHENGXI HUANG (Presenter), Pennsylvania State University, RISHIKESH PANDEY, University of Connecticut School of Medicine, ISHAN BARMAN, Johns Hopkins University, JING KONG, MILDRED DRESSELHAUS, Massachusetts Institute of Technology — Raman spectroscopy has drawn considerable attention in biomedical sensing due to the promise of label-free, multiplexed and objective analysis along with the ability to gain molecular insights into complex biological samples. However, its true potential is yet to be realized due to the intrinsically weak Raman signal. Here, we report a simple, inexpensive and reproducible signal enhancement strategy featuring graphene as a substrate. Taking key blood constituent proteins as representative examples, we show that Raman spectra acquired from biomacromolecules can be reproducibly enhanced when these molecules are placed in contact with graphene. In particular, we demonstrate that hemoglobin and albumin display significant, but different, enhancement with the enhancement factor depending on the Raman modes, excitation wavelengths and analyte concentrations. This technique offers a new strategy for label-free biosensing owing to the molecular fingerprinting capability, signal reliability, and simplicity of the enhancement method.
Effect of oxygen adsorption on electron transport in few-layer InSe FETs

ARVIND SHANKAR KUMAR (Presenter), Case Western Reserve University, RAJESH KUMAR, RAMAN SANKAR, FANGCHENG CHOU, National Taiwan University, XUAN GAO, Case Western Reserve University — The oxidation effect in 2D chalcogenides is a well-known problem in 2D materials. We investigate the adsorption of oxygen molecules on the surface of few layer InSe FETs through transconductance and time dependent conductance measurements. We observe a positive shift of threshold voltage when few-layer InSe FET devices are exposed to oxygen (corresponding to a reduction in electron density in the order of $10^{12} \text{ cm}^{-2}$ for an oxygen pressure of 60 Torr) which is partially reversible through applying gate stress. Time dependent measurements show a drop in conductivity up to a factor of 5 when exposed to 5 Torr of oxygen gas, over the time scale of the order of 1000 seconds. From these results, we characterize the oxygen sensing response of few-layer InSe devices, and discuss the implications on the underlying binding interaction between oxygen molecules and InSe. Nitrogen exposure, on the other hand, did not yield appreciable change in InSe FET’s characteristics.

*The authors thank NSF (grant number: DMR-1607631) for funding the project.

Broadband and high responsivity graphene-based photodetectors by engineering atomic-layer-deposition dielectric films

HO VINH (Presenter), YIZHOU WANG, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech, MICHAEL P. COONEY, NASA Langley Research Center, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — Ability to covert light of graphene occurs in an ultra-broadband spectral range from violet to mid-infrared region, making graphene as desirable photodetectors for various technology applications in imaging, sensing, spectroscopy and telecommunication. However, the low responsivity of graphene photodetectors about 10 mA/W, due to the ultra-fast recombination of photocarriers, limits their potential applications. Here, we have engineered the interface between graphene and atomic-layer-deposited dielectric films to introduce trapping centrals supporting the highly light reactive of photodetectors. Our graphene-based photodetectors have showed a high sensitivity up to $2 \times 10^5 \text{ A/W}$ together with a fast response time in a broadband spectral at room temperature.

*The authors gratefully acknowledge the financial support of this effort by IRAD and ESTO programs from NASA Langley Research Center’s Office of Chief Technologist.

Electronic Detection of Oxygen Adsorption and Size-Specific Doping of Few-Atom Gold Clusters on Graphene

SHUANGLONG LIU (Presenter), University of Florida, JEROEN SCHEERDER, VYACHESLAV ZHARINOV, KU Leuven, NICOLAS RECKINGER, JEAN-FRANÇOIS COLOMER, University of Namur, JORIS VAN DE VONDEL, EWALD JANSSENS, KU Leuven, HAI-PING CHENG, University of Florida — Graphene has potential application as sensor due to its sensitivity to adsorbed particles. Few-atom clusters are promising candidates as adparticles on graphene. In this joint experimental and computational work, we investigate size-selected gold clusters with 3 and 6 atoms adsorbed on graphene field-effect transistors and their interaction with molecular oxygen. We find that the doping level of graphene significantly depends on the cluster size, in the absence or presence of oxygen molecules. Furthermore, the doping of 3-atom gold cluster decorated graphene changes sign from n- to p-doping upon oxygen adsorption, directly evidencing electron transfer to the oxygen molecules and hence their activation. As such, graphene promises to be a valuable platform to investigate and exploit size-dependent cluster properties. The presentation covers mainly the theoretical aspects of the work, namely density functional theory (DFT) based simulations of adsorption site, adsorption energy, atomic configuration, and electronic structure.

*This work is supported by the KU Leuven Internal Research Fund C14/17/080. H.-P. C. acknowledges the US DOE/BES DE-FG02-02ER45995 for supporting the computational work. Part of the study received funding from the European Union H2020 program, project No 649953.

HYEONDEOK SHIN (Presenter), YE LUO, ANOUAR BENALI, Argonne National Laboratory, YONGKYUNG KWON, Physics, Konkuk University — Diffusion Monte Carlo (DMC) calculations were performed for an accurate description of the nature of the $O_2$ adsorption on a single layer graphene. We investigated the stable orientation of $O_2$ as well as its equilibrium adsorption distance and energy for a specific adsorption site. At equilibrium adsorption distances, an $O_2$ was found to prefer a horizontal orientation, where the O-O bond is parallel to the graphene surface, to the vertical orientation. However, the vertical orientation is favored at the $O_2$-graphene distance shorter than the equilibrium distance, which could be understood by their steric repulsion. Contrary to previous DFT calculations, our DMC calculations show that the most energetically-stable adsorption site for $O_2$ is not the center of a hexagonal ring but the midpoint of a C-C bond. The $O_2$ adsorption energy at a bridge site was estimated to be 0.135(4) eV, which is in good agreement with the recently-reported experimental value [1]. Finally, we have found that $O_2$ is very diffusive on the surface of graphene with the diffusion barrier along a bridge-hollow-bridge path being as small as $\sim 10$ meV.


*This work is supported by the U.S. DOE as part of the Center for Predictive Simulation of Functional Materials.

10:36AM E12.00012: Reproducible fabrication of graphene field effect transistors for detection of CA1

NARENDRA KUMAR (Presenter), Physics, Boston College, ANDREW WEBER, Giner Inc., MASON GRAY, Physics, Boston College, JUAN C. ORTIZ-MARQUEZ, Biology, Boston College, CAMERON RICHARD DESMOND, MATTHEW CATALANO, Physics, Boston College, AVNI ARGUN, Giner Inc., TIM VAN OPJNEN, Biology, Boston College, KENNETH BURCH, Physics, Boston College — The ultra-sensitivity of graphene field effect transistors (GFETs) to any chemical or biological interaction on the surface makes them a potential candidate for miniaturized label free biosensors. The reproducibility and stability remain key challenges for GFETs based biosensors as they are also sensitive to environment and chemicals used during fabrication. In this work, the reproducible GFET devices were fabricated inside a glove box in argon environment using monolayer graphene. The fabricated devices showed the charge neutrality point (CNP) of 0±10V in the back gate mode while ~0.5V in top liquid gate mode using Pt wire as pseudo reference electrode. Finally, the fabricated devices were utilized for detection of carbonic anhydrase 1 (CA1) in phosphate buffer solution (PBS) as well as CA1 spiked diluted human saliva samples using RNA aptamer as probes. I will discuss the various limits of detection and sensitivity to non-specific targets.

*Giner Inc. 89 Rumford Avenue, Newton, MA, USA 02466

10:48AM E12.00013: Fabrication of lithographic and self-organized graphene ribbons grown on SiC

BIYI WU (Presenter), NIST, Natl Taiwan Univ, YANFEI YANG, ALBERT RIGOSI, JIUNING HU, HSIN-YEN LEE, MATTIAS KRUSKOPF, HANBYUL JIN, RANDOLPH E ELMQUIST, NIST, CHI-TE LIANG, Natl Taiwan Univ — It has been shown that the edge properties play an important role in transport in narrow ribbons. In this work, we prepare two types of graphene ribbons within a few hundred nm by vastly different fabrication techniques to discuss the edge effects. The first type of samples is made by electron-beam lithography and conventional RIE etching processes. Strong negative magnetoresistance (MR) behavior is observed due to the consequence of disorder in the edge structure (e.g. chemical dopants, the resolution of e-beam lithography and so on). The second type of ribbons on SiC is self-organized, and grown “naturally” (i.e., similar to the way large-area monolayer graphene can be prepared by high-temperature Si sublimation [1]), which guarantees cleaner and more uniform edges. At low magnetic fields, the MR curve shows evidence for weak localization due to intervalley scattering from the sharp edges. With increasing magnetic field, quantum transport described by boundary scattering in the quasi-ballistic regime can be observed [2]. The scattering mechanism of self-organized ribbons is totally different from that of the etched one due to the edge effects.

References

Tuesday, March 5, 2019 8:00 AM - 10:48 AM

Session E13 DMP: 2D Materials (General) -- Growth, Mostly CVD/T
8:00AM E13.00001: Interaction of Two-Dimensional Transition Metal Dichalcogenides on Different Substrates and Nanostructures*  
ANDREW GREENSPON (Presenter), John A. Paulson School of Engineering and Applied Sciences, Harvard University, QINGQING JI, Research Laboratory of Electronics, Massachusetts Institute of Technology, MENA N GADALLA, DANQING WANG, NIAMH MULHOLLAND, John A. Paulson School of Engineering and Applied Sciences, Harvard University, JING KONG, Research Laboratory of Electronics, Massachusetts Institute of Technology, EVELYN L HU, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Two-dimensional transition metal dichalcogenides (2D TMDs) are 2D semiconductors that hold promise for a variety of optoelectronic devices, especially by harnessing the valley degree of freedom. Growth of 2D TMDs on different substrates and nanostructures provides enormous opportunities in engineering ultra-thin devices with tailored optical emission properties. We characterize the optical differences when the 2D TMD molybdenum disulfide (MoS2) is grown via chemical vapor deposition on the substrates silicon dioxide on silicon, gallium nitride (GaN), and silicon carbide (SiC). Changes in the spacing and relative intensity of the E12g and A1g Raman peaks suggest differences in the microstructure of the grown MoS2 or its interaction with the substrate. Additionally, we characterize the interaction between MoS2 and optical cavities patterned onto GaN and SiC. Preliminary results show brighter MoS2 exciton photoluminescence and shifted emission peaks on the optical cavities compared to the bulk substrate of each. We also show first results attempting to couple MoS2 emission to the resonant modes of these optical cavities.

*STC Center for Integrated Quantum Materials, NSF grant DMR-1231319.  
The Center for Nanoscale Systems at Harvard University is supported under NSF grant ECCS-1541959.

8:12AM E13.00002: The effect of multi-step Cu surface oxidization on growth of single crystal graphene by low pressure chemical vapor deposition*  
SAJITH WITHANAGE (Presenter), THARANGA NANAYAKKARA, BINUKA GUNAWARDANA, C. RASADI MUNASINGHE, U. KUSHAN WIJEWARDENA, RASANGA SAMARAWEERA, ANNIKA KRISA, RAMESH MANI, Physics & Astronomy, Georgia State University — There has been much recent interest in the growth large area single crystal graphene flakes as an approach for overcoming the relatively low carrier mobility and the multigrain structure observed in Chemical Vapor Deposition (CVD) graphene. [1] One approach for growing large-sized single crystal graphene by CVD, [2] involves limiting the nucleation density of graphene on the copper foil surface that is often used as a catalyst for the growth of CVD graphene. Here, we report the results of a study of CVD growth of graphene following surface modification of the copper foil by oxidizing the copper foil at different stages of the growth process. Thus, we detail the effect of copper surface oxidization at different steps of the growth for controlling the nucleation on the size and the quality of relatively large sized single crystal graphene flakes. The graphene layers are characterized by various methods and the results of the study are reported.

*This work was supported by the NSF under Grant No. ECCS-1710302, and by the ARO under Grant No. W911NF-15-1-0433.

8:24AM E13.00003: Tempered Dewetting of Metal Films: A platform for networked 2D crystal membranes*  
JOSE FONSECA VEGA (Presenter), JAMES CLIFFORD CULBERTSON, MAXIM ZALALUTDINOV, CORY D CRESS, JEREMY T ROBINSON, United States Naval Research Laboratory — The controlled dewetting and recrystallization of metal films with two-dimensional (2D) crystal over-layers enables the formation of highly textured metallic films, together with a network of metallic pores and suspended 2D crystal membranes. Mechanically-exfoliated and chemical-vapor deposited (CVD-grown) 2D crystals (e.g., graphene, h-BN, and transition-metal dichalcogenides (TMDs)) were transferred on top of metallic thin films on SiO2/Si substrates to modify the dewetting and recrystallization dynamics. After heat treatment, metal films capped with 2D crystals become textured and form pores that can span up to 60% of the planar surface area, depending on annealing conditions and 2D crystal quality. The network of suspended membranes was found to have significantly different optical and electronic properties than the supported regions. For example, enhancement in photoluminescence of nearly three orders of magnitude and spatial surface potential variations up to 300 mV. The process capabilities are exemplified through a series of heterostructures of different metal/2D crystal materials where the resulting properties highlight the influence of the networked topography.

*Work performed at NRL was supported through ONR. JJF acknowledges the NRC Research Associateship Programs.
8:36AM E13.00004: From Synthesis to Quantum Properties of Novel 2D Layers*

JOSHUA ROBINSON (Presenter), Pennsylvania State University — Quantum materials (QMats) are prime candidates for next-generation energy-efficient technologies, such as topological quantum computing, quantum sensing, and neuromorphic computing. 2D materials offer to drastically advance our ability to synthesize, characterize, and control QMats at the atomic scale. With graphene being the first of its kind, there are now many recent breakthrough phenomena in 2D materials, including 2D magnets (e.g. CrI3), superconductors (e.g. 2D-Ga, NbSe2), and quantum emitters (e.g. WSe2, hBN), that continue to intrigue the scientific world. Quantum phenomena needed to drive disruptive Quantum Leap technologies often require integrating dissimilar materials such as superconductors and topological insulators (SC/TI) for topological superconductivity and quantum computing; (anti)ferromagnets coupled to complex oxides for correlation-driven devices beyond Moore's Law; or coherent coupling of localized spins in SiC to magnons (magnets) and Cooper pairs (superconductors) for transduction of quantum information. In this talk I will discuss our pioneering work in confinement heteroepitaxy (CHet), which decouples the growth of disparate constituent materials, thereby enabling a new platform for creating artificial quantum lattices (AQLs) with atomically sharp interfaces and designed properties. As a specific example, we synthesize plasmonic layers and 2D-superconductors combined with topological insulators to demonstrate the first “2D” topological insulator, which opens up avenues for enabling a virtual “legoland” of hybrid quantum materials.

*Funding for this work comes from NSF, Northrop Grumman, NIST, and the Semiconductor Research Corporation.


TODD BRINTLINGER (Presenter), United States Naval Research Laboratory, TOMOJIT CHOWDHURY, BENJAMIN O STEPHENS, THOMAS J KEMPA, Chemistry, Johns Hopkins University — We characterize MoS2 nanoribbons grown using a catalyst-free vapor phase synthesis that relies on pre-treatment of a bare Si surface. This growth method leads to the spontaneous formation of long ‘nanoribbons,’ with typical diameters of 100 nm and lengths greater than 10 µm. Despite their high aspect ratio and inherent flexibility, the nanoribbons are robust upon handling and are self-supporting, rendering them stable during transfer to support structures to allow electron microscopy. We use scanning electron microscopy to characterize the ribbon morphology and aberration-corrected scanning transmission electron microscopy to identify the phase, composition, and atomic structure of the samples. We identify that the MoS2 nanoribbons (1) are predominantly 2H-phase, (2) display a ‘sawtooth’ edge structure with corrugations on the order of 2–5 nm, (3) fold to give very low radii of curvature, and (4) contain occasional nanometer-scale triangular inclusions. Intriguingly, these high aspect ratio nanoribbons exhibit a PL peak that is blue-shifted significantly relative to that of as-synthesized and transferred 2-dimensional MoS2 sheets.

*The authors acknowledge funding from the Office of Naval Research (Naval Research Laboratory Basic Research Program).

9:24AM E13.00006: Strong interlayer coupling and layer-dependent bandgap in 2D layered PdSe2 synthesized by chemical vapor deposition

LI-SYUAN LU (Presenter), HUI-YU CHENG, GUAN-HAO CHEN, Department of Electrophysics, National Chiao Tung University, CHIA-HAO CHEN, TZU-HUNG CHUANG, DER-HSIN WEI, National Synchrotron Radiation Research Center (NSRRC), MING-YANG LI, CHIH-PIAO CHUU, LAIN-JONG LI, Corporate Research and Chief Technology Office, Taiwan Semiconductor Manufacturing Company (TSMC), WEN-HAO CHANG, Department of Electrophysics, National Chiao Tung University, — Two-dimensional (2D) noble metal dichalcogenides, such as PtS2 or PdSe2, have attracted much attention due to their remarkable layer-dependent electronic structures and superior electrical properties for device applications. However, most of the demonstrated experiments thus far are based on mechanical exfoliations from bulk crystals. Here, we demonstrate that highly crystalline and air stable PdSe2, from bilayer up to few layers, can be synthesized by chemical vapor deposition. The atomic ratio and the lattice structure of PdSe2 have been confirmed by x-ray photoemission and polarization-resolved Raman spectra. Low-frequency Raman measurements of breathing vibration modes reveal the strong interlayer coupling, which can also be used for identifying the layer numbers [1]. Based on absorption measurements, we observed a strongly layer-dependent bandgap, which shows a gap shrinkage up to 0.5 eV with the increasing layer number from bilayer to 7 layers. The dramatically layer-dependent bandgap shrinkage is also consistent with the calculated energy gap based on density functional theory.[2]

9:36AM E13.00007: Synthetic Metal-Semiconductor Junctions of Transition Metal Disulfides*  WEI SUN LEONG (Presenter), QINGQING JI, NANNAN MAO, Electrical Engineering and Computer Science, Massachusetts Institute of Technology (MIT), YIMO HAN, Applied and Engineering Physics, Cornell University, HAOZHE WANG, Electrical Engineering and Computer Science, Massachusetts Institute of Technology (MIT), AARON J GOODMAN, Chemistry, Massachusetts Institute of Technology (MIT), CONG SU, YUNFAN GUO, PIN-CHUN SHEN, ZHENFEI GAO, Electrical Engineering and Computer Science, Massachusetts Institute of Technology (MIT), DAVID ANTHONY MULLER, Applied and Engineering Physics, Cornell University, WILLIAM A TISDALE, Chemical Engineering, Massachusetts Institute of Technology (MIT), JING KONG, Electrical Engineering and Computer Science, Massachusetts Institute of Technology (MIT) — Transition metal dichalcogenides (TMDs), a group of 2D materials with diverse electronic properties, are ideal candidates to build atomically thin electronics. Although critical components of an electronic device based on TMDs, such as insulator-semiconductor and semiconductor-semiconductor junctions, have been demonstrated, there is limited experimental realization of TMD-based metal-semiconductor junctions to date. Here, we report a two-step chemical vapor deposition (CVD) strategy that enables the synthesis of high-quality solely TMD-made metal-semiconductor lateral junctions. Remarkably, we discover a novel growth behavior in such lateral TMD heterojunctions: MoS2 was found to nucleate from the vertexes of multilayered VS2 flakes and evolve into monolayer polycrystals, rather than the edge epitaxy observed in other TMD lateral junctions. Furthermore, we demonstrate that lattice coherency across the lateral junction is not a necessity for low-resistance contacts, as our VS2-MoS2 junctions manifest contact resistance as low as 500 Ωµm and a Schottky barrier height as small as 30 meV, both among the best values reported to date for contacts to 2D TMDs. This work opens up a new avenue for all-2D-based synthetic electronics.

*AFOSR FATE MURI, Grant No. FA9550-15-1-0514

9:48AM E13.00008: Scaling a van der Waals quantum Hall semiconductor  KAI YUAN (Presenter), RUOYU YIN, XIAOSONG WU, YU YE, LUN DAI, School of Physics, Peking University — Indium selenide (InSe), a two-dimensional (2D) layered semiconductor material, have attracted much attention recently due to their high mobility and fascinating physical properties. Nevertheless, the preparation of few-layer InSe is limited to mechanical exfoliation which hinders their potential in the future applications. Recently reports of few-layer InSe synthesized via chemical vapor deposition (CVD) method failed to maintain high mobility characteristics of InSe. Here, we explored the controlled one-step synthesis of 2D InSe nanoflakes with chemical vapor transport (CVT) by appropriately slowing down the growth rate. Diverse growth routes were developed by using different transport agents. As-grown InSe nanoflakes with thickness down to monolayer was successfully obtained. Atomic-resolution ADF-STEM imaging revealed the high quality of the as-synthesized InSe nanoflakes. Encapsulated by BN at both sizes, the electrical transport of our InSe nanoflakes shows excellent performance with carrier mobilities larger than 1000 cm²V⁻¹s⁻¹ at room temperature and 5000 cm²V⁻¹s⁻¹ at 1.5 K, enabling us further observe the quantum Hall effect. This is the first time that a quantum Hall effect was observed in as-grown 2D semiconductor materials.

10:00AM E13.00009: Theoretical insight into the mechanism for spontaneous vertical growth in ReS2*  ANTHONY YOSHIMURA (Presenter), DEBJIT GHOSHAL, TUSHAR GUPTA, Rensselaer Polytechnic Institute, ANDREW HOUSE, New Jersey Institute of Technology, SWASTIK BASU, YANWEN CHEN, TIANMENG WANG, YANG YANG, WENJIA SHOU, Rensselaer Polytechnic Institute, JORDAN A. HACHTEL, JUAN CARLOS IDROBO, Oak Ridge National Laboratory, TOH-MING LU, Rensselaer Polytechnic Institute, SAGNIK BASURAY, New Jersey Institute of Technology, VINCENT MEUNIER, SUFEI SHI, NIKHIL KORATKAR, Rensselaer Polytechnic Institute — While vertical growth can be observed in some transition metal dichalcogenides (TMDs) under special conditions, vertical growth of rhenium disulfide (ReS2) is unique in that it is thermodynamically favorable over horizontal growth regardless of substrate. In this study, we use density functional theory (DFT) to shed light on the mechanism that initiates vertical growth in ReS2 to explain its substrate-independence. We propose that ReS2 growth has two stages. First, ReS2 grows parallel to the substrate, in a manner similar to that of conventional TMDs. However, as a growing ReS2 flake reaches a critical diameter, spontaneous vertical growth is nucleated at points near the flake’s center. At these sites, an additional Re atom binds to a cluster of “pinched” Re atoms, leaving an under-coordinated S atom protruding out of the ReS2 plane. This S atom is “reactive” and readily binds to free Re and S atoms, initiating growth in a direction perpendicular to the ReS2 surface. The resulting vertical ReS2 arrays possess high surface-to-volume ratios and can therefore accommodate a broad range of applications including surface enhanced Raman spectroscopy, field emission, and solar-based disinfection of bacteria.

*This work was supported by the National Science Foundation (Award 1608171)
10:12AM E13.00010: Stoichiometric Control of Structural Phases in Two-Dimensional NbS2 Nanoflakes* AMANDA COUGHLIN (Presenter), WENCao YANG, ZHEN LI, SHIXIONG ZHANG, Indiana University Bloomington — Two-dimensional transition metal dichalcogenides (TMDs) are known to exist in multiple structural phases (1T, 2H, and 3R etc.) each with distinct physical properties. The ability to tune the crystal structures in a controlled manner provides an effective route to engineer the respective properties and is therefore of significant technological importance. In this study, we use NbS2 nanoflakes as an example to demonstrate the control of structural phases in layered TMDs by tuning their stoichiometry. The as-grown NbS2 has a rhombohedral 3R phase which can be readily transformed into another structure via a simple annealing process. By varying the annealing conditions, we realize several different structural phases as identified by Raman spectroscopy. The reversibility and the underlying mechanism of phase transformations are also studied.

*Work supported by NSF DMR-1506460

10:24AM E13.00011: Spectroscopic Characterization of Colloidally Synthesized, Anisotropic 2D SnS ADAM BIACCHI, BRIAN ALBERDING, SON T. LE, SUGATA CHOWDHURY, JOSEPH HAGMANN, SUJITRA POOKPANRATANA, CURT A RICHTER, EDWIN HEILWEIL, ANGELA HIGHT WALKER (Presenter), National Institute of Standards and Technology — Solution routes afford scalable means of manufacturing size-, shape-, and composition-controlled nanoscale electronic materials. We have developed solution routes to monodisperse 2D semiconductor SnS nanostructures, an easily processable and cost-efficient alternative to exfoliation and gas-phase deposition techniques. These colloidal chemistries afford two distinct SnS morphologies: nanoribbons and square nanosheets. The uniformity and morphology of the nanocrystals were verified using TEM, SEM, AFM, and optical microscopy. A spectroscopic investigation of the inherent structural and electronic properties of nanocrystals showed the α-SnS polymorph adopts a layered orthorhombic crystal structure, isostructural with black phosphorus. These 2D crystals are anisotropic, with in-plane atoms adopting the armchair configuration along one axis and zigzag in the orthogonal direction. Detailed polarization-, wavelength- and temperature-dependent Raman spectroscopy provide key insight into the crystallographic details and low-frequency phonon behavior. Back-gated devices fabricated from individual crystals reveal electronic transport information and four-point probe methods show the anisotropic conductivity resulting from a black phosphorus-like bonding arrangement found in 2D SnS.

10:36AM E13.00012: Engineering Defect Transition-Levels through van der Waals Heterostructure* AKASH SINGH (Presenter), Materials Research Centre, Indian Institute of Science, Bangalore 560012, India, AADITYA MANJANATH, Institute of Chemistry, Indian Institute of Science, Bangalore 560012, India, ABHISHEK KUMAR SINGH, Materials Research Centre, Indian Institute of Science, Bangalore 560012, India — Tuning the defect transition levels in 2D semiconductors without significantly altering the integrity of the materials remains one of the most difficult challenges. Among the 2D materials, monolayer MoS2 is considered as a front-runner for device applications, does not have a single intrinsic shallow defect, thereby limiting its applications. We demonstrate that the deep defect levels created by a cation vacancy in a monolayer of MoS2, can be tuned to a shallow level by forming the van-der-Waals heterostructure of it with a monolayer of WS2, while maintaining their structural and compositional integrity intact. In result, the deep defect levels are shallowed by nearly 4(V-1Mo) and 2(V-1W) times, respectively, compared to their monolayer counterparts. The overall change in dielectric constant rescales the defect transition levels in a heterostructure. Our finding has the potential to revolutionize the doping strategy of the 2D materials and could pave the way for 2D electronics.

Akash Singh, Aaditya Manjanath, and Abhishek K. Singh, Materials Research Centre, Indian Institute of Science, Bangalore 560012, India, Engineering Defect Transition-Levels through the van der Waals Heterostructure, J. Phys. Chem. C, Article ASAP, DOI: 10.1021/acs.jpcc.8b08082

*DST-Inspire fellowship

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E14 DCMP: Graphene: Transport Properties BCEC 153C - Dongying Wang, Ohio State University
8:00AM E14.00001: Fermi surface anisotropy of graphene measured by ballistic transport experiments on antidot lattice samples  RYUTA YAGI (Presenter), TAKUSHI OKA, RYOYA EBISUOKA, TAIKI HIRAHARA, AdSM, Hiroshima Univ., KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science (NIMS) — Monolayer graphene and bilayer graphene have strikingly different properties. One such difference is the shape of the Fermi surface. Although anisotropic band structures can be detected in optical measurements, they have so far been difficult to detect in transport experiments on two-dimensional materials. Here we describe a ballistic transport experiment using high-quality graphene that revealed Fermi surface anisotropy in the magnetoresistance. The shape of the Fermi surface is closely related with the cyclotron orbit in real space. Electron trajectories in samples with triangular lattices of holes depend on the anisotropy of the Fermi surface. We found that this results in the magnetoresistance which are dependent on crystallographic orientation of the antidot lattice, which indicates the anisotropic Fermi surface of bilayer graphene which is a trigonally-warped circle in shape. While in monolayer, shape of magnetoresistance was approximately independent of the orientation of antidot lattice, which indicates that the Fermi surface is a circle in shape.

8:12AM E14.00002: Universal voltage scaling due to self-averaging of quantum corrections in graphene  NARGESS ARABCHIGAVKANI (Presenter), Department of Physics, University at Buffalo, The State University of New York, RATCHANOK SOMPHONSANE, Department of Physics, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand, HARIHARA RAMAMOORTHY, GUANCHEN HE, JUBIN NATHAWAT, SHENCU YIN, JONATHAN P BIRD, Department of Electrical Engineering, University at Buffalo, State University of New York, BILAL BARUT, Department of Physics, University at Buffalo, The State University of New York, MIAO ZHAO, ZHI JIN, High-Frequency High-Voltage Device and Integrated Circuits Center, Institute of Microelectronics of Chinese Academy of Sciences, JONAS FRANSSON, Department of Physics and Astronomy, Uppsala University — The differential conductance of graphene is shown to exhibit a zero-bias anomaly at low temperatures, arising from a suppression of the quantum corrections due to weak localization and electron interactions. A simple rescaling of these data, free of any adjustable parameters, shows that this anomaly exhibits a universal, temperature independent form. According to this, the differential conductance is approximately constant at small voltages (V<kBT/e), while at larger voltages it increases logarithmically with the applied bias, reflecting a quenching of the quantum corrections. For theoretical insight into the origins of this behavior, we formulate a model for weak-localization in the presence of nonlinear transport. According to this, the voltage applied under nonequilibrium induces unavoidable dephasing, arising from a self-averaging of the diffusing electron waves responsible for transport. By establishing the manner in which the quantum corrections are suppressed in graphene, our study will be of broad relevance to the investigation of nonequilibrium transport in mesoscopic systems in general. This includes systems implemented from conventional metals and semiconductors, as well as those realized using other two-dimensional semiconductors and topological insulators.

*DOE, NSF

8:24AM E14.00003: Uniform doping of graphene close to the Dirac point by polymer-assisted assembly of molecular dopants  YUNG PARK (Presenter), Physics and Astronomy, Seoul National University & University of Pennsylvania, HANS HE, KYUNG HO KIM, SERGEY KUBATKIN, SAMUEL LARA-AVILA, Microtechnology and Nanoscience, Chalmers University of Technology — Tuning the charge carrier density of two-dimensional (2D) materials by incorporating dopants into the crystal lattice is a challenging task. An attractive alternative is the surface transfer doping by adsorption of molecules on 2D crystals, which can lead to ordered molecular arrays. However, such systems, demonstrated in ultra-high vacuum conditions (UHV), are often unstable in ambient conditions. Here we show that air-stable doping of epitaxial graphene on SiC-achieved by spin-coating deposition of 2,3,5,6-tetrafluoro-tetracyano-quino-dimethane (F4TCNQ) incorporated in poly(methylmethacrylate)-proceeds via the spontaneous accumulation of dopants at the graphene-polymer interface and by the formation of a charge-transfer complex that yields low-disorder, charge-neutral, large-area graphene with carrier mobilities ~70,000cm²V⁻¹s⁻¹ at cryogenic temperatures. The assembly of dopants on 2D materials assisted by a polymer matrix, demonstrated by spin-coating wafer-scale substrates in ambient conditions, opens up a scalable technological route toward expanding the functionality of 2D materials.


*This work was jointly supported by the NRF-20171A2A1A18070721, Korea and the SSF No. IS14-0053, Sweden.
In conventional semiconductors, the exciton bound state (arising from the attractive Coulomb interaction between electrons and holes) can be successfully analyzed by the effective mass approximation based on the lowest-order parabolic dispersion relation at band extrema. However, parabolic dispersion is by no means the only possible outcome endowed by a periodic lattice potential, especially in two dimensional electronic materials, where weak inter-subband matrix elements suppress otherwise strong band repulsion across a forbidden gap, resulting in nonparabolic ‘Mexican hat’ or ‘caldera’-shaped bands, in which “effective mass” is ill-defined. Focusing on electrostatically-biased bilayer graphene as an example where quartic (and higher) dispersion terms are necessary, we present a semi-analytic theory used to investigate the properties of ground and excited excitonic states. This includes determination of the exciton binding energy and wavefunctions, which are further used to analyze the relative oscillator strengths and magnetic moments (g-factors) that can be directly compared to recent experimental measurements.

*National Science Foundation ECCS-1707415

In condensed matter physics, last one decade, the interesting non-monotonic behavior as a function of doping density in the vicinity of the CNP. When disorder is included, we find that the WF ratio in bilayer graphene drops below its maximal value, resulting in an extreme hydrodynamic regime. The WF ratio of the clean system reaches a maximal value at the charge-neutrality-point (CNP), and this value increases as a function of temperature. This is in contrast with a perfectly clean monolayer graphene we obtain finite electrical and thermal resistivities, even in the absence of disorder, i.e. in the extreme hydrodynamic regime. The WF ratio of the clean system reaches a maximal value at the charge-neutrality-point (CNP), and this value increases as a function of temperature. This is in contrast with a perfectly clean monolayer graphene where the WF ratio becomes infinite in the absence of disorder (requiring disorder to be observable). When disorder is included, we find that the WF ratio in bilayer graphene drops below its maximal value, resulting in an interesting non-monotonic behavior as a function of doping density in the vicinity of the CNP.

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9:24AM E14.00008: Breakdown of the law of reflection at a disordered graphene edge* ELIAS WALTER, Faculty of Physics, LMU Munich, TOMAS ÖRN ROSDAHL, ANTON AKHMEROV (Presenter), Kavli Institute of Nanoscience, Delft University of Technology, FABIAN HASSLER, Institute for Quantum Information, RWTH Aachen — The law of reflection states that smooth surfaces reflect waves specularly, thereby acting as a mirror. This law is insensitive to disorder as long as its length scale is smaller than the wavelength. Monolayer graphene exhibits a linear dispersion at low energies and consequently a diverging Fermi wavelength. We present proof that a charge-neutral disordered graphene boundary results in a diffusive electron reflection even when the electron wavelength is much longer than the disorder correlation length. Using numerical quantum transport simulations, we demonstrate that this phenomenon can be observed as a nonlocal conductance dip in a magnetic focusing experiment.

*ERC Starting Grant No. 638760, the Netherlands Organisation for Scientific Research (NWO/OCW), and the U.S. Office of Naval Research.

9:36AM E14.00009: Ultrafast Valley polarization in gapped graphene SEYYEDEH AZAR OLIAEIMOTLAGH (Presenter), VADYM APALKOV, MARK I STOCKMAN, Georgia State University — We study numerically the ultrafast valley polarization in gapped graphene that can be accessed and controlled by a single cycle of a circularly polarized intense pulse. The amplitude of the pulse is about 0.5 V/\AA and its duration is 5 fs. Depending on the polarization of the pulse, right or left handed, one valley, K or K', is significantly populated, resulting in significant residual valley polarization of gapped graphene. The unequal valley population in the reciprocal space is due to topological resonance, which is caused by the mutual cancellation of the topological and dynamic phases. The ultrafast valley polarization, generated in gapped graphene-like materials, can be used in ultrafast quantum memory devices.

9:48AM E14.00010: All-Electronic Thermal Transport With Nonlocal Noise Thermometry in Graphene JONAH WAISSMAN (Presenter), ARTEM V TALANOV, YOUNG JAE SHIN, DANIAL HAEI NAJAFABADI, Harvard University, MARINE ARINO, HUGO BARTOLOMEI, Physics, ENS Paris, PHILIP KIM, Harvard University — Ever since the measurements of Wiedemann and Franz in 1853, thermal transport has played a central role in condensed matter physics. Thermal conductance can help pinpoint neutral modes such as spin waves, non-Fermi liquid states such as hydrodynamic states and Luttinger liquids, and topological degrees of freedom such as Majorana modes. In this context, van der Waals materials now offer a rich landscape of interacting, symmetry-broken, and topological states of matter enhanced by their low dimensionality, yet thermal transport has remained a difficult probe to realize for few-atom thick materials and for many of the most delicate electronic ground states. Here, we demonstrate a new technique to achieve all-electronic thermal transport in a van der Waals material. We use graphene as a sensitive electronic heater and thermometer by implementing a new type of nonlocal noise thermometry. We show that the technique allows us to accurately extract the electronic thermal conductance of a bridge between two graphene thermometers. This new probe now allows us to study a wide array of symmetry-broken and topological states in van der Waals materials through their heat transport properties.

10:00AM E14.00011: Studying the effects of strain in graphene using a MEMS device and electronic transport measurements at low temperatures* PAUL ANDERSON (Presenter), Physics and Astronomy, California State University Long Beach, YIFAN HUANG, Mechanical and Material Engineering, University of Nebraska Lincoln, SARA QUBBAJ, Physics and Astronomy, California State University Long Beach, QIN ZHOU, Mechanical and Material Engineering, University of Nebraska Lincoln, CLAUDIA OJEDA-ARISTIZABAL, Physics and Astronomy, California State University Long Beach — Different theoretical studies have motivated experiments on strained graphene, predicting exotic behaviors such as superconductivity or the induction of gauge fields that act effectively as large magnetic fields. Up to now the study of strain in graphene has been limited to the use of substrates where wrinkles or bubbles create strain or to the use of flexible substrates that create strain when they are bent. Here we present preliminary electronic transport experiments at low temperatures on a suspended graphene where strain is applied through a sophisticated micro-electro-mechanical systems (MEMS). We observe features in the magnetoresistance that change as strain is imposed to the sample, possibly showing the effects of the superposition of a magnetic field and a time reversal symmetric pseudo-magnetic field.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences. Award number: DE-SC0018154.
10:12AM E14.00012: Conductivity and Mobility of Substitutionally Disordered Graphene under the Coherent Potential Approximation*  JACOB ROBBINS (Presenter), JORGE OSVALDO SOFO, Pennsylvania State University — We calculate the DC electrical conductivity and carrier mobility of graphene with randomly distributed impurities of boron, nitrogen, and/or carbon vacancies. Conductivity and mobility are found at the linear response level with the Kubo-Greenwood formula [1,2]. Disorder is treated in a mean field approximation, namely the Coherent Potential Approximation (CPA) [3]. Our results show a decrease in mobility for increasing disorder, which agrees with experiments on nitrogen doped graphene [4]. The CPA also captures localized states around the Dirac point whenever vacancies are included. Any amount of carbon vacancies also induce a significant decrease in conductivity, even in the presence of the softer scattering centers, boron and nitrogen. This reduction in conductivity agrees with experiments on graphene with vacancies induced by a helium ion beam [5].


*This work was funded by the Computational Materials Education and Training (CoMET) program at The Pennsylvania State University.

10:24AM E14.00013: Ballistic Transport of Epitaxial Graphene Nanoribbons on SiC  YUE HU (Presenter), YIRAN HU, DOGUHAN DENIZ, School of Physics, Georgia Institute of Technology, VLADIMIR PRUDKOVSKYI, Institut Neel/CNRS-Univ. Grenoble Alpes, JEAN-PHILIPPE TURMAUD, School of Physics, Georgia Institute of Technology, JAMES GIGLIOTTI, School of Materials Science and Engineering, Georgia Institute of Technology, LEI MA, TICNN, Tianjin University, CLAIRE BERGER, Institut Neel/CNRS-Univ. Grenoble Alpes, WALT A. DE HEER, School of Physics, Georgia Institute of Technology — Exceptional ballistic transport was observed in sidewall epitaxial graphene nanoribbons on SiC (SWGNRs) at room temperature [1]. These objects are of fundamental interest as they provide a direct access to charge neutral graphene with excellent transport properties. Here, beyond sidewalls, we fabricate epitaxial graphene nanoribbons on different crystal faces on SiC, including Si-face and non-polar facets. We introduce amorphous carbon as contact pads and high temperature annealing to reduce the edge roughness of ribbons and the contamination from resist residue. Then we discuss transport measurement and magnetoresistance results of graphene nanoribbons on Si-face as well as on non-polar SiC facets, which might reveal the nature of the ballistic channels in SWGNRs.


10:36AM E14.00014: Electron-phonon Cerenkov instability in graphene revealed by global and local noise measurements*  BO DWYER (Presenter), Harvard University, JAVIER D SANCHEZ-YAMAGISHI, Physics, University of California Irvine, TROND I ANDERSEN, JOAQUIN RODRIGUEZ NIEVA, Harvard University, KARTIEK AGARWAL, Princeton University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, EUGENE DEMLER, PHILIP KIM, HONGKUN PARK, MIKHAIL LUKIN, Harvard University —

Understanding and controlling non-equilibrium electronic phenomena is an outstanding challenge in science and engineering. Graphene presents a particularly interesting system for studying such effects because its high mobility means electrons may be accelerated very far out of equilibrium. We find that when fully encapsulated graphene is driven with a sufficiently high DC current, the drift velocity of the electrons exceeds the phase velocity of sound. This results in population inversion of the electronic system and stimulated emission of phonons becomes the dominant scattering process. This phonon Cerenkov effect leads to a runaway growth of certain phonon modes in the direction of momentum flow. Using NV centers as local noise probes, we map the exponential spatial growth of the phonon population by measuring the resulting local current fluctuations. Additionally, we measure a significantly altered global noise spectrum and AC conductivity at GHz frequencies, both of which are well described by stimulated emission of acoustic phonons. Since the amplified phonons are primarily in the THz range, the observation of a phonon Cerenkov effect in graphene is a first step towards realizing an on-chip generator of THz sound and radiation.

* DARPA
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Elastic response of the electron fluid in intrinsic graphene: The collisionless regime

JULIA LINK (Presenter), Simon Fraser University, DANIEL E. SHEEHY, Louisiana State University, BORIS N. NAROZHNY, JOERG SCHMALIAN, Karlsruhe Institute of Technology — The elastic response of an electron fluid at finite frequencies is defined by the electron viscosity $\eta(\omega)$. We determine $\eta(\omega)$ for graphene at the charge neutrality point in the collisionless regime, including the leading corrections due to the electron-electron Coulomb interaction. We find interaction corrections to $\eta(\omega)$ that are significantly larger if compared to the corresponding corrections to the optical conductivity. In addition, we find comparable contributions to the dynamic momentum flux due to single-particle and many-particle effects. We also demonstrate that $\eta(\omega)$ is directly related to the nonlocal energy-flow response of graphene at the Dirac point. The viscosity in the collisionless regime is determined with the help of the strain generators in the Kubo formalism. Here, the pseudospin of graphene describing its two sublattices plays an important role in obtaining a viscosity tensor that fulfills the symmetry properties of a rotationally symmetric system.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E15 DMP GMAG: 2D Materials (Semiconductors) -- Magnetism

BCEC 154 - Wenzhuo Wu, Purdue University

8:00AM E15.00001: Tunneling through Charge transfer heterostructure of CrI$_3$

TULA PAUDEL (Presenter), EVGENY YTSYMBAL, University of Nebraska - Lincoln — Two dimensional ferromagnetic insulator CrI$_3$ have attracted a lot of attention because of its interesting properties including tunneling magnetoresistance in a Van der Waals heterostructure. Using the first-principles methods, we calculate the spin-dependent transport through a CrI$_3$-based tunnel junction and find that the tunneling current is 100% spin polarized. In zero bias regime, switching between the ferromagnetic and antiferromagnetic configurations of CrI$_3$ leads to the tunneling magnetoresistance of 9800%. The transmission is mediated by the states located at the k-points away from the high symmetry points in the Brillouin zone and modulated by the distribution of the k-dependent decay states in the barrier. When biased, both the spin polarization and tunneling magnetoresistance are enhanced. This behavior persists even when the CrI$_3$ barrier is as thin as two monolayers. Our calculations open up the possibility achieving 100% spin polarized current using conventional metallic electrodes, thereby broadening design space beyond 2D Van der Walls heterostructures.

8:12AM E15.00002: Interplay between interlayer exchange and stacking in CrX$_3$ (X = Cl, Br, I)$^*$

CLAUDIA CARDOSO (Presenter), QuantaLab, International Iberian Nanotechnology Laboratory, Portugal, DAVID SORIANO, Institute for Molecules and Materials, Radboud University, the Netherlands, JOAQUIN FERNANDEZ-ROSSIER, QuantaLab, International Iberian Nanotechnology Laboratory, Portugal — The study of few-layer crystals with ferromagnetic (FM) order is a natural follow-up of the recent discovery of FM order in stand alone 2D crystals. And as a result, the study of the structural and magnetic interlayer interactions. Here we address the case of CrX$_3$ (X = Cl, Br, I). All of them display FM order within the layers but have different interlayer interactions. The interlayer exchange in bulk CrCl$_3$ is antiferromagnetic (AFM), whereas for CrBr$_3$ and CrI$_3$ is FM. In contrast, few-layers CrBr$_3$ and CrI$_3$ present an AFM interlayer coupling. [1] Moreover, the bulk systems undergo a crystallographic phase transitions with temperature and there is evidence of an strong interplay between the crystallographic and magnetic degrees of freedom, both for the bulk and the few layer systems. [2] In this study, we address the interplay between stacking and interlayer exchange coupling for CrX$_3$ 2D crystals using first-principles calculations and an effective interlayer coupling model. Our results shed light on the magnetic behavior of the CrX$_3$ bulk and 2D crystals.


$^*$We acknowledge FEDER project NORTE-01-0145-FEDER-000019 and the FCT grant UTAP-EXPL/NTec/0046/20177

8:24AM E15.00003: Probing interlayer magnetism and magnons in two-dimensional chromium trihalides

BOWEN YANG (Presenter), HYUN HO KIM, GEORGE NICHOLS, FRANCOIS SFIGAKIS, University of Waterloo, CHENGHE LI, SHANGJIE TIAN, Renmin University of China, DAVID CORY, GUOXING MIAO, University of Waterloo, HECHANG LEI, Renmin University of China, ADAM TSEN, University of Waterloo — We study CrX$_3$ (X = I, Br, Cl) in the atomically thin limit by incorporating them in vertical tunnel junctions with graphene electrodes. In this device geometry, we are able to characterize the interlayer magnetic coupling, tunnel magnetoresistance, magnetic anisotropy, as well as magnon excitations. I will discuss the results of these studies and show how the magnetic properties of 2D CrX$_3$ are modified when changing the halogen atom.

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Raman spectroscopy studies of spin waves in two-dimensional CrI$_3$*  
WENCAN JIN (Presenter), University of Michigan, HYUN HO KIM, University of Waterloo, ZHIPENG YE, Texas Tech University, SWEN LI, University of Michigan, POUYAN REZAIE, FABIAN S DIAZ, SAAD SIDDIQ, ERIC S WAUER, Texas Tech University, BOWEN YANG, University of Waterloo, CHENGHE LI, SHANGJIE TIAN, Renmin University of China, KAI SUN, University of Michigan, HECHANG LEI, Renmin University of China, ADAM W TSEN, University of Waterloo, RUI HE, Texas Tech University, LIUYAN ZHAO, University of Michigan — The long-range magnetic order in the two-dimensional (2D) limit at finite temperatures has recently been demonstrated in a honeycomb Ising ferromagnet CrI$_3$. It has triggered tremendous interest in 2D magnet-based applications. To achieve a complete understanding of the 2D magnetic phase, a direct measurement of the magnetic excitations, i.e., spin waves, or magnons, is pressingly in need. In this talk, we will present the experimental evidence of spin waves in the 2D honeycomb ferromagnet, CrI$_3$. Using polarized micro-Raman spectroscopy, we have identified two branches of zero-momentum spin waves in 2D CrI$_3$ with exceptionally high frequencies in the THz range, as compared to those of the conventional ferromagnets. By tracking the layer thickness dependence of both spin waves, we further show that both are surface magnons, and their lifetimes remain an order of magnitude longer than their temporal period down to the monolayer limit.

*L. Z acknowledges support by NSF CAREER Grant No. DMR-1749774. R. H. acknowledges support by NSF CAREER Grant No. DMR-1760668.
Magneto-optical Kerr effect in two-dimensional diluted magnetic transition metal dichalcogenide semiconductors*  GONÇALO CATARINA (Presenter), JOAQUIN FERNANDEZ-ROSSIER, QuantaLab.  

In this talk, I will present a theory to model the Kerr angle for two-dimensional transition metal dichalcogenide semiconductors, such as MoS2, doped with a small density of magnetic atoms. The model Hamiltonian describes the band carriers within the effective gapped Dirac theory, accounting for spin-orbit and spin-valley coupling [1]. The magnetic impurities are described within a mean-field virtual crystal approximation, leading to a band-dependent spin splitting of the spectrum [2]. We find that the transverse optical susceptibility is non-zero, leading to a finite Kerr angle, when the exchange-induced splitting in the valence and conduction bands are different. We consider the case when there are no free carriers in the bands, as well as the n-doped and p-doped regimes.


*We acknowledge financial support from FCT for the P2020-PTDC/FIS-NAN/4662/2014 project. J. F.-R. acknowledges financial support from FCT for the UTAP-EXP/NTec/0046/2017 project.

Magnetism and Distortions in Transition-Metal Dioxide Layers: On the Quest for Intrinsic Magnetic Semiconductor Layers*  FAUSTINO AGUILERA-GRANJA, Instituto de Fisica, Universidad Autonoma de San Luis Potosi, 78000 San Luis Potosi, Mexico, ANDRES AYUELA (Presenter), Donostia International Physics Center, Centro de Física de Materiales-MPC CSIC-UPV/EHU, 20018 San Sebastian, Spain — Future nanoscale technological applications in spintronics require research on two dimensional materials with combined semiconductor and magnetic properties. We investigate transition metal dioxides in the form of layers, and report on the structural and electronic properties of selected late transition metal d-elements. With half-filled d states, the MnO2 and TcO2 layers are magnetic semiconductors, and for side d-elements the CrO2 and FeO2 layers become half-metals. These magnetic materials in 2D must be synthesized in order to assess their usefulness in future electronic and spintronic devices.

*The Spanish Ministry of Economy and Competitiveness under Grant No. FIS2016-76617-P (MINECO/FEDER).

Diversified Magnetoelectric Coupling in 2D Multiferroic Materials  QING YANG (Presenter), MENGHAO WU, Huazhong University of Science and Technology — Multiferroic materials with coupled magnetism and ferroelectricity, even though scarcely exist in nature, are highly desirable for efficient “electric writing + magnetic reading”. Currently, the polarization and magnetization of traditional multiferroics with strong magnetoelectric coupling are all too weak for practical applications. Here we show first-principles evidences that strong magnetoelectric can be realized in a series of 2D multiferroics: in some intercalated bilayer systems, their “mobile” magnetism can be controlled by ferroelectric switching upon external electric field, exhibiting either “on” state with spin-selective and highly p-doped channels, or “off” state insulating for both spin and electron transport, which renders efficient electrical writing and magnetic reading; vertical polarization can be maintained against depolarizing field, rendering high-density data storage possible. In some 2D systems, the magnetization can be switched by 90 or even 180 degree upon ferroelectric switching.

10:00AM E15.00011: Negative Parabolic Magnetoresistance due to Electron-Electron Interactions in a Disordered 2D Electron Gas in InSe* KASUN PREMASIRI (Presenter), Case Western Reserve University, RAJESH KUMAR, RAMAN SANKAR, FANGCHENG CHOU, National Taiwan University, XUAN GAO, Case Western Reserve University — Magnetotransport measurements serve as a multifarious tool in understanding various phenomena involved in electron transport, among which the prevalence of the electron-electron interaction (EEI) represents a key aspect with its unique magnetoresistance (MR) signatures. Semiconductor-heterostructure-based, two-dimensional electron gases (2DEGs) have been extensively studied to extract information about the EEI. Two-dimensional (2D) materials may provide more insight into the EEI, possessing an array of materials with extreme versatility in electronic properties. We report negative parabolic MR due to the EEI in a 2DEG formed in InSe, which is a 2D monochalcogenide semiconductor. In this system, we study the EEI in the regime of $\omega_c\tau<1$, which is relatively unexplored. A logarithmic relationship between the EEI and the temperature is observed confirming the contribution from the EEI to the MR. We also compare the strength of the observed EEI with other conventional systems such as Si metal-oxide semiconductor field-effect transistors and GaAs quantum wells.

*X. G. thanks NSF (grant number: DMR-1607631) for funding the project.

10:12AM E15.00012: Ferromagnetism created from non-ferromagnetic vdW heterostructures CHENG GONG (Presenter), University of California, Berkeley, PEIYAO ZHANG, TENZIN NORDEN, Physics, University at Buffalo, State University of New York, QUANWEI LI, ZHEN GUO, University of California, Berkeley, APOORVA CHATURVEDI, School of Materials Science and Engineering, Nanyang Technological University, ARMAN NAJAFI, Physics, University at Buffalo, State University of New York, SHOUFENG LAN, XIAOZE LIU, YUAN WANG, University of California, Berkeley, HAO ZENG, Physics, University at Buffalo, State University of New York, HUA ZHANG, School of Materials Science and Engineering, Nanyang Technological University, ATHOS PETROU, Physics, University at Buffalo, State University of New York, XIANG ZHANG, University of California, Berkeley — Intrinsic long-range ferromagnetic order has recently been discovered in two-dimensional atomic crystals. However, the prospect of 2D magnets remains largely hindered by the scarcity of 2D ferromagnets with limited diversity in magnetic attributes. In this context, creative ways to bring forth ferromagnetism from non-ferromagnetic 2D materials are attractive and profitable for both fundamental physics and device applications. In this talk, I will show you the possibility of such creation based on our magneto-optical study of vdW heterostructures and discuss the underlying material physics. Our work paves the new path to harvest 2D ferromagnetism.

10:24AM E15.00013: Electrically tunable magnon bands in two-dimensional magnets* MOHAMMAD MUSHFIQUR RAHMAN (Presenter), AVINASH RUSTAGI, YONG CHEN, PRAMEY UPADHYAYA, Purdue University — Magnons, namely quanta of spin waves-coherent excitations of magnetically ordered medium-are considered as promising carriers of spin information for classical [Nat. Phys. 11, 453 (2015)] and quantum [npj Quantum Info. 3, 28 (2017)] information processing. For these applications, the ability to electrically reconfigure the bandstructure of magnons, can open novel opportunities to create dynamic magnon crystals and multifunctional high frequency, logic and quantum devices [Journal of Phys. D: Appl. Phys.50, 24 (2017)]. In this work, we propose a novel platform to realize electrically tunable magnon bands, namely recently discovered two-dimensional (2-D) magnets [Nature 546, 270(2017)]. For this purpose, we utilize the efficient electrical control of spin-spin interactions within bilayer Chromium Iodide [Nature Mat. 17, 406 (2018)] to numerically demonstrate electrically controlled sub-Terahertz magnons. This study opens the possibility of using van der Waal magnets and their heterostructures for high frequency magnon spintronics applications.

*We acknowledge NSF grant DMR-1838513.

10:36AM E15.00014: Raman phonon spectra from CrI3 atomic layers* RUI HE (Presenter), ZHIPENG YE, GAIHUA YE, ERIC S WAUER, FABIAN S DIAZ, DAVID TAUZIN, Texas Tech University, HYUN HO KIM, BOWEN YANG, ADAM TSEN, University of Waterloo, HYUN HO KIM, XIAOFENG QIAN, Texas A&M University, WENCAN JIN, LIUYAN ZHAO, University of Michigan — CrI3 has recently been demonstrated to be an Ising ferromagnet whose magnetization retains even in a single monolayer below Curie temperature. Here we report our recent Raman studies on bulk and monolayer/few-layer CrI3. Temperature-dependent Raman studies are performed to scrutinize structural phase transition and magnetic phase transition. We determine the symmetries of the phonon modes using polarized Raman spectroscopy and first-principles theoretical calculations. Our results show that Raman selection rule no longer holds in degraded CrI3 samples.

*Supported by NSF CAREER Grants No. DMR-1760668, DMR- 1753054, and DMR-1749774.
Giant excitonic and magneto-optical responses in two-dimensional ferromagnets* MENG WU
(Presenter), ZHENGLU LI, TING CAO, STEVEN G. LOUIE, University of California, Berkeley — The magneto-optical (MO) effects, such as the magneto-optical Kerr effect (MOKE) and the Faraday effect, have been intensively investigated in a variety of magnetic materials serving as a highly sensitive probe for electronic and magnetic properties. Recent experiments using MOKE have discovered a few two-dimensional (2D) magnets, and demonstrated their rich magnetic behaviors. In particular, a giant Kerr response has been measured in monolayer and few-layer CrI3. However, by far, the microscopic origin of such MO signals is still unknown, because the essential spin-orbit coupling and excitonic effects are beyond the capability of existing first-principles methods. With newly developed GW and GW-BSE methods, we show that the exceedingly large optical and MO responses in ferromagnetic monolayer CrI3 arise from the strongly bound exciton states consisting of spin-polarized electron-hole states. With a realistic experimental setup, we find that the substrate configuration and excitation frequency strongly shape the MO signals. Our first-principles results are in good agreement with recent experiments on CrI3.

*This work was supported by NSF (No. DMR-1508412 and No. EFMA-1542741), and by the U.S. DOE (No. DE-AC02-05CH11231). Computational resources were provided by XSEDE and NERSC.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E16 DMP: Transport in Nanostructures -- Nanoscale Transport I BCEC 155 - Han Htoon, Los Alamos National Laboratory - Tag(s): Focus

Nanostructured gold thermocouple for photodetection* MAHDIYEH ABBASI (Presenter), Electrical and Computer Engineering, Rice university, CHARLOTTE I EVANS, Physics and astronomy, Rice university, XIFAN WANG, Material science, Rice university, LONGJI CUI, DOUGLAS NATHELSON, Physics and astronomy, Rice university — The Seebeck coefficient of a metal depends on the energy-dependent electrical conductivity, which in turn depends on the energy-dependent electron mean free path and the material band structure. At the nanoscale, when the geometric size is comparable with mean free path of the electrons, single metal thermocouples can be fabricated by changing the material geometry across the thermocouple. By using plasmonically-resonant structures, different device geometries and sizes can be used for wavelength sensitive light detection. We will present preliminary experimental data and simulations of single metal gold nanostructures with different geometries that are plasmonically active with IR laser illumination. We will discuss how these devices can be used for photodetection and discuss future applications for these measurements.

*The authors acknowledge support from NSF-1704625.

Shot-Noise Measurements of Waveguides with Attractive Electron-Electron Interactions* MUQING YU (Presenter), YUN-YI PAI, LEENA AGGARWAL, University of Pittsburgh, HYUNGWOO LEE, JUNGWOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — Mesoscopic devices created at oxide interfaces, such as the LaAlO3/SrTiO3 heterostructure [1], exhibit a wide range of exotic behavior that is linked to a strong electron-electron interaction. Electron pairing without superconductivity [2] involves transport of charge-2e carriers and higher-order “Pascal” phases with charge \( n \) \( e \) \( (n>2) \), have been identified in quantum transport measurements. One way to gain further insight to these phases would be to verify the existence of quantized charge by measuring shot noise. Here we describe experimental efforts to reveal shot-noise characteristics in electron waveguide devices whose electronic phases can be tuned between paired and unpaired state via tuning of magnetic field and chemical potential. These shot noise measurements have the potential to confirm the charge of these exotic electron liquid phases and provide insight into their phase diagrams.


8:24AM E16.00003: Observation of 450 GHz surface acoustic waves in suspended polycrystalline films by use of time-resolved resonant soft X-ray scattering* PHOEBE TENGDIN, DMITRIY ZUSIN, JOSHUA L KNOBLOCH, Physics, University of Colorado, ANATOLY SHABALIN, STJEPAN HRKAC, NELSON HUA, Physics, University of California, San Diego, YAROSLAV KVASHNIN, Physics and Astronomy, Uppsala University, SHEENA PATEL, Physics, University of California, San Diego, TIANMIN LIU, Physics, Stanford University, JUSTIN SHAW, National Institute of Standards and Technology Boulder, HANS T. NEMBACH, JILA, University of Colorado, Boulder, DANIEL J HIGLEY, Physics, Stanford University, WILLIAM F SCHLOTTER, ALEX REID, SLAC, RAHUL NANDKISHORE, Physics, University of Colorado, OLLE ERIKSSON, Physics and Astronomy, Uppsala University, LOIC LE GUYADER, European XFEL, ERIC FULLERTON, Electrical and Computer Engineering, University of California, San Diego, OLEG SHPYRKO, Physics, University of California, San Diego, MARGARET MARY MURNANE, HENRY C KAPTEYN, JILA, University of Colorado, Boulder, HERMANN DÜRR, Physics and Astronomy, Uppsala University, THOMAS SILVA (Presenter), National Institute of Standards and Technology Boulder — We have used ultrafast optical pumping to generate nanoscale surface acoustic waves (SAWs) from 200 to 450 GHz, 10-50 nm wavelengths, in metallic films on SiN membranes. Our measurement demonstrates a novel soft X-ray elastic scattering mechanism that probes the coupling of the electronic and phononic degrees of freedom on a [Co90Fe10(0.6 nm)/Ni(0.2 nm)]x50 multilayer. The samples have an average grain size of 30 nm and a rms roughness of 1 nm. This nanostructured surface topography allows optical coupling to the in-plane SAW. In a transmission soft X-ray scattering geometry, with circular polarized X-rays tuned to the Ni L3 edge, we observe a prominent charge scatter ring with a radius of approximately 0.2 nm⁻¹. After optical pumping with fluences ranging from 24-27 mJ/cm², SAWs appeared as ripples on the charge scatter ring that oscillate at ps timescales. We use Brillouin light scattering (BLS) and modeling to identify the SAW as a dilation mode with an in-plane velocity of 5.6 km/s. Surprisingly, the SAW lifetime peaks sharply at q = 0.25 nm⁻¹ (300 GHz), with a value greater than 60 ps, suggestive of a minimum in the SAW correlation length in the case of 2-d localization.

*Support by DOE/BES X-Ray Scattering Program Awards No. DE-SC0002002, DE-SC0018237, and DE-FOA-0001664

8:36AM E16.00004: Phonon Localization in Heat Conduction MARIA N. LUCKYANOVA, JONATHAN MENDOZA, Massachusetts Institute of Technology, HONG LU, University of California, Santa Barbara, BAI SONG (Presenter), Department of Mechanical Engineering, Massachusetts Institute of Technology, SHENXIE HUANG, JIAWEI ZHOU, MINGDA LI, Massachusetts Institute of Technology, YONGQI DONG, HUA ZHOU, Argonne National Laboratory, JOSEPH A GARLOW, LIJUN WU, Brookhaven National Laboratory, BRIAN KIRBY, ALEXANDER GRUTTER, National Institute of Standards and Technology, ALEXANDER PURETZKY, Oak Ridge National Laboratory, YIMEI ZHU, Brookhaven National Laboratory, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, ARTHUR C GOSSARD, University of California, Santa Barbara, GANG CHEN, Massachusetts Institute of Technology — The departure from diffusive phonon thermal transport has been extensively observed via a reduction in thermal conductivity in nanostructures. Such non-diffusive behavior has been largely explained with classical size effects, ignoring the wave nature of phonons. Here, we report localization behavior in phonon heat conduction due to multiple scattering and interference of broadband phonon waves, observed through measurements of the thermal conductivities of GaAs/AlAs superlattices with ErAs nanodots randomly distributed at the interfaces. Near room temperature, the measured thermal conductivities increased with increasing number of superlattice periods and eventually saturated, indicating a transition from ballistic to diffusive transport. At low temperatures, the thermal conductivities of the samples with ErAs dots first increased and then decreased with an increasing number of periods, signaling phonon wave localization. This Anderson localization behavior is also validated via atomistic Green’s function simulations. The observation of phonon localization in heat conduction is surprising due to the broadband nature of thermal transport. This discovery suggests a new path forward for engineering phonon thermal transport.
profiles for desired performance of integrated semiconductor architectures. The ML framework will facilitate the development of inverse design approach to engineer interface algorithms. Our model has shown remarkable ability to predict band structures and Onsager transport coefficients of large nanostructures. The algorithm is trained on inexpensive ~200 DFT calculations of SixGe1-x substitutional alloys, by algorithms to predict electronic structure and transport of non-ideally fabricated multilayered thin film Si/Ge systems with large number of configurational degrees of freedom. In this study, we employ machine learning (ML) dimension approaches nanoscale. Ab initio methods become expensive and infeasible to predict electronic properties of broad range of applications. The contact interfaces between these components dictate performance, especially as device components are being aggressively inserted into semiconductor architectures to perform operations at high rates, for a mean free path in a network of cavities.

This departure from Casimir’s linear scaling law can be understood in terms of the geometry dependence of the phonon Casimir radiation and wavelength-dependent Rayleigh scattering. We exploit this definition to understand heat transport in newly synthesized silicon metalattices, which consist of a finely controlled, three-dimensional arrangement of nanometer-sized cavities in crystalline silicon. Through computational simulation and experimental validation, we show that the heat conductivity of metalattices exhibits a minimum as a function of the cavity diameter at constant porosity. We establish that the constants of proportionality linearly depend on SL and to determine the parameters to optimize electronic transport and therefore, thermoelectric performance of short period SL.


*This work is funded by DARPA (DSO).

9:00AM E16.00006: Controlling hot-electron thermalization in nanoscale materials*  
SRIDHAR SADASIVAM, MARIA CHAN, PIERRE DARANCET (Presenter), Argonne National Laboratory — Non-equilibrium energy transfer between hot electrons and phonons plays an important role in the design and operation of photovoltaic and nanoelectronic devices. In this talk, I will show how symmetries in low dimensional materials can impact electron-phonon coupling and the timescale of “hot” electron thermalization. Using a recently-developed first-principles Boltzmann transport equation framework accounting for electron-phonon and phonon-phonon interactions [1], I will show this effect can be used to control hot electron dynamics and phonon bottlenecks for experimentally-synthesized low-dimensional devices. In particular, I will show how such non-equilibrium dynamics can be controlled by external gate potentials.


*Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

9:12AM E16.00007: Machine Learning Electronic Transport Properties of Multilayered Semiconductor Nanostructures*  
SANGHAMITRA NEOGI (Presenter), ARTEM PIMACHEV, University of Colorado, Boulder — Computing components are being aggressively inserted into semiconductor architectures to perform operations at high rates, for a broad range of applications. The contact interfaces between these components dictate performance, especially as device dimension approaches nanoscale. Ab initio methods become expensive and infeasible to predict electronic properties of systems with large number of configurational degrees of freedom. In this study, we employ machine learning (ML) algorithms to predict electronic structure and transport of non-ideally fabricated multilayered thin film Si/Ge nanostructures. The algorithm is trained on inexpensive ~200 DFT calculations of SixGe1-x substitutional alloys, by exploiting the relationship between local atomic environments and electronic properties. The predictor variables are obtained with Voronoi tessellation approach and the response variables are calculated with decision tree regression algorithm. Our model has shown remarkable ability to predict band structures and Onsager transport coefficients of large non-ideal superlattices. The ML framework will facilitate the development of inverse design approach to engineer interface profiles for desired performance of integrated semiconductor architectures.

*The project is funded by the DARPA (DSO).

9:24AM E16.00008: Ballistic length scale of heat transport in the subwavelength limit  
WEINAN CHEN (Presenter), DISHA TALREJA, Materials Science and Engineering Department, Pennsylvania State University, HIU YAN CHENG, Department of Chemistry, Pennsylvania State University, GERALD D MAHAN, VINCENT HENRY CRESPI, Department of Physics, Pennsylvania State University, JOHN BADDING, Department of Chemistry, Pennsylvania State University, VENKATRAMAN GOPALAN, ISMAILA DABO, Materials Science and Engineering Department, Pennsylvania State University — We present a comprehensive study of phonon ballistic length scale using a Casimir–Rayleigh model of heat transport. This model incorporates temperature-dependent Casimir radiation and wavelength-dependent Rayleigh scattering. We exploit this definition to understand heat transport in newly synthesized silicon metalattices, which consist of a finely controlled, three-dimensional arrangement of nanometer-sized cavities in crystalline silicon. Through computational simulation and experimental validation, we show that the heat conductivity of metalattices exhibits a minimum as a function of the cavity diameter at constant porosity. This departure from Casimir’s linear scaling law can be understood in terms of the geometry dependence of the phonon mean free path in a network of cavities.
In contrast to established work that use the diffuse surface scattering of phonons as the physical mechanism to reduce the thermal conductivities, in this talk we show that the largest reduction of thin film heat conduction is achieved via specular surface scattering. Our results create new opportunities for heat conduction manipulation since smooth surfaces – in contrast to rough surfaces – can be more effective on suppressing thin film phonon heat conduction.

9:48AM E16.00010: Coupling of Boron Dipyrromethene Dye Excitons to Plasmonic Surface Lattice Resonances in Aluminum Nanodisk Arrays

ROBERT COLLISON (Presenter), City University of New York, JACOB TREVINO, Chemeleon Inc., VINOD M MENON, STEPHEN O'BRIEN, City University of New York — When plasmonic metal nanoparticles are arranged in extended, one- or two-dimensional periodic arrays, the localized surface plasmon resonances (LSPRs) of the individual particles will couple radiatively to form a collective, propagating photonic-plasmonic mode known as a surface lattice resonance (SLR). Currently, SLRs and their potential applications in photonic devices, such as solar cells and light-emitting diodes, are growing topics of interest in the literature. In particular, the interaction of propagating, delocalized SLRs with the highly localized excitons of organic dye molecules is being investigated, and exotic phenomena such as the Bose-Einstein condensation of polaritons composed of dye excitons coupled to SLRs was recently reported(1). We report on the fabrication of SLR-supporting arrays of aluminum nanodisks on glass, and the coupling of these SLRs to dye excitons via coating of the arrays with dye-doped poly(methyl methacrylate). In particular, the interaction of the SLRs with boron dipyrromethene (BODIPY) dyes is examined, and the resulting effects, including angle-dependent fluorescent emission and enhancement of energy transfer between two different BODIPY dyes, are reported.


*NSF, CREST IDEALS

10:00AM E16.00011: Terahertz Spectroscopy of Metallic Single-Wall Carbon Nanotubes

HENRY WLADKOWSKI (Presenter), Physics and Astronomy, University of Wyoming, SHASHANK RAM NANDYALA, Electrical and Computer Engineering, University of Wyoming, JEFFREY FAGAN, NIST - Natl Inst of Stds & Tech, JON M PIKAL, Electrical and Computer Engineering, University of Wyoming, WILLIAM RICE, Physics and Astronomy, University of Wyoming — Optically generated, Coulombically bound electron-hole pairs, known as excitons, are rarely observed in metals due to strong electrostatic screening. However, in quantum-confined systems, such as one-dimensional (1D) single-wall carbon nanotubes (SWCNTs), screening effects are suppressed giving rise to exciton-dominated optical spectra in both semiconducting and metallic SWCNTs. Because of the difficulty of creating highly isolated 1D metallic environments, these metallic excitons are poorly studied. Here, we use terahertz absorption of single-chirality enriched SWCNTs at low temperatures to examine collective phenomena in 1D. We prepared, single-chirality (5,5) metallic and enriched (6,5) semiconducting SWCNTs in high-purity using aqueous two-phase extraction and characterized these fractions by optical methods. Enriched SWCNTs were immersed in a broadly transparent polymer matrix which preserved SWCNT individualization for cryogenic measurement. Using terahertz time-domain spectroscopy, we observed low-frequency plasmon absorption in metallic SWCNTs across a broad temperature range. This work provides the foundation for in-depth study of excitonic and plasmonic phenomena in single-chirality SWCNTs.

*HVW and WDR acknowledge support from the UW School of Energy Resources.

10:12AM E16.00012: Fabrication and characterization of nanoscale devices using Local anodic oxidation technique

HYEWON DU (Presenter), TAEKWANG KIM, SOMYEONG SHIN, SEONYEONG KIM, MINHO SONG, HANSUNG KIM, DAIN KANG, SUNAE SEO, Physics, Sejong Univ. — Graphene is one of the most promising materials as a flexible transparent electrode because of its high transparency and ultrahigh carrier mobility. Up to now, there are a number of methods to pattern graphene for application as electrodes. A commonly used patterning method is a combination of lithography and plasma etching, which causes undesired graphene defects during the etching process. Attempts to develop a patterning method that can simplify the fabrication process with minimal degradation is still a challenge. Here, we applied an electrochemical process based on Atomic force microscopy (AFM), Local anodic oxidation (LAO) technique, to define graphene electrodes with minimized graphene defect by eliminating the etching process. In addition, it is easy to manufacture a short channel device because the AFM tip has a nanometer order radius. This technique paves the way for the fabrication of organic-based devices where it is difficult to fabricate with short channels.
This talk will present recent highlights from our research on two-dimensional (2D) materials. Results span from fundamental measurements and simulations, to applications taking advantage of unusual 2D material properties. We measured record velocity saturation in graphene [1], and the thermal properties of graphene nanoribbons [2]. We have also grown monolayer 2D semiconductors by CVD over large areas, including MoS$_2$ [3], WSe$_2$, MoSe$_2$ [4], and multilayer MoTe$_2$ and WTe$_2$ [5]. ZrSe$_2$ and HfSe$_2$ have native high-K dielectrics ZrO$_2$ and HfO$_2$, which are of key technological relevance [6]. Improving electrical contacts [7], we demonstrated 10 nm transistors using monolayer MoS$_2$, with the highest current reported to date (>400 µA/µm), near ballistic limits [8]. Current density in such 2D devices is ultimately limited by self-heating and phonon scattering [9], in part due to the weak van der Waals bonds between 2D materials and their environment, which lead to a large thermal resistance of this interface [10]. On the other hand, we exploited this weak interface to improve energy efficiency in phase-change memory [11], and we tuned it by Li intercalation, demonstrating MoS$_2$-based thermal transistors [12]. These studies reveal fundamental limits and some applications of 2D materials, taking advantage of their unique properties.


Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E17 DCOMP: Matter in Extreme Environments: Novel Approaches to Pressure and Synthesis

8:00AM E17.0001: Matter in Extreme Environments: Materials synthesis and crystallography at extreme pressure - revealing some remarkable materials properties [Invited] NATALIA DUBROVINSKAIA (Presenter), LEONID DUBROVINSKY, University of Bayreuth — During last decades, the impact of high-pressure studies on fundamental physics and chemistry, and especially on Earth and planetary sciences, has been enormous. Modern science and technology rely on the vital knowledge of matter which is provided by crystallographic investigations. The most reliable information about crystal structures of solids and their response to alterations of pressure and temperature is obtained from single-crystal diffraction experiments. Advances in diamond anvil cell (DAC) techniques, designs of double-stage DACs, and in modern X-ray instrumentation and synchrotron facilities have enabled structural research at multimegabar pressures.

We have developed a methodology for performing single-crystal X-ray diffraction experiments in double-side laser-heated DACs and demonstrated that it allows the crystal structure solution and refinement, as well as accurate determination of thermal equations of state above 200 GPa at temperatures of thousands of degrees. Application of this methodology resulted in discoveries of novel compounds with unusual chemical compositions and crystal structures, uncommon crystal chemistry and physical properties. It has been successful in investigations of various classes of solids - elemental materials, oxides, carbides, borides, carbonates, nitrides, and silicates. In this contribution we will report the results of our single-crystal diffraction studies of phase relations in the Fe-O system, transition metals carbonates, silicates, and nitrides at simultaneous high pressures and high temperatures. Perspectives of materials synthesis and crystallography at extreme conditions will be outlined.
8:36AM E17.00002: Investigation of Pressure Induced Formation of Diamondene* LUIZ GUSTAVO PIMENTA MARTINS (Presenter), Massachusetts Institute of Technology, DIEGO LOPEZ, Physics, Federal University of Minas Gerais, MATEUS MATOS, Physics, Federal University of Ouro Preto, LEORA EVE DRESSELHAUS-COPPER, Lawrence Livermore National Laboratory, ROBERTO MOREIRA, MARIO SERGIO MAZZONI, Physics, Federal University of Minas Gerais, JING KONG, Massachusetts Institute of Technology, LUIZ GUSTAVO CANCADO, Physics, Federal University of Minas Gerais — Pressure is a convenient thermodynamic parameter for obtaining new materials that cannot be synthesized under ambient conditions. For instance, theoretical calculations show that when two layers of graphene are compressed at high-pressures in the presence of specific chemical groups, they can be turned into a 2D diamond called diamondene: a ferromagnetic semiconductor with spin-polarized bands. Efforts to experimentally demonstrate this structure are in the initial stages, yet we have already obtained robust results [1]. In this initial work, we obtained indirect evidence of diamondene formation at room temperature by compressing two layers of graphene using water as a pressure transmitting medium (PTM) in a diamond anvil cell (DAC). The phase transition was identified by measuring the G band dispersion with laser energy as a function of pressure. We will report our progress in investigating this phase transition with new experimental evidences.


*L.G.P.M and J.K acknowledge the support from the Air Force Office of Scientific Research under the MURI-FATE program, Grant No. FA9550-15-1-0514. L.G.P.M, D.L, M.S.M, R.M, M.M acknowledge the support from CNPQ.

8:48AM E17.00003: X-Ray Diffraction Crystallization Studies on a Zr-Based Bulk Metallic Glass under High-Pressure and High-Temperature* KATHRYN HAM (Presenter), YOGESH KUMAR VOHRA, University of Alabama at Birmingham, ROSTISLAV HRUBIAK, CURTIS KENNY-BENSON, HPCAT, The Advanced Photon Source, Argonne National Laboratory, ANDREW WERESZCZAK, Materials Science and Technology Division, Oak Ridge National Laboratory — X-ray diffraction crystallization studies were conducted on bulk metallic glass, Zr_{58.5}Cu_{15.6}Ni_{12.8}Al_{10.3}Nb_{2.8}. Each sample was compressed using a Paris-Edinburgh Press at Beamline 16-BM-B, HPCAT, of the Advanced Photon Source, and heated to 800°C. MgO was used as a pressure standard for this experiment, and two constant heating rates, 2.9°C/min and 6.0°C/min were investigated. A heating rate dependence was seen in the crystallization temperature, with a faster heating rate corresponding to a higher crystallization temperature for the full pressure range tested.

*The authors acknowledge support from the US Army Research Office under grant No. W911NF-15-10614 through the University of Tennessee Knoxville. Kathryn Ham acknowledges support from the US Department of Education, Graduate Assistance in Areas of National Need program under Award P200A150001. Portions of this work were performed at HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA under award No. DE-NA0001974 with partial instrumentation funding by NSF. The Advanced Photon Source is a US Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

9:00AM E17.00004: Graphene as a Diffusion Barrier in High-Temperature Electronics* LAURA BRANDT (Presenter), Physics and Electrical Engineering & Computer Science, University of California, Berkeley, ANANTH SARAN YALAMARTH, Mechanical Engineering, Stanford University, PETER F. SATTERTHWAITE, SAM VAZIRI, SAVANNAH BENBROOK, ERIC POP, Electrical Engineering, Stanford University, DEBBIE G. SENESKY, Aeronautics & Astronautics Engineering, Stanford University — The development of high-temperature semiconductor technology for use in applications such as power plants, nuclear reactors, and on hot planets like Venus (~460°C) is severely limited by the failure of essential metal contacts in otherwise thermally robust devices. This failure, which manifests as bubbling on the metal contact, is thought to be due to inter-diffusion of metal and semiconductor layers. To test this hypothesis, we constructed a monolayer graphene barrier to see if bubble formation would be reduced. Auger electron spectroscopy was used to characterize the inter-diffusion of material layers in Pd/AlGaN/GaN and Pd/Graphene/AlGaN/GaN Schottky diodes subjected to thermal treatments over a range of temperatures from 100 to 450°C. Graphene was shown to stop bubble formation in high-temperature metal contacts up to 425°C, supporting the inter-diffusion hypothesis and demonstrating promise for use on, for example, the planet Mercury (where temperatures range from approximately -180 to 430°C).

*This work was supported by the National Science Foundation (NSF) Engineering Research Center for Power Optimization of Electro-Thermal Systems with cooperative agreements ECC-1449548, and made use of the Stanford Nano Shared Facilities, NSF grant ECCS-1542152.
MEZOUAR, ESRF — The upper pressure achievable in the conventional Diamond Anvil Cell (DAC) had been limited to approximately 400 GPa since the early 2000s. We show that by sculpting the diamond anvil tip into a toroidal shape with a ratio of 1:3, the maximum pressure can be extended toward the terapascal pressure range. Measurements similar to standard DACs are possible in terms of precision, reproducibility, sample dimensions and type of materials from gas to solids and with any atomic number. Our toroidal-DAC design will be compared to other innovative schemes recently proposed to extend the pressure limit of the DAC, such as the double-stage DAC.

**9:17AM E17.00005: In Situ Solid State Laser Refrigeration at GPa Pressures**

**ABBBIE GANAS (Presenter), ANUPUM PANT, XIAOJING XIA, ELENA DOBRETSOVA, PETER PAUZAUSKIE, University of Washington — Solid state laser refrigeration can cool a host lattice through the emission of anti-Stokes upconverted photons from rare-earth dopant ions. Recently, laser refrigeration has also been demonstrated in condensed phases, including liquid water using single-beam laser tweezers. Laser refrigeration within a diamond anvil cell would allow researchers to explore in situ temperature-dependent properties of materials without external hardware. To date, laser refrigeration at extreme pressures has not yet been demonstrated. Here, we demonstrate the cooling of 10^9 Yb^{3+}:LiYF_4 (Yb:YLF, I_{41}/a space group) micro-crystals at elevated pressures in a diamond anvil cell. In addition, we investigate the impact of a scheelite to fergusonite phase transition on laser refrigeration at pressures >10.5 GPa. Varying the irradiance of a 1020nm continuous wave laser shows that Yb:YLF can be effectively cooled with a linear dependence on laser irradiances. Cooling temperatures are quantified using a ratiometric thermometry approach involving a Boltzmann fit to f-f transitions from the Yb^{3+} ions that occur between the Stark levels within the 2F_{5/2} and 2F_{7/2} manifolds.


**9:24AM E17.00006: Magnetometry and Stress Tomography in Diamond Anvil Cells using Nitrogen Vacancy Centers**

**PRABUDHYA BHATTACHARYYA (Presenter), SATCHE HSIEH, THOMAS MITTIGA, BRYCE H KOBRIN, FRANCISCO MACHADO, CHONG ZU, Physics, University of California, Berkeley, THOMAS SMART, Earth and Planetary Science, University of California, Berkeley, TIM HOEHN, NICHOLAS Z RUI, Physics, University of California, Berkeley, MEHDI KAMRANI, Aerospace Engineering, Iowa State University, SOONWON CHOI, Physics, University of California, Berkeley, VIKTOR V. STRUZHKIN, Geophysical Laboratory, Carnegie Institute of Washington, VALERY LEVITAS, Aerospace Engineering, Iowa State University, RAYMOND JEANLOZ, Earth and Planetary Science, University of California, Berkeley, NORMAN YAO, Physics, University of California, Berkeley — The Nitrogen Vacancy (NV) center in diamond has emerged as a promising candidate for the nanoscale sensing of temperature, strain, electric and magnetic fields. The integration of NV-based sensing into diamond anvil cells (DAC), a workhorse of high pressure science, offers a means not only for making spatially resolved measurements of relevant sample properties but also for monitoring the stress distribution in the diamond anvil itself. Compared to conventional high pressure probes, key advantages of NV sensing include diffraction limited spatial resolution (~1 um) and versatility, thus enabling exploration of novel phases of matter and the transitions between them, with pressure as a tuning parameter. Additionally, imaging the stress distribution inside DACs can provide insight into the mechanical failure of anvils and inform improvements in anvil design. We describe two main results: 1) we generate a layer of NVs near the tip of the diamond anvil and use DC magnetometry to study pressure-driven magnetic phase transitions and 2) using a carefully applied bias magnetic field we map the tensorial stress distribution within the diamond anvil itself.

**9:36AM E17.00007: Sterically Controlled Solid-State Mechanochemistry Under Hydrostatic Pressure**

**HAO YAN (Presenter), Stanford University, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago, WENDY MAO, Stanford University, NICHOLAS A MELOSH, Materials Science and Engineering, Stanford University, ZHIHUN SHEN, Stanford University — Mechanical stress can modify the energy landscape of chemical reactions and enable new reaction pathways. Mechanochemical mechanisms under tensile stress have been extensively studied in one-dimensional polymers. However, bond activation has not been possible with hydrostatic pressure in three-dimensional solids. Here we show that mechanochemistry through isotropic compression is possible by molecularly engineering structures that translate macroscopic isotropic stress into molecular-level anisotropic strain. We engineer molecules with mechanically heterogeneous components consisting of a compressible mechanophore and incompressible ligands. In these ‘molecular anvils’, isotropic stress leads to anisotropic deformation of the compressible mechanophore and activating bonds. We combine experiments and computations to demonstrate hydrostatic-pressure-driven redox reactions in crystalline metal-organic chalcogenides, where bending of bond angles or shearing of adjacent chains activates the metal-chalcogen bonds. These results reveal an unexplored mechanism and enable new possibilities for high-specificity mechanosynthesis.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences, under contracts DE-AC02-76SF00515 and DE-FG02-06ER46262.

**9:48AM E17.00008: The toroidal diamond anvil cell for detailed measurements under extreme static pressures.**

**PAUL LOUBEREY (Presenter), AGNES DEWAELLE, FLORENT OCCELLI, OLIVIER MARIE, CEA de Bruyeres-le-Chatel, MOHAMED MEZOUAR, ESRF — The upper pressure achievable in the conventional Diamond Anvil Cell (DAC) had been limited to approximately 400 GPa since the early 2000s. We show that by sculpting the diamond anvil tip into a toroidal shape with a Focussed Ion Beam, the maximum pressure can be extended toward the terapascal pressure range. Measurements similar to standard DACs are possible in terms of precision, reproducibility, sample dimensions and type of materials from gas to solids and with any atomic number. Our toroidal-DAC design will be compared to other innovative schemes recently proposed to extend the pressure limit of the DAC, such as the double-stage DAC.
10:00AM E17.00009: Toroidal diamond anvils for static compression experiments beyond 5 megabar* ZSOLT JENEI (Presenter), EARL F O'BANNON, SAMUEL T WEIR, HYUNCHAE CYNN, MAGNUS J LIPP, WILLIAM J EVANS, NICK E TESLICH, Lawrence Livermore Natl Lab, YUE MENG, JESSE SMITH, HPCAT, Advanced Photon Source, ANL — The diamond anvil cell has been around for over 50 years and has been the primary tool for routinely studying materials up to pressures of ~3 Mbar. Experiments over 4 Mbar with in situ pressure determination have been reported, however these reports are scarce. This indicates that these experiments are challenging, and that the success rate of these experiments is quite low. However, critical for developing accurate fundamental physics and chemistry models, with possible applications in modeling interiors of large planets. In this presentation I will show that focused ion beam crafted toroidal single-crystal diamond anvils with ~9.0 μm culets are capable of producing pressures over 5.0 Mbar. The toroidal surface prevents gasket outflow and provides a means to stabilize the central culet. We have reached a maximum pressure of ~6 Mbar using Re as in-situ pressure marker, a pressure regime typically accessed only by double-stage diamond anvils and dynamic compression platforms.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 17-ER-038.

10:12AM E17.00010: Single Crystal X-ray Diffraction in Laser Heated DACs LEONID DUBROVINSKY (Presenter), Bayreuth University — Until recently, all DAC-laser-heating systems were stationary and could not be used for single-crystal structural studies aimed not only at determining lattice parameters, but also at structural refinements, which require measuring X-ray diffraction intensities and at least partial rotation of the DAC during experiments with monochromatic radiation. The beam of a stationary laser enters the cell at a fixed angle, so that the rotation leads to departure of the crystal from the focus position and scattering the powerful laser light in arbitrary directions by the diamond anvils that might be dangerous.

In order to overcome this problem we have developed a portable laser heating system and diamond anvils with round tables (DARTs) and implemented them in our experiments at various diffraction beamlines (ID15 and ID27 at ESRF, and P02 at PETRA III). The performance and potential of this approach have been demonstrated in simultaneous high-pressure and high-temperature powder and single-crystal diffraction studies of chemical and phase relations in transition metals oxides, carbides, hydrides, carbonates, and silicate perovskites.

10:24AM E17.00011: Carbon-based clathrates* TIMOTHY STROBEL (Presenter), Carnegie Institution for Science — Clathrate structures are found throughout nature in tetrahedral systems including water, silicates, silicon, germanium, tin and even colloids. Given similarities in bonding, it is natural to presume the existence of clathrate frameworks based on carbon, but attempts to prepare these materials have been unsuccessful thus far. If synthesized, these materials are expected to exhibit diamond-like mechanical properties due to the nature of covalent bonding, as well as strong electron-phonon coupling that could lead to high superconducting transition temperatures. We develop a stabilization principle based on the substitution of boron within the polyhedral carbon cages. Using this approach, we predict and synthesize the first carbon-based clathrate comprised of truncated octahedral C12B12 cages that trap Sr atoms in the "type-VII" structure. The mechanical properties, electronic structure and superconducting properties of this material will be discussed, as well as the potential for different structures and compositions within this new family of carbon-based materials.

*This work was supported by DARPA under Grant No. W31P4Q1310005.

Tuesday, March 5, 2019 8:00 AM - 10:36 AM
Session E18 DCOMP DCMP DAMOP: Machine Learning Quantum States I BCEC 156B - Yizhuang You, Harvard University - Tag(s): Focus

8:00AM E18.00001: Learning quantum states with generative models [Invited] JUAN CARRASQUILLA (Presenter), Vector Institute — The technological success of machine learning techniques has motivated a research area in the condensed matter physics and quantum information communities, where new tools and conceptual connections between machine learning and many-body physics are rapidly developing. In this talk, I will discuss the use of generative models for learning quantum states. In particular, I will discuss a strategy for learning mixed states through a combination of informationally complete positive-operator valued measures and generative models. In this setting, generative models enable accurate learning of prototypical quantum states of large size directly from measurements mimicking experimental data.
8:36AM E18.00002: Machine Learning Holography in Neural Network Renormalization Group  
HONGYE HU (Presenter), University of California, San Diego, SHUO-HUI LI, LEI WANG, Institute of Physics, Chinese Academy of Sciences, YIZHUANG YOU, University of California, San Diego — Previously, people have shown the close relations between renormalization group (RG) with both deep learning and holographic duality, and how holographic geometry can emerge from deep learning the entanglement feature of a quantum many-body state. Inspired by those, we propose any boundary conformal field theory can be mapped into its holographic bulk to an operator level. In our framework, renormalization group is constructed as a hierarchical unsupervised generative model. Coarse graining direction can be viewed as an emergent direction, and it pushes boundary field theory configurations to bulk field configurations. The inverse coarse graining direction generates boundary field configurations from bulk noises. The goal is to construct optimal RG that makes bulk variables as uncorrelated as possible. The leftover of correlations between bulk variables can be used to define measure of distance in the bulk. We studied two dimensional interacting bosonic system as a boundary field theory. RG network is trained to find the effective bulk field theory and we observed the emergence of hyperbolic geometry (AdS3 spatial geometry) as we tuned system towards critical point.

8:48AM E18.00003: Study of phi-4 theories with deep learning methods*  
ZHONG YUAN LAI (Presenter), XIAOPENG LI, Department of Physics, Fudan University — Field theories find wide applications from characterization of scattering processes in particle physics, to analysis of statistical models, to description of critical phenomena in condensed matter. One key problem in using field theories is to perform non-perturbative calculations, which is crucial in various places, but has remained an open question. In this talk I will present our recent work combining field theoretical and deep learning methods to systematically account for non-perturbative aspects. In calculating Green's functions, nonperturbative Feynmann diagrams are automatically taken into account in our approach. I will present applications of this new approach to phi-4 field theories in one and two dimensions. Our approach potentially offers a generic solver for nonperturbative field theory calculations, of relevance to a broad context.

*National Program on Key Basic Research Project of China under Grant No. 2017YFA0304204
National Natural Science Foundation of China under Grants No.117740067

9:00AM E18.00004: Analytic continuation by combining sparse modeling with the Pade approximation  
YUICHI MOTOYAMA (Presenter), KAZUYOSHI YOSHIMI, ISSP, University of Tokyo, JUNYA OTSUKI, Tohoku University, HIROSHI SHINAOKA, Saitama University — Numerical methods based on the imaginary-time path-integral such as the path-integral Monte Carlo method are powerful tools to investigate a quantum many-body system both at absolute zero and finite temperatures. For example, these can calculate the imaginary-time Green's function directly, and other important quantities such as spectrum function can be transformed from this by the analytic continuation (AC) or by solving the Lehmann representation as an integral equation. In practice, however, this transformation is unstable against noise of the imaginary-time Green's function.

Several methods have been developed to solve this problem so far. The noise reduction by the sparse modeling (SpM) is one of them. In this method, we transform basis by the singular matrices of the integral kernel and truncate noisy components in the new basis by the sparse modeling. However, this truncation introduces an unphysical oscillation to the obtained spectrum as a systematic error.

In this study, we have improved SpM method by combining it with AC by the Pade approximation. AC by the Pade approximation gives a stable and smooth spectrum in low frequency region, which can be used to make the SpM spectrum smooth and high accuracy.

9:12AM E18.00005: A machine learning approach to excited states of quantum many-body systems*  
DOUGLAS HENDRY (Presenter), ADRIAN FEIGUIN, Northeastern University — We present a variational Monte Carlo method for determining dynamical properties and the spectral function of quantum many-body systems. Restricted Boltzmann machines (RBMs) are used to encode the Green's function of the system. First, the ground state wave function is calculated using a standard variational approach. The dynamical correlation function is then obtained by solving two linear systems of equations. We present a variational Monte Carlo approach to do so. This process has to be repeated for each value of frequency and momentum, but it can be easily parallelized. We illustrate it with applications to the Heisenberg model in one and two dimensions. Results show remarkable agreement with exact calculations on small systems and demonstrate that RBMs can also faithfully represent excited states.

*National Science Foundation
9:24AM E18.00006: Machine Learning Spatial Geometry from Entanglement Features YIZHUANG YOU (Presenter), UCSD — Motivated by the close relations of the renormalization group with both the holography duality and the deep learning, we propose that the holographic geometry can emerge from deep learning the entanglement feature of a quantum many-body state. We develop a concrete algorithm, call the entanglement feature learning (EFL), based on the random tensor network (RTN) model for the tensor network holography. We show that each RTN can be mapped to a Boltzmann machine, trained by the entanglement entropies over all subregions of a given quantum many-body state. The goal is to construct the optimal RTN that best reproduce the entanglement feature. The RTN geometry can then be interpreted as the emergent holographic geometry. We demonstrate the EFL algorithm on 1D free fermion system and observe the emergence of the hyperbolic geometry (AdS3 spatial geometry) as we tune the fermion system towards the gapless critical point (CFT2 point).

9:36AM E18.00007: Machine learning many-body localization: Search for the elusive nonergodic metal XIAO LI (Presenter), YI-TING HSU, DONG-LING DENG, University of Maryland — The many-body localization transition in isolated quantum systems with a single-particle mobility edge is an intriguing subject that has not yet been fully understood. In particular, whether a nonergodic metallic phase associated with a many-body mobility edge exists or not is under active debate. In this Letter, we construct a neural network classifier to investigate the existence of the nonergodic metallic phase in a prototype model using many-body entanglement spectra as the sole diagnostic. We find that such a classifier is able to identify with high confidence the nonergodic metallic phase existing between the many-body localized and the thermal phase. Our neural network based approach shows how supervised machine learning can be applied not only in locating phase boundaries, but also in providing a way to definitively examine the existence of a novel phase whose existence is unclear.

9:48AM E18.00008: Machine learning of condensed-matter phases with physical interpretability MING HAN (Presenter), ZONGHUI Wei, ERIK LUIJTEN, Northwestern University — Nature displays a vast variety of phase transitions. Detecting and quantifying these often requires creative design of order parameters, which are strongly system dependent. Thanks to recent advances in machine learning (ML), it is now possible to identify phase behavior by directly analyzing atomistic configurations via modern pattern-recognition techniques. Whereas these ML approaches are universal and robust, they often suffer from the lack of physical interpretability. Here we introduce a new ML scheme, which distinguishes different condensed-matter phases by autonomously recognizing order parameters. When applied to two-dimensional Ising models, our method can accurately predict the Curie and Néel temperatures and capture the corresponding critical phenomena by recognizing ferro- and antiferro-magnetizations, respectively. Going beyond these prototypical test cases, we analyze the nonequilibrium polymeric sol-gel transition, locating not only the transition temperature, but also discovering two classes of underlying collective behavior, the condensation and network-formation modes. Compared to existing MLs, our method offers physical insights as well as high training efficiency.

10:00AM E18.00009: Interpretable Machine Learning Study of Many-Body Localization Transition in Disordered Quantum Spin Chains* WEI ZHANG (Presenter), Boston College, LEI WANG, Institute of Physics Chinese Academy of Sciences, ZIQIANG WANG, Boston College — We develop, train, and apply a support vector machine (SVM) to study the phase transition between many-body localized and thermal phases in a disordered quantum Ising chain. We use the labeled probability density of eigenstate wavefunctions in the deeply localized and thermal regimes at two different energy densities as the training set. We find that the trained SVM is then able to predict the whole phase diagram. The obtained phase boundary qualitatively agrees with previous work using entanglement entropy to characterize these two phases. We further analyze the decision function of the SVM to interpret its physical meaning and find that it is analogous to the inverse participation ratio in the many-body configuration space. Our findings demonstrate the ability of the SVM to capture potential quantities that may characterize the many-body localization phase transition. The qualitative agreement of phase boundary obtained by SVM and by scaling entanglement entropy motivates further exploration of the relation between these two different quantities in connection to many-body localization.

*U.S. Department of Energy, Basic Energy Sciences Grant No. DE-FG02-99ER45747 National Natural Science Foundation of China under Grant No. 11774398
Analytic continuation via “domain-knowledge free” machine learning*  HONGKEE YOON (Presenter), JAE-HOON SIM, MYUNG JOON HAN, Department of Physics, KAIST — We present a machine-learning (ML) approach to a long-standing issue in quantum many-body physics, namely, analytic continuation. This notorious ill-conditioned problem of obtaining spectral function from Green's function has been a focus of new method developments for past decades. Here we demonstrate the usefulness of modern ML techniques including convolutional neural networks and the variants of stochastic gradient descent optimizer. ML continuation kernel is successfully realized without any ‘domain-knowledge’, which means that any physical ‘prior’ is not utilized in the kernel construction and the neural networks ‘learn’ the knowledge solely from ‘training’. The outstanding performance is achieved for both insulating and metallic band structure. Our ML-based approach not only provides the more accurate spectrum than the conventional methods in terms of peak positions and heights, but is also more robust against the noise which is the required key feature for any continuation technique to be successful [1]. Furthermore, its computation speed is $10^4$–$10^5$ times faster than maximum entropy method.


*This work was supported by the National Research Foundation of Korea (NRF) (2017R1D1A1B03032082) and NRF (2018M3D1A1059001).

Monte Carlo Renormalization Group for Systems with Quenched Disorder*  YANTAO WU (Presenter), ROBERTO CAR, Princeton University — We extend to quenched disordered systems the variational scheme for real space renormalization group calculations that we recently introduced for homogeneous spin Hamiltonians. When disorder is present our approach gives access to the flow of the renormalized Hamiltonian distribution, from which one can compute the critical exponents if the correlations of the renormalized couplings retain finite range. Key to the variational approach is the bias potential found by minimizing a convex functional in statistical mechanics. This potential reduces dramatically the Monte Carlo relaxation time in large disordered systems. We demonstrate the method with applications to dilute Ising, random field Ising and short-range spin glass models, on the two-dimensional square lattice.

*We acknowledge support from DOE Award DE-SC0017865.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E19 DAMOP: Precision Many Body Physics IV  BCEC 156C - Tigran Sedrakyan, University of Massachusetts Amherst - Tag(s): Focus

Quantum Transport in Strongly Interacting Fermi Gases* [Invited]  MARTIN ZWIERLEIN (Presenter), Massachusetts Institute of Technology — Transport is the defining property of states of matter, but often the most difficult to understand. Strongly interacting Fermi gases are especially challenging, despite their ubiquitous presence across many fields of physics. Experiments on ultracold fermionic atoms allow the direct measurement of transport properties in ideal model systems where the hamiltonian is precisely known while transport properties are difficult to calculate theoretically. In this talk I will present transport measurements on two strongly interacting Fermi systems, the unitary Fermi gas and the Fermi-Hubbard gas, both realized in uniform box potentials. In the unitary gas, we excite first and, in the superfluid regime, also second sound waves and demonstrate a quantum limited sound diffusivity given by $\hbar c$ over the particle mass. The first and second sound diffusivities give direct access to the thermal conductivity and the viscosity of the gas. For the Fermi-Hubbard gas, realized under a quantum gas microscope, we measure spin diffusion and spin conductivity in the Mott insulator at half filling. For strong interactions, spin diffusion is driven by super-exchange and doublon-hole-assisted tunneling, and strongly violates the quantum limit of charge diffusion. The technique developed in this work can be extended to finite doping, which can shed light on the complex interplay between spin and charge in the Hubbard model.

*This work was supported by the NSF, AFOSR, an AFOSR MURI on Exotic Quantum Phases, ARO, ONR, the David and Lucile Packard Foundation and the Gordon and Betty Moore foundation.
8:36AM E19.00002: Spectra of heavy polarons and molecules coupled to a Fermi sea* DIMITRI PIMENOV (Presenter), Ludwig Maximilian University of Munich, MOSHE GOLDSTEIN, Tel Aviv University — We study the spectrum of an impurity coupled to a Fermi sea (e.g., minority atom in an ultracold gas, exciton in a solid) by attraction strong enough to form a molecule/trion. We introduce a diagrammatic scheme which allows treating a finite mass impurity while reproducing the Fermi edge singularity in the immobile limit. For large binding energies the spectrum is characterized by a semi-coherent repulsive polaron and an incoherent molecule, which is the lowest-energy feature in the single-particle spectrum. The previously predicted attractive polaron seems not to exist for strong binding.

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Israel Science Foundation (Grant No. 227/15)
US-Israel Binational Science Foundation (Grant No. 2014262)
Israel Ministry of Science and Technology (Contract No. 3-12419).

8:48AM E19.00003: Energy and short-range correlations of Bose Polarons in the strong coupling regime* CARSTEN ROBENS (Presenter), ZOE YAN, YIQI NI, ALEXANDER YU CHUANG, MARTIN ZWIERLEIN, Massachusetts Institute of Technology — The concept of the Bose polaron quasiparticle originates in Landau’s description of a crystal’s conduction electron which deforms the surrounding ionic lattice. Despite the conceptual simplicity of the Bose polaron – i.e. an impurity dressed by a surrounding bosonic bath – this quasiparticle poses remarkable challenges for both theoretical and experimental physicists. These challenges arise at strong interaction strengths where a multitude of bosons can simultaneously interact with the impurity thereby forming a complicated many-body state. We here report on the first creation of an ensemble of Bose polarons – comprised of fermionic 40K impurities immersed in a 23Na Bose Einstein condensate – in local equilibrium and in the strongly interacting regime. Using radio frequency ejection spectroscopy, we measure the Bose polaron ground-state energy and short-range correlations as a function of temperature across a variety of interaction strengths by tuning an interspecies magnetic Feshbach resonance. We further study collective oscillations between the BEC and the impurities, demonstrating strong dissipation of the impurities’ momentum at the transition from collisionless to hydrodynamic regime.

*Gordon and Betty Moore Foundation, National Science Foundation (NSF), AFOSR - MURI, ARO

9:00AM E19.00004: Polaron mobility in the \`\`beyond quasiparticles" regime* ANDREY MISHCHENKO (Presenter), Center for Emerging Matter Science (CEMS), RIKEN — In a number of physical situations, from polarons, to non-Fermi liquids, to Dirac liquids, one often faces a problem of computing particle mobility/conductivity when conditions for applicability of the kinetic equation approach are violated. The corresponding \`\`beyond quasiparticles" (or \`\`overdamped") regime is formally identified as a state in which an inelastic scattering time (computed formally within the standard perturbative approach) is exceeding the typical thermal energy of quasiparticles. We employ the Diagrammatic Monte Carlo method to study mobility of Frohlich polarons in the overdamped regime and find two effects: a substantial delay in developing an exponential law at temperatures below the optical mode frequency, and a mobility minimum at T close to optical ode frequency. Both effects should be taken into account in interpreting mobility data in materials with strong electron-phonon coupling.

*This work was funded by the ImPACT Program of the Council for Science, Technology and Innovation (Cabinet Office, Government of Japan).
9:12AM E19.00005: The contact of the Fermi gas at unitarity*  SCOTT JENSEN (Presenter), Yale University, CHRISTOPHER GILBRETH, Central Washington University, YORAM ALHASSID, Yale University — The unitary Fermi gas is a strongly correlated system with a short-range interaction that saturates the upper bound on the modulus of the two-particle s-wave scattering amplitude. It is characterized by an infinite scattering length and sits in the middle of the BCS-BEC crossover. The contact of this system is a quantity that describes short-range pairing correlations and appears in the high momentum tail of the momentum distribution and the static structure factor, as well as in the high-frequency tail of the shear viscosity spectral function. There have been a number of recent calculations and important experimental advances towards determining the contact for the unitary Fermi gas. We present results for the temperature dependence of the contact at unitarity using finite-temperature auxiliary-field quantum Monte Carlo (AFMC) methods on the lattice. Our calculations are carried out within the canonical ensemble with multiple filling factors and extrapolated to the continuum limit. We compare our results with other theoretical calculations and with experiment.

*This work was supported in part by the U.S. DOE grant Nos. DE-FG02-91ER40608 and DE-FG02-00ER41132.

9:24AM E19.00006: Signatures of pairing in the free energy of the unitary Fermi gas at finite temperature*  CHRISTOPHER GILBRETH (Presenter), Physics, Central Washington University, SCOTT JENSEN, YORAM ALHASSID, Physics, Yale University — The pseudogap regime in cold atomic Fermi gases is characterized by pairing correlations occurring above the critical temperature without the presence of superfluidity. Although this regime is easily understood to exist when there is a deep bound state in the two-particle system, its existence when there is only a zero-energy resonance, i.e., in the unitary limit of infinite scattering length, is much more difficult to verify. An accurate understanding requires precise theoretical and experimental methods at finite temperature, as well as investigating multiple observables. We discuss new quantum Monte Carlo calculations for the free energy of the unitary gas at finite temperature and their implications for pseudogap physics. In particular, we present new results for the even-odd staggering of the free energy based on canonical ensemble calculations.

*Supported in part by the US Department of Energy Grant No. DE-FG02-00ER41132.

9:36AM E19.00007: Spin Transport in a Mott Insulator of Ultracold Fermions*  MATTHEW A NICHOLS, Massachusetts Institute of Technology, LAWRENCE CHEUK, Harvard University, MELIH OKAN, THOMAS HARTKE (Presenter), ENRIQUE MENDEZ, HAO ZHANG, Massachusetts Institute of Technology, EHSAN KHATAMI, San Jose State University, MARTIN ZWERLEIN, Massachusetts Institute of Technology — Understanding transport in strongly interacting Fermi systems is among the most pressing but difficult tasks of many-body physics. The Fermi-Hubbard model serves as a prototypical example of a strongly correlated fermionic quantum system, and is believed to hold the key to high-temperature superconductivity. However, the transport properties in the various regions of its phase diagram are far from understood. We realize the Fermi-Hubbard model using a gas of fermionic atoms in an optical lattice, confined in a homogeneous box trap. In this setting, we study spin and charge transport using a quantum gas microscope, able to resolve individual atoms. In particular, at half filling, the charge degree of freedom is frozen, while spins are still able to move. Spin transport is induced by applying a spin-dependent magnetic field gradient. We observe spin dynamics which are diffusive in nature, and obtain the spin conductivity and spin diffusivity. These findings can be compared to existing theoretical approaches, such as the numerical-linked-cluster expansion (NLCE).

*This work was supported by the NSF, AFOSR, ONR, and the Gordon and Betty Moore Foundation.

9:48AM E19.00008: Excitation spectrum of dipolar Bose gases*  YOUSSEF KORA (Presenter), MASSIMO BONINSEGNI, University of Alberta — We investigate the excitation spectrum of a dipolar Bose gas in the low temperature limit across the superfluid-supersolid-crystal transition. At sufficiently low temperatures, a system of aligned dipolar bosons will undergo a quantum phase transition by tuning the range of the repulsive two-body potential. In one limit, the phase of the system is that of a classical crystal of filaments. At the other limit, the system experiences quantum melting into a superfluid phase. In the intermediate regime, the system exists in a supersolid state. We use Quantum Monte Carlo techniques to compute imaginary time correlation functions at the different regions of the phase diagram, and we use the method of Maximum Entropy to extract the dynamical structure factor, which is then used to obtain the excitation spectrum and its evolution throughout the phase diagram.

*This work was supported by the Natural Sciences and Engineering Research Council of Canada.
10:00AM E19.00009: Bose liquid in checkerboard antiferromagnet  
HAIYUAN ZOU (Presenter), Tsung-Dao Lee Institute, Shanghai Jiao Tong University, FAN YANG, School of Physics, Beijing Institute of Technology, WEI KU, Tsung-Dao Lee Institute & School of Physics and Astronomy, Shanghai Jiao Tong University — The frustrated $J_1$-$J_2$ antiferromagnet model on the checkerboard lattice, known as the two-dimensional analog of the pyrochlore lattice, provides a perfect platform for dimensional crossover effect due to competition between the two exchange constants $J_1$ and $J_2$. Using recently developed tensor network algorithm based on Projected Entangled Simplex States (PESS), we obtain a line degenerate bose liquid state without magnetic order on the whole range of $J_2 > J_1$ for both XY and Heisenberg antiferromagnetic limit. The degenerate liquid state is stable even when small anisotropy on $J_1$ bond is introduced and the interaction enhance the robustness of the bose liquid behavior.

10:12AM E19.00010: Impenetrable SU(N) fermions in one-dimensional lattices  
YICHENG ZHANG (Presenter), Department of physics, Pennsylvania State University, LEV VIDMAR, Department of Theoretical Physics, J. Stefan Institute, MARCOS RIGOL, Department of physics, Pennsylvania State University — We study SU(N) fermions in the limit of infinite on-site repulsion between all species. We focus on states in which every pair of consecutive fermions carries a different spin flavor. Since the particle order cannot be changed (because of the infinite on-site repulsion) and contiguous fermions have a different spin flavor, we refer to the corresponding constrained model as the model of distinguishable quantum particles. We introduce an exact numerical method to calculate equilibrium one-body correlations of distinguishable quantum particles based on a mapping onto noninteracting spinless fermions. In contrast to most many-body systems in one dimension, which usually exhibit either power-law or exponential decay of off-diagonal one-body correlations with distance, distinguishable quantum particles exhibit a Gaussian decay of one-body correlations in the ground state, while finite-temperature correlations are well described by stretched exponential decay. We also study the dynamics of distinguishable quantum particles after geometric quantum quenches.

10:24AM E19.00011: Efficient exact diagonalization of the n-body reduced density matrix*  
HATEM BARGHATHI (Presenter), ADRIAN DEL MAESTRO, University of Vermont — The n-body reduced density matrix provides an alternate description of a quantum-many body system that can offer considerable compression over the wavefunction while providing access to observables and correlation functions. In this talk, we present an efficient algorithm for its construction and exact diagonalization in a system of N interacting particles. In one spatial dimension, we simplify computations by exploiting translational, reflection and particle-hole symmetries. We illustrate the method by calculating the maximal particle entanglement entropy constructed from the N/2-particle reduced density matrix in the ground state of up to 13 interacting fermions on 26 sites.  

*This work was supported in part by the NSF under Grant No. DMR-1553991. Computations were performed on the Vermont Advanced Computer Core supported in part by NSF Grant No. OAC-1827314.

10:36AM E19.00012: Prethermalization and Thermalization in Generic Isolated Quantum Systems*  
KRISHNANAND MALLAYYA (Presenter), MARCOS RIGOL, Department of Physics, Pennsylvania State University, WOJCIECH DE ROECK, Instituut voor Theoretische Fysica, KULeuven — Prethermalization has been extensively studied in systems close to integrability. We propose a more general, yet simpler, setup for this phenomenon. We consider a possibly nonintegrable-reference dynamics, weakly perturbed so that the perturbation violates at least one conservation law of the reference dynamics. We argue then that the evolution of the system proceeds via intermediate (generalized) equilibrium states of the reference dynamics. The motion on the manifold of equilibrium states is governed by an autonomous equation, flowing towards global equilibrium in a time of order $g^2$, with $g$ the perturbation strength. We also describe the leading corrections to the time-dependent reference equilibrium state, in general of order $g$. The theory is well-confirmed by numerical calculations relying on the numerical linked cluster expansion.  

*NSF Grant No. PHY-1707482, PHY-1748958
Evolution of two-time correlations in strongly correlated dissipative systems: aging and hierarchical dynamics*

STEFAN WOLFF (Presenter), JEAN-SEBASTIEN BERNIER, HISKP, University Bonn, DARIO POLETTI, Science and Math Cluster and EPD Pillar, Singapore University of Technology and Design (SUTD), AMENEH SHEIKHAN, Department of Physics, Shahid Beheshti University, CORINNA KOLLATH, HISKP, University Bonn — In recent years, considerable experimental efforts have been devoted to dynamically generate complex states and monitor their evolution. Despite remarkable advances, the theoretical principles behind the non-equilibrium dynamics of strongly correlated quantum matter are still far from being fully understood. In particular, very few studies have sought to clarify the influence of environmental couplings on the propagation of correlations. We attempt here to fill this gap. To do so, we extend quasi-exact time-dependent matrix product state techniques to simulate the evolution of two-time correlations in the XXZ spin-1/2 model in contact with an environment causing local dephasing on all sites. We find this system to display hierarchical and aging dynamics. The latter dynamical regime is characterized by a breakdown of time-translation invariance, a slow non-exponential relaxation of two-time correlations and the presence of dynamical scaling.

*European Research Council, ERC (Grant Number 648166), Deutsche Forschungsgemeinschaft, DFG (TR 185 project B4, SFB 1238 project C05, and Einzelantrag)

Tuesday, March 5, 2019 8:00 AM - 11:00 AM


Time-dependent density-functional approaches for excitons: the pros and cons of long-range corrected exchange-correlation kernels*

CARSTEN ULLRICH (Presenter), University of Missouri — Time-dependent density-functional theory (TDDFT) is, in principle, more efficient than the Bethe-Salpeter equation for calculating the optical properties of semiconductors and insulators. However, finding accurate exchange-correlation (xc) kernels for describing excitons is quite challenging: standard local and semilocal approximations lack the proper long-range behavior and do not produce bound excitons. This talk presents a systematic assessment of a class of long-range corrected (LRC) xc kernels which have shown promise for excitonic effects. It is found that no existing LRC kernel is capable of simultaneously producing good optical spectra and quantitatively accurate exciton binding energies for both semiconductors and insulators. We discuss strategies to improve the TDDFT treatment of excitons via semiempirical LRC xc kernels and screened hybrid approaches.

*This work was supported by NSF Grant No. DMR-1810922

Exact exchange-correlation kernels for optical spectra

MIKE ENTWISTLE (Presenter), REX W GODBY, Physics, University of York — Time-dependent density-functional theory (TDDFT) is in principle a powerful technique for simulating the time-evolution of systems of interacting electrons. Whilst TDDFT has had notable successes, the usual adiabatic functionals within the linear response regime can fail badly when applied to problems such as optical absorption spectra. By reverse-engineering numerically exact calculations of the ground and excited many-body states, and response functions, of prototype one-dimensional systems, we obtain the exact exchange-correlation kernel $f_{xc}(x,x',\omega)$ for each system. We explore the properties of these exact xc kernels, and suggest how common approximations may be improved.
8:48AM E20.00003: Accelerating excited-state calculations in NanoGW using an interpolative separable density fitting method*  WEIWEI GAO (Presenter), JAMES CHELIKOWSKY, University of Texas at Austin — The NanoGW package implements some of the most widely used methods for calculating excited-state properties, including time-dependent density function theory (TDDFT), GW approximation, and Bethe-Salpeter equation in the single-particle orbital basis. Solving Casida's equation of TDDFT and performing GW/BSE calculations with NanoGW involve the computation of many electron-repulsion integrals. We will discuss the implementation of the interpolative separable density fitting (ISDF) method, a new density-fitting method [1] with $O(N_{\text{atom}}^3)$ computational complexity, in NanoGW. With ISDF method, we can reduce the number of electron-repulsion integrals from $O(N_{\text{atom}}^4)$ to $O(N_{\text{atom}}^2)$.


*Our supported by a subward from the U.S. Department of Energy under Contract No. DEAC02-05CH11231.

9:00AM E20.00004: Floquet theory for the electronic stopping of projectiles in solids*  NICOLO' FORCELLINI (Presenter), EMILIO ARTACHO, Physics, University of Cambridge — The problem of electronic stopping is traditionally approached and understood in the context of linear response theory[1], or a full non-linear theory for jellium[2]. First-principles quantitative simulations using time dependent density functional theory show reasonably predictive accuracy but remain computationally expensive and do not provide a clear, intuitive understanding of the stopping processes. We propose here a general (single-particle) stationary theory for the electronic excitation in crystalline solids by a constant-velocity projectile. It is based on the Floquet formalism for time-periodic systems[3], exploiting the system discrete translational space-time invariance. A change to the projectile's reference frame allows for a generalization of the treatment in Ref. [2], permitting a full study of the stopping in strong coupling for any crystalline system. Non-trivial effects such as the low-velocity threshold effect can be analyzed and understood in this framework.


*This work was supported by the EPSRC training grant EP/N509620/1 (NF) and the Leverhulme Trust Research Project Grant RPG-2018-254 (EA).

9:12AM E20.00005: Electronic stopping of protons in anisotropic weakly bound materials*  JESSICA F. K. HALLIDAY, Cavendish Laboratory, University of Cambridge, PERE ALEMANY, IQTC-UB, Universidad de Barcelona, EMILIO ARTACHO (Presenter), Cavendish Laboratory, University of Cambridge — Ions shooting through condensed matter dissipate their kinetic energy by transferring it to the target's electrons and nuclei. At high velocities (above 1% of the speed of light) the stopping is mostly electronic, in a highly non-equilibrium, non-adiabatic process. First-principles simulations of such processes have been quite successfully performed in the last decade for varied systems. Here we present results for electronic stopping power for protons in graphite and ideal crystalline polyethylene, anisotropic systems with strong bonding in two dimensions and weakly bound in the other dimension, and vice-versa, respectively. They are based on time-dependent density-functional theory in real time, and using a basis of atomic orbitals (LCAO) within the SIESTA program. Results of the effect of trajectory orientation and impact parameter will be presented, displaying a transition from electronic-structure dependence at low velocity, to a regime at higher velocities in which the particle density along the projectile's path dominates. A reformulation of the TD-LCAO formalism and its implications for numerical simulations will be also presented.

*Sabbatical stay of PA funded by the Salvador de Madariaga program, Ministerio de Educacion, Cultura y Deporte of Spain (ref. PRX17/00269)
9:24AM E20.00006: Electronic excitations in proton-irradiated ice via Real-Time TDDFT†

DANIEL MUÑOZ-SANTIBURCIO (Presenter), EMILIO ARTACHO, CIC nanoGUNE — Describing the interaction of water ice with highly energetic particles at the atomistic/electronic scale is of great importance to understand many astrophysical/chemical processes taking place in interstellar dust, comets, asteroids and satellites exposed to such particles present in solar wind, cosmic rays or strong magnetospheres.

Here I will show the results of Real-Time Time-Dependent-DFT calculations where the irradiation of ice with highly energetic protons is simulated in real time via Ehrenfest MD. This allow us not only to precisely compute the energy absorbed by the target and to follow the electronic excitations, but also to obtain an intuitive picture of which kind of electrons in the system (either ‘lone pairs’ or ‘bonding pairs’ electrons) are more likely to get excited, ultimately leading to ionization of the ice target. The influence of factors such as the trajectory and energy of the incoming proton will be also disclosed.

†This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 748673. We acknowledge PRACE for awarding us access to MareNostrum at Barcelona Supercomputing Center (BSC), Spain.

9:36AM E20.00007: Electronic stopping power from time-dependent density-functional theory in Gaussian basis

IVAN MALIYOV (Presenter), FABIEN BRUNEVAL, JEAN-PAUL CROCOMBETTE, Saclay Nuclear Research Centre — Irradiation damage in condensed matter has been identified as central to nuclear materials, electronics, nuclear medicine. The interaction between an irradiating ion and a target material is measured by the stopping power, defined as the energy transfer from the projectile to the material per penetration distance. The most important ionic energy loss channel occurs through electronic excitations. This work is devoted to the ab initio calculations of the electronic stopping power.

We have developed a real time TDDFT approach based on MOLGW code for finite systems [1]. Using localized Gaussian basis has numerous advantages, such as the cheap account of core electrons, the simple implementation of the hybrid functionals, the tunable basis accuracy and overall low computational cost.

With our tool, we explore the bulk limit, how to properly average over the impact parameters so to obtain the experimental random electronic stopping power. We perform calculations for several metallic targets and for different ionic projectiles to evaluate the so-called Barkas effect [2] and to study the wake electronic density behind the projectile.


9:48AM E20.00008: Charge equilibration and electronic stopping for self-irradiated silicon*

CHENG-WEI LEE (Presenter), ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Charged energetic particle radiation has technological interest in applications including nuclear energy, outer space, medicine, and fundamental research. As a result of irradiation, damage, including point defects, forms and ultimately determines the material properties. Therefore, understanding the underlying interactions between charged particles and a material from first principles is important. Recently, we investigated heavy (silicon) projectiles traversing crystalline bulk silicon and found a pronounced dependence of electronic stopping on the initial projectile charge state. This effect was not observed for light projectiles impacting metal or semiconductor targets. To understand this, we analyze the dynamics of charge equilibration, influence of the impact parameter, and contributions of core and valence electrons to electronic stopping. We observe that the equilibrium charge state of the Si projectile depends on the impact parameter and ultimately dominates electronic stopping. We also predict that this effect should be observable experimentally for large-Z projectiles of different charge, on hyper-channeling trajectories, e.g. in a thin film.

*Sandia National Labs – UIUC collaboration (DOE SNL 1736375)
Office of Naval Research (N00014-18-1-2605)
10:00AM E20.00009: Vicinage effects in the stopping power of molecular hydrogen in aluminum*  EDWIN QUASHIE (Presenter), XAVIER ANDRADE, ALFREDO A. CORREA, Quantum Simulation Group, Lawrence Livermore National Laboratory — Using time-dependent density functional theory (TDDFT) we calculate the electronic stopping power of the hydrogen molecule, H₂, projectile in aluminum over a wide range of velocities where we take into account the effect of the drag dynamics of excited electrons. The electronic excitations determine the stopping power and also a change the interatomic forces of the molecule during the trajectories.

We observed that the stopping power strongly depends on the orientation of the H₂ molecule and differs significantly from the stopping of He and (twice) the stopping of H. The position of the maximum stopping changes from \( \nu = 1.3 \) a.u. for H to \( \nu = 1.8 \) a.u. for H₂ projectiles. We also study the effect of the interatomic forces and equilibrium distances as a function of the projectile velocity, allowing us to make a prediction of the behavior of the molecule during the stopping process. Our results agree with the available experimental results for the stopping of H₂ molecules in aluminum thin films and allows us to understand those results.

*Prepared by LLNL under Contract DE-AC52-07NA27344. Computing support for this work came from the Lawrence Livermore National Laboratory Institutional Computing Grand Challenge program.

10:12AM E20.00010: Negative Differential Conductivity in Semiconductors from First Principles*  RAFI ULLAH (Presenter), XAVIER ANDRADE, ALFREDO A. CORREA, Lawrence Livermore Natl Lab — The negative differential conductivity (NDC) in gas-discharge tubes had been known long before [1] it was discovered in solids [2]. It was the discovery of NDC in semiconductors that invoked renewed interest in this area and opened it to applications in electronics [3]. Recently NDC has been observed in a quantum gas of neutral atoms [4]. It has been observed and predicted in different physical systems, including in normal metals [5], but the underlying physics is very different in each of those systems. In semiconductors it is mainly attributed to the electron transfer between different energy sub-bands. The transport phenomena in general and the NDC in semiconductors in particular is non-linear in nature and can not be accurately described by linear response theories. We have used time dependent density functional theory to compute the NDC in GaAs, a prototypical semiconductor. It is one of the first materials in which NDC was observed and widely used in NDC based applications.


*Prepared by LLNL under Contract DE-AC52-07NA27344

10:24AM E20.00011: Exchange and correlation effects in finite-temperature TDDFT*  JOHN REHR (Presenter), JOSHUA KAS, University of Washington — We discuss the finite-temperature (FT) generalization of time-dependent density functional theory (TDDFT) [1]. Formally the theory is analogous to that at temperature \( T = 0 \). In the local density approximation, the FT exchange-correlation kernel \( f_{xc}(T,n) \) can again be expressed as a density derivative of the exchange correlation potential \( d v_{xc}(T,n)/dn \), where \( n = N/V \) is the electron number density. An approximation for the TDDFT kernel \( f_{xc}(T,n) \) is obtained from the FT generalization of the retarded cumulant expansion applied to the homogeneous electron gas [2]. Results for \( f_{xc} \) and for the FT loss function are shown for a wide range of temperatures and densities, including the warm dense matter regime with temperatures of order \( T_F \), the electron degeneracy temperature. The FT cumulant Green’s function approach also yields a physical interpretation of the exchange and correlation contributions to the theory.


*Supported by DOE Office of Science BES Grant DE-FG02-97ER45623
10:36AM E20.00012: Real time-TDDFT study of thermal and non-thermal lattice dynamics depending on laser pulse-width*  
YOSHIYUKI MIYAMOTO (Presenter), National Institute of Advanced Industrial Science and Technology — In this work, I will discuss lattice dynamics of α-quartz conducted by femtosecond laser by performing the real-time TDDFT Ehrenfest dynamics with use of plane-wave basis set, TM type pseudopotentials, and adiabatic LDA functional. The α-quartz was expressed by a slab model with hydrogen termination. The distribution of kinetic energy for silicon and oxygen atoms was found to be nearly equal under shining the femtosecond laser with full-width of half-maximum (FWHM) 100 fs, wave length 800 nm, and fluence 10 J/cm². It is therefore concluded that this pulse width gave thermal dynamics on the lattice. By fixing the wave length and fluence of the femtosecond laser, the lattice dynamics with shorter FWHM was examined and non-equal distribution of kinetic energies among silicon and oxygen atoms was found. Furthermore, shorter pulse with FWHM=10 fs conducted ablation. I will discuss the physics behind this phenomenon.

*This work is based on results obtained from a NEDO project “Development of advanced laser processing with intelligence based on high-brightness and high-efficiency laser technologies” (TACMI project).

10:48AM E20.00013: Non-linear effects in core photoemission from Real-time TDDFT.*  
MARILENA TZAVALA (Presenter), JOSHUA KAS, JOHN REHR, Physics, University of Washington, LUCIA REINING, LSI, Ecole Polytechnique, Paris — In core photoemission spectroscopy a photon is absorbed and a core electron is emitted into the continuum, leaving behind a core hole. The remainder of the system responds to screen the core hole, significantly affecting the spectrum. State-of-the-art many-body perturbation theory (MBPT) methods such as the GW and the cumulant expansion are usually evaluated in the linear-response approximation. This requires a weak core hole; if this is not the case, one needs to go beyond linear response. This can be carried out with a non-linear cumulant derived in a MBPT framework, and evaluated from a real-time time-dependent density functional theory (TDDFT) approach. We discuss the application of this method with calculations carried out with an extension of our RT-Siesta code [1] for systems with d- and f valence electrons.


*This work was supported by the ERC grant SEED, and as part of the Computational Chemical Sciences Program funded by the U.S. Department of Energy, Office of Science, BES, Chemical Sciences, Geosciences and Biosciences Division in the Center for Scalable and Predictive methods for Excitations and Correlated phenomena (SPEC) at PNNL, and with computer support from DOE-NERSC.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E21 DCOMP DCMP GSNP: Advances in Computational Methods for Statistical Physics and Their Applications  
BCEC 157B - Ying Wai Li, Oak Ridge National Laboratory - Tag(s): Focus

8:00AM E21.00001: Parallel approaches to long-time atomistic simulations: decomposition, replication, and speculation* [invited]  
DANNY PEREZ (Presenter), Los Alamos National Laboratory — Molecular Dynamics (MD) is a workhorse of computational materials science. Indeed, MD can in principle be used to obtain any thermodynamic or kinetic quantity for a given interatomic potential. This enviable quality however comes at a steep computational price, limiting the system sizes and simulation times that can be achieved in practice. While the size limitation can be efficiently addressed with massively parallel implementations of MD based on spatial decomposition strategies, the same approach cannot extend the timescales much beyond microseconds. This is a significant issue, as this implies that the constant increase in the computing power delivered by leadership-scale machines cannot be leveraged to make long-time predictions.

In this talk, I discuss additional parallelization strategies, namely replication and speculation, that can be used to address the timescale limitation of MD for systems that evolve through rare transitions, concentrating primarily on the Parallel Trajectory Splicing (ParSplice) method and its recent developments. Using as an example the evolution of the shape of metallic nanoparticles, we show how, taken together, these ideas can significantly extend the simulation space accessible to MD in a way that can unlock the potential of current massively-parallel computing platforms.

*This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation's exascale computing imperative.
8:36AM E21.00002: Advanced computational methods for an accurate thermodynamic description of the paramagnetic state of magnetic materials from first principles  
DAVIDE GAMBINO (Presenter), BJORN ALLING,  
Department of Physics, Chemistry and Biology (IFM), Linköping University — In the past years, procedures to calculate from first principles the (Gibbs) free energy of a system with arbitrary accuracy have been established, starting in general from a simplified model and then calculating the full free energy with the use of statistical sampling techniques. These methods have been proven powerful for many materials; however, when it comes to magnetic materials at finite temperature, the system becomes more complex to be treated with ab initio techniques because of the indirect influence of magnetism on several equilibrium properties, besides its explicit contribution to the free energy.  
To improve the description of magnetic materials in the high temperature paramagnetic phase from first principles, we develop a method [Physical Review B 98, 064105 (2018)] to perform structural relaxations in the paramagnetic phase based on the disordered local moment (DLM) model, and we apply it to the case of a vacancy and a C interstitial in bcc Fe, bcc Fe$_{1-x}$Cr$_x$ random alloys, and defects in CrN. We also apply the recently developed atomistic spin dynamics-ab initio molecular dynamics approach [Physical Review Letters 121, 125902 (2018)] to defect free bcc Fe at the Curie temperature to prove the feasibility of free energy calculations on this system.

8:48AM E21.00003: Coupled spin dynamics and ab initio molecular dynamics approach for paramagnetic materials  
IRINA STOCKEM (Presenter), Department of Physics, Chemistry, and Biology (IFM), Linköping University, ANDERS BERGMAN,  
Department of Physics and Astronomy, Materials Theory Division, Uppsala University, ALBERT GLENSK, Laboratory of Computational Science and Modeling, Institute of Materials, École Polytechnique Fédérale de Lausanne, BLAZEJ GRABOWSKI, FRITZ KÖRMANN, TILMANN HICKEL, JÖRG NEUGEBAUER, Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, BJORN ALLING, Department of Physics, Chemistry, and Biology (IFM), Linköping University — Magnetic semiconductors like YMnO$_3$[1] and CrN [2] show an anomalous temperature dependence of the thermal conductivity in their paramagnetic phase: A strong suppression is observed right above the magnetic transition, followed by an almost constant conductivity at higher temperatures.  
At high temperature lattice vibrations and spin fluctuations occur simultaneously. As local effective moments still exist above the magnetic transition temperature, they interact with each other and with the lattice vibrations.  
By treating both lattice vibrations and spin fluctuations in a combined atomistic spin dynamics (ASD) – ab initio molecular dynamics (AIMD) approach, we are able to ascribe this experimentally observed effect to a mutual and dynamic spin-lattice coupling [3]. This coupling shows a strong influence on the phonon life times right above the magnetic transition.


9:00AM E21.00004: Full spin modeling and efficient mapping of the high dimensional Hamiltonian in Dy$_2$Ti$_2$O$_7$  
ANJANA SAMARAKOON (Presenter), Neutron Scattering Division, Oak Ridge National Laboratory, DAVID TENNANT, Materials Science and Technology Division, Oak Ridge National Laboratory, CRISTIAN BATISTA, Department of Physics, University of Tennessee, QIANG ZHANG, FENG YE, Neutron Scattering Division, Oak Ridge National Laboratory, HAIDONG ZHOU, Department of Physics, University of Tennessee, MARKUS EISENBACH, National Center of Computational Sciences, Oak Ridge National Laboratory, KIPTON BARROS, Theoretical Division, Los Alamos National Laboratory, SÁNTIAGO GRIGERA, School of Physics and Astronomy, University of St Andrews, YING WAI LI, National Center of Computational Sciences, Oak Ridge National Laboratory, ZHILING DUN, Department of Physics, University of Tennessee — Precise modeling of a material is a key to understand its underlying interactions and physics but also revealing the competing phases in the nearby interaction space. Highly frustrated systems are important due to the richness in physics and diversity of phases including spin liquids with exotic topological states they display.  
Here, we present a machine learning workflow to fit multi-experimental datasets to find an optimal Hamiltonian while undertaking phase classification and extracting information about the topography around the region of interest. Experimental data from a spin-ice material, Dy$_2$Ti$_2$O$_7$ including diffuse neutron scattering, heat capacity, and susceptibility are utilized. This approach is shown to provide the best model in an efficient and effective way but also is powerful at planning the best experimental strategies.
9:12AM E21.00005: Digital Alchemy Applied to Molecular Dynamics  JAMES PROCTOR (Presenter), University of Michigan, Ann Arbor, MI, GREG VAN ANDERS, Queen's University, Kingston, ON, Canada, SHARON GLOTZER, University of Michigan, Ann Arbor, MI — Recently, colloidal and nanoparticle synthesis techniques have grown in scope more quickly than the capacity to populate relevant phase diagrams, challenging the predictive ability of computer simulation. Meeting this challenge suggests the development of new techniques that simultaneously explore the dynamics of particles’ canonical degrees of freedom, and particle attributes. Here, we describe a Molecular Dynamics implementation of the “Digital Alchemy” framework. This framework extends statistical ensembles to include variation in “alchemical” degrees of freedom describing particle attributes. We apply alchemical Molecular Dynamics simulations to particles interacting via a Lennard-Jones-Gauss potential, and show that several previously known crystal structures, including a quasicrystal, exhibit stable behavior in this alchemically extended design space, allowing for optimization and exploration.

9:24AM E21.00006: Exploring the Early Stages of Corrosion with ab initio Adaptive Kinetic Monte Carlo Simulations of Non-Equilibrium Oxides  MICHAEL WATERS (Presenter), JAMES M RONDINELLI, Materials Science and Engineering, Northwestern University — The early stages of corrosion in Ni-alloys are dominated by kinetically favorable, non-equilibrium layers comprising normally immiscible oxides. The ionic transport across these highly defective layers mediates their continued growth and the oxidation the substrate alloy. While at longer time scales, the phase segregation of the non-equilibrium layer into thermodynamically stable phases is key to long term passivation of the alloy. In order to simulate the atomistic kinetics on such long-time scales in a natural manner, we employ the state-of-the-art ab initio adaptive kinetic Monte Carlo method. We detail our key findings in regards to the importance of correlation and magnetic order.

9:36AM E21.00007: Removing Lattice Constraints from Lattice Protein Models: A Wang-Landau Study  ALFRED FARRIS (Presenter), University of Georgia, DANIEL T. SEATON, Harvard University, DAVID P LANDAU, University of Georgia — We apply Wang-Landau sampling [1] to the continuum analogue of the hydrophobic-polar (HP) lattice protein model [2] to study the effects of lattice constraints on generic folding behavior in coarse-grained protein models. The continuum version is inspired by the AB polymer model [3], but incorporates potentials chosen specifically to mimic those of the lattice protein case. In this study, we compare and contrast thermodynamics during the folding process of the continuum model to the original HP lattice protein model for sequences mapped from Crambin, a 46 amino acid plant protein. We find that the folding processes for both of these coarse-grained models are quite similar, with major structural transitions occurring at almost the same temperatures. The continuum model hints at a small, additional structural transition not seen in the lattice case; the exact nature of this rearrangement is currently under investigation.


9:48AM E21.00008: Ensemble Monte Carlo Growth simulations of polymers in confined environments  GRAZIANO VERNIZZI (Presenter), Siena College (Loudonville, NY), TRUNG NGUYEN, Northwestern University (Evanston, IL), HENRI ORLAND, CEA Saclay (Gif-sur-Yvette Cedex, France), MONICA OLVERA DE LA CRUZ, Northwestern University (Evanston, IL) — We apply a recent Ensemble Monte Carlo Growth algorithm to sample the microcanonical density of states of polymers in confined geometries. The main advantage of computing the entropy directly, is that it allows to locate and characterize phase transitions accurately, while circumventing problems associated with long time scales. However, when the accessible phase space is restrained, such as in geometrically confined polymers, entropic forces exerted on the confining walls lead to changes in several statistical mechanical properties of the polymers. We test the performance of the microcanonical ensemble Monte Carlo growth algorithm for confined interacting self avoiding walks. We discuss also how to extend the model to include electrostatic interactions.
10:00AM E21.00009: Model Amyloid Protofibrils Simulated with Replica-Exchange Wang-Landau  MATTHEW S. WILSON (Presenter), GUANGJIE SHI, DAVID P LANDAU, Center for Simulational Physics, University of Georgia, THOMAS WUEST, Scientific IT Services, ETH Zurich, FRIEDERIKE SCHMID, Institute of Physics, Johannes Gutenberg University — As neurological diseases associated with toxic peptide aggregates emerge, the research of aggregate and fibril formation has become a prominent, yet extremely challenging problem. The ability to form an amyloid state has been posited as a general feature of peptide systems, and is considered in this study by simulating a collection of coarse-grained, generic model peptides. The H0P model\(^1\) adds an additional neutral polarity group to the classic hydrophobic-polar (HP) model\(^2\), and is used for simplicity and efficiency. With the replica-exchange Wang-Landau (REWL) algorithm and an efficient trial move set\(^3\), the density of states is determined for multiple interacting model peptides. We observe the formation of fibrillar structures in two continuous transitions that separate three phases: dissolved peptides, disordered oligomers, and crystalline aggregate structures. Additional structural observables are calculated in a post-simulation production run to further study the physical behavior during the observed transitions.


10:12AM E21.00010: Conformational mechanics for polymers doubly-grafted to a homogeneous substrate\(^*\)  SHENGMING ZHANG (Presenter), MICHAEL BACHMANN, Department of Physics and Astronomy, University of Georgia — Studies of linear polymer structures with their two ends anchored at a planar substrate can help to provide insights into conformational properties of biologically active systems such as myosin and kinesin. We thoroughly investigated the conformational phases of a coarse-grained flexible homopolymer model with both ends of the chain grafted to a homogeneous attractive substrate by means of parallel tempering computer simulations. For bonded monomers, we employed the FENE potential, whereas the nonbonded interaction was described by the Lennard-Jones potential. The monomer-substrate attraction was modeled using an integrated Lennard-Jones potential. Specific energetic and structural quantities were measured and used as indicator functions for the characterization of the conformational phases in this system. Based on these results, we constructed the temperature versus end-to-end separation pseudo-phase diagram. We identified unique crystalline and icosahedral solid phases in addition to a globular liquid and two geometric gas-like phases.

\(^*\)NSF Grant No. DMR-1463241

10:24AM E21.00011: Framework to track Order-Disorder Transitions - From Particles to Block Copolymers\(^*\)  ANKITA MUKHTYAR (Presenter), FERNANDO A ESCOBEDO, Cornell University — Block copolymers self-assemble into a variety of phases with highly regular patterns, depending on the ordering of molecules. Paramount to understanding and controlling this “order” is to have good “order parameters”, variables used to track changes in the system as it transitions from disorder to order. Molecular dynamics is used to simulate the growth of minimalistic versions of the lamella, cylinder and gyroid phases from an isotropic liquid using a binary nanoparticle mixture model. Based on the correlation of bonding symmetries between a particle and its neighbors, local order parameters are developed and used to track the formation and growth of specific geometric motifs along the transition pathway. They are then modified to study similar transitions in coarse-grained models of polymers and oligomers, namely the assembly of a linear symmetric diblock copolymer into the lamellar, and a branched bolaamphiphile into the single diamond phase. The framework also finds use in the estimation of free-energy barriers for such ordering transitions. These calculations are yet to be reported in literature for such systems and require the use of novel variants of nucleus-size pinning and umbrella sampling techniques.

\(^*\)Funding support from NSF award DMR-1609997 is gratefully acknowledged.
10:36AM E21.00012: Noise reduction and automated molecule detection in atomistic diffusion calculations of correlated systems

NICOLA MOLINARI, IAN LEIFER (Presenter), YU XIE, BORIS KOZINSKY, Harvard University — When using molecular dynamics to compute diffusion coefficients for correlated systems, the fully correlated analysis of molecular trajectories leads to very noisy estimates because it is based on the center of mass motion rather than motion of individual atoms. We propose a new method that systematically reduces the noise in the diffusion constant calculation. By assuming that the underlying correlation structure of a system is the same for the entire trajectory, we leverage the information learned from the well-converged short-time position-position correlation matrix to reduce the noise at longer times. The proposed method allows to significantly decrease the uncertainty of diffusivity estimates and works for both non-bonded and bonded correlation scenarios. In the latter case we are able to identify automatically the diffusing degrees of freedom of the system, i.e. identify the molecular species. Furthermore, we demonstrate that using our method the estimation of the diffusion constant is never worse than the widely-adopted center-of-mass approach.

10:48AM E21.00013: Scaling relations for the continuum limit from collisions between nanoclusters and rough surfaces*

ERIC SWITZER (Presenter), ANIKET BHATTACHARYA, University of Central Florida — Nanoclusters have wide ranges of applications for their unique size-dependent properties. We report molecular dynamics simulation studies of the coalescence of small clusters with each other and with heterogeneous surfaces, as well as bouncing and fragmentation of clusters. Specifically, we study collisions of dust particles consisting of silica and water molecules and study the aftermath immediately following the collisions. We vary cluster sizes from 10 – 1000 nm containing 1000 – 100,000 particles with an aim to derive scaling relations for the elastic limit so that the extracted elastic parameters for the extrapolated continuum models can be used to study clusters of much larger sizes beyond the scope of simulation studies.

*Supported by funds from NASA Florida Space Grant Consortium.

Tuesday, March 5, 2019 8:00 AM - 10:48 AM

Session E22 DMP: Computational Materials Design and Discovery -- Machine Learning

BCEC 157C - Xavier Gonze, Universite catholique de Louvain - Tag(s): Focus

8:00AM E22.00001: Physics-Based Machine Learning Models for Discovery of Novel Scintillator Chemistries

GHANSHYAM PILANIA (Presenter), CHRISTOPHER R. STANEK, BLAS PEDRO UBERUAGA, Los Alamos National Laboratory — Applications of inorganic scintillators—activated with lanthanide dopants, such as Ce—are found in diverse fields. As a strict requirement to exhibit scintillation, the 4f ground state and 5d1 lowest excited state levels induced by the activator must lie within the host bandgap. This talk will discuss a new machine learning (ML) based screening strategy that relies on a high throughput prediction of the lanthanide dopants’ ground and excited state energy levels with respect to the host valance and conduction band edges for efficient chemical space explorations to discover novel inorganic scintillators. Using a set of perovskite oxides and elpasolite halides as examples, it will be demonstrated that the developed approach is able to (i) capture systematic chemical trends across host chemistries and (ii) effectively screen promising compounds in a high-throughput manner. While a number of other application-specific performance requirements need to be considered for a viable scintillator, the present scheme can be a practically useful tool to systematically down-select the most promising candidate materials in a first line of screening for a subsequent in-depth investigation.
8:12AM E22.00002: Finding Novel Fast Ionic Conductors Using Combined Techniques from Density Functional Theory and Materials Informatics*  RANDY JALEM (Presenter), Center for Green Research on Energy and Environmental Materials & Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute, KENTA KANAMORI, ICHIRO TAKEUCHI, Computer Science, Nagoya Institute of Technology (NiTech), Japan, YOSHITAKA TATEYAMA, Center for Green Research on Energy and Environmental Materials & Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute, MASANOBU NAKAYAMA, Life Science and Applied Chemistry, Nagoya Institute of Technology (NiTech), Japan — Computational new material search is an ongoing hot topic for research in various fields of applications. In here, we show our works related to efficient computational methods for finding novel fast ionic conductors for potential use in solid-state batteries. One topic deals with our proposed search framework based on a Bayesian optimization algorithm with a kernel definition that is general for high dimension of material descriptors, coupled to a DFT method to calculate ion migration energy barriers (Eb) over chemical search spaces of oxides (Eb as a search criterion) (Sci. Rep. 2018, 8, 5845). The next part shows our formulation of descriptors for crystalline solids which are derived from literature data and real feature values from atom-centered Voronoi partitioning (STAM 2018, 19, 231). We validated the scheme in terms of machine learning of various DFT-calculated properties such as cohesive energy, material density, electronic band gap energy, and convex hull decomposition energy.

*This research has been supported by National Institute for Materials Science (NIMS), NIMS “Materials research by Information Integration” Initiative (MI2I), and JST-PRESTO program.

8:24AM E22.00003: Crystal structure prototype database based on machine learning classification of existing inorganic material structures*  SHULIN LUO (Presenter), BANGYU XING, JIAN LV, LIJUN ZHANG, College of Materials Science and Engineering, Jilin University — Combining high-throughput calculations with database construction and data mining offers opportunities for computational material scientists to discover new materials. Candidate materials considered in high-throughput calculations are usually from chemical substitution or structure variation based on known crystal structures. So, knowledge of crystal structure prototypes is vital for the validity of high-throughput calculations. We herein built a high quality crystal structure prototype database with the aid of machine learning classification of existing inorganic materials structures. The structure data were classified by the hierarchical clustering approach and the state-of-the-art structure fingerprinters including the bond order parameters and the smooth overlap of atomic positions were used for structure characterization. The database can generate sub-databases dynamically based on new criteria. We have integrated the database into the in-house developed infrastructure of JUMP/2, a python framework for materials discovery via high-throughput calculations, aiming at creating an automatic and high-performance computational materials discovery platform.

*Work at Jilin University is supported by National Natural Science Foundation of China under Grant Nos. 61722403 and 11674121.

8:36AM E22.00004: Development of linearly independent descriptor generation method for sparse and interpretable modeling in materials science*  HITOSHI FUJII (Presenter), National Institute for Materials Science, TETSUYA FUKUSHIMA, Institute for NanoScience Design, Osaka university, TAMIO OGUCHI, Institute of Scientific and Industrial Research, Osaka university — In recent years, researches using techniques of machine-learning have been considerably activated in the field of materials science and we focus on research for empirical law discovery to elucidate a mechanism of physical properties of target materials. We propose linearly independent descriptor generation method for increasing the expression capability of linear regression model without generating any multicollinearity and strong near-multicollinearity which are a major problem in linear regression analysis. Our method is expected to be an essential preprocessing technique for sparse and interpretable modeling in materials science.

*Materials research by Information Integration Initiative (MI2I) project of the Support Program for Starting Up innovations Hub from Japan Science and Technology Agency (JST)
At 8:48 AM E22.00005: Important descriptors and descriptor groups of Curie temperatures of rare-earth transition-metal binary alloys

HIORI KINO (Presenter), National Institute for Materials Science — We analyze Curie temperatures of rare-earth transition metal binary alloys with machine learning method. In order to select important descriptors and descriptor groups, we introduce newly developed subgroup relevance analysis and adopt the hierarchical clustering in the representation. We execute the exhaustive search and illustrate that our approach indeed leads to the successful selection of important descriptors and descriptor groups. It helps us to choose the combination of the descriptors and to understand the meaning of the selected combination of descriptors.


*This work was partly supported by PRESTO and by the "Materials Research by Information Integration" Initiative (M2I) project of the Support Program for Starting Up Innovation Hub, both from the Japan Science and Technology Agency (JST), Japan; by the Elements Strategy Initiative Project under the auspices of MEXT; and also by MEXT as a social and scientific priority issue (Creation of New Functional Devices and High-Performance Materials to Support Next-Generation Industries; CDMSI) to be tackled by using a post-K computer. The calculations are partly carried out on Numerical Materials Simulator at NIMS.

At 9:00 AM E22.00006: Supervised learning and prediction of electronic properties: Discovery and Design of Materials and Interfaces for back-end-of-line interconnects

GANESH HEGDE (Presenter), HARSONO SIMKA, CHRIS BOWEN, Advanced Logic Lab, Samsung Semiconductor Inc, Austin, TX, USA — Supervised machine learning based techniques have found notable success in the recent past in the fields of atomic structure prediction and interatomic potential generation. Such techniques, however, have not found similar success in the prediction of non-local electronic-structural quantities such as electronic transmission and total density of states.

In this work, we present approaches to accurately predict a range of electronic structure properties - from Hamiltonian Matrix elements, electronic transmission to density of states - using supervised learning. Training and test data is obtained from open materials databases and from tailored first-principles Density Functional Theory simulations of materials and material interfaces.

The key role played by structural and electronic descriptors and their impact on the accuracy of predictions is discussed. The use of simulation-based proxies for material properties accessible through experiment is also discussed.

Finally, recent progress on the discovery and design of conductor and barrier materials for back-end-of-line interconnect using supervised learning is presented.

At 9:12 AM E22.00007: Machine-Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene

ARUNKUMAR RAJAN (Presenter), AVANISH MISHRA, SWANTI SATSANGI, RISHABH VAISH, ABHISHEK KUMAR SINGH, Indian Institute of Science — MXene is a recent addition to the ever-growing family of 2D-materials, promising for optical, electronic, energy storage and photocatalytic applications. Utilizing statistical learning-based approach, we electronically characterize this vast class of materials by predicting their band gaps with GW level accuracy. Using a classification model, MXene having finite band gaps are filtered out and few of them are selected to build a machine learning model. The model is built by correlating the easily available elemental and computed properties as features with respect to calculated GW band gaps of selected MXene. Depending upon feature combinations, Gaussian process regression method resulted in optimized model yielding low root-mean-squared-error of 0.14 eV, which can be employed to estimate the accurate GW band gaps of tens of thousands of MXenes [1,2] within minutes. Our results demonstrate that machine learning model can bypass band gap underestimation problem of local and semi-local functionals used in DFT calculations, without subsequent correction using time-consuming GW approach.

References:
1. aNANt: a functional materials database. http://anant.mrc.iisc.ac.in

*KIST, Dr. D S Kothari Postdoctoral Fellowship and DST Nanomission
9:24AM E22.00008: Accelerating inorganic discovery with meta-calculation filtering via a decision classifier
CHENRU DUAN (Presenter), Chemistry, Chemical engineering, Massachusetts Institute of Technology, JON PAUL JANET, Chemical Engineering, Massachusetts Institute of Technology, ADITYA NANDY, Chemistry, Chemical engineering, Massachusetts Institute of Technology, FANG LIU, HEATHER J KULIK, Chemical Engineering, Massachusetts Institute of Technology — Machine learning (ML) has the capacity to revolutionize materials discovery with accurate property estimation at negligible computational cost. Still, most discovery workflows require computationally-demanding simulation to generate data to feed in an ML model. However, two key challenges remain at the stage of data generation: i) materials may not form a stable complex and ii) calculations may fall outside the domain of applicability of the chosen method. Usually, these two failure modes can only be detected after calculations finished, leading to a massive waste of computational resources. To address this problem, we trained a classifier to estimate the success rate of a calculation directly from topological, heuristic features prior to simulation. Inspired by the data distribution in the latent space, we designed a model confidence metric specifically for classification tasks, lowering the risk of terminating jobs that are actually fruitful. A dynamical classifier that utilizes the information generated during simulation is also developed, which directs the on-the-fly decision of whether to abandon an in-progress calculation. Our classifiers are useful in dataset generation with first-principles calculations to accelerate the ML-driven design of novel inorganic materials.

ROHIT BATRA (Presenter), School of Materials Science and Engineering, Georgia Institute of Technology, GHANSHYAM PILANIA, BLAS PEDRO UBERUAGA, Los Alamos National Lab, RAMAMURTHY RAMPRASAD, School of Materials Science and Engineering, Georgia Institute of Technology — Cost versus accuracy trade-offs are frequently encountered in materials science, where a particular property of interest can be measured at different levels of accuracy or fidelity. Naturally, the most accurate measurement is also the most resource-intensive, while the inexpensive quicker alternatives tend to be noisy. In such situations, machine learning strategies, such as multi-fidelity information fusion (MFIF), can be employed to fuse information accessible from sources with varying levels of fidelity, and allow for accelerated property predictions. In this work, we use a dataset consisting of dopant formation energies of 42 dopants in hafnia—each studied in six different hafnia phases—computed at two levels of fidelity. The performance of traditional single fidelity (SF) and three MFIF models, namely, Δ-learning, low-fidelity as a feature, and multi-fidelity (MF) co-kriging are compared. We find that the MF based learning scheme not only outperforms the traditional SF machine learning methods, such as Gaussian process regression, but also provides an accurate, inexpensive and flexible alternative to other MFIF strategies. The learning approach is expected to be general and can be readily applied to a much wider spectrum of materials discovery and optimization problems.

9:48AM E22.00010: Machine Learning for Energetic Material Detonation Performance
BRIAN BARNES (Presenter), US Army Research Laboratory — We present advances in accurate, extremely rapid prediction of detonation performance for energetic molecules. These models may be integrated into a larger effort for high-throughput virtual screening or rapid pre-screening of molecules before any hazardous synthesis is attempted. Our workflow utilizes (a) a reference dataset generated from quantum mechanical calculations and a thermochemical code, (b) a cheminformatics approach to molecular descriptors, and (c) neural network and kernel-based algorithms for nonlinear regression. This data-driven approach leverages modern “machine learning” techniques for prediction of molecular properties. We create models to predict detonation velocity and detonation pressure. Molecules evaluated are CHNO-containing organic molecules drawn from GDB datasets, and known explosives. Usefulness of a variety of feature descriptors (e.g. Morgan fingerprints), are compared. Kernel and activation functions, hyperparameter optimization, and relative accuracy of models are discussed. Algorithms evaluated include neural networks, least absolute shrinkage and selection operator regression (“Lasso”), random forest regression, and Gaussian process regression. The Python workflow for automated dataset generation and analysis is also discussed.
10:00AM E22.00011: Machine learning study of two-dimensional magnetic materials*  TREVOR DAVID RHONE (Presenter), WEI CHEN, SHAAN DESAI, AMIR YACOBY, EFTHIMIOS KAXIRAS, Harvard University — When the dimensionality of an electron system is reduced, new behavior emerges. This has been demonstrated in GaAs quantum Hall systems since the 1980’s, and more recently in van der Waals (vdW) materials. We discuss the behavior of electrons in reduced dimensions with a focus on their spin properties. We study vdW materials with intrinsic magnetic order, materials at the forefront of physics research. We use materials informatics (machine learning applied to materials science) to study the magnetic and thermodynamic properties of vdW materials. Crystal structures based on monolayer Cr2Ge2Te6, of the form A2B2X6, are studied using density functional theory (DFT) calculations and machine learning tools. Magnetic properties, such as the magnetic moment are determined. The formation energies are also calculated and used to estimate chemical stability. We show that machine learning, combined with DFT, provides a computationally efficient means to predict properties of two-dimensional (2D) magnets. In addition, data analytics provides insights into the microscopic origins of magnetic ordering in 2D. This novel approach to materials research paves the way for the rapid discovery of chemically stable 2D magnets.

*ARO MURI W911NF-14-0247; EFRI 2-DARE NSF 1542807; XSEDE NSF ACI-1548562

10:12AM E22.00012: Stochastic Discovery of Variance Mechanisms in Heterogeneous Dielectric Coatings  VENKATESH MEENAKSHISUNDARAM (Presenter), DAVID YOO, ANDREW GILLMAN, UES, Inc, JAMES DENEAULT, UTC, NICHOLAS GLAVIN, PHILIP BUSKOHL, Air Force Research Laboratory — Microscale spatial and material heterogeneities in 3D printed electrical devices present significant challenges to predictable electrical performance and device reliability. Dielectric particles are often added to dielectric inks to tailor the macro level permittivity of printed dielectric substrates and coatings. However, the combined role of particle morphology, discrete spatial arrangement and material properties on variance is difficult to distinguish experimentally, due to the large parameter space of processing variables and electrical sensitivity to local heterogeneities. We address this challenge by combining a finite element capacitor model with a neural network guided genetic algorithm (GA) to optimize the volume fraction, particle size and permittivity distributions of dielectric particles to identify systems with high capacitance variance. Classification-based machine learning techniques were also applied to the GA-created database to extract correlations between the spatial/material distributions of the dielectric particles and the capacitance variance. Collectively, the study provides a useful framework to correlate electrical performance with both macro- and microstructural variation sources, which is key to accelerating the development of 3D printing materials.

10:24AM E22.00013: Ligand Optimization for the Spin-Lattice Coupling of Single-Molecule Magnets Mn3  JIE GU (Presenter), WILLIAM PERRY, MAHER YAZBAK, DIANTENG CHEN, Department of Physics and the Quantum Theory Project, University of Florida, MARK E. TURIANSKY, University of California, Santa Barbara, HAI-PING CHENG, XIAOGUANG ZHANG, Department of Physics and the Quantum Theory Project, University of Florida — Single molecule magnets (SMM) exhibit a pseudo-multiferroicity which arises from structural changes that occur during spin state transitions. This spin-lattice coupling leads directly to magnetocapacitance which may also allow the spin state of the ground state to be tuned via strain. We propose that this tuning can be performed via replacement of the ligands which surround the SMM core atoms, and we attempt to search for a ligand which maximizes the spin-lattice coupling in the SMM Mn3 as a test case. We use density functional theory (DFT) calculations, Bayesian optimization, and slightly modified atomic environment vectors (AEVs) to perform the search. These techniques are employed in order to minimize the cost of searching through a large number of candidate ligands from the PubChem database. Following this procedure, we have obtained evidence that the spin-lattice coupling can be affected through a judicious choice of ligand.

10:36AM E22.00014: Identification of stable Cu-Pd-Ag nanoparticles using neural network interatomic potentials  SAMAD HAJINAZAR (Presenter), ERNESTO D. SANDOVAL, AIDEN J. CULLO, ALEKSEY KOLMOGOROV, Binghamton University — A neural network potential constructed with a stratified training scheme available in the MAISE package [1,2] has been used to find low-energy structures of elemental, binary and ternary Cu-Pd-Ag clusters. The efficiency of the employed unbiased global ground state evolutionary search for elemental nanoparticles was improved by co-evolving clusters across a range of sizes. We systematically compared the stability of the clusters found with the neural network model against previously reported structures found with the Gupta potential. Predictions made with the neural network show a consistent improvement in nanoparticle stability at the density functional theory level.


Tuesday, March 5, 2019 8:00 AM - 10:48 AM
8:00AM E23.00001: How do interactive physics learning environments foster Intellectual Humility (IH)?

MEAGAN SUNDSTROM (Presenter), FABIANA CARDETTI, University of Connecticut — Students often enter the physics classroom with intuitive conceptions drawn from real life experiences or former coursework, and may be hesitant or reluctant to forego these mindsets in favor of formally instructed knowledge. The goal of introductory physics courses is not only to teach and expose students to new content, but also to cultivate students' abilities to reason through and derive content knowledge through personal inquiry. This scientific process necessitates one's abilities to be open-minded in terms of hearing evidence that contradicts his or her personal opinion, to be willing to discard any original misconceptions in the face of such alternative evidence, and to identify and pay appropriate attention to one's academic limitations. Such a mindset is indicative of the quality of Intellectual Humility (IH), defined as "the owning of one's limitations." In the present study, we utilize IH surveys, reflections, conceptual knowledge assessments, and classroom observations collected for both a traditional, lecture-style physics course and an interactive environment, problem-solving based physics course. We will present our findings from the study as we attempt to examine the role of interactive learning environments in fostering IH in physics through collaboration.

8:12AM E23.00002: In-class use of clickers and clicker tests improve learning and enable instant feedback and retests via automated grading

SNEHALATA KADAM (Presenter), NANCY BURNHAM, Physics Department, Worcester Polytechnic Institute, ERIN DESILVA, Dartmouth College — An audience response system ("clickers") was gradually incorporated into introductory physics courses at Worcester Polytechnic Institute during the years 2011-14. Clickers were used in lectures, as a means of preparing for labs, and for collection of exam data and grading. Average student grades were 13.5% greater, as measured by comparing exam results with a previous year. Student acceptance of clickers was high, ranging from 66% to 95%, and grading time for exams was markedly reduced, from a full day to a few hours for approximately 150 students. The streamlined grading allowed for a second test on the same material for the students who failed the first one. These improvements have the immediate effects of engagement, learning, and efficiency, and ideally, they will also provide an environment in which more students will succeed in college and their careers.

*The authors are grateful to the continual and cheerful support of both the Academic Technology Center and the Morgan Teaching and Learning Center at WPI. We warmly thank Fred Hutson for proof-reading a draft of the manuscript.


ERIN DUFFY (Presenter), KINSEY BAIN, Department of Chemistry, Michigan State University, LYDIA BENDER, Department of Physics, Kansas State University, MARCOS DANIEL CABALLERO, Department of Physics and Astronomy, Michigan State University, JAMES T LAVERTY, Department of Physics, Kansas State University, STUART HOLDEN TESSMER, Department of Physics and Astronomy, Michigan State University, MELANIE M COOPER, Department of Chemistry, Michigan State University — In 2013, Michigan State University (MSU) launched an interdisciplinary project to transform introductory courses across chemistry, biology, and physics to three-dimensional learning (3DL) environments. As part of this effort, we have developed an observation protocol (the 3-Dimensional Learning Observation Protocol, or 3DLOP) to measure the extent to which instructors and students engage in scientific practices, disciplinary core ideas, and crosscutting concepts (the three dimensions) during class time. Simply put, the 3DLOP differs from other classroom observation protocols in that it does not only measure how active a class is, but rather, it measures how rich the activity is. Using the 3DLOP on videos of instructors, our goal is to measure the change in the amount of 3DL in gateway courses pre- and post-transformation. Protocol development and initial findings from using the 3DLOP on physics lecture courses will be discussed.

*This material is based upon work supported by the National Science Foundation under Grant No. 1725520.
8:36AM E23.00004: Exploring the relationship between students' online LMS performance and attitudes in an intro physics course  
MICHELLE TOMASIK (Presenter), Physics, MIT, ANINDYA ROY, Open Learning, MIT — Many educational institutions have adopted a variety of online learning platforms to offer online content. As students use these learning platforms, they leave behind digital footprints. We can construct a better understanding of students' behaviors and practices if we complement this observational clickstream dataset with other data sources -- such as the data obtained from survey instruments. In this project we combine CLASS (Colorado Learning Attitudes about Science Survey)[1] results with the online learning activities on the MITx platform (a modified version of the edX platform[2]) for an on-campus introductory physics course at MIT. CLASS is a validated and popular survey instrument, which probes students' problem-solving sophistication, confidence and their conceptual understanding, among other categories. From the edX platform, we get a detailed record of students' problem-solving efforts, and the use of posted video resources. By combining these datasources and tying them to their overall course performance, we get improved insight into student behavior and motivation that could inform the course-design process and the science of teaching and learning.


8:48AM E23.00005: Calculus-based Physics students' understanding on vectors: a comparison between engineering students and life-science students*  
DIEGO VALENTE (Presenter), XIAN WU, University of Connecticut — Students' understanding of vector concepts affects their learning outcome of introductory physics courses. We administered a research-based vector survey to test how well students understood eight essential vector concepts. Students from two calculus-based physics course sequences were recruited: engineering students from a traditional physics for engineers course sequence and life-sciences students from a general physics with calculus course. We found that even though engineering students outperformed life-sciences students, these two groups of students had difficulties answering 2D vector subtraction, dot product and cross product questions correctly. We have also analyzed whether dressing a vector problem with physical context affected student performance in the vector survey and have found that physical context had a stronger impact on the questions with lower student performance than on questions where students performed better: adding a physical context made students do worse in the 2D vector subtraction question, while for questions evaluating the dot product and the cross product, adding physical context improved student performance on these questions.

*The authors acknowledge funding from the Center for Excellence in Teaching and Learning at the University of Connecticut.

9:00AM E23.00006: Transforming the introductory physics laboratory using Jupyter Notebooks*  
EMILY WALL (Presenter), CADE SCHURZ, PAUL NAKROSHIS, University of Southern Maine — Many colleges and universities have large introductory physics lectures and a correspondingly large number of laboratory sections that are taught using a cookbook style laboratory wherein students typically gather data in one week and turn in the report the next, with no opportunity to revise or revisit the experiment. A recent article by Natasha Holmes and Carl Wieman in Physics Today (Physics Today 71, 1, 38 (2018); https://doi.org/10.1063/PT.3.3816) concluded that the standard introductory lab section did not have any measurable positive effect on student's learning in lecture. Armed with the results of their work, we have begun the process of transforming our introductory laboratory by piloting an experimental section to focus on the process of doing science, and modelling reproducible research principles by using python-based Jupyter Notebooks to analyze data and write lab reports. We will report on the results of this trial, including student learning, attitudes, and a comparison to a non-reformed section. This talk will be presented by the two upper level physics Learning Assistants that were instrumental in the design and implementation of this introductory laboratory reform.

*Funding for this project comes from the University of Southern Maine Learning Assistant Program.
9:12AM E23.00007: The power of physics to demonstrate the physics of power  SAAMI SHAIBANI (Presenter), Instruction Methods, Academics & Advanced Scholarship — The promise of nuclear fusion as a viable means of generating electricity remains elusive, even after more than half a century of effort. One reason for this lies in a low level of public awareness of the enormous potential of fusion, whereas greater awareness might lead to appropriate pressure on policymakers to cause an increase in funding. Educational resources developed to help encourage societal participation include material originally designed for the classroom[1], which is extended here by a new construct involving the D-T reaction. Use of this tool identifies how so much (energy) is available from so little (fuel), and an instructional approach to present the solution is also described. The definitive nature of the methodology produces successful student learning and it is readily adaptable to reach a broader audience in the public arena. A concomitant benefit of this strategy is the addition of another scenario to the library of real-world events[2-5], which are vastly superior to standard textbook problems but which are still accessible with standard principles.


9:24AM E23.00008: Primetime learning: collaborative and technology-enhanced studying with genuine teacher presence  PEKKA KOSKINEN (Presenter), Department of Physics, University of Jyväskylä, JONI LÄMSÄ, Department of Education, University of Jyväskylä, JUSSI MAUNUKSELA, Department of Physics, University of Jyväskylä, RAJJA HÄMÄLÄINEN, Department of Education, University of Jyväskylä, JOUNI VIIRI, Department of teacher education, University of Jyväskylä — While physics education research has introduced several effective instructional strategies, most of them still rely on traditional teacher roles, depend on the presence of classrooms, and cling to a summative assessment. Here we summoned all the lessons learned from science education research and developed a new, practical, and transformational instructional strategy, the primetime learning model.(1) We devised the model by organizing the basic elements of active learning into a theory-based four-step study process. The model is based on collaborative and technology-enhanced learning, on versatile formative assessment without a final exam, and on genuine teacher presence through intimate meetings between students and teachers. We piloted the model on two university physics courses on thermodynamics and optics and observed persistent student activity, improved retention, enjoyable learning experience, and robust learning outcomes. The model suits particularly well for courses that, in addition to the teaching subject itself, focus on teaching balanced study routines and strengthening social integration.


9:36AM E23.00009: Replacing traditional final exams with project-building in advanced undergraduate physics classes  PRATHEESH JAKKALA (Presenter), Illinois College — This paper presents the implementation of project-building replacing traditional final exams in advanced undergraduate physics classes at a small liberal arts college. Students from 'Circuits' class and 'Dynamics' class built projects using the concepts learnt throughout the semester. Projects for Circuits class were built in teams of three and projects for Dynamics class were built by individual students. Majority are original projects. A total of 18 students built 11 projects. Students were required to present their findings, conclusions and data in a scientific paper format and an oral presentation. Students were presented with challenging and open-ended real-life problems. This paper also presents the learning outcomes, and how students successfully used the classroom concepts to solve the challenging real-life problems. This paper also presents the details of all the students projects under consideration.

9:48AM E23.00010: Introducing the strong nuclear interaction and many-body physics in undergraduate quantum mechanics  BRANDON INSCOE (Presenter), JARRETT LANCASTER, High Point University — The standard treatment of spin in undergraduate quantum mechanics provides all the essential ingredients for introducing a number of exciting and contemporary topics which are of great interest to the condensed-matter and high-energy physics community but which are also rarely addressed in a meaningful way at the undergraduate level. Specifically, the color charge of quantum chromodynamics possesses a structure which is quite similar to the electron's spin degree of freedom. By considering a system of three color charges at fixed positions with Heisenberg-like interactions, one is able to construct a toy model of a baryon with tunable interaction strength in which the color charge components exhibit dynamics similar to those of interacting spin components. The system of three particles leads naturally to an exploration of three-body interactions, which are highly relevant to quantum chromodynamics. Moreover, the overall approach to investigating the system's nontrivial dynamics provides a digestible introduction to the technique of exact diagonalization in a novel, few-body quantum system. VPython is used to visualize the emergent dynamics, providing an interesting demonstration which is appropriate for a course on modern physics.
**10:00AM E23.00011: Modernizing the Undergraduate Dynamics Curriculum**  
DAVID NOLTE (Presenter), Purdue University  
— The best parts of physics are the last topics that our students ever see. These are exciting topics like the bending of light by black holes, traffic on the World Wide Web, or the synchronization of global economies. A new method for teaching upper-division mechanics provides an introduction to modern dynamics by generalizing state-space and metric-space approaches at a mathematically accessible level. Given the growing importance of dynamical systems in science and technology, this approach gives students an up-to-date foundation for their future careers, embedding topics of modern dynamics—chaos, synchronization, network theory, neural networks, evolutionary change, econophysics and relativity—within the context of traditional physics founded on Lagrangian and Hamiltonian physics. The goal is to modernize the teaching of junior-level dynamics, responsive to a changing society, while retaining the core traditions and common language of the physics of dynamics.

**10:12AM E23.00012: A program to encourage underrepresented high school students to study STEM through hands-on University-level research experience: its impact, how we did it, and what we learned**  
TREVOR GRANDPRE (Presenter), Science Education, Graduate Division, University of California, Berkeley, MIGUEL DAAL, Physics, UC Santa Barbara, KAYLEIGH A CASSELLA, DA AN, Science Education, Graduate Division, University of California, Berkeley, DANIELLE H SPELLER, Physics, Yale University, BERNARD SADOULET, RACHEL WINHELD, MATTHEW CHOW, FRANK WANG, ALVARO A LOYA VILLALPANDO, Science Education, Graduate Division, University of California, Berkeley, ARRAN TJ PHIPPS, Physics, Stanford University, TAMMIE VISINTAINER, Science Education, Graduate Division, University of California, Berkeley — Since 2007, we have offered a course that pairs small groups of ninth grade high schoolers from historically underrepresented backgrounds with graduate student researchers from STEM disciplines to complete a five week long summer research project of the graduate students' design. Our course, 'Topics in Current Research', is located at UC Berkeley and administered with the SMASH Academy, a Bay Area non-profit. In this presentation, we detail the structure of the course; discuss lessons learned in its administration; and, present findings from 10 years of data collected from the high school and graduate students showing, among other things, that after participating in the program high schoolers were more likely to feel like they belonged in STEM and more likely to consider it for a career. We hope that this program will serve as a model and motivation for other institutions to do something similar.

*This work is supported in part by the National Science Foundation Particle Astrophysics/Underground Physics Program, under Grant Number PHY-1408597.

**10:24AM E23.00013: Observation of relativistic corrections to Moseley’s law at high atomic number**  
DUNCAN C WHEELER, EMMA BINGHAM (Presenter), MICHAEL WINER, JANET MARIE CONRAD, SEAN ROBINSON, Department of Physics, Massachusetts Institute of Technology — Transitions between low-lying electron states in atoms of heavy elements lead to electromagnetic radiation with characteristic discrete energies between about 0.1 keV and 100 keV (x rays). Moseley’s law is an empirical relation, described in 1914, that supported predictions of the Bohr model of the atom. It predicts that the energy of these x rays scales as $Z^2$ while also identifying the atomic number $Z$ as the measure of nuclear charge. The foundational nature of Moseley’s experiment has led to popularity in undergraduate advanced laboratory physics subjects. We report observations of deviations from Moseley’s law in the K-alpha x-ray emission of 13 elements from $Z = 29$ to $Z = 92$. While the deviations follow the square-law predictions of the Bohr model fairly well at low Z, they become larger with increasing Z. We find that relativistic models of atomic structure are necessary to fit the full range of elements observed ($p = 0.23$ for the relativistic Bohr model). As has been argued by previous authors, measurements of relativistic deviations from Moseley's law are pedagogically valuable at the advanced lab level and accessible with modern but modest apparatus. Here, we show this value can be extended by using higher Z elements, where the effects are more dramatically observable.

**10:36AM E23.00014: In-situ differential thermal analysis and crystal growth**  
YURI JANSSEN (Presenter), KEMAR DUDLEY, Department of Physics, Farmingdale State College — Differential thermal analysis (DTA) can give valuable information on melting and freezing of mixtures that are used for flux or solution growth of single crystals for materials research, and increasing the success rate of crystal growth attempts. DTA is especially valuable as a tool for undergraduate research involving crystal growth, as it can quickly give a realistic and easy-to-understand picture at what is happening inside a growth crucible as it is hiding the cooling crystal-growth mixture from view. In the past, we have performed DTA in a dedicated instrument, with small crucibles containing exactly the same composition as the larger growth crucible in the larger growth furnace. Recently, we have started to perform in-situ DTA inside the growth furnace and on as-prepared growth samples, quickly improving crystal growth performed by undergraduate students with limited time dedicated to lab, and, moreover, on very inexpensive equipment. Here, we will present first results on these developments, and provide an outlook at possible enhancements of this in-situ technique, used by undergraduate students.

*Funding was provided by the Office of the Provost of Farmingdale State College.
Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E24 DAMOP DQI: Hybrid/Macroscopic Quantum Systems, Optomechanics, and Interfacing AMO with Solid State/Nano Systems I  BCEC 159 - Tian Zhong, Univ of Chicago - Tag(s): Focus

8:00AM E24.00001: Measuring Electromagnetic and Gravitational Responses of Photonic Landau Levels* [Invited]
NATHAN SCHINE (Presenter), University of Chicago — Topology describes global properties insensitive to local perturbation or manipulation. Mathematical examples include knots in strings, where no manipulation of a closed loop besides cutting it can change its knottedness, and the genus (number of handles) of a closed surface, where no smooth deformation can change its number of handles. Topological materials have recently become a distinct focus in condensed matter physics, appearing famously in the quantum Hall effect and topological insulators.

Synthetic materials in which the constituent particles are photons trapped in an optical resonator offer an exciting platform on which to study topological materials. Recent efforts have realized broad control over the single-photon Hamiltonian, including a strong synthetic magnetic field for photons, and strong photon-photon interactions. In this talk, I will present how a nonplanar resonator can harbor a quantum Hall system in curved space. I will then discuss measurements of three distinct topological indices, offering insight onto their physical meaning and application. We measure the Chern number via real-space local projectors: non-reciprocal products of transmission amplitudes reveal an Aharanov-Bohm phase associated with a non-zero Chern number. Two additional topological invariants, the mean orbital spin and chiral central charge, are encoded in the variation of the local density of states near a singularity of spatial curvature, revealing a complex interplay between geometry and topology. I will conclude with a view towards the experimental introduction of interactions and the role these invariants play in characterizing topological phases of matter.

*This work was supported by DOE grant DE-SC0010267 for apparatus construction/data collection and MURI grant FA9550-16-1-0323 for analysis.

8:36AM E24.00002: Dynamically Generated Synthetic Electric Fields for Photons* PETR ZAPLETAL (Presenter), University of Cambridge, STEFAN WALTER, FLORIAN MARQUARDT, Max Planck Institute for the Science of Light, Staudtstrasse 2, 91058 Erlangen, Germany — Static synthetic magnetic fields give rise to phenomena including the Lorentz force and the quantum Hall effect even for neutral particles, and they have by now been implemented in a variety of physical systems. Moving towards fully dynamical synthetic gauge fields allows, in addition, for backaction of the particles’ motion onto the field. If this results in a time-dependent vector potential, conventional electromagnetism predicts the generation of an electric field. Here, we show how synthetic electric fields for photons arise self-consistently due to the nonlinear dynamics in a driven system. Our analysis is based on optomechanical arrays, where dynamical gauge fields arise naturally from phonon-assisted photon tunneling. We study open, one-dimensional arrays, where synthetic magnetic fields are absent. However, we show that synthetic electric fields can be generated dynamically. The generation of these fields depends on the direction of photon propagation, leading to a novel mechanism for a photon diode, inducing nonlinear unidirectional transport via dynamical synthetic gauge fields.

*This work was supported by the European Union's Horizon 2020 research and innovation programme under grant agreement No 732894 (FET Proactive HOT).

8:48AM E24.00003: A polarization-selective cavity inside a hollow-core optical fiber* JEREMY FLANNERY (Presenter), BEHROOZ SEMNANI, MICHAL BAJCSY, University of Waterloo — We fabricate and characterize a polarization-selective cavity inside a hollow-core optical fiber by attaching photonic-crystal (PC) membranes acting as metasurface mirrors to the end faces of a segment of such fiber. These slabs are comprised of a thin film of a dielectric material (silicon nitride) perforated with a pattern of holes where the reflective properties are dictated by the type and dimensions of the hole pattern. By breaking the x-y symmetry of the photonic crystal pattern using a rectangular lattice of elliptical holes, the mirrors become polarization-selective, i.e., the mirrors are highly reflective for one linear polarization and almost fully transparent for the orthogonal polarization. The holes of the PC slab allow injection of gasses into the hollow core of the fiber, which would not be possible if the fiber was capped with a dielectric stack mirror. The polarization selectivity is also a unique feature not possible with conventional mirrors.

This novel type of polarization dependent fiber-integrated cavity can enhance quantum optics schemes with atomic ensembles relying on cavity field and single-pass field with the ensemble by choosing the appropriate polarizations of the fields.

*Industry Canada, Ontario’s Early Researcher Award, NSERC's Discovery grant, OGS.
9:00AM E24.00004: Quantum Noise Free Thermal Noise Measurements of a Fabry-Perot Cavity  TORREY CULLEN (Presenter), Physics, Louisiana State University — As gravitational wave measurements become more sensitive, they will start to be limited by quantum back action noise. Because effects like quantum radiation pressure noise have been previously measured, the next step is to remove these effects from measurement in a process called back action cancellation. Our system, consisting of a Fabry Perot cavity with a microfabricated movable mirror, is used to demonstrate cancellation of quantum back action. We first verify the presence of this back action by measuring the light in reflection of the cavity. The cancellation is then performed by splitting the transmitted light from the cavity, sending it to two photo detectors, and cross correlating the outputs. By showing that the cross correlated output and previous measurements of thermal noise are the same, we confirm that these quantum effects have been eliminated from the measurement (because thermal noise is the next limiting noise source). These cancellations demonstrate a significant step towards the reduction of quantum radiation pressure noise effects in aLIGO and future generation detectors.

9:12AM E24.00005: Multimode Cavity Optomechanics in superfluid Helium droplets*  ANDREA AIELLO (Presenter), Marquardt's division, Max Planck Institute for the Science of Light — The “minimal” optomechanical system consists in an optical cavity with a vibrating end mirror. There is, in this case, one optical mode coupled via radiation-pressure force to one mechanical mode [1]. Recently, it was proposed a novel optomechanical system based upon millimeter-size droplets of liquid Helium magnetically levitated in vacuum where the droplet serves both as optical and mechanical resonator [2]. The optical resonances are given by the whispering-gallery modes of light and the mechanical resonances by the vibrational surface modes. These about $10^3$ resonances ranges from $2\pi \times 23$ Hz to $2\pi \times 219$ kHz [3].

In this presentation we illustrate the principal unusual characteristics of the multimode dynamics [4] of the optically excited Helium droplet and we present some preliminary results about nonlinear effects.


*This project has received funding from the European Unions Horizon 2020 research and innovation programme under grant agreement No 732894 (Hybrid Optomechanical Technologies)

9:24AM E24.00006: Towards two spin-mechanical hybrid quantum systems  EMMA ROSENFELD (Presenter), JAN GIESELER, AARON N KABCENELL, ARTHUR D SAFIRA, MARTIN SCHUETZ, MIKHAIL LUKIN, Harvard University — Hybrid quantum systems combine complimentary phenomena to enable breakthroughs in quantum mechanics, information processing, and simulation - from preparation of non-thermal states of mechanical objects, to quantum buses for long-distance entanglement of qubits. A particular hybrid quantum system with such potential can be achieved by combining the spins with a magnetic mechanical oscillator. Creating such a platform with high cooperativity is both desirable and challenging to implement: we need a large resonator zero-point motion and magnetic field gradient to maximize the coupling, while both the resonator and spin are isolated from the environment.

To address this challenge, we investigate two mechanical resonators, each of which are coupled to a spin: (i) high-Q nanobeam SiN resonators and (ii) levitated mechanical oscillators. In both cases, the small mass results in a large zero-point motion, and the geometry reduces coupling to the environment, thereby minimizing dissipation. For the spin, we use a nearby nitrogen-vacancy (NV) center defect in diamond, which features long coherence times. In this talk, we demonstrate progress towards these hybrid systems, each of which could open doors to unexplored regions of parameter space in the physics of quantum optics.
THIBAUD RUELLE, MARTINO POGGIO, FLORIS BRAAKMAN (Presenter), University of Basel — In recent years, techniques have been developed to realize concave mirror templates on the tips of optical fibers. These can be used to define tunable open-access Fabry-Perot microcavities with high finesse. The combination of spectral tunability, high finesse, intrinsic fiber coupling and uniquely small dimensions offered by these optical cavities has led to their widespread adoption in the cavity quantum electrodynamics (CQED) community and to a lesser extent in the optomechanics community.

We realize mirror templates on the tips of optical fibers using a single-shot CO2 laser ablation procedure. We perform a systematic study of the influence of the pulse power, pulse duration, and laser spot size on the radius of curvature, depth, and diameter of the mirror templates. We find that these geometrical characteristics can be tuned to a larger extent than has been previously reported, and notably observe that compound convex-concave shapes can be obtained. This detailed investigation should help further the understanding of the physics of CO2 laser ablation processes and help improve current models. We additionally identify regimes of ablation parameters that lead to mirror templates with favorable geometries for use in cavity quantum electrodynamics and optomechanics.

*Swiss SNF

TIRTH SHAH (Presenter), Physics, Friedrich Alexander Universität Erlangen Nurnberg, VITTORIO PEANO, CHRISTIAN BRENDEL, Max Planck Institute for the Science of Light, OSKAR PAINTER, Applied Physics, California Institute of Technology, HANNES PFEIFER, FLORIAN MARQUARDT, Max Planck Institute for the Science of Light — We present the design of and numerical simulations for an on-chip optomechanical device that supports helical vibrations and allows all-optical excitation and read-out thereof. The device is based on a so-called optomechanical crystal, i.e. a nanostructure that supports both mechanical and optical bulk band gaps. The optomechanical crystal of interest is a patterned silicon slab. The pattern of holes has been engineered to give rise to i) topologically distinct domains separated by a domain wall of chosen shape supporting a broadband mechanical helical edge state, ii) high quality factor optical cavities that are localized close to the domain wall and display a good coupling to the helical states. As usual in optomechanics, the optomechanical coupling can be boosted by driving the optical cavities using a laser. This allows the excitation and the high-precision read out of the helical vibrations propagating along the domain wall.

*Tirth Shah acknowledges support from the European Union's Horizon 2020 Programme for Research and Innovation under grant agreement No. 722923 (Marie Curie ETN - OMT).

VICTOR BITTENCOURT (Presenter), VERENA FEULNER, SILVIA VIOLA-KUSMINSKIY, Max Planck Institute for the Science of Light — Cavity optomagnonics is an emergent field where photons couple to elementary magnetic excitations in solid state systems. For optical photons, the coupling is parametric and the magnetic material is both the optical cavity and the host of the magnetic excitations (magnons). These systems are promising for integration in hybrid quantum platforms. In this context, we propose a magnon heralding protocol to generate a magnon Fock state by detecting a cavity photon. We analyze the constraints imposed by the magnonic decay rate and by the strength of the optomagnonic coupling. We show that the detrimental thermal effects can be overcome by initially actively cooling the magnon mode. We discuss the feasibility of the proposed protocol for state of the art YIG cavity optomagnonic systems.

*The authors acknowledge the support from the Max Planck Gesellschaft through an independent Max Planck Research Group
10:12AM E24.00010: Faddeev-Kulish Asymptotic States in Cold Atom Quantum Physisorption on 2D Materials
SANGHITA SENGUPTA (Presenter), Physics, Institut quantique de l’Université de Sherbrooke — Theories with long-range interactions like QED or perturbative gravity exhibit severe infrared divergences in their scattering rates due to the emission of infinitely many soft quanta. Remarkably, a low-energy condensed matter analogue of this infamous infrared problem in QED is realized in a hybrid system of cold atoms coupled to a vibrating elastic membrane. We focus on the atom-phonon coupling of the vibrating membrane and provide procedures to address the infrared divergences. Our methods include non-perturbative techniques that can be broadly categorized into two schemes: (1) inclusion of emission of infinitely many soft-phonons and (2) dressing of asymptotic states which is similar in essence to the Faddeev-Kulish treatment of the infrared divergences in QED. We provide results for both the schemes in the spirit of the well-known exact solution of the independent boson model and discuss the validity of the results corresponding to the different scales of the infrared. In particular, we present the results of our resummation procedures for the physisorption rate of cold atomic hydrogen as function of membrane sizes and temperature.

10:24AM E24.00011: Cavity Superconductor-Polaritons
ANDREW ALLOCCA (Presenter), ZACHARY RAINES, JONATHAN CURTIS, VICTOR GALITSKI, University of Maryland, College Park — Following the success of realizing exciton-polariton condensates in cavities, we examine the hybridization of cavity photons with the closest analog of excitons within a superconductor, states called Bardasis-Schrieffer modes. Though these modes do not typically couple linearly to light, one can engineer a coupling with an externally imposed supercurrent, leading to the formation of hybridized Bardasis-Schrieffer-polariton states, which we obtain both as poles of the bosonic Green's function and through the derivation of an effective Hamiltonian picture for the model. These new excitations have nontrivial overlap with both the original photon states and d-wave superconducting fluctuations. We conjecture that their condensation could produce a finite d-wave component of the superconducting order parameter -- an $s\pm id$ superconducting state.

*This work was supported by NSF DMR-1613029 (Z.R.), DOE-BES (DESC0001911) and the Simons Foundation (V.G.), US-ARO contract No. W911NF1310172 (A.A.), the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE1322106 (J.C.)

10:36AM E24.00012: Cavity superconductor Higgs-polaritons
ZACHARY RAINES (Presenter), ANDREW ALLOCCA, VICTOR GALITSKI, University of Maryland, College Park — Motivated by the dramatic success of cavity exciton-polariton physics we consider the formation of a polariton from cavity photons and the amplitude mode of a disordered superconductor. Enabled by the recently predicted and observed supercurrent-induced coupling between these excitations we find that significant hybridization between cavity photons and Higgs excitations in a quasi-2D superconductor can occur. We analyze the character and damping of the hybrid modes.

10:48AM E24.00013: Investigating Light-Matter Interactions Through the Coupling of Single Emitters to Bowtie Nanoantennas
NATHAN KIMMITT (Presenter), ESTHER A WERTZ, Rensselaer Polytechnic Institute — Metallic nanoparticles, which confine light into very small volumes and greatly enhance fields, have many exceptional and tunable optical properties. Nanodimers known as bowtie nanoantennas are known to have strong field enhancements and confinement to the gap between the triangles. However, due to intrinsic ohmic losses, obtaining strong coupling between an emitter and the cavity remains an issue. In this study, to elucidate the effects of the nanometric positioning of the emitter, we employ super-resolution single-molecule fluorescence techniques to study the effects of detuning, polarization, orientation, nanometer gap size, and adhesion layer have on the fluorescence properties of the dye, as well as the trapping dynamics of the system. A clear set of optimal parameters has been found, aided by finite element simulations, hinting towards obtaining the maximal coupling for single emitters in this geometry.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E25 DAMOP DCMP: Disorder and Localization in AMO Systems I: Time Crystals, Diffusion, Quantum Chaos 8CEC 160A - Anushya Chandran, Boston University - Tag(s): Focus
Discrete time crystals in long-range interacting systems

NORMAN YAO (Presenter), University of California, Berkeley — A generic periodically driven, isolated system will absorb energy until it looks, locally, like an infinite-temperature state. However, when the drive frequency is large compared with the local energy scales of the system, then the system can only absorb energy from the drive by spreading it out over many excitations. Consequently, heating occurs very slowly, and there is a long-lived quasi-steady state - a so-called "pre-thermal" state - in which ordered phases of matter can occur. In this context, I will describe how long-range interactions can stabilize pre-thermal time-translation symmetry breaking in one dimensional systems (even in the absence of disorder). I will begin by motivating a new definition for light-cones in power-law interacting quantum systems and using this definition, I will prove that long-range, pre-thermal time crystals naturally exhibit exponentially long lifetimes. Finally, an experimental realization of a one dimensional, pre-thermal time crystal in trapped atomic ions will be discussed.

NMR observations of discrete time crystalline signatures in an ordered crystal of ammonium dihydrogen phosphate

ROBERT BLUM (Presenter), JARED ROVNY, SEAN BARRETT, Physics, Yale University — The discrete time crystal (DTC) is a recently-described phase of driven quantum systems that breaks the discrete time translation symmetry of its drive. If the Hamiltonian has period T, the signature of a DTC is a response of period nT that is robust to "error" in the drive. Two experiments recently reported this signature in trapped ions [1] and in diamond NV centers [2]. We present signatures of DTC order [3,4] in an NMR system of 31P spins in an oriented crystal of ammonium dihydrogen phosphate (ADP), a clean sample with multiple dipolar-coupled spin species (1H, 31P, 14N). By varying the pulse angle θ and delay time τ of the DTC pulse sequence, we observe robust DTC oscillations across a much greater range in (θ, τ) than has been observed in earlier experiments [1,2], both with and without 1H decoupling.

Beyond discrete time crystal signatures: hidden coherence, causes of decay, and the first "discrete time crystal echo"

JARED ROVNY (Presenter), ROBERT BLUM, SEAN BARRETT, Physics, Yale University — The phase structure of driven quantum systems can include exotic phenomena, including the recently-described discrete time crystal (DTC). The key signature of a DTC is a response with period nT (n=2,3,...) for drive period T, even when the drive is imperfect. Two experiments recently demonstrated this signature, one in trapped ions [1] and the other in diamond NV centers [2]. We have shown this signature in an NMR system of 31P spins on a crystal lattice, with little to no disorder [3,4]. We study the decay of the DTC oscillations, with two main results. First, we use a novel "DTC echo" sequence to demonstrate that the decay is caused in part by coherent evolution. Second, we demonstrate that the observed decay for perfect pi pulses (ε = 0) can be produced by the action of the internal Hamiltonian during the pulses.
9:00AM E25.00004: Spatial-Translation-Induced Discrete Time Crystals  KAORU MIZUTA (Presenter), KAZUAKI TAKASAN, Department of Physics, Kyoto University, MASAYA NAKAGAWA, CEMS, RIKEN, NORIO KAWAKAMI, Department of Physics, Kyoto University — Time crystals, where time translation symmetry is spontaneously broken, are novel phases of matters in that they are proved to exist only in nonequilibrium[1]. In particular, time crystals in Floquet systems, called discrete time crystals (DTCs), have attracted much interest because of theoretical developments[2] and recent experimental realization[3].

In many of conventional DTCs, symmetry operation and its symmetry breaking are utilized [2], but only on-site symmetries are focused on. Therefore, we propose new DTCs named "spatial-translation-induced DTCs"(STI-DTCs), which is realized by spatial translation and its symmetry breaking[4]. By focusing on spatial translation symmetry, STI-DTCs have notable properties which do not exist in conventional DTCs - high controllability of DTC orders and nontrivial oscillation of local transport. We have also proposed a new way to realize DTCs in quantum circuits as an experimental platform.

References

9:12AM E25.00005: Quantum diffusion in the strong tunneling regime*  NISARGA PAUL (Presenter), ARIEL AMIR, Harvard University — We discuss the dynamics of a quantum-mechanical wavepacket in a noisy environment (i.e., time-dependent disorder), modeled using a tight-binding Hamiltonian. It has been found that the fluctuating environment may give rise to diffusive behavior (rather than Anderson localization, which occurs for time-independent disorder). We develop a new approach to this problem by considering the dynamics as arising from multiple Landau-Zener crossing events. We find the conditions for the validity of the approach, and use it to calculate how the diffusion constant depends on the noise. The analytical results are corroborated numerically. The results may be applicable to exciton diffusion in photosynthesis and electronic transport in solid-state physics.

*NP was supported by the Harvard College Research Program and Herchel Smith fellowship. AA thanks the Harvard Society of Fellows for support during the early stages of this work.

9:24AM E25.00006: Quantum-Spin Diffusion Driven by Ergodic and Non-Ergodic Finite Spin Baths  WALTER HAHN (Presenter), VIATCHESLAV DOBROVITSKI, TU Delft, QuTech — We investigate spin diffusion driven by a finite quantum spin bath in a system accessible for solid-state NMR experiments; namely polycrystalline L-alanine. The direct spin transport within the subsystem consisting of dipolar coupled carbon spins is suppressed due to disorder given by different Larmor frequencies. Spin diffusion is, therefore, governed by the surrounding network of proton spins-1/2. This proton network consists of strongly coupled groups which are weakly interacting among each other. By means of numerical simulations, we model realistic solid-state NMR experiments. We show that nearby proton spins govern the local magnetic field for carbon spins, while the farther proton spins determine dynamics within the proton bath. In particular, the farther proton spins provide ergodicity in the proton bath and, thereby, drastically change the spin diffusion in the carbon subsystem. We also consider deuterated alanine with all proton spins-1/2 replaced by deuteron spins-1. For deuterated L-alanine, we show that the local magnetic fields created by deuterons is insufficient to allow for spin diffusion due to the small magnetic dipole moment of deuterons. Instead, spin diffusion is governed by the spin-lattice relaxation of deuteron spins on much larger time scales.

9:36AM E25.00007: Signatures of Quantum Chaos in Classically Non-Chaotic Systems  EFIM ROZENBAUM (Presenter), University of Maryland, College Park, LEONID BUNIMOVICH, School of Mathematics, Georgia Institute of Technology, VICTOR GALITSKI, University of Maryland, College Park — One of the original goals in the field of quantum chaos was to establish a correspondence between the dynamics of chaotic classical systems and their quantum counterparts. The general issue is that quantum-mechanical interference washes out classical chaos after a very short (logarithmic) time, and the correspondence breaks down. Recently, out-of-time-ordered correlator, a universal tool to study quantum chaos, has received a lot of attention due to its versatility and natural interpretation. We use this diagnostic to show that a new kind of drastic disagreement can occur between quantum and classical counterparts of the same model. Remarkably, quantum mechanics appears capable of playing the opposite to its usual role. In particular, it brings chaos to a family of classically non-chaotic systems, where on the quantum side, we demonstrate the Lyapunov-like exponential growth of OTOC.
9:48AM E25.00008: The longest-lived current in a quantum chaotic spin chain  ARNOLD K. MONG (Presenter), DAVID HUSE, Princeton University — To explore issues of numerically capturing dissipative dynamics in closed many-body quantum systems, we have studied the relaxation of nonconserved current operators in a certain quantum chaotic spin chain. The Hamiltonian is a translationally-invariant spin-1/2 chain with nearest-neighbor XY interactions and a tilted field that breaks the conservation of total Z magnetization. We look at an infinite chain and examine the relaxation of all “current” operators that have total momentum zero and are odd under spatial inversion. The relaxation is via operator spreading; a unitary flow in operator space from simple short Pauli strings to long (and thus nonlocal) Pauli strings. To approximate this numerically, we limit the length of the Pauli strings and introduce an artificial nonunitary damping that acts only on the longest Pauli strings that we keep, and solve exactly for the longest-lived current operator in this approximation. We find that there is a regime of this artificial damping where we obtain a good approximation to the correct unitary dynamics, while in other regimes the artificial damping causes a blockage of the proper unitary flow in operator space and, as a result of this “bad plumbing”, gives incorrect results.

10:00AM E25.00009: Quantum Chaos for the Unitary Fermi Gas from the Generalized Boltzmann Equations  PENGFEI ZHANG (Presenter), Tsinghua University — we study the chaotic behavior of the unitary Fermi gas in both high and low temperature limits by calculating the Quantum Lyapunov exponent defined in terms of the out-of-time-order correlator. We take the method of generalized Boltzmann equations derived from the augmented Keldysh approach. At high temperature, the system is described by weakly interacting fermions with two spin components and in the low temperature limit, the system is a superfluid and can be described by phonon modes. By comparing these to existing results of heat conductivity, we find that $D \ll v^2 \tau_L$. We argue that this is related to conservation laws for such systems with quasi-particles.

10:12AM E25.00010: Chaos and integrability in experimentally accessible all-to-all spin models*  GREGORY BENTSEN, Stanford University, THOMAS SCAFFIDI, VIR BULCHANDANI (Presenter), IONUT-DRAGOS POTIRNICHE, University of California, Berkeley, MONIKA SCHLEIER-SMITH, Stanford University, EHUD ALTMAN, University of California, Berkeley — In recent years, models of disordered fermions with random, all-to-all couplings have emerged as prime candidates for studying the limit of strong chaos in quantum mechanical systems. However, such models are prohibitively difficult to realize experimentally. By contrast, spin models with random, all-to-all couplings can be engineered in the context of cavity QED and could provide an opportunity to probe strongly interacting, disordered physics in the laboratory. We show that the class of models most naturally realized in this system has the unusual property of possessing two integrable points in its phase diagram. We construct the integrals of motion explicitly and propose a method to directly measure their characteristics in the experiment. This scheme raises the possibility of tuning the system between classical and quantum physics on the one hand, by varying the effective spin per site, and between integrable and chaotic physics on the other, by varying the effective cavity interactions.

*EPIQS initiative of the Moore Foundation (T. S.), NSF, DoE (M. S.-S.), ERC Synergy Grant UQUAM (E. A.)

10:24AM E25.00011: Scrambling in the Dicke model*  YAHYA ALAVIRAD (Presenter), SEYED ALI HOSSEINI LAVASANI, University of Maryland, College Park — The scrambling rate $\lambda_L$ associated with the exponential growth of out-of-time-ordered correlators can be used to characterize quantum chaos. Here we use the Majorana Fermion representation of spin $1/2$ systems to study quantum chaos in the Dicke model. We take the system to be in thermal equilibrium and compute $\lambda_L$ throughout the phase diagram to leading order in $1/N$. We find that the chaotic behavior is strongest close to the critical point. At high temperatures $\lambda_L$ is nonzero over an extended region that includes both the normal and super-radiant phases. At low temperatures $\lambda_L$ is nonzero in (a) close vicinity of the critical point and (b) a region within the super-radiant phase. In the process we also derive a new effective theory for the super-radiant phase at finite temperatures. Our formalism does not rely on the assumption of total spin conservation.

*Y.A. was supported by JQI-NSF-PFC and the National Science Foundation NSF DMR-1555135. A.L. was supported by JQI-PFC-UMD.
Quantum inverse freezing and mirror-glass order* THOMAS IADECOLA (Presenter), MICHAEL SCHECTER, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland — It is well known that spontaneous symmetry breaking in one spatial dimension is thermodynamically forbidden at finite energy density. Here we show that mirror-symmetric disorder in an interacting quantum system can invert this paradigm, yielding spontaneous breaking of mirror symmetry only at finite energy density and giving rise to "mirror-glass" order. The mirror-glass transition, which occurs via the energetic activation of a finite density of emergent Ising degrees of freedom, is enabled by many-body localization and appears to occur simultaneously with the localization transition. This counterintuitive manifestation of localization-protected order can be viewed as a quantum analog of inverse freezing, a phenomenon that occurs, e.g., in certain models of classical spin glasses.


*We acknowledge support from the Laboratory for Physical Sciences and Microsoft. T.I. acknowledges a JQI postdoctoral fellowship.

Out of Time Ordered Correlators in the Random Field XX Spin Chain* JONATHON RIDDELL (Presenter), ERIK SORENSEN, Physics and Astronomy, McMaster University — We study out of time order correlations, $C(x,t)$ and entanglement growth in the random field XX model with open boundary conditions using the exact Jordan-Wigner transformation to a fermionic Hamiltonian. For any non-zero strength of the random field this model describes an Anderson insulator. Two scenarios are considered: A global quench with the initial state corresponding to a product state of the Néel form, and the behaviour in a typical thermal state at $\beta=1$. As a result of the presence of disorder the information spreading as described by the out of time correlations stops beyond a typical length scale, $\xi_{\text{OTOC}}$. For $|x|<\xi_{\text{OTOC}}$ information spreading occurs at the maximal velocity $v_{\text{max}}=J$ and we confirm predictions for the early time behaviour of $C(x,t)-t^2|x|$.

*This research was supported by NSERC and enabled in part by support provided by (SHARCNET) (www.sharcnet.ca) and Compute/Calcul Canada (www.computecanada.ca).

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E26 DQI: Driven and Dissipative Superconducting Circuits BCEC 160B - Shyam Shankar, Yale Univ

Observation of the parity-time symmetry breaking transition in a dissipative superconducting qubit* MAHDI NAGHILOO (Presenter), MARYAM ABBASI, Physics, Washington University in St. Louis, YOGESH N JOGLEKAR, Physics, Indiana University-Purdue University Indianapolis (IUPUI), KATER MURCH, Physics, Washington University in St. Louis — Non-Hermitian systems that exhibit parity-time (PT) symmetry have been recently studied in electrical, optical, and mechanical classical systems revealing applications in non-reciprocal devices and sensing. While questions have remained as to whether PT-symmetric systems are realizable in the quantum regime due to the role of quantum noise in amplifiers, the topological features associated with PT-symmetric Hamiltonians are shared by dissipative systems with selective losses, which can be realized at the quantum level. We employ bath engineering techniques to realize a non-Hermitian Hamiltonian that has effective PT symmetry for a superconducting circuit. We use quantum state tomography to observe the PT symmetry breaking transition as manifested in the evolution of both diagonal and off-diagonal elements of the qubit density matrix.

*This work was supported by the John Templeton Foundation grant ID 58558 and the NSF Grant No. PHY-1607156.
8:12AM E26.00002: An experimental implementation for stabilizing Schrödinger cat states in a Kerr nonlinear resonator - Basic concepts* NICHOLAS FRATTINI (Presenter), ALEXANDER GRIMM, SHANTANU O. MUNDHADA, SHRUTI PURI, STEVEN TOUZARD, Applied Physics, Yale University, MAZYAR MIRRAHIMI, INRIA Paris and Yale University — Schrödinger cat states of microwave light based on superpositions of coherent states in a superconducting resonator can be used as error-protected qubits as well as auxiliary systems for fault-tolerant quantum computation. It has recently been shown that such states can be stabilized by applying a two-photon drive to a Kerr nonlinear resonator. In this talk, we will give an introduction on this type of qubit and its potential uses in quantum computation before discussing an experimental implementation. Our system is based on a modified, low-anharmonicity, transmon qubit. Instead of a Josephson junction, we use a Superconducting Nonlinear Asymmetric Inductive eLement (SNAIL) providing us with both three- and four-wave-mixing terms. This simultaneously implements the required nonlinearity and gives us access to a strong two-photon drive. We will report on the details of this implementation and present our progress towards the realization of this stabilization scheme. Part one of this two-part presentation will introduce the basic concept of this qubit and its uses in quantum information. 

*Work supported by: ARO, NSF, and YINQE

8:24AM E26.00003: An experimental implementation for stabilizing Schrödinger cat states in a Kerr non-linear resonator - Part 2: Experiment.* ALEXANDER GRIMM (Presenter), NICHOLAS FRATTINI, SHANTANU O. MUNDHADA, SHRUTI PURI, STEVEN TOUZARD, Applied Physics, Yale University, MAZYAR MIRRAHIMI, INRIA Paris and Yale University — Schrödinger cat states of microwave light based on superpositions of coherent states in a superconducting resonator are useful as error-protected qubits as well as auxiliary systems for fault-tolerant quantum computation. In this talk, we will give an introduction on this type of qubit and its potential uses in quantum computation before discussing an experimental implementation of this idea. Our system is based on a modified, low-anharmonicity, transmon qubit. Instead of a Josephson junction, we use a Superconducting Nonlinear Asymmetric Inductive eLement (SNAIL) providing us with both three- and four-wave-mixing terms. This simultaneously realizes the required non-linearity and gives us access to a strong two-photon drive. We report on this implementation and present preliminary results towards the realization of a stabilization scheme.

*Work supported by: ARO, NSF, and YINQE

8:36AM E26.00004: Directional Quantum State Transfer by Dissipation I – Conceptual Overview* CHEN WANG (Presenter), JEFFREY GERTLER, University of Massachusetts Amherst — Quantum state transfer from an information-carrying qubit to a receiving qubit is ubiquitous for quantum information technology. In a closed quantum system, this task requires precisely-timed control of coherent qubit-qubit interactions that are intrinsically reciprocal. Here, breaking reciprocity by dissipation in an open system, we propose a type of cascaded quantum systems where a quantum state can be spontaneously transferred between stationary qubits without time-dependent control. We show that the minimum system dimension for transferring one qubit of information in this way is 3x2 (between one physical qutrit and one physical qubit), plus one auxiliary reservoir. We discuss general requirements and strategies for such autonomous quantum state transfer as well as its connection with autonomous quantum error correction. We further discuss physical implementation schemes, with our experimental progress in a superconducting circuit QED platform to be described in a following presentation.


*This research was supported by the U.S. Air Force Office of Scientific Research and the U.S. Army Research Office.
**8:48AM E26.00005: Directional Quantum State Transfer by Dissipation II – Implementation in Circuit QED**

JEFFREY GERTLER (Presenter), CHEN WANG, Physics, University of Massachusetts Amherst, XIAOWEI DENG, Physics, University of Massachusetts Amherst and Southern University of Science and Technology, China — Dissipation is a remarkable resource in quantum information processing that can be used to stabilize and manipulate quantum states or manifolds. Here we utilize dissipation to implement an autonomous technique for quantum state transfer, with built-in directionality, that eliminates the need for time dependent external control. We report experimental progress towards this state transfer in a 3D superconducting circuit QED system between a three-level transmon (Alice) and a coaxial storage cavity (Bob). The quantum state is irreversibly transferred from Alice to Bob via dissipation of a coupled axillary transmon reservoir, activated by two four-wave mixing processes produced by off-resonant drives. Using virtual states of the reservoir to compensate for unwanted dispersive frequency shift, we show that quantum coherence can be maintained throughout the dissipative process, leading to high-fidelity state transfer which is limited by inherent qubit/cavity decoherence.


*This research was supported by the U.S. Air Force Office of Scientific Research and the U.S. Army Research Office.

**9:00AM E26.00006: Reconstructing Josephson Current-Phase Relations with Intermodulation Spectroscopy**

SHAN JOLIN (Presenter), THOMAS WEISSL, RICCARDO BORGANI, DAVID HAVILAND, Nanostructure Physics, KTH Royal Institute of Technology — When driving with multiple tones, a nonlinear system will give rise to intermodulation, or frequency mixing. Two drive tones placed near a nonlinear resonance produces a comb of intermodulation products. We present a method based on matrix inversion to reconstruct the nonlinearity from a measurement of this comb [1, 2]. We apply this method to a microwave frequency comb generated from a Nb-coplanar waveguide resonator with Josephson weak-links. This method is useful for accurate characterization of nonlinearities in superconducting quantum circuits.


*The authors acknowledge financial support from Knut and Alice Wallenberg Foundation.

**9:12AM E26.00007: Dissipation-free non-Hermitian physics using quantum parametric amplifiers**

YUXIN WANG (Presenter), AASHISH CLERK, Institute for Molecular Engineering, University of Chicago — There has been considerable interest in driven-dissipative systems governed by non-Hermitian effective Hamiltonians. These systems can exhibit a range of unusual phenomena, such as the spontaneous breaking of parity-time (PT) symmetry [1], and chiral effects associated with encircling exceptional points [1]. Quantum versions of these effects are however often compromised by their dissipative nature. Here, we show that many of these non-Hermitian effects can be realized in a completely non-dissipative setting, by exact unitary mappings to parametrically-driven bosonic setups. Applications of these mappings include enhanced quantum sensing using exceptional points, and chiral switching based on encircling of exceptional points. Our approach could be implemented experimentally using superconducting quantum circuits, or in optomechanical systems.


**9:24AM E26.00008: Driven Kerr resonators: new regimes of solvability and quantum bistability**

DAVID ROBERTS (Presenter), Physics, University of Chicago, AASHISH CLERK, Institute for Molecular Engineering, University of Chicago — The driven Kerr resonator is one of the most iconic solvable models in cavity QED [1]. When subject to two-photon (parametric) driving it can exhibit bistability, something that has been exploited in several recent experiments in circuit quantum electrodynamics and proposals for protected quantum memories [2, 3]. Here, we develop a more physically transparent method for finding analytic solutions to driven Kerr resonators. This allows us to solve for a wider class of systems than in previous work, and also allows us to derive closed-form expressions for steady-state Wigner functions. More intriguingly, our approach also uncovers a new class of previously-overlooked points of quantum bistability in the resonator's phase diagram. Our work could open up new avenues for using nonlinear driven superconducting quantum circuits as quantum processors.

Motivation and modelization*  JAYAMEENAKSHI VENKATRAMAN (Presenter), XU XIAO, CLARKE SMITH, Applied Physics, Yale University, ZAKI LEGHTAS, Centre Automatique et Systèmes, Mines ParisTech, LUCAS VERNEY, QUANTIC, INRIA, Paris, MAZYAR MIRRAHIMI, QUANTIC, INRIA, Paris; YQI, Yale University, SHYAM SHANKAR, Applied Physics, Yale University, IOAN-MIHAI POP, Physics, Karlsruhe Institute of Technology, MICHEL H. DEVORET, Applied Physics, Yale University — The transmon is ubiquitous in circuit QED experiments due to its remarkable coherence properties and simplicity of design and fabrication. However, when strongly driven at microwave frequencies, the transmon exhibits various kinds of instabilities. Floquet-Markov theory indeed predicts such instabilities. Shunting the transmon with a linear inductance qualitatively changes the potential seen by the phase, thus increasing the device stability under certain conditions. We call the resulting qubit the inductively-shunted transmon (IST) to distinguish it from the RF SQUID. Comparison of driven transmons and ISTs with different implementations offers insights in eliminating these instabilities, and also sheds light on the fundamental problem of chaos in a strongly driven dissipative quantum system. This talk will focus on the motivation and modelization.

*ARO, ONR, AFOSR and YINQE

9:48AM E26.00010: Quantum Electrodynamic Modeling of Superconducting Circuits* [Invited]  HAKAN TURECI (Presenter), Princeton University — The demand for rapid and high-fidelity execution of initialization, gate and read-out operations casts tight constraints on the accuracy of quantum electrodynamic modeling of superconducting integrated circuits. Attaining the required accuracies requires reconsidering our basic approach to the quantization of the electromagnetic field in spatially inhomogeneous waveguides and the notion of normal modes. I will discuss a computational framework based on the Heisenberg-Langevin approach to address these fundamental questions. This framework allows the accurate determination of the quantum dynamics of a superconducting qubit in an arbitrarily complex electromagnetic environment infinite in extent, for any coupling strength and any degree of openness. This includes the regime of overlapping resonances and the “ultra-strong coupling” regime. I will also discuss the effectiveness of this computational approach in meeting the demands of present-day quantum computing research.

This work has been carried out with Moein Malekakhlagh, Alex T. Petrescu and Saeed Khan.

*Parts of this work was supported by the Department of Energy and the Army Research Office.

10:24AM E26.00011: Suppressing the instabilities of RF driven transmon by a kinetic inductive shunt - Part 2: Experimental results*  XU XIAO (Presenter), JAYAMEENAKSHI VENKATRAMAN, CLARKE SMITH, Applied Physics, Yale University, ZAKI LEGHTAS, Centre Automatique et Systèmes, Mines ParisTech, LUCAS VERNEY, QUANTIC, INRIA, Paris, MAZYAR MIRRAHIMI, QUANTIC, INRIA, Paris; YQI, Yale University, SHYAM SHANKAR, Applied Physics, Yale University, IOAN-MIHAI POP, Physics, Karlsruhe Institute of Technology, MICHEL H. DEVORET, Applied Physics, Yale University — The transmon is ubiquitous in circuit QED experiments due to its remarkable coherence properties and simplicity of design and fabrication. However, when strongly driven at microwave frequencies, the transmon exhibits various kinds of instabilities. Floquet-Markov theory indeed predicts such instabilities. Shunting the transmon with a linear inductance qualitatively changes the potential seen by the phase, thus increasing the device stability under certain conditions. We call the resulting qubit the inductively-shunted transmon (IST) to distinguish it from the RF SQUID. Comparison of driven transmons and ISTs with different implementations offers insights in eliminating these instabilities, and also sheds light on the fundamental problem of chaos in a strongly driven dissipative quantum system. This talk will focus on recent experimental results for such investigations.

*ARO, ONR, AFOSR and YINQE

10:36AM E26.00012: Bistability and Critical Slowing Down in Superconducting Circuits  PAUL BROOKES (Presenter), University College London, GIOVANNA TANCREDI, Chalmers University of Technology, THEMIS MAVROGORDATOS, Stockholm University, ANDREW D PATTERTON, JOSEPH RAHAMIM, MARTINA ESPOSITO, PETER LEEK, University of Oxford, ERAN GINOSSAR, University of Surrey, MARZENA HANNA SZYMANSKA, University College London — We carry out an experimental and numerical examination of bistability and critical slowing down in the strongly driven non-linear regime of circuit QED. The system under study is a 3D microwave cavity coupled to a transmon qubit. By measuring the response of the cavity to a step function drive pulse, we see that in the bistable regime the time required for the system to reach equilibrium is far longer than both the cavity and qubit relaxation times. We observe that this equilibration time saturates at high drive powers. Through careful modelling we are able to attribute this saturation to phase noise of the transmon. In addition we demonstrate that the equilibration time is highly sensitive to the temperature of the cavity.
Sizeable photon-photon interactions in networks of nonlinear oscillators enable the study of strongly correlated photons in non-equilibrium quantum many-body systems. We present a system composed of two superconducting resonators, coupled nonlinearly by a superconducting quantum interference device (SQUID). By applying a parametrically modulated magnetic flux we control the linear photon hopping rate between the two resonators and its ratio with the cross-Kerr rate. When increasing the hopping rate we observe a fully controllable crossover in the spatial correlations of the photonic fields of the two resonators, from photon self-ordering to delocalization of photons. The presented parametric coupling scheme is intrinsically robust to frequency disorder and may therefore prove useful for realizing larger-scale resonator arrays, and in turn facilitate active control of extended correlated quantum gases for the purpose of emulating other less accessible quantum systems.

*This work is supported by the National Centre of Competence in Research "Quantum Science and Technology" (NCCR QSIT), a research instrument of the Swiss National Science Foundation (SNSF) and by ETH Zurich. M. J. H. acknowledges support by the EPSRC under grant No. EP/N009428/1.

Tuesday, March 5, 2019 8:00 AM - 10:48 AM

Session E27 DQI DQI: Quantum Machine Learning I BCEC 160C - Daniel Kyungdeock Park, KAIST - Tag(s): Focus

8:00AM E27.00001: Improved Training of Quantum Boltzmann Machines
ERIC ANSCHUETZ (Presenter), YUDONG CAO, Zapata Computing — Quantum Boltzmann machines (QBMs) are a natural quantum generalization of restricted Boltzmann machines (RBMs) that, at least under numerical simulation, perform better than their classical counterparts in learning generic data distributions. However, training QBMs using gradient-based methods requires sampling observables in quantum thermal distributions, a problem that generically is NP-hard. In this work, we find that the locality of the gradient observables that must be sampled gives rise to an efficient sampling method based on the Eigenstate Thermalization Hypothesis (ETH), and thus an efficient method for training QBMs on quantum devices. Furthermore, we demonstrate a hybrid gradient-based/black box optimization procedure that outperforms strictly gradient-based training methods.

8:12AM E27.00002: Measurement-based adaptation protocol with quantum reinforcement learning
LUCAS LAMATA (Presenter), University of the Basque Country, FRANCISCO ALBARRÁN-ARRIAGADA, JUAN CARLOS RETAMAL, Universidad de Santiago de Chile, ENRIQUE SOLANO, University of the Basque Country — Machine learning employs dynamical algorithms that mimic the human capacity to learn, where the reinforcement learning ones are among the most similar to humans in this respect. On the other hand, adaptability is an essential aspect to perform any task efficiently in a changing environment, and it is fundamental for many purposes, such as natural selection. Here, we propose an algorithm based on successive measurements to adapt one quantum state to a reference unknown state, in the sense of achieving maximum overlap. The protocol naturally provides many identical copies of the reference state, such that in each measurement iteration more information about it is obtained. In our protocol, we consider a system composed of three parts, the "environment" system, which provides the reference state copies; the register, which is an auxiliary subsystem that interacts with the environment to acquire information from it; and the agent, which corresponds to the quantum state that is adapted by digital feedback with input corresponding to the outcome of the measurements on the register. F. Albarrán-Arriagada, J. C. Retamal, E. Solano, and L. Lamata, Phys. Rev. A 98, 042315 (2018).
8:24AM E27.00003: Improving training of Boltzmann machines with error corrected quantum annealing* RICHARD LI (Presenter), DANIEL A LIDAR, University of Southern California — Boltzmann machines, a class of machine learning models, are the basis of several deep learning methods that have been successfully applied to both supervised and unsupervised machine learning tasks. Quantum annealing may help lead to future advances in the development of these learning algorithms, but its usefulness is determined in part by the effective temperature. We have applied nested quantum annealing correction (NQAC) to do unsupervised learning with a small bars and stripes (BAS) dataset, and to a coarse-grained MNIST dataset, which consists of black-and-white images of hand-written integers, to do supervised learning. For both datasets, we demonstrate an effective temperature reduction with NQAC that leads to an increase in learning performance. We also find better performance overall with longer annealing times and offer some interpretation of the results based on comparison to simulated quantum annealing (SQA) simulations.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.

8:36AM E27.00004: Opportunities and Challenges in Quantum-Assisted Machine Learning [Invited] ALEJANDRO PERDOMO (Presenter), Rigetti Computing — With quantum computing technologies nearing the era of commercialization and quantum advantage, machine learning (ML) is promising as one of the promising "killer" applications. Despite significant effort, there has been a disconnect between most quantum ML proposals, the needs of ML practitioners, and the capabilities of near-term quantum devices towards a conclusive demonstration of a meaningful quantum advantage in the near future. In this talk, we provide concrete examples of intractable ML tasks that could be enhanced with near-term devices. We argue that to reach this target, the focus should be on areas where ML researchers are struggling, such as generative models in unsupervised and semi-supervised learning, instead of the popular and more tractable supervised learning tasks. We focus on hybrid quantum-classical approaches and illustrate some of the key challenges we foresee for near-term implementations.

9:12AM E27.00005: Quantum generative adversarial learning in a superconducting quantum circuit HU LING, Tsinghua University, SHUHAO WU, USTC, WEIZHOU CAI, YUWEI MA (Presenter), XIANGHAO MU, YUAN XU, HAIYAN WANG, YIPU SONG, DONG-LING DENG, Tsinghua University, CHANG-LING ZOU, USTC, LUYAN SUN, Tsinghua University — Generative adversarial learning is one of the most exciting recent breakthroughs in machine learning—a subfield of artificial intelligence that is currently driving a revolution in many aspects of modern society. It has shown splendid performance in a variety of challenging tasks such as image and video generations. More recently, a quantum version of generative adversarial learning has been theoretically proposed and shown to possess the potential of exhibiting an exponential advantage over its classical counterpart. Here, we report the first proof-of-principle experimental demonstration of quantum generative adversarial learning in a superconducting quantum circuit. We demonstrate that, after several rounds of adversarial learning, a quantum state generator can be trained to replicate the statistics of the quantum data output from a digital qubit channel simulator, with a high fidelity (98.8% on average) that the discriminator cannot distinguish between the true and the generated data. Our results pave the way for experimentally exploring the intriguing long-sought-after quantum advantages in machine learning tasks with noisy intermediate-scale quantum devices.

9:24AM E27.00006: Noncommutative Boltzmann Machines* MARK NOVOTNY (Presenter), Mississippi State University — Building on the 2018 paper on quantum Boltzmann Machines (qBM) by Amin et al [1], the concept of noncommutative Boltzmann Machines (ncBM) is introduced. ncBM contain qBM as a subset, but can be viewed, for example, as machine learning with superoperators. In particular, we study ncBM with the Liouvillian superoperator, and show the negative phase of machine learning becomes easy to calculate in a particular limit. Both Bernoulli data sets [1] and quantum dragon datasets [2] are utilized for both generative and discriminative learning. Possibilities of using near-term adiabatic quantum annealing machines for ncBM will be discussed.


*Based on work supported by the Air Force Research Laboratory (AFRL) under agreement number FA8750-18-1-0096. The views and conclusions herein are those of the authors, and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of AFRL or the US Government.
9:36AM E27.00007: Hybrid quantum-classical schemes for generative adversarial learning: HQGANs*  JHONATHAN ROMERO (Presenter), Harvard University, ALAN ASPURU-GUZIK, University of Toronto, Department of Chemistry, and Computer Science — Quantum computing and machine learning are two fast-growing research areas. Recently, these two areas have been merged into the field of quantum machine learning (QML), seeking to find ways in which quantum computers can offer advantages at solving machine learning problems over classical computers. Here, we propose to use quantum computers to learn models that mimic observed data distributions, a type of task known as generative learning, by substituting neural networks with variational quantum circuits in the generative adversarial networks (GANs) framework. GANs are statistical models that learn to sample from an observed data distribution by looking at individual samples. They consist of two neural networks, known as the discriminator and the generator, competing against each other in a minimax game. We propose a hybrid-quantum classical scheme that trains two variational quantum circuits, playing the role of discriminator and generator, to perform the same task on classical data. The proposed hybrid quantum GANs (HQGANs) might benefit machine learning by improving the ability to model more complex data distributions and could offer a new niche of applications for near-term quantum computers.

*Sponsoring Agency: Office of Naval Research (ONR)
Award Number: N00014-16-1-2008

9:48AM E27.00008: Variational circuits for machine learning with near-term devices  MARIA SCHULD (Presenter), University of KwaZulu-Natal and Xanadu — Variational circuits are parameter-dependent quantum algorithms that can be optimized for a certain task. One approach in quantum machine learning is to interpret these circuits as machine learning models that can be trained to generalise from data. Such models are often referred to as variational quantum classifiers. This talk will focus on various issues around this approach, for example how to think about the power of variational quantum classifiers, how we can train them and what they might be good for.

10:00AM E27.00009: Quantum Manifold Learning Algorithms for Dimensionality Reduction  XI HE (Presenter), LI SUN, XIAOKAI HOU, XIAOTING WANG, University of Electronic Science and Technology of China — Manifold learning is a kind of method which discusses the machine learning problems under the manifold hypothesis. It assumes that the sampled high-dimensional data actually comes from the embedding of some low-dimensional manifold structure. Manifold learning has wide range of applications in dimensionality reduction and data visualization. In the field of manifold learning, two most representative and commonly used algorithms are isometric mapping and locally linear embedding. Using techniques of quantum computing, we research out two quantum algorithms in correspondence to them. Compared with corresponding classical algorithms, the two quantum algorithms proposed in this paper can be implemented on a quantum computer with quantum speed-up. Quantum isometric mapping provides at least quadratic acceleration and quantum locally linear embedding takes logarithmic resources. In addition, we attempt to find out a common process to deal with quantization of manifold learning algorithms.

10:12AM E27.00010: Differentiable Quantum Circuits and Generative Modeling*  JINGUO LIU (Presenter), LEI WANG, Institute of Physics, Chinese Academy of Sciences — We present a fresh approach to quantum machine learning by using quantum circuits as probabilistic generative models. The proposed QCBM overcomes the challenging problem in training implicit density models with discrete outputs in deep learning. The key component of our gradient-based learning algorithm is to measure the gradient of the two sample test loss function on a quantum computer unbiasedly and efficiently. With the inspiration of matrix product state, we are able to train a Born machine to generate intermediate-scale images with number of qubits much less than pixel numbers. We demonstrate the generative power of these learning schemes with our new Julia quantum circuit simulator Yao.jl [1]. With Yao.jl, one can simulate quantum machine learning models, quantum optimization algorithms and quantum chemistry problems efficiently and easily. We combined our framework with state of art machine learning framework like Zygote.jl, aiming for quantum software 2.0: "Automatic Differentiable Quantum Circuits".

[1] https://github.com/QuantumBFS/Yao.jl

*The authors are supported by the National Natural Science Foundation of China under the Grant No. 11774398, research program of the Chinese Academy of Sciences under Grant No. XDPB0803 and HuaWei Quantum Computing.
10:24AM E27.00011: Machine-learned QCVV for distinguishing single-qubit noise*  
TRAVIS SCHOLTEN (Presenter), T. J. Watson Research Center, IBM, YI-KAI LIU, NIST, KEVIN YOUNG, Sandia National Laboratories, ROBIN BLUME-KOHOUT, Center for Computing Research, Sandia National Laboratories — We investigate the use of machine learning (ML) algorithms for developing new QCVV protocols. ML algorithms learn approximations to functions that relate experimental data to some property of interest. As an example, we show ML algorithms can successfully learn separating surfaces for distinguishing coherent and stochastic noise affecting a single qubit. The performance of various ML algorithms depends strongly on the geometry of experimental data (in this case, data from gate set tomography experiments). We show performance can be boosted by hyperparameter tuning and feature engineering.

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10:36AM E27.00012: Quantum optical neural networks for next generation quantum information processing*  
GREGORY R STEINBRECHER, Research Laboratory of Electronics, Massachusetts Institute of Technology, JONATHAN OLSON (Presenter), Zapata Computing, DIRK R. ENGLUND, JACQUES CAROLAN, Research Laboratory of Electronics, Massachusetts Institute of Technology — Physically motivated quantum algorithms for specific near-term quantum hardware will likely be the next frontier in quantum information science. Here, we show how many of the features of neural networks for machine learning can naturally be mapped into the quantum optical domain by introducing the quantum optical neural network (QONN). Through numerical simulation and analysis we train the QONN to perform a range of quantum information processing tasks, including protocols for quantum optical state compression, reinforcement learning, and black-box quantum simulation. Our results indicate QONNs are a powerful design tool for quantum optical systems and a promising architecture for next generation quantum processors.

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Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E28 DQI: Quantum Control of Open and Tracked Quantum Systems  
Yale Univ - Tag(s): Focus

8:00AM E28.00001: Quantum dynamics and fluctuating Hamiltonians: controlling many-body decoherence  
AURELIA CHENU (Presenter), AVADH SAXENA, Los Alamos National Laboratory, ADOLFO DEL CAMPO, University of Massachusetts — Beating decoherence and dissipation is a core problem to develop quantum computation and quantum technologies. While tailoring the environment-system coupling has been proposed as a solution, techniques to engineer the required many-body decoherence in the laboratory remain to be developed. Instead, the stochastic fluctuations naturally present on any platform can be harnessed as a resource to tailor the dynamics. I will present a versatile scheme for the quantum simulation of the open dynamics of a many-body system embedded in an environment to which it couples via arbitrary many-body interactions. This approach exploits current technology for digital and analog quantum simulation of unitary dynamics harnessing noise as a resource, and can be readily implemented in various quantum experimental platforms such as trapped ions, superconducting circuits and cold atoms, thus finding widespread applications in quantum simulation and computation, quantum chemistry and biology.
Gradient-based optimal control of open systems using quantum trajectories and automatic differentiation* MOHAMED ABDELHAFEZ (Presenter), DAVID SCHUSTER, University of Chicago, JENS KOCH, Northwestern University — We present a gradient-based optimal-control technique for open quantum systems that utilizes quantum trajectories. Using trajectories allows for optimizing open systems with less computational cost than the regular density matrix approaches. In addition, we propose an improved sampling algorithm to minimize the required number of trajectories needed per optimization iteration. Together with employing stochastic gradient descent techniques, this reduces the complexity of optimizing realistic open quantum systems. Our optimizer harnesses automatic differentiation to provide flexibility in optimization and to suit the different constraints and diverse parameter regimes of real-life experiments. The optimizer is utilized in a variety of applications to demonstrate how the use of quantum trajectories significantly reduces the computation complexity while achieving a multitude of simultaneous optimization targets. Demonstrated targets include high state transfer fidelities despite dissipation, and maximizing the readout fidelities of a qubit while maintaining the quantum non-demolition nature of the measurement and allowing for subsequent fast resonator reset.

*This research was supported by the Army Research Office through Grant No. W911NF-15-1-0421

Dissipative self-interference and robustness of continuous error-correction to miscalibration VICTOR ALBERT (Presenter), Caltech, KYUNGJOO NOH, Yale, FLORENTIN REITER, Harvard — We derive an effective equation of motion within the steady-state subspace of a large family of Markovian open systems (i.e., Lindbladians) subject to perturbations of their Hamiltonians and system-bath couplings [1]. We derive a set of conditions under which competing dissipative processes destructively interfere, producing no dissipation within the steady-state subspace. Due to the mildness of the conditions, such destructive interference turns out to be much more generic than expected. For quantum error-correction, these effects imply that continuously error-correcting Lindbladians are robust to calibration errors, including miscalibrations consisting of operators undetectable by the code. A similar interference is present in more general systems if one implements a particular Hamiltonian drive, resulting in a coherent cancellation of dissipation. On the opposite extreme, instead of suppressing dissipation, we provide a simple implementation of universal Lindbladian simulation.


A Quantum Law of Requisite Variety* DAVIDE GIROLAMI (Presenter), Los Alamos National Laboratory — The Law of Requisite Variety was the first attempt to quantify the ability of a controller to shield information-processing systems against error sources. It was then rediscovered in classical control theory, complexity science and computational mechanics. I here extend it to the quantum domain, establishing information-theoretic limits to the controllability of open quantum systems in terms of the resources available to the controller, quantum coherence and correlations. I also introduce a measure of controllability to capture the influence exerted on a system by a controlling device. I verify the result by implementing a control protocol in the IBM 5-qubit chip "ibmqx4".

LA-UR-18-29964

*Los Alamos National Laboratory, project 20180702PRD1

Conditions allowing error correction in driven qubits* ROBERT THROCKMORTON (Presenter), University of Maryland, College Park — We consider a qubit that is driven along its logical z axis, with noise along the z axis in the driving field Ω proportional to some function f(Ω), as well as noise along the logical x axis. We establish that whether or not errors due to both types of noise can be canceled out, even approximately, depends on the explicit functional form of f(Ω) by considering a power law form, f(Ω) ∝ Ω^k. In particular, we show that such cancellation is impossible for k = 0, 1, or any even integer. However, any other odd integer value of k besides 1 does permit cancellation; in fact, we show that both types of errors can be corrected with a sequence of four square pulses of equal duration. We provide sets of parameters that correct for errors for various rotations and evaluate the error, measured by the infidelity, for the corrected rotations versus the naive rotations. We also consider a train of four trapezoidal pulses, which take into account the fact that there will be, in real experimental systems, a finite rise time, again providing parameters for error-corrected rotations that employ such pulse sequences. Our dynamical decoupling error correction scheme works for any qubit platform as long as the errors are quasistatic.

*This work is supported by the Laboratory for Physical Sciences.
9:00AM E28.00006: Parametrically-mediated Dissipative Entanglement Generation  EMERY DOUCET (Presenter), Physics and Applied Physics, University of Massachusetts Lowell, FLORENTIN REITER, Physics, Harvard University, LEONARDO M RANZANI, Raytheon BBN Technologies, RAYMOND SIMMONDS, JOSE AUMENTADO, NIST - Boulder, ARCHANA KAMAL, Physics and Applied Physics, University of Massachusetts Lowell — Dissipative state preparation provides a powerful alternative to traditional gate-based state preparation protocols. Rather than generating the desired state through a sequence of unitary operations, dissipative protocols engineer always-on interactions with the environment such that the system autonomously converges to the desired state. Such an approach allows improved robustness to initialization errors and decoherence. Nonetheless, dissipative state preparation methods realized thus far have the limitation that the preparation time and error are anti-correlated, meaning that accurate preparation requires long stabilization times. In this talk, I will present a novel scheme which makes use of parametric qubit-qubit and qubit-resonator interactions to avoid this issue. This scheme allows high-fidelity preparation of arbitrary maximally-entangled two-qubit states with stabilization times in the few hundred nanosecond range. Uniquely, it also enables continuous in-situ control of the target state in a specified parity manifold. I will discuss the robustness of the scheme to experimental imperfections and qubit decoherence, and an implementation which is readily achievable with current circuit-QED technology.

9:12AM E28.00007: To catch and reverse a quantum jump mid-flight* [Invited]  ZLATKO MINEV (Presenter), SHANTANU O. MUNDHADA, SHYAM SHANKAR, PHILIP REINHOLD, Applied Physics, Yale University, RICARDO GUTIERREZ, The Dodd-Walls Centre for Photonic and Quantum Technologies, Department of Physics, University of Auckland, ROBERT SCHOELKOPF, Applied Physics, Yale University, MAZYAR MIRRAHIMI, QUANTIC, INRIA Paris, HOWARD J CARMICHAEL, The Dodd-Walls Centre for Photonic and Quantum Technologies, Department of Physics, University of Auckland, MICHEL H. DEVORET, Applied Physics, Yale University — Quantum physics differs fundamentally from classical physics in that the measurement of a quantity cannot always give certain results, even in the ideal case where both the preparation and the measurement of the system is perfect. This idea is epitomized in the phenomenon of quantum jumps, first hypothesized by Bohr in his description of the radiation emitted by an excited hydrogen atom, and now routinely observed in the laboratory on a single quantum entity. Quantum jumps are fundamentally random: the time at which they occur cannot be predicted. However, modern measurement theory stipulates that it is possible to obtain an advance warning signalling the imminent occurrence of jump, before its full completion. Consequently, it is possible to reverse the jump if it is initiated by a coherent drive. We have successfully caught and reversed jumps by implementing the indirect QND measurement of a superconducting artificial atom that undergoes a transition from its ground state G to a dark state D. This is achieved by monitoring the occupancy of an auxiliary bright level B coupled to G through a Rabi drive. Our experimental results, in agreement with the predictions of quantum trajectory theory with essentially no adjustable parameters, provide new ground for the exploration of real-time intervention techniques in the control of quantum systems, such as early detection of error syndromes for computation and sensing. More generally, our results provide support to the point of view that a single system under continuous, efficient observation is characterized by a time-dependent wave-function inferred from the record of previous measurement outcomes, and whose meaning is that of an objective, generalized degree of freedom.

*Work supported by ARO, AFOSR, ONR and YINQE

9:48AM E28.00008: Adaptive Rotating-Wave Approximation for Driven Open Quantum Systems* BRIAN BAKER (Presenter), Department of Physics and Astronomy, Northwestern University, ANDY C. Y. LI, Fermi National Accelerator Laboratory, NICHOLAS IRONS, Department of Physics and Astronomy, Northwestern University, NATHAN D EARNEST, The James Franck Institute and Department of Physics, University of Chicago, JENS KOCH, Department of Physics and Astronomy, Northwestern University — In this talk, I will present a numerical method to approximate the long-time asymptotic solution \( \rho_{\infty}(t) \) to the Lindblad master equation for an open quantum system under the influence of an external drive. The proposed scheme uses perturbation theory to rank individual drive terms according to their dynamical relevance, and adaptively determines an effective Hamiltonian. In the constructed rotating frame, \( \rho_{\infty} \) is approximated by a time-independent, nonequilibrium steady-state. This steady-state can be computed with much better numerical efficiency than asymptotic long-time evolution of the system in the lab frame. I will illustrate the use of this method by simulating recent transmission measurements of the heavy-fluxonium device, for which ordinary time-dependent simulations are severely challenging due to the presence of metastable states with lifetimes of the order of milliseconds.

*This research was supported by the Army Research Office through Grant No. W911NF-15-1-0421 and by the NSF Graduate Research Fellowship Program through grant No. DGE-1144082.
10:00AM E28.00009: Exploring topological features of a dissipative qubit near an exceptional point* MARYAM ABBASI (Presenter), MAHDI NAGHILLOO, Physics, Washington University in St. Louis, YOGESH N JOGLEKAR, Physics, Indiana University-Purdue University Indianapolis (IUPUI), KATER MURCH, Physics, Washington University in St. Louis — We study the behavior of a single dissipative qubit which is described by a non-Hermitian Hamiltonian that has effective space-time reflection (PT) symmetry. We use quantum state tomography to observe the PT-symmetry breaking transition as we cross the exceptional point by varying the coupling strength between the two quantum states. By changing the detuning of the coupling, we probe the topological features associated with encircling the exceptional point. In addition, we introduce a time-modulated coupling strength where the resulting Floquet Hamiltonian provides a richer phase diagram where the PT broken phase can occur for dissipations levels that are much smaller than the PT symmetry threshold in the static case. Here we observe multiple transitions breaking and restoring the PT-symmetric phase.

*This work was supported by the John Templeton Foundation grant ID 58558 and the NSF Grant No. PHY-1607156

10:12AM E28.00010: Experimental repetitive quantum channel simulation WEIZHOU CAI (Presenter), HU LING, XIANGHAO MU, YUWEI MA, YUAN XU, HAIYAN WANG, YIPU SONG, Tsinghua University, CHANG-LING ZOU, University of Science and Technology of China, LUYAN SUN, Tsinghua University — Universal control of quantum systems is a major goal to be achieved for quantum information processing, which demands thorough understanding of fundamental quantum mechanics and promises applications of quantum technologies. So far, most studies concentrate on ideally isolated quantum systems governed by unitary evolutions, while practical quantum systems are open and described by quantum channels due to their inevitable coupling to environment. Here, we experimentally simulate arbitrary quantum channels for an open quantum system, i.e. a single photonic qubit in a superconducting quantum circuit. The arbitrary channel simulation is achieved with minimum resource of only one ancilla qubit and measurement-based adaptive control. By repetitively implementing the quantum channel simulation, we realize an arbitrary Liouvillian for a continuous evolution of an open quantum system for the first time. Our experiment provides not only a testbed for understanding quantum noise and decoherence, but also a powerful tool for full control of practical open quantum systems.

10:24AM E28.00011: Measurement-induced phase transition in the dynamics of entanglement BRIAN SKINNER (Presenter), Massachusetts Institute of Technology, JONATHAN RUHMAN, Bar-Ilan University, ADAM NAHUM, Oxford University — We study the dynamics of quantum entanglement in a many-body system that undergoes unitary evolution punctuated by projective measurements. We show that when these measurements occur randomly with a finite rate per degree of freedom, there is a critical measurement rate that separates "entangling" and "disentangling" phases. The entangling phase is characterized by a linear growth of the entanglement entropy with time that leads to volume-law entanglement, while in the disentangling phase the entanglement entropy takes a constant, area-law value. We demonstrate this dynamical transition using numerics and a mapping to classical percolation that becomes exact in certain limits.

10:36AM E28.00012: Controlling the dynamics across a quantum phase transition* ADOLFO DEL CAMPO (Presenter), LUIS PEDRO GARCIA-PINTOS, DIEGO TIELAS, FERNANDO GÓMEZ-RUIZ, University of Massachusetts Boston — When a quantum phase transition is crossed in finite time, critical slowing down leads to the breakdown of adiabatic dynamics and the formation of topological defects. The average density of defects scales with the quench rate following a universal power-law predicted by the Kibble-Zurek mechanism (KZM). The scaling theory of phase transitions can however be used to determine the full counting statistics of topological defects, beyond the KZM. Knowledge of the distribution of topological defects provides new insights into the breakdown of adiabaticity. In addition, the quantum critical dynamics can be controlled. One approach relies on quantum monitoring via continuous quantum measurements. A second approach is based on local driving of the phase transition. We shall present theoretical and experimental progress based on these approaches.


*Funding support from the John Templeton Foundation is acknowledged.
Quantum Tracking Control of Molecular Rotor Orientation is Singularity-free

ALICIA MAGANN (Presenter), TAK-SAN HO, HERSCHEL A RABITZ, Princeton University — Quantum tracking control aims to identify applied fields to steer particular observable expectation values along desired paths in time. The fields can be identified by inverting the underlying dynamical equations for the observables. However, fields found in this manner are often plagued by undesirable singularities. In this talk I will consider a planar molecular rotor and derive singularity-free expressions for the fields that steer the expectation value of the rotor's orientation along desired trajectories in time. Simulations will be presented that utilize two orthogonal control fields to drive the orientation of the rotor along a series of designated tracks.

*This work was supported by funding from the DOE CSGF, Grant No. DE-FG02-97ER25308.

Tuesday, March 5, 2019 8:00 AM - 10:36 AM

Session E29 DFD GSNP: Turbulence and Instabilities

BCEC 162A - Li Xi, McMaster University

Stability of an accelerated hydrodynamic discontinuity

DANIIL ILYIN, WILLIAM GODDARD, California Institute of Technology, SERGEI I. ANISIMOV (Presenter), Landau Institute for Theoretical Physics, Russia, SNEZHANA ABARZHI, Univ of Western Australia — While looking from a far field, we analyze the evolution of an accelerated discontinuity separating ideal incompressible fluids of different densities. We develop and apply a general matrix method and identify a new hydrodynamic instability that occurs when the acceleration magnitude exceeds a critical threshold value. The flow dynamics conserves mass, momentum and energy in the fluid bulk and at the interface, has potential velocity fields in the fluid bulk, and is shear-free at the interface. The interface stability is set by the interplay of inertia and buoyancy. Surface tension also stabilizes the dynamics by a distinct mechanism. The growth rate and the flow fields' structure of the unstable dynamics depart substantially from those of other interfacial hydrodynamic instabilities, thus suggesting new opportunities for stabilization, diagnostics, and control of the interfacial dynamics.

*The work is supported by the University of Western Australia (AUS), the California Institute of Technology (USA), and the National Science Foundation (USA).

Detonation Initiation in Type Ia Supernovae

GABRIEL CASABONA (Presenter), University of Massachusetts Dartmouth, PRITOM MOZUMDAR, Physics, UC Davis, UMass Dartmouth, ROBERT FISHER, University of Massachusetts Dartmouth — Type Ia supernovae play a crucial role as standardizable candles for cosmology, but their stellar progenitors remain mysterious. Underlying this mystery is a crucial physical process: the mechanism of detonation initiation in Type Ia supernovae. Early suggestions for detonation initiation, based upon a detonation initiation mechanism originally proposed by Zel'dovich, cannot apply in the highly-turbulent conditions prevalent in major Type Ia supernova channels, in which the burning is disrupted into the distributed burning regime. We demonstrate, for the first time, using both analytic estimates and three-dimensional numerical simulations, how a carbon detonation may arise in a realistic three-dimensional turbulent electron-degenerate flow. We term this new mechanism turbulently-driven detonation. The turbulently-driven detonation initiation mechanism leads to a wider range of conditions for the onset of carbon detonation than previously thought possible, with important ramifications for SNe Ia models.

*We acknowledge support from NASA ATP Award 80NSSC18K1013.

A Numerical Study of the Richtmyer–Meshkov Instability in a Relativistic Fluid using Multi-Directional Riemann Solvers and High-Order WENO Schemes

JAMIE TOWNSEND (Presenter), LÁSZLÓ KÓNÖZSY, KARL JENKINS, Cranfield University — The present work focuses on relativistic hydrodynamic (RHD) simulations of the Richtmyer–Meshkov (RM) instability in 2D and assesses the performance of different numerical schemes. The RM instability is known to occur in various high-energy phenomena such as supernovae detonations and relativistic jets. The RHD equations are solved using the finite volume method (FVM) via a third-order TVD Runge–Kutta scheme for time integration and WENO reconstructions for spatial discretization. The effect of the imposed Riemann solver is studied via the comparative use of a Rusanov, HLL, and HLLC Riemann solver. A novel multi-directional approach has been used in which all fluxes have been computed by taking into account information propagation from all spatial directions. In particular, we investigate the linear growth-rate of the instability under a parameter space consisting of positive and negative Atwood numbers and varying shock-speed for a perfect gas. The growth-rate in the linear regime has been reported to peak in the mildly relativistic limit. We aim to shed light on the numerical influence and predictive capability of computational modelling relativistic fluids.

*Fully-funded studentship provided by the Centre for Computational Engineering Sciences, Cranfield University.
8:36AM E29.00004: Evaluation of the turbulence velocity skewness factor in a detonation-turbulence interaction
SARAH HUSSEIN (Presenter), FRANK K LU, Mechanical and Aerospace Engineering, University of Texas at Arlington — In physical and computational studies of turbulence, the velocity skewness factor is a property of interest quantifying the development of the turbulence. Tavoularis (1978) defined the velocity skewness for fully-developed turbulence as a negative ratio of the average partial derivative of streamwise velocity with respect to the axial position, \( S(u,x) \). This definition is used in the direct numerical simulation of homogeneous isotropic turbulence. The skewness factor, in this study, is evaluated for a turbulent fluid flow as it interacts with a detonation wave. The analysis extends the long-standing definition to include the variation of the transverse velocities in all three Cartesian spatial coordinates. The skewness components are evaluated and compared to assess significance in a detonation-turbulence interaction.

*I acknowledge that this material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program (2014). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

8:48AM E29.00005: Correlating ocean vertical transport and surface coherent structures
ARAVIND HARILAL MEENAMBIKA (Presenter), MICHAEL ALLSHOUSE, Mechanical Engineering, Northeastern University — Vertical transport in the upper ocean impacts the transport of nutrients, surface mixing, and the ocean energy budget. Observing regions of significant vertical transport has proven to be difficult since vertical velocities in the ocean are often orders of magnitude smaller than horizontal velocities. What is available, however, is HF radar and satellite altimetry, which provide ocean surface velocities. While an Eulerian analysis of this field can yield some information, Lagrangian coherent structures prove to be more robust to noisy observational data. We correlate these structures on the surface to vertical transport below the surface. In particular, we compute the finite-time Lyapunov exponent (FTLE) field from just the surface velocity and compare this with the FTLE field for a full three-dimensional analysis and the corresponding vertical subduction. These correlations are tested on a high-fidelity simulation of a sheared submesoscale flow.

9:00AM E29.00006: Vegetation-generated turbulence in combined wave-current canopy flows
JIARUI LEI (Presenter), HEIDI NEPF, Massachusetts Institute of Technology — Laboratory experiments are conducted in combined waves and current to measure turbulence structure and intensity in arrays of wooden cylinders, a model for submerged rigid aquatic vegetation. For dense canopies, drag leads to velocity reduction within canopy. The velocity gradient at the top of canopy generates a shear layer which results in coherent vortices traveling downstream. The canopy-scale vortices control the transport of mass and momentum and penetrate into the canopy with a length of \( \delta_e \). In pure current, near-bed TKE (turbulent kinetic energy) is elevated as turbulence is transported from the shear region to the bed. TKE increases as the vortices develop downstream. In combined wave-current conditions, the turbulence within canopy is mainly set by the waves as the mean current is small compared to wave velocity. The near-bed turbulence is not significantly elevated by the shear-generated vortices and can be predicted using existing empirical model of stem-generated turbulence. As the ratio of wave velocity to current speed increases, the shear layer diminishes and \( \delta_e \), as well as the magnitude of Reynolds stress, decreases. In pure waves, no shear layer is observed and stem-generated turbulence dominates the turbulence structure and intensity within canopy.

9:12AM E29.00007: Electron Contribution in Mirror mode Instability in Quasi-linear Regime
NAILA NOOREEN (Presenter), Forman Christian College — The solar wind is characterized by proton temperature anisotropies. The plasma compression generates the perpendicular anisotropy, which may lead to the mode instability for high beta situation. In the present paper the mirror mode instability is discussed in the framework of simplified and reduced quasi-linear kinetic theory, which includes the contribution of electrons. It is found that the linear growth rate associated with the electron mirror mode can be much higher than that the proton mirror mode, and the electron mirror instability operates over a range of carrying out the quasi-linear analysis, it is shown that for the proton mirror instability. However, upon carrying out the quasi-linear analysis, it is shown that for the high initial growth rate does not necessarily imply dynamical importance, since the saturated magnetic field intensity associated with electron mirror instability is extremely low and that the influence on the particle temperature is minimal. The present finding shows that under some circumstances, the dynamical consequences of a system cannot simply be estimated on the basis of the linear prediction alone and that nonlinear analysis must be taken into account.
KEQING XIA (Presenter), Department of Mechanics and Aerospace Engineering, Southern University of Science and Technology, KAI LEONG CHONG, GUANG-YU DING, The Chinese University of Hong Kong — We study numerically the dynamical and structural properties of columnar vortices in rotating Rayleigh-Bénard convection. Our results show that the vortices form clustered structures with a characteristic length scale when their density becomes sufficiently large. Dynamically, their motion is ballistic in short time scale and crosses over to diffusive in longer time scale. We further found that the ratio of the Brownian time scale for vortex diffusion and the relaxation time scale given by the normal stress among vortices may be the key parameter that determines the structural formation of vortices.

*We acknowledge the support of this work from the Hong Kong Research Grants Council (RGC) under grant CUHK 14301115 and CUHK14302317.

SAMAR ALQATARI (Presenter), Mechanical Engineering, Massachusetts Institute of Technology, THOMAS ERIK VIDEBÆK, Physics, University of Chicago, IRMGARD BISCHOFBERGER, ANETTE E. HOSOI, Mechanical Engineering, Massachusetts Institute of Technology, SIDNEY ROBERT NAGEL, Physics, University of Chicago — A hydrodynamic instability can develop at the interface between a denser fluid placed atop a less dense one. We investigate this Rayleigh-Taylor instability between two miscible liquids in a confined Hele-Shaw geometry. Surprisingly, we find that the typically unstable interface between the dense and less-dense liquids is stabilized below a critical confinement, set by the gap spacing of the Hele-Shaw cell. This critical confinement shows power law scaling with the difference in densities between the liquids. We also discuss the dependence of the characteristic wavelength of the instability on fluid parameters and the gap spacing. Our measured wavelength in this confined geometry deviates strongly from theoretical predictions for unconfined systems, suggesting an important effect of geometry on the onset of the instability.

RYAN MCKEOWN (Presenter), Harvard University, RODOLFO OSTILLA MONICO, University of Houston, ALAIN JACK PUMIR, ENS Lyon, MICHAEL PHILLIP BRENNER, SHMUEL RUBINSTEIN, Harvard University — The turbulent cascade, or the means by which the energy of a flow is conveyed from large to small scales, is governed by the interactions between vortices over many scales. In order to better understand the mechanisms that govern the close-range interactions between vortices, we experimentally examine the head-on collision of two vortex rings. By seeding the vortex rings with fluorescent dye and imaging their collision with a high-speed scanning laser sheet, we visualize the breakdown dynamics of the flow in full 3D. For weak collisions at low Reynolds numbers, the colliding rings stretch radially, develop long-wavelength perturbations, and reconnect into a tiara of secondary vortex rings. Conversely, for violent collisions at high Reynolds numbers, the rings rapidly develop short-wavelength perturbations as they stretch radially before erupting into a turbulent cloud of fine-scale vortex filaments. Initiated by these instabilities, the colliding vortices break down through various distinct processes and lead to the generation of small-scale flow structures. Thus, the close-range interactions of the colliding vortices could provide new insights into the mechanistic underpinnings of the turbulent cascade.

LU ZHU (Presenter), LI XI, Department of Chemical Engineering, McMaster University — Study of turbulent vortices in DNS relies heavily on visual inspection, anecdotal observations, and intuitive arguments. Quantitative analysis is limited by the lack of computational tools for the objective detection and extraction of vortex structures. Despite much progress in the development of vortex identification criteria (which shows the vortices without distinguishing their individualities), vortex tracking requires a separate step and existing techniques only targeted quasi-linear vortices. In this study, a new tracking algorithm is proposed which propagates along the vortex axis-lines and iteratively search for new directions for growth. It is the first tracking method designed for general three-dimensional vortices. The method is tested in transient flow fields with specific vortex types as well as DNS. A new procedure is also proposed that classifies vortices into commonly-observed shapes, including quasi-streamwise vortices, hairpins, hooks, and branches, based on their axis-line topology. This new method is then applied to both viscous and viscoelastic turbulent channel flows for analyzing the distribution of vortex size, shape, and location. Introducing polymer additives suppresses vortex lift-up process and fundamentally change the vortex regeneration dynamics.
10:12AM E29.00012: Realization of Confined Turbulence Through Multiple Vortex Ring Collisions* TAKUMI MATSUZAWA (Presenter), NOAH P MITCHELL, STEPHANE PERRARD, WILLIAM T. M. IRVINE, University of Chicago — We report a method to generate a steady, localized blob of turbulence by colliding multiple vortex rings successively. Our system supplies vorticity to a turbulent region through vortex rings, which enables us to create controlled turbulent flows far from boundaries. The state of turbulence can be controlled by altering properties of the injected rings. We present spatial structures and turbulence characteristics of the blobs by varying strength, size and shape of the vortex rings. This novel method provides an ideal system to study both generation and decay of turbulence absent from any boundary effects.

*The authors gratefully acknowledge financial support from the U.S. Army Research Office through Grant No. W911NF-18-1-0046.

10:24AM E29.00013: Numerical Analysis of Iron-Zeolite Based Emission Control Device for Two-Wheelers NAFEES AHMAD (Presenter), MEHUL VARSHNEY, ANCHAL VARSHNEY, SS ALAM, Aligarh Muslim University — The present work involves numerical simulation of a novel emission control device (Indian Patent Publication Number: 41/2018) for about 30 million two-wheeled vehicles running on Euro3/BS III norms without a catalytic converter across the Asia Pacific. The governing equations for turbulent fluid flow and species transport with eddy dissipation and PDF models have been solved on commercial package FLUENT® to predict the behavior of oxides of nitrogen (at different engine loads) in presence of Iron-Zeolite. Substrates of Iron Zeolites with high viscous resistance provide ample residence time for adsorption of exhaust gas molecules and reduction of inorganic oxides. The findings show that the concentration of harmful oxides of Nitrogen in exhaust gases gets reduced by approximately 50% by conversion to harmless nitrogen gas. Furthermore, the geometry is optimized in a way to ensure invariance in standard speed-torque characteristics of the engine by generating negligible back pressure. The device provides an optimal business and environmental solution by controlling emissions through extremely cheap and innovative Iron-Zeolite at places where ultra-expensive Platinum/Palladium/Rhodium based catalysts are not feasible.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E30 DPOLY: Polymer Networks, Gels, and Elastomers I: Dynamics BCEC 162B - John Kieffer, University of Michigan Ryan Toomey, University of South Florida - Tag(s): Focus

8:00AM E30.00001: Polymer Physics Prize Talk Break —

8:06AM E30.00002: Soft ionic diodes formed at the interface of ionic liquid networks* [Invited] RYAN HAYWARD (Presenter), University of Massachusetts Amherst — Soft elastic materials capable of conducting ionic charge carriers offer numerous opportunities for the design of new classes of highly deformable electronic devices. Our group has recently studied the formation of ionic ‘diodes’ at the interface between two single-ion conducting elastomers with oppositely signed charge carriers formed by polymerization and crosslinking of ionic liquid monomers. We characterize the properties of these interfaces using a variety of techniques, in particular AC impedance spectroscopy, and show that they act as stretchable rectifying junctions based on capacitive, rather than electrochemical, effects. Further, such soft ionic diodes possess a number of potentially useful characteristics, including strain sensitive electrical signals and reversibly switchable electro-adhesion. Finally, we have explored templating methods to generate high surface area ionic diodes, which are expected to yield further improvements in properties.

*This work was supported by the National Science Foundation through grant DMR-1609972.
Neutron Spin Echo Insight into Dynamic Networks Formed by Ionomers

DVORA PERAHIA (Presenter), Chemistry, Physics, Clemson University, SIDATH WIJESINGHE, Chemistry, UNC Chapel Hill, MANJULA SENANAYAKE, SUPUN S. MOHOTTALALAGE, CHATHURIKA KOSGALLANA, Chemistry, Clemson University, PIOTR ADAM ZOLNIERCUZUK, Jülich Centre for Neutron Science at SNS, ORNL, Oak Ridge, TN

Association of ionic groups strongly affects the rheology of ionomers in melts and in solutions. The constraint arises from formation of ionic clusters affects the macroscopic dynamics. While the network is constrained, the chains remain dynamic on the length scale of the network mesh. Using NSE we probe chain dynamics in networks formed by polystyrene sulfonate (PSS) as the physical crosslinks are perturbed by addition of ethanol. Solutions of 20Wt% PSS, 11,000 g/mol (PD=1.02) with 3 and 9% mole sulfonation were studied. S(q,t) measured across a broad temperature range, was analyzed in terms KWW and characteristic times extracted. At length scales that correspond to the ionic domains, the motion is constrained in both solvents; however, ethanol enhances the dynamics. While the ionic domains expand, the dynamics remain restricted, pointing to formation of "ionic clouds" where the ionic clusters are swollen with alcohol, but remain segregated, retaining the physical crosslinks of the network. At smaller dimensions, the dynamics becomes significantly faster and no differences are observed as ethanol was added. Increasing the temperature results in equal acceleration of the motion across all q values, indicative of retaining the dynamic, swollen, physical crosslinks.

Solvent Polarity Effects on Segmental Dynamics in Ionic Polymer Networks: Quasi Elastic Neutron Scattering Study

SUPUN SAMINDRA MOHOTTALALAGE (Presenter), SIDATH WIJESINGHE, MANJULA SENANAYAKE, CHATHURIKA KOSGALLANA, Department of Chemistry, Clemson University, Clemson, SC, United States., NARESH OSTI, Oak Ridge National Laboratory, Oak Ridge, TN, United States., DVORA PERAHIA, Department of Chemistry/Department of Physics, Clemson University, Clemson, SC, United States.

Incorporating ionic groups into polymers drives formation of physical networks that affect the dynamics of the macromolecules. Here, using quasi elastic neutron scattering (QENS), segmental dynamics of slightly sulfonated (3mol%) polystyrene (PSS) networks formed in cyclohexane, a non-polar environment and a theta solvent for PS was studied, followed by tracking the polymer motion as the association of the sulfonated groups is disrupted by ethanol. Specifically, a 10%(w/w) PSS in cyclohexane/ethanol solutions was studies in the q range of 0.3 Å⁻¹ to 1.3 Å⁻¹ corresponding to 5 Å⁻²1 Å. The relaxation times and segmental motion were extracted from a Kohlrausch-Williams-Watts (KWW) analysis. As expected for PSS in cyclohexane, the dynamics is constrained at larger dimensions but the polymer remains mobile on smaller length scales. Addition of less than 5%(v/v) of ethanol is enough to release the constrains. Surprisingly however, further increase in ethanol results in decrease in segmental motion. This reduction could be attributed to overall plasticization of the polymer in presence of ethanol.

Dynamics of Ionomer Networks Studies by Pulse Field Gradient (PFG) NMR

SHALIKA D. K. MEEDIN (Presenter), MANJULA SENANAYAKE, SUPUN S. MOHOTTALALAGE, CHATHURIKA KOSGALLANA, Department of Chemistry, Clemson, SC, 29634, United States, Clemson University, DVORA PERAHIA, Department of Chemistry, Clemson, SC, 29634, United States, Clemson University, Department of Physics, Clemson, SC, 29631, United States, Clemson University — Ionomer networks are formed in solutions at extremely low concentrations. Tuning these networks offers a means to control the structures that remain trapped as the solvents evaporate to form membranes. Here, we probe the diffusion of the polymers and the solvents in networks formed by polystyrene sulfonate (PSS) by pulse field gradient NMR. The diffusion of the polymer reflects the properties of the network and that of the solvent. Specifically, PSS networks with sulfonation levels of 0, 3 and 9 mole % were studied in toluene and cyclohexane neat and mixed with ethanol. Toluene is a good solvent for polystyrene and cyclohexane is a theta solvent at room temperature. We find that with increasing sulfonation levels, both the polymer and the solvent motions decrease in both solvents. Regardless of sulfonation level, the diffusion of PSS is almost same in cyclohexane and toluene at room temperature. With increasing temperature, the diffusion of all components increases in both solvents however it is more pronounced in cyclohexane. The solvents diffuse faster than the polymers but follow similar trends. While perturbing the ionic clusters affect the overall network dynamics, the polar solvent also affects the hydrophobic network rigidity.

DOE funding DE-SC0019284
9:48AM E30.00006: Solvent Effects on the Structure of Sulfonated Polystyrene Networks* CHATHURIKA KOSGALLANA (Presenter), SIDATH WIJESINGHE, MANJULA SENANAYAKE, SUPUN S. MOHOTTALALAGE, Department of Chemistry, Clemson University, Clemson, SC, United States, LILIN HE, Oak Ridge National Laboratory, Oak Ridge, TN, United States, DVORA PERAHIA, Department of Chemistry/Department of Physics, Clemson University, Clemson, SC, United States — Driven by ionic association, ionomers form dynamic sparse networks in solutions at extremely low ionic content. Here we probe the factors that affect the structure of these types of networks formed by lightly sulfonated polystyrene (PSS) using small angle neutron scattering (SANS). Measurements were carried out in 0.25-10Wt% PSS in toluene/ethanol solutions, across a broad temperature range. In toluene, a good solvent for the PS, the SANS patterns consist of a broad signature at intermediate q, attributed here to an average network mesh size, determined by the distance between ionic physical crosslinks. At low q, a network characteristic upturn is observed. With increasing concentrations, the characteristic dimension, calculated from Rg of a Gaussian chain, decreases by ~1nm due to increasing cluster size and numbers. The long-range correlations of ~20nm, were captured by the Beacuge model. The PS chains assume an overall Gaussian configuration around the ionic clusters. Surprisingly, while the long-range correlations diminish with addition of ethanol, the mesh size decreases. While the ionic clusters become less defined, the PS chains are concurrently affected, assuming a more constrained chain configuration.

*DOE DE-SC0019284

10:00AM E30.00007: Dissipative Particle Dynamics Computational Modeling of Structurally Tailored and Engineered Macromolecular (STEM) Gels TAO ZHANG (Presenter), SANTIDAN BISWAS, ANNA CHRISTINA BALAZS, University of Pittsburgh — Structurally tailored and engineered macromolecular (STEM) gels are polymer networks containing latent initiator sites available for post synthesis modifications, with the networks acting as a backbone grafted with secondary polymer side chains. Here we use dissipative particle dynamics (DPD) simulations to study the mechanical response of the modified STEM gels under compression. We observe lower compressional modulus of the networks after adding secondary side chains and the mechanical properties are tunable by varying the grafting density and side chain length. To gain insight into the microscopic origin of observed mechanical behaviors, we measure the chain entanglements density, conformational entropy change, and conduct 3D structural domain analysis during the compression process. Furthermore, we show that attaching the initiator sites to the primary networks through labile links allows the links to break/rearrange, and thus relieves local stress concentrations.

10:12AM E30.00008: Internal Fracture in Tough Double Network Hydrogels Revealed by Various Modes of Stretching THANH-TAM MAI (Presenter), Kyoto Institute of Technology, TAKAHIRO MATSUDA, TASUKU NAKAJIMA, JIAN PING GONG, Hokkaido University, KENJI URAYAMA, Kyoto Institute of Technology — The cyclic stretching measurements in various geometries including uniaxial, planar, unequal and equal biaxial extension, reveal the distinctive features of the internal fracture in the double network (DN) hydrogels. The modulus reduction, dissipated energy (D), dissipation factor (Δ, the ratio of dissipated energy to input strain energy) in each loading-unloading cycle are evaluated as a function of the imposed maximum elongation (λi,m) in i-direction (i=x,y) in each cycle. The modulus reduction and Δ depend on the stretching mode when compared at the same λx,m, but each of them exhibits a universal relation independently of the stretching mode when the magnitude of left Cauchy-Green deformation tensor is used as a variable. In contrast, Δ in filled elastomers shows the corresponding universal relation when the first strain invariant is used as a variable (Mai et al., Soft Matter 13, 1966–1977, 2017). The difference in governing variable indicates that the influence of the cross-effect of strains (λλj; ij =x,y,z and i ≠ j) on the dissipation factor is pronounced in the DN gels whereas it is minimal in the filled elastomers. (Mai et al., Macromolecules 51, 5245–5257, 2018)
10:24AM E30.00009: Design and Control of Finite Conformational Changes in Mechanical Networks* JASON KIM (Presenter), DANIELLE BASSETT, University of Pennsylvania — Conformational changes in physical networks play a crucial role in many systems, enabling error correction in DNA replication, cooperativity in hemoglobin, and mechanical capacities in metamaterials. Important work has begun to delineate the relationship between network structure and instantaneous conformational change. However, these efforts have failed to address finite conformations, which are critical for the successful function of most physical networks. Here we establish a simple framework for the design and control of mechanical spring networks in 2 and 3 dimensions. Specifically, for a set of nodes with arbitrarily specified initial and final positions, we characterize all bipartite networks with zero energy at these positions, demonstrate transitions between these positions, and design multi-stable networks for information storage. Finally, we use hysteresis and bi-stability to design networks demonstrating cooperativity.

*JZK acknowledges support from NIH T32-EB020087, PD: Felix W. Wehrli, and the NSF GRFP No. DGE-1321851. DSB acknowledges support from the John D. and Catherine T. MacArthur Foundation, the ISI Foundation, the Alfred P. Sloan Foundation, an NSF CAREER award PHY-1554488, and from the NSF through the University of Pennsylvania MRSEC DMR-1720530.

10:36AM E30.00010: Quantifying force-induced bond dissociation in metal-coordinate gels under steady shear flow* IRINA MAHMAD RASID (Presenter), BRADLEY DAVID OLSEN, NIELS HOLTEN-ANDERSEN, Massachusetts Institute of Technology — The dynamic nature of the bonds in associating polymer networks has led to its use in the design of tough and self-healing hydrogels. While the ability of the materials to regain its original stiffness after a recovery period has been documented, such data provides no information on the molecular level processes occurring as the network is damaged, and subsequently as it heals. In this work, the non-linear response of a model associative network, consisting of linear side-functionalized chains, with nickel-terpyridine complexation as the crosslinking group was investigated. With a custom-built setup, force-induced bond dissociation was quantitatively measured through fluorescence measurements, as the network was strained under steady shear. The measured fraction of dissociated bonds is compared to predictions of several models from transient network theory.

*Funding sources:
-Institute for Soldier Nanotechnologies (ISN)
-Office of Naval Research (ONR)
-Center for Materials Science and Engineering (CMSE)

10:48AM E30.00011: The Dynamics of Bulk Polymers with Metal-ligand Coordination Crosslinking* JOY ZHANG (Presenter), YUVAL VIDAVSKY, MEREDITH SILBERSTEIN, Cornell University — The dynamics of polymer networks consisting of metal-ligand coordination as crosslinks have been widely studied in solution and gel systems. However, understanding the dynamics of bulk polymers with metal-ligand coordination crosslinking remains a challenge because it is hard to decouple the polymer relaxation and association/dissociation of the dynamic bonds. To address this problem, we carefully designed both the polymer structure and the intramolecular dynamic bond in the system. A series of copolymers containing ethyl acetoacetate ligands have been synthesized by RAFT polymerization. The ethyl acetoacetate ligands can form coordination complexes with different metal ions (Ni(II), Cu(II), and Zn(II)) and act as reversible crosslinks. We investigated the dynamic responses of these polymer networks by rheometer and DMA. These lightly crosslinked networks have behavior that varies both with choice of metal and quantity of metal, thereby revealing the kinetic differences due to the metal-ligand coordination bonds in bulk polymers. We show that these non-covalent dynamic bonds in the bulk polymer networks play an important role in determining their mechanical properties.

*This work is supported by the office of Naval Research under Grant No. N00014-17-1-2989.

Tuesday, March 5, 2019 8:00 AM - 10:48 AM

Session E31 DCP GMAG: Design and Control of Molecular Magnets (QIS2) BCEC 203 - Mark Pederson, United States Department of Energy - Tag(s): Focus
8:00AM E31.00001: The power of molecular chemistry in nanoscale materials research: from quantum physics properties to water oxidation catalysis [Invited] GEORGE CHRISTOU (Presenter), Department of Chemistry, University of Florida — Molecular chemistry brings many powerful advantages to the study of nanoscale materials of various kinds, and this area of 'molecular nanoscience' is therefore a rapidly growing field. The advantages include monodisperse (single-size) products and a monolayer shell of organic ligands that imparts solubility and crystallinity, allowing structural characterization of molecular crystals to atomic resolution by X-ray crystallography. The ligands can usually also be modified as desired, allowing tuning of redox properties and atom/isotope labelling (²H, ¹⁹F, etc.) for studies in the solid state and solution, such as NMR spectroscopy. In the molecular nanomagnetism arena, these advantages have been absolutely crucial in the study of single-molecule magnets (SMMs), molecules that function as individual ultra-small nanomagnets. They have greatly assisted the synthesis and study of numerous SMMs, leading to discovery of new quantum physics phenomena important to new 21st century technologies, such as exchange-biased quantum tunneling of the magnetization vector and quantum superposition states. Giant (~4 nm) SMMs have also bridged the gap between the 'top-down' world of traditional magnetic nanoparticles and the 'bottom-up' world of molecular nanomagnets. Recently we have developed controlled ways to form supramolecular [Mn₃]ₙ oligomers of 2 or more linked Mn₃ SMMs to study the resulting quantum properties, introduced by the weak inter-SMM exchange coupling, in more detail, including in solution for the first time. Some of our larger magnetic molecules, such as [Mn₁₂O₁₂(O₂CR)₁₆(H₂O)₄] and others, can be described as a small piece of metal oxide within an organic shell, and recent work has established that they can also function as homogeneous electrocatalysts for water oxidation to O₂ gas with low overpotentials. A selection of these materials and studies will be described.

8:36AM E31.00002: Controlling Anisotropy in the Presence of Magnetic Coupling in Molecular Magnets* [Invited] JEFFREY RINEHART (Presenter), JEREMY HILGAR, MAXIMILIAN BERNBECK, AARON BUTTS, Chemistry and Biochemistry, University of California, San Diego — The control of magnetic anisotropy and magnetic coupling are crucial to the design of devices utilizing molecular materials for both spintronic and quantum information processing. Generally, theoretical models and synthetic approaches exist for optimizing these parameters independently to a very high degree. However, design principles for either orthogonal or synergistic, predictable control of anisotropy and coupling are far more complex. This presentation will focus on our efforts to address the challenge of designing molecules that can effectively preserve the orientation and magnitude of their anisotropy upon introducing coupling interactions that necessarily alters the local crystal field.

*We thank the Office of Naval Research Young Investigator Award N00014-16-1-2917 for supporting this research.

9:12AM E31.00003: Magnetic properties of actinide complexes from first principle calculations. [Invited] HÉLÈNE BOLVIN (Presenter), Université Toulouse 3, LCPQ-IRSAMC — Magnetic properties of actinides are often analyzed using models devoted to lanthanides. But due to the higher covalency of the former, those models are not adequate and a more precise description of the complexes is necessary in order to get the full understanding of those properties. The calculation of the magnetic properties of open-shell 5f molecules is a challenge for the methods of quantum chemistry: actinide complexes have many low lying configurations, spin-orbit effects are important and correlation effects must be taken into account. The first principle SO-CASPT2 method gives results that compare well to experimental data and permits to analyze the different contributions to the magnetic properties.

On monomers, calculations enable to
- determine crystal field parameters
- analyze the effect of covalency
- scrutinize the contributions above the LS coupling scheme.

On dimers, they permit to
- analyze the magnetic coupling between the two magnetic centers
- propose Spin Hamiltonians which permit to model the magnetic behavior of those complexes
9:48AM E31.00004: Theoretical Investigation of Actinides Based Single Molecule Magnets  CARLO ALBERTO GAGGIOLI (Presenter), LAURA GAGLIARDI, Department of chemistry, University of Minnesota — Single molecule magnets (SMMs) are highly appealing for reducing the length scale of magnetic materials that have potential applications in information storage and spin electronics.\(^1\) SMMs show slow relaxation of the magnetization of purely molecular origin. The actinides elements are promising for the design of SMMs and examples have emerged.\(^2\)

In this contribution, the electronic structure of plutonium based SMMs\(^3\) have been computationally examined by means of multiconfigurational calculations. A modified ligand has also been studied in order to modify the electronic properties.\(^4\)

We are currently investigating other actinide-based SMMs, namely \(\text{[Np(COT)2]}\)\(^5\) and \(\text{AmFe}_2\).\(^6\) We are also analyzing the inclusion of dynamical correlation by means of multiconfiguration pair-density functional theory (MC-PDFT),\(^7\) a new method developed in our group. These results will be discussed.


10:00AM E31.00005: Self-interaction effects in the density functional description of iron(II) spin-crossover molecules  TORSTEN HAHN (Presenter), SEBASTIAN SCHWALBE, JULIA RICHTER, Theoretical Physics, Technical University Freiberg — Spin-crossover metal complexes are one of the paradigmatic examples of magnetic molecular materials showing switching and bistability at the molecular level. Octahedral Fe\(^{2+}\) molecules are particularly interesting as they often exhibit such a spin-crossover transition. Many efforts were made to assess the performance of density functional theory for such systems. However an exchange-correlation functional able to account accurately for the energetic of the various possible spin-states has not been identified yet.

We present results on different Fe\(^{2+}\) ions using self-interaction corrected semilocal exchange-correlation functionals \([1,2,3]\) within the FLO-SIC DFT framework and we focus on the energy differences between the various spin states. Further we compare our data to high level quantum chemical calculations.


10:12AM E31.00006: Molecular Geometries of Fe (II) Spin-Crossover Complexes  BRIAN FINNEY (Presenter), BESS VLAISAVLJEVICH, University of South Dakota — Spin-crossover (SCO) complexes are a class of inorganic compounds in which external stimuli facilitate a change in geometry and spin state from a diamagnetic low spin state to a paramagnetic high spin state or vice versa. Due to this bistability, they are an important class of molecules for new energy technologies and molecular electronics\(^1\). The multiconfigurational nature and large number of electrons of these molecules make it difficult to provide accurate theoretical descriptions of the electronic structure. To date, density functional theory (DFT) has been the foundation for the study of these complexes' geometries\(^2\). Recent advances in computing has made it now possible to produce geometries with methods beyond DFT.

Octahedral Fe(II) (d\(^6\)) molecules are among the most well studied of this class of compound. Here, an accurate description of the multiconfigurational electronic structure of several Fe(II) SCO complexes using the CASPT2 method is presented. The convergence of geometry with respect to active space and basis set size as well as differences with the traditional DFT approach and the refined CASPT2 structures are noted.


10:24AM E31.00007: Coupled-Cluster Valence Bond Theory for Exact Treatment of Spin-Fluctuation  JOONHO LEE (Presenter), DAVID SMALL, MARTIN HEAD-GORDON, College of Chemistry, University of California, Berkeley — We present a valence bond approach for treating spin-fluctuation called coupled-cluster valence bond (CCVB). In particular, we will discuss the three-pair extension of CCVB, CCVB+i3, and its application to spin-frustrated systems such as molecular magnets. CCVB+i3 can describe spin-fluctuation exactly without invoking neither an exponential wall nor spin contamination. We also discuss a future direction on including charge-fluctuation into this model.
Molecular Magnetism and Quantum Information  MARK PEDERSON (Presenter), United States Department of Energy — Quantum Information Science and instrumentation for next-generation computing, information, and other fields is evolving quickly into an interdisciplinary field that intersects strongly with the missions, interests and portfolios of basic energy sciences. The fundamental research in chemical physics, quantum chemistry, inorganic chemistry, and magnetism is strongly synergistic with applications such as sensing, navigation, communications, simulation and computing. Researchers in these fields must play a role in enabling and understanding manipulation of uniquely quantum phenomena that arise from the entanglement of electrons, spins, and low-energy excitations in actual molecular systems. This talk will summarize emerging possibilities for chemical sciences based upon DOE Basic-Energy-Sciences rountable reports. It will focus on activities targeting the fundamental design, manipulation, or addressing of molecular-scale quantum-chemical qubits, the use of early quantum processors for chemical simulation, and synergistic prospects for the near-term quantum- systems and algorithms research supported by BES. To address the aims of this focused session, specific contact to the chemistry, magnetism, and optical response of molecular magnets and organic poly-radicals will be featured.

Tuesday, March 5, 2019 8:00 AM - 10:12 AM

Session E32 DCP: Time-dependent and Time-independent Approaches (B) BCEC 204A - Tucker

Towards the calculation of multidimensional vibrational spectra* [invited] KENNETH RUUD (Presenter), Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, UiT The Arctic University of Norway — Great advances are being made in the experimental realization of multiphoton spectroscopy, such as the experimental confirmation of four- and five-photon absorption in the visible energy range as well as two-dimensional Raman spectra.

The complexity of these nonlinear processes means, however, that computational studies are important for unraveling the full information content of the experimentally recorded spectra. Furthermore, many of the unique responses that can be observed in multidimensional vibrational spectroscopies are directly related to electric and/or mechanical anharmonicities. These methods therefore provide a unique window into molecular vibrational responses that would otherwise be difficult to disentangle from the dominant harmonic contributions.

In this presentation, I will in particular focus on the evaluation of the vibrational response functions that determine a wide class of multidimensional vibrational spectroscopies. Our approach takes as its starting point the Liouville equation, from which a sum-over-states expression for the response function at the appropriate order for an in principle arbitrary number of incident laser pulses is derived. The vibrational contributions to these response functions are determined recursively and the results are evaluated for a general setup of polarization vectors and time-ordering of the incident lasers. For selected numbers of independent variables (i.e. frequencies or frequency differences/sums in the IR range), the program generates spectra of the appropriate dimensionality.

I will provide some illustrations of the code to different multidimensional vibrational spectra. I will also present a benchmark study of the accuracy of density functional theory for the calculation of harmonic and fundamental vibrational frequencies.

*Research Council of Norway, Grant No 262695 and Grant No 250743.
Norwegian Supercomputing program NOTUR, Grant No NN4654K.
8:36AM E32.00002: Anharmonicity and vibrational coupling from ab-initio molecular dynamics* [invited] NADIA REGA

(Presenter), Department of Chemical Sciences, University of Napoli Federico II — We discuss on going advances in developing methods based on ab-initio molecular dynamics to simulate and understand vibrational dynamics, with focus on anharmonicity and vibrational coupling. This achievement is essential to understand at molecular level photoinduced processes on fast and ultrafast scale (femtoseconds to picoseconds). To this aim, we adopt time resolved vibrational analysis designed to follow equilibrium and transient vibrational dynamics extracted from ground and excited state trajectories.[1-5] We present results obtained for charge transfer complexes and photochromic reactions. We also discuss perspectives, limits and future challenges of these methods.

References


*We gratefully acknowledge fundings from Gaussian, Inc. (Wallingford, CT)

9:12AM E32.00003: UV Photodissociation Dynamics of Bromoform Studied by Ultrafast Inner-Shell Transient Absorption Spectroscopy* HAN WANG (Presenter), BENJAMIN W TOULSON, MARIO BORGWARDT, OLIVER GESSNER, Chemical Sciences Division, Lawrence Berkeley National Laboratory, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory — Small bromoalkanes have been the focus of multiple studies owing to the importance of bromine chemistry in the atmosphere as bromine is ~60 times more destructive towards stratospheric ozone than chlorine. Here we study the photochemistry of the low-lying electronically excited states of bromoform (CHBr3). To understand the physical mechanism of UV-induced C-Br bond breaking, fewest switches surface hopping (FSSH) calculations are performed to simulate the dynamics of CHBr3 after photon excitation. Using intermediate geometries and electronic structures from the FSSH simulation, XUV absorption spectra are calculated with the linear-response time-dependent DFT method for comparison with femtosecond time-resolved inner-shell absorption measurements. The combined theoretical-experimental study indicates that C-Br bond scission proceeds on a timescale of ~30-40 fs, followed by continued electronic interaction between the departing Br atom and the remaining CHBr2 fragment on an ~80-90 fs timescale. The study demonstrates how photochemical processes may be probed through a combination of ultrafast XUV/X-ray transient absorption spectroscopy, excited state molecular dynamics simulations, and core-level near-edge XUV/X-ray absorption calculations.

*Department of Energy

9:24AM E32.00004: Probing Ultrafast Dissociation Dynamics of Pentafluorobenzene Cation (C₆F₅H⁺) with Electrons* MING-FU LIN (Presenter), XIAOZHE SHEN, SLAC National Accelerator Laboratory, PEDRO NUNES, Department of Physics and Astronomy, UNIVERSITY OF NEBRASKA–LINCOLN, JIE YANG, RENKAI LI, STEPHEN WEATHERSBY, SLAC National Accelerator Laboratory, ROB PARRISH, TODD MARTINEZ, Department of Chemistry, Stanford University, MARTIN CENTURION, Department of Physics and Astronomy, UNIVERSITY OF NEBRASKA–LINCOLN, THOMAS JACOB ARCANGELO WOLF, XIJIE WANG, MICHAEL MINITTI, SLAC National Accelerator Laboratory — Real-time observation of a structural change of photoexcited molecular ion is important to understand the fundamental reaction mechanism. Here, we use mega-electronvolt ultrafast electron diffraction technique (MeV-UED) to directly construct a molecular movie of photogenerated pentafluorobenznen cation. The molecular cation was produced by multiphoton ionization of C₆F₅H at 269 nm. This cation dissociates into fragment ions within ~10 ps time scale through statistical internal energy redistribution prior to the following bond dissociation and ring opening. Parit distribution function (PDF) analysis allows us to pin down the specific chemical bond dissociation process in this unimolecular dynamics.

*The UED work was performed at SLAC MeV- UED, which is supported in part by the DOE BES SUF Division Accelerator & Detector R&D program, the LCLS Facility, and SLAC under contract Nos. DE-AC02-05-CH11231 and DE-AC02-76SF00515.
9:36AM E32.00005: State-resolved thermal reaction rate from ring-polymer surface hopping* XUECHENG TAO (Presenter), PHILIP SHUSHKOV, THOMAS MILLER, Caltech — Employing the recently developed isomorphic Hamiltonian framework for including nuclear quantum effects in mixed quantum-classical non-adiabatic dynamics, [J. Chem. Phys., 148, 102327 (2018)] we present a flux-side formulation of state-resolved thermal reaction rates for ring-polymer surface hopping. The method is shown to be robust and straightforwardly implemented, and numerical results reveal that RPSH in the isomorphic Hamiltonian framework leads to excellent dividing-surface independence, due to improved preservation of the path-integral statistics. The method is further applied to investigate F+H2 reactive scattering with an ab initio multi-level potential energy surface and its effectiveness is demonstrated with preliminary results.

*We acknowledge support from the Office of Naval Research, Air Force Office of Scientific Research. Computational resources were provided by the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the US Department of Energy.

9:48AM E32.00006: Mapping of the Excited State Potential Energy Surface during Molecular Photo-isomerization to Control Chemical Reactions RACHEL GLENN (Presenter), Michigan State, Virginia Tech — We present a new perspective of light matter interaction with molecules. When using shaped pulses, we explain fundamentally how our understanding of absorption and dispersion changes. We show how the phase of the pulse can change an absorption line-shape to a dispersion-like line-shape. Contrary to conventional belief, we show that the first-order polarization is sensitive to the phase of the electric field. We show that by performing single pulse experiments that it is possible to "map" out the propagation of the wave packet in the excited state potential energy surface. In addition, we describe how to measure the momentum dependent lifetime of the wave packet through a conical intersection. We use these fundamental ideas to answer the question of finding an optimum coherent pulse(s) that will maximize the formation of a desired chemical species.

10:00AM E32.00007: Modeling Molecular Spectra with Interpretable Atomistic Neural Networks* MICHAEL GASTEGGER (Presenter), KRISTOF T SCHÜTT, HUZIEL SAUCEDA, KLAUS-ROBERT MÜLLER, Technical University of Berlin, ALEXANDRE TKATCHENKO, University of Luxembourg — Deep neural networks are emerging as a powerful tool in quantum chemistry, combining the benefits of high-level electronic structure methods with excellent computational efficiency. The recently developed SchNet model provides an accurate description of molecules and materials across chemical compound space, as well as easy access to energy conserving force fields [1]. Here, we demonstrate that the modular nature of deep models can also be exploited to enhance their versatility and offer insights beyond the basic relationships learned by the network. First, we adapt existing architectures to model different spectroscopic quantities, such as molecular infrared spectra [2]. Going beyond the simple prediction of properties, we then explore modifications of SchNet in the form of latent features. Although these variables are inferred, they correspond to readily interpretable physical concepts, such as molecular charge distributions [3].


*This work was supported by the European Union's Horizon 2020 program under the Marie Sklodowska-Curie grant No 792572.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E33 FIAP: Devices for Biological Applications and Biological Materials BCEC 204B - Alan Johnson, Univ of Pennsylvania
8:00AM E33.00001: Laser-activated Polymer Devices for Intracellular Delivery  WEILU SHEN (Presenter), ERIC MAZUR, School of Engineering and Applied Physics, Harvard University, STEFAN KALIES, Institut für Quantenoptik, Gottfried Wilhelm Leibniz Universität Hannover, MARINNA MADRID, School of Engineering and Applied Physics, Harvard University, ALEXANDER HEISTERKAMP, Institut für Quantenoptik, Gottfried Wilhelm Leibniz Universität Hannover — A challenge in the biomedical field to advancing fundamental studies of biologically interesting molecules for clinical use is the direct delivery into the cytoplasm in an efficient way. Established methods such as electroporation and viral transduction each come with respective strengths and weaknesses that fit different application needs. We present a delivery method that combines 11-ns laser pulses of 1064 nm wavelength and polymer substrates to create transient pores in cells. These polymer devices are low-cost, biocompatible, and have simple fabrication techniques. Adherent cells are grown on the substrates, and pores only form on the cells in localized regions excited with the laser pulses, allowing spatial selectivity. The medium surrounding the cell contain the cargos, and they diffuse into the cell before the transient pores self-seal. We are able to deliver membrane-impermeable cargos of sizes up to 40 kDa. We obtained efficiencies of up to 40% with viabilities of 60% for calcein green in HeLa and Panc-1 cells. Scanning electron microscopy and optical profilometry are used to study the substrate surface morphology. This laser-activated polymer device can deliver important material directly into cells, furthering the field of nanomedicine in a cost-effective manner.

8:24AM E33.00003: A high-sensitivity 16-channel magnetic sensor for magnetocardiographic experiments*  YOUNG JIN KIM (Presenter), IGOR M SAVUKOV, Los Alamos National Laboratory — Multichannel parallel magnetic measurements are required for various applications in many fields such as neuroscience and biomedical research. We recently constructed a portable, low-cost, high-sensitivity 16-channel magnetic sensor for magnetocardiography (MCG) applications. The sensor is based on a high-sensitivity atomic magnetometer (AM) with a novel configuration of nearly parallel pump and probe laser beams. The AM-based 16-channel magnetic sensing is realized in a single module by using a single large rubidium vapor cell, two broad laser beams, and a 16-channel photodiode matrix, leading projected 10-fold reduction of the cost of sensors. For MCG experiments with the sensor, its main components except lasers are located inside a magnetically shielded room. We describe the basic principle and the design of the 16-channel magnetic sensor. We also present human heart signals directly recorded by the sensor.

*This work was supported by the U. S. DOE through the Los Alamos National Laboratory LDRD program.

8:36AM E33.00004: Detection of Biofilm Infections in Human Fluid Samples using DNA-Functionalyzed Carbon Nanotube Vapor Sensors*  EMILIE BENSON (Presenter), CHRISTOPHER KEHAYIAS, ALAN T JOHNSON, University of Pennsylvania — Human fluid samples collected from individuals suffering from various biofilm-related infections were analyzed using single-stranded DNA-functionalized carbon nanotube (ssDNA-CNT) vapor sensors. Fluids from infected individuals were collected and categorized by infection type: staph infections and non-staph infections. The samples were placed in individual flasks that were heated in a water bath, and a vapor handling system was used to sequentially deliver the headspace of the samples to an array of CNT devices configured as an “electronic nose”. Each array comprised up to 100 sensors, with each sensor functionalized with one of ten unique sequences of ssDNA, thereby yielding a ten-dimensional output response characteristic of the volatile odor signature of the samples. The resulting data space was dimensionally reduced using linear discriminant analysis (LDA), resulting in a differentiation of staph versus non-staph data clusters.

*This work was supported by the Kleburg Foundation.
8:48AM E33.00005: Triggered gelation of microfluidic polymer droplets to identify and isolate viable antigen-specific immune cells* BRENDA DEVENEY (Presenter), JULIE BROUCHON, JOHN HEYMAN, YUAN YUAN, DAVID A WEITZ, Harvard University — The isolation of antigen-specific immune cells is fundamental to the study of autoimmune diseases and to the development of effective immunotherapies, yet practical technologies for doing so are lacking. We present here a new method for the triggered gelation of polymeric microfluidic assay droplets that enables the isolation of viable antigen-specific T-cells in microfluidic devices. Specifically, T-cell/target cell pairs are coencapsulated in liquid droplets prior to droplet conversion into gel microspheres compatible with fluorescence activated cell sorting. We aim to use this platform to perform high-throughput cell-cell interaction assays and isolate individual immune effector cells together with their cognate target cells for future immunotherapy development.

*This is work is supported by AmfAR.

9:00AM E33.00006: Emergence of quantized vortices in microfluidic devices* JEREMIAS GONZALEZ (Presenter), BIN LIU, Physics, UC Merced — Structured vortices in microfluidic flows are often associated with suspensions of active matter that move in a collective fashion. For instance, vortical flows at microscales have been observed in bacterial swarms, with their forming mechanisms attributed to the self-propulsion of individuals and the cell-cell interactions. Here, we demonstrate that an array of microscale vortices can emerge purely due to the geometry and dimensionality in a steady flow. Specifically, we show that a chain of vortices can be induced in a rectangular cavity that is sheared under a steady flow. Interestingly, these vortices have an intrinsic aspect ratio, with their numbers quantized by the length of the cavity. We also elucidate that such intrinsic flow structures can be generalized to a wide class of confining geometries, indicating a fundamental mechanism of vortex formation in microscale flows.

*The authors thank the support of National Science Foundation NSF, CREST: Center for cellular and Biomolecular Machines (NSFHRD1547848).

9:12AM E33.00007: Graphene Probes for Detecting Electrical Activity of Individual Synapses* YUCHEN ZHANG (Presenter), RUI WANG, MINGJIAN SHI, BRYSON BREWER, LIJIE YANG, DONNA WEBB, DEYU LI, YAQIONG XU, Vanderbilt University — Complex neural circuits connected by billions of neurons with trillions of synapses require techniques that map the electrical activity of neural networks with extraordinary temporal and spatial resolution to decipher the underlying mechanisms for multiple aspects of neuroscience. By combining graphene transistors with scanning photocurrent microscopy, we can detect the local electrochemical environment changes induced by electrical activity of individual synapses of primitive hippocampal neurons, enabling us to estimate extracellular potential variations of individual synapses during depolarization. The ultrafast nature of graphene photocurrent response allows decoding of the activity patterns of individual synapses with sub-millisecond temporal resolution. As such, our new neurotechnology will offer promising potential for recording the electrical signals of a large population of synapses in neural networks.

*This work was supported by the National Institutes of Health (1R01EY027729, 1R21EY026176, and 1R21NS095323) and the National Science Foundation (ECCS-1055852 and 1810088, CBET-1264982, and BIO-1450897). Device Fabrication was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

9:24AM E33.00008: Development of a Mass Spectrometer for Sequencing Single Protein Molecules* BENJAMIN WIENER (Presenter), NICHOLAS DRACHMAN, Brown University, MATHILDE LEPOTTEVIN, Chemistry, École normale supérieure, WILLIAM MAULBETSCHE, OLIVER G ISIK, DEREK STEIN, Brown University — I will describe a new nanopore-based mass spectrometer designed to sequence proteins. The instrument will combine a nanopore ion source capable of extracting ionized amino acids directly from solution into a vacuum chamber using electric fields[1] with a magnetic sector for separation by charge-to-mass ratio. The mass-separated ions will travel into an array of channeltron-style detectors capable of continuously monitoring the full mass range of interest and tagging each detected ion with its precise arrival time. In addition, our design features tunable hardware which will allow us to precisely align and adjust the position of our ion source to achieve the detection efficiency necessary for sequencing.


*We acknowledge support from Oxford Nanopore Technologies.
Microfluidic calorimetric immunosensor: experimental results and COMSOL simulations of heat transfer in microchannel

SAIF MOHAMAD ISHRAQ BARI, LOUIS REIS, GERGANA NESTROVA (Presenter), Louisiana Tech University — Recent years have witnessed significant progress in the development of detection technologies for lab-on-a-chip immunoassays that provide increased sensitivity and specificity. The calorimetric technique allows the detection of reactions that are not compatible with other methods. Optimization of thermal transport through the microchannel relates to increasing sensitivity and high-throughput of sample analysis. This study presents the design and fabrication of calorimetric immunosensor for quantification of TNF-α. The impact of channel height (100μm, 500μm, 1000μm), lower channel wall thickness (170μm, 500μm, 1000μm), and MEMS materials (PDMS, glass) were simulated using COMSOL Multiphysics® to investigate the effect of these parameters on the heat transfer within the microchannel. Computational analysis indicates that reducing the channel height and the thickness of the lower channel wall results in an increased temperature difference. The simulations results were validated experimentally in a microfluidic immunosensor with an integrated antimony/ bismuth thermopile for quantification of TNF-α. The accuracy of the developed technology was validated using conventional ELISA.

Detection of Early-Stage Ovarian Cancer using DNA-Decorated Carbon Nanotube Vapor Sensors

CHRISTOPHER KEHAYIAS (Presenter), EMILIE BENSON, ALI GHORASHI, WILLIAM WATKINS, ALAN T JOHNSON, University of Pennsylvania — We propose an “electronic nose” technology based on arrays of carbon nanotube field-effect transistors (CNT-FETs) as a minimally invasive diagnostic for ovarian cancer. We measured the real-time electrical response of the sensor arrays to volatile organic compounds (VOCs) in the headspace of blood plasma samples collected from 21 patients with malignant ovarian cancer (six of whom had early-stage cancer), 16 patients with benign ovarian lesions, and 21 age-matched healthy subjects. Sensor arrays comprised 100 CNT-FETs, where each device was functionalized with one of ten different sequences of single-stranded DNA, providing a ten-dimensional output for each sample tested. A linear discriminant analysis tool was used to dimensionally reduce the ten-dimensional data space. A machine-learning package was then used to classify samples as malignant, benign, or healthy based on a training subset of the data, leading to correct classification of 88% of the samples in the test set. Moreover, all early-stage samples were correctly classified as malignant. This signifies a promising step towards a reliable diagnostic for ovarian cancer in the early stage, when standard therapeutic procedures are highly effective.

Prediction of crystal structure and study of transport and optoelectronic properties of NH2 substituted trans-stilbene derivative: A new promising ambipolar organic semiconductor

DWAIPAYAN CHAKRABORTY (Presenter), PRIYA JOHARI, Shiv Nadar University — Organic Semiconductor (OS) is an emerging class of energy materials, for its several advantages over its inorganic counterpart, such as large area, flexibility, low cost and most importantly their environment friendly manufacturing process. This class of materials can start a new electronic era, if their charge transport properties can be improved. Computational designing and study of new semiconducting organic molecules has come up as a great support in this regard. In this effort, we therefore rationally designed a promising Donor(D)-π-Acceptor(A) type molecule NNDM-NH2, a trans-stilbene derivative. We first calculated the molecular properties of this newly designed molecule and found important characteristics of molecule to exhibit high charge carrier mobility in solid. Further, on predicting its crystal structure and calculating the corresponding properties, we found that this new organic semiconductor owns a high charge carrier mobility of \(~ 2.11 \text{ cm}^2/\text{Vs}\) for hole and \(~ 0.64 \text{ cm}^2/\text{Vs}\) for electron, together with desirable electronic and optical properties. Thus, revealing NNDM-NH2 as a potential candidate for the application in opto-electronic devices. In addition, it has found to have remarkable non linear optical (NLO) properties.

We acknowledge Shiv Nadar University for funding.
**10:12AM E33.00012: XAS signature of ferroelectricity in Croconic Acid**  
FUJIE TANG (Presenter), PRATIKKUMAR H DHU Vad, Temple University, XUANYUAN JIANG, University of Nebraska, Department of Physics and Astronomy, MEHMET TOPS AKAL, DEYU LU, Brookhaven National Laboratory, Center for Functional Nanomaterials, XIAOSHAN XU, University of Nebraska, Department of Physics and Astronomy, XIFAN WU, Temple University — Molecular ferroelectrics (FE) based on ordering hydrogen bonds have potentially high electric polarization and ordering temperature compared with the conventional oxide FE materials. In particular, croconic acid (C₅O₅H₂) has a FE polarization of 26 μC/cm², in which the polar mode is strongly coupled to the intermolecular proton transfer. We applied X-ray absorption spectroscopy (XAS), a characterization technique that is sensitive to local structural and chemical properties, to probe the hydrogen bond structures of the croconic acid. First-principles simulations were used to interpret oxygen K-edge XAS features of croconic acid. The calculated XAS spectra semi-quantitatively agree with the three main experimental features at ~531.2 eV, 533.6 eV and 541.1 eV, respectively. The electron excitations in the two low-energy spectral features are found to be closely associated with the proton transfer, which gives rise to the FE polarization and can be recognized as a spectral signature of the FE in the croconic acid.

**10:24AM E33.00013: Conformation of DNA in periodic temperature gradient created by plasmonic heating**  
RYOKO SHIMADA (Presenter), HITOMI SAKAI, Japan Women's University — Different molecules in mixed solutions can be separated from each other along a temperature gradient. This phenomenon, so-called Soret effect, is quite important for molecular manipulation in various research fields. Among various techniques, plasmonic heating from periodic metal domains is one of the effective ways to create a periodic temperature gradient for observation of the Soret effect. In this work, we utilized the plasmonic heating from periodic silver (Ag) domains under emission of blue light (400 – 440 nm) to create the periodic temperature gradient (with a large amplitude of ~ 0.5 K/mm), thereby attempting to observe the Soret effect of DNA mixed in polyethylene glycol (PEG) solutions. The DNA molecules, labeled with fluorescent dyes, were concentrated in high temperature zones, confirming the positive Soret effect. In addition, for large DNA molecules (~166 Kbp), the conformation appeared to be distorted possibly because of the microscopic Soret effect within the molecule. Details of this observation will be discussed on site.

*This work was supported by JSPS KAKENHI grant number 18K03570.

**10:36AM E33.00014: Excess heat capacity measurement of nano/bio-materials by photo-thermal conversion calorimetry**  
XING LI (Presenter), CHIA-CHING CHANG, Department of Biological Science and Technology, National Chiao Tung University, Taiwan, DAR-BIN SHIEH, CHENG-YANG TSAI, Institute of Oral Medicine, National Cheng Kung University, Taiwan — Photothermal therapy in medical care including cancer is gradually being valued. We modified Thermal activity monitor to measure the heat generated by the photothermal reaction of nanoparticles. The thermal Activity Monitor is a freestanding multichannel microcalorimeter. We use this system to measure the photothermal reaction excess heat and calculate the specific heat of the photothermal nanoparticles. Furthermore, We can calculate the elevated net temperature. In addition, this method can also measure the excess heat generated by various nanoparticles and proteins excited by laser at a specific wavelength. According to this result, we can accurately know the thermal reaction effect of the nanoparticles to achieve better treatment.

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

**10:48AM E33.00015: Para-phenylenediamine crosslinked alginate gels and their mechanical properties**  
ROSA MARIA BADANI PRADO (Presenter), RANGANA WIJAYAPALA, SANTANU KUNDU, Chemical Engineering, Mississippi State University — Alginate hydrogels are widely applicable in bioengineering and pharmaceutical applications due to their biocompatibility. Conventionally, calcium ions are used to crosslink alginate chains. However, gel modulus decreases in physiological solutions due to ion exchange with the medium, leading to a deterioration of their microstructure. This can be overcome by replacing the crosslinking calcium ions with covalent bonds. Here, we investigate chemically crosslinked alginate hydrogels using para-phenylenediamine (PPD) as a crosslinker. PPD binds the carboxylic groups present in β-D-mannuronic acid and α-L-guluronic acid residues of alginate chains. The gel modulus is tuned by changing polymer and crosslinker concentrations. These gels show higher moduli and are more brittle as compared to ionic alginate gels for the same crosslinker concentration. A comparison of mechanical properties with respect to the ionic alginate gels will be presented.

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**Tuesday, March 5, 2019 8:00 AM - 11:00 AM**

**Session E34 GMED: Radiation Detection and Monitoring in Medical Imaging and Therapy**

BCEC 205A - Wojciech Zbijewski, Johns Hopkins University - Tag(s): Invited

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Recent advances in medical imaging include the development of large-area flat-panel x-ray detectors for radiography, fluoroscopy, mammography, and cone-beam CT as well as multi-detector and photon counting systems for diagnostic CT. Such advances have enabled new capabilities (for example, improved spatial resolution and reduced radiation dose) and propelled a revolution in 3D imaging systems over the last two decades. Quantitative understanding of the performance of various detector technologies - and optimizing their performance for a particular clinical application - benefits tremendously from mathematical models of imaging performance, including analytical models of spatial resolution, noise, and detective quantum efficiency. Such models give insight on the performance of each element of the imaging chain in terms of its spatial-frequency-dependent transfer characteristics. In turn, these characteristics can be related to the performance of a particular imaging task by considering spatial-frequency-dependent signal and noise with respect to the spatial-frequencies associated with performance of a particular task - i.e., "task-based" models. Such analysis has provided a foundation for imaging chain optimization (including scintillator thickness, pixel pitch, and electronic readout noise) and helped to accelerate the development of new imaging systems for 2D (projection) and 3D (volumetric) imaging systems for a variety of applications in medical diagnosis and interventional guidance. In this presentation, we review the essentials of such task-based models of imaging performance, study examples of model-based design of new imaging systems, and consider future challenges in modeling of nonlinear imaging systems.

Research supported by the National Institutes of Health and academic-industry partnership with Siemens Healthineers, Carestream Health, Philips Healthcare, and Elekta Oncology.
Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E35 DQI: Exchange-Based Spin Qubits BCEC 205B - Pascal Cerfontaine, RWTH Aachen University - Tag(s): Focus

8:00AM E35.00001: Spin qubits made of quantum dots and donors in silicon [Invited] PATRICK HARVEY-COLLARD (Presenter), Sandia National Laboratories — In this talk, I will present our recent work on control and readout of electron spin qubits in silicon MOS. Valley splitting is an issue that can induce control variability or limit readout fidelity. We show how this splitting is tunable in MOS devices [1], and introduce a shell-filling trick to overcome potential readout challenges. Readout fidelity has lagged behind that of control. We demonstrate that an enhanced latching mechanism can be used to improve the signal and lifetime of the spin-blockade readout while preserving its speed, achieving single-shot readout fidelities of > 99.86% [2]. The best spin qubit in the solid state is the nuclear spin of donors, but it is difficult to couple it to other qubits. We show coherent coupling of a donor to a quantum dot, a milestone for nuclear spin quantum computing [3]. We also study spin-orbit interaction for electrons in silicon quantum dots. We show that it is sufficiently large to drive a singlet-triplet qubit, allowing universal control without external elements [4]. We study the mechanisms behind this interaction and find three different effects [5]. Our work identifies crystallographic and magnetic field anisotropies that can be used to enhance or suppress these effects.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the DOE's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.


8:36AM E35.00002: Decoherence of a donor-dot hybrid qubit in Si* JOHN TRUONG (Presenter), XUEDONG HU, University at Buffalo, The State University of New York — A recent proposal for a scalable donor-based quantum computer scheme promises excellent coherence properties and fast qubit couplings [1]. The system consists of two types of qubits per donor: a flip-flop qubit consisting of the electron and nuclear spins, and a charge qubit of the donor electron tunneling between the donor and an interface quantum dot. The proposal identifies a parameter regime where flip-flop qubit dephasing due to electrical noise is strongly suppressed.

We study the decoherence properties of the flip-flop qubit when positioned near this sweet spot. In particular, we study the effect of charge noise that is coupled to the flip-flop qubit via the dependence of the hyperfine interaction and the electron gyromagnetic ratio on the charge qubit state. We find that zero frequency noise is indeed suppressed at the sweet spot. In the meantime, finite-frequency contributions from the qubit coupling to the excited charge states come into play at shorter time scales, although their effects average out over longer times. We also explore the decoherence dependence on external control parameters such as the applied magnetic field and tunnel coupling between the donor and dot.


*We acknowledge support by US ARO, grant W911NF1710257.
Probing exchange interaction for gate-defined double quantum dots

PATRICK BETHKE (Presenter), JARA-FIT Institute Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, MICHAEL A WOLFE, Department of Physics, University of Wisconsin, Madison, ROBERT P. G. MCNEIL, Niels Bohr Institute, University of Copenhagen, ARNE LUDWIG, ANDREAS D. WIECK, Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, HENDRIK BLUHM, JARA-FIT Institute Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University — The exchange interaction $J$ is vital for gating in electron-spin qubits. Therefore, understanding its behavior is crucial for high-fidelity gating, especially at low $J$ where an inability to turn it off completely may impact the fidelity of parallel qubit operations. Historically, the exchange interaction (controlled via detuning $\varepsilon$ between dots) measured in experiment, $J(\varepsilon) \propto \exp(-\varepsilon/\varepsilon_0)^{1-2}$, has deviated from Hubbard-based predictions, $J(\varepsilon) \propto 1/|\varepsilon|$.

We present measurements of $J$ down to values below 1MHz by controlling the nuclear magnetic field gradient $\Delta B_z$ in a GaAs double quantum dot. When $\Delta B_z$ becomes comparable to $J$ the visibility of the S-T0 precession is reduced. Fitting the relation between oscillation amplitude and frequency allows the extraction of $J(\varepsilon)$. In combination with Ramsey-like experiments we measure $J(\varepsilon)$ over three orders of magnitude.

Our results can be reproduced by a microscopic model including excited states in each dot and state-dependent tunnel coupling. Some parameters in the Hamiltonian, e.g. ground-state tunneling, excited-state tunneling, S-T0 splitting, can be measured independently and are found to be reasonably consistent with the model.


Computational modeling of exchange splitting in Si/SiO₂ double quantum dots

HARSHAD SAHASRABUDHE (Presenter), Department of Physics and Astronomy, Purdue University, West Lafayette, IN, RAJIB RAHMAN, School of Physics, University of New South Wales, Sydney, Australia — One and two qubit operations have been demonstrated using electrons trapped in quantum dots at the interface of isotopically purified Si/SiO₂ materials. We present a computational study of Si/SiO₂ based double quantum dot qubits which could help in scaling the device design. Exchange splitting between the lowest singlet and triplet states, which plays an important role in two qubit operations, is calculated using the full configuration interaction (FCI) method. The single electron wavefunctions used in FCI are calculated using 20-band $sp^3d^5s^*$ tight binding (TB) Hamiltonian, which accurately represents the conduction-band X valley and spin orbit coupling in quantum dots. The electrostatic potential needed in TB is calculated using self-consistent effective-mass Schroedinger-Poisson (S-P) simulations on finite element meshes resembling the actual device geometry. Energy spectrum of S-P and TB simulations shows a good match at low detuning between the dots. At high detuning close to the (1,1)-(0,2) transition, where the two qubit operations take place, higher X-valleys along x, y and z axes are found to play a role in the exchange splitting, which could impact the response to charge noise.

Achieving A High Fidelity Controlled-NOT Gate Between A Pair Of Exchanged-Coupled Silicon Double-Quantum-Dot Hybrid Qubits

YUAN-CHI YANG (Presenter), MARK G FRIESEN, SUSAN COPPERSMITH, University of Wisconsin - Madison — It has been shown that operating qubits by varying exchange couplings while operating at sweet spots against detuning noise can improve gate fidelities. For double-quantum-dot hybrid qubits, this requires keeping the system in the large-detuning regime where dephasing is greatly suppressed. Here we show that, in a pair of exchange-coupled double-quantum-dot hybrid qubits, it is possible to exploit the large-detuning regime to achieve a sizeable exchange interaction between the qubits while suppressing leakage and dephasing, yielding a high-fidelity controlled phase gate with a gate time less than 1 ns. We find that the fidelity of a CNOT gate can be above 99.9%, in the presence of charge noise typical for semiconductor devices.

*This work has been supported in part by ARO (W911NF-17-1-0274), the University of Wisconsin-Madison, and the Vannevar Bush Faculty Fellowship program sponsored by the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering and funded by the Office of Naval Research through grant N00014-15-1-0029. The views and conclusions contained in this work are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Army Research Office (ARO), or the U.S. Government.
MAXIMILIAN RUSS (Presenter), Department of Physics, University of Konstanz, JASON R PETTA, Department of Physics, Princeton University, GUIDO BURKARD, Department of Physics, University of Konstanz — We propose a quadrupolar exchange-only (QUEX) spin qubit that is highly robust against charge noise and nuclear spin dephasing, the dominant decoherence mechanisms in quantum dots [1]. Building on ideas developed for the exchange-only qubit [2], the hybrid qubit [3], and the exchange-only singlet-only spin qubit [4], the QUEX qubit consists of four electrons trapped in three quantum dots, and operates in a decoherence-free subspace to mitigate dephasing due to nuclear spins. To reduce sensitivity to charge noise, the qubit can be completely operated at an extended charge noise sweet spot that is first-order insensitive to electrical fluctuations. Due to on site exchange mediated by the Coulomb interaction, the qubit energy splitting is electrically controllable and can amount to several GHz even in the “off” configuration, making it compatible with conventional microwave cavities. A symmetric readout and initialization protocol can be used to perform fast and high fidelity measurements.


*RResearch was sponsored by Army Research Office grant W911NF-15-1-0149.

JONNE KOSKI (Presenter), ANDREAS LANDIG, PASQUALE SCARLINO, Department of Physics, ETH Zurich, MAXIMILIAN RUSS, Department of Physics, University of Konstanz, DAVID VAN WOERKOM, CHRISTIAN REICHL, WERNER WEGSCHEIDER, Department of Physics, ETH Zurich, GUIDO BURKARD, Department of Physics, University of Konstanz, ANDREAS WALLRAFF, THOMAS IHN, KLAUS ENSSLIN, Department of Physics, ETH Zurich — The implementation of circuit quantum electrodynamics (cQED) allows coupling of distant qubits by microwave photons hosted in on-chip resonators. Typically, the qubit-photon interaction is realized by coupling the photons to the electrical dipole moment of the qubit. A recent proposal [1] suggests storing the quantum information in the quadrupole moment of an electron in a triple quantum dot. This type of qubit is expected to have an improved coherence since the qubit does not have a dipole moment and is consequently better protected from electric noise. We report the experimental realization of such a quadrupole qubit hosted in a triple quantum dot in a GaAs/AlGaAs heterostructure. A high-impedance microwave resonator is capacitively coupled to the middle of the triple dot to realize interaction with the qubit quadrupole moment. We demonstrate strong quadrupole qubit-photon coupling with a qubit-photon coupling strength of $g / 2\pi \approx 130$ MHz and a qubit decoherence rate of $\gamma_2 / 2\pi \approx 30$ MHz. Furthermore, we observe improved coherence properties of the qubit when operating in the parameter space where the dipole coupling vanishes.


GUO XUAN CHAN (Presenter), XIN WANG, City University of Hong Kong — The relatively weak coupling between spin states in spin qubits has spurred a revival of interest in charge qubits, which promises stronger coupling between multiple charge qubits due to stronger long-range Coulomb interaction. Among the proposed charge qubits, charge quadrupole (CQ) qubit is suggested to provide a relatively robust quantum computation by virtue of the logical bases residing in a decoherence free subspace such that leakage state decouples from the manifold [1]. Conventionally, CQ qubit is realized with an electron residing in a lateral triple quantum dot device, yet any fluctuation in tunneling and detuning control causes significant leakage. We propose a strategy to mitigate such destructive coupling by simply implementing the CQ qubit in a triangular triple quantum dot, where the tunneling between the two dots on the edge strongly suppresses leakage, eliminating the need of complex pulse sequences. The reduction of leakage is demonstrated from molecular orbital calculation, in corporation with numerical simulations.


*This work is supported by the Research Grants Council of the Hong Kong Special Administrative Region, China (No. CityU 21300116, CityU 11303617).
10:00AM E35.00009: A High-Fidelity Gateset for Exchange-Coupled Singlet-Triplet Qubits

RENE OTTEN (Presenter), PASCAL CERFONTAINE, JARA-FIT Institute Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, MICHAEL A WOLFE, Department of Physics, University of Wisconsin, Madison, HENDRIK BLUHM, JARA-FIT Institute Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University — A key ingredient for a quantum computer is the accurate manipulation of qubits in order to generate high-fidelity gates. For S-T0 qubits in semiconductor quantum dots, which allow purely electric control with moderate bandwidth requirements, single-qubit gates with fidelities above the error correction threshold were demonstrated, whereas two-qubit operations have not reached the required fidelity [1-2]. Here, we numerically optimize a complete two-qubit gate set under realistic experimental constraints, exploiting exchange coupling while also accounting for capacitive coupling. We obtain fidelities of 99.9% for GaAs, while about 99.99% are achieved with vanishing magnetic field noise as in Si. We suppress leakage to $10^{-5}$ by choosing high inter-qubit magnetic field gradients.

For optimized parallel single-qubit gates, we find that inter-qubit capacitive coupling needs to be considered to avoid undesired entanglement, but is mitigated by interleaved operation. Realistic levels of residual inter-qubit exchange coupling are compensated for by our gates.

We will also report on progress of the realization of such gates in a GaAs device with two exchange-coupled S-T0 qubits.


10:12AM E35.00010: Fast high-fidelity entangling gates in Si double quantum dots

FERNANDO CALDERON-VARGAS (Presenter), GEORGE BARRON, XIUHAO DENG, EDWIN BARNES, SOPHIA ECONOMOU, Virginia Tech — High-fidelity two-qubit gates remain a challenge for spin qubits in quantum dots, partly due to the exchange coupling’s sensitivity to charge noise and relatively longer gate times. Here we show that, by using simple smooth pulses to control the amplitude of the oscillating magnetic field, entangling gates locally equivalent to control-NOT and control-Z gates can be implemented in times as low as 26 ns and with fidelities up to 99.99%. Moreover, we provide the particular single-qubit gates necessary to make the two-qubit gates exactly equal to the CNOT and CZ gates.

*This work is supported by the Army Research Office (W911NF-17-0287).

10:24AM E35.00011: Robust implementation of one-qubit gates despite always-on exchange coupling in silicon double quantum dots

UTKAN GUNGORDU (Presenter), JASON PAUL KESTNER, University of Maryland, Baltimore County — In a silicon two-qubit device, bandwidth constraints on exchange coupling and limitations on ESR power are important obstacles for the realization of strictly local gates, which are themselves necessary components of robust non-local gating schemes [1]. Here we show that, even in the presence of an exchange coupling stronger than one-qubit Rabi frequencies, spins can be addressed separately to implement a particular class of one-qubit gates optionally surrounded by exchange gates, and the crosstalk between them can be eliminated stroboscopically. We also show how to make such gates robust against quasistatic charge- and hyperfine-noise.


*This research was sponsored by the Army Research Office (ARO), and was accomplished under Grant Number W911NF-17-1-0287.

10:36AM E35.00012: Adiabatic two-qubit gates of capacitively coupled quantum dot hybrid qubits

ADAM FREES (Presenter), University of Wisconsin - Madison, JOHN GAMBLE, Quantum Architectures and Computation Group, Microsoft Research, MARK G FRIESEN, SUSAN COPPERSMITH, University of Wisconsin - Madison — Semiconductor quantum dot qubits have progressed greatly over the past several years, with two-qubit gates realized by several groups. So far, the fidelities reported for these gates are still below the error correction threshold. Here, we model a system consisting of two capacitively-coupled quantum dot hybrid qubits, and optimize the adiabatic electrical pulses used to entangle these qubits. We find a simple pulse that yields a CZ gate with greater than 99% fidelity in the presence of a quasistatic charge noise distribution with standard deviation 1 µeV. Further, we introduce the concept of a "dynamical sweet spot" which can be used to develop pulses that decrease the infidelity by a factor of >5.

*Support by ARO (W911NF-12- 1-0607, W911NF-17-1-0274), and NSF (PHY-1104660) is acknowledged. The views and conclusions reported here are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of ARO or the U.S. Government. The authors acknowledge support from the Vannevar Bush Faculty Fellowship program, funded by the Office of Naval Research through Grant No. N00014-15-1-0029.
10:48AM E35.00013: Minimal non-orthogonal gate decomposition for qubits with limited control*  XIAOMING ZHANG (Presenter), City University of Hong Kong, JIANAN LI, Department of Physics, Southern University of Science and Technology, XIN WANG, City University of Hong Kong, MAN-HONG YUNG, Shenzhen Institute for Quantum Science and Engineering and Department of Physics, Southern University of Science and Technology — How an arbitrary unitary transformation can be decomposed into minimum number of elementary rotations, subject to particular physical constraints, is a fundamental and practical question. Here, we consider two important scenarios. The first one is when rotation axes are allowed to vary in a range of a plane, which corresponds to the Singlet-Triplet (ST) qubit in quantum-dot systems; the second one is when rotation axes can only along two fixed directions, corresponding to the Exchange-Only (EO) qubits. For both scenarios, we provide the criteria for determining the minimal number of pieces and explicit gate construction procedure for each unitary gate. Our results analytically explain the four-gate decomposition of EO qubits, previously determined numerically by Divincenzo et al. Moreover, our approaches can reduce both gate time and gate fidelity dramatically for ST qubits, compared with Ramon sequence and its variant.

*This work is supported by the Research Grants Council of the Hong Kong Special Administrative Region, China (No. CityU 21300116, CityU 11303617)

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E36 DBIO: Physics of the Cytoskeleton Across Scales I  BCEC 205C - Megan Valentine, University of California, Santa Barbara - Tag(s): Invited

8:00AM E36.00001: Controlling Epithelial Cell Shape [Invited]  MARGARET GARDEL (Presenter), University of Chicago — I will discuss my lab's recent work to study the biophysical mechanisms regulating control of cell shape in epithelial tissue. In particular, we have used optogenetics to locally regulate Rho activity at cell junctions to uncover how local Rho pulses drive junction contraction and stabilization via a ratcheting mechanism. We find that at short timescales, Rho activation drives junction contraction that reverses upon Rho reduction. Sustained RhoA activity shows a similar initial rapid contraction followed by a slow contractile phase. Upon removal of RhoA activation, the junction does not fully recover back to its original length, similar to junctional ratcheting observed in vivo. We find that this ratchet is dependent on both trans E-cadherin interactions and Formin activity. To understand these data, we model junction length in response to variable tension. In contrast to existing vertex models, our data argues that a junction has a rest length that is determined by the force-dependent junctional remodeling under acute periods of tension. This model then predicts that the slow contractile phase will eventually saturate to limit the amount of junction length changes and this is indeed what we see experimentally. We can overcome this saturation by inducing multiple activation periods, recapitulating junctional ratcheting seen in vivo. Altogether, these data provide insight into the underlying molecular and biophysical mechanisms of junction length changes seen in development.

8:36AM E36.00002: Posttranslational modification of microtubule mechanics* [Invited]  LOREN HOUGH (Presenter), Department of Physics and BioFrontiers Institute, University of Colorado, Boulder, TAVIARE L HAWKINS, Department of Physics, University of Wisconsin, La Crosse, KATHRYN P. WALL, Department of Biochemistry and BioFrontiers Institute, University of Colorado, Boulder, HAROLD HART, Department of Physics, University of Wisconsin, La Crosse — Microtubules are built from tubulin dimers, which contain an intrinsically disordered C-terminal tail that makes up approximately 4% of the mass of a dimer. These tails coat the microtubule surface, and affect microtubule bending (the persistence length) and binding of other proteins. C-terminal tails are post-translationally modified by addition of chains of glycine or glutamate residues. We have developed methods for purifying tubulin with distinct levels of these modifications to study how tail modification affects microtubule behavior. We combine nuclear magnetic resonance spectroscopy with fluorescence measurements of the microtubule bending rigidity to determine the atomic and mechanical effects of varying post-translational modifications. Remarkably, we find that posttranslational modification that adds a small number of additional residues to the tubulin tail can lead to increase the microtubule persistence length by almost 50%.

*NIGMS R35GM119755
9:12AM E36.00003: Active Stresses and Stress Relaxation in Cytoskeletal Networks* [Invited] FRED C. MACKINTOSH (Presenter), Department of Chemical and Biomolecular Engineering, Rice University — Living systems must operate out of thermodynamic equilibrium at the molecular scale. This lack of equilibrium results in directed fluxes through chemical states or phase space, corresponding to violations of the principle of detailed balance at the molecular scale. We explore consequences of such active, nonequilibrium dynamics at the meso and macro scales, with particular emphasis on cytoskeletal networks, which are driven by a variety of internal stresses. These stresses are often due to molecular motors, such as myosin that generates tension in the actin networks. These stresses can result in active remodeling of the networks and self organization of stress, particularly in networks near marginal stability. Active processes can also govern stress relaxation in such networks, through treadmilling and severing of filaments. We show how severing can lead to a surprising molecular weight independent relaxation in actin gels. We also show how transient crosslinking, together with prestress can lead to very slow, glassy relaxation in actin gels. Moreover, transient nonequilibrium (un)binding can also generate contractile stress in the absence of molecular motors.

*This work was supported in part by the National Science Foundation (Grant DMR-1826623) and Center for Theoretical Biological Physics (NSF Grant PHY-1427654).

9:48AM E36.00004: Dynamics and mechanics of actin cytoskeleton networks in vitro and in cellulo* [Invited] OLIVIA DU ROURE (Presenter), JULIEN HEUVINGH, PMMH UMR 7636, CNRS ESPCI Paris, PIERRE BAUÉR, Hospital, Institut Curie, Paris, REDA BELBAHRI, PMMH UMR 7636, CNRS ESPCI Paris, ALPHÉE MICHELOT, IBDM UMR 7288, CNRS AMU, VALENTIN LAPLAUD, PMMH UMR 7636, CNRS ESPCI Paris, MATTHIEU PIEL, UMR 144, Institut Curie, Paris, ANA-MARIA LENNON-DUMENIL, U932, Institut Curie, Inserm — Actin is a protein which self-assembles into highly dynamic filaments organized, within the cells, in different kinds of structures: bundled, crosslinked, contractile or branched networks. Actin interacts with a large number of partners either regulating the meshwork dynamics (polymerization, depolymerization and contractility) or the meshwork architecture (bundling, branching or crosslinking proteins). The architecture dictates the mechanics of the network and combines to its dynamic properties to enable the cell to achieve essential processes like migration, deformation or integration of external signals. I will show in this talk how we take advantage of the self-assembly of magnetic micro-particles to study simultaneously dynamic and mechanical properties of different actin networks. Results on actin cortex directly in living cells as well as on in vitro Arp2/3 actin networks resembling the ones at play in lamellipodia or in endocytosis will be discussed.

*This work benefited from the support of the French Agence Nationale de la Recherche (ANR) under the grant MuScActin (ANR-15-CE13-0004), of ITMO Cancer (VL, PhD fellowship), and of ERC grant SegregActin (ERC-StG-2014 638376).

10:24AM E36.00005: What can we learn from self-organization for the understanding of the spatio-temporal dynamics of the cytoskeleton* [Invited] EBERHARD BODENSCHATZ (Presenter), ALEXEI KREKOV, MARCO TARANTOLA, HSIN-FANG HSU, Max Planck Institute for Dynamics and Self-Organization, CARSTEN BETA, University of Potsdam — The response of the actin cytoskeleton to external chemical stimuli plays a fundamental role in numerous cellular functions. One of the key players that governs the dynamics of the actin network is the motor protein myosinII. Here we report on experiments and modeling on the interplay between myosinII and filamentous actin in Dictyostelium discoideum. In chemotactically competent cells, upon uniform stimulation with the chemoattractant cAMP, myosinII is first released from the cortical region and then translocated back to the cortex with a time delay relative to the rapid increase of cortical actin. After the initial release of myosinII, the freshly formed filamentous actin pushed the membrane outward resulting in a change of cell morphology. By comparing with myosinII-null cells, we found that in the last stage of the cell response the coupling between myosinII and actin determines contraction dynamics. I shall also report on our approaches using phase field modeling.

*Supported by Deutsche Forschungsgemeinschaft SFB 937 “Collective Behavior of Soft and Biological Matter“ and the Max Planck Society.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E37 GMAG DCMP DMP: Kagome Lattices BCEC 206A - Jeffrey Quilliam, Universite de Sherbrooke - Tag(s): Focus
8:00AM E37.00001: NMR Investigation of the Breathing Kagome Lattice in Li$_2$In$_{1-x}$Sc$_x$Mo$_3$O$_8$  AIME VERRIER
(Presenter), MARIAM EL-AMINE, XAVIER BAZIER-MATTE, Institut Quantique, Université de Sherbrooke, HAIDONG ZHOU, RYAN P
SINCCLAIR, University of Tennessee, JEFFREY QUILLIAM, Institut Quantique, Université de Sherbrooke — We report $^7$Li NMR
measurements on Li$_2$In$_{1-x}$Sc$_x$Mo$_3$O$_8$ at concentrations $x=0$, 0.6 and 1. The results are compared with those of other groups
on the end members of the series [1] and with previous work using muon spin rotation ($\mu$SR) [2]. The sample dependence
and the effects of pressure on the NMR spectra and on the temperature dependence of the spin-lattice relaxation will be
discussed, as well as their implications for possible spinon excitations in the spin liquid regime at intermediate Sc
concentration.

(2018).

8:12AM E37.00002: Thermal transport properties of S = 1/2 Cd-kapellasite  MASATOSHI AKAZAWA (Presenter), HAYATO
DOKI, KAORI SUGII, MASAAMI SHIMOZAWA, MINORU YAMASHITA, HYUN-YONG LEE, NAOKI KAWASHIMA, RYUTARO
OKUMA, ZENJI HIROI, ISSP, University of Tokyo, JUNG HOON HAN, Sungkyunkwan University — In recent years the thermal Hall
effect has gained a great interest as an important signature of the topology. This effect has been observed in
paramagnetic phase of kagome antiferromagnets, volborthite and Ca-kapellasite [1]. These thermal Hall conductivities ($\kappa_{xy}$)
are shown to be well reproduced by Schwinger-boson mean field theory by tuning the Dzyaloshinskii-Moriya
interaction D and the exchange energy J as fitting parameters. In this talk, we report further evidence supporting the
agreement between the experiment and theory from thermal Hall measurements in Cd-kapellasite CdCu$_3$(OH)$_6$(NO$_3$)$_2$H$_2$O
which has a smaller J/k$_B$ ~ 45 K than that of Ca-kapellasite. We find not only that $\kappa_{xy}$ of Cd-kapellasite is also well
reproduced by the theory, but also that the peak temperature in $\kappa_{xy}$ is shifted to a lower temperature with a larger value in
$\kappa_{xy}$ as expected by the theory. The good scaling of these kagome materials strongly indicates that a kagome

8:24AM E37.00003: Structural Phase Transitions in the S=1/2 Kagome Antiferromagnets Barlowite and
Claringbullite*  ALYSSA HENDERSON (Presenter), LIANYANG DONG, Florida State University, SANANDA BISWAS, Institut für
Theoretische Physik Goethe Universität Frankfurt am Mai, HANNAH I REVELL, YAN XIN, National High Magnetic Field Laboratory,
JOHN SCHLUETER, Division of Material Research, National Science Foundation, ROSER VALENTI, Institut für Theoretische Physik
Goethe Universität Frankfurt am Mai, THEO SIEGRIST, National High Magnetic Field Laboratory — Barlowite (Cu$_4$(OH)$_6$FBr)
and claringbullite (Cu$_4$(OH)$_6$FCl) are atacamite minerals related to the quantum spin liquid (QSL) candidate herbertsmithite
ZnCu$_3$(OH)$_6$Cl$_2$, the popular S = ½ antiferromagnet with a geometrically perfect kagome lattice. The kagome lattices of
claringbullite and barlowite are stacked perfectly on top of one another and show promise as QSL candidates.
Experiments suggest that at room temperature both materials have a hexagonal crystal structure with P6$_3$/mmc symmetry and
undergo temperature-dependent phase transitions. Ab-initio density functional theory calculations were performed to
explain these structural phase transitions. The transitions are likely influenced by the presence of defects, so it is expected
that the transition temperature varies from sample to sample and will be different for crystals grown by different
methods.

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Advanced Photon Source, a User Facility operated for the U.S. Department of Energy Office of Science by Argonne National
Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.
ARASH AKBARI-SHARBAF (Presenter), Institut Quantique and Département de Physique, Université de Sherbrooke, RYAN P. SINCLAIR, Department of Physics and Astronomy, University of Tennessee, AÎMÉ VÉRRIER, DJAMEL ZIAT, Institut Quantique and Département de Physique, Université de Sherbrooke, HAIMDONG ZHOU, Department of Physics and Astronomy, University of Tennessee, XUEFENG SUN, Department of Physics, Hefei National Laboratory for Physical Sciences at the Microscale, JEFFREY QUILLIAM, Institut Quantique and Département de Physique, Université de Sherbrooke — A promising approach to understanding the complexities of experimental quantum spin liquid candidates is to search for a way to tune the microscopic Hamiltonian and study changes in the resulting magnetic phases. In this talk I will present recent developments in a new class of highly tunable Mo$_3$O$_{13}$ cluster Mott insulators. This family of materials can be viewed as a breathing kagome lattice (BKL) of Mo ions, where the corner-sharing up and down triangles have two different sizes. In the compounds Li$_2$In$_{1-x}$Sc$_x$Mo$_3$O$_8$ the breathing parameter ($\lambda$) changes non-monotonically with Sc concentration ($x$), tuning the system from an antiferromagnetic Mott insulator for large $\lambda$, to a quantum spin liquid for small $\lambda$.[1]. For large breathing parameter electrons become confined on the small triangles forming spin-1/2 Mo$_3$ clusters on a triangular lattice with antiferromagnetic exchange coupling between them, leading to long range antiferromagnetic order. On the other hand, for small breathing parameter electrons are no longer confined to individual Mo$_3$ clusters but can tunnel between adjacent clusters, leading to a novel long range plaquette charge order (PCO) [2]. Our thermodynamic and muon spin rotation ($\mu$SR) measurements, suggest that the PCO coincides with a high degree of spin frustration and leads to a quantum spin liquid ground state, with gapless spinon excitations. The tunability of these materials can be extended to lower and higher breathing parameter in several related Mo-oxide materials, revealing additional quantum spin liquids and even ferromagnetism.


*We acknowledge funding from CFREF, NSERC, and FRQNT

9:12 AM E37.00005: Pressure and doping effects on the low-field anomalous magnetism in kagome Co$_3$Sn$_2$S$_2$  
HUNG-CHENG WU (Presenter), Texas Center for Superconductivity, University of Houston, Texas 77204, USA, PO-JUNG SUN, DONG-JIE HSIEH, Department of Physics, National Sun Yat-sen University, Kaohsiung, 80424, Taiwan, D CHANDRASEKHAR KAKARLA, Center of Crystal Research, National Sun Yat-sen University, Kaohsiung, 80424, Taiwan, CHING-WU CHU, Texas Center for Superconductivity, University of Houston, Texas 77204, USA, HUNG-DUEN YANG, Department of Physics, National Sun Yat-sen University, Kaohsiung, 80424, Taiwan — Polycrystalline samples Co$_3$Sn$_2$S$_{2+x}$ (0 ≤ x ≤ 0.34) and (Co$_{1-x}$M$_x$)$_3$Sn$_2$S$_{2.26}$ (M = Ni and Fe, 0 ≤ x ≤ 0.05) have been synthesized using solid-state-reaction and characterized by X-ray diffraction (XRD) and electron probe microanalyzer (EPMA). Basically, we are able to reproduce the phase diagram (so-called A' phase) as previously reported with negligible sample dependent effect. Furthermore, following the similar procedure and analysis, a so-called A' phase within phase can be sketched in H-T phase diagram of Co$_3$Sn$_2$S$_2$. Under the effects of external high-pressure and chemical substitutions, the anomalous magnetisms (A and A') in low magnetic field show a significant change. The possible origin of the field-induced A' phase could be ascribed to the non-collinear skyrmion-like phenomena. These striking findings provide a new candidate in spin-frustrated systems to explore the complexity of magnetic-field-induced magnetism.

*This work was supported by the Ministry of Science and Technology, Taiwan, under Grant Nos. MOST 106–2112–M–110–013–MY3 and MOST 107–2917–I–564–008

9:24 AM E37.00006: Spin dynamics in the antiferromagnetic Heisenberg model on a pyrochlore slab  PREETHA SAHA (Presenter), DEPEI ZHANG, GIA-WEI CHERN, University of Virginia — Unconventional magnetic states such as spin liquids and spin glasses continue to attract the interest of researchers in magnetism. Recently, considerable effort has been focused on understanding their dynamical signatures.[1-2]. We present our study on deterministic spin precession dynamics using energy conserving Landau-Lifshitz equation on a geometrically frustrated magnet. The lattice constitutes of a triangular arrangement of bipyramids with classical antiferromagnetic Heisenberg interaction. Such a lattice structure is realized in frustrated SrCr$_9$Ga$_{2.9}$P$_{0.19}$[SCGO(p)] compounds [3]. Monte Carlo simulations are used to thermalize the system, which is then used as the initial state for the dynamical studies. We explore the temperature, wave vector and frequency dependence in the dynamical structure factor and the corresponding time dependent correlation functions of the model. Dynamics simulations is further used to estimate the extent to which transport of spin excitations in the lattice conform with phenomenological concept of spin diffusion.

9:36AM E37.00007: Chiral superconductivity with full Bogoliubov Fermi surface in a doped Kagome spin-liquid state.* FAN YANG (Presenter), Beijing Institute of Technology, YIFAN JIANG, Stanford University, HONG YAO, Tsinghua University — We employ a large-scale variational Monte-Carlo simulation to investigate the lightly doped t-J model on the Kagome lattice. We propose several new variational states which smoothly connect to the previously studied uniform 0-flux or U(1) π-flux states. By comparing the energies of a variety of trial-states at several system-sizes, we find that the state with lowest energy is a chiral superconducting state with full Bogoliubov Fermi surface, which can be analogous to the Fulde-Ferrell-Larkin-Ovchinnikov state. The physical properties of this new state and the experimental consequences of the existence of Bogoliubov Fermi surface in this superconducting state are discussed.

*Supported by NSFC under the grant No.11674025, 11334012

9:48AM E37.00008: A single-layer infinite projected entangled-pair state study of the chiral antiferromagnetic Heisenberg model on Kagome lattice* REZA HAGHSHENAS (Presenter), DONNA SHENG, SHOUSHU GONG, California State University, Northridge — In this talk, we present the study of the chiral antiferromagnetic Heisenberg model on Kagome lattice by using the infinite projected entangled-pair state ansatz. We discuss how to develop an efficient optimization algorithm in the framework of the single-layer tensor network with reduced computation cost O(D^9), where D is the so-called bond dimension of local tensors. We show that the algorithm is stable, providing accurate results similar to previous double-layer tensor network ansatz. We compare the extracted phase diagram with previous DMRG study and additionally show that only for strong chiral couplings the correlation length, extracted from the transfer matrix, reaches a fixed value for the largest bond dimensions, representing a gaped chiral state.

*This research is supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515 through SLAC National Accelerator Laboratory

10:00AM E37.00009: Magnetic clustering in frustrated Heisenberg magnets TOMONARI MIZOGUCHI (Presenter), Department of Physics, University of Tsukuba, LUDOVIC JAUBERT, University of Bordeaux, RODERICH MOESSNER, Max-Planck-Institut fur Physik komplexer Systeme, MASAFUMI UDAGAWA, Department of Physics, Gakushuin University — Fractionalization is one of the fundamental properties of magnets with nontrivial topological character. For example in spin ice, fractionalized degrees of freedom take the form of magnetic monopoles which serve as elementary excitations with a conserved quantum number, their magnetic charge. Recently, it has been pointed out that the clustering of such topological charges leads to characteristic patterns in static structure factors, which we named half moons, distinct form the pinch points that serve as indicators of a Coulomb phase.

In this presentation, we present a theory of clustering of spins in a more general framework. For this purpose, we employ J1-J2-J3 Heisenberg models on kagome and pyrochlore lattices. By investigating the magnetic structure factor with a large-N approximation, we find that the pinch points turn into different characteristic patterns, namely half moons and stars. Those are the sign of the clustering of spins in the real space whose structures are similar to that in the Ising models. We also reveal by solving the Landau-Lifshitz equation that the characteristic patterns are also found in the dynamical structure factor, indicating that those patterns serve as a clue to find clustering states through inelastic neutron scattering spectra.

10:12AM E37.00010: Phases of the Chiral-Heisenberg Kagome Antiferromagnet* JACKSON PITTS (Presenter), Univ of California - Riverside, FINN BUSSSEN, Univ Cologne, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, Dresden, SIMON TREBST, Univ Cologne, KIRILL SHTENGEL, Univ of California - Riverside — The ground state degeneracy of the classical kagome Heisenberg antiferromagnet (KHAFM) is remarkably similar to that of the kagome chiral model (KCM) whose Hamiltonian consists of the scalar spin chiralities on the triangles of the lattice. However, models containing both types of interactions have reduced degeneracies. If chiral terms are introduced uniformly, the v3×v3 state lifts from the ground state manifold, but if they are introduced with staggered sign, the q=0 state is excluded instead. Only once the Heisenberg terms are entirely eliminated are states of both types again ground states. This has drastic effects on the order-by-disorder mechanism that drives coplanar ordering in the KHAFM. Our Monte Carlo simulations demonstrate a more discriminating selection effect in the intermediate models. Furthermore, even in the case of the pure KCM, only the v3×v3 structure is observed. We explain this by counting the soft modes of the KCM’s ground states. Only states of v3×v3 structure have sufficient populations of soft modes to drive the system to order. Due to an extra degeneracy of the KCM this structure exists on a large set of states forming a classical spin liquid.

*The authors acknowledge partial funding through DFG research center SFB 1238 and NSF DMR-1411359.
A mechanism for thermal Hall effect in Mott insulating spin liquid

YONGHAO GAO (Presenter), GANG CHEN, Fudan University — We study the origin of thermal Hall effect from the spinon transport in a U(1) spinon metal. The external magnetic field, that polarizes the spins, effectively generates an internal U(1) gauge flux for the spinons and twists the spinon motion through the antisymmetric interaction. Such a mechanism for Lorentz force generation differs fundamentally from the induction of the internal U(1) gauge flux in the weak Mott insulating regime from the charge fluctuations. We apply this understanding to the specific cases of spinon metals in Kagome lattice and hyperkagome lattice. We carry out a numerical calculation of the thermal Hall conductivity within the linear response theory and discuss the relevance with the thermal transport measurement in Kagome materials volborthite and kapellasite.
8:12AM E38.00002: Mapping of a thin-film ferromagnet to electrodynamics: quantum statistics of vortices

SHU ZHANG (Presenter), SAYAK DASGUPTA, MICHAEL BJERNGAARD, OLEG TCHERNYSHYOV, Johns Hopkins University — We consider a field-theoretic description of a thin-film ferromagnet with easy-plane anisotropy. The system can be mapped to the electrodynamics theory in (2+1)-dimensional space-time. The low-energy description is the familiar Maxwell electrodynamics. Spin waves become electromagnetic waves, whereas vortices turn into particles whose electric charge equals the vortex number n. A careful analysis of the high-energy theory reveals that these particles also carry a magnetic flux equal to the net spin of the vortex core $S_z$. Braiding two identical vortices yields an Aharonov-Bohm phase $\exp(2\pi i n S_z)$, which may lead to a nontrivial quantum statistics of vortices.

*U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, Award DE-FG02-08ER46544.

8:24AM E38.00003: Mapping of a thin-film ferromagnet to electrodynamics: emission of spin waves by vortices

MICHAEL BJERNGAARD (Presenter), SAYAK DASGUPTA, SHU ZHANG, OLEG TCHERNYSHYOV, Johns Hopkins University — We consider a field-theoretic description of a thin-film ferromagnet with easy-plane anisotropy. An extension of the well-known duality with electrostatics in 2-dimensional space to (2+1)-dimensional spacetime maps this system to a theory of electrodynamics. The low-energy description is the familiar Maxwell electrodynamics. Spin waves become electromagnetic waves, whereas vortices turn into particles whose electric charge equals the vortex number. This analogy allows us to compute the emission of spin waves by a rotating vortex-antivortex pair. Energy dissipation from this process becomes noticeable when the pair separation decreases below a characteristic length scale of order $a^{-1/2}R$, where $R$ is the radius of the vortex core and $a$ is the Gilbert constant.

*The research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544.

8:36AM E38.00004: Calculation of nonlinear susceptibility in magnetic systems

YURIY SIZYUK (Presenter), PETER P. ORTH, Physics and Astronomy, Iowa State University — Coherent nonlinear optical spectroscopy has been a successful tool to probe interactions between excitations in NMR and semiconductor experiments. Recent advances of optical experiments in the terahertz range allows the realization of similar measurements for localized magnetic systems. Anticipating this, we are calculating nonlinear magnetic susceptibilities for well known models, such as the transverse field Ising model, and Kitaev honeycomb model. The information about the magnetic excitations can then be used as a probe to experimentally identify complex, yet elusive magnetic ground states, such as quantum spin liquids.

8:48AM E38.00005: Energy-momentum tensor of a ferromagnet

SAYAK DASGUPTA (Presenter), OLEG TCHERNYSHYOV, Johns Hopkins University — The energy-momentum tensor provides valuable information about a physical system. Deriving this quantity for a ferromagnet runs into a conceptual difficulty associated with the presence of gyroscopic forces, which are represented by spin Berry-phase terms in the Lagrangian. Their gauge dependence and lack of rotational symmetry lead to paradoxes. E.g., the adiabatic spin torque exerted on a domain wall by a spin-polarized current is either missing or contains unphysical glitches, depending on the gauge choice. It is therefore desirable to derive a gauge-invariant and rotationally symmetric version of the energy-momentum tensor. We achieve this by using the gauge-invariant and symmetric Wess-Zumino action for spins at the expense of introducing an extra dimension, with the ferromagnet living on its boundary. The energy-momentum tensor defined in this (d+2)-dimensional spacetime yields correct physical answers.

*U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544.

9:00AM E38.00006: A measurable form of Bell's correlation of spin currents across a double dot in the Kondo regime

RUI SAKANO (Presenter), ISSP, University of Tokyo, AKIRA OGURI, YUNORI NISHIKAWA, Physics, Osaka city university, EISUKE ABE, Spintronics Research Center, Keio university — We investigate Bell-state correlations of quasiparticle pairs that are excited within nonlinear current through a double dot in the Kondo regime. Using the renormalized perturbation expansion in the residual interaction of the local Fermi liquid, we calculate an asymptotically exact form of Bell's correlation at low energies. We find that the exchange interaction of the double dot violates Bell's inequality. We especially suggest a measurable form of Bell's inequality that is given by correlations of the full current across the double dot. We illustrate the exchange interaction dependence of upper limits of the suggested Bell's correlation in the quantum theory and the hidden variable theory, using the numerical renormalization group calculation.

*This work was partially supported by JSPS KAKENHI Grant Numbers JP26220711, JP15K05181, JP16K17723, and JP18K03495.
9:12AM E38.00007: Evolution of magnetic Dirac bosons in a Kagome lattice* DANIEL BOYKO (Presenter), University of North Florida, ALEXANDER BALATSKY, Institute for Material Science, Los Alamos National Laboratory, AVADH SAXENA, Theoretical Division - T4, Los Alamos National Laboratory, JASON HARALDSEN, University of North Florida — We examine the magnetic properties and spin dynamics of Dirac nodes in a Heisenberg kagome lattice. Using linear spin theory, the phase diagrams and the evolution of exchange interactions in various magnetic configurations of the Kagome lattice are numerically calculated and produce spin waves that contain bosonic Dirac and Weyl points. Through the frustration of the magnetic geometry, we see a connection to the symmetry properties of the kagome lattice and the various antiferromagnetic configurations, where further study of external frustrations from a magnetic field, temperature, and anisotropy may reveal a controllability of the exchange interactions and nodal points.

*Institute for Materials Science at Los Alamos National Laboratory.

9:24AM E38.00008: How many tunable parameters to attain a spin degeneracy between Landau levels? CHONG WANG (Presenter), DUAN WENHUI, Tsinghua University, LEONID GLAZMAN, ARIS ALEXANDRADINATA, Yale University — The spin degeneracy of Landau levels is generically lifted by the Zeeman interaction, and also by the spin-orbit coupling in non-centrosymmetric solids. In the absence of any crystalline point-group symmetry, such a spin degeneracy can only be found by tuning three real parameters; we have exhaustively identified all symmetry classes of solids for which this number is reduced from three. In particular, only one parameter is needed in the presence of rotational symmetry; this parameter may be the magnitude or orientation of the field, or the bias voltage in tunneling spectroscopy. Signatures of single-parameter tunability include: (i) a smooth crossover between period-doubled and -undoubled quantum oscillations in the low-temperature Schubnikov-de Haas effect, and (ii) "magic angle" magnetoresistance oscillations. Case study is discussed for the Rashba-Dresselhaus two-dimensional electron gas subject to an arbitrarily oriented magnetic field.

9:36AM E38.00009: Implementation and application of a real-space pseudopotential method for calculating magnetocrystalline anisotropy* MASAHIRO SAKURAI (Presenter), JAMES CHELIKOWSKY, University of Texas at Austin — We present a real-space pseudopotential method for calculating magnetocrystalline anisotropy within relativistic density-functional theory. Our formalism is implemented in our real-space pseudopotential code, PARSEC, which is explicitly designed for an efficient implementation on a parallel computing platform (Phys. Rev. Materials 2, 084411 (2018)). We demonstrate that our formalism works well for prototypical transition-metal compounds, such as YCo5 and Mn2Ga, yielding an accurate magnetization and a magnetocrystalline anisotropy constant consistent with previous work. We also use our method to explore possible candidate materials for rare-earth-free permanent magnets. We find that ZrCo5 compounds can provide moderate magnetocrystalline anisotropy and sufficient work is supported by the National Science Foundation (NSF), DMREF-1729202. HPC resources were provided by the Texas Advanced Computing Center (TACC).saturation magnetization (Phys. Rev. Materials 2, 084410 (2018)).

*Our work is supported by the National Science Foundation (NSF), DMREF-1729202. HPC resources were provided by the Texas Advanced Computing Center (TACC).

9:48AM E38.00010: Strain control of the Néel vector in L10-type Mn-based antiferromagnetic materials: a first principles study* IN JUN PARK (Presenter), ROGER LAKE, University of California, Riverside — Mn-based antiferromagnetically ordered L10-type crystals such as MnIr, MnRh, MnNi, MnPd, and MnPt are of interest for possible electronic or spintronic applications. We used first-principles calculations to study the effect of strain on the magnetic anisotropy of those materials. The strain is applied along one axis (a) of the basal plane, and the structure and lattice vectors in the other two directions (b,c) are fully relaxed. We found that by applying strain, the direction of the Néel vector can be rotated by 90° for all materials. For MnIr, MnRh, MnNi, and MnPd, the Néel vector rotates within the basal plane. The sign of the effect, whether compression along the a-axis leads to a parallel or perpendicular Néel vector, depends on the specific material. MnPt is unique among this material family, since, at zero strain, its Néel vector lies along the c-axis, and strain along the a-axis rotates it into the basal plane.

*This work was supported as part of the Spins and Heat in Nanoscale Electronic Systems (SHINES) an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0012670.
10:00AM E38.00011: First-principles calculations of magneto-optical Kerr effect in high Neel temperature antiferromagnetic Metals*  KRITHIK PUTHALATH (Presenter), Physics, University of Illinois at Urbana-Champaign, KISUNG KANG, ANDRE SCHLEIFE, Materials Science and Engineering, University of Illinois at Urbana-Champaign — Recent developments in spintronics have suggested the use of high Neel temperature antiferromagnetic (AFM) materials in memory devices due to their vanishing stray fields and robust magnetic structure for ultra-fast spin dynamics in the terahertz regime. In particular, the optical response of these magnetic materials via the Kerr effect (MOKE) provides an excellent method to probe surface magnetization and elucidate the AFM state under external magnetic fields. In this work, we use first-principles density functional theory calculations to obtain the fully relativistic dielectric tensor to predict MOKE signals for Cr$_2$As, Mn$_2$As, Fe$_2$As, MnPt and Mn$_2$Au under external magnetic fields. We further corroborate experimental measurements by obtaining the magnetic susceptibility from first principles using a spin-tilting method. Finally, we explore the implications of applying external magnetic bias in AFMs by interpreting the electronic band structure and its evolution with respect to spin-orbit coupling and magnetization, to better understand the origins of the predicted MOKE signals.

*Illinois MRSEC NSF DMR-1720633

10:12AM E38.00012: Geometrical indicators for magnetism in Pt clusters*  ROBERTO D'AGOSTA (Presenter), University of the Basque Country, CONO DI PAOLA, FRANCESCA BALETT, Physics, King's College London — With "There is plenty of room at the bottom", Feynman points at the nanoscale where new phenomena take place, in particular when the behaviour of "a few" influences "many" particles. In particular, in nanoparticle physics, the lack of periodicity stabilises isomers whose morphology is impossible in crystalline bulk. At the same time, the physical properties of a mono-metallic nanocluster depend strongly on its shape and size. For example, catalytic properties rely on the presence of specific and diverse adsorption sites. By playing with size and shape of the nanocluster, we modify its properties towards tailored applications. We show that magnetism arising in nano-sized Pt objects is due to an effect present in the second coordination shell [1]. We demonstrate how magnetism is affected by the surrounding environment in the case of small Pt-nanoclusters embedded in zeolite pores [2]. Hopefully, we can identify geometrical indicators that help in designing clusters.


* C.D.P. and F.B. have been supported by the U.K. research council EPSRC (Grant No. EP/G003146/1). R.D'A. acknowledges support by Select-DFT (Grant No. FIS2016-79464-P).

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E39 GMAG DMP: Magnetic Nanostructures and Nanoparticles BCEC 207 - Katrin Schultheiss, Helmholtz-Zentrum Dresden-Rossendorf - Tag(s): Focus
8:00AM E39.00001: Topological Magnetic Writing: Controlling the magnetic state of nanostructures∗ [Invited] JACK C GARTSIDE, DAAN M ARROO, ALEXANDER VANSTONE, LESLEY COHEN, WILL BRANFORD (Presenter), Physics, Imperial College London — Networks of magnetic nanostructures are of broad interest from novel data storage and computation to magnonic crystals. One family of nanomagnetic arrays, characterized by strong and frustrated magnetic interactions are the artificial spin ices (ASI).1 ASI structures have provided vast amounts of physical insight in recent years in part due to their ability to model complex systems and exhibit exotic phenomena such as ‘magnetic monopole’-like states.2 The power of these networks stems from the extraordinary number of unique microstates, even in systems comprising relatively few nanostructures. However, magnetic nanoarrays in general, and ASI structures in particular, have yet to realise their full potential as the majority of microstates remain inaccessible due to the rudimentary state-writing tools currently available. An experimental means to prepare all potential microstates has huge implications, including realising ASI as a tunable-bandgap magnonic crystal3 or reconfigurable neural-network4. We present a novel MFM-tip based state writing technique,5 building on our previously demonstrated domain-wall injection process.6 It requires no global fields and is applicable to all nanostructure architectures, providing control over the spin-configuration and access to every possible microstate. We demonstrate our method via realisation of several exotic and thus-far unobserved states, unachievable via global field-protocols: ‘magnetic monopole-defect’ chains and the spin-crystal ground state of kagome ASI.


*The work was funded by Leverhulme Trust Research Project Grant RPG-2017-257

8:36AM E39.00002: Enhanced interaction strength in perpendicular artificial spin ice arrays∗ SUSAN KEMPINGER (Presenter), YU-SHENG HUANG, PAUL EDWARD LAMMERT, Pennsylvania State University, MICHAEL VOGEL, JOHN E. PEARSON, AXEL F HOFFMANN, Argonne National Lab, VINCENT HENRY CRESPI, Pennsylvania State University, PETER E SCHIFFER, Yale University, NITIN SAMARTH, Pennsylvania State University — Perpendicular implementations of artificial spin ice are appealing as a custom designed, frustrated system due to the optical accessibility of the magnetic components. This allows for complete microstate characterization in situ with an applied field using magneto-optical Kerr effect microscopy. We have fabricated arrays of lithographically patterned, single-domain Pt/Co multilayer islands. Studies on this system thus far have been limited by the weak interactions between islands that fit the constraints necessary for optical accessibility. New samples fabricated with a permalloy underlayer show an enhancement in correlation and allow for studies beyond the weakly interacting regime. We study both the quasi-dynamic hysteresis and demagnetized states of these systems to gain an understanding of how the coupling is affected by the soft underlayer.

*This project was funded by the US Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under Grant No. DE- SC0010778

8:48AM E39.00003: Role of Lattice Defects in Artificial Spin Ice Studied with Coherent X-ray Scattering and XMCD-PEEM∗ XIAOQIAN M CHEN (Presenter), Lawrence Berkeley National Laboratory and University of Kentucky, BARRY W FARMER, JUSTIN WOODS, LANCE DE LONG, Physics, University of Kentucky, SUJOY ROY, ALS, Lawrence Berkeley National Laboratory, JEFFREY T HASTINGS, Electrical and Computer Engineering., University of Kentucky — Magnetically frustrated materials are unable to satisfy all competing interactions simultaneously. The introduction of a small defect in such a system can completely alter the ground state. We used coherent x-ray scattering and XMCD-PEEM to investigate the role of lattice defects in artificial spin ice. We observed reduced blocking temperature and the broadening of the phase coexistence region with increased doping. In addition, we observed defect pinnings of superdomain walls in a nontrivial manner as the temperature is varied through the transition.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0016519.
From ordering piles of sand [1] to comprehending the human mind [2], spin glass systems continue to inspire theorists and experimentalists alike. Artificial nanomagnet fabrication [3] offers a unique opportunity to directly visualize the dynamics of glassy systems. However, spin glass phases have only been discovered at finite temperature in systems embedded in dimensions greater than or equal to 3 [1,4]. In this study we fabricate Nanomagnet arrays such that the network of their interactions possesses an effective dimension [5] higher than 2. Dubbed the Bethe glass, this is first finite temperature spin glass embedded in two dimensions. Using XMCD [6] the time scale free relaxation of magnetic moments is filmed in real space, directly observing the supermetric qualities of [1] spin glass. Further, the effective dimension is varied to show the tunability of glass properties.


The fabrication of three-dimensional (3D) magnetic nanostructures is currently a central topic in nanomagnetism [1]. Ferromagnetic nanowires (NWs) and nanotubes (NTs) are potential candidates for magnetic data storage, logic and sensing, and Focused Electron Beam Induced Deposition (FEBID) could play a crucial role in the fabrication of these architectures [2].

We have developed a new approach to grow core-shell heterostructures by FEBID [3], obtaining Co@Pt and Fe@Pt NWs, and Co NTs [4]. In addition, annealing treatments of Co NWs have been found to increase metal purity, crystallinity and magnetic induction [5].

Furthermore, we report on the fabrication of Magnetic Force Microscopy (MFM) tips by FEBID, showing great performance. Tailored Co and Fe MFM tips have been tested, both in ambient conditions and liquid environment, getting outstanding mechanical stability, resolution and sensitivity [6,7]. In particular, Fe tips with a 7 nm-wide sharp end exhibit low sample-tip magnetic interaction, which has been useful to measure complex magnetic states such as skyrmions [7].


We have observed asymmetric electrical transport in macroscopic samples of artificial magnetic honeycomb lattice of Permalloy having ultra-small elements with length scales of sub - 10nm to 30nm. The unidirectional enhancement of conductivity, analogues to a semiconductor diode, is dependent on thickness of the Permalloy as well as the order of honeycomb and can persist up to room temperature. The Permalloy honeycomb lattice exhibit very small rectification voltage and power dissipation compared with semiconductor diodes, which could have strong implication for spintronics. We will present detailed investigation done on the system and shed some light on the possible mechanism behind the asymmetric transport phenomena.

*The research at MU is supported by the US Department of Energy, Office of Basic Energy Sciences under grant no. DE-SC0014461.
10:00AM E39.00007: Field and current control of the electrical conductivity of an artificial two-dimensional honeycomb lattice* YIYAO CHEN (Presenter), BROCK T SUMMERS, ASHUTOSH DAHAL, Department of Physics and Astronomy, University of Missouri, VALERIA LAUTER, Neutron Scattering Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, GIOVANNI VIGNALE, DEEPAK K SINGH, Department of Physics and Astronomy, University of Missouri — The conductivity of a neodymium-based artificial honeycomb lattice undergoes dramatic changes upon application of magnetic fields and currents. We attribute these changes to a redistribution of magnetic charges that are formed at the vertices of the honeycomb due to the non-vanishing net flux of magnetization from adjacent magnetic elements. We suggest that the application of a large magnetic field or a current causes a transition from a disordered state, in which magnetic charges are distributed at random, to an ordered state, in which they are regularly arranged on the sites of two interpenetrating triangular Wigner crystals.

*The research at MU is supported by DOE, Office of Basic Energy Sciences under grant no. DE-SC0014461.

10:12AM E39.00008: Dynamic hysteresis loops of iron oxide nanoflowers ZOE BOEKELHEIDE (Presenter), JACKSON MILLER, Lafayette College, CORDULA GRÜTTNER, micromod Partikeltechnologie GmbH — Iron oxide nanoparticles have many potential applications in biomedicine, including magnetic hyperthermia and magnetic particle imaging. These applications depend sensitively on the magnetization ($M$) of the particles under a rapidly oscillating applied field $H$. The internal structure of nanoparticles strongly affects the magnetic behavior. Iron oxide nanoflowers, particles composed of several small crystallites fused together with an irregular surface, are promising for magnetic hyperthermia due to their large loss power [1]. We present dynamic measurements of $M(H)$ at 230 kHz for iron oxide nanoflowers. The nanoflowers were synthesized by a polyol method described previously [2]. The cores are 22 ± 9 nm and are coated in dextran (synomag®-D). The particles are suspended in H$_2$O at 14.2 mg(Fe)/mL. The resulting $M(H)$ curves show linear behavior (open ellipsoidal loops) at low fields, transitioning to nonlinear behavior at a field of 6 kA/m. These results show directly the magnetic reversal behavior of iron oxide nanoflowers in the linear and nonlinear regimes, and will help guide applications of these particles.

References:


10:24AM E39.00009: Room temperature ferromagnetic MnCr2O4 spinel chromite nanoparticles EDUARDO MARTÍNEZ-TERÁN (Presenter), RAJU BARAL, HARIKRISHNAN NAIR, AHMED EL-GENDY, University of Texas, El Paso — MnCr2O4 spinel is a non-collinear ferrimagnet with transition temperature around 43 K. By means of reducing the particle size to nanoscale regime, the magnetic behavior changes to long-range ferromagnetic order and the transition temperature shifts to above 400 K. MnCr2O4 nanoparticles were synthesized successfully using supercritical conditions of liquid. Changing the reaction conditions, in particular, increasing the reaction time leads to reducing the particles size as well as increasing the magnetic properties of the formed MnCr2O4 nanoparticles. Crystal structures of the synthesized bulk and their nano-sized candidates were investigated using XRD revealing the same spinel cubic symmetry Fd-3m. Morphology of all samples has been identified using SEM yielding average size of 535±75 nm for bulk sample and 223±50, 195±40, 172±30, 148±27 nm for nanoparticles prepared at reaction time of 2, 4, 6, and 8 hours respectively. The results yield room temperature ferromagnetic behavior at 300 K with magnetization of 6.5, 8.4, 10.8, 17 emu/g, for 223±50, 195±40, 172±30, 148±27 nm respectively. The obtained results confirm the role of reducing the particles size in enhancing the magnetic properties and open new route to probe the ferroelectricity as well as multiferroicity of this system.

10:36AM E39.00010: Coercivity Distributions in BiFeO3 nanoparticles* EDWIN RAMOS (Presenter), ALEXANDER CARDONA, JUAN RAMIREZ, Department of physics, University of the Andes — We study the effect of distribution of coercivities with the calcination temperature, using the first order reversal curves (FORC) treatment in BiFeO3 nanoparticles prepared by sol-gel method. We varied the calcination temperature in order to control the NP size. XRD measurements suggest that at lower temperatures (450°C and 550°C) the BFO NPs are single phase. At higher temperatures an impurity phase at higher appears with magnetic contribution. The FORC treatment was built as a linear combination for each temperature value. The coercivity distributions were obtained extracting the central ridge of the resultant FORC diagrams and contrasted with magnetization as a function of magnetic field measures. These results evidence a decreasing in the coercivity average that we associate to a decrease of magnetic domain size; then, suggesting a transition from single domain to superparamagnetic particles.

*Partial Funding provided by Vicerrectoria de Investigaciones Universiad de los Andes.
Magnetically controlled geometry of flexible ferromagnetic rings

KOSTIANTYN YERSHOV (Presenter), Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01171 Dresden, Germany, DENIS D. SHEKA, Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine, VOLODYMYR P. KRAVCHUK, Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01171 Dresden, Germany, AVADH SAXENA, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, YURI GAIIDIDEI, Bogolyubov Institute for Theoretical Physics of National Academy of Sciences of Ukraine, 03143 Kyiv, Ukraine — We propose a minimal extension of the anisotropic Heisenberg model in order to describe flexible magnetic wires (rings) [1]. Flexible ferromagnetic wires are spin-chain magnets, in which the magnetic and mechanical subsystems are coupled. The coupling between the magnetic and mechanical subsystems is driven by uniaxial anisotropy with the easy-axis oriented along the tangential direction. First, we show that depending on the magnetic and elastic parameters and the size of the system one can obtain two different states: the onion state with the quasi-uniform magnetization is typical for small enough rings, while the vortex state with the magnetization oriented tangential to the wire is preferable for large systems. Second, we demonstrate that according to the system symmetry there can appear normal modes with zero frequency (i.e. zero modes) on the background of equilibrium states. [1] Yu. Gaididei et al, arXiv:1809.10622 (2018).

Tuesday, March 5, 2019 8:00 AM - 10:48 AM

Session E40 GMAG DMP: Magnetic Excitations in Oxides

8:00AM E40.00001: Optical signatures of a 3D electronic liquid crystal in Cd2Re2O7 [invited] DAVID HSIEH (Presenter), Physics, California Institute of Technology — In the presence of strong interactions, the fluid of mobile electrons in a metal can spontaneously break the point group symmetries of its underlying host lattice, forming an electronic analogue of a classical liquid crystal. The experimental discovery of 2D electronic liquid crystals (ELCs) was first made nearly 20 years ago in semiconductor heterostructures and has since been reported in many other systems including the copper- and iron-based high-temperature superconductors. However whether or not a 3D version of an ELC can exist has remained unclear. In this talk, I will present signatures of a 3D ELC in the strongly spin-orbit coupled metallic pyrochlore Cd2Re2O7 detected using ultrafast coherent phonon spectroscopy and a recently developed spatially-resolved nonlinear optical polarimetry technique.

8:36AM E40.00002: Nature of magnetic excitations in the spin-1/2 triangular antiferromagnet Ba3CoSb2O9 in applied magnetic field* LUWEI GE (Presenter), School of Physics, Georgia Institute of Technology, QING HUANG, Department of Physics and Astronomy, University of Tennessee, Knoxville, TAO HONG, Oak Ridge National Laboratory, HAILONG ZHOU, Department of Physics and Astronomy, University of Tennessee, Knoxville, JIE MA, Department of Physics and Astronomy, Shanghai Jiao Tong University, MARTIN MOURIGAL, School of Physics, Georgia Institute of Technology — Ba3CoSb2O9 is one of the very few experimental realizations of the spin-1/2 triangular antiferromagnets. Despite the model being extensively studied, a unified understanding of the compound’s zero-field magnetic excitations has not yet been achieved. Spin-wave theory up to 1/S correction clearly failed to describe the whole picture. However, whether this is indeed due to the intrinsic nature of the spin Hamiltonian remains debatable. Seeking more experimental evidence, we investigated the system’s field-induced states with inelastic neutron scattering, particularly in the low-field regime. While revealing some yet unexplained features, our results show some strong damping of the excitation branch around K point, consistent with the field-induced magnon decay scenario. Our results are expected to help obtain a better understanding of the system.

*The work at Georgia Institute of Technology was supported by NSF-DMR-1750186. The work at University of Tennessee, Knoxville was supported by NSF-DMR-1350002.
modes in the 2500 – 3500 cm⁻¹ range in Fe₂Mo₃O₈ at low temperatures. We attribute them to optical transitions from the analysis and complimentary DFT and DMFT lattice dynamics calculations. At temperatures below and below the magnetic transitions. Experimental data for optical phonons are compared to group theoretical mode studied in a wide temperature range by means of infrared (IR) reflectivity and Raman scattering at the temperatures above and below the magnetic transitions. Experimental data for optical phonons are compared to group theoretical mode transitions. We attribute them to optical transitions from the ground state to the split levels of the ⁵T₂ state of Fe²⁺ ions in the tetrahedral coordination.

*T.N.S., A.A.S., Y.W. and S.W.C. were supported by U.S. Department Energy DOE DE-FG02-07ER46382. Z.L., NSLS-II, BNL acknowledges DE-AC98-06CH10886 and CDAC DE-NA-0002006 support. A.P.L. was supported by the State of Texas via the Texas Center for Superconductivity.

**8:00AM E40.00004: Non-Reciprocal Directional Dichroism of THz Radiation in Multiferroic Sr₂CoSi₂O₇**

JOHAN VIROK (Presenter), URMAS NAGEL, TOOMAS ROOM, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, DÁNIEL GERGELY FARKAS, Department of Physics, Budapest University of Technology and Economics and MTA-BME, Budapest, Hungary, PETER BALLA, Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary, DÁVID SZALLER, Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria, VILMOS KOCSIS, YUSUKE TOKUNAGA, YASUJIRO TAGUCHI, YOSHINORI TOKURA, RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan, BENCE BERNÁTH, DMYTRO KAMENSKYI, High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, The Netherlands, ISTVAN KEZSMARKI, Experimental Physics 5, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, Germany, SANDOR BORDACS, KARLO PENC, Department of Physics, Budapest University of Technology and Economics and MTA-BME, Budapest, Hungary — Directional dichroism (DD) is the effect when material absorbs light beams travelling in opposite direction differently. At THz frequencies DD has been found in multiferroics with magnetic and charge order. In these materials the spin waves are coupled to the oscillations of electric polarization. A spin wave acquires electric dipole activity due to optical magnetoelectric (ME) coupling and therefore interacts with the electric component of the THz radiation in addition to magnetic component. We studied spin excitations in Sr₂CoSi₂O₇ below 2 THz between 3 and 100 K and in magnetic fields up to 30 T. Almost one-way transparency is seen in some spin wave modes. What is more, the DD increases above the Neel temperature (7 K) in high magnetic field. This is unusual in multiferroics but is explained by the ME coupling on a single spin site [1]. This study demonstrates that DD exists in multiferroics with the single spin site ME interaction even above the magnetic ordering temperature when sufficiently strong polarizing external magnetic field is applied [2].


*This research was supported by the Estonian Ministry of Education and Research Grant IUT23-3 and by the European Regional Development Fund project TK134.

**9:12AM E40.00005: Resonant inelastic x-ray scattering study the evolution of spin and charge excitations in La₂₋ₓCeₓCuO₄ combi-films**

JIAQI LIN (Presenter), JIE YUAN, Institute of Physics, Chinese Academy of Sciences, SCHMITT THORSTEN, Paul Scherrer Institute, KEJIN ZHOU, Diamond Light Source, KUI JIN, Institute of Physics, Chinese Academy of Sciences, XUERONG LIU, School of Physical Science and Technology, ShanghaiTech University — We present resonant inelastic x-ray scattering (RIXS) study of spin and charge excitations in La₂₋ₓCeₓCuO₄ combi-films. The doping level of the film changes continuously from one tip to the other, nominally x=0.10 to x=0.19. Doping dependence is accomplished by simply translating the film in a fine step along the doping gradient direction. We explored the evolution of spin and charge excitations from an optimal doped superconductivity at x=0.11 to an overdoped fermi liquid at x=0.18. As doping, the energy of both spin and charge excitations is hardening. For the width, the spin excitation is broadening, and the charge excitation becomes sharpening. In addition, we performed L and incident energy dependence measurements to examine the characteristics of two excitations. Spin excitation does not have L dependence nor incident energy dependence, while charge excitation has L dependence and slightly incident energy dependence. This indicates spin and charge excitations are not the two faces of the coin. Instead, spin and charge excitations are derived from short-range correlation and long-range Coulomb interaction, respectively.
polarization configuration $h_\omega \parallel c$ and $e_\omega \parallel b$ and observed a significant change in the spectrum between 80 K and 120 K ferroelectric phase below $T_C \approx 833$ K, there is a strong continuous change in phonon profiles involving the two non-mid-infrared spectral range. While up to 300 K our measurements are in agreement with known spectra, in the THz dielectric permittivity shows hysteresis between 80 K and 120 K that does not occur for any other orientations. In addition, we have observed a magnon with a frequency of 840 GHz at 10 K that red shifts with increasing temperature until 70 K. At which point, its spectral weight decreases rapidly, while at the same time a lower frequency magnon gains intensity. This behavior is only observed for $h_\omega \parallel c$ irrespective of the direction of the electric field of the THz pulse. These behaviors seem to be associated with the decrease in the population of the B magnetic phase and simultaneous increase in the population of the A phase around 100 K.


9:36AM E40.00007: Hysteresis of THz dielectric permittivity below $T_{\text{Neel}}$ in CaFe$_2$O$_4$*  

DANIEL HELIGMAN (Presenter), THUC MAI, Physics, Ohio State University, LUNYONG ZHANG, Laboratory for Pohang Emergent Materials and Max Plank POSTECH Center for Complex Phase Materials, Pohang University of Science and Technology, Pohang 790-784, Korea, JAE WOOK KIM, Physics and Astronomy, Rutgers University, SANG-WOOK CHEONG, Rutgers University, Physics and Astronomy, and Laboratory for Pohang Emergent Materials and Max Plank POSTECH Center for Complex Phase Materials, Pohang University of Science, ROLANDO VALDES AGUILAR, Physics, Ohio State University — CaFe$_2$O$_4$ is a quantum antiferromagnet that exhibits an interplay between two different magnetic phases below $T_{\text{Neel}} \sim 200$ K. We have analyzed the terahertz (THz) response of CaFe$_2$O$_4$ for the polarization configuration $h_\omega \parallel c$ and $e_\omega \parallel b$ and observed a significant change in the spectrum between 80 K and 120 K for frequencies above 900 GHz. The THz dielectric permittivity shows hysteresis between 80 K and 120 K that does not occur for any other orientations. In addition, we have observed a magnon with a frequency of 840 GHz at 10 K that red shifts with increasing temperature until 70 K. At which point, its spectral weight decreases rapidly, while at the same time a lower frequency magnon gains intensity. This behavior is only observed for $h_\omega \parallel c$ irrespective of the direction of the electric field of the THz pulse. These behaviors seem to be associated with the decrease in the population of the B magnetic phase and simultaneous increase in the population of the A phase around 100 K.

*Funding for this research was provided by the Center for Emergent Materials: an NSF MRSEC under award number DMR-1420451.

9:48AM E40.00008: H-ErMnO$_3$ electrodynamics from far-infrared emission, reflectivity, and absorption in the ferroelectric and paraelectric phases  

NESTOR MASSA (Presenter), CEQUINOR, CONICET- UNLP, La Plata, Argentina, LEIRE DEL CAMPO, CNRS-CEMHTI, Orléans, France, KARSTERN HOLLDACK, HZB, BESSY II, Berlin, Germany, VINH TA PHUOC, GREMAN, Tours, France, PATRICK ETCHEGUT, CNRS-CEMHTI, Orléans, France, PAULA KAYSER, CSEC-UE, Edinburgh, UK, JOSÉ ANTONIO ALONSO, ICMM-CSIC, Madrid, Spain — We report on the temperature evolution of ambient non-centrosymmetric hexagonal H-ErMnO$_3$ -P6$_3$cm-(Z=6) from 2 K to decomposition as seen in absorption, near normal reflectivity, and emission spectra in the THz to mid-infrared spectral range. While up to 300 K our measurements are in agreement with known spectra, in the ferroelectric phase below $T_C \sim 833$ K, there is a strong continuous change in phonon profiles involving the two non-equivalent Er sites and bipyramids tilting. Three weak but sharp lowest frequency-lower temperature hybrid modes also melt into the background at about $T_C$. In emission spectra, toward the paraelectric centrosymmetric (P6$_3$ /mmc, Z=2) phase, an optical conductivity mid-infrared intraband becomes distinctive. It peaks at ~5000 cm$^{-1}$ and has the energy and profile fingerprint of small polarons (bipolarons). Its intensity depends on electric dipole ordering. At 900 K, just above $T_C$, this pronounce band starts a continuous weakening shifting to lower frequencies up to the temperature triggering hopping conduction onset of decomposition. We propose that oxygen polarizability (partially delocalized 2p-electrons) is a main dynamical constituent for bipolarons in cooperative driven MnO$_5$ bipyramids and thus in spontaneous ferroelectric polarization.
Managing magnon transport properties in bulk magnetic oxides within mesoscopic Boltzmann methods*  
YANXIA WANG, TAO LIU, WEI WANG, YUHENG LI, JIANWEI ZHANG (Presenter), School of Physics Science and Engineering, Tongji University — The bulk transport properties of magnon in magnetic oxides layers demand precise physical understanding of magnon diffusion, scattering and relaxation processes. In this work, we invent a novel magnon Boltzmann equation from full quantum magnon Hamiltonian. With changing thickness of magnetic oxide film (YIG), our numerical results on magnon accumulation and current show there are two different processes in bulk magnon transport: diffusion region and relaxation region. Furthermore, we theoretically discover physical origin for decreasing of magnon diffusion length with increasing magnetic field $H$, it was only observed in previous experimental works. And since magnon relaxation closely related to many magnons scattering, a new spatial dependent draft field was introduced, similar to anisotropy, which was describing collective local motion of magnon. More importantly, our results show magnon current can be manipulated by varying of anisotropy in magnetic oxides, especially in strong anisotropic energy materials, such as NiFe$_2$O$_4$ or CoFe$_2$O$_4$. In this framework, we also provide the methods to adjust the magnon transport with applying gradient magnetic field and gradient $T$ field.

*This work was supported by NSFC grant No. 51471119 & 51331004 and by MNSRP grant No. 2015CB921501.

Spin Structure Models of YFeO$_3$ from THz Spectroscopy Study*  
KIRILL AMELIN (Presenter), URMAS NAGEL, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, RANDY FISHMAN, Materials Science and Technology Division, Oak Ridge National Lab, Oak Ridge, Tennessee, USA, YOSHIYUKI YOSHIDA, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, Japan, HASUNG SIM, KISOO PARK, JE-GUEN PARK, Department of Physics & Astronomy, Seoul National University, Seoul, Korea, TOOMAS ROOM, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia — In YFeO$_3$ iron spins $S=5/2$ arrange in an antiferromagnetic (AFM) canted state $\Gamma_4(G_a F_{c} A_{1b})$ well above room temperature. With four spins per unit cell, its spin structure is described by a combination of exchange interactions, Dzyaloshinskii-Moriya (DM) interactions, and single-ion anisotropies (SIA). Since only Fe ions have the non-zero magnetic moment, this compound is a perfect modelling system for spin interactions and a step towards understanding more complex materials, possibly those with multiferroic properties.

We measured absorption of THz radiation in single crystals at the temperature 3 K in magnetic fields up to $B = 17$ T. THz spectroscopy can measure two out of four spin wave (SW) modes in YFeO$_3$, those with zero-field energies 1.2 and 2.4 meV. Combining the $B$ dependence of the SW modes with earlier inelastic neutron scattering results, we were able to quantify the parameters of DM interactions and SIA more precisely than was previously possible. We then evaluated different models of the spin structure and determined the one that represents magnetic interactions most accurately.

*We acknowledge the Estonian Ministry of Education and Research under Grant No. IUT23-03, and the European Regional Development Fund project TK134.

Terahertz emission spectroscopy of YIG | topological insulator bilayers*  
EVAN JASPER (Presenter), Department of Physics, The Ohio State University, JOHN S JAMISON, Materials Science and Engineering, The Ohio State University, TIMOTHY PILLSBURY, ANTHONY R. RICHARDELLA, NITIN SAMARTH, Department of Physics and Materials Research Institute, Pennsylvania State University, ROBERTO MYERS, Materials Science and Engineering, The Ohio State University, ROLANDO VALDES AGUILAR, Department of Physics, The Ohio State University — Building on the demonstration of terahertz (THz) emission spectroscopy (TES) in metallic ferromagnet | normal metal heterostructures, recent works have now observed the THz emission from heterostructure bilayers of both yttrium iron garnet (YIG) | Pt and Co | Bi$_2$Se$_3$. We examine the energy dependence of the spin-charge conversion efficiency of THz emission in samples of a few quintuple layers of Bi$_2$Se$_3$ and (Bi$_{24}$Sb$_{76}$)$_2$Te$_9$ grown on YIG(100) and YIG(111) substrates. We excite the samples with ultrafast femtosecond light pulses of both 1.55 eV and 3.10 eV. At 1.55 eV, no electrons in YIG are excited above the band gap of 2.85 eV. When we double the photon energy to 3.10 eV, electrons in the YIG are excited into the conduction band. Since both photon energies emit THz radiation, we expect that in each case the mechanism of emission will be attributed to different effects. Specifically, with excitations of 1.55 eV, the spin current process should be predominately generated by the spin-Seebeck effect. With excitations of 3.10 eV, the generation of spin current should be dominated by the direct photoexcitation of spin-polarized charge carriers.

*Funded by NSF through 2DCC-MIP (DMR-1539916) and CEM-MRSEC (DMR-1420451)
10:36AM E40.00012: Temperature dependent infrared spectroscopy on single crystals of YIG and Bi:YIG* RODICA MARTIN (Presenter), VALERIE AVENDANO, KEVIN SANTIAGO, CASEY KERKHOF, Physics and Astronomy, Montclair State University, IHOR SYDORYK, CATALIN MARTIN, Ramapo College — The insulating ferrimagnet yttrium iron garnet (YIG) has long been the material of choice for various optical and magneto-optical applications. Of particular interest is the use of YIG in optical isolators due to its large Faraday effect and good transparency over a broad spectral range in near/mid infrared. Bismuth doping has been shown to further increase the Faraday rotation. In this talk, we present temperature dependent (300 K to 4 K), broadband (10 meV to 3 eV) optical reflectance and transmittance on single crystals of YIG and Bi:YIG. We discuss the temperature dependence of vibrational modes in connection with magneto-optical properties, and assess the potential for using YIG and Bi:YIG in low temperature optical isolators.

*National Science Foundation - Major Research Instrumentation Grant 1625882

Tuesday, March 5, 2019 8:00 AM - 10:48 AM

Session E41 GMAG: Spin Hall effects BCEC 209 - Hailong Wang, Massachusetts Institute of Technology - Tag(s): Focus

8:00AM E41.00001: Unidirectional spin-Hall and Rashba–Edelstein magnetoresistance in topological insulator-ferromagnet layer heterostructures* [Invited] YANG LV (Presenter), Electrical and Computer Engineering, University of Minnesota, JAMES KALLY, Department of Physics, The Pennsylvania State University, DELIN ZHANG, Electrical and Computer Engineering, University of Minnesota, JOON SUE LEE, Department of Physics, The Pennsylvania State University, MAHDI JAMALI, Electrical and Computer Engineering, University of Minnesota, NITIN SAMARTH, Department of Physics, The Pennsylvania State University, JIANPING WANG, Electrical and Computer Engineering, University of Minnesota — The large spin–orbit coupling in topological insulators results in helical spin-textured Dirac surface states that are attractive for topological spintronics. These states generate an efficient spin–orbit torque on proximal magnetic moments. However, memory or logic spin devices based upon such switching require a non-optimal three-terminal geometry, with two terminals for the writing current and one for reading the state of the device. An alternative two-terminal device geometry is now possible by exploiting the recent discovery of the unidirectional spin Hall magnetoresistance in heavy metal/ferromagnet bilayers and unidirectional magnetoresistance in magnetic topological insulators. Here, we report the observation of such unidirectional magnetoresistance in a technologically relevant device geometry that combines a topological insulator with a conventional ferromagnetic metal. Our devices show a figure of merit (magnetoresistance per current density per total resistance) that is more than twice as large as the highest reported values in all-metal Ta/Co bilayers.

*This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.

8:36AM E41.00002: Giant Spin Hall Effect in Magnetron sputtered W3Ta thin films* MOHSIN ZAMIR MINHAS (Presenter), ILYA KOSTANOVSKIY, STUART S PARKIN, MAZHAR NAWAZ ALI, Max Planck Institute for Microstructure Physics — The spin Hall effect (SHE), in non-magnetic (NM) metals with strong spin-orbit coupling (SOC) has received much attention due to potential technological applications like magnetic random-access memory (MRAM) and spin-logic devices. Large spin Hall angles (SHA, the ratio of $J_S/J_C$) have been observed in materials like Pt and β-W (a.k.a. W3W in the A15-structure), particularly when doped with oxygen reaching a peak value of 0.45. Recently, W3Ta (and other A15 compounds) was theoretically predicted to host an even larger intrinsic SHE than β-W, originating from the large spin Berry curvature of its electronic band structure. Here we present experimental results on magnetron sputtered W3Ta thin films, fabricated in Hall bar geometries using standard lithography and deposition techniques. The SHA was measured using ST-FMR on films of various thicknesses. Also, SHAs of various $W_{4-x}Ta_x$ compositions will be presented and compared with theoretical predictions.

*Alexander von Humbolt Foundation Sofia Kovalevskaja Award Max Plank Society
Giant intrinsic orbital Hall effects in weakly spin-orbit coupled metals

DAEGEUN JO (Presenter), DONGWOOK GO, HYUN-WOO LEE, Department of Physics, Pohang University of Science and Technology — Recently, it was proposed that the intrinsic orbital Hall effect (OHE) can emerge from momentum-space orbital texture in centrosymmetric materials [1]. In searching for real materials with strong OHE, we investigate the intrinsic OHE in metals with small spin-orbit coupling (SOC) in face-centered cubic (Al, Mn, and Ni) and body-centered cubic structures (Li, V, Cr, and Mn). We find that these materials can have the giant orbital Hall conductivities (OHCs) $\sim 10^3 - 10^4 \,(h/e)(\Omega \text{cm})^{-1}$, which are comparable or larger than spin Hall conductivity (SHC) of Pt. We also show SHCs in these materials are sizable and the spin Hall angles may be of the order of 0.1, although SHCs are smaller than OHCs due to small SOC. We discuss implications on recent spin-charge interconversion experiments on materials having small SOC.


Ab initio calculation of intrinsic anomalous and spin Hall conductivity using localized pseudoatomic orbitals

JUWON OH (Presenter), HYOUNG JOON CHOI, Department of Physics, Yonsei University, Seoul 03722, Korea — For first-principles calculation of intrinsic anomalous Hall conductivity (AHC) and spin Hall conductivity (SHC), we implemented AHC and SHC formulas into the SIESTA code, which uses localized pseudoatomic orbitals to expand electronic wavefunctions. We calculate AHC from the Brillouin zone integration of the Berry curvature, and SHC by replacing a velocity operator in the AHC formula with a symmetrized product of spin and velocity operators. For AHC and SHC calculations, it is crucial to perform noncollinear-spin calculations including the spin-orbit coupling. We conduct AHC calculations of Fe, Co and SHC calculations of Pd, Pt and Ta. We compare our calculations with experimental results. We also investigate Berry curvature along high symmetry k points and the energy dependence of AHC and SHC.

Real-space Picture of the Intrinsic Anomalous Hall Effect

FEI XUE (Presenter), PAUL HANEY, National Institute of Standards and Technology — The intrinsic anomalous Hall effect is commonly expressed as the integral of Berry curvature in the reciprocal space. It has been shown that this intrinsic effect can also be computed in real space for systems which lack periodicity (e.g. finite or open systems). Motivated by this, we study a tight-binding toy model to show that the intrinsic anomalous Hall effect could be interpreted in terms of an electric field-induced change in the charge quadrupole moment. We additionally present a first-principle calculation of bcc Fe and demonstrate how the charge quadrupole moments changes in the presence of electric field. We also consider a real space interpretation of intrinsic anti-damping torques in a ferromagnet/heavy metal bilayer system.

Intrinsic spin Hall effect in nonmagnetic compounds

YANG ZHANG (Presenter), QIUNAN XU, Max Planck Institute for Chemical Physics of Solids, JAKUB ZELEZNY, TOMAS JUNGWIRTH, Institute of Solid State Physics, Czech Academy of Sciences, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, JEROEN VAN DEN BRINK, Leibniz Institute for Solid State and Materials Research, YAN SUN, Max Planck Institute for Chemical Physics of Solids — The spin Hall effect (SHE), i.e., conversion of charge current to spin current without magnetic moment, has gained intensive interests over the last decade since the study of its intrinsic mechanism and the observation of it in experiments. Owing to its natural functions of spin current generation, detection, and manipulation, SHE meets the fundamental requirements for the spintronics. In this work, we performed an extensive study of the intrinsic SHE for all the existing non-magnetic materials, and provide an intrinsic SHC database including approximately 20000 compounds. From this database, we extracted a universal origin for strong SHE, the mirror symmetry protected nodal lines that are gapped out by spin-orbit coupling. This extensive study of intrinsic SHE in materials via numerical predictions offers a good platform to experimental design strong SHE, and it is helpful for the comprehensive understanding of the SHE via statistical analysis.

This work was financially supported by the ERC Advanced Grant No. 291472 `Idea Heusler’, ERC Advanced Grant No. 742068–TOPMAT, Deutsche Forschungsgemeinschaft DFG under SFB 1143, and EU FET Open RIA Grant No. 766566 grant (ASPIN).
9:36AM E41.00007: Large spin Hall conductivity in Pt as measured with non-contact microwave spectroscopy
ANDREW BERGER (Presenter), Stanford Research Systems, ERIC EDWARDS, HANS T. NEMBACH, National Institute of Standards and Technology Boulder, ALEXY KARENOWSKA, Department of Physics, University of Oxford, MATHIAS WEILER, Walther-Meissner-Institut, OLOF KARISS, Department of Physics and Astronomy, Uppsala University, MARK KELLER, THOMAS SILVA, National Institute of Standards and Technology Boulder — By use of microwave spectroscopy, we have measured the spin Hall effect (SHE) and spin transparency in bilayers of Ni80Fe20/Pt. The method uses a phase-sensitive amplitude analysis of FMR spectra with unpatterned thin films that are proximate to, but not electrically connected with a coplanar waveguide [1]. Both SHE and iSHE are measured simultaneously, as mandated by Onsager reciprocity. The method does not require the samples to have an easy axis, nor knowledge of the precession angle. Damping is simultaneously measured, permitting self-consistent fitting of the SHE and spin pumping signals [2]. In agreement with previous reports [3], the spin transport efficiency between Ni80Fe20 and Pt is << 1, presumably due to interfacial spin memory loss. Also, the transparency is a strong function of deposition order, with a 3x reduction when Ni80Fe20 is grown on Pt. While the effective SHE signal and spin diffusion length are comparable to previous reports [4], substantial spin memory loss implies a larger value for the intrinsic SHE ratio of Pt (~ 0.4) than previously reported. [1] Berger, A. J., et al. (2018). PRB 97 094407. [2] Berger, A. J., et al. (2018). PRB 98 024402. [3] Rojas-Sánchez, J.-C., et al. (2014). PRL 112 106602. [4] Nguyen, M.-H., et al. (2016). PRL 116 126601

9:48AM E41.00008: Anisotropic and spin Hall magnetoresistance in FeRh/Pt bilayers* JOSEPH SKLENAR (Presenter), University of Illinois at Urbana-Champaign, HILAL SAGLAM, Materials Science Division, Argonne National Laboratory, JUNSEOK OH, GREG HAMILTON, University of Illinois at Urbana-Champaign, YI LI, Materials Science Division, Argonne National Laboratory, WEI ZHANG, Oakland University, MATTHEW GILBERT, University of Illinois at Urbana-Champaign, AXEL F HOFFMANN, Materials Science Division, Argonne National Laboratory, NADYA MASON, University of Illinois at Urbana-Champaign — We have sputtered epitaxial films of BCC FeRh with thicknesses between 7.5-35 nm on (100) MgO, capped with 5-nm Pt. Magnetometry and magnetotransport measurements indicate a first-order transition from ferromagnetic to antiferromagnetic order below room temperature. We have structured lithographically the films into Hall bars and nano-wires, such that the current is directed along different crystalline orientations. The angular-dependent magnetoresistance of all devices is measured in both the ferromagnetic and antiferromagnetic phase, and there is evidence for both intrinsic anisotropic magnetoresistance as well as spin Hall magnetoresistance contributing to the measured signal. In the antiferromagnetic phase we measure drastically different angular signals depending on whether the current is along the (100) or (110) direction.

*Work at The University of Illinois at Urbana-Champaign was supported by the National Science Foundation MRSEC program under NSF award number DMR-1720633. Work at Argonne was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division.

10:00AM E41.00009: Spin hall effect in SrIrO3 measured by spin torque ferromagnetic resonance XIAOXI HUANG (Presenter), Department of Materials Science and Engineering, University of California, Berkeley, ARNOUD EVERHARDT, Materials Science Division, Lawrence Berkeley National Laboratory, MAHENDRA DC, School of Physics and Astronomy, University of Minnesota, CHRISTOPH KLEWE, Advanced Light Source, Lawrence Berkeley National Laboratory, R RAMESH, Department of Physics, University of California, Berkeley, JIANPING WANG, School of Physics and Astronomy, University of Minnesota — A lot of research focus on spin Hall effect for the use of spintronic devices has been put on heavy metals such as Pt and topological insulators but there is rare research on spin Hall effect in complex oxide systems with strong spin orbit coupling effects. Complex oxides such as SrIrO3 with strong spin orbit coupling effects have drawn considerable research interest. We have studied spin torque ferromagnetic resonance (ST-FMR) induced by spin Hall effect in SrIrO3. Spin Hall angle of SrIrO3 as large as 0.36 is determined by ST-FMR, which is almost the same order as Ta. More interestingly, as thickness of SrIrO3 increases, spin Hall angle of SrIrO3 increases, while resistivity decreases.
10:12AM E41.00010: Detecting end states of topological quantum paramagnets via spin Hall noise spectroscopy*
DARSHAN G. JOSHI, ANDREAS P SCHNYDER, Max Planck Institute for Solid State Research, SO TAKEI (Presenter), Queens College — We theoretically study the equilibrium spin current fluctuations and the corresponding charge noise generated by the inverse spin Hall effect (ISHE) in a metal with strong spin-orbit coupling deposited on top of a quantum paramagnet. It is shown that the charge noise power spectra measured along different spatial axes can directly probe the different spin components of the boundary dynamic spin correlations of the quantum paramagnet. We report the utility of this ISHE-facilitated spin noise probe as a tool to unambiguously detect topological phase transitions in an $S = 1/2$ quantum spin ladder that hosts a trivial ground state of singlet product states, but topologically protected fractional spin excitations localized at its ends. Our work demonstrates the general usefulness of ISHE-mediated spin noise spectroscopy for the detection of topological phases in quantum paramagnets.

*S.T. acknowledges support from The Research Foundation of The City University of New York, Start-up Fund #90922-07 10.

10:24AM E41.00011: Electrical detection of Spin Hall effect in Tungsten films using a compact device geometry*
ARPITA MANDAL, SOUMIK AON, PARTHA MITRA (Presenter), Indian Institute of Science Education and Research, Kolkata — Direct detection of Spin Hall Effect (SHE) using electrical schemes continues to be an experimental challenge as there is no electrical voltage associated with the accumulation of electron spins of opposite signs at the edges of a standard Hall bar sample. We present a simple yet elegant measurement scheme that allows detection of spin accumulation using the well known concepts of non-local detection proposed by Johnson and Silsbee. We fabricated devices with pairs of voltage leads consisting of a ferromagnet (FM: Co or Py) and a normal metal (NM: Cu) suitably placed in contact with one of the spin accumulation edge of Tungsten (W) bar shaped films, so that other competing effects like ordinary Hall effect and magnetoresistance are minimised. We show that voltage difference measured between the FM and NM leads are a manifestation of the spin accumulation due to SHE. We present detailed temperature and magnetic field dependent study of the spin Hall conductivity extracted from the spin accumulation voltage.

*Ministry of Human Resources Development, Govt of India

10:36AM E41.00012: Temperature dependence of side-jump contribution to anomalous/spin Hall conductivities*
CONG XIAO (Presenter), Department of Physics, University of Texas at Austin, YI LIU, ZHE YUAN, The Center for Advanced Quantum Studies and Department of Physics, Beijing Normal University, SHENGYUAN YANG, Research Laboratory for Quantum Materials, Singapore University of Technology and Design, QIAN NIU, Department of Physics, University of Texas at Austin — The side-jump contribution to anomalous/spin Hall conductivities is conventionally understood to be a constant independent of both the scattering strength and density of scatterers, even though it depends on the type of scatterer. In this work, we reveal that the side-jump contribution due to electron-phonon scattering, the primary source of scattering in clean samples, can in fact acquire substantial temperature dependence when the temperature drops below the high-temperature classical regime of equipartition law. We demonstrate this phenomenon in an analytic model, supplemented by a first-principles calculation for pure Pt. Experimentally accessible high-purity Pt is proposed to be suitable for observing the predicted prominent variation of the spin Hall conductivity below 80 K.

*C.X. and Q.N. are supported by DOE (DE-FG03-02ER45958, Division of Materials Science and Engineering), NSF (EFMA-1641101) and Welch Foundation (F-1255). S.A.Y. is supported by Singapore Ministry of Education AcRF Tier 2 (MOE2017-T2-2-108). Y. Liu and Z. Yuan is supported by the NSFC (Grants No. 61604013, No. 61774018, and No. 11734004), the Recruitment Program of Global Youth Experts, and the Fundamental Research Funds for the Central Universities (Grants No. 2016NT10 and No. 2018EYT03).

Tuesday, March 5, 2019 8:00 AM - 10:12 AM

Session E42 DQI: Applications of Noisy Intermediate Scale Quantum Computers II BCEC 210A
- Andras Gyenis, Princeton University - Tag(s): Focus
8:00AM E42.00001: Algorithm-Centric Error Mitigation*  ED YOUNIS (Presenter), Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, WIM LAVRIJSEN, Computational Research Division, Lawrence Berkeley National Laboratory, KOUISHIK SEN, Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, AYDIN BULUC, MIROSLAV URBANEK, WIBE A DE JONG, COSTIN IANCU, Computational Research Division, Lawrence Berkeley National Laboratory — We derive algorithm-specific error mitigation procedures for VQE. The core idea is to determine which part of a circuit contributes most to the final output error and then harden only these sub-circuits. Using simulation with gate level noise injection, our results indicate that VQE is most sensitive to errors on the source qubit of CNOT gates, and relatively insensitive to errors on any other qubits or single gates, irrespective of the noise distribution. We then devise an algorithm that attempts to increase the fidelity of qubits that appear as sources of CNOT gates. Given a circuit, we determine the qubits that appear in most CNOT gates (contribute most to error) and use ancilla qubits to mimic their operations (same state) and periodically switch between the original and ancilla qubit during circuit operation. Simulation results indicate that the technique is able to improve the quality of the solution from the quantum circuit. This is confirmed by experiments on the IBM hardware, where for a 4-qubit VQE with one ancilla qubit we observe fidelity improving from 46% to 52%.

*This work was supported by the Office of Advanced Scientific Computing Research, Quantum Algorithms Team Program, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

8:12AM E42.00002: Implementation of Grover's quantum search algorithm with error mitigation at IBM Q computers  YULUN WANG (Presenter), ROBERT J HARRISON, PREDRAG KRSTIC, Institute for Advanced Computational Science, State University of New York at Stony Brook — We have constructed the quantum circuits for implementation of the N=4 qubits Grover algorithm at IBM Q quantum computers. The circuit efficiency was achieved by explicit use of the qubits topology, specific for the used machines. For comparison, we implemented the same approach for the 2 and 3 Grover's algorithms. While the classical simulation led to a high probability of finding the searched object, the running at the IBM Q quantum machine resulted to the search probability below the recognition. This was a consequence of the decoherence errors, which has grown with the number of the circuit elements. We have experimented with zero-noise extrapolation method as well as error correction codes to mitigate and correct the errors of the circuit, leading to improvements in the implemented search.

8:24AM E42.00003: Fundamental limitations for measurements in quantum many-body systems  THOMAS BARTHEL (Presenter), JIANFENG LU, Duke University — Dynamical measurement schemes are an important tool for the investigation of quantum many-body systems, especially in the age of quantum simulation. Here, we address the question whether generic measurements can be implemented efficiently if we have access to a certain set of experimentally realizable measurements and can extend it through time evolution. For the latter, two scenarios are considered (a) evolution according to unitary circuits and (b) evolution due to Hamiltonians that we can control in a time-dependent fashion. We find that the time needed to realize a certain measurement to a predefined accuracy scales in general exponentially with the system size – posing a fundamental limitation. The argument is based on the construction of ε-packings for manifolds of observables with identical spectra and a comparison of their cardinalities to those of ε-coverings for quantum circuits and unitary time-evolution operators. The former is related to the study of Grassmann manifolds.

Postponing the orthogonality catastrophe: efficient state preparation for electronic structure simulations on quantum devices*  
NORM TUBMAN (Presenter), CARLOS MEJUTO ZAERA, JEFFREY EPSTEIN, DIPTARKA HAIT, DANIEL LEVINE, WILLIAM HUGGINS, University of California, Berkeley, ZHANG JIANG, JARROD MCCLEAN, Ryan BABBUSH, Google, MARTIN HEAD-GORDON, BIRGITTA K WHALEY, University of California, Berkeley — Many proposals for efficiently simulating eigenstates of physical systems on quantum computers require that one can easily initialize wavefunctions with non-vanishing overlap on eigenstates of interest. Though there is now a large body of work exploring the costs of simulating electronic structure systems on a quantum computer, the challenge of preparing states with sufficient ground state support has so far been largely ignored. In this work we demonstrate that the adaptive sampling configuration interaction technique can be used to investigate the overlap issue. Using this technique, we find that easy-to-prepare single Slater determinants such as the Hartree-Fock state often have surprisingly robust support on the ground state for many applications of interest. For the most difficult systems, we introduce a method for preparation of multi-determinant states on quantum computers. We investigate several prominent applications of quantum simulations including organic molecules, transition metal complexes, the uniform electron gas, Hubbard models, and the quantum impurity models arising from embedding formalisms such as dynamical mean-field theory.

*This work was supported by the U.S. Department of Energy, Quantum Algorithm Teams Program.

Testing, analysis, and refinement of the quantum Metropolis algorithm  
JONATHAN MOUSSA (Presenter), Molecular Sciences Software Institute — The classical Metropolis algorithm has been adapted into a quantum algorithm [Temme et al., Nature 471, 87 (2011)] with three important drawbacks: (1) long-time Hamiltonian evolution is needed for precise phase estimation of system energies, (2) many repetitions are needed to successfully reject a Metropolis update with a low failure rate, and (3) thermal-state observables are not measured during the thermalization process. We present a revised quantum Metropolis algorithm that partially mitigates these drawbacks as evidenced by a combination of numerical experiments and theoretical analysis.

Simulating strongly interacting fermionic systems in a quantum computer  
ALEXANDRE CHOQUETTE-POITEVIN (Presenter), Univeristé de Sherbrooke, PANAGIOTIS BARKOUTSOS, IBM Research - Zurich, AGUSTIN DI PAOLO, ALEXANDRE FOLEY, DAVID SENECHAL, Univeristé de Sherbrooke, IVANO TAVERNELLI, IBM Research - Zurich, ALEXANDRE BLAIS, Univeristé de Sherbrooke — Noisy intermediate-scale quantum computation has the potential to be useful for the quantum simulation of small fermionic systems using variational quantum algorithms (VQA). Applications of hybrid quantum-classical approaches provide proof that VQAs are robust against noise and can handle limited qubit connectivity. In this talk, we approach a class of strongly interacting fermionic Hamiltonians formulated in the variational cluster approach by means of VQAs. More precisely, we tackle the problem of a 1D lattice to study the Mott transition. This work is a first step towards quantum simulation of larger and higher-dimensional strongly interacting electronic systems.

End-to-end quantum chemistry simulations with reduced errors*  
MIROSLAV URBANEK (Presenter), WIM LAVRIJSEN, WIBE A DE JONG, Computational Research Division, Lawrence Berkeley National Laboratory — Error reduction through suppression, mitigation, or correction is essential to enable quantum chemistry applications on a larger number of qubits accessible in Noisy Intermediate-Scale Quantum (NISQ) computers. We focus on the development of quantum chemistry algorithms running within the hybrid classical-quantum Variational Quantum Eigensolver (VQE) approach. VQE has been successfully demonstrated on quantum computers with a small number of qubits, but its performance on larger systems is currently limited by various sources of experimental noise. Our target is to develop quantum algorithms and computational circuits that exploit various error mitigation and correction techniques for initialization, gate operations, and measurement. This is necessary to reduce errors introduced by experimental conditions in NISQ systems. We compare theoretical and simulation results with results obtained in experiments.

*This work was supported by the Office of Advanced Scientific Computing Research, Quantum Algorithms Team Program, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
9:24AM E42.00008: Trotter Error Scaling with System Size in Quantum Simulations*  MATTHIAS TROYER (Presenter), Microsoft, NATALIE PEARSON, Theoretical Physics, ETH Zurich, DAVID POULIN, Université de Sherbrooke — A main concern when implementing digital quantum simulation on quantum computers or simulators is the number of gate operations required. The most common implementation uses the Trotter decomposition to map an arbitrary Hamiltonian onto realisable gates. However, the proven upper bounds on the error introduced using this method grows with the system size. In order to maintain the same accuracy this would imply that the time step has to shrink with system size, leading to a sharp increase in the number of gates required. We show empirically that for local Hamiltonians the error for local observables and their correlation functions is independent of system size. This results is obtained by simulating large one-dimensional quantum Ising model at and away from the critical point using a Trotter decomposition in imaginary time. We find that the Trotter errors saturate with increasing system size even at the critical points. We finally discuss long-range models and correlations in time.

*This work was supported by the Swiss National Science Foundation through the NCCR QSIT

9:36AM E42.00009: Improved optimization algorithm for use in variational quantum eigensolvers*  TITUS MORRIS (Presenter), Oak Ridge National Laboratory — Quantum algorithms for treating nuclear and electronic structure problems face a host of challenges in order to run successfully on both near-term and future fault tolerant quantum computers. For variation quantum eigensolvers (VQE), one such challenge is how to optimize parameters dictating the wavefunction efficiently i.e. with few function evaluations in the presence of noisy energy evaluation. This has typically been done with classic optimizers, but these will begin to pose problems as the parameter sets required to treat larger realistic systems grow. Here I present an algorithm that, at the cost of extra Pauli expectation values, allows for a faithful estimation of the parameter gradient of several classes of wavefunctions. I apply this algorithm to the treatment of the deuteron and H_2, and show that it gives a much faster convergence in terms of overall function evaluations when compared to classic optimizers, and this advantage increases with parameter set size. This presents a promising step forward in pushing for treating realistic systems with quantum computers.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR) quantum algorithms and testbed programs.

9:48AM E42.00010: Characterization of Training Circuits for Hybrid Quantum-Classical Algorithms*  SUKIN SIM (Presenter), Chemistry and Chemical Biology, Harvard University, PETER D. JOHNSON, Zapata Computing, Inc., ALAN ASPURU-GUZIK, Chemistry and Computer Science, University of Toronto — Performing useful computations with current and near-term quantum computers is becoming increasingly viable due to rapid advances in both algorithms and hardware. A class of algorithms that are promising candidates for demonstrating the utility of near-term quantum computers is the so called hybrid quantum-classical (HQC) algorithms. A common ingredient that plays a crucial role in the algorithmic performance of many HQC algorithms is the parametrized quantum circuit that is tuned to prepare quantum states relevant for (approximately) solving the problem of interest. Despite the importance of these circuits, they are often generated in the absence of a robust theoretical framework. In this work, we introduce several descriptors to characterize a set of parametrized circuits, including a measure of a circuit's expressibility and how it correlates with algorithmic performance. Ultimately, having a deeper understanding of the qualities associated with an effective parametrized circuit can lead to significant improvements in the overall development of HQC algorithms.

*Sukin Sim is supported by the DOE Computational Science Graduate Fellowship under grant number DE-FG02-97ER25308.
Error mitigation by symmetry verification on a variational quantum eigensolver*  

RAMIRO SAGASTIZABAL (Presenter), QuTech and Kavli Institute of Nanoscience, Delft University of Technology, XAVIER BONET-MONROIG, Lorentz Institute, Leiden University, MALAY SINGH, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, THOMAS E O’BRIEN, Lorentz Institute, Leiden University, MICHEL ADRIAAN ROL, CORNELIS CHRISTIAAN BULTINK, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, XIANG FU, QuTech and Quantum Computer Architecture Lab, Delft University of Technology, NANDINI MUTHUSUBRAMANIAN, ALESSANDRO BRUNO, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Current efforts to increase the accuracy of quantum algorithms focus on the design and implementation of low-cost techniques to mitigate the impact of errors while avoiding fully-fledged error correction schemes. Both simple and comprehensive, variational quantum eigensolvers provide an excellent platform for exploring error and accuracy trade-offs. We present the implementation of our own low-cost error detection scheme, named symmetry verification (SV). We demonstrate an order of magnitude improvement in accuracy while solving the hydrogen molecule in a transmon quantum processor. Furthermore, by matching measurements to simulations, we report a breakdown of noise sources with which we quantify the error mitigating effects of SV and its limitations.

*This research is funded by an ERC Synergy Grant, the Netherlands Organization for Scientific Research (NWO/OCW), the China Scholarship Council, and IARPA (U.S. Army Research Office grant W911NF-16-1-0071).

Tuesday, March 5, 2019 8:00 AM - 11:00 AM


Rotationally Controlled Atomic Layer Heterostructures*  

EMANUEL TUTUC (Presenter), University of Texas at Austin — Heterostructures of atomic layers such as graphene, hexagonal boron-nitride, and transition metal dichalcogenides (TMDs) can serve as testbed for novel quantum phenomena in two-dimensions (2D). A key ingredient that can add a new dimension to the atomic layer heterostructures palette is the rotational control and alignment of different 2D layers. We review here an experimental technique that enables rotationally controlled heterostructures with accurate alignment of individual layer crystal axes [1]. We illustrate the applicability of this technique to the realization of tunable moiré patterns in twisted bilayer graphene [2], and rotationally aligned double layers of graphene [3], or TMDs [4] separated by a tunnel barrier, which display resonant, energy- and momentum-conserving tunneling in vertical transport. Rotationally aligned double bilayer graphene separated by a WSe2 tunnel barrier, designed to study equilibrium indirect exciton formation, display a strongly enhanced tunneling at low temperatures when the two graphene bilayers are populated with carriers of opposite polarity and equal density [5]. The enhanced tunneling at overall neutrality departs markedly from single-particle model calculations, and suggests the emergence of a many-body state with when electrons and holes of equal densities populate the two layers.


*This work was supported by the National Science Foundation Grant EECS-1610008, Semiconductor Research Corp. Nanoelectronics Research Initiative SWAN center, and the Army Research Office under Grant No. W911NF-17-1-0312.*
**8:36AM E43.00002: Strain-induced Pseudo-Magnetic Fields and flat band in Graphene** [Invited] YUHANG JIANG (Presenter), Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, Piscataway, NJ 08855 USA — The discovery of free-standing 2D atomic layers ushered in a new era of materials whose properties can be shaped controlled and engineered by unconventional means such as strain, bend or twist. An externally imposed periodic potential breaks up the electronic band structure into a series of mini-bands which, under certain circumstances, become almost dispersionless. Such flat bands can occur naturally in the presence of a vector potential generated by a strain-induced periodic pseudo-magnetic field (PMF). Within these flat bands, the strongly suppressed kinetic energy favors the formation of interaction-driven exotic phases which can give rise to novel electronic properties. In this talk, I will present experimental results demonstrating two pathways to generate strain induced PMFs and flat bands. In the first method, a graphene membrane is supported and strained by a two-dimensional (2D) periodic array (~1mm) of Au nano-pillars grown on a hexagonal Boron Nitride (hBN) substrate. A direct measure of the local strain is achieved by scanning tunneling microscopy (STM) through the magnifying effect of the Moiré pattern formed against the hBN substrate. The strain-induced PMF (~10T) is obtained from the pseudo-Landau level spectra observed in scanning tunneling spectroscopy (STS). The second method utilizes the buckling transition of a compressed graphene membrane to generate a 2D periodic strain pattern. This produces spatially modulated PMFs with periods of order ~10nm and amplitudes exceeding 100T. Using STM, STS and numerical simulations we find that the pseudo-Landau levels associated with the strain-induced periodic PMF give rise to a flat-band at charge-neutrality, providing a pathway to engineering correlated phases by non-chemical means.  


**9:12AM E43.00003: Superconductivity in twisted graphene layers: electronic structure and interactions.** [Invited] FRANCISCO GUINEA (Presenter), Imdea Nanoscience, Madrid, Spain and School of Physics and Astronomy, University of Manchester, UK — A special feature of the states in the low energy bands of twisted graphene bilayers is that their charge distribution shows a significant momentum dependence. As a result, the filling of these bands leads to electrostatic potentials, which, in turn, modify the energy levels and the structure of the bands. The dependence of the band shape on the band filling can be described in terms of the emergence of new electron-electron interactions. We quantify and analyze these interactions, and discuss their relation with the observed superconducting and insulating states.

*This work was supported by the European Commission under the Graphene Flagship, contract CNECTICT-604391.

**9:48AM E43.00004: Transport in Twisted Bilayer Graphene at Extreme Angles** [Invited] PETER RICKHAUS (Presenter), Physics, ETH Zürich, JOHN WALLBANK, Centre for Ecology and Hydrology, Oxfordshire, SERGEY SLIZOVSKII, NRC Kurchatov Institute, Russia, RICCARDO PISONI, HISKE OVERWEG, YONGJIN LEE, MARIUS EICH, Physics, ETH Zürich, MING-HAO LIU, Department of Physics, National Cheng Kung University, Taiwan, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, Japan, KLAUS ENSSLIN, THOMAS IHN, Physics, ETH Zürich — Two misaligned layers of graphene exhibit intriguing transport properties that depend drastically on the twist angle. At very large twists, the system behaves similar to two decoupled graphene layers. Upon reduction of the angle, the graphene layers begin to couple, leading to a decrease in Fermi velocity. At a magical angle of 1.1°, superconductivity emerges [1]. Finally, at tiny twist angles, large regions of strongly coupled bilayer graphene dominate the transport. By gating, these regions can become insulating leading to a triangular network of topological channels [2]. An intriguing probe for transport phenomena in graphene consists in the formation of an electronic Fabry-Pérot interferometer [3,4]. P-n junctions serve as semi-transparent mirrors and exhibit relativistic phenomena such as Klein-tunneling and we discuss how they can be used to access the interesting physics twisted bilayer graphene at tiny [5] and at very large twist angles.


*European Graphene Flagship
NCCR QSIT: Quantum Science and Technology
SNF: Swiss National Foundation
10:24AM E43.00005: Electrically tunable frustrated lattices and magnetism in twisted bilayer graphene* [Invited]
JOSE LADO (Presenter), ETH Zurich, ALINE RAMIRES, ICTP-SAIFR, Brazil, LUIS ALBERTO GONZALEZ-ARRAGA, IMDEA Nanoscience, Madrid, Spain, FRANCISCO GUINEA, IMDEA Nanoscience, Madrid, Spain and School of Physics and Astronomy, University of Manchester, UK, PABLO SAN-JOSE, ICMM-CSIC, Madrid Spain — Twisted graphene bilayers have become a powerful solid-state platform to realize a plethora of electronic states, stemming from the emergence of controllable moire superlattices and their electrical tunability. Here we theoretically show that twisted bilayer graphene is a versatile platform to realize tunable frustrated magnets, by realizing triangular and Kagome lattices of localized modes in two dramatically different regimes [1,2]. First, for rotation angles around 1.5 degrees, we show that the magnetic instabilities of the emergent triangular AA lattice can be electrically controlled [1]. In particular, we show that the ferromagnetic and antiferromagnetic ordering inside the AA regions can be electrically switched, giving rise to superlattice spin spirals in the emergent triangular moire superlattice. Second, we show that in the tiny angle regime of 0.2 degrees, an emergent Kagome lattice of localized modes can be electrically generated, stemming from an artificial gauge field created by the interlayer bias [2]. In particular, we show that the microscopic properties of these Kagome modes are controlled by the magnitude of the electrically generated gauge field, yielding a powerful solid-state platform to experimentally engineer a paradigmatic model of frustrated magnetism. These rich and electrically controllable frustrated lattices provide a potential route to experimentally explore frustrated magnetism and quantum spin liquid physics in twisted graphene bilayers.


*J.L. acknowledges financial support from the ETH Fellowship program

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Tuesday, March 5, 2019 8:00 AM - 9:48 AM

Session E44 DCMP: New Developments in STM on Surfaces of Unconventional Superconductors and Related Systems BCEC 210C - Ilya Eremin, Ruhr University Bochum - Tag(s): Invited

8:00AM E44.00001: Determination of the superconducting gap sign by the phase referenced method: successful practice in cuprate and several iron based superconductors* [Invited] HAI-HU WEN (Presenter), Nanjing University — In many unconventional superconductors, the superconducting gap will change sign along the Fermi surface. The fundamental reason for this behavior is that the Cooper pairing may be established through a repulsive interaction, instead of the attractive interaction in phonon mediated pairing picture. However to detect this gap sign is not easy at all. The usual method for solving this problem is to measure the behavior of phase difference or supercurrent through a Josephson junction. However, this method seems not working well in systems with multi-Fermi pockets and with the same sign in individual pocket. Such circumstances happen in many iron based superconductors. In the superconducting state, quasi-particles (QPs) will be generated by thermal or pair breaking. These QPs with Bogoliubov dispersion are scattered from one momentum $k_1$ to another $k_2$ forming a standing wave with wave vector $q = k_1 - k_2$. All these standing waves interfere each other and form a particular pattern in the real space (QPI). By using STM we can measure these patterns. Through the Fourier transform on QPI patterns we can not only get the Fermi surface contour, but also obtain the gap feature, including the magnitude and sign for different $q$ vectors. This was called as the phase referenced QPI. Following this idea we have successfully detected the gap sign reversal in several iron based superconductors with and without the hole pockets. We can also directly visualize the d-wave gap in the typical cuprate superconductor Bi-2212.

References

*This work has been supported by the Chinese National Science Fouadation and the Ministry of Science and Technology of China.

8:36AM E44.00002: Pairing gap symmetry in optimally doped NaFeAs [Invited] ABHAY PASUPATHY (Presenter), Columbia University — TBD
9:12AM E44.00003: Lessons from modeling of tunneling spectroscopy on FeSe [Invited]  BRIAN ANDERSEN (Presenter), Niels Bohr Institute — Iron-based superconductors have been extensively studied both experimentally and theoretically over the last decade, with great progress in our understanding of these materials. Recent focus on FeSe has been centered on the connection between nematicity and superconductivity, and the possibility of enhancing Tc in monolayers on STO, or by pressure. In this talk, I will focus on two aspects of the theoretical study of tunneling spectroscopy on unconventional superconductors, 1) the physics of disorder generated local order, and 2) the understanding of recent scanning tunneling experiments mapping out the detailed spectroscopic features of FeSe by the Davis group at Cornell University. I will explain the recent evidence for orbital selective superconducting pairing, and the direct detection of orbital selective quasiparticles by quasi-particle interference. This highlights the correlated nature of FeSe, more specifically its Hund's metal nature with coexisting orbital-dependent coherent and incoherent low-energy states. I then proceed to discuss the theoretical modelling of these phenomena and the implications for our understanding of the magnetic properties of FeSe. This is relevant for understanding the origin of superconductivity in FeSe in particular, and in the iron-based superconductors in general.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E45 DCMP: Complex Oxide Surfaces, Interfaces, and Thin Films I BCEC 211 - David Lederman, UC Santa Cruz

8:00AM E45.00001: Mechanical strain-tuned magnetism and AFM Neel temperature by 90 K in PrVO3 thin films* WILFRID PRELLIER (Presenter), Laboratoire CRISMAT, CNRS/ENSICAEN/UNICAEN — The transition-metal oxides with ABO3 type perovskite structure show a strong coupling between spin-orbital and lattice degrees of freedom. Here, we present an experimental study of magnetic response to the residual strain in PVO thin films by growing PVO films on a variety of single crystal substrates and by varying PVO film thickness on a single crystal substrate. PrVO3 in bulk, being a strong antiferromagnet shows TN~ 130 K [1]. Our study reveals that the lattice distortion via misfit strain pave the way towards tuning the anti-ferromagnetic ordering temperature in PrVO3 thin films, resulting in a non-trivial evolution of the Neel temperature (TN) with substrate pseudo-cubic lattice parameter and PVO film thickness. We demonstrate that the strain produced via mechanical strain engineering, tune TN of PVO films in the range of 90 K. Moreover, we also show that PVO thin films show low temperature ferromagnetic behavior along with the insulating properties irrespective of the substrate. [1] Sage M H et. al. Phys. Rev. B 76 195102 (2007)

*This work is supported by ANR, LABEX and Region Normandie.

8:12AM E45.00002: Unusual Electronic Phase Separation Phenomena in Manganite Ultrathin Films  HONGYAN CHEN (Presenter), YANG YU, BAI YU, HANXUAN LIN, Fudan University, XIAOLONG LI, Chinese Academy of Sciences, HAO LIU, TIAN MIAO, YUNFANG KOU, Fudan University, YONGSHENG ZHANG, YAN LI, JIN TANG, Chinese Academy of Sciences, ZECHAO WANG, Tsinghua University, PENG CAI, YINYAN ZHU, ZHE WANG, Fudan University, ZHAOHUA CHENG, Chinese Academy of Sciences, XIAOYAN ZHONG, Tsinghua University, WENBIN WANG, Fudan University, XINGYU GAO, Chinese Academy of Sciences, RUQIAN WU, LIFENG YIN, JIAN SHEN, Fudan University — Ultrathin films often exhibit two-dimensional characteristics that are distinctly different from their bulk counterpart. In this work, we show an unusual behavior in La0.7Sr0.3MnO3 (LSMO) ultrathin films grown on SrTiO3 (001) (STO) substrate. Combining scanning tunneling microscopy and magneto-optical Kerr effect measurements, we have obtained the evolution of the magnetic state of the LSMO ultrathin films as a function of thickness. Strikingly, the LSMO ultrathin films are electronically phase separated in both lateral and vertical directions in thickness range between 4 and 7 unit cells. Specifically, the films are formed by 3 unit cell thick antiferromagnetic base layers, on top of which the layers consist of ferromagnetic metallic nanodisks in antiferromagnetic matrix. At 8 unit cells, an abrupt shear strain relief occurs by forming twinning patterns along [010] and [100] directions. After the shear strain is relieved, the whole films transform into a uniform ferromagnetic metallic state. Our observation reveals the richness of electronic and magnetic phases for strongly correlated systems even in their two-dimensional limit.
YOUNG MO KIM (Presenter), YOUJUNG KIM, JUYEON SHIN, KOOKRIN CHAR, Seoul National University — In order to identify the origin of the large conductance enhancement in the polar interface of LaInO$_3$/BaSnO$_3$, we studied the variation of the conductance enhancement in LaIn$_{1-x}$Ga$_x$O$_3$/BaSnO$_3$ interface. We found that the magnitude of the conductance enhancement decreased as Ga ratio increased and eventually completely disappeared in the case of LaGaO$_3$/BaSnO$_3$. The conductance of the interface, when present, reached its maximum values when LaIn$_{1-x}$Ga$_x$O$_3$ was about 4 unit cell thick, beyond which the conductance started to decrease slowly. Based on such findings, we developed a model for interface polarization in LIO, in which the polarization exists only in the 4 unit cell thick LIO near the interface. Such a model, when aided by 1D Poisson-Schrödinger equation, produces the $n_{2D}$ consistent with the experimental results. In addition, by introducing a deep donor density in LIO, we are able to fit the slow relaxation of the interface conductance. Our complete model, comprised of interface polarization in the 4 unit cell thick LIO and the resulting 2DEG state in BSO with 2 nm confinement length, also explains in a consistent way the entire experimental data of the recent doping dependence of the LIO/BSO interface conductance on both SrTiO$_3$ and MgO substrates.

Tuning the physical properties via Sr doping in the 4d transition metal oxide LaRhO$_3$ JUAN JIANG (Presenter), SANGJAE LEE, FREDERICK J WALKER, CHARLES H AHN, Applied Physics, Yale University — Perovskite transition metal oxides exhibit various novel properties due to the interactions of strongly correlated electrons. We discuss the physical properties of Rhodate thin film in this talk. We grow high quality La$_{1-x}$Sr$_x$RhO$_3$ thin films (up to $x=0.5$) on LaAlO$_3$ substrates by molecular beam epitaxy, and characterize their electrical and magnetic properties. Electrical anomalies and ferromagnetic signatures are observed. Strain effects are discussed, which might play a role in determine the physical properties of our thin films.

Modulation of manganite thin-film properties by strontium titanate excitons* CHI SIN TANG (Presenter), NUS Graduate School of Integrative Sciences & Engineering, National University of Singapore, XINMAO YIN, Department of Physics, National University of Singapore, LE WANG, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, ANDREW THYE SHEN WEE, Department of Physics, National University of Singapore, JUNLING WANG, School of Materials Science and Engineering, Nanyang Technological University, ANDRIVO RUSYDI, Department of Physics, National University of Singapore — A comprehensive investigation of the optical, electronic and magnetic properties of La$_{0.7}$Sr$_{0.3}$MnO$_3$ films on SrTiO$_3$ (LSMO/STO) and other substrates is conducted using multiple experimental techniques. There is a significant difference in the optical properties of LSMO/STO even in the case of 87.2nm-thick LSMO/STO as compared to those of LSMO on other substrates. We observed interesting excitonic features in the LSMO/STO thin-film at ~4eV. This could be due to formation of anomalous charged excitonic complexes. Based on spectral-weight transfer analysis, anomalous excitonic effects from STO strengthen the electronic-correlation in LSMO films. This results in optical spectral changes related to intrinsic Mott-Hubbard properties in the manganite films. While lattice strain influences the optical properties of the LSMO thin-films, strong e-e and e-h interactions from the substrate play a significant role as well.

*This work is supported by Singapore Ministry of Education (MOE2015-T2-2-065, MOE2015-T2-1-099, MOE2015-T2-2-147, and MOE2016-T2-1-054), Singapore National Research Foundation under its Competitive Research Funding (NRF-CRP 8-2011-06 and NRF-CRP15-2015-01), NUS-YIA, FRCs (R-144-000-379-114 and R-144-000-368-112), and NUS Core Support C-380-003-003-001.

Thickness-dependent metal-to-insulator transition in La-doped SrTiO$_3$ thin films YEONGJAE SHIN (Presenter), CLAUDIA LAU, SANGJAE LEE, FREDERICK J WALKER, CHARLES H AHN, Department of Applied Physics, Yale — The electronic and structural properties of La-doped SrTiO$_3$ (LSTO) films grown by molecular beam epitaxy are studied as a function of film thickness and La doping. We demonstrate that electronic transport is highly affected by the insulating dead layers inside LSTO films, whose thickness depends on La doping. As the film thickness is reduced below the dead layer thickness, an abrupt metal-to-insulator transition occurs. We attribute the existence of insulating layers to the surface structure of LSTO. The reduced conductivity of LSTO films due to dead layers can be counteracted by growing additional capping layers on top of the LSTO surface, indicating the strong relationship between insulating dead layers and surface structure of LSTO films. Synchrotron-based X-ray scattering analysis is used to test this hypothesis. Our results emphasize the importance of surface structure studies for functional oxides in the thin film limit and provide a guiding principle to fabricate oxide nanoscale devices.
9:12AM E45.00007: Thickness-dependent oxygen octahedral distortions in perovskite thin films as an adaption to the heterointerface 
JENNIFER FOWLIE (Presenter), CÉLINE LICHTENSTEIGER, University of Geneva, MARTA GIBERT, University of Zurich, HUGO MELEY, University of Geneva, PHILIP WILLMOTT, Paul Scherrer Institut, JEAN-MARC TRISCONE, University of Geneva — Distortions of the oxygen octahedral network of ABO₃-type perovskites are one of the most common features that develop in oxide heterostructures as a response to the epitaxial strain imposed by the substrate. This behaviour, which can be characterised as rigid tilts and rotations of the octahedra themselves, is readily studied quantitatively by synchrotron x-ray diffraction at half-integer Bragg positions [1].

In this study, we analyse the thickness-dependence of the octahedral tilts and rotations of thin films of LaNiO₃. We find a striking difference between films grown on SrTiO₃ and LaAlO₃ substrates, which appears to stem not only from the difference in epitaxial strain state but also from the level of continuity at the heterointerface. In particular, the highly discontinuous LaNiO₃/SrTiO₃ interface causes a large variation in the octahedral network as a function of film thickness whereas the rather continuous LaNiO₃/LaAlO₃ interface seems to allow the immediate formation of a stable octahedral pattern corresponding to simply the applied biaxial strain from just a few unit cells.

The scope for structural engineering by exploitation of these interfacial effects is tangible.


9:24AM E45.00008: The spin texture in a SrTiO₃(111) two-dimensional electron gas 
PAN HE (Presenter), Department of Electrical and Computer Engineering, National University of Singapore, SIQBHAN MCKEOWN WALKER, Department of Quantum Matter Physics, University of Geneva, SHULEI ZHANG, Materials Science Division, Argonne National Laboratory, F. Y. BRUNO, Department of Quantum Matter Physics, University of Geneva, M. S. BAHRAMY, Quantum-Phase Electronics Center, The University of Tokyo, JONGMIN LEE, RAJAGOPALAN RAMASWAMY, KAIMING CAI, Department of Electrical and Computer Engineering, National University of Singapore, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, FELIX BAUMBERGER, Department of Quantum Matter Physics, University of Geneva, HYUNSOO YANG, Department of Electrical and Computer Engineering, National University of Singapore — We report the observation of a bilinear magnetoelectric resistance (BMER) signal in the d-orbital two-dimensional electron gas (2DEG) at the SrTiO₃ (STO) (111) surface, demonstrating a spin-splitting. We show that our BMER measurements reveal a three-fold symmetric out-of-plane spin component that breaks the six-fold symmetry of the 2DEG subband dispersion, and an in-plane spin component locked perpendicularly to the momentum. By performing tight-binding supercell calculations based on the relativistic density functional theory of the STO bulk band structure, we find that this 3D spin texture is fully described by the effects of confinement of the STO t₂g conduction band in the (111) plane. We also show that the BMER can be substantially tuned through oxygen vacancy doping, electrostatic gating and temperature variation. Our findings highlight the untapped potential of SrTiO₃ (111) based 2DEGs as a playground for spintronic applications.

9:36AM E45.00009: Atomic-scale observation of large lattice bending and ferroelectric phase transition in freestanding BiFeO₃ thin films* 
DIANXIANG JI (Presenter), SONGJIA CAI, YIPENG ZANG, HAOLANG SUN, LU HAN, MIN GU, ZHENGBIN GU, PENG WANG, YUEFENG NIE, National Laboratory of Solid State Microstructures, College of Engineering and Applied Sciences, and Collaborative Innovation Center of Advanced Microstructures, Nanjing Univ, XIAOQING PAN, Department of Chemical Engineering and Materials Science and Department of Physics and Astronomy, University of California, Irvine, 916 Engineering Tower, Irvine, CA 92697, U — Novel electronic phases emerge in the growing family of two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides. Recent realization of freestanding perovskite films could open the door to a rich spectrum of exotic 2D correlated phases. Moreover, the inherent flexibility at reduced dimensionality makes 2D materials more promising to achieve strong electromechanical coupling and novel functionalities. Here, using reactive molecular beam epitaxy and aberration-corrected transmission electron microscopy, we provide an atomic-scale demonstration of a large lattice bending in ionic crystals. In addition, a tetragonal phase was observed in bended freestanding BiFeO₃ films with a giant c/a of 1.3, which exceeds the largest reported value. Our work indicates that freestanding oxide perovskite is a promising platform to investigate electromechanical effects and their potential applications.

*We thank the National Basic Research Program of China (2015CB654901) and the National Natural Science Foundation of China (51772143, 11574135, 51672125, 11774153, 11474147, 11874199), and the Fundamental Research Funds for Central Universities (0213-14380058).
9:48AM E45.00010: Anomalous behaviour of phonon modes – Magnetic properties correlations in La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrRuO$_3$ superlattices

ROSHNA S H (Presenter), P PADHAN, Indian Institute of Technology Madras, WILFRID PRELLIER, CRISMAT Laboratory, CNRS — Artificial superstructure of (111) oriented La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO)/SrRuO$_3$ (SRO) were grown on (111) oriented SrTiO$_3$ substrate using pulsed laser deposition. Microstructure quality and coherency of interafaces were studied using high resolution transmission electron microscopy. The growth epitaxy, crystalline quality, crystal structure and artificial bilayer periodicity of these superlattices were studied using x-ray diffraction. The cumulative strain in these superlattices was studied from the reciprocal space mapping (RSM). The RSM image of these superlattices indicates relaxation in some crystallographic directions. The magnetic exchange coupling at the interfaces of the LSMO-SRO has been investigated with the in-plane and the out-of-plane oriented magnetic field. The phonon mode anomaly of these superlattices were observed in the temperature dependent frequencies of the Raman lines. The observed peak at around 160 K and step like anomaly at around 350 K of the Raman peak frequencies provide strong evidence of magnetic phase transition of SRO and LSMO respectively. The observed anomalies in phonon modes in Raman scattering are discussed in terms of spin phonon coupling and delocalization of polaronic states in the vicinity of magnetic phase transition temperature of LSMO and SRO.

10:00AM E45.00011: Induced ferromagnetism due to oxygen vacancies at the YBa$_2$Cu$_3$O$_7$/SrTiO$_3$ Interface

KYRO BOOM, Department of Physics, University of North Florida, MI HE, EE MIN CHIA, Department of Physics and Applied Physics, Nanyang Technological University, JIAN-XIN ZHU, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, JASON HARALDSEN (Presenter), Department of Physics, University of North Florida — Complex oxide heterostructures provide a large playground of order parameters that can introduce a wide range of emergent phenomena. In the study, we set out to explain the emergent magnetic properties at the interface between YBa$_2$Cu$_3$O$_7$/SrTiO$_3$. Using density functional theory, we determined the electronic and magnetic properties for a simulated heterostructure with and without oxygen vacancies. It is shown that the sheer presence of the interface is not enough to produce a magnetic response. However, with the introduction of oxygen vacancies, we show that there is a shifting of the d orbital electron energies on the transition-metal atoms that induces a magnetic moment at the interface. This work details the effects of oxygen vacancies on complex oxide heterostructures, which has the ability to provide critical insight into future applications of oxide electronics.

*Center for Integrated Nanotechnologies at Los Alamos National Laboratory

10:12AM E45.00012: Mechanism of the irreversible back gate doping at the LaAlO$_3$/SrTiO$_3$ Interface

CHUNHAI YIN (Presenter), Huygens – Kamerlingh Onnes Laboratory, Leiden University, SANDER SMINK, MESA+ Institute for Nanotechnology, University of Twente, INGE LEERMAKERS, LUCAS TANG, High Field Magnet Laboratory (HFML-EMFL), Radboud University, NIKITA LEBEDEV, Huygens – Kamerlingh Onnes Laboratory, Leiden University, ULI ZEITLER, High Field Magnet Laboratory (HFML-EMFL), Radboud University, HANS HILGENKAMP, MESA+ Institute for Nanotechnology, University of Twente, JAN AARTS, Huygens – Kamerlingh Onnes Laboratory, Leiden University — The two-dimensional electron gas (2DEG) formed at the LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface exhibits rich physical properties such as superconductivity and magnetism. Additionally, due to the large dielectric constant of STO, the 2DEG can be controlled by a back gate voltage ($V_G$). When applying $V_G$ to the system, a commonly observed phenomenon is that the sheet resistance follows an irreversible route when $V_G$ is swept first forward and then backward. The explanation as given by Biscaras et al. [1] is that the Fermi energy is close to the top of the quantum well (QW) and high mobility electrons escape the QW and get trapped in STO when the carrier density goes beyond a critical value. In this work, we study the mechanism of the irreversible field-effect doping by means of a back gate. By combining magnetotransport data and self-consistent Schroedinger-Poisson calculations, we come to a different picture. There is no critical carrier density for electron trapping but rather applying any positive $V_G$ triggers it. Moreover, the analysis shows that it is not the mobile charges which get trapped but that the additionally injected electrons immediately find defects. This appears to be a universal phenomenon in STO-based heterostructures.

**10:24 AM E45.00013: Influence of defects on surface morphology and electronic structure in BiVO₄**

WENNIE WANG (Presenter), Institute for Molecular Engineering, University of Chicago, MINGZHAO LIU, Center for Functional Nanomaterials, Brookhaven National Laboratory, KYOUNG-SHIN CHOI, Department of Chemistry, University of Wisconsin-Madison, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Bismuth vanadate (BiVO₄) has several electronic properties that make it a promising candidate as a photoanode for water photocatalysis; these include strong absorption across much of the visible spectrum and a conduction band edge near the hydrogen evolution potential. However, charge transport and interfacial charge transfer have been reported to be limiting factors for PEC performance. Understanding the connections between surface morphology and PEC performance remains in its nascent stages, and building an accurate structural model is key. Here, we use density functional theory calculations to study the surface morphology and electronic structure of BiVO₄, and compare them with experiment. We investigate pristine surfaces and compare with those that have defects, and discuss the implications on PEC performance.

*This work is supported by the NSF-DMR.

**10:36 AM E45.00014: Electronic Symmetry of La₀.₆₇Sr₀.₃₃MnO₃/SrTiO₃ Interfaces as a Function of Film Thickness**

JOEL E TAYLOR (Presenter), KUN ZHAO, MOHAMMAD SAGHAYEZHIAN, JIANDI ZHANG, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LOUIS H HABER, Department of Chemistry, Louisiana State University, Baton Rouge, E WARD PLUMMER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge — Second harmonic generation (SHG) is a well known optical technique for probing electronic symmetry originating from regions of broken symmetries. For La₀.₆₇Sr₀.₃₃MnO₃/SrTiO₃ (LSMO/STO) buried interfaces, rotational anisotropic SHG is capable of characterizing interfacial electronic symmetry. Using film thickness and growth conditions to control the interface structure for LSMO/STO buried interfaces, induced changes in the electronic symmetry are detected with rotational anisotropic SHG. Data accumulated for LSMO/STO demonstrates thickness-dependent enhanced four-fold electronic symmetry patterns which are contrary to the measured C₄ᵥ electronic symmetry measured using atomically resolved electron microscopy and spectroscopy. Furthermore, the relative angles of the peak intensities between in-plane and out-of-plane polarization geometries varies with film thickness. Rotational anisotropy SHG of LSMO/STO thin films will be presented from <5 unit cell to 300+ unit cell LSMO/STO heterostructures.

*Supported by U.S. NSF through grant No. DMR-1504226. Thin films are grown by DoE grant No. DE-SC0002136.

**10:48 AM E45.00015: Decoupling carrier concentration and electron-phonon coupling in oxide heterostructures**

DEREK MEYERS (Presenter), Materials Science and Engineering, University of California, Berkeley, KEN NAKATSUKASA, Department of Physics and Astronomy, University of Tennessee, SAI MU, Department of Condensed Matter Physics and Materials Science, Oak Ridge National Laboratory, LIN HAO, JUNYI YANG, Department of Physics and Astronomy, University of Tennessee, YUE CAO, Materials Science Division, Argonne National Laboratory, GILBERTO F L FABBRIS, Advanced Photon Source, Argonne National Laboratory, HU MIAO, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, JONATHAN PELLICIALI, Department of Physics, Massachusetts Institute of Technology, DANIEL MCNALLY, MARCUS DANTZ, EUGENIO PARIS, Research Department Synchrotron Radiation and Nanotechnology, Paul Scherrer Institute, EVGUENIA KARAPETROVA, YONGSEONG CHOI, DANIEL HASKEL, Advanced Photon Source, Argonne National Laboratory, PADRAIC SHAFER, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, SCHMITT THORSTEN, Research Department Synchrotron Radiation and Nanotechnology, Paul Scherrer Institute, TOM BERLIJN, Center for Nanophase Materials, Oak Ridge National Laboratory, STEVEN JOHNSTON, JIAN LIU, Department of Physics and Astronomy, University of Tennessee, MARK DEAN, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — We present the results of resonant inelastic x-ray scattering at the O K-edge on superlattices of form nSrIrO₃/mSrTiO₃. Multiple phonon satellite peaks are observed corresponding to the 4th longitudinal optical mode of SrTiO₃ allowing direct extraction of the electron-phonon coupling strength. As the values of n and m are varied a systematic change in the relative intensity of the satellite features is observed indicating large changes to the electron-phonon coupling strength. In the absence of significant carrier doping this result shows the heterostructure morphology is able to independently tune this important interaction. Theoretical calculations indicate the Fröhlich mechanism dominates the electron-phonon coupling in these superlattices, with the reduced polarity and increased ε∞ driving the observed changes in the electron-phonon coupling.

*This material is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Early Career Award Program under Award No. 1047478 and the Office of Basic Energy Sciences under Contract No. DE-SC0012704.

Tuesday, March 5, 2019 8:00 AM - 10:48 AM
8:00AM E46.00001: Investigation of LaVO3/PrVO3 superlattices as geometric ferroelectrics  STEFANO GARIGLIO (Presenter), HUGO MELEY, University of Geneva, DUNCAN ALEXANDER, EPFL, PHILIPPE GHOSEZ, Université de Liège, JEAN-MARC TRISCONE, University of Geneva — Structural distortions in orthorhombic perovskite structures have been suggested as a source of ferroelectricity in layer-by-layer grown heterostructures of transition metal oxides. Here we explore the idea to achieve a multiferroic state by epitaxial growth in superlattices of LaVO3 and PrVO3. Heterostructures were synthesised by pulsed laser deposition and investigated by X-ray diffraction in order to determine the pattern of the oxygen octahedra. Cation polar distortions were measured by scanning tunnelling electron microscopy in order to confirm the prediction that superlattices with odd repetitions of LaVO3 and PrVO3 layers present a macroscopic ferroelectric state.

8:12AM E46.00002: Domain-wall ferroelectric tunnel junction with triple resistance states  MING LI (Presenter), LINGLING TAO, EVGENY Y TSYMBAL, University of Nebraska - Lincoln — The tunneling electroresistance (TER) effect in ferroelectric tunnel junctions (FTJs) has attracted interest due to potential applications in non-volatile memory devices. TER represents dramatic change in resistance of FTJ upon polarization reversal in ferroelectric barrier. A new type of TER's proposed, utilizing a head-to-head ferroelectric domain wall in La1-xSr_xMnO3(LSMO)/BaTiO3(BTO)/LSMO FTJ with the wall parallel to the plane. Domain wall state has higher conductance than uniformly polarized states, but is metastable and thus not reversible. This work, using first-principles DFT calculations, explores stability of the wall in this FTJ, by considering different La1-xSr_xO/TiO2 terminations at LSMO/BTO interfaces. Due to polar nature of the interface, appearance of the wall depends on doping level x. For x<0.4 domain wall state becomes global minimum, and DFT calculations demonstrate a triple-well energy profile with respect to net polarization. Using an electric field, the FTJ can be switched reversibly between domain wall and two uniformly polarized states. Using a phenomenological model based on Landau-Devonshire free energy and parameters obtained from DFT calculations, we analyze the hysteresis loops of this FTJ demonstrating the emergence of the triple resistance states.

8:24AM E46.00003: Design of a new polar metal via 6s lone pair electrons*  HANGHUI CHEN (Presenter), Physics, NYU Shanghai, YUEWEN FANG, Material Science and Engineering, Kyoto University — Polar metals are extremely rare because mobile electrons within a metal eliminate internal dipoles that may arise owing to asymmetric charge distributions. In this work we combine first-principles calculations and crystal structural search (CALYPSO) method to design a new polar metal. We show that an ordered double perovskite oxide BaBiTi2O6 undergoes a continuous transition from a high-temperature centrosymmetric P4/mmm structure to a low-temperature non-centrosymmetric Pmm2 structure. The material is conducting throughout the structural phase transition. The underlying mechanism is that the 6s lone-pair electrons in Bi3+ leads to polar instability and simultaneously donates electrons to empty Ti-d states, which results in conduction. Our work demonstrates that the lone-pair electrons are effective to induce polar instability in metals as they induce ferroelectric instabilities in insulators. This provides a robust design principle for new polar metals.

*We acknowledge financial support from NSFC.
8:36AM E46.00004: Dynamical Multiferroicity [Invited] NICOLA SPALDIN (Presenter), ETH Zurich — An appealing mechanism for inducing multiferroicity in complex oxides is the generation of electric polarization by a spatially varying magnetization that is coupled to the lattice through the spin-orbit interaction. Here, I will describe the reciprocal effect, in which a time-dependent electric polarization induces a magnetization, even in a material composed only of non-magnetic ions [1]. Two predicted consequences of dynamical multiferroicity will be illustrated using the example of strontium titanate as a model material: A Phonon Zeeman Effect, in which previously degenerate optical phonons split in the presence of a magnetic field, and a Quantum Critical Multiferroicity, manifesting as an anomalous magnetic susceptibility in the vicinity of the ferroelectric quantum critical point [2]. Finally, I will discuss possibilities for engineering and optimizing the behaviors using heteroepitaxial strain.


9:12AM E46.00005: Interface induced polar metals by multi-mode coupling* SAURABH GHOSH (Presenter), AAFREEN FATHIMA, Dept. of Physics and Nanotechnology, SRM Institute of Science and Technology, India, HANGWEN GUO, E WARD PLUMMER, Dept. of Physics and Astronomy, Louisiana State University, USA, SOKRATES T PANTELIDES, Dept. of Physics and Astronomy, Vanderbilt University, USA — Multi-mode coupling between various phonon modes in ABO3 perovskite oxides can be tuned by forming heterostructures, which can lead to precise control of their functionalities [1]. Considering the interest in ferroelectric properties in a metal i.e., in polar metals [2], an efficient way to induce ferroelectric-like (FEL) displacements in the centrosymmetric phase is by interface-induced coupling [3]. Here, using first-principles density functional theory (DFT) and DFT+U (static d-d Coulomb interaction) we have investigated (BaTiO3)m/(Metal)p/(BaTiO3)m' heterostructures [(m/p/m')= 6/3/7, 7/2/7, 7/1/8, m+p+m'= 16] to explore a new family of polar metals. We have chosen various metal blocks in a way that can represent a BTO/3dn/BTO system, where n= 1-6. We found that a FEL phase coupled with in-plane rotation of BO6 octahedra (a0a0c+) can be induced in the centrosymmetric ‘metal’ block when BaTiO3 is in the ferroelectric phase. The properties are found to depend strongly on the relative polarization direction of BTO units. [1]. S. Ghosh et. al. Phys. Rev. B. 92, 184112, (2015), [2] S. Ghosh et. al. Phys. Rev. Lett. 119, 177603 (2017), [3] H. Guo, PNAS, 114, E5062-E5069 (2017).

*DOE-DE-FG02-09ER46554 (S.G., S.T.P.), DOE-DE-SC0002136 (H.G., E. W. P)

9:24AM E46.00006: Electrically-Tuned Strain Fields in a Ferroelectric/Ferromagnetic (PZT/LSMO) Heterostructure NELSON HUA (Presenter), University of California, San Diego, SYLVIA MATZEN, THOMAS MAROUTIAN, GUILLAUME AGNUS, University of Paris-Sud, MARTIN HOLT, Argonne National Laboratory, PHILIPPE LECOEUR, DAFINE RAVELOSONA, University of Paris-Sud, OLEG SHPYRKO, University of California, San Diego — Manipulating the magnetic properties of complex materials can be achieved by varying the temperature or composition (doping), but alternative methods like strain-induced modification of magnetic domains has been less explored. Nanostructures can accommodate larger values of strain, and can be applied using various epitaxial growth methods and dynamically altered by an external stimulus. Therefore, lattice strain can be used as a tuning parameter to modify magnetic properties on the nanoscale. To explore this possibility, we investigated the response from multiferroic materials that uses an intermediary strain field as a coupling mechanism. Specifically, we performed x-ray nanodiffraction to spatially resolve the coupled strain field between PZT and LSMO, a ferroelectric/ferromagnetic heterostructure, as a function of an applied electric field in the ferroelectric PZT layer. Our results reveal this interfacial strain transfer with 30nm spatial resolution and uncover the details of confined size effects associated with nanoscale structural domains.
Correlated oxides often exhibit the presence of intertwined phases of long-range order. The rare-earth nickelates (RNiO3) serve as a model transition metal oxide platform to understand and engineer the electronic structure of such phases. For several ‘strange’ metals whose properties cannot be described within the paradigm of conventional Fermi liquids, heterostructures incorporating such metals also have properties that are distinct from those found in similar structures based heterostructures resulting from the influences of dimensional confinement and interfacial coupling. We focus on the AF ground state in (NNO)m-(NdAlO3)n heterostructures: enhancement of AF domain dynamics and spin fluctuations in reduced dimensions appear to hinder spin ordering. We employ x-ray photon correlation spectroscopy (XPCS) measurements via coherent x-ray scattering of the heterostructures to elucidate dimensionality-driven spin dynamics. Speckle patterns arising from AF domains are investigated for different thickness of confined nickelate layers and their dynamics are studied across the charge and spin ordering transitions. This study demonstrates an approach to characterize dimensional effects on long-range order and the ability to control the AF domain configurations in oxide heterostructures.

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*The work was primarily funded by the Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division. The use of facilities at the Center for Nanoscale Materials, an Office of Science user facility, was supported by the US Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-06CH11357. Work at Brookhaven National Laboratory is supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-SC0012704. We acknowledge the support of the National Institute of Standards and Technology, U.S. Department of Commerce, in providing the neutron research facilities used in this work.
Comparing Bulk and Layer Confined RNiO$_3$ to Disentangle Lattice and Electronic Effects in the Metal-Insulator Transition

ALEXANDRU BOGDAN GEORGESCU (Presenter), Center for Computational Quantum Physics, Flatiron Institute, NY, NY, 10010, OLEG E. PEIL, Materials Center, Leoben, Austria, ANKIT S DISA, Max Planck Institute, Hamburg, Germany, ANTOINE GEORGES, ANDREW MILLIS, Center for Computational Quantum Physics, Flatiron Institute, NY, NY, 10010 — The metal-insulator transition (MIT) of transition metal oxides is often associated with a simultaneous lattice and electronic symmetry breaking. We disentangle the effects of the electronic and lattice structure in the MIT of rare earth nickelates (RNiO$_3$) by comparing bulk and layer-confined NdNiO$_3$, using a combination of electronic structure and many-body methods[1,2,3]. We find that electronic confinement leads to an increase in the relative role of local interactions that favor an insulating symmetry-broken state. However, heterostructuring with another material leads to an increase in the lattice stiffness with respect to structural disproportionation caused by the interfacial octahedral coupling. Our work explains why nickelate heterostructures can have both a higher MIT temperature despite a weaker structural signature of the insulating state[4]. These results are of general relevance to the physics of transition-metal oxides.


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Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E47 GERA: Energy Storage: Electrolytes and Ionic Conductors

BCEC 213 - Nancy Haegel, National Renewable Energy Laboratory

Nuclear Magnetic Resonance Investigation of Lithium Ion Transport in a Highly Conducting Solid Polymer Electrolyte: The Enabling Effect of High Salt Concentration

SAHANA BHATTACHARYYA (Presenter), Physics, CUNY Graduate Center, New York, NY 10016, MOINESHA GARAGA, STEVEN GARRY GREENBAUM, Physics and Astronomy, Hunter College of the City University of New York, New York, NY 10065, MATTHEW D WIDSTROM, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20740, PETER KOFINAS, Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20740 — Solid polymer electrolytes based on poly(ethylene oxide) (PEO) for rechargeable lithium ion batteries significantly lack sufficiently high ionic conductivity for practical use at ambient temperature. Recent reports of high ionic conductivity and an expanded electrochemical window of aqueous electrolytes enabled by very high salt concentration (~20m) as well as earlier work on the “salt-in-polymer” concept have inspired this investigation of a solid PEO-salt-water system, where the dissolved salt (LiTFSI) concentration approaches its solubility limit and in combination with water association succeeds in inhibiting crystallization of the PEO matrix leading to higher conductivity. Room temperature ionic conductivity in these solid-like polymer electrolytes is about 2 mS-cm$^{-1}$, which is sufficiently high for battery application. Characterization of the ion transport process by NMR pulsed field gradient diffusion measurements ($^7$Li and $^{19}$F for the cation and anion, respectively) and electrochemical impedance spectroscopy demonstrate an acceptable degree of salt ion dissociation and a lithium transport number, i.e. the Li ionic fraction of the current, exceeding 0.6, which is unusually high for polymer electrolytes. Additional electrochemical testing results will also be presented.
Computational and experimental investigation of Na₄P₂S₆ as a promising solid electrolyte material for sodium metal batteries

YAN LI (Presenter), NATALIE A HOLZWARTH, Department of Physics, Wake Forest University, ZACHARY DAVID HOOD, Department of Materials Science and Engineering, MIT — Recent experiments¹ have shown that Na₄P₂S₆, prepared from a hydrated precursor Na₄P₂S₆·6H₂O by heating under vacuum to 175 deg. C, has good ionic conductivity and stability with respect to metallic Na anodes, suggesting its promise as a solid state electrolyte for Na ion batteries. Examining the experimental results, we have extended previous computational work² on this material to further understand its structural, conductivity, and interface properties. Of particular interest is the observation¹,³ that Na₄P₂S₆ crystallizes to form monoclinic crystals having the space group C2/m which is distinct from the hexagonal or trigonal structures⁴-⁶ analyzed for the related material Li₄P₂S₆. Computer modeling results suggest that the C2/m structure of Na₄P₂S₆ is stabilized by lattice vibrations.


*Computer simulations supported by NSF grant DMR-1507942.

First-principles prediction of potentials and space-charge layers in all-solid-state batteries

MICHAEL W. SWIFT (Presenter), YUE QI, Chemical Engineering and Materials Science, Michigan State University — As all-solid-state batteries (SSBs) develop as an alternative to traditional cells, a thorough theoretical understanding of driving forces behind battery operation is needed. We present a fully first-principles-informed model of potential profiles in SSBs and apply the model to the Li/LiPON/LiₓCoO₂ system. These profiles, especially the interface dipoles, yield valuable information about lithium distribution and transport and the nature of interfacial electrical double layers. The results suggest design rules to minimize interfacial lithium transport resistance and optimize device performance.

*This work was supported by the Nanostructures for Electrical Energy Storage (NEES) center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award number DESC0001160.

Structural Characterization of a Solid Electrolyte for 3D Microbatteries

DAVID CLARKSON (Presenter), MOUNESHA GARAGA, STEVEN GARRY GREENBAUM, Department of Physics & Astronomy, Hunter College of the City University of New York, MORAN LIFSHITZ, ELAZAR COHEN, DIANA GOLODNITSKY, School of Chemistry, Tel Aviv University — Three-dimensional (3D) microbatteries have gained attention as viable compact power sources with applications in wearable and implantable microelectronics, and IoT functions. A key innovation from our lab is electrophoretic deposition (EPD) of all thin-film layers, enabling conformal deposition of electrodes and solid electrolytes on complex-shape, high-aspect-ratio perforated silicon and polymer substrates. This leads to a large capacity gain per footprint area of battery, compared with wafer surface deposition.

Using EPD, we prepared a novel composite polymer-in-ceramic electrolyte composed of 87% lithium aluminum germanium phosphate (Li₁.₅Al₀.₅Ge₁.₅(PO₄)₃, LAGP), 13% polyethyleneimine (LAGP–PEI), saturated by LiI salt to produce high concentrations of mobile Li⁺ and I⁻ ions.

Solid state ⁶,⁷Li, ²⁷Al, and ³¹P magic angle spinning nuclear magnetic resonance (MAS NMR) measurements showed structural changes the LAGP-PEI-LiI composite compared with base LAGP material, including the conversion of about 1/3 of the crystalline compound into an amorphous phase containing both two-fold and three-fold coordinated P, and a change in the ratio of five-fold to six-fold coordinated Al. ⁷Li NMR diffusometry revealed faster Li ion diffusion in the LAGP-PEI-LiI composite than in base LAGP.
8:48AM E47.00005: Sol-gel synthesis of a Fe-doped cubic phase Li$_2$La$_3$Zr$_2$O$_{12}$ Solid State Electrolyte  
ANDRES VILLA PULIDO (Presenter), MAI TAN, ERNESTO MARINERO, School of Materials Engineering, Purdue University — Cubic Li$_2$La$_3$Zr$_2$O$_{12}$ (LLZO) exhibits high ionic conductivity, chemical stability and thermal stability and a high transference number. These characteristics make it a promising material for integration in solid state batteries. Doping LLZO with certain elements like bismuth, gallium, aluminum and tantalum increases the ionic conductivity and reduces the stabilization temperature of the cubic phase. In this work a sol-gel method is used to synthesize Fe-doped LLZO (Li$_{7-2x}$Fe$_x$La$_3$Zr$_2$O$_{12}$), wherein a low calcination temperature of 700°C in air is used. XRD is used to characterize the cubic phase and presence of other impurity phases. SEM is used to determine the microstructure of the powder and the prepared pellets with different Fe stoichiometric content. Electrochemical impedance spectroscopy is used to determine the bulk conductivity of the Fe-doped LLZO pellets. The low synthesis and calcination temperature combined with the high ionic conductivity (and other favorable characteristics of the LLZO garnet) make this synthesis method and material highly attractive for lithium-ion solid state batteries. Future work will involve fabrication of polymer composite electrolytes with this material, looking for positive synergy of polymer and garnet characteristics.

9:00AM E47.00006: Theoretical modelling of lithium environment in composite solid electrolyte batteries investigated through x-ray absorption near edge spectroscopy*  
EMILY BEEN (Presenter), FEIFEI SHI, Materials Science & Engineering, Stanford, SRI CHAITANYA DAS PEMMARAJU, SLAC, Stanford, YI CUI, Materials Science & Engineering, Stanford, THOMAS DEVEREAUX, SLAC, Stanford — Liquid electrolytes in conventional batteries are volatile, flammable, and cause many of the fires and explosions of lithium ion batteries. Moving to solid state electrolytes not only removes these instabilities but also suppress dendritic growth of lithium that can short a battery. Ion transport is a main limitation in these solid-electrolytes. Composite electrolytes made of nanostructured combinations of ceramics and polymers show promise to increase ion transport at the ceramic-polymer interface[1]. To investigate the mechanisms that preferentially transport lithium ions at this interface, x-ray absorption near edge spectroscopy (XANES) of lithium K-edge was performed experimentally and elucidated through theoretical simulation. The solid-electrolyte system investigated is lithium perchlorate (ClO$_4^-$) dissolved in poly(ethylene oxide) (PEO) in nanopores of anodized aluminum oxide. Simulation results explicate a complex relationship between the XANES edge shift and lithium environment, going beyond the preliminary expectation that coordination number of lithium with oxygen causes the XANES shift.


*This research is funded by U.S. Department of Energy, Stanford University, and SLAC National Accelerator Laboratory.

9:12AM E47.00007: Effects of solvent-salt charge-transfer complexes on oxidative stability of Li-ion battery electrolytes*  
ERIC FADEL (Presenter), Materials Science and Engineering, Massachusetts Institute of Technology, FRANCESCO FAGLIONI, Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia, GEORGY SAMSONIDZE, Robert Bosch LLC Research and Technology Center, NICOLA MOLINARI, John A. Paulson School of Engineering and Applied Sciences, Harvard University, BORIS V MERINOV, WILLIAM GODDARD, Materials and Process Simulation Center, California Institute of Technology, JEFFREY C GROSSMAN, Materials Science and Engineering, Massachusetts Institute of Technology, JONATHAN P MAILOA, Robert Bosch LLC Research and Technology Center, BORIS KOZINSKY, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Electrochemical stability windows of multi-component electrolytes, both solid polymer and organic liquid, largely determine the operating regime limits of Li-ion batteries. In order to increase energy densities and lifetimes of batteries, new electrolyte materials need to be discovered and optimized which requires better understanding of their degradation and oxidation. Using computational tools, we present new insights into the oxidation mechanism that governs stability of multi-component polymer and liquid electrolytes. We find that explicitly including solvent molecules in the computation of the anion stability has a strong impact, and we show that this effect stems from electrostatic interactions between the molecules. Particularly, we find that across all chemistries studied, only one molecule in the system is oxidized. Building on this, we construct a model where two oxidation scenarios lead to different stability behaviors for the anion-solvent pairs, depending on their relative strength and geometry. This understanding of the microscopic details of oxidation allows one to formulate design rules and provides a good framework for screening electrolyte materials.

*Funding for E. R. F. was provided by Robert Bosch LLC, partly through the MIT Energy Initiative fellowship.
The Role of Ion Correlation on Transport Properties of Concentrated Ionic Liquids for Battery Electrolytes

Nicola Molinari (Presenter), Harvard University, Jonathan P Mailoa, Nathan Craig, Jake Christensen, Robert Bosch LLC, Boris Koziński, Harvard University — Recent pioneering work on Na batteries has drawn attention on ionic liquid electrolytes, yet most published works ignore the effects of ion-ion correlation. Using classical all-atom molecular dynamics and fully-correlated theory we highlight the drastic differences in fundamental understanding when using the systematically overlooked correlated approach. As a case study, we look at the promising Na/bis(fluorosulfonyl)imide (NaFSI) in room temperature ionic liquid N-propyl-N-methylpyrrolidinium/FSI. A previously undetected negative transference number emerges for sodium molar fractions lower than 0.2, effectively hinting to high degrees of ion-ion correlation that should not be dismissed. The spatial correlation is explored further by employing a variant of the single-linkage clustering algorithm. The approach we use enables us to explain the concentration-driven trends in ionic conductivity and transference numbers, and is generally able to correctly capture the transport physics of highly-correlated systems such as concentrated electrolytes.

First-Principles Replica Monte Carlo Sampling of Dopant Disorder in Solid Electrolyte

Shusuke Kasamatsu (Presenter), Osamu Sugino, Univ of Tokyo-Kashiwanoha — Oxides such as ZrO₂ and BaZrO₃ are promising candidates for the electrolyte material in medium to high-temperature solid oxide fuel cells. In these materials, aliovalent cation doping is used to introduce ionic defects which act as ionic charge carriers. Optimization of doping conditions is imperative for obtaining sufficient and stable ionic conductivity, but it is yet unclear how dopants are distributed in the material under various processing conditions and how the details of the distribution affect the total conductivity. Since the experimentally found optimal doping concentration can run up to 20%, the degrees of freedom in substitutional dopant placement is enormous (for example, choosing 10 substitutional sites out of 50 corresponds to 50C10~10 billion degrees of freedom). In this work, we harness the power of modern-day supercomputers and perform thermodynamic sampling of dopant placement in BaZrO₃ by directly combining first-principles calculations and the replica exchange Monte Carlo method. We show that dopant-carrier association decreases with increasing dopant concentration, in contrast to popular belief that association effects are responsible for conductivity decrease at high dopant concentrations.

Polyethylene oxide-Li₇La₃Zr₂O₁₂ composite solid-state electrolyte for advanced Li-ion batteries (LIBs)

Parisa Bashiri (Presenter), Prasada Rao Talakonda, Wayne State University, Vaman M Naik, University of Michigan Dearborn, Gholamabbas Nazri, Ratna Naik, Wayne State University — Recently, conformal solid-state polymer-based electrolytes have been considered as promising alternatives for liquid electrolytes in LIBs because of their fire safety and ease of fabrication in thin film form with desirable mechanical, thermal and high electrochemical stability. Several researchers have investigated polyethylene oxide (PEO) based films complexed with Li-salts, such as LiClO₄, as polymer electrolytes. However, these electrolytes exhibit low ionic conductivity (~10⁻⁶ - 10⁻⁷ S cm⁻¹) at room temperature due to high degree of crystallinity. This issue has been addressed by adding plasticizers such as ethylene carbonate (EC) or using inorganic fillers. We have studied PEO based polymer electrolyte with Li₇La₃Zr₂O₁₂ (LLZO) as an inorganic filler, which is also a Li-ion conductor. We show that the addition of LLZO (20 wt%) and EC (20 wt%) increases the ionic conductivity of PEO-LLZO composite electrolyte by an order of magnitude, lowers the activation energy from 0.6 eV to 0.5 eV, and maintains a high voltage stability (5 V). The results of electrochemical impedance spectroscopy, linear sweep voltammetry, and chronoamperometry measurements will be presented.

Investigate the mobility of Lithium-sulfur batteries via ab initio molecular dynamic with external force

Guoping Gao (Presenter), Lawrence Berkeley National Laboratory — Even though tremendous achievement has been made experimentally in the performance of Li-S battery, theoretical studies in this area are lagging behind due to the complexity of the Li-S systems. For this purpose, we have developed a new molecular dynamic method with external force applied on the Li atom to investigate the mobility. Our proposed computational framework not only opens a new avenue for understanding the key role played by solution and liquid electrolytes in Li-S battery, but also can be generally applied to other processes with liquids involved.
The development of safe high energy density rechargeable lithium (Li) ion batteries is crucial for meeting the goal of clean sustainable energy. A major limiting factor in these batteries is the electrolyte — organic liquids are typically flammable and have limited electrochemical stability while most solid electrolytes have lower ionic conductivity and limited stability. Here, we focus on design principles for ionic transport in multicomponent solid electrolytes, either artificially created or naturally generated at the electrode-electrolyte interface. General tradeoffs prevent single component solid electrolytes from achieving the desired properties simultaneously [1] but may be broken through a multicomponent system by a careful use of the phase boundaries through the generation of space charge regions [2], confinement, ion adsorption etc. Together with the descriptors for ionic conduction, our design principles will be supplemented by theoretical spectroscopy studies based on x-ray absorption and emission to assist in experimental validation of samples with the required composition.

8:00AM E48.00001: Enhancement of lift to drag ratio for a wing using thermal forcing ANchal VARshney, MeHuL VARshney (Presenter), MF Baig, Aligarh Muslim University — The aim is to enhance the lift to drag ratio produced by a wing with a cambered profile by thermal forcing its partial lower surface. Reynolds number is considered in the laminar regime. The efficacy of control technique has been checked at various Mach number and angle of attack. The overheat factor, which is the ratio of the temperature of the heated portion to free stream temperature has also been varied to study its role in the control technique. The governing equations of continuity, momentum, and energy have been solved using commercial package Fluent®. As of now, the proposed mechanism for the enhancement of lift to drag ratio is the increase in vorticity generation near the trailing edge because of the variation in viscosity. This brings about a net increase of circulation about the wing which results in higher lift. The other possible mechanism for the phenomenon is further being explored such that advancement in Micro-Air Vehicles technology can be done.

8:12AM E48.00002: Turbulent Drag Reduction on an Aircraft Wing MEHUL VARSHNEY (Presenter), MF BAIG, Aligarh Muslim University — The aim of the present work is to reduce the turbulent drag induced on a supercritical aircraft wing at commercial flight scale conditions of Reynolds number and Mach number by using jets installed on the upper and lower surface of the wing. The present method is an active technique of viscous drag reduction. To the best of author’s knowledge, no such control technique has been explored at such conditions. The analysis considers jets in the stream-wise and span-wise direction incorporated on suction and pressure surfaces of the wing which tend to form a pair of colliding-jets in the span-wise direction. The efficacy of the control technique has been checked for jets with various emerging mass flux and inclination angle of the streams. The governing equation of continuity, RANS (using Spalart Allmaras as turbulence model) and the energy have been solved numerically using the commercial package Fluent®. The mechanism behind the control technique is the lifting of the boundary layer which brings about a reduction in the skin-friction component of the drag and the cross-diffusion of the near-wall streaks which brings about a decrease in the turbulent kinetic energy and hence viscous drag. Role of vorticity variation will also be explored.

8:24AM E48.00003: Stable flight of meteors* PEJMAN SANAEI (Presenter), New York University - Courant Institute, MICHAEL JOHN SHELLERY, New York University - Courant Institute, Flatiron Institute, LEIF RISTROPH, New York University - Courant Institute — The atmospheric erosion of meteors is a splendid example of the reshaping of a solid object due to its motion through a fluid. Motivated by meteorite samples collected on Earth that suggest fixed orientation during flight—most notably the strikingly conical shape of so called oriented meteorite—here the hypothesis that such forms result from an aerodynamic stabilization of posture that may be achieved only by specific shapes, is explored. The laboratory- scale experiment is conducted for exploring systematic static stability tests on cones of varying apex angles in fast flows, and the resulting map of the orientational equilibria and their stability. A 2D mathematical model has been developed, and is compared with the experimental results. Armed with the simplified 2D model of oriented meteorites (with a conical shape), an isosceles triangle is considered in order to calculate its flow wake structure using free streamline theory and conclude that meteors are self-stabilizing in the sense that they seem to reshape themselves through erosion into a flight-stable form.

*RTG/DMS-1646339
NSF CBET-1805506

8:36AM E48.00004: Vortex streets behind triangular objects ILDOO KIM (Presenter), Brown University — When a triangular object, instead of a circular object, is used to produce a vortex street, an exotic vortex arrangement is observed in addition to the commonly observed mushroom-like structure. The exotic structure is morphologically distinctive from the classical von Karman vortex street and is characterized by a thin layer of irrotational fluid that separates two rows of vortices. This structure appears when a dimensionless ratio between the thickness of the boundary layer and the size of the object is less than a certain value, which is measured to be 0.4 in our experiment. The experiment is modeled by a double shear layer profile, whose linear stability is solved numerically. The theoretical consideration shows a rough agreement with the measurement.
ALEXANDRE VILQUIN (Presenter), Laboratoire de Physique et Mécanique des Milieux Hétérogènes, VINCENT PAGNEUX, Université du Mans, AGNÉS MAUREL, PHILIPPE PETITJEANS, ESPCI — The vortex rings are torus-shaped vortices existing in many different situations in fluid mechanics. They are involved in the locomotion of numerous animals like birds and fish. The understanding of their formation process is essential to optimize the propulsion in engineering. They also play a major role for blood pumping in left ventricle and are considered as an index of cardiac health in the human heart. As proof of the phenomenon diversity, the presence of charged vortex ring with a quantized circulation has also been identified in superfluid helium.

The first part of this talk will give a short overview about interest and properties of the vortex rings. In a second part, I will present an experimental study on a semi vortex ring connected to a free surface, notably involved in the locomotion of water striders. This U-shaped object is here generated by the circular motion of a flat circular disc in water. Digital particle image velocimetry provides velocity fields and vortex properties. The formation process highlights not only the existence of a classical rolling up at the rear of the disk, but also a shedding phenomenon on the leading edge of the disc. The created small vortices affect final properties of the semi vortex ring.

POOJA CHOPRA (Presenter), DAVID A QUINT, AJAY GOPINATHAN, BIN LIU, University of California, Merced, CA, United States. — Transport through complex environments is paramount to microorganism propagation and survival. At the scale of a single bacterium, there can be environmental physical features that dramatically alter transport properties at the population level. In this work, we study the transportation of individual bacteria, here *Escherichia coli* (*E. coli*), through a lattice of micropillars which serve as structured obstacles with well-defined geometries. To fully account for single cell kinematics, we employ a 4D (3D+time) tracking microscope while imaging in the micropillar environment. Interestingly, we found that the micropillar arrays promote the dispersal of bacteria rather than serving as simple obstacles. We explore the mechanisms of such enhanced transport by studying the spatial dependence of the run-and-tumble statistics of *E. coli*, in part due to the hydrodynamic interactions between the bacteria and solid surfaces.

*The authors thank the support of National Science Foundation NSF, CREST: Center for cellular and Biomolecular Machines (NSF-HRD-1547848).

AMANDINE LECHANTRE (Presenter), University of Mons, ALEJANDRO RICO GUEVARA, University of California at Berkeley, PASCAL DAMMAN, University of Mons — Hummingbirds have a high metabolic rate requiring to feed on a very energetic resource: the nectar. For this purpose, they have developed a truly specialized nectar-feeding method. During the capture of the nectar, the hummingbird's bill goes into the corolla of the flower. Then the tongue is protruded out and plunges into the nectar. After the loading, the tongue retracts and is unloaded in the bill. The mechanism of the tongue's loading is still unresolved. At first, it was suggested that the tongue was composed of two thin tubes which was filled because of a capillary suction mechanism (Martin 1833, Scharnke 1931). But the morphological study of the tongue reveals that it is composed of two folded sheets and no closed tubes. In this talk, we will tackle the question: how a sheet can fold into a tube to capture viscous fluid. Several mechanisms were proposed: self-assembling capillary syphon (W. Kim et al. 2012) or elastic micropumps (A. R. Guevara et al. 2005). Based on elasto-capillary experiments and recording of living hummingbirds, the relevance of both models will be discussed.

GIUSEPPE PUCCI, IAN HO, DANIEL M HARRIS (Presenter), School of Engineering, Brown University — A body in motion tends to stay in motion but is often slowed by friction. We investigate the friction experienced by centimeter-sized bodies sliding on water. We show that their motion is dominated by skin friction due to the boundary layer that forms in the fluid beneath the body. We develop a simple model that considers the boundary layer as quasi-steady, and is able to capture the experimental behaviour for a range of body sizes, masses, shapes and fluid viscosities. We define a dimensionless sliding number as the ratio between the fluid inertia and the body inertia, which allows us to assess the regime of validity of our model. Furthermore, we demonstrate that friction can be reduced by modification of the body's shape or bottom topography. Our results are significant for understanding natural and artificial bodies moving at the air-water interface, and can inform the design of aerial-aquatic microrobots for environmental exploration and monitoring.

*The authors would like to thank the Brown OVPR Seed Award for partial support of this work. G. P. thanks the program CNRS Momentum for its support.
We study the effect of shape-polarity on the Stokesian sedimentation dynamics of particles by experiments in which isosceles triangles of varying apex angles are placed in a vertical plane and sedimented at low Reynolds number in a quasi-two-dimensional container. Unlike a nonpolar shape, the triangle rotates as it sediments - due to coupling between the orientational and translational degrees of freedom - and asymptotically approaches a stable configuration either pointing along or away from gravity [Jayaweera, Mason, J. Fluid Mech. 22 (1965)]. For small apex angles the triangle is stable with apex pointing down. As the apex angle is increased we find a transition at $\pi/3$ for which all orientations of the triangle are stable and for apex angles greater than $\pi/3$, the triangle is stable with apex pointing up. We understand the experimental results with a model of three stokeslets fixed to the vertices of a triangle. Adding polarity to the particles introduces an effective damping term in the equations of motion, thus making it not amenable to an effective Hamiltonian treatment constructed for apolar particles [R. Chajwa et. al. arXiv:1803.10269 (2018)].

*NM, AC acknowledge funding through NSF DMR 1507650.
9:00AM E49.00004: Mechanical Properties and Crazing Behavior in Model Polymer-Grafted Nanoparticle Thin Films*

JEFFREY ETHIER (Presenter), LISA HALL, William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University — Thin films comprised of inorganic-organic polymer-grafted nanoparticles (PGNs) show promise for use in flexible electronics and high energy density materials. Recently, there has been significant interest in tuning the properties of the polymer-grafted layers to optimize entanglement formation between neighboring PGNs and improve mechanical performance. In this work, we show how graft density and polymer length affect inter-PGN entanglements and mechanical properties using coarse-grained molecular dynamics (MD) simulations. Specifically, we simulate twelve PGNs organized in a hexagonal spacing on a smooth, attractive surface. We rigidly attach the first monomer of every chain to the surface of a nanoparticle (using rigid body constraints) and model the polymers as bead-spring chains. We first quantify the number of interparticle entanglements between PGNs and show that moderate graft density particles have increased interparticle entanglements per chain and better mechanical toughness compared to high graft density particles in the melt state. We then cool the monolayer below the glass transition and compare the crazing behavior of PGN thin films to their analogous homopolymer thin films.

*This work is supported by the AFRL/DAGSI Ohio Student-Faculty Research Fellowship program.

9:12AM E49.00005: Microscopic origins of caging and hyperdiffusive relaxations in hairy nanoparticle fluids*

[Invited]

LYNDEN ARCHER (Presenter), Cornell University — Nanocomposites formed from well-dispersed suspensions of solvent-free silica nanoparticles tethered with flexible polymers are known to exhibit jamming behavior due to interpenetrated chains in the confined space between nanoparticle cores. This talk discusses equilibration processes in such materials by means of small-angle X-ray scattering (SAXS), dielectric relaxation, and rheology measurements. In so doing the talk we explore the microscopic processes responsible for caging and show how cages emerge on the nanoparticle cores. The talk also considers consequences of caging, including hyperdiffusive particle dynamics and yielding. A simple microscopic model for caging and particle clustering is shown to explain both the yielding transition and onset of hyperdiffusive relaxations.

*National Science Foundation, Division of Materials Research, Award No. DMR–1609125

9:48AM E49.00006: Polymer-Grafted Nanoparticle (PGN) Assemblies: Supramolecular Dynamic Bonds for Enhanced Toughness*

ANDREW TIBBITS (Presenter), ALI JAWAID, JASON STREIT, LAWRENCE DRUMMY, RICHARD VAIA, Materials and Manufacturing Directorate, Air Force Research Laboratory — The targeted design of PGNs has significant ramifications in the design of scalable and tough coatings, flexible electronics, and functional inks. Studies of the nanomechanics of polystyrene grafted nanoparticles have shown a strong dependence of PGN architecture on plasticity. Nonetheless, toughness at high NP fraction is impeded by the inherently high entanglement molecular weight (MWe) of amorphous polymer grafts. The incorporation of supramolecular dynamic bonds (e.g. hydrogen bonding) into the canopy provides dynamic crosslinks that enhance viscoelasticity and dissipative processes at lower molecular weights. The modification of pendant olefins in poly(1,2-butadiene) with supramolecular dynamic bonds and subsequent grafting onto gold nanoparticles permits directed self-assembly into ordered superlattice structures at high core volume fraction (>30 vol%). The modular chemistry and grafting approach facilitates development of a comprehensive phase space correlating PGN architecture, dynamic bond strength and content, morphology, and nanomechanics to direct optimal engineered canopy designs to maximize robustness in PGN assemblies.

*Air Force Office of Scientific Research (AFOSR)

10:00AM E49.00007: Structure and dynamics of architecturally engineered all-polymer nanocomposites*

ERKAN SENSES (Presenter), Koc University, MADHUSUDAN TYGAI, ANTONIO FARAOE, NCNR, NIST — We present nanocomposites formed by using glassy star-shaped polymers as nanofillers and dispersing them in soft matrices. The resulting 'architecturally engineered' nanocomposites structurally reside between the linear homopolymer blends and the conventional polymer nanocomposites with solid fillers. We observed that the star polymers can induce reinforcement that can be as strong as that of solid nanoparticles, or softening depending on the compactness and concentration of the nanoparticles. We showed that the remarkable influence of filler architecture on the rheological properties can be traced back to the dynamical features at the segmental and the chain level which we investigated using neutron scattering over a wide range of time and lengths scales in the glassy and melt states of the nanocomposites. The local and segmental dynamics as well as chain-chain entanglements are all modified by polymer architecture, offering a novel approach for tuning the physical properties of all-polymer based composites.

*This work utilized facilities supported in part by the National Science Foundation under Agreement No. DMR-1508249
10:24AM E49.00009: Deformation Mechanism of Mechanochromic Polymer Nanocomposites Fabricated by Self-Assembly of Colloidal Particles  
CHAO-HUNG CHENG (Presenter), SHUHEI NOZAKI, SHIORI MASUDA, NATTANEE DECHNARONG, Graduate School of Engineering, Kyushu University, KAZUTAKA KAMITANI, TOMOYASU HIRAI, KEN KOJIO, ATSUSHI TAKAHARA, Institute for Materials Chemistry and Engineering, Kyushu University — A novel polymer nanocomposite consisting of polymer-grafted nanoparticles have attracted great attention due to their properties of self-assembling to an ordered colloidal crystal structure. However, the deformation mechanism of this colloidal crystal has not been clarified yet. In this study, the structural evolution of a colloidal crystal with rubbery/glassy block copolymer-grafted silica particles (BCP-g-SiO$_2$) was investigated by in situ ultra small-angle X-ray scattering (USAXS) under deformation. Poly(butyl acrylate) (PBA) and poly (methyl methacrylate) (PMMA) were chosen as inner and outer layers of BCP-g-SiO$_2$, respectively. The heat-pressed film consisting of BCP-g-SiO$_2$ exhibited structural color due to the formation of photonic colloidal structure. The color changed under uniaxial stretching. The first order ring of USAXS pattern changed from circle to ellipsoid under elongation, indicating the lattice distance increased along the elongation direction but decreased in the direction perpendicular to elongation. Moreover, the BCP-g-SiO$_2$ with higher PBA ratio had larger transverse strain which was calculated from the $d$-spacing of the first order ring of structure factor, because the polymer layer was compressed more in the transverse direction under uniaxial stretching.

10:36AM E49.00010: Polymer-grafted Nanoparticle Membranes with Exceptional Gas Separation Performance*  
CONNOR BILCHAK (Presenter), SANAT KUMAR, CHRISTOPHER JAMES DURNING, Columbia University, YUCHENG HUANG, BRIAN C BENICEWICZ, Department of Chemistry and Biochemistry, University of South Carolina, JACQUES JESTIN, CEA/CNRS — There is considerable interest in developing novel gas separation membranes that improve on current, pure polymer-based technologies. Pure polymer grafted nanoparticle based membranes offer the exciting opportunity to tuneable small gas permeabilities but are still limited compared to current exotic polymers. Here, we discuss gas transport in GNP integrating small amounts of ungrafted polymer chains with judiciously chosen chain lengths. We find that the addition of homopolymer allows us to almost independently increase membrane gas selectivity, and thus exceed the Upper Bound representing the best currently available membrane materials. X-Ray and neutron scattering suggest that gas transport in GNP is spatially inhomogeneous with solutes bigger than a critical size being moved primarily through the interstitial spaces between the NPs, while small solutes are carried more homogeneously through the whole layer. High molecular weight free chains segregate into these interstitial regions and preferentially hinder large solute motion, thus greatly improving selectivity. Controllably manipulating transport in these inhomogeneous materials thus offers the opportunity to construct gas-separation membranes with exceptional performance.

*NSF CBET-16959502

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E50 DPOLY GSOFT DBIO: Chirality in Polymers and Soft Matter II: Liquid Crystals and Liquid Crystalline Polymers  
BCEC 252B - Mohan Srinivasarao, Georgia Institute of Technology - Tag(s): Focus

8:00AM E50.00001: E50 POLYMER PHYSICS PRIZE BREAK  —
8:36AM E50.00002: Programming Emergent Chiral and Polar Symmetries with Saddle-Splay Elasticity  YU XIA  (Presenter), Chemical and Biological Engineering, Princeton University, ANDREW DEBENEDICTIS, Tufts University, DOUG J CLEAVER, Sheffield Hallam University, TIM ATHERTON, Tufts University, SHU YANG, University of Pennsylvania — Emergent chiral symmetries in liquid crystals (LCs) are usually achieved by symmetry breaking in close boundary confinements. Gaining precise control over the location, creation and manipulation of broken symmetries remains a formidable challenge. In this work, we achieve pre-programming of broken chiral symmetries in the nematic phase of two achiral LCs (5CB and 8CB) through a ubiquitous but oft-neglected property of LCs: the “saddle-splay” elasticity. Using combinations of lithographic patterning and selective surface functionalization, we create surface patterns with spatially defined geometry and precisely controlled surface chemistry. Through this, we characterize broken symmetry regimes on a variety of surface patterns, including arrays of circular, trefoil, and annulus posts, in which saddle splay-driven effects gain physical expression. In turn, we unlock the resultant director field patterns, and identify spontaneously broken symmetries within domains exhibiting chiral and polar regimes. By fine-tuning the patterning geometry, we then program the location, energy landscape, and means of manipulation of the symmetry breaking processes. As a result, we demonstrate a multi-state stable LC display device that can be switched at an extremely low voltage density (~0.5 V/µm).

8:48AM E50.00003: Twist-bend-like phases and elastic response of model bent-core liquid crystals*  JIALE SHI  (Presenter), Department of Chemical and Biomolecular Engineering, University of Notre Dame, HYTHEM SIDKY, Institute for Molecular Engineering, University of Chicago, JONATHAN WHITMER, Department of Chemical and Biomolecular Engineering, University of Notre Dame — Bent-core liquid crystals have recently attracted significant attention because of their novel mesostructure and the intriguing behavior of their elastic constants, which are strongly anisotropic and have an unusual temperature dependence. For instance, experiments report an abnormally low bend elastic constant, which dips near the nematic-twist-bend transition, and increases again as the transition is crossed; the molecular mechanisms responsible for these behaviors are unclear. Here, we utilize Density of States algorithms in Monte Carlo simulation applied to a bent-core variant of the Lebwohl-Lasher model to analyze the mechanism behind elastic response in this novel mesostructure and understand the temperature dependence of its Frank-Oseen elastic constants.

*Department of Energy, Basic Energy Sciences (MICCoM)

9:00AM E50.00004: Chiral helical nanofilament and nanocylinder phases and a new type of polymorphism in liquid crystals*  SASAN SHADPOUR (Presenter), AHLAM NEMATI, Advanced Materials & Liquid Crystal Institute, Kent State University, LIN LI, Department of Chemistry and Biochemistry, Kent State University, SAMANTHA WAKERLIN, JULIE VANEGAS, Advanced Materials & Liquid Crystal Institute, Kent State University, MIROSLAW SALAMONCZYK, CHENHUI ZHU, Advanced Light Source, Lawrence Berkeley National Laboratory, ANTAL ISTVAN JAKLI, TORSTEN HEGMANN, Advanced Materials & Liquid Crystal Institute, Kent State University — Helical nanofilaments, consisting of bundles of twisted smectic layers with a helical pitch of 200 nm, are formed by achiral bent-core liquid crystal (BC-LC) molecules due to an intralayer mismatch between top and bottom molecular halves relieved by local saddle-splay. Here, by introducing a chiral center to one of the sides of asymmetric BC-LCs (shorter side, called meta-side), we observed the first example of the polymorphism in liquid crystalline materials. They form a not heretofore helical microfilament (HF) phase upon rapid cooling and an oblique columnar upon slow cooling. Interestingly, another not reported morphology observed when the chiral center migrates to the longer para-side). In this case, the BC-LC molecules form layers that are rolled up into coaxial cylinders resulting in the formation of heliconical-layered nanocylinders (HLNCs). HLNCs form within 80-100 nm width and micrometer lengths. This optically active cylinders form feather-like structures, braid, and assemble into hollow structures totaling six levels of hierarchical self-assembly.


*(NSF, DMR-1506018 and DMR 1307674)
9:12AM E50.00005: Indication of a Twist-Grain-Boundary-Twist-Bend Phase of flexible bent-shape chiral dimers.*

MATTHEW MURACHVER (Presenter), AHLAM NEMATI, Chemical Physics Interdisciplinary Program, Kent State University, CARSON BULLOCK, Department of Physics, College of Wooster, ZACHARY SABATA, Department of Physics, University of Nebraska, Omaha, HAUMED RAHMANI, TETIANA VOROBIOVA, Chemical Physics Interdisciplinary Program, Kent State University, MIROSLAW SALAMONCZYK, Faculty of Chemistry, University of Warsaw, ALAIN IZADNEGHADAR, Advanced Precision Systems, SEYYED SALILI, Department of Physics & Astronomy, University of Pennsylvania, VICTORIA NORMAN, CHENHUI ZHU, Advanced Light Source, Lawrence Berkeley National Laboratory, TORSTEN HEGMANN, Chemical Physics Interdisciplinary Program, Kent State University, SAMUEL N SPRUNT, JAMES GLEESON, Department of Physics, Kent State University, ANTAL ISTVAN JAKLI, Chemical Physics Interdisciplinary Program, Kent State University — Flexible bent-core oligomers with odd-numbered methylene spacers exhibit a “twist-bend” nematic (NTB) phase characterized by a nanoscale heliconical pitch. We designed mixtures of achiral dimers, which exhibit the NTB phase, with a chiral additive. By differential scanning calorimetry, resonant soft X-ray scattering, polarized optical microscopy, and induced circular dichroism studies on condensed phases of these mixtures, we find, while in the nematic phase the micron-scale pitch of the additive-induced helical structure decreases with increasing additive concentration, in the N phase both the micron-scale and the nanoscale pitch of the ambidextrous spontaneous heliconical structure increase. At chiral additive concentrations above ~2% by weight, a new phase appears between the N* and NTB* phases, which we propose to be analogous to the twist-grain-boundary (TGB) phase of chiral smectics; we designate this new phase by TGBTB.

*This work was supported by U.S. National Science Foundation (NSF) DMR-1506018 and DMR 1307674 and NSF REU CHE-1659571. Beamline 11.0.1.2 at Advanced Light Source at Lawrence Berkeley National Laboratory are supported by Director of the Office of Science, Office of Basic Energy Sciences, of U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

9:24AM E50.00006: Nano-confinement of chiral liquid crystals gives rise to exotic blue phases* VIVIANA PALACIO-BETANCUR (Presenter), Institute for Molecular Engineering, University of Chicago, JULIO C. ARMAS-PÉREZ, División de Ciencias e Ingenierías, Universidad de Guanajuato, JUAN P HERNANDEZ-ORTIZ, Departamento de Materiales y Minerales, Universidad Nacional de Colombia, JUAN DE PABLO, Institute for Molecular Engineering, University of Chicago — Blue phases (BPs) arise spontaneously in chiral liquid crystals (ChLCs) as a means to minimize the global free energy, by forming networks of defects with specific cubic symmetries. By confining BPs we introduce an approach to manipulate their structure through geometrical frustration. In this work, we present a new family of BPs by modeling ChLCs in toroidal and cylindrical cavities. The configurations are obtained following a theoretically-informed Monte Carlo relaxation of the free energy functional, which is described in the framework of the Landau-de Gennes formalism. We vary temperature and chirality to build phase diagrams and summarize the portfolio of chiral morphologies, which can be classified into twisted cholesterics, and BPs with helical and cubic symmetries. We also study the effects of surface anchoring and curvature to highlight the stability of these new phases. The formation of these new kind of morphologies offers interesting opportunities to direct the assembly of macromolecules and colloids at the nanoscale.

*Fulbright Commission in Colombia and COLCIENCIAS

9:36AM E50.00007: Temperature Dependence of the Pitch in Chiral Lyotropic Chromonic Liquid Crystals* TIMOTHY OGOILLA, Kent State University, ROBERT PALEY, Swarthmore College, PETER COLLINGS (Presenter), Swarthmore College & University of Pennsylvania — Molecular chirality is a subtle symmetry-breaking operation, yet its presence can produce profound macroscopic effects. One example is the nematic phase of liquid crystals, in which the presence of molecular chirality causes the preferred direction of molecular orientation to rotate in helical fashion resulting in striking optical effects. The pitch of the helix is sensitive to many parameters, including the type of molecules, concentration of chiral molecules, and temperature. Most liquid crystals studied to date consist of molecules or strongly bonded molecular assemblies that are not affected by experimental conditions. One exception is a lyotropic chromonic liquid crystal (LCLC), in which the size of the assemblies depends strongly on concentration and temperature. Investigation of the pitch of the helix in such systems reveals a highly unusual temperature dependence in which the pitch diverges as the temperature increases and the assemblies decrease in size. Theoretical considerations both explain this effect and allow the basic chiral interactions to be explored.

*We gratefully acknowledge funding support from the National Science Foundation through a grant to the University of Pennsylvania (MRSEC-DMR17-205030), and from Swarthmore College.
9:48AM E50.00008: Inducing chirality in homeotropic nematics via confinement geometry  JAMES MCINERNEY (Presenter), Georgia Institute of Technology, PERRY W ELLIS, Harvard University, ALBERTO FERNANDEZ-NIEVES, D. ZEB ROCKLIN, ELISABETTA MATSUMOTO, Georgia Institute of Technology — The configuration of liquid crystalline phases, in particular nematics, are controlled by both the microscopic properties of their constituents and the macroscopic boundary conditions. Past work has shown that microscopically achiral chromonic liquid crystals, which have a small twisting modulus in comparison to splay and bend moduli, form chiral textures when embedded in cylindrical geometries with homeotropic boundary conditions. We show that when the cylinder is bent into a torus, these chiral configurations form at higher relative twisting moduli than it would in a straight cylinder. We use a boundary preserving Möbius transformation to shift the escaped core region toward the inner walls of the torus, yielding energetically favorable configurations. In order to match the homeotropic boundary conditions, these configurations are necessarily twisted independent of the elastic constants of the achiral mesogens. We experimentally verify the existence of such twisted textures with 5CB in toroidal droplets.

10:00AM E50.00009: Mesogen-free Liquid Crystalline Poly(ethylene oxide) with Sulfonyl Side Chains: Effects of Tacticity and Alkyl Side Chain Length  MAN HIN KWOK (Presenter), Macromolecular Science and Engineering, Case Western Reserve University, BRYAN T SEYMOUR, BIN ZHAO, Chemistry, University of Tennessee, LEI ZHU, Macromolecular Science and Engineering, Case Western Reserve University — Atactic and isotactic poly(ethylene oxide) possessing alkylsulfonfylmethyl side chains were synthesized. Because of the strong dipolar interactions among sulfonyl groups in the side chains, they have a tendency of forming self-assembled mesophases even without the presence of aromatic mesogens. These polymers were characterized by size-exclusion chromatography (SEC), differential scanning calorimetry (DSC), and X-ray diffraction (XRD) at various temperatures. These PEO-based comb-like polymers are capable of forming liquid crystals with a double layer structure, which has been determined by temperature dependent XRD. In this presentation, effects of the tacticity and alkyl chain length on the mesophase structure and dielectric properties will be discussed.

10:12AM E50.00010: Ionic Liquid Crystalline Elastomers Actuated by Low Electric Field  CHENRUN FENG (Presenter), C.P.HEMANTHA RAJAPAKSHA, Liquid Crystal Institute, Kent State University, CAMILO PIEDRAHITA, JINWEI CAO, Polymer Engineering, University of Akron, ANTAL ISTVAN JAKLI, Liquid Crystal Institute, Kent State University, THEIN KYU, Polymer Engineering, University of Akron — Over the past two decades Liquid Crystalline Elastomers (LCEs) with anisotropic properties attracted immense interest for their superior responsibility to various external stimuli. Hybrid aligned LCE films have anisotropy of thermal extension coefficient and dielectric properties in top and bottom sides, leading to large thermally and/or optically induced bend. Electric field induced bending via Maxwell stress from dielectric coupling of insulating LCEs requires electric fields close to electric breakdown, thus limiting their applications. In ionic electroactive polymers (IEAPs), ion flow causes asymmetric volume change and generates large bending even at low (~1V) voltages. In this work ionic liquids (ILs) are introduced into hybrid aligned LCE films to combine spatial anisotropic properties of hybrid alignment in LCEs with charge separation dynamics of ionic EAPs. We demonstrate that charge separation in LCE-IL system is capable for low electric field induced flexing or flexing-induced electricity effect. Additionally, ion motion induced electro-thermomechanical effects that enable spatial deformations by varying directors of LCEs are also presented.

10:24AM E50.00011: Backfolding Transitions in a Liquid Crystalline Polymer Brush*  STEVEN BLABER (Presenter), Physics and Astronomy, University of Waterloo, NASSER ABUKHDEIR, Chemical Engineering, University of Waterloo, MARK W MATSEN, Physics and Astronomy, University of Waterloo — Liquid crystalline (LC) polymer brushes offer a convenient way of modifying surface properties for LC materials in, for example, LC displays. With this motivation in mind, we begin by studying LC polymer brushes in a simple solvent using self-consistent field theory. The polymers are modeled as worm-like chains with Maier-Saupe interactions. For good solvent conditions, the isotropic interactions favor a stretched brush while the anisotropic LC interactions favor folding into a high-density nematically collapsed brush. The brush undergoes first-order transitions as the number of folds increases. The folding transitions can be qualitatively understood through a simple analytic model balancing the energetic benefit from increased LC alignment and the cost associated with the bending energy of hairpin folds.

*This work was supported by NSERC of Canada and computer resources were provided by SHARCNET of Compute Canada.
10:36AM E50.00012: Tension-induced nematic phase separation in homopolymer melts  
WENLIN ZHANG (Presenter), RONALD LARSON, Chemical Engineering, University of Michigan — The nematic coupling parameter $\alpha$, which quantifies the interactions between backbone tangents and nematic fields, governs the nematic phase behaviors and polymer alignment in bulk and at interfaces. Together with external tension, the nematic interactions can also drive phase separation of long chains from short ones in bidisperse homopolymer melts. Combining molecular dynamics (MD) simulations and analytical theory, we extract $\alpha$ for polyethylene (PE) oligomers under applied tension, and construct a mean-field free energy to predict the phase boundary for bidisperse melts in which the longer chains are stretched by uniaxial tension. Phase separation occurs when sufficient tension is applied, consistent with a previous prediction by Olmsted and Milner. By directly observing phase separation in MD simulations, we validate the phase diagram. Using non-equilibrium MD (NEMD) simulations, we also show that extensional and shear flow may lead to nematic phase separation in molten PE oligomers, because the flow can impose a stronger tension on the longer chains than the short ones. We expect the tension-induced nematic phase separation may affect chain configurations for polydisperse polymer melts under flow, and in turn affect flow-induced crystallization.

10:48AM E50.00013: Entanglement in the isotropic-nematic crossover regime: does Edwards' primitive path picture still apply?*  
ROBERT HOY (Presenter), University of South Florida, MARTIN KRÖGER, ETH Zurich — Edwards defined entanglements in polymer melts in terms of contacts between individual chains' primitive paths (PPs). This picture breaks down in the rigid-rod-like limit: while there are no inter-PP contacts, systems remain entangled in the sense that every chain's transverse motion remains highly constrained by the other chains. How it breaks down as chains approach this limit is largely unknown. Using molecular dynamics simulations and topological analyses, we characterize how entanglement in polymer melts varies and the Edwards picture breaks down as chain stiffness and nematic order increase. We find that the diffusivity and the entanglement length $N_e$ measured by topological analyses are minimized at two different chain stiffnesses $k_1$ and $k_2$ (with $k_1 < k_2$). Both of these are below the stiffness $k_3$ at which the isotropic-nematic transition occurs. We relate these phenomena to both the gradual onset of local nematic order and the inherent limitations of Edwards’ PP picture for quantifying entanglement in semiflexible polymer melts.

*Support from NSF Award No. DMR-1555242 is gratefully acknowledged.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E51 DPOLY: Polymer Physics Prize Symposium  
BCEC 253A - Sharon Glotzer, University of Michigan - Tag(s):
Invited

8:00AM E51.00001: Polymer Physics Prize Talk: Getting the kinks out: extensional flow in polymer solutions, melts, and glasses*  
[Invited] RONALD LARSON (Presenter), Chemical Engineering, University of Michigan, SOROUSH MOGHADAM, Mechanical Engineering, University of Michigan, WEIZHONG ZOU, Chemical Engineering, University of Michigan, ROBERT HOY, Physics, University of South Florida — Using molecular dynamics and Brownian dynamics, and “kink dynamics” simulations, polymer chains under extensional flow at high stress and strains are found to unravel through folded states, wherein highly stretched strands connected by kinks, or fold points, bear most of the stress. This process occurs universally at high stresses in polymer solutions, melts, and glasses, and is responsible for the strain hardening seen in extensional flows in all these states, regardless of whether the polymer is entangled or not. We show that experimental data for stress and local orientation can be explained semi-quantitatively or even quantitatively with models that capture these dynamics.

*The support of the National Science Foundation under grant DMR 1403335 is gratefully acknowledged.
8:36AM E51.00002: Accessing the Unexplored Regions of the Glassy State to Test Paradigms of the Glass Transition*
[Invited] GREGORY MCKENNA (Presenter), HEEDONG YOON, Texas Tech University — A major challenge in glass physics is the determination of the temperature dependence of the relaxation times in the equilibrium state well below the laboratory glass temperature $T_g$. This is because the times required to achieve equilibrium in this regime become of geological/astronomical scale [1,2]. To finesse this problem, we are using materials with extremely low fictive temperature $T_f$ relative to $T_g$, hence unlocking an unexplored region of the glassy state to investigation. First, we measured the viscoelastic response of a 20 million year old amber with $T_f \sim 43.6$ K below $T_g$. The relaxation times deviated strongly from the expected VFT or WLF-behaviors turning towards an Arrhenius-response, albeit with a high activation energy. Though convincing as evidence that the dynamics of the glass do not diverge at a finite temperature, often linked to the Kauzmann [3] temperature $T_K$, the amber work is complicated because the natural origins of amber make reproducing the experiments difficult. We also built on the ultra-stable glasses exploited by Ediger and co-workers [4] and made an amorphous Teflon material with $T_f \sim 55$ K below $T_g$ and close to the putative $T_K$. Made only in microgram quantities, we needed the TTU bubble inflation [5] method to measure the creep response in the range between $T_f$ and $T_g$, expanding the amber work to $T_K$. The observed relaxation times deviate from the extrapolated WLF-line challenging the view that there is an "ideal" glass transition as posited by multiple theories and commonly considered an important aspect of glass-formation and glassy behavior.


*The authors acknowledge support from National Science Foundation under grant DMR-1610495.

9:12AM E51.00003: Edge fracture in polymeric fluids*
[Invited] SUZANNE FIELDING (Presenter), EWAN HEMINGWAY, Physics, Durham University — We study theoretically edge fracture in sheared polymeric fluids, using linear stability analysis and nonlinear simulations. We derive an exact analytical expression for the onset of edge fracture in terms of the shear-rate derivative of the second normal stress difference, the shear-rate derivative of the shear stress, the jump in shear stress across the interface between the fluid and the outside air, the surface tension of that interface, and the rheometer gap size. We provide a full mechanistic understanding of the edge fracture instability, and validate this against our simulations. These findings also suggest a possible route to mitigating edge fracture, potentially allowing experimentalists to achieve and accurately measure flows stronger than hitherto. We then consider the interaction of edge fracture with the fluid bulk. For fluids with a rather flat (but still monotonically increasing) bulk constitutive curve of shear stress as a function of shear rate, we show that edge fracture can cause a pronounced apparent shear banding that invades the fluid bulk to a distance of many gap widths in from the sample edge. To paraphrase this first scenario: "edge fracture causes (apparent) shear banding". For fluids that have a non-monotonic constitutive curve and therefore show bulk shear banding (even in the absence of any edge instabilities), we show that the jump in the second normal stress difference between the shear bands causes strong edge fracture at the fluid-air interface, consistent with the earlier intuition of Skorski and Olsmited. To paraphrase this second scenario: "shear banding causes edge fracture".

*EU 7th Framework Programme (FP7/2007-2013) / ERC grant number 279365.
9:48AM E51.00004: Statistical Field Theory of Inhomogeneous Polarizable Soft Matter* (Invited) GLENN FREDRICKSON (Presenter), DOUGLAS GRZETIC, KRIS T DELANEY, JONATHAN MARTIN, University of California, Santa Barbara — Standard approaches to modeling the electrostatic properties of inhomogeneous soft matter systems involves either neglecting dielectric contrast entirely, or imposing an ad-hoc dielectric constitutive law that is not consistent with pairwise van der Waals (VDW) interactions included elsewhere in the model. We recently developed a framework for building statistical field theories from coarse-grained particle models where the force centers can optionally carry monopole charges, dipoles, and/or classical Drude oscillators that confer polarizability. The resulting polarizable field theories self-consistently embed dielectric constitutive laws, VDW interactions, and a rich variety of charge and structure correlation physics. This talk will report on recent analytical results from loop expansions and numerical results from complex Langevin simulations that address: 1) the VDW contribution to the Flory interaction parameter in polymer blends and block copolymers, 2) the dielectric decrement or increment on adding salt to a polar or polarizable solvent, and 3) the electric-field induced shift in the critical temperature of a binary dielectric fluid mixture.

*This work was partially supported by the NSF CMMT Program through Award No. DMR-1822215 and by the MRSEC Program of the National Science Foundation under Award No. DMR 1720256.

10:24AM E51.00005: Fast but Inaccurate or Slow but Accurate: The Dilemma of Tubes and Slip Links* (Invited) SACHIN SHANBHAG (Presenter), Florida State University — The tube model for entangled polymers projects a complex multi-body problem of interacting chains onto a mean-field representation. This popular framework has been enormously successful at predicting the rheology of model (and even some industrial) polymers. However, its success cloaks several fundamental problems that become obvious when it is subjected to strong tests. One such example is binary blends with well-separated relaxation times. In such cases, slip link models which retain the multi-body character of the original problem offer a more accurate and robust alternative. However, slip link models are computationally demanding. Here, I resuscitate a super-fast slip link model that Ron Larson and I first introduced over 15 years ago. With a few small modifications, it predicts the linear rheology of binary blends with remarkable accuracy and speed.

*This material is based partially upon work supported by the National Science Foundation under Grant No. DMR 1727870.

Tuesday, March 5, 2019 8:00 AM - 9:48 AM

Session E53 GSNP DCMP: Heineman and Oppenheim Award Session B6EC 253C - Greg Huber - Tag(s): Invited

8:00AM E53.00001: Dannie Heineman Prize for Mathematical Physics Talk: Solvable systems of nonlinear ODEs: old and new results (Invited) FRANCESCO CALOGERO (Presenter), Physics & Sezione di Roma 1, Universita' di Roma "La Sapienza" & Istituto Nazionale Fisica Nucleare — Some old and new "exactly solvable" dynamical systems will be tersely reviewed.

8:36AM E53.00002: Irwin Oppenheim Award Talk: The Thermodynamic Uncertainty Relation: Theoretical Introduction* [Invited] TODD GINGRICH (Presenter), Chemistry, Northwestern University, JORDAN HOROWITZ, Biophysics and Complex Systems, University of Michigan — In thermodynamic equilibrium, molecular motions cannot generate a non-vanishing average current—of particles, mass, charge, etc. This fact is elegantly seen as a consequence of the time-reversible nature of equilibrium dynamics, which obeys detailed balance. It is well known that detailed balance can be broken by external driving, either with a time-dependent protocol (as in flashing ratchets) or by coupling a system to multiple incommensurate reservoirs (say a high-chemical-potential bath on one side of a membrane and a low-chemical-potential bath on the other side). In this latter case, the system coupled to the baths experiences a time-independent thermodynamic driving force causing the system to relax into a nonequilibrium steady state (NESS) that generates current. Since the current is made up of individual transport events, it will fluctuate around the steady state value, and the scale of these fluctuations is constrained by the typical rate of dissipation into the reservoirs, a constraint which has been labeled a Thermodynamic Uncertainty Relation (TUR). In this talk I will outline this TUR and illustrate the large-deviation-theoretic arguments underlying its derivation.

*Gordon and Betty Moore Foundation

9:12AM E53.00003: Irwin Oppenheim Award Talk: The Thermodynamic Uncertainty Relation: Applications And Extensions* [Invited] JORDAN HOROWITZ (Presenter), Biophysics, University of Michigan, TODD GINGRICH, Chemistry, Northwestern — At the mesoscale, thermal noise is an unavoidable nuisance interfering with the function of molecular devices, from molecular motors to chemical clocks. For these devices to operate, they must constantly consume energy to suppress these fluctuations. Remarkably, the recently discovered thermodynamic uncertainty relation offers a universal bound on the energetic cost to attain precision in the face of such noise. In this talk, I will discuss examples drawn from the literature of how one can apply the thermodynamic uncertainty relation to gain insight into the design principles underpinning the function of such molecular-scale devices as stochastic heat engines, molecular motors, self assembly, chemical kinetics and nonlinear response. I will then turn to extensions and generalizations of the thermodynamic uncertainty relation to highlight new opportunities for applications and insight.

*This work was support by the Gordon and Betty Moore Foundation through Grant GBMF4513.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E54 DPOLY GSOFT: Dielectric Relaxation and Charge Transport of Soft Materials
BCEC 254A - Andreas Schoenhals - Tag(s): Focus

8:00AM E54.00001: E54 POLYMER PHYSICS PRIZE BREAK —

8:36AM E54.00002: Morphology and Conductivity in Sulfonated Polyphenylenes* AMALIE FRISCHKNECHT (Presenter), Center for Integrated Nanotechnologies, Sandia National Laboratories, ERIC SORTE, Dept of Organic Materials Science, Sandia National Laboratories, BENJAMIN PAREN, Dept of Materials Science and Engineering, University of Pennsylvania, CY FUJIMOTO, LAUREN J ABBOTT, NASA Ames Research Center, KAREN WINEY, Dept of Materials Science and Engineering, University of Pennsylvania, TODD ALAM, Dept of Organic Materials Science, Sandia National Laboratories — Proton conduction in hydrated, proton-conducting polymer membranes is highly affected by hydration level and membrane morphology. Here we examine morphology and dynamics in a promising proton-conducting polymer, a sulfonated Diels-Alder polyphenylene (SDAPP). We performed atomistic molecular dynamics (MD) simulations on a series of SDAPPs, systematically varying the degree of sulfonation and water content to determine their effect on the nanoscale structure, particularly for the hydrophilic domains formed by the ionic groups and water molecules. The static structure factors calculated from simulation are in good agreement with X-ray scattering data. NMR and impedance spectroscopy measurements show that the proton conduction mechanism evolves from being dominated by vehicular transport at low hydration and sulfonation levels to including a significant contribution from the Grötthuss mechanism at higher hydration and sulfonation levels.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
8:48AM E54.00003: Phase Transition and Dynamics in Imidazolium-Based Ionic Liquid Crystals through a Metastable States*
KOJI FUKAO (Presenter), TOSHIHARU YAMANE, JUN YOSHIOKA, Department of Physics, Ritsumeikan University — The phase transition behavior and dynamics of ionic liquid crystals, 1-methyl-3-alkylimidazolium tetrafluoroborate with various alkyl chain lengths, were investigated by X-ray scattering, differential scanning calorimetry, optical microscopy, and dielectric relaxation spectroscopy to elucidate the mechanism of their structural and phase changes. A metastable phase was found to appear via a supercooled smectic phase on cooling. In the metastable phase, disorder in the smectic phase is partially frozen; thus, the phase has order higher than that of the smectic phase but lower than that of the crystalline phase. During the subsequent heating process, the frozen disorder activates, and a crystalline phase appears in the supercooled smectic phase before entering the smectic phase. The relationship between the phase behavior and the dynamics of charge carriers such as ions is also discussed.

*This work was partially supported by a Grant-in-Aid for Scientific Research (B) (No. 25287108 and No.16H04036) from the Japan Society for the Promotion of Science. The synchrotron radiation experiments were performed at the BL40B2 of SPring-8 with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) (Proposals 2014A1230, 2017B1119, and 2018B1454).

9:00AM E54.00004: Revealing the fine features of charge transport mechanism in ionic glass-forming liquids by dielectric spectroscopy*
YANGYANG WANG (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — By examining the fine features of the dielectric spectra of a variety of ionic glass-forming materials, including ionic liquids and poly(ionic liquids), we show that the derivative of their real permittivity progressively broadens on the low-frequency side when the glass transition is approached from above. This phenomenon, ubiquitous and yet difficult to ascertain in the widely-used conductivity or modulus representation, is reminiscent of the spectrum broadening in supercooled dipolar liquids. Our finding provides direct evidence of heterogenous dynamics in ac conduction of ionic glasses and calls for a reconsideration of the classical models that predict a steep, Debye dispersion at low frequencies.

*This research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT Battelle, LLC, for the U.S. Department of Energy.

9:12AM E54.00005: Dielectric Relaxation and Conductivity in Polyelectrolyte Systems*
KHATCHER O. MARGOSSIAN (Presenter), MURUGAPPAN MUTHUKUMAR, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Using Electrical Impedance Spectroscopy, we have monitored the dynamical relaxations of polyelectrolytes in concentrated solutions and in charged materials. Here, we explore the effects of chain length, ionic strength, cross-link density, and pH on the dynamics of charged macromolecular assemblies. We also report experimental results on the ionic conductivity of these systems. This research builds our understanding of the parameters necessary for tuning functional properties of polyelectrolyte-based systems, and motivates further work in logically designing electrically-responsive materials.

*National Science Foundation (DMR-1504265)
National Science Foundation, SMLS National Research Traineeship (Grant No. 1545399)

9:24AM E54.00006: Dielectric Spectroscopy on Choline Chloride based Deep Eutectic Solvents
DANIEL REUTER (Presenter), PETER LUNKENHEIMER, ALOIS LOIDL, Experimental Physics V, University of Augsburg — Deep eutectic solvents (DES) have caught the attention of the scientific community in recent years and are discussed as a promising new class of ionic liquid analogues [1]. Prominent examples are mixtures based on choline chloride (ChCl) with various hydrogen-bound donors like, e.g., glycerol [2]. Although dielectric spectroscopy is an ideal tool to investigate ionic-conductivity mechanisms, until now only a few DES were studied by this method. In this talk, we present dielectric spectroscopy data for three ChCl based DES, covering a broad frequency and temperature range. Our evaluation focuses on the often neglected molecular reorientational dynamics and its correlation with the ionic mobility, as also found in ionic liquids [3].

9:36AM E54.00007: Molecular Dynamics Simulations of Ion Transport in High Transference Number Polyelectrolytes for Li-ion Batteries  
KARA FONG (Presenter), Chemical and Biomolecular Engineering, University of California, Berkeley, JULIAN SELF, Materials Science and Engineering, University of California, Berkeley, KYLE DIEIDERICHSEN, Chemical and Biomolecular Engineering, University of California, Berkeley, KRISTIN PERSSON, Materials Science and Engineering, University of California, Berkeley, BRYAN MCCLOSKEY, Chemical and Biomolecular Engineering, University of California, Berkeley — Conventional liquid electrolytes for Li-ion batteries suffer from low Li\(^+\) transference numbers, which limit mass transport in porous electrodes and thus reduce the battery's energy density and rate capability. It has been proposed that replacing traditional Li-ion battery salts with lithium-neutralized polyanions dissolved in solution could be a means to increase the Li\(^+\) transference number while only modestly sacrificing ionic conductivity. While initial experimental studies have demonstrated the promise of this approach, rational design of optimal polyelectrolytes requires more fundamental, atomistic-level understanding of the ion transport mechanisms in these systems. To this end, we use classical molecular dynamics simulations to investigate the behavior of poly(allyl glycil ether-lithium sulfonate); this polyanion has been thoroughly characterized experimentally for this application, enabling validation of the computational model. By characterizing the Li\(^+\) diffusion mechanism as well as ion aggregation behavior in the system, we elucidate the atomistic phenomena that most strongly govern experimentally-measured conductivity and transference numbers.

9:48AM E54.00008: Temperature dependent vibrational modes of Ammonium Nitrate in terahertz regime*  
ABDUR RAHMAN (Presenter), Physics and Technology, Edinboro University, TOWFIQ AHMED, DAVID S. MOORE, ABUL K AZAD, Los Alamos National Laboratory — Ammonium Nitrate (AN), often used as an ingredient for making improvised explosives, does not show any spectral feature at room temperature. We employed terahertz time domain spectroscopy (THz-TDS), a non-invasive technique, in the range of 0.30 THz to 2.50 THz to measure the effective dielectric properties of AN embedded in a polytetrafluoroethylene (PTFE) binder in the temperature range 5K to 300K. We extracted the dielectric constants of AN using effective medium theories and fitted them using Lorentz dispersion model combined with Huang equation. We identified six low frequency vibrational modes of pure AN at low temperature (<240 K). These lattice vibrations in the low frequency range agree reasonably well against our first principles Density Functional Theory (DFT) simulation of molecular AN, that reveals four low frequency vibrational modes within 3THz.

*Los Alamos National Laboratory LDRD program.

10:00AM E54.00009: Low-frequency dielectric response of a periodic array of charged spheres in an electrolyte solution  
CHANG-YU HOU (Presenter), JIANG QIAN, DENISE FREED, Schlumberger-Doll Res Ctr — We study the low-frequency dielectric response of charged spheres arranged in a cubic lattice and immersed in an electrolyte solution. We focus on the influence of the out-of-phase current in the ionic charge neutral regime. In the thin double-layer limit, we use Fixman's boundary condition at the outer surface of the double layer to capture the direct interaction between the electric field and the flow of the ions. For periodic conditions, we combine the methods developed by Lord Rayleigh and by Korringa, Kohn and Rostoker. When the charged spheres occupy a very small volume fraction, smaller than one percent, our solution becomes consistent with the Maxwell Garnett mixing formula together with the single particle polarization response, as expected, because inter-particle interactions become less prominent in the dilute limit. By contrast, the inter-particle interaction, computable in the periodic geometry, greatly alters the dielectric response when charged spheres occupy even a slightly higher volume fraction, as low as two percent. Our results imply that the signature of the dielectric response of a system consisting of densely packed charged spheres immersed in the electrolyte can differ drastically from a dilute suspension.

10:12AM E54.00010: Low-frequency dielectric response of charged oblate spheroidal particles immersed in an electrolyte*  
CHANG-YU HOU, DENISE FREED (Presenter), PABITRA N SEN, Schlumberger-Doll Res Ctr — We studied the low-frequency polarization response of an oblate spheroidal particle with surface charge immersed in an electrolyte. Because the charged spheroid attracts counterions which form an electric double layer around the particle, the dielectric response involves an interplay between the motion of these counterions and the spheroidal shape of the particle. For two different counterion distributions in the thin electric double-layer limit, we obtained analytic expressions for the polarization coefficients to the first nontrivial order in frequency. We find that the polarization response normal to the symmetry axis depends on the total amount of charge carried by the oblate spheroid, while that parallel to the symmetry axis is suppressed when there is less charge on the edge of the spheroid. We then show that a dilute suspension of charged particles has an enhancement in the low-frequency dielectric response which is suppressed by high ion concentrations in the electrolyte. Both higher aspect ratios and smaller sizes of the spheroids lead to a stronger dielectric enhancement. The characteristic frequency associated with the dielectric enhancement scales inversely with the particle size, and it has a weak dependence on the shape of spheroid.

*Supported by Schlumberger.
Dielectric Study of Soft Materials at High Electric Fields [Invited]  RANKO RICHERT (Presenter), Arizona State University — The area of nonlinear dielectric effects began with Debye's work on saturation, its signature being a reduction of the dielectric constant, \( \varepsilon_s \), as the electric field is increased [1]. The work of Piekara [2] added the chemical effect, an increase in \( \varepsilon_s \) that originates from the equilibrium of two species with different dipole moments. Dielectric hole burning and similar techniques demonstrated that the energy absorbed from a field can accelerate dynamics, even when the temperature remains constant. Moreover, strong external fields can slow down the dynamics of polar liquids, a feature that may be associated with entropy reduction. The overall reversible field effects amount to amplitudes increasing and/or decreasing, and the loss spectrum being shifted to the left and/or right along the logarithmic frequency scale [3]. Additionally, crystallization outcomes can be modified by static fields of moderate amplitude [4]. The aim of this talk is to provide an outline of the various experimental approaches used with high fields and to present the different field protocols can be exploited to discriminate among the different sources of nonlinear polarization in soft materials. We will discuss the level of our understanding for each of the effects, and the progress of modeling the observed features. The results of time-resolved (with respect to the time at which the high field is applied) experiments will be connected to structural recovery and physical aging.


Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E55 GSNP: Statistical Mechanics of Social Systems  BCEC 254B - Michel Pleimling, Virginia Tech

Statistical mechanics of Twitter*  GAVIN HALL (Presenter), Feinberg School of Medicine, Northwestern University, WILLIAM BIALEK, Physics, Princeton University and The CUNY Graduate Center — From fads to residential segregation, social processes depend on interactions among many individuals. Social phenomena are prototypically emergent, leading some to ask if we can build a statistical mechanics for these systems. We construct such models directly from data on individual participation in Twitter communities. We identify communities and topics of conversation within those communities, allowing the definition of binary (tweet/silent) variables for each individual during each conversation. We then build maximum entropy models that match the pairwise correlations among these variables, predicting the joint distribution of the binary variables across the entire community. These simple Ising-like models give an accurate quantitative description of many higher order features in the data, and lie near a critical surface in the space of possible models. Finally, we systematically coarse-grain the observed network states, finding hints that the macroscopic behavior is controlled by a non-trivial fixed point in the sense of the renormalization group.

*Supported in part by the NSF Center for the Physics of Biological Function (PHY-1734030), Center for the Science of Information (CCF-0939370), and grant PHY-1607612.
Empirical scaling and dynamical regimes for GDP: challenges and opportunities

HAROLD HASTINGS, TAI YOUNG-TAFT (Presenter), CHRIS COGGINS, THOMAS WANG, Bard College at Simon’s Rock — Analysis of GDP data and per capita GDP data from 1980 and 2016 finds three scaling regions. The GDP of the largest ~25 economies (nations, EU) follows a power law GDP ~ 1/rank; this is followed by a second scaling region in which GDP falls off exponentially with rank and finally a third scaling region in which the GDP falls off exponentially with the square of rank. The distribution of per capita GDP also displays these three scaling regions. Both patterns hold despite significant changes in technology, the size of the world economy, emergence of new economic powers such, and world trade (almost free communication, containerized shipping yielding sharp declines in shipping costs). Thus, empirically, these patterns may be universal [1-5]; in which case one of the targets for growth of those in the second and third scaling regions may be to identify and target causative differences between these economies and those in the first (power law) scaling region.

References

8:48AM E55.00005: Coarse-graining armed conflict*  EDWARD LEE (Presenter), Cornell University, BRYAN DANIELS, Arizona State University, VEIT ELSER, Cornell University, DAVID KRAKAUER, JESSICA FLACK, Santa Fe Institute — Large-scale armed conflict between groups is a defining phenomenon of modern human civilization, but the absence of a compelling model of conflict that agrees with the data means that prediction of conflict remains rudimentary. In a simple model, the spread of conflict might be described as a propagating avalanche or percolating component that extends across time and space and through a network of related actors. The presence of near power-law statistics in the sizes, durations, and actor network components of conflict suggests that such an abstracted model could provide both useful intuition and quantitative predictions about the structure of conflict on large scales. We explore this perspective in detail by performing a renormalization scheme on the surface of the Earth to generate statistics of conflict avalanches along coarse-grained spatiotemporal scales. We show that some kinds of armed conflict may obey scaling laws that could provide a basis for a predictive theory of conflict based on ideas from statistical physics.

*We acknowledge funding from the John Templeton Foundation (no. 60501), St. Andrews (no. 13337), National Science Foundation (no. 0904863, no. DGE-1650441). J.C.F. acknowledges The Proteus Foundation.

9:00AM E55.00006: Impact Factors and the Central Limit Theorem: Why citation averages are scale dependent MANOLIS ANTONOYIANNAKIS (Presenter), Applied Physics and Applied Mathematics, Columbia University — We apply the Central Limit Theorem to study how citation averages, and Impact Factors (IFs) in particular, depend on scale. For a journal of \( n \) papers randomly selected from a population, we expect from the Theorem that its IF fluctuates around the population average \( \mu \), and spans a range of values proportional to \( \sigma / \sqrt{n} \), where \( \sigma^2 \) is the variance of the population's citation distribution. The \( 1/\sqrt{n} \) dependence has profound implications for IF rankings: The larger a journal, the narrower the range around \( \mu \) where its IF lies. IF rankings therefore allocate an unfair advantage to smaller journals in the high IF ranks, and to larger journals in the low IF ranks. This implies a scale-dependent stratification of journals in IF rankings, whereby small journals occupy all ranks, mid-sized journals occupy the middle ranks, and very large journals have IFs that asymptotically approach \( \mu \). We confirm these predictions by analyzing 20 years of Impact-Factor and journal-size data, and the citation distributions of 11,000 journals. We propose the \( \Phi \) index, a rescaled IF that accounts for size effects, and which can be readily generalized to account also for different citation practices across research fields [1].


9:12AM E55.00007: Higher-Order Correlations in Bursty Temporal Patterns  HANG-HYUN JO (Presenter), TAKAYUKI HIRAOKA, Asia Pacific Center for Theoretical Physics, MIKKO KIVELÄ, Aalto University — Temporal inhomogeneities in event sequences of natural and social phenomena have been characterized in terms of interevent times and correlations between interevent times. The inhomogeneities of interevent times have been extensively studied, while the correlations between interevent times, correlated bursts (CB), are far from being fully understood. Firstly, we numerically show that the strong CB, depicted by power-law burst size distributions, violates the well-established scaling relation between the power-law decaying autocorrelation function and the power-law interevent time distribution (PRE 2017). Next, for understanding empirical data sets for human activities showing power-law burst size distributions but negligible memory coefficient, we derive an analytic form of the memory coefficient between consecutive interevent times as a function of parameters describing interevent time and burst size statistics, to conclude that the memory coefficient might have some limits in quantifying CB (PRE 2018). Finally, in order to completely characterize the event sequence, we develop a detection method of the hierarchical burst structure by exactly mapping the event sequence onto a rooted tree, implying no loss of information on the original event sequence (in preparation).

9:24AM E55.00008: A Generalized Asset Exchange Model With Economic Growth and Wealth Distribution  HARVEY GOULD (Presenter), Physics, Clark University, KANG LIU, Physics, Boston University, NICHOLAS LUBBERS, Computer, Computational, and Statistical Sciences Division, Los Alamos National Laboratory, W. KLEIN, Physics, Boston University, JAN TOBOCHNIK, Physics, Kalamazoo College, BRUCE M BOGHOSSIAN, Mathematics, Tufts University — An agent-based yard-sale model of the economy is generalized to incorporate economic growth and its distribution to the agents according to their wealth as determined by a parameter \( \lambda \). In addition to providing insight into the relation between the nature of economic growth and wealth inequality, we find that the model has a phase transition at \( \lambda = 1 \) between a equilibrium phase with economic mobility and a non-stationary phase for which there is no mobility and wealth is concentrated among a few agents. We show that the critical exponents obtained for a fixed number of agents do not obey the usual scaling laws. However, the critical exponents are consistent with the scaling laws and mean-field theory if the Ginzburg parameter, which controls the accuracy of the mean-field approximation, is held fixed as the transition is approached and is much greater than one. The transition raises questions about whether the methods of equilibrium statistical mechanics can be applied to economic systems. We also discuss possible implications of our results for economic systems and for understanding critical point behavior in systems with long, but finite, range interactions such as metals, biological systems and polymers.
9:36AM E55.00009: Statistical Mechanics of Intractable Conflicts  MIRON KAUFMAN (Presenter), Cleveland State University, HUNG T. DIEP, University of Cergy-Pontoise, SANDA KAUFMAN, Cleveland State University — We extend a statistical physics model of two-group conflicts (H. T. Diep, et al Physica A 469, 183 (2017) to three conflicting groups. We apply mean field theory (for long range interactions) and Monte-Carlo simulations (for short range interactions) to study the time dependence of the mean attitudes in each group. Using the mean field approach, we observe that at some intermediate temperatures the means of group attitudes oscillate in time. Independent of initial conditions, attitude trajectories converge over time to an attractor in the three-dimensional space of group mean attitudes. In contrast, chaotic unpredictable time variation of attitudes is observed for short range interactions. This model with attractors and chaos is proposed as a tool for understanding intractable conflict dynamics. It can be used to generate scenarios of possible trajectories in time, which can be employed for managing intractable conflicts.

9:48AM E55.00010: Understanding the extreme Thouless effect in a simple, dynamic social network - the XIE model*  ROYCE ZIA (Presenter), Physics, Virginia Tech, WEIBIN ZHANG, MOHAMMADMEHDI EZZATABADIPOUR, KEVIN EBASSLER, Physics, University of Houston — A system undergoing a phase transition which exhibits the characteristics of both first and second order transitions is said to display the Thouless effect, e.g., the order parameter suffering a discontinuity and fluctuates through all values within the jump. In a simple model extreme introverts and extraverts, the former/latter cuts/adds a random link when chosen to act (the XIE model, EPL 100, 66007 and PRE91, 042102). The steady state consists of a networks of crosslinks between the i's and e's. The fraction of these, f, serves as an order parameter jumping from ~0 to ~1 as the ratio of i's to e's drops through unity. At unity, f wanders between "soft walls" at f0 and 1-f0. With f0 →0, the system is said to exhibit an "extreme Thouless effect." We present a novel approach based on a self-consistent mean field theory. The predictions agree spectacularly well with all simulation data. Further, we obtain the analytic form of the asymptotic behavior of f0 : It vanishes as [(lnL2/L)]1/2, where L is the size of each subgroup. Though this form sets in as late as L->2000, very good bounds (e.g., ~1%) for more accessible L's (e.g., 2000) can be found by solving a transcendental equation: x+lnx = ln(L^2/2π).

*This research is supported in part by NSF DMR-1507371.

10:00AM E55.00011: Price Measurement in Financial Markets and Quantum Coupled-Wave Model of Price Dynamics*  JACK SARKISSIAN (Presenter), Managing Director, Algostox Trading — We present a theory of bid and ask price dynamics in financial markets where the two prices form as a result of quantum-chaotic interaction between buy and sell orders. In this model the two prices are represented by eigenvalues of a 2x2 price operator corresponding to "bid" and "ask" eigenstates. We will present the trading process from physics point of view, discuss how each trade represents an elementary act of price measurement and demonstrate how the theory is built from this argument. We will show that the coupled-wave theory reflects important characteristics of bid and ask price dynamics and order density in the limit order book. Calibration examples will be provided for stocks at various time scales. This theory opens a new dimension in financial modeling providing a framework for liquidity pricing, illiquidity risk evaluation, position management, as well as brings up a discussion about the nature of processes in financial markets.

*The work was not funded by any external sources.

10:12AM E55.00012: Congested Equilibria in Large-Scale Traffic Networks: Existence, Stability and Robustness through Chemical Reaction Network Analogues  S SIVARANJANI (Presenter), VIJAY GUPTA, University of Notre Dame — Discrete fluid-like models such as the Cell Transmission Model (CTM) have proven successful in modeling traffic networks. In general, these models employ discontinuous dynamics or nonlinear terms to describe phenomena like shock waves and phantom jams. Given the complexity of the dynamics, it is not surprising that the stability properties of these models are not yet well characterized. Recent results prove the existence of a unique equilibrium in the free flow regime for certain classes of networks modeled by the CTM; however, these results restrict network demands and hold only for acyclic network topologies. Further, it is of interest to understand network behavior in congested regimes, since practical networks are often congested. We propose a new modeling paradigm for traffic networks, where an analogy between discrete fluid-like traffic models and a class of chemical reaction networks is constructed by suitable relaxations of key conservation laws in the CTM. Using this analogy, we provide structural conditions on the network graph topology for the existence of equilibria in congested regimes. Drawing upon entropy-like Lyapunov functions from chemical reaction network theory, we prove that the network admits multiple stable and robust congested equilibria.
Understanding the underlying mechanism of collaborative network formation is highly relying on the property of assortative/disassortative mixing patterns. Recent studies have shown that both of assortative and disassortative mixing patterns are widely existing in many social networks. However, it’s not always been well-confirmed that people tend to connect with someone who has similar or dissimilar individual traits. In this study, we build a scientific collaboration network by the common publishing relationship with the APS journal papers and measure the scholars’ degree assortativity and research interest assortativity. Our study has shown that the extent of assortative mixing behaviors of scholars may diversify from the different physics fields, or the social ties. In addition, the middle-level degree scholars play a vital role in bridging the collaborative communities and research fields, while this large group of members have not received adequate attention in the study of the science of science.

*This work is supported by the NNSFC under grant Nos. 71871042 and 71371040.

Most existing works modeling influence propagation assume that there is only one content spreading over networks. However, an influence propagation process could have multiple correlated contents spreading simultaneously and exhibiting positive (e.g., opinions on same-sex marriage and gun control) or negative (e.g., opinions on universal healthcare and tax-relief for the ‘rich’) correlation. In a nutshell, few researchers model an influence propagation with the simultaneous spread of multiple correlated contents. Thus, for this scenario, we first propose a new model, the vector threshold model. For this model, we analyze the expected size of global cascades and find the condition of the existence of global cascades. Then, we confirm the correctness of our analysis by numerical studies. Next, we discuss how the correlation among contents affects the expected size of global cascades. In particular, when the mean degree of nodes is at a low level, the competitive, independent, and cooperative relationships produce global cascades with similar size. Only when the mean degree is at a high level do we see significant differences between these relationships on the expected size of global cascades.

*Research was sponsored by the ARO and was accomplished under Grant Number W911NF-17-1-0587.

We present a stochastic microscopic model that exhibits the same properties as the Generalized Voter Model in its Langevin description. Building on a model introduced in 2011 by Blythe et al. for the investigation of ordering dynamics in the presence of symmetric absorbing states, we show that our model exhibits phase transitions belonging to three different universality classes: Voter, Ising, and Directed Percolation. These different universality classes are identified through a systematic investigation of various static and dynamic quantities. We also present some data on the aging processes taking place at Voter critical points and show that, depending on the values of some system parameters, properties of linear or non-linear voter models are recovered.

*Research was sponsored by the US Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.
Emergence of a crystalline phase in sheared granular matter

HARRY SWINNEY (Presenter), CHARLES RADIN, University of Texas at Austin, FRANK RIETZ, MATTHIAS SCHROETER, Max-Planck-Institute for Dynamics and Self-Organization — One-half century ago a classic experiment by G.D. Scott (Nature 188, 908, 1960) showed that pouring steel balls into a rigid container filled the volume to an upper limit volume fraction of 0.64, which is well below the volume fraction 0.74 filled by spheres in a hexagonal close-packed (HCP) or face-centered cubic (FCC) lattice. Subsequent experiments confirmed a “random closed-packed” (RCP) volume fraction of about 0.64. However, the physics of the RCP limit has remained a mystery. We have conducted an experiment on a cubical box filled with 49400 precision glass spheres under weak shear imposed by a small slow angular oscillation of two opposite sidewalls. A phase transition occurred at a volume fraction of 0.645, from a disordered to an ordered state, consisting of crystallites of mixed FCC and HCP symmetry that coexist with the amorphous bulk. The transition is initiated by homogeneous nucleation. In the shearing process small crystallites with about ten or fewer spheres dissolve, while larger crystallites grow.

doi.org/10.1103/PhysRevLett.120.055701, JSP doi.org/10.1007/s10955-018-2144-4).

Jamming by shear in a dilating granular system

MEIMEI WANG (Presenter), Civil Engineering, University of Science and Technology Beijing, DONG WANG, JOSHUA SOCOLAR, HU ZHENG, ROBERT P BEHRINGER, Physics Department, Duke University — Jamming can occur in frictional granular materials undergoing shear at a fixed packing fraction, $\phi$, for $\phi$ within a range of packing fractions below the isotropic jamming point, and the amount of strain required to induce jamming, $\gamma$, increases with decreasing $\phi$. We are interested in how the shear jamming process is affected if the system is dilating as it is sheared. We conduct experiments to shear a 2D granular system while continuously increasing the system volume. Below a certain dilation rate, the system is still able to jam at packing fraction, $\phi_c$, smaller than the initial $\phi$. We measure $\gamma$ for different dilation rates and initial packing fractions by monitoring the coordination number of non-rattlers and the system pressure. We find that $\gamma$ is the same as the $\gamma$ required to jam a system with fixed packing fraction $\phi_c$ via pure shear.

*This work was supported by NSF DMR-1206351, NSF DMR-1809762, NASA NNX15AD38G, DARPA 4-34728 and the W. M. Keck Foundation.

System Size Dependence in Shear Jamming of 2D Frictional Grains

DONG WANG (Presenter), HU ZHENG, Duke University, JONATHAN BARES, CNRS, ROBERT P BEHRINGER, Duke University — Jamming jamming (SJ) occurs for frictional granular materials with packing fractions (\(\Phi\)) in a finite range below the isotropic jamming point, when the material is subject to a sufficiently large shear strain, $\gamma_{SJ}$, starting from a force-free state. Here we report experimental studies on the system size dependence for a quasi-2D frictional system composed of bidisperse photoelastic disks. The number of particles in the system ranges from 60 to 3000 by varying particle diameters while maintaining the number and size ratio between big and small disks the same. We observe that $\gamma_{SJ}$ increases with system size at the same $\Phi$ for systems with less than 1000 particles, reminiscent of a recent simulation work (Baity-Jesi et al., J. Stat. Phys. 167, 735 (2017)). However, such a dependence is much weaker comparing systems with 1000 and 3000 particles. Our results imply that SJ still exists in frictional granular materials in the thermodynamic limit.

*We acknowledge support from NSF DMR1206351 and DMR1809762, NASA NNX15AD38G, DARPA 4-34728, the W. M. Keck Foundation and a Research Triangle MRSEC Fellowship.

Granular jamming transition: induced by shearing and compressing

HU ZHENG (Presenter), Duke University/Hohai University, DONG WANG, YIQIU ZHAO, ROBERT P BEHRINGER, Duke University — Jamming of a granular system can be achieved by either isotropically increasing the packing fraction (isotropic jamming) or applying pure shear over a range of packing fractions below the isotropic jamming point (shear jamming). We experimentally study jammed configurations obtained by isotropic biaxial compression or pure shear in a quasi-2D granular system composed of photoelastic disks. A density matching method is applied to avoid basal friction. The fabric anisotropy and stress anisotropy are clearly different in the two cases. However, studies of the scaling behavior near the jamming transition reveal that, as the transition is approached, the scaling exponent of the pressure is the same for the isotropic jamming and shear jamming cases.

*This work was supported by NSF grants DMR-1809762 and DMR-1206351, the William M. Keck Foundation, DARPA grant 4-347281, and a Triangle MRSEC fellowship for DW. HZ thanks NSFC(Jiangsu) Grant No. BK20180074 for financial support.
8:48AM E56.00005: Experimental observation of shear jamming in 3D granular materials* DAVID Z CHEN (Presenter), RYAN KOZLOWSKI, ROBERT P BEHRINGER, Duke University — Frictional granular media can shear jam over a range of packing fractions below the isotropic jamming packing fraction. We experimentally study shear jamming in 3D by applying cyclic shear at fixed volume for a granular packing submerged in a density-matched solution; the effects of gravity are minimized in this environment, preventing compaction by grain weight. We observe signatures of shear jamming in the macroscopic pressure signal with a variety of packing fractions and shear amplitudes over many (on the order of 100) shear cycles. We report on analysis of particle positions (tracked via refractive index matched scanning [1]) from cycle to cycle that show correlations between microscopic rearrangements and changes in peak pressure across cycles.


*The following grants support this work: DARPA 4-34728, NSF-DMR1206351, NASA NNX15AD38G, Army Research Office Grant W911NF-18-1-0184.

9:00AM E56.00006: Nontrivial plasticity of a shear-jammed granular system* YIQIU ZHAO (Presenter), Duke University, JONATHAN BARES, Laboratoire de M‘(e)canique et G‘(e)nie Civil, Universit‘(e) de Montpellier, HU ZHENG, AGHIL ABED ZADEH, JOSHUA SOCOLAR, ROBERT P BEHRINGER, Duke University — We report shear experiments on a layer of photo-elastic disks in which shear is applied through basal friction with 21 independently controllable concentric rings below the granular layer in a Couette geometry. The rings rotate at different rates to make the local shear strain uniform inside the system. By applying this uniform shear in small steps, we create an ensemble of static shear jammed (SJ) configurations with different packing fractions (\(\phi\)) below the isotropic jamming packing fraction (\(\phi_J\)). We find that the average size and radial profile of plastic deformations between steps vary with packing fraction. A transition at \(\phi_c<\phi_J\) is observed. When \(\phi_c<\phi_c\), the plastic deformation is localized to a narrow shear band close to the inner boundary of the shear cell. When \(\phi_c>\phi_c\), the plastic deformation is spread through the entire system. We report power-law dependence of deformation amplitude on packing fraction close to \(\phi_c\). We also find similar behavior for non-uniform applied shears.

*This work is funded by NSF DMR-1809762, NSF-DMR1206351, NASA NNX15AD38G, the William M. Keck Foundation and DARPA grant 4-34728.

9:12AM E56.00007: Experiments on jamming with oil droplets instead of photoelastic disks* ERIC WEEKS (Presenter), YONGLUN JIANG, CARLOS S ORELLANA, XIA HONG, Emory University — We use quasi-two-dimensional emulsions as experimental models to study the flow of jammed materials. Our emulsions are oil droplets in water and are compressed between two parallel glass plates so that the droplets are deformed into pancake-like disks. We use microscopy to observe these droplets as they flow. From the deformed outlines of the droplets, we can measure all of the inter-droplet forces to within 10%. In this talk I’ll present some of the experiments we’ve done that were directly inspired by Behringer group experiments, and also briefly mention some recent results on flowing samples.

*Funded by NSF (earlier work by CBET-1336401, recent work by CBET-1804186)

9:24AM E56.00008: Dynamic Measurements of Normal and Tangential Coefficients of Restitution for an Inelastic Billiard JEFFREY OLAFSEN (Presenter), KAI YANG, Department of Physics, Baylor University — Driven granular media dissipate a large amount of energy in their particle-particle and particle-boundary interactions. As such, our understanding of the fundamental dynamics in these systems is complicated by the velocity-dependent nature of the coefficient of restitution. Even how a driven granular flow jams necessitates a better understanding of the details of this dissipative mechanism. Very sophisticated experiments have sought to better understand and characterize the velocity dependence of the coefficient of restitution by attempting to constrain and control aspects of the collisions. A careful and in-depth analysis for an inelastic billiard moving within a confining boundary allows the velocity-dependence to be measured as the dynamics freely evolve over multiple collisions in the driven system. The shape of the geometry can be varied to tease out details of the dynamics as well as the differences between the normal and tangential coefficients of restitution. The large amount of data generated in this experiment allows the contributions from both the normal and tangential velocity components in the particle-boundary interactions to be examined. Two derivative experiments, one for particle-boundary and the other for particle-particle collisions will also be discussed.
9:36AM E56.00009: Nontrivial power-law scaling of impact forces into granular materials  NASSER KRIZOU
(Presenter), ABE CLARK, Naval Postgraduate School — When an intruder strikes a granular material, the grains exert a force which decelerates and stops the intruder. Existing ballistic models can successfully describe much of the intruder-material interaction using a macroscopic force law, but these models often fail near the moment of impact. Here, we show results from experiments and numerical simulations, focusing on microscopic intruder-grain interactions during the early stages of impact. We record high-speed videos of intruders (of varying size and density) impacting assemblies of photoelastic disks, and we quantify both the intruder dynamics and the forces in the material. We show nontrivial power law scaling of peak forces during the initial transient phase of the impact into granular materials. Experiments and simulations indicate that this scaling is insensitive to many system details, such as friction, grain stiffness, and whether grain-grain interactions are linear (Hookean) or nonlinear (Hertzian). We also find important similarities to impact forces in dense suspensions, suggesting that our results may be generic for impacts into many kinds of soft, deformable materials.

9:48AM E56.00010: Experimental seismicity and avalanches in sheared granular media*  AGHIL ABED ZADEH
(Presenter), JONATHAN BARES, University of Montpellier, JOSHUA SOCOLAR, ROBERT P BEHRINGER, Duke University — We report on experiments investigating the dynamics of a 2D granular medium, consisting of a vertical layer of photo-elastic disks sheared by a slider that is pulled by a spring. The motion of the slider proceeds through a sequence of discrete events, analogues to seismic shocks, in which elastic energy stored in the spring is rapidly released. We measure the statistics of several properties of the individual events: the energy loss in the spring, the duration of the movement, and the temporal profile of the slider motion. We also study certain conditional probabilities and the statistics of mainshock-aftershock sequences. At low driving rates, we observe crackling with Omori-Utsu, Bath, and waiting time laws similar to those observed in seismic dynamics. At higher driving rates, where the sequence of events shows strong periodicity, we observe scaling laws and asymmetrical event shapes that are clearly distinguishable from those in the crackling regime.


10:00AM E56.00011: Dynamics of a grain-scale intruder in a granular system with and without basal friction*  RYAN KOZLOWSKI (Presenter), DAVID Z CHEN, HU ZHENG, JOSHUA SOCOLAR, Physics, Duke University, LOU KONDIC, Mathematical Sciences, New Jersey Institute of Technology, KAREN DANIELS, Physics, North Carolina State University, ROBERT P BEHRINGER, Physics, Duke University — When a granular medium is sheared by a spring-driven mechanism, the system can exhibit stick-slip dynamics: The grains form a rigid solid as the spring loads (stick event) which plastically deforms when the spring load exceeds the yield stress of the stable configuration (slip event). We experimentally investigate the dynamics of a single grain-scale intruder driven by a spring through a 2D annular bed of photoelastic disks. We vary the grain packing fraction, the interparticle friction, and the basal friction between grains and the table surface, and we measure the azimuthal force on the intruder. For grains resting on a dry surface, where basal friction is present, the system undergoes aperiodic stick-slip motion; when the grains are floating on a fluid and basal friction is negligible, the intruder flows unimpeded through the medium but occasionally clogs. These qualitative behaviors do not seem to depend on packing fraction and interparticle friction coefficient. We report on measurements of the intruder force and speed distributions as well as particle displacements.

*The following grants support this work: DARPA 4-34728, NSF-DMR1206351, NASA NNX15AD38G, and Army Research Office Grant W911NF-18-1-0184.

10:12AM E56.00012: Tears of wine and shock dynamics*  YONATAN DUKLER, Mathematics, University of California, Los Angeles, ANDREA BERTOZZI (Presenter), Mathematics and Mechanical and Aerospace Engineering, University of California, Los Angeles, ANDREAS MUENCH, Mathematical Institute, Univ. of Oxford, HANGJIE JI, Mathematics, University of California, Los Angeles — We revisit the classical problem of “tears of wine” and discuss the role of the geometry of the wine glass in regards to the formation of tears. Transport of a thin liquid up the side of the glass is instigated by a Marangoni stress due to a combination of thermal gradient and surface tension gradient. This effect is balanced by both normal and tangential components of gravity. When gravity effects are non-negible the possibility of undercompressive shocks enters the picture. We discuss this implications of compressive versus undercompressive shocks for film morphologies and compare with prior experiments on the tears of wine problem and experiments on thermally driven films.

*This work is supported by Simons Math + X Investigator Award number 510776. YD is supported by an NSF graduate research fellowship.
10:24AM E56.00013: Vibration can enhance stick-slip behavior for granular friction* JACQUELINE KRIM (Presenter), Physics, North Carolina State University, ROBERT P BEHRINGER, Physics, Duke University, ABE CLARK, Physics, Naval Postgraduate School — We experimentally study the frictional behavior of a two-dimensional slider [1] pulled slowly over a granular substrate comprised of photoelastic disks while being vibrated at frequencies ranging from 0 to 30 Hz in a direction parallel to sliding. Measurements are performed at constant peak acceleration amplitude, which results in constant average friction levels, but varying frictional behaviors. Surprisingly, we find that stick-slip behavior, where stress slowly builds up and is released in intermittent slips, is enhanced as the frequency of vibration is increased. Our results suggest that increasing the frequency of vibration may help to combine many smaller rearrangements into fewer, but larger, avalanche-like slips. We also examine the manner in which the self-affine character of the force curves evolves with frequency, and find additional support for this interpretation.


*NSF DMR0805204 and NSF DMR0906908

10:36AM E56.00014: Nonlocal rheology of a dense granular flow in annular shear experiments KAREN DANIELS (Presenter), ZHU TANG, North Carolina State University, THEODORE ANTHONY BRZINSKI, Haverford College, MICHAEL SHEARER, North Carolina State University — The flow of dense granular materials at low inertial numbers cannot be fully characterized by local rheological models; several nonlocal rheologies have recently been developed to address these shortcomings. To test the efficacy of these models across different particle shapes, packing fractions and shear rates, we perform experiments in a quasi-2D annular shear cell using photoelastic particles. The apparatus is designed to measure both the stress ratio \( \mu \) and the inertial number through the use of a torque sensor, laser-cut leaf springs, and particle-tracking. We observe that across several different packing fractions and rotation rates, a single set of model parameters is able to capture the full range of data collected once we account for frictional drag with the bottom plate. While the model's local parameter is always approximately unity, the nonlocal parameter varies sensitively on both the particle shape and material. Our measurements confirm the prediction that there is a growing lengthscale at a finite value \( \mu_s \), associated with a frictional yield criterion. Finally, we newly identify the physical mechanism behind this transition at \( \mu_s \) by observing that it corresponds to a drop in the susceptibility to force chain fluctuations.

10:48AM E56.00015: Non-local effects in intermediate granular avalanching flows* NATHALIE VRIEND (Presenter), AMALIA L THOMAS, University of Cambridge, KAREN DANIELS, North Carolina State University — In this work we showed that photoelastic analysis allows the quantification of rheologies in an intermediate chute flow. We characterize stresses and velocities in a flow layer with regions below and above the yield ratio \( \mu_s \). We compare our experimental results with a nonlocal rheology. Preliminary results show that the timescale over which the force chains decorrelate is strongly associated with the inverse of the fluidity, a viscosity-like quantity. This provides a physical interpretation of its particle-scale origins.

*This work was made possible by the support of an IFPRI collaborative grant. NMV is supported by a Royal Society Dorothy Hodgkin Research Fellowship RG 70273, ALT is funded by a Royal Society Research Grant RG 73329 and the Cambridge International Trust and KED acknowledges support from the James S. McDonnell foundation.

Tuesday, March 5, 2019 8:00 AM - 9:48 AM

Session E57 GSNP: Physics of Liquids III BCEC 256 - Yang Zhang, University of Illinois at Urbana-Champaign - Tag(s): Focus
8:00AM E57.00001: Can Statistical Physics Concepts Shed Some Light on the 73 Anomalies of Liquid Water?* [Invited]

H STANLEY (Presenter), Boston University — We focus on recent progress in understanding the 73 anomalies of water, by combining information provided by recent experiments and simulations on water in bulk, nanoconfined and biological environments designed to test the hypothesis that liquid water has behavior consistent with the novel phenomenon of “liquid polymorphism” in that low-temperature water can exist in two distinct phases [1,2]. We will utilize the properties of the Widom line—the locus of maximum correlation length—which can be measured experimentally at temperatures well above the critical temperature. Finally, we will discuss how the general concept of liquid polymorphism is proving useful in understanding anomalies in other liquids, such as silicon, silica, and carbon which have in common that they are characterized by two characteristic length scales in their interactions.


* This work has been supported by the NSF Chemistry Division grant CHE-1213217 and was performed in collaboration with, among others, C. A. Angell, S. V. Buldyrev, S.-H. Chen, D. Corradini, P. G. Debenedetti, G. Franzese, P. Kumar, E. Lascaris, F. Mallamace, O. Mishima, P. H. Poole, S. Sastry, F. Sciortino, and L. Xu. The Boston University Center for Polymer Studies is supported by NSF Grants PHY-1505000, CMMI-1125290, and CHE-1213217, and by DTRA Grant HDTRA1-14-1-0017.

8:36AM E57.00002: Liquid-Liquid Phase Transition in Metallic Alloy Melts Detected by Nuclear Magnetic Resonance*

EN-YI CHEN (Presenter), WEI-MING YANG, ALFRED KLEINHAMMES, YUE WU, Department of Physics and Astronomy, University of North Carolina at Chapel Hill — Liquid-liquid phase transition (LLPT) is thought to be exotic as it is not obvious what order parameters could be associated with qualitative changes in liquid structures. In some special cases where the valency of the element and bonding characters change substantially with pressure and temperature, such as the case of phosphorus and cerium, LLPT could take place accompanied by clear changes of the density. Here we show that non-density-driven LLPT can actually be common in metallic alloys, taking place above the liquidus temperature $T_{\text{liq}}$. High-temperature NMR is shown to be an effective tool for revealing such LLPT facilitated by its high sensitivity and high resolution. Subtle changes are detected that are difficult to detect by conventional thermodynamic measurement techniques. We will discuss the observation of LLPT in La-based alloys and Al-based alloys. We will show that the corresponding density change is exceedingly small. In addition, the kinetics of the transition process is also characterized systematically by NMR. This shows that the LLPT should have a profound influence on alloy solidifications.

*This work was supported by the US Army Research Office under the contract W911NF-17-1-0224.

8:48AM E57.00003: Liquid lipid phase separation on curved surfaces*

MELISSA RINALDIN (Presenter), PIERMARCO FONDA, LUCA GIOMI, DANIELA JUTTA KRAFT, Leiden University — By using colloid supported lipid bilayers of designed shape we proved how the interplay of the shape and the composition of a closed membrane determines the likelihood, the position and the composition of liquid domains [1]. Here, we show that if we open the membrane by connecting it to a reservoir of lipids, all these three properties are deeply affected. In particular, the pinning of the softer domains in high curvature regions is enhanced, leading to a consistent pattern on all colloids.


*This work was supported by the Netherlands Organisation for Scientific Research (NWO/OCW), as part of the Frontiers of Nanoscience program, VENI grant 680-47-431 and the VIDI scheme.
Genetic Competition in Weakly Compressible Turbulent Flows

ROBERTO BENZI, Tor Vergata University, GIORGIA GUCCIONE, Eindhoven University of Technology, ABIGAIL PLUMMER, DAVID ROBERT NELSON, Harvard University, FEDERICO TOSCHI (Presenter), Eindhoven University of Technology — The genetic competition for biological species living in marine environments can be severely influenced by fluid advection. Very often, in oceans and in lakes, cell generation times are precisely in the inertial range of eddy turnover times and therefore the influence of turbulence must be properly taken into account. We employ both an off-lattice agent-based simulation as well as an on-site density-based model to describe two competing populations in one and in two spatial dimensions under the influence of advecting (turbulent) velocity fields. The novel on-site density-based model allows us to accurately and efficiently describe the dynamics of the population and the genetics of a large number of individuals, making this the ideal tool to study populations in two dimensions. We find that the presence of compressible turbulent velocity fields can have a strong effect on genetic competitions. Even in regimes where the overall population structure is approximately unaltered, the flow can significantly diminish the effect of a selective advantage on fixation probabilities. We explain this effect in terms of the enhanced survival of organisms born at the sources in the flow and the influence of Fisher genetic waves.

Structure and Dynamics of Water Interacting with Hydrophilic, Nanostructured CuO Coatings

JAMES TORRES (Presenter), ZACHARY BUCK, HELMUT KAISER, XIAOQING HE, TOMMI WHITE, ROBERT WINHOLTZ, HASKELL TAUB, University of Missouri, MADHUSUDAN TYAGI, NIST Center for Neutron Research, KENNETH W HERWIG, EUGENE MAMONTOV, LUKE L DAEMEN, MICHELLE KIDDER, Oak Ridge National Laboratory, FLEMMING Y HANSEN, Technical University of Denmark — We have used neutron scattering and electron microscopy to investigate how the structure, dynamics, and phase transitions of water near a bare copper surface are affected by coating it with strongly hydrophilic CuO nanostructures. Our high-energy-resolution elastic neutron scattering measurements show the abrupt freezing transition of water near a bare Cu surface is spread into a continuous transition spanning a temperature range of ~80 K upon coating with the CuO nanostructures. From these elastic scans, we infer the presence of at least two distinct water populations, differing in their freezing behavior and their proximity to the nanostructures. Quasielastic neutron scattering measurements support this interpretation by providing evidence of three water components diffusing on different time scales. Our environmental-SEM images reveal micron-size water droplets wet to the nanostructures. In addition, neutron diffraction measurements indicate that the water closest to the CuO nanostructures freezes into an amorphous solid, while more distant water freezes into crystalline ice. The presence of the two forms of ice is consistent with vibrational spectra observed by inelastic neutron scattering.

The molecular description of amorphous ices and the mechanism governing their pressure induced interconversion

FAUSTO MARTELLI (Presenter), IBM Research, ROBERTO CAR, Princeton University, NICOLAS GIOVAMBATTISTA, Brooklyn College — We employ classical molecular dynamics simulations to investigate the molecular-level structure of water during the isothermal compression of hexagonal ice (Ih) and low-density amorphous (LDA) ice at low temperatures to high-density amorphous ice (HDA) [1], and the isothermal decompression of HDA by employing a sensitive local order metric [2]. Our results confirm that LDA and HDA are indeed amorphous, i.e., they lack of polydisperse ice domains. Interestingly, HDA contains a small number of domains that are reminiscent of the unit cell of ice IV, although the hydrogen-bond network (HBN) of these domains differ from the HBN of ice IV. Both nonequilibrium LDA-to-HDA and Ih-to-HDA transformations are two-steps processes where a small distortion of the HBN first occurs at low pressures and then, a sudden, extensive re-arrangement of hydrogen bonds at the corresponding transformation pressure follows.

9:36AM E57.00007: Multiple Protonic Kinetic Energy Band Models of Melted Ice Periodic Lattice for Pure Liquid Water  BIN JIE (Presenter), Physics Department, Xiamen University, TIANHUI JIE, Institution applied, CHIH-TANG SAH, Physics Department, Xiamen University — Existence of long-range order in fluid water under numerous daily conditions led us to extend the 1933 Bernal-Fowler Hexagonally Close Packed (HCP) crystalline ice lattice to model pure liquid water as Melted Ice. The 8 protons in the primitive unit cells (PUC) of the HCP lattice vibrate about their lattice positions, jump among the 16 possible proton sites, half empty and half occupied in the PUC and transport among the PUC’s. Propagating and localized proton vibrations are respectively the Protonic Fermions and Bosons, described by the Bloch and Wannier eigenfunctions, which are perturbed to form localized states (protonic traps) by rare random localizations. The eigenvalues of the frozen periodic lattice give the kinetic energy-band landscapes of the protonic Fermions and Bosons, while the long-range order in fluid water led us to model the proton transport by our 3-step (A, B, C) collision dynamics (DDGRT). The observed 3 thermal activation energies of pH and positive and negative ion electrical mobilities, are in excellent agreement with Slinky Toy Model of the proton vibration frequencies of dilute vapor water, providing the existence proof for this new two-phase approach to model liquid water, employing ice lattice and random distribution of water molecules in vapor.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E58 GSOFT: Colloids I BCEC 257A - Vivek Sharma, University of Illinois at Chicago

8:00AM E58.00001: Impact of extreme softness on the crystallization of ultra-low crosslinked microgels in two and three dimensions*  STEFFEN BOCHENEK (Presenter), ANDREA SCOTTI, MONIA BRUGNONI, Institute of Physical Chemistry, RWTH Aachen University, LUCIO ISA, Department of Materials, ETH Zurich, WALTER RICHTERING, Institute of Physical Chemistry, RWTH Aachen University — Ultra-low crosslinked poly(N-isopropylacrylamide) microgels are used to elucidate the effect of softness on crystallization in two- and three-dimensions. 2D systems are produced by compressing and depositing microgels from oil-water interfaces. Ex-situ analysis by atomic force microscopy reveals that no crystals form upon compression, as opposed to the case of stiffer microgels. Once adsorbed at a fluid interface, microgels spread into disk-like objects whose size and stiffness are a strong function of polymer content and crosslinking. Consequently, interfacial confinement exacerbates size and mechanical polydispersity, effectively suppressing crystallization. In contrast, in 3D, the microgels crystallize at high concentrations, indicating that softness per se is not sufficient to suppress the liquid-solid phase transition, unless it is coupled to induced polydispersity. Furthermore, small-angle neutron scattering with contrast matching reveals that interpenetration is dominant over deswelling and deformation when these microgels are in 3D-overcrowded environments.

*The authors acknowledge the Deutsche Forschungsgemeinschaft within the SFB 985 “Functional Microgels and Microgel Systems” for financial support. A. S. thanks Alexander von Humboldt Foundation for financial support.

8:12AM E58.00002: Influence of Softness and Internal Architecture on Microgel Deswelling in Concentrated Suspensions*  ANDREA SCOTTI (Presenter), MONIA BRUGNONI, RWTH Aachen University, JUDITH HOUSTON, Forschungszentrum Juelich GmbH, FRIEDERIKE SCHULTE, STEFFEN BOCHENEK, WALTER RICHTERING, RWTH Aachen University — Microgels are soft polymeric networks swollen in a good solvent. They can be compressed, deformed or interpenetrated in concentrated suspensions. The prevalence of one of these mechanisms depends on both the softness and the architecture of the polymer network. By probing regular, ultra-low crosslinked, and hollow-poly(N-isopropylacrylamide) based microgels we show that for the same architecture, a decrease in the amount of crosslinker during the synthesis produces a more pronounced deswelling. Small-angle neutron scattering is used to directly access the form factors of the different microgels embedded within a matrix of regular crosslinked ones. This work clarifies that to obtain compressible microgels that adapt their size in concentrated suspensions, the presence of a cavity produces higher deswelling than decreasing the amount of crosslinker during the precipitation polymerization. The latter option leads to the opposite effect and interpenetration is dominant.

*Alexander von Humboldt Foundation, Deutsche Forschungsgemeinschaft (SFB 985 \` Functional Microgels and Microgel Systems") and the International Helmholtz Research School of Biophysics and Soft Matter (IHRS BioSoft)
8:24AM E58.00003: Influence of Softness on the Stability of Binary Crystals  RONALD LACOUR (Presenter), CARL SIMON ADORF, SHARON GLOTZER, Chemical Engineering, University of Michigan — Binary systems of spherical colloids have shown the ability to self-assemble into many more superlattice structures than comparable monodisperse systems. Understanding the nature of the interparticle forces in such self-assembly is critical to target specific structures for self-assembly. Here we computationally investigate the influence of "softness", the steepness of the interaction potential, on the solid phase behavior of particles interacting with a purely repulsive, isotropic pair potential. We determine the ground state phase diagram for our model using a basin-hopping algorithm to optimize candidate structures for low enthalpy. The phase behavior of repulsive particles is often understood by looking at the packing fraction of different phases; however, we find that a very small amount of softness can change the stable ground state phase of a system away from the densest packing structure. We also find softness increases the stability of many experimentally observed structures. Our results provide further insight into why particular structures self-assemble and will be useful as a reference for experimentalists working with softly repulsive particles.

8:36AM E58.00004: Spontaneous deswelling of microgels controlled by counterion clouds  URS GASSER (Presenter), Paul Scherrer Institut, ANDREA SCOTTI, RWTH Aachen, Germany, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Microgels based on poly(N-isopropylacrylamide) (pNIPAM) show a unique, spontaneous deswelling behavior at constant temperature below the deswelling transition of pNIPAM at 32C when brought above a critical concentration. We have shown that counterion clouds of pNIPAM microgels provide the mechanism for this spontaneous deswelling [A. Scotti et al., PNAS 113, 5576 (2016)]. Although pNIPAM is uncharged, charged groups are incorporated on the particle surface during synthesis. Counterions not bound by the surface charge set the osmotic pressure of the microgel suspension. At high concentration, the overlap of counterion clouds of neighboring particles causes an increase of the osmotic pressure in the space between the particles, while the pressure in the interior of the microgels does not increase. The resulting pressure difference deswells the microgels, if it exceeds their bulk modulus. Measurements of the microgel size at high concentrations using small-angle neutron scattering show that the volume fraction remains below random close packing up to effective volume fractions of about 1.0. We show that the essential aspects of the observed deswelling are captured with a Poisson-Boltzmann model of the microgels and without direct interaction of the microgels.

8:48AM E58.00005: Self-inflating Colloidal Microcapsules  ZHE XU (Presenter), STEFANO SACANNA, New York University — Hollow-structured particles have attracted great attention in both nanomaterials and colloidal science due to their high surface area and unique spatial confinement. Here I will present a self-inflation method to produce 3-(trimethoxysilyl)propyl methacrylate(TPM) based colloidal microcapsules with versatile design and tunability of structures. Detailed mechanistic study revealed the process is the result of a fine balance between surface tension and osmotic pressure from partial hydrolysis of TPM network. Microcapsule sizes can be accurately controlled by adjusting the osmotic pressure due to the semipermeable property of the membrane. We further demonstrate the feasibility of introducing an opening hole onto the capsules by hard-templating on a removable seed, and the whole network can be solidified to maintain stable and rigid morphology. Large-scale synthesis of monodisperse polymeric microcapsules with tunable and uniform hole can be easily obtained. As a result, these model particles laid solid foundation for studying fluid mechanics, self-assembly, packing and jamming in confinement, and showed great potential in dynamic transport, storage, separation and delivery of drugs or particles.

9:00AM E58.00006: Designing plasmonic-based colloidal pH microsensors*  REMI DREYFUS (Presenter), CNRS, CELINE BUREL, Solvay, BERTRAND DONNIO, CNRS — Many natural processes start with an alteration of their immediate environment at the microscopic level. Therefore there is a need to develop pH microsensors that can easily reveal local changes in pH in any heterogeneous system. In this presentation, we show that with a careful design of colloids made of closely packed gold nanoparticles embedded in a thin pH-responsive polymeric shells, we can synthesize sensors at the micron scales that can be dispersed into heterogeneous systems and from which we can read sensitive information on local pH. We found that at low pH, close-packed jammed gold nanoparticles experience strong coupling in their plasmonic resonance, changing the plasmonic resonance to the red part of the spectrum, and giving a strong blue color to the microparticles. As pH is increased, the polymeric crust of the particles gets charged and swells, increasing the distance between the nanoparticles, thus suppressing the plasmonic correlations and inducing a strong color change with an absorption in the blue part of the spectrum, changing the microcapsules into red. Our results demonstrate that these colloidal capsules provide us with an easy way to unambiguously detect local pH changes at the microscale level in heterogenous systems.

*ANR-15-PIRE-0001-06 and CIFRE
9:12AM E58.00007: Improved generative models for colloidal specimens in digital holographic microscopy*
RONALD ALEXANDER (Presenter), BRIAN LEAHY, VINOTHAN N MANOHARAN, Harvard University — Digital holographic microscopy (DHM) is an important tool for characterizing colloidal specimens. Traditionally, the inverse problem of determining the size, shape, orientation and composition of an object from a hologram obtained by DHM is approached by numerical reconstruction of the incident and scattered electromagnetic fields. Recently, we have made advances by comparing holograms to predictions of a forward model for hologram formation. For systems colloidal spheres and cylinders in which multiple scattering is negligible, the scattering problem is solvable analytically and/or numerically. These calculations provide the basis for a model of image formation in DHM. We present progress highlighting improvements to a generative model for DHM of systems of colloidal particles. In particular, we show that explicit modelling of the scattering and diffraction effects in a microscope's optical train increase the model's predictive power. We also investigate the challenges for extending our technique of characterization through fitting of a forward model to biological systems such as bacteria and and animal cells.

*This work is partially funded by an NSF MRSEC under award number DMR-1420570.

9:24AM E58.00008: A Quick Method to determine ensemble averaged Translational and Rotational Diffusion coefficients
NAMITA SHOKEEN (Presenter), ASHIS MUKHOPADHYAY, Wayne State University — The ensemble averaged translational diffusion of isotropic particles and coupled translational-rotational diffusion of anisotropic particles inside water and various polymer solutions were determined using dynamic differential microscopy (DDM). Initially, we applied this technique to characterize the dynamics of 25 nm radius particles within entangled high molecular weight, \( M_w = 600 \) kg/mol polyethylene oxide-water solutions, which extended the scope of DDM to study the dynamics and rheological properties of soft matter at nanoscale. We will demonstrate the application of this method to characterize the motion of colloidal ellipsoids of different aspect ratios.

9:36AM E58.00009: Dynamic properties of liquid states in systems with a short-range attraction and long-range repulsion*
PAUL D GODFRIN, Massachusetts Institute of Technology, PETER FALUS, LIONEL PORCAR, Institut Laue–Langevin, KUNLUN HONG, Oak Ridge National Laboratory, STEVEN HUDSON, National Institute of Standards and Technology, NORMAN J. WAGNER, University of Delaware, YUN LIU (Presenter), National Institute of Standards and Technology — Colloidal systems with a short-range attraction and long-range repulsion have been intensively studied in the past decade. A generalized phase diagram has been proposed with multiple liquid states. Using lysozyme as a model system, we have identified different liquid states of previous experimentally studied lysozyme samples within this generalized state diagram and explore the dynamic properties of each liquid state. Most lysozyme samples studied previously at low and intermediate concentrations are dispersed fluid states while a few high concentration samples are randomly percolated liquid states. In the dispersed fluid state, the short-time diffusion coefficient measured is found insensitive to the attraction strength, while it is very sensitive to the attraction strength in random percolated fluids. At high enough concentrations, the mean square displacement can be as slow as those of many glassy colloidal systems at time scales near the characteristic diffusion time even though these lysozyme samples remain in liquid states at the long-time limit. A localized glassy state is further identified by the mean square displacement.

*NSF: DMR-1508249
NIST: 70NANB12H239 and 70NANB10H256

9:48AM E58.00010: Hyperuniform defects in an isotropic liquid
RODRIGO GUERRA (Presenter), PAUL M CHAIKIN, New York University — The concentration and organization of topological lattice defects form the basis of our theoretical understanding of the two-step melting process of two-dimensional solids, as described by Kosterlitz, Thouless, Halperin, Nelson, and Young (KTHNY). In this description, particles surrounded by anything but six nearest neighbors act as topologically charged quasi-particles, called disclinations, that interact via Coulombic pair potentials when the material is in the liquid-crystalline hexatic phase. This description is presumed to break down in the fully-isotropic liquid phase, but we find that the spectrum of topological charge density fluctuations in the liquid obeys the same spatial and temperature scaling relationships, \( S(q \to 0) \sim k_B T q^2 \), expected for an idealized fluid of oppositely charged particles: except for temperatures much larger than the isotropic-hexatic transition temperature. This suggests that the quasi-particle description may provide valuable insights into the behavior of the fluid too, particularly to the coupling of Gaussian curvature and topological charge in the fluid.
10:00AM E58.00011: Colloidal gelation as a nonequilibrium continuous phase transition  JOEP ROUWHORST (Presenter), Institute of Physics, University of Amsterdam, CHRIS NESS, ALESSIO ZACCONE, Department of Chemical Engineering and Biotechnology, University of Cambridge, PETER SCHALL, Institute of Physics, University of Amsterdam — A new view on gelation as a second-order nonequilibrium phase transition is presented using combined experiments on critical Casimir colloidal suspensions, simulations, and analytic solutions to a simplified master kinetic equation. The critical Casimir forces provide effective, short-ranged colloidal interactions that can be tuned with temperature, allowing to study gelation over a range of moderate attractive strength (bond energy between 3 and 6kBT). The experiments and simulations show cluster sizes and correlation lengths diverging with exponents ~1.6 and 0.8, respectively, consistent with growth exponents in percolation theory. Cluster masses exhibit power-law distributions with exponents -3/2 and -5/2 before and after gelation, respectively, as predicted by a master kinetic equation with single-bonded particle detachment. As detailed balance is violated in this process, our results indicate that the observed gelation is a nonequilibrium continuous phase transition (nonequilibrium percolation). These results suggest that the observed gelation process, in which fluid particles aggregate and percolate into rigid structures, is an analogue, mirror-image process of yielding, where emerging fluid-like particles percolate within a rigid matrix.

10:12AM E58.00012: Evolution of a sedimenting colloidal sheet  RUO-YU DONG (Presenter), IBS Center for Soft and Living Matter, WEI WANG, Harbin Institute of Technology, SHANKAR GHOSH, Tata institute of fundamental research, STEVE GRANICK, IBS Center for Soft and Living Matter — A sedimenting 2D colloidal sheet shows curious stability and nonlinear behavior at small Re around 10^{-3}, which should be in the linear Stokes regime. Small-scale mechanical instabilities develop in the form of dynamic swirling of particles in transient clusters, which generate multiple critical points and highly entangled vortex lines. This nonlinearity results from the topological nature of the fluid flow. Spatial organization of swirling motions determines the overall shape. The observed phenomena may challenge our notion of a low Reynolds number hydrodynamic problem, and holds value for understanding other dissipative dynamical systems.

10:24AM E58.00013: Electrical resistance fluctuations as a probe to monitor colloidal flows*  CAGATAY KARAKAN (Presenter), KAMIL EKINCI, Mechanical Engineering, Boston University — Impedance measurements are widely used to detect particles or cells in a flow and to measure their various properties. The approach typically focuses on individual cell counting and sizing by passing the cells through artificial constrictions in which the channel diameter D is comparable to particle size d (D~d). Here, we explore the electrical impedance sensing technique to characterize colloidal flows in microchannels at different D/d limits. Our measurement is based on a standard four-wire probe of the mean electrical resistance R_m and its fluctuations ΔR(t) across the channel. We have applied this approach to measure flows with microbead and red blood cell suspensions in microchannels with different diameters. Flow properties such as flow rate, shear stress, concentration and composition are varied while monitoring the microchannel optically and electrically. Our results suggest that concentration can be inferred from R_m, while ΔR/R_m and its probability distribution contains information about other flow parameters, such as flow rate, particle composition and its properties. Based on our preliminary data, we will discuss how impedance sensing can be used to monitor flow parameters in vasculature networks.

*This work is supported by NSF CELL-MET ERC award no. 1647837.

10:36AM E58.00014: Solvent coarsening around laser-heated colloids and related effective forces  SUTAPA ROY (Presenter), Max-Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany, and 2 IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 5, JUAN RUBEN GOMEZ-SOLANO, Universität Nacional Autonoma de Mexico, CHRIS NESS, ALESSIO ZACCONE, Department of Chemical Engineering and Biotechnology, University of Cambridge, PETER SCHALL, Institute of Physics, University of Amsterdam — Laser illuminating a Janus colloid which is suspended in a near-critical binary solvent leads to the formation of the concentration gradient and coarsening patterns around the colloid, which leads to its phoretic motion. Using analytical theory and numerical simulations, we investigate this non-equilibrium phenomenon under the influence of a time-dependent temperature gradient. Our predictions are also confirmed by experiments with Gold-capped Janus particles immersed in PnP-water binary liquid mixture. Time-dependent properties of the coarsening patterns for various surface adsorption properties of the Janus colloid are analyzed. We also present results for structure formation around colloidal particles kept confined in thin films with confining surfaces preferring one species of the binary liquid mixture over the other. Confinement leads to the formation of a bridge connecting the colloid and both the confining walls. It is observed that the particle starts to move much before the stationary state is achieved. Results will also be presented on the time-dependent effective interactions between two such heated colloidal particles.
investigate the effects of using cell-cell alignment is necessary to generate the observed correlation length scales. In this context, we additionally vary trends in cell density, cell shape, and cell motility observed in our monolayers, and that a coupling mechanism like to include both cell alignment and proliferation. We find that shape-based models quite naturally generate the time-
tissue rheology changes dramatically as cells proliferate, with interesting dynamical correlation length scales that depend
remains unclear. Moreover, our recent observations of cell monolayers that undergo extensive cell division indicate that
tissue rheology changes dramatically as cells proliferate, with interesting dynamical correlation length scales that depend on the mechanical environment. To understand these observations, we extend shape-based models of confluent tissues to include both cell alignment and proliferation. We find that shape-based models quite naturally generate the time-varying trends in cell density, cell shape, and cell motility observed in our monolayers, and that a coupling mechanism like cell-cell alignment is necessary to generate the observed correlation length scales. In this context, we additionally investigate the effects of using metric vs topological alignment rules in active matter systems where the interaction potential is itself explicitly topological.

We acknowledge support from NSF DMR16-07378, PENN MRSEC Grant DMR-1720530, and NASA Grant NNX08AOOG.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E59 GSOFT: Rheology and Flow of Soft Matter II BCEC 257B - Scott Franklin, Rochester Institute of Technology

8:00AM E59.00001: Dynamical correlation lengths in shape-based models of confluent tissue DANIEL SUSSMAN (Presenter), Syracuse University, JOHN DEVANY, MARGARET GARDEL, University of Chicago, M. LISA MANNING, Syracuse University — It has become increasingly clear that the rheology of densely packed cells in confluent tissue helps control processes ranging from multicellular development to wound healing to cancer tumor development. However, the impact on tissue rheology of cell-autonomous active processes, such as active alignment of cell motility and cell proliferation, remains unclear. Moreover, our recent observations of cell monolayers that undergo extensive cell division indicate that
tissue rheology changes dramatically as cells proliferate, with interesting dynamical correlation length scales that depend on the mechanical environment. To understand these observations, we extend shape-based models of confluent tissues to include both cell alignment and proliferation. We find that shape-based models quite naturally generate the time-varying trends in cell density, cell shape, and cell motility observed in our monolayers, and that a coupling mechanism like cell-cell alignment is necessary to generate the observed correlation length scales. In this context, we additionally investigate the effects of using metric vs topological alignment rules in active matter systems where the interaction potential is itself explicitly topological.

8:12AM E59.00002: Perclosures induced by quasistatic shear in athermal systems with weak attraction* YUCHUAN WANG (Presenter), YOUJIN DENG, NING XIU, Department of Physics, University of Science and Technology of China — When quasistatically shearing athermal particulate systems with weak attraction, we observe both connectivity percolation and solidlike transitions over a wide range of packing fractions below the jamming transition point. It is already known that without shear connectivity percolation for the same system occur at specific packing fraction, \( \varphi_{cp} \). It is interesting that driven by shear the system undergoes percolation transition even far below \( \varphi_{cp} \). We find that \( \varphi_{cp} \) and another specific packing fraction approximately separate the whole packing fraction regimes into three parts, in which the connectivity percolation exhibits apparent differences. Combining the static structure factor, we come up with a novel phase diagram with percolation transitions, and regimes of phase separation, gelation, shear jamming, and jamming.

*This work is supported by the National Natural Science Foundation of China (Grants No. 11734014)

8:24AM E59.00003: Pressure Decay in 2D Molecular Dynamics Simulation with Varied Filter Pore Width and Fluid Impurity Diameter KEVIN VANSLYKE (Presenter), SURAJIT SEN, University at Buffalo, The State University of New York — Time dependent pressure in a 2D molecular dynamics model using Lennard-Jones Argon atoms is studied in a semi-periodic chamber containing a simple porous filter. In each case an initial velocity bias towards the filter leads to the buildup of pressure in a region adjacent to the filter. The pressure in this region is shown to exhibit damped oscillatory behavior as the pulse is reflected and travels across periodic boundary conditions. The effects of pore width and fluid impurity diameter on the exponential decay time constant are evaluated in detail. Our results demonstrate a negative linear relation between time constant and pore width for systems with a fixed impurity diameter, and a positive linear relation between time constant and impurity diameter in systems with a fixed pore width.
2d Shear of Granular Annular Sector Particles (ASPs)*

SCOTT FRANKLIN (Presenter), ELYSE ROOD, Rochester Institute of Technology, THEODORE ANTHONY BRZINSKI, SYKES CARGILE, Physics, Haverford College — We study the shear of granular annular sector particles (ASPs), open semi-circular rings that have previously been studied at colloidal scales. ASPs can be characterized by two dimensionless numbers: the subtended opening angle and the ratio of inner and outer radii. We place granular ASPs in an annular-planar Couette shear cell and visualize the entire 360° with six cameras. Particle tracking software identifies the position and orientation of each ASP and enables measurement of large-scale motion and particle-particle interactions. ASPs can entangle to form dimers, trimers and other structures and we measure the distribution, creation and annihilation of these structures. Dimers can be characterized by the dot product of constituent ASP orientations. I will describe our initial experiments and compare with collaborative experiments in avalanching geometries.

*This material is based upon work supported by the National Science Foundation under Grant No. CBET-#1438077

Effect of Acid Hydrolysis on the Rheology of Phytoglycogen Nanoparticles

HURMIZ SHAMANA (Presenter), MICHAEL GROSSUTTI, JOHN DUTCHER, University of Guelph — Phytoglycogen is a natural polysaccharide produced in the form of compact 35 nm diameter nanoparticles by some varieties of plants such as sweet corn. The highly-branched, dendrimeric structure of phytoglycogen leads to interesting and useful properties that make the particles ideal as unique additives in personal care, nutrition and biomedical formulations. One such property is the unusual polysaccharide rheology of aqueous dispersions of phytoglycogen nanoparticles [1]. When added to water, the zero-shear viscosity of the dispersions remains small up to large concentrations (~20% w/w). For higher concentrations, the zero-shear viscosity increases dramatically, reaching values that exceed that of water by more than a factor of $10^6$ at the highest concentrations of 30% w/w. We have used acid hydrolysis to partially digest the phytoglycogen nanoparticles, which not only reduces their diameter, but also removes the hairy chains on the outer surface of the particles thereby altering the interaction between particles. We compare the concentration dependence of the zero-shear viscosity of the smaller, acid hydrolyzed particles to that of the native particles. These results suggest new applications for the acid hydrolyzed particles.


Biased Brownian motion in a channel with symmetry and anisotropy*

KI WING TO (Presenter), Institute of Physics, Academia Sinica, WEI-HSUAN TSENG, National Taiwan Normal University, Department of Physics — We study biased Brownian motion of a bead in a quasi-two-dimensional horizontal channel consists of identical cells with asymmetric walls and anisotropic base connected in a circular loop. When the channel is shaken vertically, energy is injected to the bead by collisions with the base and converted to kinetic energy in the horizontal direction. Asymmetry and anisotropy of channel induce a driving force on the bead so that the bead performs biased Brownian motion along the channel axis with the drift velocity being proportional to the diffusivity. Furthermore, the distribution function of the escape time from a cell is found to be an exponentially decay function. These experimental results can be explained by the continuous time random walk theory (CTRW).

*MOST 106-2112-M-001-026 R.O.C. (Taiwan)

Tuning the Shear Thickening Response using Acoustic Perturbations*

PRATEEK SEHGAL (Presenter), Sibley School of Mechanical and Aerospace Engineering, Cornell University, MEERA RAMASWAMY, ITAI COHEN, Department of Physics, Cornell University, BRIAN J. KIRBY, Sibley School of Mechanical and Aerospace Engineering, Cornell University — Shear thickening behavior of dense particle suspensions is generally not considered an externally tunable response. In this work, we present a novel method to dynamically tune the rheological response of a non-Brownian shear thickening suspension using local acoustic perturbations. We apply resonant perturbations in two different directions orthogonal to the primary shear flow and show a tunable viscosity response of the suspension in the transitioning regime and the shear-thickened regime of the flow curve. We find that the acoustic perturbations increase the onset strain rate of shear thickening in addition to decreasing the viscosity (de-thickening) of the suspension. We attribute the mechanism of de-thickening to the breaking of shear-induced force chains and disruption of solid-solid frictional contact between the particles by local acoustic perturbations. With the temporal amplitude modulation of the perturbations, we further demonstrate a periodic thickening/de-thickening of the suspension and show that the response is dynamically tunable.

*This work is supported by the National Science Foundation (Award Number - 1804963)
We discuss the applications of our results to experimental nanopore systems, and within cells. We identify and characterize a new non-Fickian regime of anomalous transport. We characterize flux and fluctuations in this pore of finite length \( L \). We recover our earlier hydrodynamic regime for large \( L \), with Fickian transport. For smaller \( L \), we density-dependent length-scale determined by the transition rates. Here we consider the anomalous transport within a pore of finite length \( L \). We recover our earlier hydrodynamic regime for large \( L \), with Fickian transport. For smaller \( L \), we identify and characterize a new non-Fickian regime of anomalous transport. We characterize flux and fluctuations in this regime. We discuss the applications of our results to experimental nanopore systems, and within cells.

This research was funded by the Natural Sciences and Engineering Research Council (NSERC) of Canada with operating grant number RGPIN-2014-06245. Computational resources were provided by ACENET and Compute Canada.

In this study, we use the lattice Boltzmann method coupled with the coarse-grained spring network model for RBCs to simulate aggregating RBCs in a rectangular microchannel under Poiseuille flow. The effect of polymer additives is modeled by an attractive potential. We investigate the cell free layer thickness, the aggregate size and distribution, as well as the suspension viscosity in various shear rates and different strength of the attraction interaction.

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Geometric frustration induces the transition between rotation and counterrotation in swirled granular media

LISA LEE, Harvard University, JOHN PAUL RYAN, Department of Computer Science, Cornell University, MIRANDA HOLMES-CERFON, Courant Institute of Mathematical Sciences, New York University, SHMU EL RUBINSTEIN (Presenter), Harvard University — Marbles in a swirled teacup exhibit a curious dynamical transition: at small densities, the marbles circulate in the same direction as the container, but at larger densities, they transition to circulating in the opposite direction. This phenomenon occurs in a range of swirled and vibrated granular systems, from industrial vibration mills to baby rattles, each observation challenging our intuitive understanding of angular momentum conservation. Using an accelerating coordinate system, we use experiments and simulations to identify the cause for the transition to counterrotation. At low densities, the grains roll freely in the container, but as density increases, antiferromagnetic-like frictional interactions between beads lead to geometrical frustration, resolved only via global circulation. I will furthermore show that in the new frame of reference this system resembles a rotating drum.

*NSF (DMR-1420570).

Harvard Kavli Institute for Bionano Science and Technology

Predicting and measuring shear rheology of soft interfaces

ADITYA RAGHUNANDAN (Presenter), NICHOLAS DEBONO, NICHOLAS PEARSON, PATRICK UNDERHILL, Rensselaer Polytechnic Institute, JUAN MANUEL LOPEZ, Arizona State University, A HIRSA, Rensselaer Polytechnic Institute — Measuring the non-Newtonian shear responses of monomolecular films or macromolecules like proteins at fluid-fluid interfaces has been limited by using linear (Newtonian) constitutive equations to determine rheological properties. Predicting this nonlinear behavior is integral to comprehending many biophysical processes such as breathing and in the pathology of diseases such as Alzheimer’s, which are marked by protein denaturation in vivo. We present a generalized 2-D constitutive equation for interfaces under steady shear with the interfacial shear viscosity generalized to be a function of the imposed shear-rate. We introduce non-Newtonian material properties that control nonlinear and linear shear responses of an interfacial system. Combining flow field predictions from the new equation and experiments in a knife-edge flow geometry, we demonstrate that monomolecular films of DPPC – the primary constituent of mammalian cell walls and pulmonary surfactant – are shear-thinning at near-physiological surface packing over six decades of shear-rate. Also, the role of interfacial rheology of an adsorbed protein film of insulin in the process of denaturation and subsequent amyloid fibril formation at the air/water interface is delineated.

Slip-link Simulations under Fast Flows: Effect of the Stretch/Orientation-Induced Reduction of Friction

TAKESHI SATO (Presenter), TAKASHI TANIGUCHI, Kyoto University — Macroscopic flows of entangled polymer melts are tightly connected with the microscopic polymer chain dynamics. One possible solution to this problem could be obtained with a multiscale simulation (MSS) approach, where a microscopic model is combined with a macroscopic model. To develop the MSS technique that can address polymer processing conditions, we need to develop a microscopic model that can correctly predict rheological behaviors under fast flows. However, the molecular mechanisms of entangled polymer chains under fast flows have not been fully understood. Yaoita et al. have introduced the concept of the stretch/orientation-induced reduction of molecular friction (SORF) to their slip-link (SL) model and found that SORF can improve the predictions of rheological behaviors under fast uniaxial elongational flows [Yaoita et al., 2012]. In this study, we have investigated the effect of SORF on the more coarse-grained SL model [Doi et al., 2003]. As a result, we have found that SORF can improve the rheological properties obtained from our SL model especially under uniaxial elongational flows. This result will help us to develop the MSS technique for fast entangled polymer melt flows.

*This work was supported by JSPS KAKENHI Grant No. 1810643.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E60 FOEP: Sharing Science: How to Communicate with the Public

Fermilab - Tag(s): Invited, Outreach, Undergraduate

Science Blogs and Talking Dogs: Reflections on 17 Years in Social Media [Invited] CHAD ORZEL (Presenter), Union College — In this talk I will discuss lessons learned about physics and science communication in the online world, drawing on my experiences since starting a weblog to discuss physics in 2002. This will include pros and cons of various media, including blogs, Twitter, and Facebook, and a discussion of the opportunities and risks these technologies offer for physicists interested in engaging with a broad public audience.
8:36AM E60.00002: Science News Online: Finding the Signal in the Noise [Invited]  ALLISON ECK (Presenter), NOVA —
You've been working in the lab for a long time, but you want to experiment with writing physics stories—or any kind of science story—for the public. So how do you do it? This session, led by Allison Eck, a digital editor for the award-winning PBS science documentary series NOVA, will introduce attendees to the vast and evolving landscape of digital science news. Attendees will also learn how to identify good science news stories, pitch them to editors, build a "beat," and more. Get ready to think like a reporter!

9:12AM E60.00003: Adventures in Podcasting [Invited]  SEAN CARROLL (Presenter), Caltech — Podcasts are a relatively new, but already popular and rapidly-growing, means of outreach and communication. They are essentially radio shows with episodes that are put on the internet rather than broadcast. I will describe my experiences as someone who listens to and appears on podcasts, as well as the creator and host of a new podcast, Mindscape.

9:48AM E60.00004: Science Festivals, Live Events, and the Importance of Face-to-Face Interaction* [Invited]  BEN WIEHE (Presenter), Science Festival Alliance, MIT Museum —
Since at least the dawn of agriculture, humans have gathered in the public square to celebrate what brings them together as a community. Even in our digital age, there is something special about festivals and live events. There is an immediacy to being there in-person: a unique don't-miss-out buzz and a compelling urgency. Events offer the chance to quickly develop real human relationships, and are rich with the potential for genuine dialogue and exchange. Events need not be tied to one location or venue, and can be quickly adapted to be meaningful and energizing for different audiences. Events can also work at any scale, budget, institutional backing, and level of professionalism, so anyone and any organization can get involved.

As they have for millennia, festivals and events still have the power to energize a community and then periodically reaffirm and renew that energy. What happens when that power is used in the name of science? Over the past two decades, there has been an explosion of experimentation with live public science events in the United States. From intimate discussions of science in a neighborhood pub, to science festival main events that draw tens of thousands in a single day, there is much to learn from these experiments.

Examples of past and ongoing events set the context for a presentation of notable evaluation and research findings related to science events, with a special emphasis on the direct participation of professional scientists. By situating these specific findings within the vast and multi-disciplinary literature dedicated to festival and event studies, a case is made for the importance of face-to-face interaction in every initiative seeking to share science with the public.

*The Science Festival Alliance is currently supported by funding from Science Sandbox (an initiative of the Simons Foundation), and the Alfred P. Sloan Foundation

10:24AM E60.00005: Tough crowd: Reaching beyond the usual science-interested audiences [Invited]  RAY JAYAWARDHANA (Presenter), Cornell University — For those involved in science communication and outreach, engaging with audiences who usually do not seek out science events/media/venues presents interesting challenges. I will reflect on those challenges, drawing upon a few attempts bring science content to unexpected places.

Tuesday, March 5, 2019 8:00 AM - 10:24 AM

Session E61 GSOFT DBIO GSNP: Active Matter II BCEC 258B - M Cristina Marchetti, University of California, Santa Barbara - Tag(s): Focus
8:00AM E61.00001: Defect loops in 3D active nematics [Invited] DANIEL BELLER (Presenter), Department of Physics, University of California, Merced, GUILLAUME DUCLOS, Martin A. Fisher School of Physics, Brandeis University, DEBARGHYA BANERJEE, Max Planck Institute for Dynamics and Self-Organization, Göttingen, MINU VARGHESE, MATTHEW PETERSON, ARVIND BASKARAN, APARNA BASKARAN, MICHAEL F HAGAN, Martin A. Fisher School of Physics, Brandeis University, FEDERICO TOSCHI, Department of Applied Physics, Eindhoven University of Technology, SEBASTIAN STREICHAN, Department of Physics, University of California, Santa Barbara, VINCENZO VITELLI, James Franck Institute and Department of Physics, University of Chicago, ZVONIMIR DOGIC, Department of Physics, University of California, Santa Barbara, ROBERT PELCOVITS, Department of Physics, Brown University, THOMAS POWERS, School of Engineering and Department of Physics, Brown University — In 2D active nematics, internally driven chaotic flows are characterized by the continual production, motion, and annihilation of point defect pairs. We investigate the behavior of active nematics in 3D, for which we have developed an experimental model system of microtubules and molecular motors, as well as numerical modeling approaches. The defects characterizing chaotic flow are here curvilinear rather than point-like. We present a theoretical model predicting a certain class of closed disclination loops to be the system's generic singularities. Through detailed analysis of experimental and numerically generated configurations, we show how our predictions of defect topology, geometry, and dynamics provide important insights into this highly complex 3D system.

8:36AM E61.00002: Synchronization and pattern formation in chiral active matter DEMIAN LEVIS (Presenter), Ecole Polytechnique Federale de Lausanne, BENNO LIEBCHEN, Heinrich-Heine-Universitat Dusseldorf, IGNACIO PAGONABARRAGA, Ecole Polytechnique Federale de Lausanne — The emergence of synchronized states in populations of mobile entities is widely observed in different contexts: from animal groups - like flocks of birds moving coherently or crowds of people walking cooperatively on the London's Millenium bridge - to synthetic colloidal systems. However, previous studies on synchronization have focused on, either immobile oscillators, or mobile oscillators which phase does not directly influence the way they move in space [1]. Here we focus on active oscillators - circle swimmers which rotate with an intrinsic frequency - and show that self-propulsion, induces a qualitatively new and generic synchronization scenario which generates two novel phases: (i) a phase where oscillators move collectively along a given direction; a phase showing long-range order in 2D (akin to the celebrated Toner-Tu flocking phase [2]). (ii) a second phase where particles of opposite chirality segregate into rotating clusters. Both phases feature activity-induced synchronization in 2D, which is not achievable for immobile oscillators in low dimensional systems [3].


8:48AM E61.00003: Active mixing, manifolds and barriers in imposed, laminar flows* CHRISTINA YU (Presenter), MICHAEL GERBER, BREE MCCULLOUGH, Dept. of Physics & Astronomy, Bucknell University, KEVIN MITCHELL, Dept. of Physics, UC-Merced, THOMAS SOLOMON, Dept. of Physics & Astronomy, Bucknell University — We present experiments and simulations on the motion of self-propelled tracers in imposed laminar fluid flows. The flows used are hyperbolic and vortex-dominated flows, generated in microfluidic (PDMS) cells and in laboratory-scale, magnetohydrodynamically-driven systems. The tracers are either brine shrimp (for large-scale flows) or bacillus subtilis (for microfluidic flows). Two types of bacillus subtilis are studied: a wild-type -- characterized by run-and-tumble trajectories in the absence of a flow -- and a mutated "smooth swimmer" strain in which the tumbling is suppressed. We analyze the results in conjunction with a theory that predicts the existence of "Swimming Invariant Manifolds" (SwIMs) that act as one-way barriers that impede the trajectories of self-propelled tracers. We explore how the shape and location of the SwIMs vary with the imposed flow, along with the different ways in which the swimming behavior of the organism affect these SwIMs.

*Supported by NSF Grants DMR-1361881, DMR-1806355 and DUE-1317446.
9:00AM E61.00004: Stability of interfaces in active fluids* WAN LUO (Presenter), HARSH SONI, ROBERT ALAN PELCOVITS, THOMAS POWERS, Brown University — We study the linear stability of an active nematic fluid at rest in its isotropic phase in the following geometries: (1) a membrane immersed in the fluid, (2) a fluid film of finite height, (3) a spherical droplet of fluid, and (4) a cylindrical thread of fluid. In all four cases, we observe two frequency modes due to the coupling between the dynamics of the interface of the fluid and the dynamics of the nematic molecules. Propagating waves are seen above a value of activity which is independent of surface tension and has the same value in all four cases. For the first three cases, the fluid becomes unstable as the activity is further increased. In cases (1) and (2) the critical activity for instability is the same as for an unconfined active fluid and independent of surface tension. For case (3), the critical activity is larger than that for an unconfined fluid, and increases with increasing surface tension. A cylindrical thread of radius $R$ is always unstable against harmonic perturbations of wavenumber $k$ if $kR<1$, but the growth rate can be controlled by varying the activity. Perturbations with $k>1/R$ become unstable above a critical activity which changes with $k$ and surface tension.

*National Science Foundation through Grants Nos. MRSEC-1420382 and CBET-1437195.

9:12AM E61.00005: 1D condensation and onset to collective motion of swimming droplets* PIERRE ILLIEN (Presenter), CHARLOTTE DE BLOIS, MARJOLEIN VAN DER LINDEN, OLIVIER DAUCHOT, Gulliver lab, ESPCI Paris, CNRS — We observe that swimming droplets confined in a 1D channel spontaneously develop clustering and collective motion. A careful examination of the individual and interaction dynamics suggest that it can be described by effective inelastic collisions followed by a relaxation to the nominal velocity prescribed by activity. Starting from these experimentally observed features, and inspired by paradigmatic lattice models of interacting particles, we develop a theoretical framework in which alignment rules emerge from the microscopic interactions between the particles. This model reveals a rich phase diagram, in which the onset to collective motion results from the competition between inelasticity and activity, and can be preceded by very long-lived but transient macroscopic clustered states. We provide quantitative arguments that account for the formation of clusters in the system, and for the emergence of collective motion.

*Agence Nationale de la Recherche (MiTra project)
Marie Curie Actions/PRESTIGE programme (PCOFUND-GA-2013-609102)

9:24AM E61.00006: Odd viscosity in a chiral active fluid* EPRAIM BILILIGN (Presenter), VISHAL H SONI, University of Chicago, SOFIA MAGKIRIADOU, École Polytechnique Fédérale de Lausanne (EPFL), STEFANO SACANNA, New York University, DENIS BARTOLO, ENS de Lyon, MICHAEL JOHN SHELLEY, New York University, WILLIAM T. M. IRVINE, University of Chicago — We spin a system of colloidal magnets in an external magnetic field, forming a cohesive material that behaves like a liquid. Along a boundary of the fluid, we observe lively dynamics, including unidirectional surface waves that propagate due to an interplay of viscous stresses and surface tension. Through broken time-reversal and parity symmetries, this system allows the emergence of an anomalous transport coefficient known as odd (or Hall) viscosity. Unlike ordinary viscosity, this coefficient is dissipationless and absent in simple fluids. By reducing substrate drag, we are able to experimentally observe odd viscosity through the decay of free surface waves.

*National Science Foundation MRSEC Program at The University of Chicago (Grant DMR-1420709) and a Packard Fellowship

9:36AM E61.00007: Universal scaling in defect-free active turbulence* RICARD ALERT (Presenter), Princeton University, JEAN-FRANCOIS JOANNY, ESPCI, JAUME CASADEMUNT, University of Barcelona — Active fluids exhibit turbulent flows at low Reynolds numbers. In active liquid crystals, these flows are strongly constrained by topological defects, whose density defines a characteristic length that prevents the scale invariance typical of turbulence. Here we show that, at zero Reynolds number, defect-free active nematics exhibit a new type of turbulence with a distinctive scaling regime at large length scales. The system self-organizes into a disordered spatiotemporal pattern of orientation domains with a characteristic wavelength selected by the nonlinear dynamics, at which the active energy injection is maximal. In contrast to inertial turbulence, the energy is entirely dissipated at the scale where it is injected, without energy transfer to other scales. Nevertheless, arbitrarily large flow vortices are generated by the instantaneous, long-range kernel of Stokes hydrodynamics. Hence, instead of the Kolmogorov $\sim q^{-5/3}$ scaling of inertial turbulence, the velocity power spectrum scales as $\sim q^{-1}$, with $q$ being the wave number. Thus, in the absence of the screening effects due to topological defects, active nematic fluids exhibit turbulence without energy cascades and with a new universal scaling.

*R.A. acknowledges Fundació ‘La Caixa’ and the HFSP (LT000475/2018-C).
9:48AM E61.00008: Polar active suspensions - stability, waves, turbulence  RAYAN CHATTERJEE (Presenter), Tata Institute of Fundamental Research Hyderabad, ADITI SIMHA, Madras, Indian Institute of Technology, SRIRAM RAMASWAMY, Department of Physics, Indian Institute of Science, PRASAD PERLEKAR, Tata Institute of Fundamental Research Hyderabad — We study the hydrodynamics of self-propelled fluids with polar orientational order, using linear stability analysis and direct numerical simulations. We show that inertia and system dimension lead to a threshold for the instability of such systems to spontaneous distortion, with a diffusive growth rate at small wavenumber, and we confirm numerically the prediction (Simha & Ramaswamy 2002) of long-wavelength propagating modes. We illustrate the varieties of disturbance growth and explore the effects of self-propulsion and fluid inertia on active turbulence.

10:00AM E61.00009: Shear-induced transitions in passive and active polar liquid crystals: A novel shear-elongation parameter*  TOMER MARKOVICH (Presenter), CTBP Bioscience Research Collaborative, MS 654, Rice University, 6500 Main S, Rice University, ELSN TJHUNG, MICHAEL E CATES, DAMTP, University of Cambridge — Polar order in molecular liquid crystals is relatively rare, hence, it was not thoroughly investigated as other liquid crystalline phases. Recently, it has been discovered that suspensions of magnetic platelets in nematic liquid crystals show polar order at room temperature. Furthermore, polar order is ubiquitous in biology. It is seen in cell migration, swimming bacteria, the cytoskeletal etc. The growing interest in active matter and these recent experimental advances call for further theoretical investigations of polar liquid crystals. In the presence of external shear, polar particles tend to align with the shear flow at the Leslie angle, much like nematics. However, unlike the nematic director, the polar order parameter is not of fixed size. In this talk I will introduce the shear elongation parameter. This often neglected parameter, give rise to new physics such as shear-induced first order transition and significantly changes the rheological properties of the fluid. Active fluids can further exhibit yield stress and negative apparent viscosity.

*Work funded in part by the ERC, EU’s Horizon 2020 Programme (Grant 760769). TM is funded by the Blavatnik fellowship and the NSF CTBP (Grant PHY-1427654). MEC is funded by the Royal Society.

10:12AM E61.00010: Active fluid of self-rotating particles*  CODY REEVES (Presenter), Applied Math, Northwestern, IGOR S ARONSON, Biomedical Engineering, Pennsylvania State University, PETIA M. VLAHOVSKA, Applied Math, Northwestern — Suspensions of self-propelled particles, such as bacteria, have received considerable attention. Recently there has been increased interest in suspensions of self-rotating particles, such as Quincke rotors in electric fields and ferromagnetic colloids in alternating magnetic fields. While the individual particles are governed by relatively simple dynamics, the interaction of the particles can result in incredibly complex and interesting phenomena. Experiments show phase separation, macroscopic directed motion, and structure formation (e.g. vortices and asters). Modeling these systems as discrete particles at the micro-scale is computational expensive and limits the study of the rotors collective dynamics. We develop a continuum model for such rotor systems based on derivation for dielectric fluids with internal rotation This model allows us to study properties of the fluid and the existence of active turbulence caused by the rotors. To study the effect of confinement, we include phase parameter to restrict the rotors inside a region with a defined diffuse interface. We then can study the interaction between the rotors and the interface for both a fixed and deformable interface.

*This work was supported by a NSF graduate fellowship and NSF grants 1544196 and 1704996.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E62 DCOMP: Dealing With Spin-Orbit Coupling  BCEC 258C - David Vanderbilt, Rutgers Univ - Tag(s): Invited
Spin-orbit-proximitized ferromagnetic metals in spintronic phenomena: A first-principles Green's function approach

BRANISLAV NIKOLIC (Presenter), University of Delaware — The talk reviews first-principles Green's function methodology to obtain spectral function and spin texture at an arbitrary plane around interfaces within multilayers of different materials [1]. When applied to ultrathin ferromagnetic layer in contact with a material with strong spin-orbit coupling—such as topological insulators, heavy metals, monolayer transition metal dichalcogenides and Weyl semimetals (all of which have been utilized very recently to develop novel spintronic devices and they will be discussed in the talk)—this methodology reveals dramatic modification of ferromagnet electron and spin structures which acquire properties of the adjacent layer due to hybridization of their wave functions. In particular, such spin-orbit-proximitized ferromagnetic layer acquires spin textures that are noncollinear to its own magnetization. Passing unpolarized charge current parallel to the interface generates nonequilibrium spin density [2] in the presence of such textures, which becomes resource for spintronic devices operated by spin-orbit torques [3]. On the other hand, passing spin-polarized charge current or pure spin current perpendicular to the interface leads to spin memory loss due to the same spin textures [4] (even in the absence of disorder, intermixing and magnons at the interface) which adversely affects spintronic device operation. The talk will explain how to model spin-orbit torques and spin memory loss by employing first-principles Green's functions to construct relevant nonequilibrium density matrices [3,4].

References:


Comprehensive modeling of band gaps and absorption spectra of complex semiconductors for solar applications

JULIA WIKTOR (Presenter), EPFL — The performance of photosorbing materials is closely related to their band gaps and absorption spectra. In the fields of solar cells and photocatalysis, search for novel materials is ongoing. To identify optimal compounds, a modelling approach yielding accurate predictions for their electronic and optical properties is highly desirable. We recently applied the quasiparticle self-consistent QSGW method, efficiently accounting for the vertex correction, to study the electronic structure of halide perovskites and complex oxides. In the calculations, we included effects such as spin-orbit coupling, electron-hole interaction, magnetic ordering, nuclear quantum motions, and thermal vibrations. I will show that when an accurate electronic structure method is applied, and the significant effects are correctly accounted for, the band gaps and absorption spectra of complex materials can be reliably determined.

Carrier recombination in materials with strong spin-orbit coupling

XIE ZHANG (Presenter), University of California, Santa Barbara — Materials that have large spin-orbit coupling and no inversion symmetry can display interesting spin texture. The hybrid perovskites, which are receiving a lot of attention for photovoltaic applications, are prominent examples in which the spin texture exhibits unexpected patterns. Based on model calculations, it has been suggested that due to mismatched spins the radiative recombination is severely suppressed. We have performed first-principles calculations to compute the spin texture in the prototypical hybrid perovskite, CH3NH3Pbl3. We find that the spin texture is dynamically evolving in various patterns with the rotation of the organic molecule [1]. However, the spin-orbit coupling always leads to spin-allowed optical transitions and the momentum splitting affects the radiative recombination coefficient by less than a factor of two [2]. The spin-orbit coupling does, however, significantly enhance the Auger coefficient due to a coincidental resonance between the band gap and interband transitions to spin-orbit-split conduction bands [3]. These insights demonstrate the importance of accurate treatment of spin-orbit coupling in describing materials properties, and also offer new computational approaches to quantitatively calculate the spin texture and its impact on carrier recombination.


*This work was performed in collaboration with Jimmy-Xuan Shen, Wennie Wang, and Chris G. Van de Walle, and supported by DOE.
9:48AM E62.00004: The role of temperature in spin-orbit materials† [Invited]  BARTOMEU MONSERRAT (Presenter), Physics, University of Cambridge — The spin-orbit interaction underlies multiple physical phenomena, including topological order and the spin splitting of bands in inversion asymmetric crystals, which could be harnessed in novel technologies including spintronics or quantum computers. However, for any practical device, the spin-orbit driven properties need to survive all the way to room temperature, and therefore understanding the role of electron-phonon coupling and thermal expansion in spin-orbit materials becomes central.

In this talk, I will describe our work exploring the role of temperature in spin-orbit materials. I will describe the temperature dependence of the bulk Rashba splitting in the bismuth tellurohalides [1], temperature induced topological transitions in the bismuth selenide family [2], and structural stabilization driven by spin-orbit coupling in superconducting InSbBi3.


†Winton Programme for the Physics of Sustainability and Robinson College, Cambridge, and the Cambridge Philosophical Society for a Henslow Research Fellowship.

10:24AM E62.00005: Impact of spin-orbit coupling on the magnetic phase diagram of the iron pnictides† [Invited]  MORTEN HOLM CHRISTENSEN (Presenter), University of Minnesota — Experimental research over the past few years has shown the presence of sizeable spin-orbit coupling (SOC) in the iron pnictides [1]. Here, we focus on the impact of SOC on the magnetic phase diagram of the iron pnictides and in particular the implications for competing magnetic states and quantum criticality. Magnetism in the pnictides occurs in three distinct types. The prevalent magnetic phase is the C2 symmetric stripe magnetism, with moments parallel to the ordering vector. Additionally, there are two tetragonal, or C4r, magnetic phases, one with out-of-plane moments observed close to optimal doping in several compounds [2], and another with in-plane moments forming a spin-vortex structure [3]. The intimate relation between the ordering vectors and the moment direction is a direct consequence of SOC. Interestingly, a proliferation of different magnetic phases in close proximity in the phase diagram is observed in different pnictide materials as the putative magnetic quantum critical point is approached, e.g. by changing doping or pressure. We demonstrate, using a renormalization group approach, that such a behavior is a natural consequence of the interplay between magnetic quantum fluctuations and SOC. Formally, this is due to the emergence of a Gaussian fixed point leading to an enhanced magnetic degeneracy. This leads to an increase in the phase space of fluctuations which can enhance the transition temperature of superconductivity. Furthermore, we show how a rich landscape of magnetic phases emerges as a result of frustration between spin-anisotropic and spin-isotropic interactions. These novel phases consist of admixtures of the known C2 and C4 orders, and provide possible candidates for experimental observations [4].


†Work supported by the U.S. DOE, BES, under Award number DE-SC0012336.
Dynamics of microbiota communities during physical perturbation.* [Invited] CAROLINA TROPINI (Presenter), School of Biomedical Engineering, Microbiology & Immunology, University of British Columbia, JUSTIN SONNENBURG, Stanford University — The consortium of microbes living in and on our bodies is intimately connected with human biology and deeply influenced by physical forces. Despite incredible gains in describing this community, and emerging knowledge of the mechanisms linking it to human health, understanding the basic physical properties and responses of this ecosystem has been comparatively neglected. Most diseases have significant physical effects on the gut; diarrhea alters osmolality, fever and cancer increase temperature, and bowel diseases affect pH. Furthermore, the gut itself is comprised of localized niches that differ significantly in their physical environment, and are inhabited by different commensal microbes. Understanding the impact of common physical factors is necessary for engineering robust microbiota members and communities; however, our knowledge of how they affect the gut ecosystem is poor.

As a model of a biophysical perturbation, we are investigating how changes in osmolality affect the host and the microbial community and lead to mechanical shifts in the cellular environment. Osmotic perturbation is extremely prevalent in humans, caused by the use of laxatives, lactose intolerance, or celiac disease. In our studies we monitored osmotic shock to the microbiota using a comprehensive and novel approach, which combined in vivo experiments to imaging, physical measurements, computational analysis and highly controlled microfluidic experiments. By bridging several disciplines, we developed a mechanistic understanding of the processes involved in osmotic diarrhea, linking single-cell biophysical changes to large-scale community dynamics. Our results indicate that physical perturbations can profoundly and permanently change the competitive and ecological landscape of the gut, and affect the cell wall of bacteria differentially, depending on their mechanical characteristics.

*This work was funded in part by a James S. McDonnell Postdoctoral Fellowship.

Evolution of Multicellular Specialization in Dynamic Fluids* GURDIP UPPAL (Presenter), DERVIS CAN VURAL, University of Notre Dame — Multicellularity and division of labor mark a major transition in the development of life. In this study, we determine the conditions for multicellular specialization to occur starting with a system of generalists that secrete two public goods. We look at two different fitness functions where either both public goods are necessary for any fitness gain or where either one is sufficient for a fitness gain. We denote these by AND and OR respectively, to resemble the logical AND and OR functions. Social structures arise naturally from our advection-diffusion-reaction model as self-replicating Turing patterns. We see that an AND structure is necessary for the specialists to stay together in the same social structure. Specialists in the OR case dissociate into separate groups of pure specialists. We look at the effects of varying the cost of cooperation and mutation rate on the emergence of specialization. When trade-off costs are small, we see that spatial structure can help facilitate the transition to specialization for either fitness function. At larger trade-offs in the AND case, we see that generalists are more stable.

*This material is based upon work supported by the Defense Advanced Research Projects Agency under Contract No. HR0011-16-C-0062.

Pinning and pulsed expansion in a spatially expanding bacterial mutualism AROLYN CONWILL (Presenter), JEFFREY GORE, Massachusetts Institute of Technology — Range expansions occur when a population expands in space due to dispersal and growth. These expansions can result from environmental change, introduction of invasive species, or evolutionary adaptation that enables a population to move into previously unoccupied territory. Theoretical work has shown that fragmented habitats and seasonal growth (discrete space and discrete time) can result in pinning and pulsed invasions in expanding populations with an Allee effect. However, it is not clear how underlying population dynamics such as limit cycle oscillations influence these phenomena. We probe this question in an experimental model system consisting of an oscillating bacterial mutualism inhabiting discrete population patches and subject to periodic growth cycles. For low nearest-neighbor migration rates, the mutualism cannot expand, and the population is pinned in place. For high nearest-neighbor migration rates, the mutualism expands at pulsed speeds. Furthermore, our experimental results are consistent with a mechanistic model prediction that the period of population oscillations locks into specific values during pulsed invasion, emphasizing the interplay between ecological interactions and spatial structure.
9:00AM E63.00004: Survival probabilities of mutants with antagonistic interactions  MAXIM O LAVRENTOVICH (Presenter), Physics and Astronomy, University of Tennessee, DAVID R NELSON, Department of Physics, Harvard University — Strains within a population interact not only via competition due to varying growth rates, but also via secretion of toxins, predation, parasitism, and other adaptations which result in frequency-dependent selection. These dynamics often play out in a spatial context, such as at the frontier of a growing spherical cell mass, or on the surface of a Petri dish. We study how a mutant, interacting antagonistically with a wild-type strain (i.e., the mutant grows more slowly in the presence of the wild-type), survives in two-dimensional populations with flat and curved geometries, representing, for example, the Petri dish surface and cell mass frontier, respectively. The antagonistic interactions significantly diminish the survival probability of the mutant even when, in isolation, the mutant grows much faster than the wild-type strain. We show that the survival probability can be thought of as a kind of “nucleation rate” of the mutant strain. The predictions of classical nucleation theory agree with our simulation results and provide an important modification, due to the antagonistic interactions, of the classic Kimura formula for the survival probability. We comment on both the effects of small-number fluctuations and the curved population geometry.

9:12AM E63.00005: Measuring cellular memory and heterogeneity at the single-cell level  TAMAS SZEKELY (Presenter), ZHIHAO CAI, MARTIN SAUZADE, ERIC BROUZES, GABOR BALAZSI, Stony Brook University — Microbial populations live in a wide range of ecological settings. In changing environments, survival is improved by heterogeneity. In contrast, in stable environments the population is best off when cells adopt the single optimal phenotype. In a clonal population, heterogeneity occurs at the phenotypic (protein) level; as cellular protein levels vary over time, phenotypes can change dynamically, with the timescale given by “cellular memory”. However, the population-level distribution of phenotypes remains stable, optimised by evolution to its ecological setting. An interesting situation occurs when a population moves from one setting to another. In this case, one can encounter a bimodal population in a constant environment for which it is not adapted. How does evolution shape this population? We examine this in yeast containing a synthetic gene circuit that gives a phenotypically bimodal population. We expose cells to a stable environment and observe changes in heterogeneity. Using a microfluidic platform, we measure the cellular memory of many single cells. Thus, we investigate the relationship between fitness, cellular memory and phenotype distribution during evolution in a constant environment.

*NIH #R35GM122561 and Laufer Center for Physical & Quantitative Biology to GB.

9:24AM E63.00006: Bet-hedging strategies in expanding populations  PAULA VILLA MARTÍN, Okinawa Institute of Science and Technology, MIGUEL ANGEL MUÑOZ, Physics, University of Granada, SIMONE PIGOLOTTI (Presenter), Okinawa Institute of Science and Technology — Ecological species can spread their extinction risks in uncertain environments by adopting a bet hedging strategy, i.e. by diversifying individual phenotypes. We present a theory of bet-hedging for populations colonizing unknown environments that fluctuate either in space or time. We find that diversification is more favorable strategy in this scenario than for well-mixed populations, supporting the view that range expansions promote diversification. For slow rates of variation, spatial fluctuations open more opportunities for bet-hedging than temporal variations. Opportunities for bet-hedging reduce In the limit of frequent environmental variation, regardless of the nature of these fluctuations. These conclusions are robust against stochasticity induced by finite population sizes.


9:36AM E63.00007: Competition in dense bacterial biofilms through killing and replication  GABI STEINBACH (Presenter), MICHAEL SIULUNG, BRIAN K. HAMMER, PETER YUNKER, Georgia Institute of Technology — Typically, biofilms feature many different microbial species and strains. This diversity presents a challenge, as individuals must compete for resources and space. In response, microbial species have evolved antagonistic mechanisms such as the Type VI secretion system (T6SS). This is a contact-dependent toxin-delivery system that enables the injection of fatal toxins into other bacteria as well as eukaryotic cells. Previous studies have shown that such an antagonistic one-on-one interaction causes an initially well-mixed culture to phase separate, providing protection by number. We study biofilms consisting of V. cholerae, which express T6SS, as an experimentally controllable and practically relevant system of mutual killers. While we observe phase separation, the typical size of clonal patches stops changing much earlier than expected. In experimental and numerical studies of mutual killing strains of V. cholerae, we show that a protective layer of debris forms at the interface between patches, which slows down further killing. This poses major consequences for the role of antagonistic interactions and the survival dynamics in biofilms.

*Funding by the German Academy of Sciences Leopoldina is acknowledged.
Phase Transition Behavior in Yeast Populations Under Stress*  
STEPHEN W. ORDWAY, Physics & Astronomy, University of Missouri -- St. Louis, DAWN M. KING, Slalom Consulting, DAVID FRIEND, Illinois Institute of Technology, CHRISTINE NOTO, Biology, Saint Louis University, SNOWLEE PHU, WENDY OLIVAS, Biology, University of Missouri -- St. Louis, SONYA BAHAR (Presenter), Physics & Astronomy, University of Missouri -- St. Louis — Nonequilibrium phase transition behavior has recently been observed in computational models of evolutionary dynamics (Scott et al., 2013; King et al. 2017). Dynamical signatures predictive of population collapse have been observed in yeast populations under stress (Dai et al., 2012). We experimentally investigate the population response of *Saccharomyces cerevisiae* to biological stressors (temperature and salt concentration) in order to investigate the dynamical behavior of the system in the vicinity of population collapse. While both conditions lead to population decline, the dynamical characteristics of the population response differ significantly depending on the stressor. Under temperature stress, the population undergoes a sharp change with significant fluctuations within a critical temperature range, indicative of a continuous absorbing phase transition. In the case of salt stress, the response is much more gradual.

*This work was supported in part by a University of Missouri IDIC (Inter-disciplinary Inter-campus) Grant.

A neural network model predicts the consequences of crosstalk in bacterial quorum sensing*  
JAMES BOEDICKER (Presenter), KALINGA PAVAN T SILVA, TAHRIR YUSUFALY, University of Southern California — Many bacteria use chemically similar molecules to communicate, resulting in crosstalk between bacterial signaling networks. Such crosstalk can have unexpected consequences for decision making in heterogeneous communities of cells. Here we examine crosstalk within a community composed of five strains of *Bacillus subtilis*, with each strain producing a variant of the quorum sensing peptide ComX. Co-cultures of these strains create in a mixture of ComX variants, resulting in variable levels of gene expression in each strain. To predict gene regulation in communities producing multiple signals, we implement a neural network model. Experimental quantification of crosstalk between pairs of strains parametrized the model, enabling the accurate prediction of activity within the full five-strain network. Interactions weights between the five signaling networks were both positive and negative, of variable magnitude, and asymmetric. Signal crosstalk within the five-strain community results in multiple community-level quorum sensing states, each with a unique combination of quorum sensing activation among the five strains. The community-level signaling state was influenced by the ratio of strains as well as dynamics of community composition.

*NSF CAREER: PHY-1753268

Production of a biofilm polymer can benefit bacteria when grown in co-culture under low iron conditions*  
VERNITA GORDON (Presenter), JAIME B HUTCHISON, KARISHMA S KAUSHIK, CHRISTOPHER A RODESNEY, THOMAS LILIEHOLM, LAYLA BAKHTIARI, University of Texas at Austin — Biofilm formation is associated with resistance to antibiotics and the immune system. The opportunistic human pathogen *Pseudomonas aeruginosa* forms biofilm infections in lungs, wounds, and on medical devices. However, its ability to form biofilms originated in this bacterium's native environment, primarily plants and soil. Such environments are polymicrobial and resource-limited. The *P. aeruginosa* extracellular polysaccharide Psl can bind iron and, for the strain PAO1, is also the dominant "glue" holding together multicellular aggregates and biofilms. Here, we quantify early biofilm growth using time-lapse confocal microscopy. We find that aggregates of *P. aeruginosa* have a growth advantage over single cells of *P. aeruginosa* in the presence of *Staphylococcus aureus* in low-iron environments. This growth advantage is linked to aggregates' high Psl content and to the production of an active factor by *S. aureus*. We posit that this may have been linked to the evolutionary development of the strong biofilm-forming tendencies of *P. aeruginosa*.

*Human Frontier Science Program (HFSP-RGY0081/2012 – GORDON); Cystic Fibrosis Foundation (Gordon 201602808-001); National Science Foundation (727544, BMMB, CMMI); National Institutes of Health (1R01AI121500-01A1, NIAID)
10:24AM E63.00011: Oxygen dynamics in a two-dimensional microbial ecosystem* ALEXANDER PETROFF (Presenter), Clark University, FRANK TEJERA, ALBERT J LIBCHABER, Rockefeller University — Ecosystems persist over geological timescales by continuously cycling nutrients. However, we lack a quantitative model of how diverse organisms organize with respect to one another. We observe these dynamics in a quasi-two-dimensional microbial ecosystem, in which all microbes live within the penetration depths of oxygen and light. This community is composed of both photosynthetic bacteria, which produce sugars and oxygen, and aerobic bacteria, which consume oxygen and sugars. Shining a light on the community drives a nutrient cycle between these two groups of microbes. Illuminating a spot, we measure the resulting distribution of oxygen. Under normal conditions, diffusion alone stabilizes oxygen gradients. However, at freezing temperatures or low atmospheric oxygen concentration, the kinetics of microbial oxygen production and consumption dominate. Surprisingly, after three weeks, the initially uniform distribution of oxygen in the spot becomes an annulus. We present a robust method to invert the measured oxygen concentration for the distribution of oxygen sources and sinks.

*HFSP RGP003

10:36AM E63.00012: Thermodynamic constraints on cross-feeding in bacterial population TONG WANG (Presenter), University of Illinois at Urbana-Champaign, CHEN LIAO, Memorial Sloan Kettering Cancer Center, SERGEI MASLOV, University of Illinois at Urbana-Champaign — Overflow metabolism refers to the strategy of cells using fermentation instead of the more energetically-efficient respiration, even when the oxygen is available. Cross-feeding between two bacterial strains growing on a single primary carbon source can be established when one bacterial strain consumes overflow metabolites excreted by the other bacterial strain. Many overflow pathways are thermodynamically controlled and thermodynamic constraints on them are not included to consider the cross-feeding of overflow metabolites between two strains in the past. Motivated by experimental results of acetate cross-feeding polymorphism, in this paper, we developed a single cell growth model with coarse-grained metabolic pathways including proteome allocation and thermodynamic constraints on the overflow pathway. The model can accurately capture the flux of thermodynamically controlled overflow pathway and growth rate of cells under different growth conditions. Moreover, when it is applied to study the cross-feeding, the model can reveal the short-term dynamics and long-term dynamics of cross-feeding stable polymorphism seen in experiments.

10:48AM E63.00013: How can unsuccessful invaders drive long-term shifts in community state?* DANIEL R. AMOR (Presenter), CHRISTOPH RATZKE, JEFFREY GORE, Massachusetts Institute of Technology — The stability of virtually all microbial communities is frequently challenged by the arrival of new individuals that could potentially invade the system. This urges for a deeper understanding of how invasions can interfere the dynamics of microbial communities. I will present a bistable model system to study the dynamics between alternative stable states in microbial ecosystems. By introducing additional species into the system, we observed induced transitions between stable states. Interestingly, in many cases the invading species did not survive in the final community state, making these species what we call a “transient invader.” This suggests that short-term invasions (such as infections) could be a common mechanism driving transitions between stable states in microbial communities.

*TGNational Institutes of Health New Innovator Award (NIH DP2)

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E64 DBIO GSNP: Physics of the Brain: Structure and Dynamics 8CEC 259B - Mukesh Dhamala, Georgia State University; Peter Robinson, University of Sydney - Tag(s): Focus

8:00AM E64.00001: Oscillation onset and wave propagation in neocortex* [Invited] TIMOTHÉE PROIX (Presenter), University of Geneva — In this talk, I will present recent findings on spatiotemporal patterns and wave propagation in neocortex based on intracortical microelectrode array recordings in primates during various states including optogenetic stimulation to probe neural dynamics, movement preparation and execution, and human epileptic seizures. I will follow with results based on neural-field models to account for the observed oscillation onset and wave propagation phenomena.

*This research was supported by the National Institute of Neurological Disorders and Stroke (NINDS), grant R01NS079533; the Department of Veterans Affairs, Merit Review Award I01RX000668; and the Pablo J. Salame ’88 Goldman Sachs endowed Assistant Professorship of Computational Neuroscience.
STEVEN J. SCHIFF (Presenter), Pennsylvania State University — There is a several decade history demonstrating that electrical polarization of neurons can modulate neuronal firing, and that such polarization can suppress (or excite) spiking activity and seizures. In recent years, we uncovered a unification in the computational biophysics of spikes, seizures, and spreading depression (Wei et al, Journal of Neuroscience 34:11733-11743, 2014). These findings demonstrated that the repertoire of the dynamics of the neuronal membrane encompasses a broad range of dynamics ranging from normal to pathological, and that seizures and spreading depression are manifestations of the inherent properties of those membranes. Most recently, we have demonstrated that neuronal polarization can suppress (or enhance), block, or prevent spreading depression (Whalen et al, Scientific Reports, 8:8769, 2018), the physiological underpinning of migraine auras. Remarkably, this suppression requires qualitatively different stimulation from that required to suppress spikes and seizures, and is fully consistent with the computational biophysical models of spreading depression. Further unexpected findings from these experiments were that suppression of spreading depression does not generate seizures, and vice versa, that when the brain is in seizure activity suppression does not generate spreading depression. The implications are that in controlling brain dynamics from different states of the brain, there can be state dependent control which is qualitatively very different from that required in other states.

*Funding: NIH 1R01EB014641, 1R21EY026438.

SPASE PETKOSKI (Presenter), VIKTOR JIRSA, Aix-Marseille University — Neural network oscillations are a fundamental mechanism for cognition, perception and consciousness. Consequently, perturbations of network activity play an important role in brain disorders. Customization of healthcare with medical decisions tailored to the individual patient is a key aspect of personalized medicine.

When structural information from non-invasive brain imaging is merged with mathematical modelling, then generative brain network models constitute personalized in silico platforms for the exploration of causal mechanisms of brain function and clinical hypothesis testing. In partial epilepsy seizures originate in a local network, the so-called epileptogenic zone, before recruiting other brain regions. We build a Virtual Epileptic Patient (VEP) brain model that integrates patient-specific information, and we demonstrate that VEP derived from diffusion magnetic resonance imaging have sufficient predictive power to improve diagnosis and surgery outcome [1]. Individual brain models for 15 patients are validated against the presurgical electroencephalography data and the standard clinical evaluation, and are used to show that VEP brain models account for the patient seizure propagation patterns and explain the variability in postsurgical success [2]. Finally, we demonstrate how to develop novel personalized strategies towards therapy and intervention, by the example of applying linear stability analysis to the VEP in order to identify the minimal number of links that need to be removed for stopping the seizure propagation [3]. This suggests a less invasive paradigm of surgical interventions to treat and manage partial epilepsy.

References

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9:48AM E64.00004: Influence of the Human Amyloidogenic precursor on Epithelial and Neuronal Cell Membrane*
IZABELA STROE (Presenter), BIBI NAJMA, Physics, Worcester Polytechnic Institute, AMITY MANNING, Biology & Biotechnology, Worcester Polytechnic Institute — The pathology of Alzheimer's disease (AD) is correlated with the amyloid fiber formation. The Aβ (1-42) amyloid fragment is the principal species associated with senile plaque. There is evidence that the Aβ (1-42) amyloid precursors, such as the monomers, dimers, oligomers, and the proto-fibrils are toxic to the neuronal cell. It is believed that the Aβ (1-42) amyloid precursors perturb the neuronal cell membrane integrity leading to its death; however, the molecular mechanism by which the neuronal cell death occurs is not yet understood. Dielectric relaxation spectroscopy was used to study the interaction of the oligomeric Aβ (1-42) with the cell membrane of epithelial and neuronal cells. We incubated both cell types with the Aβ (1-42) solution of monomers, oligomers, and fibrils. We measured the dielectric response of the incubated cells at different concentrations over a wide range of frequencies (from 10⁻² Hz to 10⁷ Hz). Two dispersion processes (α, β) can be observed for all concentrations of the cell suspensions. We observed changes in the conductivity and permittivity of the neuronal cells when incubated with Aβ (1-42), which suggests the toxicity of the precursors causing marked alterations in the electrical properties of the cell membrane.

*Fulbright educational foundation

10:00AM E64.00005: Impact of Damaged Neurons on Continuous Attractor Network Models of Grid Cells. YUDUO ZHI (Presenter), DANIEL COX, Department of Physics, University of California, Davis — Grid cells in the dorsolateral band of the medial entorhinal cortex(dMEX) display strikingly regular firing responses to animal’s position in 2-D space. This helps animals be able to encode relative spatial location without reference to external cues. Within a continuous attractor model of grid cell activity[1,2], we focus on the question of how two different kinds of damage to the dMEX that can arise from neurodegenerative diseases affect grid cell performance: I) randomly distributed discrete damage and II) diffusing damage that can arise from propagation of neurofibrillary tangles. Drawing on models from the existing literature, we employ 1- and 2-dimensional neural networks with background excitation sensitive to motion and a ring of inhibitory couplings modeled as a difference of Gaussians around each firing neuron. For sufficiently strong inhibition, the model always produces a stable 1-dimensional or 2-dimensional lattice. We will study the impact of the two damage types on the attractor model and contrast this with the impact of damage on an oscillatory grid cell model[3].

10:12AM E64.00006: Molecular Underpinnings of Postsynaptic Calmodulin-dependent Calcium Signaling*
MARGARET CHEUNG (Presenter), University of Houston — Calcium (Ca²⁺) signaling is a dynamic system where Ca²⁺ concentration fluctuates in range of 0.1-10μM with time. These short transient Ca²⁺ around the entry sites activate Ca²⁺-binding proteins such as calmodulin (CaM). The prototypical pathway describes CaM as encoding a Ca²⁺ signal by selectively activating downstream CaM-dependent proteins through molecular binding. However, CaM’s intrinsic Ca²⁺-binding properties alone appear insufficient to decode rapidly fluctuating Ca²⁺ signals. It has been proposed that the temporally varying mechanism for producing target selectivity requires CaM-target interactions that directly tune the Ca²⁺-binding properties of CaM through reciprocal interactions. I will focus on two unique and distinct CaM binding targets, neurogranin (Ng) and CaM-dependent kinase II (CaMKII), which are abundant in postsynaptic neuronal cells and are biochemically known to tune CaM’s affinity for Ca²⁺ in opposite directions. By employing an integrative approach of quantum mechanical calculations, all-atomistic molecular dynamics, and coarse-grained molecular simulations, we have revealed the molecular mechanisms of CaM’s reciprocal interaction between target binding and Ca²⁺binding.

*We thank the support from the National Science Foundation (MCB 1412532, PHY 1427654).

10:24AM E64.00007: Dynamics of neuronal growth on surfaces with controlled geometries* ILYA YURCHENKO (Presenter), CRISTIAN STAII, Tufts University — Detailed knowledge of how the surface physical properties, such as mechanics, topography and texture influence neuronal growth and guidance is essential for understanding the processes that control neuron development, the formation of functional neuronal connections and nerve regeneration. I will present experimental results that demonstrate directional neuronal growth imparted by the surface geometry. We quantify axonal alignment and growth dynamics using a general stochastic model based on the Langevin equation. We relate the observed alignment in axonal growth to cellular contact guidance behavior, which results in an increase in the cell-substrate coupling on surfaces with micro-patterned structures. These results provide new insight into the role played by geometrical cues in neuronal growth and could lead to new methods for stimulating neuronal regeneration and the engineering of artificial neuronal tissue.

*Tufts Summer Scholars and Tufts Faculty Research Award
Non-parametric discovery of population dynamics from large-scale neural activity recordings*

MIKHAIL GENKIN (Presenter), TATIANA A. ENGEL, Neuroscience, Cold Spring Harbor Laboratory — Recent advances in neurotechnology enabled activity recordings from many neurons simultaneously, allowing us to study how neural populations are coordinated to drive behavior. Current population-analysis methods are based on fitting parametric models to data. However, these ad hoc models often distort dynamical features and result in ambiguous model comparisons. To overcome these limitations, we develop a non-parametric framework for discovering population dynamics directly from the data without a priori model assumptions. Our framework is based on latent Langevin dynamics, in which driving forces are directly optimized to effectively search the entire space of possible dynamics. The framework incorporates diverse, non-linear relationships between population-dynamics and firing-rates of single neurons. We derive a gradient descent algorithm for optimization over the space of continuous functions and use cross-validation and early stopping for regularization. Our framework accurately recovers qualitatively different population-dynamics simultaneously with diverse firing-rate profiles of single neurons.

*This work was supported by the Swartz Foundation and NIH grant 1R01EB026949-01.

Tracking multineuronal activity in unrestrained animals with a random access two photon microscopy*

AKIHIRO YAMAGUCHI (Presenter), DOYCHO P KARAGYOZOV, MIRNA MIHOVILOVIC SKANATA, RUI WU, MARC H GERSHOW, Department of Physics, New York University — Optical recordings of neuronal activity in freely behaving animals can reveal the correlation between the neural activity and behavioral outcome, such as decision making, learning, and multisensory integration. Such recordings require a microscopy that can overcome motion artifacts that accompany behavior. We recently developed a two-photon tracking microscope capable of recording activity from neurons in freely behaving larval fruit flies without motion artifacts[1]. However, due to the inertia of the scanning elements, the current technique is limited to recording only two neurons at a time. In order to study the correlation between neural activities and behavioral outcome across a range of neurons - sensory to motor neurons, it is essential to track multiple neurons at a time.

We extended the microscope using acousto-optic deflectors to relocate the laser beam in a constant time regardless of the distance between the two positions. Combined with improved feedback algorithms implemented in field-programmable gate arrays, this allows us to track and record the activities of many neurons at a high spatio-temporal resolution.


*NSF 1455015, NIH 1DP2EB022359

Tuesday, March 5, 2019 8:00 AM - 10:48 AM

Session E65 DBIO DPOLY GSNP: Physics of Genome Organization I

8:00AM E65.00001: Complexity in transcription factor – DNA recognition [Invited] MARTHA BULYK (Presenter), Harvard Medical School — TBD
8:36AM E65.00002: Quantifying sequence readout by transcription factors through principled analysis of high-throughput SELEX data* [Invited] HANS RUBE (Presenter), CHAITANYA RASTOGI, JUDITH F KRIBELBAUER, XIAOTING LI, BACH-VIET DO, HARMEN J BUSSEMAKER, Columbia University — Transcription factors (TFs) control gene expression by binding to genomic DNA in a sequence-specific manner. In recent years, hundreds of TFs have been characterized using high-throughput in vitro DNA binding assays coupled with deep sequencing. Variations of these assays can characterize binding by TF complexes and by RNA-binding proteins, or binding to chemically modified DNA. However, no unified method for analyzing all these data yet exists. We recently developed an algorithm named No Read Left Behind or NRLB (Rastogi et al., PNAS, 2018), which infers biophysical binding specificity models across the full affinity range from single-round SELEX data. It predicts human MAX homodimer binding in near-perfect agreement with existing low-throughput measurements, captures the specificity of the full-length p53 tetramer, and distinguishes multiple binding modes within a single sample. In addition to the chemical identity of the DNA bases, TF binding affinity is sensitive to the local three-dimensional shape of the DNA double helix. We demonstrate that linear models based on mononucleotide features alone can account for 60–70% of the variance in the DNA shape parameters minor groove width, roll, helix twist, and propeller twist. We also show that NRLB binding models implicitly encode DNA shape readout. Building on these observations, we developed a post hoc analysis method that interprets NRLB models in terms of DNA shape readout (Rube et al., MSB, 2018). Finally, we will discuss our latest algorithm, ProBound, which, unlike NRLB, allows principled modeling of multiple SELEX rounds, chemically modified DNA, and complexes with variable spacing between the DNA binding domains. ProBound works on all currently available data and allows us to build a resource of DNA binding specificity models for hundreds of TFs.

*This research was supported by NIH grant R01HG003008.

9:12AM E65.00003: Heterodimer Transcription Factors as Novel Gene Regulators KYLE NAUGHTON (Presenter), JAMES BOEDICKER, University of Southern California — Synthetic bacterial communities often incorporate quorum sensing (QS) networks to enable cell-cell communication. An intrinsic component of most QS networks is dimerization of receptor proteins around QS signals. Dimers of receptors act as transcription factors, modulating gene expression in the presence of high signal concentration. For example, LuxR binds a signal, forms a homodimer, and activates an operon in a feed-forward manner that makes more signal, more receptors, and invokes bioluminescence in Vibrio fisheri. In cells with more than one type of receptor protein, homodimers and heterodimers may form. The role of heterodimers and the conditions for their formation, however, remains murky. Some authors suggest heterodimers mute genes by competitively binding QS signals or forming inactive dimers. It remains possible, however, that heterodimer formation occurs in a purposeful way. We explore the possibility that heterodimers directly regulate gene expression based on experiments with tethered dimers. From a theoretical perspective use simple thermodynamic models to examine under what conditions heterodimers might form. Using MCMC and QS receptor position weight matrices we suggest DNA binding sites may exist which favor the heterodimers over either homodimer.

9:24AM E65.00004: Gene clustering drives co-regulation of disparate biological pathways in eukaryotes RICHARD JOH (Presenter), MICHAEL LAWRENCE, MARTIN ARYEE, MO MOTAMEDI, Center for Cancer Research, Massachusetts General Hospital — The establishment of distinct transcriptional states in response to developmental or environmental cues is critical for survival. This involves the concordant or discordant transcriptional regulation of several distinct biological pathways, often involving thousands of genes. How these system-level changes to transcriptionomes are coordinated is an understudied problem in eukaryotic biology. Here, using computational and experimental approaches in eukaryotes ranging from yeast to human, we report that this coordination is in part achieved by the genic proximity of the regulatory nodes of disparate biological pathways whose co-regulation drives the transcriptional coherence of their respective pathways. Overall, our data identifies transcriptional co-regulation of hundreds of discreet biological pathways and suggest that genomic clustering of their transacting factors such as transcription factors create operon-like regulation in eukaryotes.

9:36AM E65.00005: Liquid-liquid phase separation driven organization of nuclear chromatin domains RABIA LAGHMACH (Presenter), DAVIT POTYOYAN, Chemistry department, Iowa State University — Chromatin of eukaryotic cells folds within few micrometers of nuclear space while still retaining dynamism and accessibility needed for function. Latest experiments have revealed a liquid like behavior of chromatin manifested in epigenetically mediated phase separation into micro-droplets with distinct transcriptional states. Motivated by these experiments we have devised a mesoscale liquid like model of nucleus (MELON) with chromatin states resolved as a viscoelastic fluid fields of type A and B corresponding to transcriptionally active and silent states. The model allows direct comparison with imaging experiments of different cell lines and during various stages in cell cycle. Using MELON framework, we investigate the roles of chromatin droplet diffusion, fluctuations and impact of phase separation kinetics on non-equilibrium processes of growth and inversion. We show that ideas based on classical theories of nucleation and phase separation can have a broad predictive power in capturing several salient features of intra-nuclear chromatin dynamics.
9:48AM E65.00006: Polymer Models of S. pombe Chromatin  PETER WILLIAMS (Presenter), Applied Physics, Yale University, SIMON G MOCHRIE, Physics and Applied Physics, Yale University, MEGAN KING, Cell Biology, Yale University, COREY SHANE O’HERN, Mechanical Engineering & Material Science, Physics, and Applied Physics, Yale University — Recent advances in Hi-C studies have laid the groundwork for understanding the organization of the genome at different points in the cell cycle. We present a coarse-grained polymer model with short-ranged attractions and volume exclusion that quantitatively recapitulates experimental Hi-C maps for the yeast strain, S. pombe. The polymer model gives rise to an ensemble of transient clusters corresponding to topologically associated domains. Insight on the dynamics of chromatin can be obtained from single particle tracking experiments on fluorescently tagged transgenic loci at strategic points in the genome. Transcription inhibitors have been shown to dramatically suppress the mean square displacements of the loci. These results imply that transcription is the source of activity within the nuclear envelope. We have also developed a coarse-grained model of polymerase translocating along a polymer. We model portions of the genome to identify the effect of activity on loci proximal and distal to regions of high gene expression.

10:00AM E65.00007: Bacterial chromosome organization: few special cross-links, cell confinement, and molecular crowders play the pivotal roles.*  TEJAL AGARWAL (Presenter), Department of Physics, Indian Institute of Science Education and Research, Pune, MANJUNATH G. P., Department of Biochemistry and Molecular Pharmacology, NYU Langone Medical Center, FARHAT HABIB, Inmobi, APRATIM CHATTERJI, Department of Physics, Indian Institute of Science Education and Research, Pune — Using a coarse-grained bead-spring model of bacterial chromosomes of C. crescentus and E. coli we show that just 33 and 38 effective cross-links in 4017 and 4642 monomer chain at special positions along the chain contour can lead to the large length-scale organization of the DNA polymer, where confinement effects of the cell walls play a crucial role in the organization. The positions of the 33/38 cross-links along the chain contour are chosen from the Hi-C contact map of bacteria C. crescentus and E. coli. We represent 1000 base pairs as a coarse-grained monomer in our bead-spring flexible ring polymer model of the DNA. Thus 4017/4642 beads on a flexible ring polymer represent the C. crescentus/ E. coli DNA polymer with ~4 million base pairs. Choosing suitable parameters from our preceding study, we also incorporate the role of molecular crowders and the ability of the chain to release topological constraints. We also validate our prediction of the organization of the bacterial chromosomes with available experimental data.

Ref:

*DST, DBT India.

10:12AM E65.00008: Spatial proximity coordinates histone modification and expression of multiple genes*  JINGYU ZHANG, YAN ZHANG, IVET BAHAR, JIANHUA XING (Presenter), University of Pittsburgh — A cell type transition process requires temporally orchestrated global changes of gene expressions despite existence of large extrinsic and intrinsic stochasticity. One such major source of stochasticity is transcriptional bursting, where even under constant levels of trans-regulatory elements genes stochastically switch between a transcriptionally active and an inactive state. Such bursting dynamics may destroy temporal coordination of genes. We integrated datasets of gene expression, histone modification, and chromosome conformation for the mouse nervous system development and TGF-β treated MCF10A cells. We identified that genes having related functions and regulated by common TFs tend to cluster spatially and share similar histone modification patterns. Through a polymer-based model that describes cooperativity in histone modification dynamics, we predict that genes in proximity synchronize their transcriptions by synchronizing their stochastic switching between histone modification states with different transcriptional activities. This hypothesis is supported by analysis of allele-specific single cell RNAseq data, and we are further testing it with single cell FISH and superresolution imaging.

*This work is funded by NSF.
**10:24AM E65.00009: Interphase chromatin as a self-returning random walk: Can DNA fold into liquid trees?**

KAI HUANG (Presenter), VADIM BACKMAN, IGAL G SZLEIFER, Northwestern University — We introduce a self-returning random walk to describe the structure of interphase chromatin. Based on a simple folding algorithm, our de novo model unifies the high contact frequency discovered by genomic techniques, and the high structural heterogeneity revealed by imaging techniques, which two chromatin properties we theoretically prove to be irreconcilable within a fractal polymer framework. Our model provides a holistic view of chromatin folding, in which the topologically associated domains are liquid-tree-like structures, linked and isolated by stretched out, transcriptionally active DNA to form a secondary structure of chromatin that further folds into a "3D forest" under confinement. The model pivots an unprecedentedly wide array of experimental observations and suggests the existence of a universal chromatin folding principle. Based on a global folding parameter, the model reveals a unique structure-function relation of chromatin, which is abnormal from a polymer point of view but explains some experimental observations of how chromatin responses to stress.

*We gratefully acknowledge funding from National Science Foundation Grants: Biol & Envir Inter of Nano Mat 1833214, EFRI RESEARCH PROJECTS 1830961.*

**10:36AM E65.00010: Investigating dynamic chromatin states in a model cell organism**

MARY LOU BAILEY (Presenter), Applied Physics, Yale University, JESSICA F WILLIAMS, MEGAN KING, Cell Biology, Yale University, SIMON G MOCHRIE, Applied Physics, Yale University — Chromatin's biological functions are inextricably linked to its spatial organization and real-time dynamics. I will describe research aimed at gaining new insight into chromatin organization and dynamics, focused on the emerging model of Topologically-Associated Domains (TADs) – 50-100 kb-length regions of the genome that show unusually high contact probability. To date, approaches capable of linking the physical TAD structure to chromatin dynamics have been lacking. I will present a novel data acquisition and analysis pipeline and preliminary results: We label specific gene loci within a model cell organism, *S. pombe*, with lacO arrays bound by fluorescent LacI-GFP proteins. We then image cell populations over time on a widefield microscope. These movies are used to track the motions of loci for large populations of single cells. Next, we analyze the diffusive behavior of the chromatin loci by determining the mean-square displacement and velocity autocorrelation function. To further investigate the underlying biology that contributes to locus motion, we compare perturbations to a variety of biological inputs, including temperature, the cytoskeleton, and proteins that are hypothesized to have key roles in TAD formation.

*We acknowledge support from the NSF EFMA 1830904 and NSF GRFP.*

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**Tuesday, March 5, 2019 8:00 AM - 10:24 AM**

Session E66 DBIO GSNP GSOFT: Growth and Shapes 8CEC 261 - Karen Kasza, Columbia University - Tag(s): Focus

**8:00AM E66.00001: Tissue fracture and healing dynamics govern extreme plastic shape changes in the *Trichoplax adhaerens*, a simple, early divergent animal**

VIVEK N. PRAKASH (Presenter), Department of Bioengineering, Stanford University, MATTHEW S BULL, Department of Applied Physics, Stanford University, MANU PRAKASH, Department of Bioengineering, Stanford University — While epithelial tissues provide robust mechanical support, they also exhibit local ‘flows’ during morphogenesis and development. In adults, epithelial tissues undergo repeated stretching (e.g. lungs), and an inability to withstand stretch can cause fractures leading to diseases. Tissue fractures so far have been associated with negative consequences, and we do not yet know if fractures can be beneficial. Here, we have discovered a novel fracture-based mechanism by which epithelial tissues can exhibit fast and extreme plastic shape changes in a simple, early divergent animal - the *Trichoplax adhaerens* (phylum Placozoa). Fracture dynamics play a critical role in the lifecycle of Placozoans by dictating asexual reproduction by binary fission. Using innovative experimental in-toto imaging and tagging techniques, we quantitatively demonstrate that innate mechanical forces (shear and tension) arising from organismoal motility govern tissue fracture dynamics. These physiological fractures can either enlarge or ‘heal’ rapidly – leading to dramatic tissue shape change. These tissues exemplify a novel paradigm in soft-active-living-matter since they ‘fluidize’ by creating transient, local, stochastic ‘soft zones’ that exhibit glassy dynamics and a yield stress behavior in living animals.
8:12AM E66.00002: Cell Shape Dependent Motility During the Establishment of Tissue Structure  JOHN DEVANY
(Presenter), Physics, The University of Chicago, DANIEL SUSSMAN, M. LISA MANNING, Physics, Syracuse University, MARGARET
GARDEL, Physics, The University of Chicago — Mature epithelial tissues have distinct cellular architecture, which is maintained
despite externally applied forces, wounding, and cell division or death. Here we investigate how a model tissue develops and
maintains cellular structure by quantifying single cell dynamics and cell shape in newly formed MDCK monolayers. Over time cells in
the monolayer become increasingly hexagonal and arrest at a final structure resembling a mature epithelium. Throughout this process we observe glassy dynamics controlled by cell shape, as predicted by vertex models. Varying substrate stiffness causes monolayers to form and evolve with different cell density, but a similar relationship between cell shape and dynamics. This suggests the changes in cell density often observed in tissue development may not directly impact cell motility. We find that inhibiting regulators of the actin cytoskeleton cause monolayers to arrest with elongated cell shapes. Interestingly, across a diverse set of conditions we find a relationship between the final cell shapes and velocity correlation length which we explore in vertex models by including cell alignment coupling. Our results demonstrate that multicellular coordination of motility affects the regulation of cell shape and determination of final tissue structure.

8:24AM E66.00003: Relationship between cell force, shape, and motion in collective cell migration  AASHRITH
SARASWATHIBHATLA (Presenter), JACOB NOTBOHM, University of Wisconsin - Madison — In biological tissues, collective cell
groups exhibit a transition from a solid-like state, wherein cell positions remain fixed, to a fluid-like state, wherein cells flow freely and rearrange their positions with their neighbors. Recent theoretical models and experiments have demonstrated that this transition can be predicted by average cell shape, with cells having more elongated shapes and greater perimeters more easily sliding past their neighbors. Cell perimeter is hypothesized to be controlled by the cell surface tension which is an interplay of the cell’s cortical actomyosin contractility and cell-cell adhesions. However, the hypothesis is still experimentally unexplored. Here, we investigate the factors affecting cell perimeter, and we quantify the corresponding effects on collective migration. For this, we perturb actin and myosin-II in epithelial (MDCK) cell monolayers and study the effects on force, shape, and motion. We employ traction force microscopy, fluorescent imaging, and quantitative image analysis to measure forces, cell perimeters, and migration respectively. By combining these experimental measurements, our study provides experimental testing of the theoretical models and establishes new principles relating cell force, shape, and motion.

8:36AM E66.00004: Embryonic Inversion in Volvox carteri: The Flipping and Peeling of Elastic Lips  PIERRE HAAS
(Presenter), RAYMOND E GOLDSTEIN, Department of Applied Mathematics and Theoretical Physics, University of Cambridge — The
embryos of the green alga Volvox are spherical sheets of cells that turn themselves inside out at the close of their
development through a program of cell shape changes. This process of inversion is a simple model for the mathematical
analysis of morphogenesis [1], yet shares many features with processes such as gastrulation in higher organisms. In Volvox
carteri, inversion starts with four lips opening up at the anterior pole of the cell sheet, flipping over and peeling back to
invert the embryo. Experimental studies have revealed that inversion in V. carteri is arrested if some cell shape changes
are inhibited, but the mechanical basis for these observations has remained unclear. We analyse the mechanics of this
inversion by deriving an averaged elastic theory for these lips and we interpret the experimental observations in terms of
the mechanics and evolution of inversion [2].


8:48AM E66.00003: Morphogenesis of termite mounds*  ALEXANDER HEYDE (Presenter), Harvard University, SAMUEL A
OCKO, Stanford University, L MAHADEVAN, Harvard University — Several species of termites across Africa, Asia, Australia, and
South America collectively construct meter-sized porous mound structures that regulate mound temperature, humidity,
and gas concentrations. These mounds display varied yet distinctive morphologies that range widely in size and shape. To
explain this morphological diversity, we introduce a mathematical model that couples environmental physics to insect
behavior: the advection and diffusion of heat and pheromones through a porous medium are modified by the mound
geometry and in turn modify that geometry through a minimal characterization of termite behavior. Our model captures
the range of naturally observed mound shapes in terms of a minimal parameter set and suggests several simple scaling
laws for mound morphology and construction time. An elaboration of our model that incorporates 3D internal nest
structure gives rise to regularly spaced floors and pillars, as well as the spontaneous generation of helical ramps, as have
been observed in scanned mounds across termite species. This framework makes testable hypotheses for the response of
mound morphology to external temperature oscillations and internal odors.

*This material is based on work supported by NSF Grant DGE 1144152 (A.H.) and the MacArthur Foundation (L.M.).
9:00AM E66.00006: Pattern Selection in Brine Shrimp Swarms  ANDREA WELSH (Presenter), FLAVIO FENTON, Georgia Institute of Technology — Swarming is a ubiquitous self-organization phenomenon which occurs in many biological systems such as flocks of bird and insect, schools of fish, and collections of bacteria. This sort of behavior emerges spontaneously, arising without any sort of centralized control or leadership. Many crustaceans such as brine shrimp produce swarms, in which individuals cluster together rather than spreading out uniformly in their environment. The size and distribution of these swarms are governed by local interactions between individuals. We will discuss the three-dimensional patterns that can be observed in brine shrimp swarms, specifically of the Great Salt Lake strain of Artemia franciscana, at high concentration. These patterns can be easily observed with simple tabletop experiments; however, the causes of these patterns are unknown. We experimentally test the effects of certain environmental conditions on the development of these swarms. We then develop a model an agent based model of shrimp which yields the same sort of spatial patterns as those that are observed. The model reproduces the basic length and times scales of the patterns, the type patterns selected, and the stability of those patterns.

9:12AM E66.00007: Social insect aggregations as inspiration for mesoscopic active matter*  SHANKAR LALITHA SRIDHAR (Presenter), TONG SHEN, KANGHYEON KOO, Mechanical Engineering, University of Colorado, Boulder, ROBERT JAMES WAGNER, Material Science and Engineering Program, University of Colorado Boulder, FRANCK J VERNEREY, Mechanical Engineering, University of Colorado, Boulder — Social insects such as ants and bees exhibit extraordinary co-operative behavior to form aggregations and are often called super-organisms due to their ability to achieve complex structures and functionalities. Individual interactions include attachment and detachment of legs, bodies and mandibles that result in active re-organization of the network that can drastically transform the aggregation from a solid-like to fluid-like material and vice-versa. As the interactions in these aggregations operate in the mesoscale, they are easily observable and are attractive candidates to emulate in synthetic systems. Drawing inspiration from insects, we have designed a synthetic mesoscopic aggregation in our lab made of particles resembling mini gears and interact through magnetic and shear forces to self-organize into a network. The aggregation is infused with leader particles containing battery powered motors that induce motion and activity in the entire network. The aggregation behavior can be tuned by varying the magnetic strength, motor activity of leaders and their positions and diversity in particle size. Using statistical mechanics, we show that the aggregation can be programmed to achieve specific shapes and even transport solid metal objects through them.

*NSF Career Award 1350090

9:24AM E66.00008: Surface-mediated cell alignment using polymerized liquid crystal nanostructures*  GRETA BABAKHANOVA (Presenter), JESS KRIEGER, MIN-HO KIM, O D LAVRENTOVICH, Kent State University — The microenvironment of cells affects their morphology and alignment. The physical characteristics of a cell are of extreme importance as the function and viability of a cell is closely linked to its morphology. In this work, we demonstrate the control of the orientation of cultured human dermal fibroblasts (hDFs) using polymerized liquid crystal (LC) periodic nano- and microstructures. The desired pattern is created by controlling the boundary conditions of the LC molecules which exhibit a smectic-A phase. Doping the LC with a small amount of reactive monomers allowed us to fix the molecular orientation and preserve the nano- and microstructures after photopolymerization and subsequent washing. The plated hDFs respond to the polymerized LC topography by changing their shape and aligning their long axis parallel to the patterned grooves. Though fibronectin treatment promotes proliferation of the cells, when comparing the hDFs grown on fibronectin and fibronectin-free patterned surfaces, the cells on fibronectin-free surface show improved alignment and elongation. The demonstrated LC-based surfaces will potentially find practical applications to preprogram cells to form specific kinds of tissues.

*The work was supported by Office of Sciences, DOE, grant DE-SC0019105.
9:36AM E66.00009: Fluid to solid transition in muscles*  KHOI NGUYEN (Presenter), NEELIMA SHARMA, MADHUSUDHAN VENKADESAN, Yale Univ — Roboticists have long sought to develop actuators that emulate the performance of muscle. These have mostly centered on the power and force capacity of muscle and more recently on muscle’s stiffness and damping characteristics. However, a critical aspect that remains missing in muscle-inspired actuators, and also poorly studied in muscle, is an activation-dependent fluid-to-solid transition in muscle’s mechanical response. For example, a highly activated muscle resembles a solid-like material that maintains posture and provides stiffness, whereas muscle under low activation yields like a fluid without much resistance against rapid motions. Understanding how this transition may arise in muscle could guide the development of new muscle-like actuators that use similar principles as muscle to achieve a fluid-to-solid transition. Current understanding of the sarcomere is based on mean-field models of Huxley-based crossbridge cycles. We find that models of varying complexity, from two- to five-state models of actomyosin, all fail to capture the fluid-to-solid transition. In analogy with jamming transitions in disordered solids, we postulate potential nonequilibrium dynamics that may underlie the fluid-to-solid transition in muscle.

*Supported by NIH Training Grant, T32EB019941

9:48AM E66.00010: A web-based application of the Cellular Force-Inference Toolkit (CellFIT)*  XIAOJIA XU (Presenter), W. TYLER MCCLEERY, SHANE HUTSON, Physics and Astronomy, Vanderbilt University — Given an image of an epithelial cell sheet, CellFIT can infer cellular forces by segmenting the image into individual cells, constructing equilibrium equations for the points where cells meet at triple junctions, and finding a least-squares solution for the tensions at cell-cell interfaces. Similarly, cellular pressures can be estimated by constructing Laplace equations that relate the edge tensions, curvatures and cellular pressure differences. Despite these capabilities, the accessibility of CellFIT to scientists of all backgrounds is not yet optimized. We will present an updated web-based application of CellFIT that allows users to access the software from a browser. The updated version includes improved error handling and the implementation of additional functionality for reading and processing image stacks. Application of the web-based CellFIT to time-resolved image stacks of wound healing in Drosophila epithelia demonstrates spatial and temporal variations in cellular forces as the wounds close.

*Supported by NIH/NIGMS grant 1R01GM130130.

10:00AM E66.00011: Mechanical and Biochemical Simulations of Atherosclerosis*  NAVID MOHAMMAD MIRZAEI (Presenter), PAK-WING FOK, University of Delaware — Atherosclerosis is a disease considered to be one of the leading causes of death. Understanding the behavior and dynamics of the vessel wall before and after atherosclerosis has been a motivation for many studies. We investigate this phenomenon as a combination of mechanical deformation of the vessel wall along with the cell and chemical dynamics that happen inside of it. We consider the vessel wall as a growing hyperelastic material with three layers, each having a different set of mechanical properties. To describe tissue growth we use morphoelasticity as the mathematical framework. To include the stiffening effect of collagen fibers we employ a Holzapfel-Gasser-Ogden anisotropic strain energy function. In addition, we explore the distribution of oxidized lipids, macrophages, foam cells, oxygen and necrotic cells in the intima at each growth step via a system of PDEs. All numerical simulations are carried out via the finite element method on the FENICS framework. Altogether, this allows us to observe intimal thickening as a result of vessel growth along with histological changes within the wall such as the development of necrotic zones. Our simulations show results similar to the images acquired from ultrasounds scans.

*DE-CTR ShoRe pilot grant (NIGMS IDeA U54-GM104941)

10:12AM E66.00012: Pattern formation and ecological feedback in antigen-immunity co-evolution  HONGDA JIANG (Presenter), SHENSEN WANG, California State University, Los Angeles — Immune systems manifest self-tolerance and respond to foreign invaders. Despite our knowledge of the molecular mechanisms involved in immune response and tolerance, an intuitive understanding of the immune-antigen relationship that determines the overall efficacy of immune control is lacking. We suggest that both features of natural immunity can be described by immune-antigen co-evolution. Extending ecological insights, we consider predator-prey interactions between immune cells and foreign or self antigen that can reach a dynamic balance through mutual adaptation. We present a minimal model of the co-evolutionary dynamics as a pair of reaction-diffusion processes in a phenotypic shape space, coupled by reciprocal interactions with finite cross-reactivity. We find that asymmetry in cross-reactivity can lead to pattern formation, indicating the emergence of antigen niches. We show in a phase diagram the regimes of balance breaking caused by pattern-forming instability: antigen extinction occurs as a result of co-localized population densities, whereas antigen escape follows the formation of alternating patterns under immune homeostasis. Thus, it is important to consider the feedback between population dynamics and pattern formation in understanding immune function and abnormality.
8:00AM E67.00001: Complexity and Fly Swarms*  TROY TAYLOR (Presenter), JOELLE L MURRAY, Linfield College — A system is considered complex if it is composed of individual parts that abide by a set of simple rules while the system, as a whole, exhibits more elaborate, unexpected properties. The motivation for studying complexity stems from the fact that it is a feature of many different systems. We are particularly interested in fly swarms and the possible complex properties that swarms exhibit, arising from individual fly interactions. To better understand the nature of complexity exhibited by fly swarms, a simple stochastic fly swarm model was created to investigate the relationship between the average radius of the swarm and the number of individuals within it, as experimental data shows a power-law scaling of the number of flies to the average radius. In addition, the model will be used to explore the difference between swarming and non-swarming behavior.

*Linfield College Student-Faculty Collaborative Research Grant

8:12AM E67.00002: Quasiperiodic Earthquake Events in an Olami-Feder-Christensen Model  JACOB OWENS (Presenter), RACHELE DOMINGUEZ, Randolph - Macon College — We simulated an earthquake fault system using a variation of the OFC cellular automata model. The fault is represented by a 2D lattice structure wherein each site holds some amount of stress. Our model increases the stress on the system in a more realistic way and allows multiple sites to fail simultaneously. The model generates data that produces Gutenberg-Richter scaling, which is consistent with real earth data. Additionally, the model incorporates “asperity” sites into the lattice; these asperities have a much higher failure threshold relative to other sites in the lattice. The introduction of asperities to the system generates a characteristic period according to which we observe very large events. These main shocks are preceded by a gradually increasing number of large events (foreshocks) and followed by a gradually decreasing number of large events (aftershocks). By introducing multiple distinct failure thresholds for the asperity sites, we were able to identify characteristic periods related to the respective failure thresholds. In varying these parameters we can control the periodicity of large earthquake events. These results suggest that the spatio-temporal clustering observed in real seismic data is related to the physical structure of the fault system involved.

8:24AM E67.00003: Quantum Coherence Enhanced Phototherapy: A Step Towards Quantum Medicine  ZACHARY WITHERS (Presenter), DMITRI VORONINE, University of South Florida — Irradiation and phototherapy involves the application of electromagnetic radiation to infected or tumorous tissues. Historically, radiation dosage, energy, and specificity have been of significant research areas, but with the evolution of quantum optics, plasmonics, and nanotechnology new devices and enhancement schemes are being realized. We propose the use of aluminum SPASERs as an ultraviolet phototherapeutic treatment mechanism and discuss the role quantum coherence plays in treatment enhancement, efficiency, effectiveness, and specificity. We further discuss optimization of temporal nonlinear regimes and potential application of laser pulse shaping.

8:36AM E67.00004: Protein-Based Drug Delivery Nanoparticles*  TY NAQUIN (Presenter), Department of Physics and Chemistry, Department of Chemical and Biomedical Engineering, Troy University, Cleveland State University, KIRIL STRELETZKY, Department of Physics, Cleveland State University — Elastin-like polypeptides (ELPs) are a class of biopolymers that undergo a reversible phase transition occurring at a transition temperature. Recently, six-armed star polymers (G10 and G19) have been synthesized with arms composed of ELPs, namely repeats of the amino acid sequence GVGVP. Each arm of the G10 contains 10 repeats of this sequence, whereas the G19 contains 19 repeats. Above a certain temperature, these proteins aggregate due to the hydrophobic nature of ELP chains. They form specific aggregation structures, which may prove suitable for drug delivery applications. The proteins may collapse into individual molecules or assemble into nanoparticles that could be used to transport and protect slightly hydrophobic drug compounds. We have characterized the solution properties of G10 and G19. The transition temperatures of the proteins were measured using spectrophotometry for various protein concentrations, salt concentrations, and pH values. The samples were also investigated using light scattering. In particular, dynamic light scattering was used to probe the size of the aggregates above and below the transition temperature. Further measurements illustrate the effects of salt concentration and pH on particle dimensions.

*This work was supported by NSF REU award #1659641.
Biocompatible Exchange-Coupled Magnetic Nanoparticles for Advanced Hyperthermia*

ELIZABETH FULLER (Presenter), Ohio State University, JOSHUA L ROBLES, MANH-HUONG PHAN, HARIHARAN SRIKANTH, Physics, University of South Florida — Exchange-coupled bimagnetic nanoparticles describe a potential for advanced hyperthermia treatment of cancer with an increased heating capability. The feasibility of magnetic hyperthermia in humans warrants magnetic nanoparticles (MNPs) with an Fe3O4 shell to meet biocompatibility standards. In our study, we compare the heating efficiency and magnetic properties of CoFe2O4@Fe3O4 MNPs with the inverse system, Fe3O4@CoFe2O4. We calculate the Specific Absorption Rate (SAR) values of both nanoparticle systems when dispersed in hexane, water, and agar in addition to proper morphological and magnetic characterization using TEM, XRD, and DC Magnetometry. At 80mT, we report SAR values of our CoFe2O4@Fe3O4 MNPs to be 62% greater in water and 2% greater in agar than the inverse MNPs. We observe a significant coercive field of the CoFe2O4@Fe3O4 MNPs when taking DC Magnetometry measurements at 10K, to which we attribute its superior heating power over the inverse system in media that limit Brownian movement. We anticipate an increase in saturation magnetization of the CoFe2O4@Fe3O4 system with negligible effect on coercive field with increased Fe3O4 shell thickness.

*Funding for this research was provided by the NSF REU Grant No. 1560090.

Computer simulation of a finite-time Carnot engine working under ecological conditions

DAVID A. ROJAS-GAMBOA (Presenter), JUAN I. RODRÍGUEZ, Escuela Superior de Física y Matemáticas, Instituto Politécnico Nacional, JULIAN GONZALEZ-AYALA, Departamento de Física Aplicada, Universidad de Salamanca, F. ANGULO-BROWN, Escuela Superior de Física y Matemáticas, Instituto Politécnico Nacional — In the context of finite-time thermodynamics some optimization criteria for heat engines have been proposed, such as the maximum power [1] or the ecological criterion [2], being the later the best compromise between high power output and low entropy production. In order to study these criteria, we present a molecular dynamics simulation of a hard-disk gas performing a finite-time cyclic process that is near to a Carnot one. While previous works analysed the maximum power regime [3], in the present work we discuss the ecological case. When the gas is in contact with a stochastic thermal wall (or heat reservoir), we show that the speeds distribution is well described by a Maxwell-Boltzmann function with an effective temperature that is lower/higher than the source/sink temperature (as in the endoreversible model). By obtaining the power output and total entropy production, the ecological efficiency of such an engine was computed via molecular simulations for the first time, showing good agreement with analytical approaches. Our results were reported in D. A. Rojas-Gamboa et al., Phys. Rev. E 98, 022130 (2018).


Higher-Order Numerical Solutions of the Quarter Car Suspension Model

ALBERT MATERDEY (Presenter), Roxbury Community College — Applying Newton’s second law to the sprung and un-sprung masses, the Quarter Car Suspension mathematical model was derived as a system of two coupled second-order differential equations. This system was rearranged into a system of four coupled first-order differential equations. Algorithms were derived to solve this system in the time domain using the Euler’s, second-order Runge-Kutta , and fourth-order Runge-Kutta methods. For larger values of the suspension and tire spring constants, for example in heavier vehicles with large tires such as utility, crane, and backhoe trucks, higher order algorithms are essential to describe the high-frequency oscillations of the vehicle suspension system.

Synchronization of Mid-Frequency Engines for Energy Harvesting.*

SEO YOUNG AHN (Presenter), University of Utah — Thermoacoustic engines convert heat to electricity by producing sound, which generates electricity by a piezo electric device. Multi-device arrays of such mid-frequency (2.5 kHz) thermoacoustic energy converters have been studied in order to raise the power output. Devices with 2 and 3 engines were investigated, eventually leading up to 6 engines. Being self-sustained oscillators with random phase, their synchronizations are crucial in attaining maximum power. Indeed, synchronization was observed; coupling between the engines is attributed to their radiation impedance and reflections from the acoustic cavity supporting them. The observed increased output levels substantiate synchronization through the absence of beats between engines, Fast Fourier Transforms, where a peak due to a common frequency is observed, and resultant common, lowered frequency. A benefit of the array is the reduction of onset temperature such as 50°C for 3 engines, and similarly onset times for oscillations.

*University of Utah Department of Physics and Astronomy
University of Utah Undergraduate Research Opportunities Program
Wearable textile-based energy harvester designed for human motion.*

REBECA GURROLA (Presenter), Physics and Mathematics, St. Mary's University, JANNA EAVES, CARY L PINT, Mechanical Engineering, Vanderbilt University — While there are many different methods of generating sustainable energy, small quantities of energy otherwise wasted in the pursuit of everyday activities are often overlooked. Recently, electrochemical energy harvesters joined the ranks of piezoelectric and triboelectric harvesters to convert mechanical energy into electrical energy. Here, we use materials with mechanochemical response to seamlessly integrate motion harvesting into textiles for wearable applications.

This study presents a novel class of safe and non-toxic “smart” energy harvesters which can be activated via sweat, simulated here by a solution of NaCl. The harvester comprised of a sodium tin alloy on copper fabric exploits ambient motion at frequencies of 0.1 Hz. In bend tests, the harvester generates a peak power of ~36.4 μW/cm² and energy of ~131.1μJ/cm² with each bend. Additionally, it is sensitive to changes in salt concentration, suggesting applications in hydration-monitoring. These results emphasize the exciting possibilities for a new class of wearable harvesters.

*We gratefully acknowledge the National Science Foundation under the grant numbers of 1560414 and 1400424.

Increasing the Number of Sides of a Luminescent Solar Concentrator can Increase its Power Output*

BAILEY HOPKINS (Presenter), BRUCE PAUL WITTMERSHAUS, Penn State Erie — Luminescent Solar Concentrators (LSCs) are fluorescent sheets of glass or plastic that absorb sunlight and concentrate their fluorescence using total internal reflection onto a small area of photovoltaic solar cells for energy conversion. LSCs have the potential to generate electricity at a lower cost than standard solar panels. Current LSCs are designed as squares. This shape can cause non-uniform illumination along its edges leading to current mismatch in the solar cells resulting in loss of power output. We present results showing that changing the LSC’s shape closer to that of a circle decreases current mismatch by improving the uniformity of illumination.

*This material is based upon work supported by the National Science Foundation under Grant Number NSF-ECCS-1306157 and a Penn State Behrend Undergraduate Research Grant.

Pretreatment of rice straw for enhancing fermentable sugar yield using a high-pressure reactor

PRATHAM GUPTA (Presenter), BAHIRU TSEGAYE, CHANDRAJIT BALOMAJUMDER, Chemical Engineering, Indian Institute of Technology Roorkee — Rice straw has proved to be a potential renewable energy source due to its high polysaccharide contents and abundance availability. Fermentable sugars are easily obtained on hydrolysing rice straw using different pretreatment techniques. In this study, organosolv was used to pretreat rice straw in high-pressure autoclave reactor, under different conditions, for the removal of lignin and release of trapped polysaccharides. The composition of rice straw was analyzed as per National Renewable Energy Laboratory (NREL) guidelines. The temperature was varied as 120, 140 and 160 degree Centigrade and the exposure time was varied as 15, 30 and 60 minutes. The amount of sugar and lignin were greatly affected by temperature and time. It was found that sugar yield was maximum at 140 degree Centigrade and 15 minutes. At this pretreatment condition, it was observed that almost all of the hemicellulose was solubilized and 73% and of lignin was removed and 82% cellulose was released from the biomass. The removal of the high amount of lignin facilitates the release of the cellulose from the biomass matrix. Overall, this study showed the possibility of a high-pressure reactor for effective removal of lignin, which enhances the yield of fermentable sugars.

Thermal Expansion in 3D Printing Materials for Interferometric Devices

THEODORE MORIN (Presenter), LUISA VELASCO, CATHERINE HAND, MICHAEL EWNETU, University of Dallas — 3D printed optomechanics offers a cheaper alternative to conventional machined parts with the potential for customization. Examples include the kinetic mounts, precise linear movement, and integrating sphere described by Salazar-Serrano et al (2017). When considering the use of 3D printed parts to make high precision interferometric instruments, thermal expansion becomes an important consideration. We present an inexpensive interferometric measurement of thermal expansion in 3D printed materials. Tests are performed with ABS and PLA plastics. We also explore variation with different colors of the plastics and different printing conditions. Finally, we present a design for a low-cost, 3D printed scanning Fabry-Perot interferometer with minimal thermal sensitivity and an anticipated finesse of about 50.
10:24AM E67.00013: Electrode Coatings for Neurostimulation and Cardiac Pacing Applications*  
SIERRA DUTKO (Presenter), ANTHONY VALENTI, NATALIE PAGE, ROBERT LOWE, RHANDY PALADINES, JEFFREY HETTINGER, Physics and Astronomy, Rowan University — Neurostimulation and cardiac pacing electrodes have many applications each requiring biocompatibility and the ability to exchange charge between the underlying metallic electrode and the ionic fluid surrounding it. The trend toward smaller electrodes as well as higher current applications has resulted in the need for improved charge transfer. With this goal, cubic nitride coatings with columnar microstructure have been added to the electrodes using reactive magnetron sputtering in a nitrogen rich atmosphere. These coatings which provide capacitive coupling between the electrode and the biological solutions increase the surface area improving the required charge transfer. Coating performance is measured electrochemically using cyclic voltammetry with the coated metal as the working electrode, a platinum coiled wire as the counter electrode, and phosphate buffered saline as the electrolyte. We report on the thickness dependence of the coating performance and delineate important parameters influencing this performance.

*This research has been funded in part by a grant from New Jersey Health Foundation.

10:36AM E67.00014: Hygroscopic Nature of Solution Processed Al2O3 Thin Film Dielectric and Impact on Electrical Characteristics*  
JAMES TRAN (Presenter), TREY B DAUNIS, JULIA WAN-PING HSU, University of Texas at Dallas — Metal oxides are a good candidate for gate dielectrics because of their high dielectric constant and low leakage current. Solution deposition is a favorable method for thin film fabrication due to its low cost and high throughput. Here, we compare the property and stability of solution-processed Al2O3 and ZrO2 films. Fourier transform infrared spectroscopy (FTIR) and electrical characterization reveal that Al2O3 absorbs moisture from air, while ZrO2 remains stable with no moisture gain. This conclusion is established by comparing Al2O3, ZrO2, and bilayers of Al2O3/ZrO2 and ZrO2/Al2O3. FTIR spectra show increased intensity in the water -OH region (3700-2500 cm⁻¹) when Al2O3 is exposed to air or purposely soaked in water. The change in surface contact potential indicates that the adsorbed water molecules’ dipoles point away from the surface. Effects of the moisture gain on electrical characteristics are studied with metal-insulator-metal capacitors and field effect transistors. Absorption of water in Al2O3 results in higher capacitance and dissipation at low frequencies and show a counter-clockwise hysteresis in transistor drain current vs. gate voltage curves.

*This work is supported by the National Science Foundation (NSF DMR-1305893) and the University of Texas at Dallas.

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E68 APS/SPS: Undergraduate Research V  
BCEC 051 - Brad Conrad, American Institute of Physics - Tag(s):
Undergraduate

8:00AM E68.00001: Golf ball simulation and aerodynamic characteristics*  
EDUARDO RIVERA (Presenter), MARCO FATUZZO, Xavier University — The flight trajectory of a golf ball depends upon the net effect of gravity, lift, and drag. The latter two forces result from the complex interaction between the ball surface and the air through which it moves, and are characterized in terms of drag and lift coefficients that depend upon the geometry, speed and spin rate of the ball as well as the density of the air. Our research focused on using both wind-tunnel results and ANSYS software analysis to obtain reliable lift and drag coefficients for different flight condition and ball dimple-pattern, and use the results to inform a robust flight simulation MATLAB program.

*John Hauck Foundation Summer Research Program
Waves crashing in the ocean generate large numbers of bubbles, which burst and can produce jets that break up into sea spray aerosol droplets. Wind can carry these aerosol drops into the atmosphere and seed cloud formation. Much of the research on bursting bubbles focuses on isolated bubbles; however, bubbles from breaking waves normally exist in close proximity to other bubbles. We therefore investigate how the presence of a neighboring bubble affects jet drop formation from a bursting bubble. Combining high-speed imaging experiments with numerical simulations, we show that a bubble bursting near another bubble ejects drops angled away from the neighbor bubble. We relate this ejection angle to the asymmetry in the collapsing bubble cavity and explore how bubble separation and bubble size affect the process. The observed effects could eventually help to improve aerosol production models and clarify the accuracy of previous assumptions.

*National Science Foundation Award #1351466

The printability regimes in inkjet bioprinting are the sets of printing conditions described using the , in which a stable . Previous experimental and simulation works of printability have mainly focused on millimeter-sized nozzles, while it is uncertain whether their conclusions can be applied to micrometer-sized nozzles. Because the capillary effect is significantly enhanced in the micrometer scale, the printability regimes in the micrometer scale are likely to differ greatly from that in the millimeter scale. In this study, the printability regimes in the micrometer scale are calibrated through three-dimensional computational fluid dynamics simulations. Our works are expected to be critically helpful in design of inkjet bioprinting with micrometer-sized nozzles.

Nanoparticles have been extremely useful in the treatment of diseases, such as cancer and bacterial infections, as well as for cleaning up pollutants like oil or minerals from water. Since it is hard to image any water-based solution in electron microscope, the behavior of charged nanoparticles in water is not well understood. This has been a barrier to the development of applications for nanoparticles.

The focus of the work presented here is to examine charge screening of positive and negatively charged gold nanoparticles (+/- AuNP) in water with different concentrations of salt. Aggregation and flocculation will be studied using a combination of transmission electron microscopy (TEM) and scanning transmission electron microscope (STEM), using liquid cells fabricated from nanoparticles in various solutions encapsulated by graphene. The degree of aggregation is determined by measuring the radial distribution function (RDF) of a field of particles in an image. RDF is directly related to the surface charges of nanoparticles. This information yields a much better understanding of the aggregation behavior of nanoparticles in water.

*Supported by the Chancellor's Undergraduate Research Award. This work made use of Electron Microscopy Services at Research Resources Center, UIC.

We seek to understand the dynamics of micro-swimmers by quantifying the stochastic forces generated by their motion. We are currently working with Chlamydomonas Reinhardtii—a green algae commonly used to study microscopic locomotion. Our approach is to use optical tweezers and a direct force calibration known as the photon momentum method (PMM) to measure micro-swimmer forces. The power spectral density (PSD) of the force dynamics is analyzed, providing information about the frequency content of the force signals. A simple stochastic model based on the generalized Langevin equation predicts the power spectral density to have a Lorentzian-type curvature. We compare our experimental data to the theoretical model to test if the model can predict our experimentally measured PSD. This approach allows the calculation of thermodynamic quantities such as work, power, efficiency, etc. to describe the microscopic motion. Our analysis seeks to apply concepts from stochastic thermodynamics to understand micro-swimmer dynamics.

*CSUF Dan Black Fellowship
9:00AM E68.00006: Pattern Formation in Driven Particulate Suspensions  WEI LU (Presenter), PRASHANT SHARMA, Suffolk University — Systems that are driven by energy from external sources are ubiquitous, and the rich phenomenology they display (e.g., ordered phases and pattern formation of bacteria, or nanoparticles in a fluid) is described by physical models that do not rely on conventional equilibrium physics. We study theoretically and computationally a class of such active-matter models with self-propelled motion and interactions and classify the resulting non-equilibrium ordered states using techniques from statistical physics.

9:12AM E68.00007: Density Driven Instability during Proppant Injection in a Hele-Shaw Cell*  RAM SUDHIR SHARMA (Presenter), RAUSAN JEWEL, ARSHAD KUDROLLI, Department of Physics, Clark University — We report an experimental investigation of granular matter suspended in a liquid injected between two parallel plates with a constant separation distance called a Hele-Shaw cell. These experiments are motivated by proppant injection in hydraulic fracturing of shale used to extract hydrocarbons. The cell is fully filled in with a similar ambient fluid to avoid capillary effects and pinning and dipinning dynamics of the front. We image the dynamics and deposition of the grains as they spread inside the cell as a function of injection rate and volume fraction of the grains. A finger-like instability is observed for sufficiently density difference between the particles and the ambient fluid. We will discuss the observed phase diagram as a function of the injection-rate of the fluid, its packing fraction and time. We demonstrate a correlation between the timescale for the sedimentation of the particles and for the onset of fingers as well as subsequent bifurcations. Corresponding length scales are studied as well, i.e. the finger lengths and widths as a function of the packing fraction of the injected fluid. Early analysis suggest that for a fixed packing fraction, regardless of the flow-rate, the sedimentation time determines the onset of the instability.

*Supported by DOE DE-SC0010274

9:24AM E68.00008: The Missing Model of the Liquid State, from Crystalline Solid State to Random Gas State  TIANHUI JIE (Presenter), Institution applied — Liquid state of materials has not had a successful physics-based model, for example, water, the most abundant and life-dependent, although the components of a successful model have been well-developed and successfully employed in applications, for examples, semiconductor physics-based solid-state electronics in communication (stereo, TV, PC, cell phone) and control (simple to complex robotics). The two missed culprits in physics are the long range order in the crystalline solid state which continues persistently into the higher kinetic energy fluidic liquid state, and also the dynamics of isolated molecules in a random ensemble of the gas phase at higher kinetic energies which continue persistently into the lower kinetic energy fluidic liquid state. The recent success of this new approach of combining the solid-state and gas-state to model the liquid state of pure water (such as the 80+ mega-ohm pure drinking water sold at the grocery stores for 75 cents) is described and extended to all the liquid states of materials in this presentation. [1] Binbin Jie, Tianhui Jie and Chihtang Sah, Studies of Water VI. Journal of Semiconductors, 2018, 39(11):111001. [2] Bin Jie, Tianhui Jie, Chih-Tang Sah, submitted to APS March Meeting 2019.

9:36AM E68.00009: Exploring self-organized criticality in driven cold gases  KAI KLOCKE (Presenter), GIL REFAEL, MICHAEL BUCHHOLD, Department of Physics and Institute for Quantum Information and Matter, California Institute of Technology — Recent experiments with strongly interacting, driven Rydberg ensembles have unambiguously demonstrated aspects of self-organized criticality (SOC) in the dynamics of the Rydberg pseudospins. Such experiments present a means for precise control of the microscopics from which SOC emerges and offer a new playground for the exploration of SOC with cold atoms. Here we simulate the dynamics of such Rydberg ensembles through numerical integration of the corresponding effective field theory. In particular, we discuss an experimentally feasible loading scheme by which the prototypical avalanche dynamics can be maintained and controlled. This gives access to three distinct dynamical regimes: i) a subcritical regime of periodically occurring avalanches, ii) an extended SOC regime featuring scale invariance and fractal real-space structures, and iii) a supercritical regime with constant avalanche activity. This relates Rydberg atom dynamics with SOC in neural networks, where similar scenarios have been observed. We sharpen this connection by analyzing the dependence of SOC on the size and dimensionality of the ensembles.

9:48AM E68.00010: Head-on Collisions of Vortex Rings with Solid Bodies*  MARY AGAJANIAN (Presenter), RYAN MCKEOWN, SHMUEL RUBINSTEIN, Harvard University — The head-on collision of vortex rings with slender wires creates complex vortex reconnection and breakdown behavior. Specifically, the interaction results in the rapid emergence of secondary vortical structures. These structures suggest that vortex lines are being created in the fluid; however, as, in the finite Reynolds number regime, vorticity must either close in on itself or begin or end on a boundary, the origin of the secondary structures is not well understood. We experimentally investigate the emergence and evolution of this behavior by varying the vortex ring dyeing technique, geometry of the wire, and Reynolds number. This allows us to characterize the interaction of the vortex core with the secondary vortical structures.

*Supported by DOE DE-SC0010274
10:00AM E68.00011: Nonequilibrium power-law correlations in a system of tight-binding fermions with gapped spectrum  
JOSEPH GODOY (Presenter), JARRETT LANCASTER, High Point University — A quantum quench is explored in a system of tight-binding fermions in which a smooth, linearly-varying chemical potential is rapidly switched off at the same time a staggered chemical potential is turned on. The initial particle density profile is a “domain wall” shape and evolves unitarily under a Hamiltonian which possesses a gap in its spectrum. In the ground-state of the Hamiltonian generating time evolution, correlations decay exponentially with distance, while in this non-equilibrium setting, a steady state quickly forms within a central subsystem in which power-law correlations persist. The long-time average of the particle density, current and various correlation functions are shown to be obtainable from an effective momentum distribution which depends on the details of the Hamiltonian and the initial state. Intriguing similarities between the results in this model of free fermions and similar results obtained within interacting systems are discussed.

10:12AM E68.00012: Stochastic Simulations of Single-Cell Circadian Oscillations in Arabidopsis thaliana*  
YIAN XU (Presenter), ORRIN ABRAHAM BRUN SHINDELL, Trinity University — Chemical oscillations are a universal feature of living systems. In plants, for example, the daily periodicity of many functions is regulated by the oscillatory expression of circadian gene networks present in each cell. We analyze the chemically reacting system that controls the circadian rhythms in cells of the plant Arabidopsis thaliana by numerically solving a continuous kinetic model whose parameters were deduced from experimental data [1]. We find that the model exhibits slowly decaying oscillations and is situated near a Hopf bifurcation in parameter space. Then we implement Gillespie’s Stochastic Simulation Algorithm to simulate the system at the single-cell level and account for random fluctuations in particle numbers [2]. Finally, we comment on the relationship between the two approaches and on the possible biological significance of the model’s mathematical features.


*This work was supported by Murchison Fellowship from Trinity University.

10:24AM E68.00013: NSF IRES: Exploring the Effects of Single Point Mutations of Arabidopsis thaliana Cryptochrome 1 (AtCry1), a Plant Protein Involved in Blue Light Response*  
LILLIAN HAERR (Presenter), EMILY SHOCKLEY, JOHN STERNEN, JOHN KAVANAGH, JUSTIN J LINK, STEPHEN MILLS, DOROTHY ENGLE, Xavier University, MARGARET AHMAD, Sorbonne University — Cryptochromes are proteins that act as photoreceptors regulating development and the circadian clock in plants. It has been shown that mutations in cryptochromes, specifically AtCry1, alter the functionality of the proteins. These flavoprotein photoreceptors mediate growth, leaf expansion, and floral initiation. They act through blue-light dependent photoreduction of flavin adenine dinucleotide (FAD) via an electron transport chain. In the dark state, the flavin is oxidized and when stimulated with blue light, it is semi-reduced and in the active state which arguably causes protein conformational change and signal transduction. This photoreduction of FAD can be tracked using visible light absorption as the spectra of the oxidized and semi-reduced forms differ. Specifically, the oxidized FAD has an absorption at 450nm and once semi-reduced, the 450nm peak decreases and there is an increase in absorption at 550nm. Mutants studied show significant difference in appearance and plant growth in blue light when compared to native plants. Differences in absorption between mutant and native proteins were used to analyze potential differences in the photochemistry involved in plant growth.

*This material is based upon work supported by the National Science Foundation under Grant No.1658640.

10:36AM E68.00014: Membrane Simulations with Amyloid Beta*  
TYLER JENKINS (Presenter), GUOPING ZHANG, Indiana State University — Amyloid Beta is a misformed protein that is a key characteristic of Alzheimer’s disease. A plethora of research has been carried out to determine the structure of amyloid beta and mechanisms behind the plaque formation. We model 1-3 amyloid beta peptides in 3 different configurations inside a 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) membrane in order to simulate a key step in the formation of amyloid plaques: the formation of pores in the cell wall of neurons due to amyloid beta. Our preliminary findings identify a configuration of amyloid beta in the membrane that appears to promote the formation of pores.

*US Department of Energy, contract no. DE-FG02-06ER46304
Focused Ultrasound as a Replacement for Endodontic Therapy

TALISI MEYER (Presenter), Chemistry and Physics, Simmons College, PHILLIP JASON WHITE, Radiology, Brigham and Women, MICHAEL JORDAN, Chemistry and Physics, Simmons College — Focused ultrasound has exhibited promising results as a therapeutic modality in its ability to minimize the invasiveness of a number of medical treatments that are physically and mentally traumatic to the patient. We propose the investigation of its use for non-invasive endodontic therapy (a.k.a. a “root canal”), with the ultimate goal of removing microbial infection from the root canal system of a contaminated tooth.

To avoid thermal damage to adjacent healthy tissues, we considered using the mechanical effects created by ultrasound, specifically that of cavitation. To generate proof-of-concept data, we designed, constructed, and tested a series of ultrasound transducers that delivered sufficiently low frequencies operating below 300 kHz and pressures below -30MPa to induce cavitation in degassed water with less than 3ppm. Our initial experiments have shown that sufficient ultrasound energy can be transmitted through intact ex vivo human teeth to elicit nonlinear streaming in the root canal of intact ex vivo human teeth. We have also demonstrated the use of equivalent parameters to kill bacteria. We will further determine and refine the optimal ultrasound parameters for eliciting bactericide in the intact tooth.

SCARP at Simmons College

Tuesday, March 5, 2019 8:00 AM - 11:00 AM

Session E69 FHP FIP: History of Contemporary Chinese Physics BCEC 052A - Yuanrong Lu, Peking University -

Creating A Center of Theoretical Physics at Christian Yenching University in Peking: British physicist William Band’s endeavor in the 1930s

DANIAN HU (Presenter), History, The City College of The City University of New York — William Band (1906-1993) was a practical physicist from Liverpool, who came to Yenching University in 1929. Having taught several years in Peking (Beijing) and worked mostly on experimental projects, Band had realized by the mid-1930s that “many Chinese students have a considerable natural aptitude for theoretical work,” and that there was no place in China where students could receive adequate training in theoretical physics. Thus he was determined to concentrate on theoretical study and aspired to build a center at Yenching to explore modern theoretical physics and its philosophical basis. For this purpose, he spent his sabbatical leave at Cambridge University, studying with Ralph Fowler, Arthur Eddington, Paul Dirac, and Rudolf Peierls. Based on extensive archival research, I examine in this paper Band’s endeavors in both China and England, demonstrating significant contributions of both Band and the American funded Yenching University to Chinese physics development and revealing a missed opportunity for Band to propose independently the effect of gravitational lensing.

Creating A Center of Theoretical Physics at Christian Yenching University in Peking: British physicist William Band’s endeavor in the 1930s

This project is in part supported by PSC-CUNY Research Awards and research grants from the Division of H & A at The City College of New York.

From Binoculars to Cinetheodolite: The Development of Applied Optics and the Optical Industry in China

LIE SUN (Presenter), Department of History of Science and Technology in Modern China, Institute for the History of Natural Sciences, Chinese Academy of Sciences — The emergence of the applied optics and the optical industry in China primarily started during the Second World War and the Cold War periods, while the applied optics and the optical industry in China mainly developed through three ways: setting up plants, sending students to study overseas, and engaging in mission-oriented disciplinary development. In the Anti-Japanese War (1937-1945), Gong Zutong and his colleagues, who had studied at the Technical University of Berlin, started to learn German optical technology. In 1939, the first batch of 6*30 Type Zhongzheng (Chiang Kai-shek) Binoculars were manufactured at the No. 22 Arsenal (Kunming) on a trial basis. The optical glass and accessories used by the binoculars were imported from Europe. From 1950s, industrial demand largely dominated the objectives and missions of China's sciences and industrial technologies. The mission-oriented disciplinary development model – the state's needs led the establishment and expansion of underlying disciplines – had direct impacts on the development of applied optics in China. Among others, an symbolic achievement was China's first large optical equipment developed by Wang Daheng and his colleagues in 1965 – a large cinetheodolite for observing satellite trajectories, fostering both a number of specialized research and development institutions on applied optics and the optics and instrument disciplines of some universities, and directly formulating one of the major features of the optics-related disciplines in China in the following decades, i.e., preferring development for practical purposes to fundamental researches.

This work is supported by the “Significant Breakthrough Project”of the Institute for the History of Natural Sciences (IHNS), Chinese Academy of Sciences (No. Y821101003).
9:12AM E69.00003: Entangled Worldlines: Four Physicists Whose Transnational Trajectories Reshaped Physics in China and the United States [invited] ZUOYUE WANG (Presenter), California State Polytechnic University — Chen Ning Yang and Tsung-Dao Lee are eminent Chinese American physicists who not only shared the 1957 Nobel prize in physics for their breakthrough on parity conservation, but also made other important discoveries as well as played active roles in promoting US-China scientific exchanges. Less well-known were Deng Jiaxian and Zhu Guangya, close friends to Yang and Lee respectively who also received their PhDs in physics in the US but who made the choice to return to China in 1950 and became prominent leaders in Chinese science and technology. This talk explores the entangled trajectories of these American-educated Chinese physicists in an attempt to present a nuanced picture of the transnational characters of both Chinese and American science.

9:48AM E69.00004: Chinese Physicists’ Construction of Straton (or Mao-particle) in the 1960s: the Chinese search for the structure of Hadrons under the guidance of Maoist philosophy* [invited] JINYAN LIU (Presenter), Chinese Academy of Sciences — Particle physics developed rapidly between the 1950s and the 1960s. The discovery of new particles at that time left particle physicists with an urgent need to make classification of them, to figure out their underlying relations and to put forward new conceptual and theoretical models. This brought about the proposition of the well-known Sakata model, Eight-fold way and quark model. What is rarely known is that Chinese particle physicists independently put forward a structure model of hadrons——straton model in 1966 inspired by Mao Zedong's philosophy. Mao Zedong explicitly supported Shoichi Sakata, a Japanese physicist, in applying materialistic dialectics to physics research, which influenced Chinese physicists in their study of particle physics. Starting in the early 1960s, Chinese particle physicists engaged in the theoretical research of elementary particles. From 1965 to 1966, they analyzed the experimental results and existing theories available to them, made a connection between their work and Mao Zedong's philosophy and proposed the straton model. In July 1966, the straton model was presented at the Summer Physics Colloquium of the Peking Symposium. Unfortunately, scientific research in China soon came to a halt due to the Cultural Revolution (1966–1976), the academic exchange between Chinese scientists and their foreign peers became even more difficult than before. The calculation results of the hadron model failed to be formally published in English as Chinese scientists had wanted. As a result, the straton model did not have the kind of influence upon the development of particle physics at the international level that these scientists had expected.

*Research and Teaching Project for youth of Chinese Academy of Sciences

10:24AM E69.00005: Physics and Politics Intertwined -- The manipulative moves in the 2016 supercollider controversy in China [invited] TIAN YU CAO (Presenter), Boston University — The controversy in 2016 over the worthiness of building an extremely expensive supercollider in China was both scientific and political. The intricacies of the asymmetrical manipulative moves on the science-politics interface by the pro-side and the con-side will be analyzed. The talk will end with some general remarks on the determinants in agenda-setting for fundamental researches in China, which will be compared with those in the US.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F01 DCMP: Exotic Electronic States in Topological Systems BCEC 106 - Predrag Nikolic, George Mason University

11:15AM F01.00001: Exactly Solvable Majorana-Anderson Impurity Models SHANKAR GANESH (Presenter), JOSEPH MACIEJKO, University of Alberta — Majorana fermions emerge in topological superconductors as end zero modes in one dimension, and vortex-trapped zero modes or chiral edge modes in two dimensions. A question of much recent interest is the effect of electron-electron interactions on such Majorana fermions. We introduce exactly solvable Majorana-Anderson impurity models that describe an interacting Anderson impurity (i) immersed in tight-binding lattices of Majorana modes in one and two dimensions, (ii) coupled to the Majorana end mode of a Kitaev chain, and (iii) coupled to the edge mode of a chiral p-wave superconductor. The Ising slave-spin representation is used to map our interacting models to models of free auxiliary Majorana fermions. In each case, we calculate exact spectral functions for the impurity fermions and observe a nontrivial temperature dependence as a signature of interactions. Spectral functions for the host fermions are also calculated to study the feedback effect of the impurity on the superconducting host. We compare our exact results to those obtained from strong-coupling perturbation theory.
11:27AM F01.00002: Tuning Many-Body Interactions in a Thin Topological Insulator  NICHOLAS DALE (Presenter), ALEXANDER NGUYEN, DREW W LATZKE, University of California, Berkeley, NIKEH KOIRALA, Massachusetts Institute of Technology, PAVEL P SHIBAYEV, JISOO MOON, SEONGSHIK OH, Rutgers University, ALESSANDRA LANZARA, University of California, Berkeley — The conical dispersion of spinless Dirac fermion systems can become renormalized upon introduction to electron-electron interactions. It is an open question whether or not this behavior extends to the spin-momentum locked surface states of Topological Insulators. We investigate in Photoemission Spectroscopy the surface states of a thin Topological Insulator Bi2Se3 on SrTiO3 using temperature as a knob to tune electron-electron interactions.

11:39AM F01.00003: Surface band bending on cleaved strongly correlated topological insulators* CHRISTIAN MATT (Presenter), HARRIS PIRIE, Department of Physics, Harvard University, Cambridge, MA, United States, WENDEL S. PAZ, JUAN JOSE PALACIOS, Departamento de Fisica de la Materia Condensada, Universidad Autónoma de Madrid, DANIEL LARSON, MOHAMMAD H HAMIDIAN, JENNIFER HOFFMAN, Department of Physics, Harvard University, Cambridge, MA, United States — Strongly correlated topological surface states are promising platforms for next-generation quantum applications, but they remain elusive in real materials. Although angle-resolved photoemission (ARPES) experiments on the correlated insulator SmB6 appear to show spin-textured surface states, the Dirac point – the hallmark of any topological system – has not been resolved by ARPES. A key challenge is that SmB6 lacks a natural cleaving plane, thus limiting the ordered surface domains to tens of nanometers, with local energy band features shifted by tens of meV as observed by our scanning tunneling microscopy experiments. Here we simulate the full spectral function as an average over multiple domains with different surface potentials and band-bending. We thus explain the discrepancy between large-area measurements that average over multiple band-shifted domains and atomically-resolved measurements.

*Experiments were supported by National Science Foundation DMR-1410480. HP and MHH were funded by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4536. CEM is supported by the Swiss National Science Foundation under fellowships P2EZP2_175155

11:51AM F01.00004: Band topology in twisted bilayer graphene* HOI CHUN PO (Presenter), Physics, Massachusetts Institute of Technology, LIUJUN ZOU, Physics, Harvard University, SENTHIL TODADRI, Physics, Massachusetts Institute of Technology, ASHVIN VISHWANATH, Physics, Harvard University — Superconductivity and correlated insulators have been observed in "magic-angle" twisted bilayer graphene when the nearly flat bands close to charge neutrality are partially filled. The observed phenomenology resembles that of high-temperature superconductors like cuprates. Yet, the building blocks of the two systems are vastly different, since the states in TBG descend from graphene's Dirac dispersion. We argue that the Dirac character of the relevant states endows the nearly flat bands with a nontrivial band topology, which forbids any fully symmetric tight-binding description for the nearly flat bands alone. Extended models incorporating the higher energy bands, however, are possible. We constructing a family of such tight-binding models, and from them establish that the band topology is "fragile" in nature, in that it can be dissolved simply by adding additional atomic bands. Our models pave the way to developing a theoretical understanding of twisted bilayer graphene from a strong-coupling perspective.

*TS is supported by a US Department of Energy grant DE-SC0008739, and in part by a Simons Investigator award from the Simons Foundation. AV was supported by a Simons Investigator award and by NSF-DMR 1411343.

12:03PM F01.00005: Magnetic structure of the antiferromagnetic Weyl semimetal candidates Mn3(Ge/Sn)* YOUZHE CHEN (Presenter), JONATHAN GAUDET, GUY G MARCUS, Johns Hopkins University, NAOKI KIYOHARA, AGUSTINUS A. NUGROHO, U Tokyo, ISSP, YANG ZHAO, NIST, SATORU NAKATSUJI, U Tokyo, ISSP, COLLIN BROHOLM, Johns Hopkins University — The recent discovery of Anomalous Hall Effect in Mn3X (X=Sn,Ge) suggests the existence of Weyl nodes in the electronic band structure of these non-colinear antiferromagnets. The magnetic structure of Mn3X is crucial to Weyl physics, but is still under debate due to the lack of experimental studies. To determine the structure, we report polarized neutron diffraction studies on Mn3X (X=Sn,Ge). In Mn3Ge, a k=0 antichiral structure was determined, which naturally explains the origin of a net in-plane magnetization along the [110] direction. In Mn3Sn, an additional incommensurate phase was discovered and further characterized with polarization analysis. The magnetic ground state selection of Mn3X (X=Sn,Ge) will be discussed in terms of exchange, Dzyaloshinskii-Moriya and crystal electric field interactions.

*This work is funded by DOE under DE-SC0019331.
12:15PM F01.00006: A topological classification of molecules and chemical reactions with and without interactions* LUKAS MUECHLER (Presenter), Center for Computational Quantum Physics, Flatiron Institute — In this talk, we propose a topological classification of molecules and their chemical reactions with and without many-body interactions. We consider 0-dimensional molecular Hamiltonians in a real-space tight-binding basis with time-reversal symmetry and an additional spatial reflection symmetry. On a single particle level, the reflection symmetry gives rise to a perplectic structure which can be probed by a Wilson loop after a flux-insertion. The classification in terms of Wilson loops remains stable in the presence of many-body interactions, which can be explained by the presence of zeros of the interacting single particle Green's function.

We argue that this topological classification has a universal contribution to the rate constants of chemical reactions and apply our model to a class of chemical reactions studied by Woodward and Hoffmann, where a reflection symmetry is preserved along a one-dimensional reaction path.

*The Flatiron Institute is a division of the Simons Foundation

12:27PM F01.00007: Spin-wave excitations in the antiferromagnetic Weyl semimetal candidates Mn3Ge and Mn3Sn* JONATHAN GAUDET (Presenter), YOUZHE CHEN, GUY G MARCUS, IQM, Johns Hopkins University, IKHLAS MUHAMMAD, NAOKI KIYOHARA, AGUSTINUS A. NUGROHO, SATORU NAKATSUJI, ISSP, U Tokyo, MATTHEW BRANDON STONE, Oak Ridge National Lab, MINORU SODA, TAKATSUGU MASUDA, ISSP, U Tokyo, COLLIN BROHOLM, IQM, Johns Hopkins University — Mn3X (with X = Ge or Sn) are semimetal antiferromagnets with large anomalous Hall and Nernst effects. These anomalous transport properties have been attributed to the presence of electronic Weyl nodes near the Fermi energy of these materials [1,2]. The magnetism of Mn3X remains relatively unexplored. For example, a detail knowledge of their magnetic excitations is still lacking. In this talk, we report the inelastic neutron scattering spectra of Mn3Ge and Mn3Sn. Our analysis reveals linear dispersive modes that are gapped by ~ 5 meV and have an energy bandwidth of ~ 80 meV. Spin Hamiltonians for both Mn3Sn and Mn3Ge have been derived and will be presented along with a detailed comparison between the two sister compounds. [1] S. Nakasutji et al., Nature 527, p.212–215 (2015) [2] M. Iklhas et al., Nature Physics 13, p. 1085–1090 (2017)

*Support from DOE EFRC (DE-SC0019331) and CMHC-NSERC Postdoctoral Fellowship.

12:39PM F01.00008: Field theory of incompressible topological quantum liquids in higher dimensions PREDRAG NIKOLIC (Presenter), George Mason University — I will discuss a derivation of field theories that describe quantum dynamics of topological defects in a broad range of topologically ordered phases. Beyond quantum Hall liquids in two dimensions, the obtained Lagrangians hint at the existence of stable topologically ordered states with fractional excitations in higher dimensions - involving defects such as monopoles and hedgehogs. I will outline some properties of these topological phases (e.g. fractionalized magnetoelectric effect), and touch upon the prospects for their observation in three-dimensional topological materials.

12:51PM F01.00009: Possible 3-dimensional Topological Excitonic Insulator in a Semimetal under Magnetic Field ZHIMING PAN (Presenter), RYUICHI SHINDOU, Peking University — Motivated by a recent graphite experiment under high magnetic field, we introduce an interacting electron model with a pair of electron pocket and hole pocket under magnetic field. We use a fermionic renormalization group (RG) method and study a parquet RG equation of the model for various types of effective electron-electron interactions. We found that, for a screened Coulomb interaction, the one-loop level RG equation exhibit an instability of the excitonic pairing, while, for a short-ranged repulsive interaction case, the excitonic instability and a charge-density wave instability appear simultaneously. We further argue that, depending on the sign of the interaction, the excitonic insulator phase can be either a symmetry-protected topological excitonic insulator or topologically trivial excitonic insulator. In the former case, an odd-parity excitonic pairing in the bulk reconstruct a chiral Fermi arc state of electron type and that of hole type into a helical surface state with gapless Dirac cone. The reconstructed surface state may provide a simple explanation for a mysterious in-plane transport behaviour observed in the graphite experiment under high magnetic field.

*The Flatiron Institute is a division of the Simons Foundation
Coexistence of metallic edge states and antiferromagnetic ordering in correlated topological insulators

GIORGIO SANGIOVANNI (Presenter), University of Wurzburg, ADRIANO AMARICCI, ANGELO VALLI, MASSIMO CAPONE, SISSA - Trieste, JAN CARL BUDICICH, TU Dresden, BJÖRN TRAUZETTEL, University of Wurzburg — We investigate the emergence of antiferromagnetic ordering and its effect on the helical edge states in a quantum spin Hall insulator, in the presence of strong Coulomb interaction [1-5]. Using dynamical mean-field theory, we show that the breakdown of lattice translational symmetry favors the formation of magnetic ordering with nontrivial spatial modulation. The onset of a nonuniform magnetization enables the coexistence of spin-ordered and topologically nontrivial states. An unambiguous signature of the persistence of the topological bulk property is the survival of bona fide edge states. We show that the penetration of the magnetic order is accompanied by the progressive reconstruction of gapless states in subperipheral layers, redefining the actual topological boundary within the system.


Kondo Hole Scattering in the Strongly Correlated Topological Insulator SmB6

HARRIS PIRIE (Presenter), YU LIU, Harvard University, SAGEN C COCKLIN, ERIC MASCOT, University of Illinois at Chicago, PENGCHENG CHEN, Harvard University, SHANTA SAHA, XIAOFENG WANG, JOHNPIERRE PAGLIONE, University of Maryland, MOHAMMAD H HAMIDIAN, Harvard University, DIRK MRR, University of Illinois at Chicago, JENNIFER HOFFMAN, Harvard University — Quantum materials combining strong correlations and spin-orbit coupling are predicted to generate multiple exotic ground states. For example, in topological Kondo insulators, interactions within a lattice of local moments open a hybridization gap in the conduction band, within which topologically protected heavy Dirac surface states emerge. When a lattice moment is removed, the resulting Kondo hole is predicted to create oscillations in the electron screening cloud, with accompanying magnetic fluctuations. Here we use scanning tunneling microscopy and spectroscopy to image the interaction between a Kondo hole and the topological surface state in SmB6. We show that Sm vacancies induce oscillations in the hybridization gap and electrochemical potential, matching predictions for Kondo holes [1], while B-site defects do not. Furthermore, we find that only Sm-site defects cause significant scattering of the topological surface state. Our results demonstrate how intrinsic, nominally nonmagnetic defects can generate magnetic fluctuations that provide a new mechanism for scattering topological surface states.


Pulsed field studies of Kondo insulator YbB12

ZIJI XIANG (Presenter), University of Michigan, YUICHI KASAHARA, Department of Physics, Kyoto University, TOMOYA ASABA, BENJAMIN LAWSON, COLIN TINSMAN, LU CHEN, University of Michigan, YUKI SATO, Department of Physics, Kyoto University, FUMITOSHI IGA, College of Science, Ibaraki University, JOHN SINGLETON, Los Alamos National Laboratory, YUJI MATSUDA, Department of Physics, Kyoto University, LU LI, University of Michigan — The Shubnikov-de Haas (SdH) effect, quantum oscillations in the electrical conductivity, have been detected in Kondo insulator YbB12 [1]. Such an observation suggests a highly exotic ground state in this material. Here we show the results of magnetoresistance and proximity detector oscillator (PDO) measurements in YbB12 in pulsed magnetic fields up to 65 T. SdH oscillations are observed both above and below the field-induced insulator-metal (I-M) transition. An abrupt increase in the oscillation frequency takes place at the transition. A unique angular dependence of the SdH frequencies is also revealed, which is related to the angle-dependent I-M transition field. The origin of the SdH effect in the insulating phase of YbB12 is discussed based on the pulsed field studies.

1:39PM F01.00013: Coupled-wire models of non-Abelian topological orders in 3D  
SYED RAZA (Presenter), JEFFREY C.Y. TEO, University of Virginia — Topological order corresponds to patterns of long-range entanglement in ground-states. The point-like and line-like excitations in 3D topologically ordered states can have fractional charge and spin degrees of freedom giving rise to fractional quantum statistics. In this work, we study 3D non-Abelian topological order via coupled-wire construction. By putting the wire configuration on a closed manifold, we study the properties of ground states and the Wilson algebra of various excitations. We study the topological order of previously proposed coupled-wire models of symmetry-preserving gapped Dirac (semi)metal and Dirac superconductor. We also study new non-Abelian topologically ordered states that inherit their topological properties from conformal field theories like SO(3)$_3$.

1:51PM F01.00014: Study of hysteretic magnetotransport of SmB$_6$ using local and non-local Corbino disk techniques.*  
YUN SUK EO (Presenter), TRISTIN E METZ, HYUNSOO KIM, Department of Physics, University of Maryland, College Park, WESLEY T. FUHRMAN, Schmidt Science Fellows, in partnership with the Rhodes Trust, SHANTA SAHA, Xiangfeng Wang, Department of Physics, University of Maryland, College Park, JUAN CHAMORRO, Department of Chemistry, Johns Hopkins University, SEYED KOOHPAEH, TYREL MCQUEEN, Henry A. Rowland Department of Physics and Astronomy, Johns Hopkins University, MICHAEL FUHRER, School of Physics & Astronomy, Monash University, JOHNPIERRE PAGLIONE, Department of Physics, University of Maryland, College Park — Recent experiments that have been reported during the past several years suggest that samarium hexaboride (SmB$_6$) is a true topological Kondo insulator (TKI). Particularly, the hysteretic magnetotransport at low temperatures is a remarkable feature that seems to be consistent with the TKI picture, but distinct from other topological insulators. Motivated by the growing interest in the role of disorder and impurities in bulk SmB$_6$, we revisit the surface transport, including the hysteresis features, using Corbino disk structures on flux- and floating zone-grown samples with small impurity concentrations (e.g., Gd, Ni, and Fe). Also, using bulk probing techniques such as non-local (inverted) Corbino transport and heat capacity, we investigate if the bulk channel has an influence on the hysteresis signals we observe in standard transport configurations.

*The work at IQM supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0019331.

2:03PM F01.00015: Correlation Driven Topological Insulator to Weyl Semimetal Transition in Actinide System UNiSn  
VSEVOLOD IVANOV, SERGEY SAVRASOV (Presenter), Physics, UC Davis — We use a modern electronic structure method combining density functional theory of band electrons with dynamical self-energies of strongly correlated states to predict that two well known phases of actinide compound UNiSn, a paramagnetic semiconducting and antiferromagnetic metallic, correspond to Topological Insulator (TI) and Weyl semimetal (WSM) phases of topological quantum matter. Thus, the famous unconventional insulator-metal transition observed in UNiSn is also a TI to WSM transition. Driven by a strong hybridization between U f-electron multiplet transitions and band electrons, multiple energy gaps open up in the single-particle spectrum whose topological physics is revealed using the calculation of Z2 invariants in the strongly correlated regime. A simplified physical picture of these phenomena is provided based on a periodic Anderson model of strong correlations and multiple band inversions that occur in this fascinating compound. Studying the topology of interacting electrons reveals interesting opportunities for finding new exotic phase transitions in strongly correlated systems.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F02 DMP DCOMP: Dielectric & Ferroic Oxides -- Structure, Phase Stability, and Competition I  
BCEC 107A - Jason Hoffman - Tag(s): Focus
11:15AM F02.00001: Diffuse scattering and the local structure of relaxors* [Invited] MATTHEW KROGSTAD, Argonne National Laboratory, PETER M GEHRING, National Institute of Standards and Technology, STEPHAN ROSENKRANZ, RAYMOND OSBORN, Argonne National Laboratory, FENG YE, YAOHUA LIU, Oak Ridge National Laboratory, JACOB RUFF, CHESS, Cornell University, WENZHI CHEN, Simon Fraser University, JUSTIN WOZNIAK, Argonne National Laboratory, YE ZUO-GUANG, Simon Fraser University, DANIEL PHELAN (Presenter), Argonne National Laboratory — Anomalous dielectric and electromechanical properties make relaxor ferroelectrics fundamentally and technologically appealing. We have used three dimensional diffuse scattering measurements (x-ray and neutron) to investigating several classes of relaxor ferroelectrics, including pseudo-cubic Pb-based perovskites and uniaxial tungsten bronze systems. We discuss the different components that are observed in these measurements and how they relate to the physics and material properties of these systems.

*Work at the Materials Science Division at Argonne National Laboratory was supported by the US Department of Energy, Office of Science, Materials Sciences and Engineering Division.

11:51AM F02.00002: Effects of Substrate Orientations on Phase Stability of Epitaxial HfO2 Thin Films* SHI LIU (Presenter), BRENDAN HANRAHAN, US Army Rsch Lab - Adelphi — The discovery of ferroelectricity in both pure and doped HfO2 thin films have revitalized the interest in using ferroelectrics for nanoscale device applications. Previous studies on epitaxial strain engineering of ferroelectricity have mostly focused on thin films grown on (001)-oriented substrates. There is increasing interest in applying biaxial strain along other crystallographic planes such as (101) and (111) by growing thin films on substrates of different cuts. In this work, we focus on the effects of film orientations on the phase stability of HfO2 thin films. We start by examining the ideal transition barriers between different phases of HfO2 with first-principles methods. We find that the three phases, P21/c, Pca21 , and Pbc are separated by relatively large barriers. We calculate the energetics of different polymorphs of hafnia with epitaxial constraints imposed on the {100}, {110}, and {111} planes. Our calculations suggest that the two orthorhombic phases can become the ground state in (111)-oriented thin films. This work suggests the possibility to better stabilize the ferroelectric phase in HfO2 thin films through substrate orientation engineering.

*Shi Liu is supported by SEDD Distinguished Postdoc Fellowship at US Army Research Laboratory

12:03PM F02.00003: Competing phases of HfO2 in applied electric field: A first principles insight* YUBO QI (Presenter), KARIN RABE, Rutgers University, New Brunswick — The recent discovery of ferroelectricity in doped HfO2 thin films has generated intense experimental and theoretical interest, with a particular focus on the precise nature of the HfO2 ferroelectric phase and the factors promoting the observation of ferroelectric switching. In this talk, I present first principles results and analysis to demonstrate how phases of HfO2 evolve under applied electric field as a function of field magnitude and direction. In particularly, the symmetry breaking of yttrium dopants is shown to open new reaction pathways for structural transformation, leading to an electric-field-driven transition from a metastable nonpolar tetragonal phase to the polar ferroelectric orthorhombic phase. The implications of the results for interpreting recent experimental observations will be discussed.

*This work was supported by ONR N00014-17-1-2770.

12:15PM F02.00004: Unconventional Stability of Subloop Behavior for Neuromorphic Computing in a Ferroelectric HfO2 KYOUNGJUN LEE (Presenter), SEUNG CHUL CHAE, Physics Education, Seoul National University — Recent discovery of ferroelectricity in HfO2 film has attracted not only as a conventional non-volatile memory application but as a neuromorphic analogue device. Multiple intermediate state in ferroelectric switching is one of good candidate for neuromorphic application. Though ferroelectric HfO2 have CMOS compatibility and ferroelectricity in thin film thickness, due to its large coercive field which can induce uncertainty in multi-level switching process, multilevel switching process research is needed. In this study, we present the stability of multi-level polarization states in terms of large activation energy and small critical domain volume. We measured switching dynamics and temperature dependence hysteresis of HfO2 thin films. The characteristic switching time and temperature dependence of hysteresis showed that ferroelectric HfO2 has large activation energy while the critical ferroelectric domain volume is small compared to the conventional perovskite materials. PFM results showed large domain wall activation energy due to stable small critical volume. Due to small critical size of ferroelectric domain in HfO2, the enhanced accuracy for the access of multiple states can be used for the analogue ferroelectric HfO2 memory for the neuromorphic memory application.
The need for efficient energy utilization is driving research into ways to harvest ubiquitous waste heat. Here, we explore pyroelectric energy conversion (PEC) from low-grade thermal sources that exploits strong field- and temperature-induced polarization susceptibilities in the relaxor ferroelectric 0.68Pb(Mg1/3Nb2/3)O3–0.32PbTiO3 (PMN-PT). Relaxors have attracted considerable attention due to their intriguing dielectric and piezoelectric properties including high reversible strains and high-temperature operation, but there has been only minimal study of their electrothermal effects. Here, we develop a comprehensive picture of the relationship between epitaxial strain, structure, properties, and local polar order in relaxor thin films. We will discuss how high-quality, coherently-strained films of PMN-PT provide new understanding of structure and properties which opens doors for new applications. In particular, we explore how the electric-field-driven enhancement of the pyroelectric response (−550 μC m−2 K−1) and suppression of the dielectric response (by 72%) yield substantial figures of merit for PEC. Field- and temperature-dependent pyroelectric measurements highlight the role of polarization rotation and field-induced polarization in mediating these effects. Solid-state, thin-film devices that convert low-grade heat into electrical energy are demonstrated using pyroelectric Ericsson cycles, and optimized to yield maximum energy density, power density, and efficiency of 1.06 J cm−3, 526 W cm−3 and 19% of Carnot, respectively; the highest values reported to date and equivalent to a thermoelectric with an effective ZT = 1.16 for a temperature change of 10 K. We will also explore the potential for electrocaloric effects and routes to enhance the energy conversion potential of materials.


Electrode material effect on the switching behavior of ferroelectric HfO2-based thin films

Application of HfO2-based films to ferroelectric memory and logic devices has generated considerable interest as they allow overcoming significant problems associated with poor compatibility of perovskite ferroelectrics with CMOS processing. However, detailed studies of such application-relevant properties as imprint and polarization switching dynamics with respect to the electrode material and processing condition are still sparse in literature. Here, we use a combination of Piezoresponse Force Microscopy (PFM) and pulse switching techniques to analyze the time- and field-dependent evolution of the domain structure in Hf0.5Zr0.5O2 thin film capacitors with oxygen rich/deficient electrodes. Switching spectroscopy-PFM (SS-PFM) maps revealed the electrode-dependent spatial variations in the local potential landscape, which strongly affect the domain switching kinetics. It is shown that stronger oxidation reduces the internal imprint bias while also leading to an increase in the remanent polarization.

1:15PM F02.00007: ABSTRACT WITHDRAWN

Probing short-range polar order in PZN-xPT and PMN-xPT relaxor ferroelectrics with neutron scattering

We have performed neutron scattering measurements on single crystal PZN-xPT and PMN-xPT samples. One of the key issues in these materials is the role of polar nano-regions (PNR), how the short-range orders coexist with long-range polar order and influence the bulk property. With diffuse scattering measurements carried out under external field along different directions, we were able to monitor how the dominant part of the diffuse scattering of “butterfly diffuse” that extends along <110> directions change with field. We observe an anormal suppression of diffuse scattering in Tetragonal phase near 400K and recover in Rhombohedral phase. We also investigate acoustic phonon, which are also affected in the same narrow temperature range. Our results suggest that the polar nano-regions are robust local orders that are locked in within the surrounding polar environment below Tc, and also strongly interact with acoustic phonon modes that induces instability in these systems.
1:39PM F02.00009: New approaches to understanding the ferroic properties of perovskite oxide solid solutions*  
[invited]  ANDREW RAPPE (Presenter), University of Pennsylvania — The dielectric properties of ferroelectric materials are a key driver of smart materials applications. In this talk, two key aspects of anomalous dielectric enhancement will be analyzed: domain walls and relaxor ferroelectrics. A comprehensive theoretical viewpoint will be sketched that unifies these aspects, based on multi-scale materials modeling.

Incorporating quenched Coulombic disorder in ferroelectrics disrupts and changes the character of this transition; instead of a sharp transition in a small temperature range, these oxide alloys exhibit "relaxed" transitions over 100-200 K and are called "relaxor ferroelectrics." I will describe how a first-principles based multi-scale model can reveal the dynamic and statically correlated motions of ions that lead to relaxor behavior, and I will discuss their promise for next-generation piezoelectric and dielectric material systems, with emphasis on the emergent stabilization of a high density of low-angle domain walls.

I will also present molecular dynamics simulations of 90° domain walls (separating domains with orthogonal polarization directions) in the ferroelectric material PbTiO3 to provide microscopic insights that enable the construction of a simple, universal, nucleation-and-growth-based analytical model that quantifies the dynamics of many types of domain walls in various ferroelectrics. This new model illuminates domain wall influence on the dielectric responses of conventional and relaxor ferroelectrics.

*This work was supported by the Office of Naval Research under grant N00014-17-1-2574.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F03 DCMP: Novel Transport Properties of Weyl and Dirac Semimetals BCEC 107B -
Dmytro Pesin, University of Virginia

11:15AM F03.00001: Fermi arc induced vortex structure in Weyl beam shifts  UDVAS CHATTOPADHYAY (Presenter), Nanyang Technological University, Singapore, LI-KUN SHI, Institute of High Performance Computing, A *STAR, Singapore, BAILE ZHANG, JUSTIN SONG, YIDONG CHONG, Nanyang Technological University, Singapore — In periodic media, despite the close relationship between geometrical effects in the bulk and topological surface states, the two are typically probed separately. We have recently found that when beams in a Weyl medium reflect off an interface with a gapped medium, the trajectory is influenced by both bulk geometrical effects and the presence of Fermi arc surface states. The reflected beam experiences a displacement, analogous to the Goos-Hänchen or Imbert-Fedorov shifts, that forms a half-vortex in the two-dimensional surface momentum space. The half-vortex structure is centered at the point where the Fermi arc of the reflecting surface touches the Weyl cone, and the magnitude of the shift scales as the inverse square root of distance from the touching-point. This striking feature provides a way to use bulk transport to probe the topological characteristics of a Weyl medium.

11:27AM F03.00002: Magnetotransport in Weyl nanowires*  VARDAN KALADZHYAN (Presenter), JENS BARDARSON, Department of Physics, KTH Royal Institute of Technology — We study longitudinal magnetotransport in Weyl semimetal nanowires. We show that depending on radii of nanowires and magnetic field amplitudes there exist two qualitatively and quantitatively different regimes of transport. It is demonstrated that in the strong magnetic field regime (magnetic length much smaller than the radius of the nanowire), Landau level spectrum contains the chiral 0-th Landau level, and thus the transport properties resemble that of a bulk Weyl semimetal. On the contrary, in the weak magnetic field regime (magnetic length much larger than the radius of the nanowire), the lowest-energy band is a Fermi arc surface-bulk state with a non-chiral dispersion, hence there appear transport features distinct from those attained at larger radii or larger magnetic fields. We argue that both regimes are relevant for the ongoing experiments. We also demonstrate that the contribution of Fermi arc surface states is salient and, therefore, crucial for understanding transport properties of finite-size Weyl semimetal systems.

*This work was funded by ERC Starting Grant No. 679722.
11:39AM F03.00003: Chirality in Weyl semimetals in strong circularly-polarized electric field FATEMEH NEMATOLLAHI (Presenter), VADYM APALKOV, JHIH-SHENG WU, MARK I STOCKMAN, Georgia State University — We theoretically study the interaction of three-dimensional topological Weyl semimetals with a single oscillation femtosecond long circularly-polarized pulse. The chiral pulse causes a finite electron population of the conduction band which is highly structured and is determined by the topological resonance. These textures can be probed by a linear pulse applied after the circularly-polarized pulse. The response of the system to the linear probe pulse is highly sensitive to the chirality of the circular pulse. Also, the pulse which consists of two oscillations of different chiralities causes conduction band population distribution in the reciprocal space which is highly chiral and is related to the intrinsic chirality of Weyl semimetals.

11:51AM F03.00004: Topological Nodal Lines from Crystalline Symmetry HEQUIU LI (Presenter), Physics, University of Michigan, CHEN FANG, Institute of Physics, Chinese Academy of Sciences, KAI SUN, Physics, University of Michigan — Topological nodal lines protected by the time-reversal symmetry and space-inversion symmetry $T$ and space-inversion symmetry $P$ can be classified into two categories, depending on the value of the $Z_2$ monopole topological index. Nodal lines with trivial (non-trivial) monopole charge can (cannot) be gapped out via shrinking the nodal line into a point. In this study, we show that for four-band models with $T^2=+1$, there are two special points in phase space where the system has a $Z_2$ symmetry, and any Hamiltonian can be adiabatically connected to one of these points. Utilizing this result, we provide a general principle for finding topological nodal lines with nontrivial monopole charge based on the interplay between lattice crystalline symmetries and the time-reversal symmetry. In addition, this study also reveals a new family of topological nodal lines, protected by the time-reversal symmetry and point group symmetries.

12:03PM F03.00005: Strong disorder in nodal semimetals: Schwinger-Dyson–Ward approach* BJOERN SBIERSKI (Presenter), FU Berlin — The self-consistent Born approximation quantitatively fails to capture disorder effects in semimetals. We present an alternative, simple-to-use non-perturbative approach to calculate the disorder induced self-energy. It requires a sufficient broadening of the quasiparticle pole and the solution of a differential equation on the imaginary frequency axis. We demonstrate the performance of our method for various paradigmatic semimetal Hamiltonians and compare our results to exact numerical reference data. For intermediate and strong disorder, our approach yields quantitatively correct momentum resolved results. It is thus complementary to existing RG treatments of weak disorder in semimetals.

12:15PM F03.00006: Parity anomaly in the nonlinear response of nodal-line semimetals* ALBERTO MARTIN-RUIZ, Centro de Ciencias de la Complejidad, Universidad Nacional Autonoma de Mexico, ALBERTO CORTIJO (Presenter), Theory and simulation department, Instituto de Ciencia de Materiales de Madrid — Nodal-line semimetals (NLSM) are topological semimetals where conduction and valence bands touch each other at one dimensional lines in the Brillouin zone. We will focus on the the PT-symmetric version of NLSM and see how adding and removing a PT symmetry-breaking parameter leaves scars in the electromagnetic response of these systems. Tilting breaks $P$ and $T$ but leaves their product invariant, not modifying the symmetry breaking procedure, but allows the parity anomaly to appear both in the linear and non-linear response. In the case of the linear response, we will show that the tilted NLSM display an axionic electromagnetic response, but with a different origin of the one appearing in Weyl semimetals.

*The authors acknowledge CONACyT postdoctoral Grant No. 234774, MINECO/AEI/FEDER, UE Grant No. FIS2015-73454-JIN, and Comunidad de Madrid MAD2D-CM Program (S2013/MIT-3007) for funding.

12:27PM F03.00007: Topological Amorphous Metals* YANBIN YANG (Presenter), TAO QIN, DONG-LING DENG, LUMING DUAN, YONG XU, Tsinghua University — A Weyl semimetal, a crystalline material with translational symmetry, possesses pairs of Weyl points in momentum space band structures and its topology is characterized by the first Chern number defined over a closed surface in momentum space. Here, we study amorphous systems with completely random sites and find that, through constructing and exploring a concrete model Hamiltonian, such a system can host an exotic phase of topological amorphous metal in three dimensions. In contrast to the traditional Weyl semimetals, topological amorphous metals break translational symmetry, and thus cannot be characterized by the first Chern number defined based on the momentum space band structures. Instead, their topological properties will manifest in the Bott index and the Hall conductivity as well as the surface states. Moreover, by studying the energy band and quantum transport properties, we find that topological amorphous metals exhibit a diffusive metal behavior. Our results open a door for exploring topological gapless phenomena in amorphous systems.

*This work was supported by the start-up fund from Tsinghua University, the National Thousand-Young-Talents Program, the Ministry of Education and the National Key Research and Development Program of China (2016YFA0301902).
12:39PM F03.00008: Adiabatic dechiralisation and thermodynamics of Weyl semimetals  SERGEY SYZRANOV  
(Presenter), Physics Department, University of California, Santa Cruz, USA, YAROSLAV I RODIONOV, Institute for Theoretical and 
Applied Electrodynamics RAS and National Institute for Science and Technology MISIS, Moscow, Russia, BRIAN SKINNER, Department 
of Physics, Massachusetts Institute of Technology, Cambridge, USA — We study thermodynamic manifestations of the chiral 
anomaly in disordered Weyl semimetals. We focus, in particular, on the effect which we call "adiabatic dechiralisation", the 
phenomenon in which a change in temperature and/or an absorption or release of heat results from changing external 
electric and magnetic fields that change the imbalance of quasiparticles with different chiralities (at different Weyl nodes). 
This effect is similar to that of adiabatic demagnetisation, which is commonly used as a method of low-temperature 
refrigeration. We describe this phenomenon quantitatively and discuss experimental conditions favourable for its 
obervation. A related phenomenon, which we analyse and which is readily observable in experiment, is the dependency 
of the heat capacity of a Weyl semimetal on parallel electric and magnetic fields.

12:51PM F03.00009: Dynamical density response and optical conductivity in topological metals*  ANTON BURKOV  
(Presenter), University of Waterloo — Topological metals continue to attract attention as novel gapless states of matter. While 
there by now exists an exhaustive classification of possible topologically nontrivial metallic states, their observable 
properties, that follow from the electronic structure topology, are less well understood. Here we present a study of the 
electromagnetic response of three-dimensional topological metals with Weyl or Dirac nodes in the spectrum, which 
systematizes and extends earlier pioneering studies. In particular, we argue that a smoking-gun feature of the chiral 
anomaly in topological metals is the existence of propagating chiral density modes even in the regime of weak magnetic 
fields. We also demonstrate that the optical conductivity of such metals exhibits an extra peak, which exists on top of the 
standard metallic Drude peak. The spectral weight of this peak is transferred from high frequencies and its width is 
proportional to the chiral charge relaxation rate.

*Financial support was provided by Natural Sciences and Engineering Research Council (NSERC) of Canada.

1:03PM F03.00010: Two-particle collisional coordinate shifts and hydrodynamic anomalous Hall effect in systems 
without Lorentz invariance*  DMYTRO PESIN (Presenter), University of Virginia — We show that electrons undergoing a 
two-particle collision in a crystal experience a coordinate shift that depends on their single-particle Bloch wave functions, 
and derive a gauge-invariant expression for such shift, valid for arbitrary band structures, and arbitrary two-particle 
interaction potentials. As an application of the theory, we consider two-particle coordinate shifts for Weyl fermions in 
space of three spatial dimensions. We also demonstrate that such shifts in general contribute to the anomalous Hall 
conductivity of a clean electron liquid.

*National Science Foundation Grant No. DMR-1738384.

1:15PM F03.00011: Optical responses of chiral multifold fermions*  MIGUEL ANGEL SANCHEZ-MARTINEZ, Neel Institute 
(CNRS), FERNANDO DE JUAN, DIPC, San Sebastian, ADOLFO GRUSHIN (Presenter), Neel Institute (CNRS) — Multifold fermions are 
generalizations of two-fold degenerate Weyl fermions with three-, four-, six- or eight-fold degeneracies protected by crystal 
symmetries, of which only the last type is necessarily non-chiral. Their low energy degrees of freedom can be described as 
higher spin generalizations of Weyl semimetals. In this talk I will discuss their linear and non linear optical responses 
including optical activity, linear optical conductivity and photogalvanic effects. These are typically enhanced compared to 
Weyl fermions of the same Fermi velocity and can be quantized in the case of the circular photogalvanic effect. We use 
these results to qualitatively predict optical responses in multifold materials such as RhSi or CoSi.

*Financial support from the Marie Curie programme under EC Grant agreement No. 653846 (AGG), No. 705968 (FdJ) and 
754303 (MASM).
1:27PM F03.00012: Intrinsic magnetoresistance in three-dimensional Dirac materials with low carrier density*
HUANWEN WANG (Presenter), BO FU, SHUNQING SHEN, The University of Hong Kong — Negative longitudinal and positive in-plane transverse magnetoresistance have been observed in most topological Dirac/Weyl semimetals and some other topological materials. Here we present a quantum theory of intrinsic magnetoresistance for three-dimensional Dirac fermions at a finite and uniform magnetic field B. In the semiclassical regime, it is shown that the longitudinal magnetoresistance is negative and quadratic of a weak field B while the in-plane transverse magnetoresistance is positive and quadratic of B. The relative magnetoresistance is inversely quartic of the Fermi wave vector and only determined by carrier density, irrelevant to the external scatterings in the weak scattering limit. This intrinsic anisotropic magnetoresistance is measurable in systems with low carrier density and high mobility. In the quantum oscillation regime, a formula for the phase shift in Shubnikov-de Haas oscillation is present as a function of the mobility and the magnetic field, which is helpful for experimental data analysis

*This work was supported by the Research Grants Council, University Grants Committee, Hong Kong under Grants No. 17301116 and No. C6026-16W.

1:39PM F03.00013: Novel Planar Hall Effect in Tilted Weyl Semimetals*
DA MA (Presenter), International Center for Quantum Materials, Peking University, HUA JIANG, School of Physical Science and Technology, Soochow University, HAIWEN LIU, Department of Physics, Beijing Normal University, XINCHENG XIE, International Center for Quantum Materials, Peking University — In addition to the chiral anomaly, the planar Hall effect has been proposed in the magnetotransport of the Weyl semimetals. We investigate the transport of the tilted Weyl semimetals semiclassically in an in-plane magnetic field. The results show that the longitudinal and the Hall conductivities in this system each has a linear term in magnetic field besides the quadratic terms and the angular dependence of them are different from the case without the tilt. The unusual magnetotransport is induced by the Berry curvature, either through the axial chemical potential or the anomalous velocity. The correction of the phase space volume factor is also presented, which has effects on both the angular and the magnetic field dependence of the conductivities.

*This work is financially supported by NBRPC and NSFC.

1:51PM F03.00014: WITHDRAWN ABSTRACT —

2:03PM F03.00015: Spin-to-charge conversion in magnetic Weyl semimetals.* SHULEI ZHANG (Presenter), Materials Science Division, Argonne National Laboratory, Lemont, Illinois, USA, ANTON BURKOV, Dept. of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, Canada, IVAR MARTIN, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory, Lemont, Illinois, USA — Weyl semimetals (WSM) are a newly discovered class of quantum materials which can host a number of exotic transport properties in bulk, such as the chiral magnetic effect, negative magnetoresistance, and the anomalous Hall effect. In this work, we investigate theoretically the inverse Edelstein effect (IEE) in a magnetic WSM, i.e., a charge current induced by spin accumulation at the interface between a magnetic WSM and a normal metal. Formally, the induced current is obtained by solving for the scattering wave functions and the nonequilibrium distribution functions in each layer. We find that both surface and bulk states contribute to the IEE, and that the induced current exhibits strong anisotropy: It vanishes along the direction parallel to the line connecting the two Weyl nodes, regardless of the direction of the injected spin. We also determined the dependence of the current on the position of the Fermi level as well as the separation between the two Weyl nodes, which provide extra knobs for controlling the spin-charge conversion in these topological materials.

*Work by S. Z., A. B. and O.H. was supported by the U.S. DOE, Office of Science, Office of BES EFRC program; work by I. M. was supported by the U.S. DOE, Office of Science, BES, Mater. Science and Engineering Division.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F04 DMP: Dirac/Weyl Semimetals -- Transport II (including STM, etc) BCEC 107C - Hsu Liu, Univ of Cambridge - Tag(s): Focus
11:15AM F04.00001: Shubnikov-de Haas oscillations of topological metal Pd$_3$Pb  
NIRMAL GHIMIRE (Presenter), Department of Physics and Astronomy, George Mason University, MOHAMMED ALAM KHAN, Argonne National Laboratory, ANITA S. BOTANA, Arizona State University, J. SAMUEL JIANG, JOHN MITCHELL, Argonne National Laboratory — The recent realization of topological electronic states such as Dirac and Weyl fermions in real materials and their potential for future energy and electronics applications has motivated interest in the study of new forms of topological behavior embodied through new materials. Pd$_3$Pb is one such candidate predicted recently to host unique topological features, including a dispersionless band near the Fermi level and triple nodal points hosting Dirac fermions and open Fermi arcs. Here, we report the crystal growth and electric transport properties of Pd$_3$Pb. Our low field magnetoresistance measurements indicate an anisotropic Fermi surface. We found that Pd$_3$Pb manifests a large transverse magnetoresistance, which reaches 650% at 1.8 K and 14 T, and pronounced Shubnikov-de Haas (SdH) oscillations. Preliminary analysis of the field dependence of the SdH oscillations points to the likelihood of nontrivial Berry phase in Pd$_3$Pb. Further studies in high field limit are desirable to extend the realization of the topological properties of the predicted novel fermions in this material.

11:27AM F04.00002: Quantum oscillations in topological semimetal candidate CaSn$_3$  
K A M HASAN SIDDIQUEE (Presenter), RIFFAT MUNIR, CHARUNI DISSANAYAKE, University of Central Florida, XINZHE HU, SWAPNIL YADAV, YASUMASA TAKANO, University of Florida, EUN SANG CHOI, Florida State University, YASUYUKI NAKAJIMA, University of Central Florida — Binary stannide CaSn$_3$ with a centrosymmetric cubic structure is theoretically predicted to be a topologically non-trivial semimetal, and undergoes superconductivity at $T_c \approx 4.2$K, providing an excellent platform for the understanding of interplay between topology and superconductivity. Here, we report a detailed study of de Haas–van Alphen (dHvA) quantum oscillations for CaSn$_3$ single crystals via torque magnetometry in high magnetic fields up to 35T. Analyzing the dependence of dHvA oscillation frequency and amplitude on temperatures and field angles, we will review the effective carrier masses and the normal state fermiology, and also discuss the non-trivial Berry phase in CaSn$_3$.

11:39AM F04.00003: Vector field STM study on transition metal based kagome magnet*  
JIAXIN YIN (Presenter), SONGTIAN SONIA ZHANG, GUOQING CHANG, ZURAB GUGUCHIA, Princeton University, SHUANG JIA, Peking University, HECHANG LEI, Renmin University of China, TITUS NEUPERT, University of Zurich, ZIQIANG WANG, Boston College, HSIN LIN, Academia Sinica, ZAHID HASAN, Princeton University — We recently found that the kagome magnet can have giant spin-orbit tunability (Nature 562, 91–95 (2018)). We use STM/S to elucidate the atomically resolved electronic states and their magnetic response in another transition metal based kagome magnet. We determine the chemical nature of the surface by atomic imaging of the native defects and surface step edges. On different surface terminations, we have observed different types of tunneling spectra, which corresponds well with our first principle calculation. Surprisingly, we find the tunneling signal has systematic magnetic field response, demonstrating an intriguing coupling of electronic structure and magnetism in a frustrated setting. We further discuss the connection of these results with the topological fermions and Berry phase theory.

*Work at Princeton was supported by the US DOE under Basic Energy Sciences programme (grant number DOE/BES DE-FG-02-05ER46200) and the Gordon and Betty Moore Foundation (GBMF4547/ Hasan)

11:51AM F04.00004: Evidence for edge states in trigonal layered PtBi$_2$  
XIAOANG NIE (Presenter), Shanghai Jiao Tong University, YOUGUO SHI, Institute of Physics, Chinese Academy of Sciences, HAO ZHENG, JINFENG JIA, Shanghai Jiao Tong University — PtBi$_2$ is predicted to be a 3D topological semimetal which possesses triply degenerate point close to Fermi level. Here, we observe that unpredicted edge states exist at the edge of PtBi$_2$ using scanning tunneling microscopy at 4.2K. More importantly, due to the inversion symmetry breaking, PtBi$_2$ features two inequivalent top and bottom surfaces. We detect the edge states at the step edges on both surfaces. Our experiment results, together with calculations, reveal the interesting physics of monolayer PtBi$_2$. 

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12:03PM F04.00005: Evidence of Charge density wave in Re doped MoTe\textsubscript{2}  SUMAN KAMBOJ (Presenter), ANSHU SIROHI, AASTHA VASDEV, Indian Institute of Science Education and Research, Mohali, MANASI MANDAL, SOURAV MARIK, RAVI PRAKASH SINGH, Department of Physical Sciences, Indian Institute of Science Education and Research Bhopal, Bhopal, 462066, India, GOUTAM SHEET, Indian Institute of Science Education and Research, Mohali — Transition metal dichalcogenides exhibit interesting structural and intercalation chemistry and consequent exotic physical properties. Superconductivity with a very low transition temperature of 0.1 K was earlier discovered in the orthorhombic MoTe\textsubscript{2}. MoTe\textsubscript{2} also shows a charge density wave (CDW) phase when grown in thin film form, but a CDW phase in bulk MoTe\textsubscript{2} has not been reported. It is also known that Re substitution for Mo sites leads to an increase in superconducting transition temperature. Mo\textsubscript{0.8}Re\textsubscript{0.2}Te\textsubscript{2} shows a high critical temperature $T_c$ of 3.8 K. Based on our transport and scanning tunneling microscopy experiments we will discuss that the compound Mo\textsubscript{0.8}Re\textsubscript{0.2}Te\textsubscript{2} also supports a CDW phase with an onset temperature of 150 K. Our results suggest that CDW and superconductivity may compete with each other in Re doped MoTe\textsubscript{2}.

12:15PM F04.00006: Topological Appearances between Two Type-II Weyl Semimetals  CHUNLIANG LIN (Presenter), National Chiao Tung University — Topology in abstract mathematics has revolutionized our conventional understanding of condensed matter physics, resulting in the emergence of exotic quantum phases such as topological insulators (TIs). Current realizations of the Weyl semimetals (WSMs) leads us to further study the topological phases of matter beyond TIs. WSMs have gathered great attentions because the quasiparticles in WSMs behave as Weyl fermions, massless chiral fermions. WSMs are classified into Type I and II, according to the topology of the Weyl point, where the electron and hole pockets touch each other. Quasiparticle interference (QPI) study with STM has shown the evidence that a T\textsubscript{d} phase Tungsten Ditelluride (WTe\textsubscript{2}) is type-II WSM\textsuperscript{1}, agreeing with the prior theoretical predictions. A similar measurement has also been performed to a T\textsubscript{d} phase Molybdenum Ditelluride (MoTe\textsubscript{2})\textsuperscript{2}. The difference in the topological appearance (i.e. the positions of the Weyl points and the Fermi arc surface states) of MoTe\textsubscript{2} from that of WTe\textsubscript{2} is clearly revealed.


12:27PM F04.00007: Andreev reflection and Josephson currents on the surface of line Weyl semimetals*  XIANG HU (Presenter), Physics, William and Mary, DMITRY PIKULIN, Microsoft Quantum, Microsoft Station Q, University of California, Santa Barbara, ENRICO ROSSI, Physics, William and Mary — We study the Andreev reflection of line Weyl semimetals' surfaces drumhead states. Drumhead states are expected to have a very large effective mass. We show that the measurement of the Andreev reflection can be a very effective way to detect such mass experimentally. We then investigate Josephson junctions in which the surface of a line Weyl semimetal is placed between two superconducting regions. Using a transfer matrix method we obtain the dependence of the Josephson current on the phase difference between the superconducting leads for long and short junctions. We then study how the interplay of drumhead and bulk states affects the Josephson current-phase relation.

*Work supported by NSF, ONR, and ARO.
**Observation of the nonlinear Hall effect in bilayer WTe$_2$**

SU Yang Xu (Presenter), Qiong Ma, Shen Huitao, David MacNeill, Valla Fatemi, Massachusetts Institute of Technology, Tay-Rong Chang, Physics, National Cheng Kung University, Andres M. Mier Valdivia, Sanfeng Wu, Massachusetts Institute of Technology, Zongzheng Du, Department of Physics, Southern University of Science and Technology, Chuang-Han Hsu, Department of Physics, National University of Singapore, Shiang Fang, Department of Physics, Harvard University, Quinn Gibson, Department of Chemistry, Princeton University, Kenji Watanabe, Takashi Taniguchi, National Institute for Materials Science, Robert Cava, Department of Chemistry, Princeton University, Efthimios Kaxiras, Department of Physics, Harvard University, Haizhou Lu, Department of Physics, Southern University of Science and Technology, Hsin Lin, Department of Physics, National University of Singapore, Liang Fu, NuH GediK, Pablo Jarillo-Herrero, Massachusetts Institute of Technology — The electrical Hall effect is the production of a transverse voltage under an out-of-plane magnetic field. In nonmagnetic materials without external magnetic fields, the electrical Hall effect is rarely explored because of the constraint by time-reversal symmetry. However, only the Hall effect in the linear response regime identically vanishes due to time-reversal symmetry. The Hall effect in the non-linear response regime, on the other hand, may not be subject to such symmetry constraints. Here, we report the observation of the nonlinear Hall effect (NLHE) in the electrical transport of the nonmagnetic 2D quantum material, bilayer WTe$_2$. The NLHE exhibits unusual properties sharply distinct from the AHE in metals: The NLHE shows a quadratic I-V characteristic; it strongly dominates the nonlinear longitudinal response, leading to a Hall angle of about 90 deg. We further show that the NLHE directly measures the “dipole moment” of the Berry curvature, which arises from layer-polarized Dirac fermions in bilayer WTe$_2$. Our results demonstrate a new Hall effect and provide a powerful methodology to detect Berry curvature in a wide range of nonmagnetic quantum materials in an energy-resolved way.

NG and SYX acknowledge support from DOE, BES DMSE (data taking and analysis), the Gordon and Betty Moore Foundations EPiQS Initiative through Grant GBMF4540 (manuscript writing) and National Science Foundation under Grant No. DMR-1809815 (modeling). Work in the PJH group was partly supported by the Center for Excitonics, an Energy Frontier Research Center funded by the US DOE, Office of Science, BES under Award Number DESC0001088 (fabrication and measurement) and partly through AFOSR grant FA9550-16-1-0382 (data analysis), as well as the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4541 to PJH. This work made use of the Materials Research Science and Engineering Center Shared Experimental Facilities supported by the NSF (Grant No. DMR-0819762).

**Giant anomalous Hall and planar Hall effect in magnetic Weyl semimetal Co$_3$Sn$_2$S$_2$ nanoflakes**

Shuo-Ying Yang (Presenter), Max Planck Institute of Microstructure Physics, Enke Liu, Institute of Physics, Chinese Academy of Science, Claudia Felser, Max Planck Institute for Chemical Physics of Solids, Stuart S Parkin, Max Planck Institute of Microstructure Physics — Weyl fermions are chiral massless fermions manifested in crystalline solids by spin split conduction and valence bands crossing at discrete points. Magnetic Weyl semimetals with spontaneous time-reversal-symmetry-breaking are predicted to host large Berry curvature and resulting in a large intrinsic anomalous Hall effect (AHE). In this work, we perform detailed transport studies on the nanoflake devices of magnetic Weyl semimetal, Co$_3$Sn$_2$S$_2$. The two-dimensional nature of its Kagome-lattice allows Co$_3$Sn$_2$S$_2$ to be grown into nanoflakes as thin as 180 nm via the chemical vapor transport method. Through magneto-transport measurements, we observe a large intrinsic anomalous Hall conductivity (AHC) and anomalous Hall angle (AHA) generated by the Weyl-related Berry curvature that is robust against both temperature and charge conductivity. The AHC and AHA simultaneously reach 1422 S/cm and 23%, even higher than recent reports in single crystals [1]. Furthermore, we discuss the observation of the planar Hall effect (PHE) in Co$_3$Sn$_2$S$_2$ which can be caused by the chiral anomaly. Other possible origins of the PHE, including contributions from orbital magnetoresistance and interaction of the electrons with the magnetic order will also be discussed.

1:27PM F04.00010: Origin of the finite-temperature violation of the Wiedemann-Franz law in semi-metals*
ALEXANDRE JAOUÍ (Presenter), BENOIT FAUQUE, KAMRAN BEHNIA, ESPCI ParisTech — We present a study of the electrical and thermal conductivities of the semimetals WP₂, WTe₂ and Sb in the 2K-40K temperature range. At low temperature, the Wiedemann-Franz law holds (κ/T = L₀/ρ with κ the thermal conductivity, ρ the electrical resistivity and L₀ the Lorenz number). However, upon warming, a downward deviation from the Wiedemann-Franz law is observed. In the case of the Weyl semimetal WP₂ [1], the difference reaches an exceptionally large value compared to what we determined in WTe₂ and Sb and what was previously reported in other metals [2]. We identify electron-electron scattering as the origin of this departure [3]. We were further able to quantify the mismatch in the frequency of inter-electronic collisions which conserve momentum (i.e. electric current) but degrade energy (as in the case of normal-state liquid ³He). This sets a narrow temperature window between the ballistic and diffusive regimes where the hierarchy of scattering times corresponds to the hydrodynamic requirements for charge carriers [4].


*This work was funded by Fonds-ESPCI and by Agence Nationale Recherche.

1:39PM F04.00011: Low-dissipation edge currents without edge states*
GIOVANNI VIGNALE (Presenter), Department of Physics and Astronomy, University of Missouri, JUSTIN C. W. SONG, Division of Physics and Applied Physics, Nanyang Technological University — We show that bulk free carriers in topologically trivial multi-valley insulators with non-vanishing Berry curvature give rise to low-dissipation edge currents, which are squeezed within a distance of the order of the valley diffusion length from the edge. This happens even in the absence of edge states [topological (gapless) or otherwise], and when the bulk equilibrium carrier concentration is thermally activated across the gap. Physically, the squeezed edge current arises from the spatially inhomogeneous orbital magnetization that develops from valley-density accumulation near the edge. While this current possesses neither topology nor symmetry protection and, as a result, is not immune to dissipation, in clean enough devices it can mimic low-loss ballistic transport.

*J.C.W.S. was supported by the Singapore National Research Foundation (NRF) under NRF fellowship award NRF-NRF2016-05. G.V. was supported by NSF Grant DMR-1406568.

1:51PM F04.00012: Microwave electrodynamics of WP₂
JAMES DAY (Presenter), GRAHAM BAKER, Stewart Blusson Quantum Matter Institute, VICKY SÜSS, CHANDRA SHEKHAR, CLAUDIA FELSER, Max Planck Institute, DOUGLAS BONN, Stewart Blusson Quantum Matter Institute — We report on measurements of the microwave conductivity of WP₂ from 0.5 to 20 GHz and at low temperatures by way of bolometric broadband microwave spectroscopy. WP₂ is a recently discovered type-II Weyl semimetal that has been reported to host several anomalous transport properties, including a record-high residual resistivity ratio and magnetoresistance. Recent studies of the temperature-dependent electrical and thermal conductivities of WP₂ show that, at certain temperatures, electronic transport is in the hydrodynamic regime – in stark contrast to the diffusive transport found in most metals. Identification of the various scattering rates has thus far relied on measurement of DC quantities, whereas key signatures of charge dynamics are also manifested in the frequency dependence of these quantities. We will discuss our measurements of the microwave-frequency electrical conductivity in the context of hydrodynamic electronic transport in WP₂.
2:03PM F04.00013: NMR Investigation of the Weyl Semimetal TaAs* ARASH AKBARI-SHARBAF (Presenter), AIMÉ VERRIER, Department of Physics, Institut Quantique, Université de Sherbrooke, Sherbrooke, QC, NITAY NAIR, JAMES G. ANALYTIS, Department of Physics, University of California, Berkeley, California, JEFFREY QUILLIAM, Department of Physics, Institut Quantique, Université de Sherbrooke, Sherbrooke, QC — Weyl semimetals are expected to host topologically protected bulk states. Recently $^{181}$Ta nuclear quadrupolar resonance (NQR) was used as a bulk probe to investigate the band structure of the Weyl semimetal TaP near the Weyl nodes. [1] This is possible because nuclear spins couple to Weyl fermions via an anomalous hyperfine coupling influencing the temperature-dependent nuclear spin relaxation time $T_1$. [2] Depending on the position of the chemical potential with respect to the Weyl nodes, the temperature-dependent relaxation rate is expected to deviate from the Korringa relation, where $1/T_1 T = constant$. In this work we present $^{181}$Ta nuclear magnetic resonance (NMR) study of a single crystal TaAs Weyl semimetal, a material in which the chemical potential is typically closer to the Weyl nodes. The $1/T_1 T$ dependence of the $\pm 3/2 \leftrightarrow \pm 5/2$ transition is measured using progressive saturation, and results are compared to theoretical calculations [2] and results on TaP [1]. The $^{181}$Ta quadrupole parameters and Knight shift are also determined from the field and temperature dependence of the resonance frequency. [1] H. Yasuoka et al., Phys. Rev. Lett. 118, 236403 (2017). [2] Z. Okvátovity et al., Phys. Rev. B 94, 245141 (2016). *We acknowledge grants from the CFREF and FRQNT.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F05 DMP: Topological Superconductivity: 3D Materials 8CEC 108 - Tag(s): Focus

11:15AM F05.00001: Observation of Topological Surface State in High Temperature Superconductor MgB2* [Invited] XIAOQING ZHOU (Presenter), KYLE GORDON, University of Colorado, Boulder, KYUNG-HWAN JIN, Physics, University of Utah, HAOXIANG LI, DUSHYANT M NARAYAN, HENGDI ZHAO, HAO ZHENG, University of Colorado, Boulder, HUAQING HUANG, Physics, University of Utah, GANG CAO, University of Colorado, Boulder, NIKOLAI D ZHIGADLO, University of Bern, FENG LIU, Physics, University of Utah, DANIEL DESSAU, University of Colorado, Boulder — Most topological superconductors known-to-date suffer from low transition temperatures ($T_c$) and/or high fragility to disorder and dopant levels, which greatly hamper the progress in this promising field. In this work, we suggest BCS superconductor MgB2 as a superior candidate: not only is its superconducting $T_c=39K$ nearly triple the current record of all candidate topological superconductors, but it also has topological Dirac nodal line states which are highly tolerant against disorder and inadvertent doping variations. Our density functional theory (DFT) calculation and Angle-resolved Photoemission Spectroscopy (ARPES) measurements locate the topological Dirac Nodal Lines and their corresponding topological surface states on the [010] faces of MgB2, which could host topological superconductivity via the proximity effect to the bulk.

*This work was funded by DOE project DE-FG02-03ER46066 (Colorado) and by the DOE project DE-FG02-04ER46148 (Utah). Work in the Stanford Synchrotron Radiation Lightsource is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

11:51AM F05.00002: Termination-dependent Superconducting Topological Surface States in Non-centrosymmetric PbTaSe2 TIEN-MING CHUANG (Presenter), SYU-YOU GUAN, PENG-JEN CHEN, Institute of Physics, Academia Sinica, MING-WEN CHU, Center for Condensed Matter Sciences. National Taiwan University, RAMAN SANKAR, Institute of Physics, Academia Sinica, FANGCHENG CHOU, Center for Condensed Matter Sciences, National Taiwan University, HORNG-TAY JENG, Department of Physics, National Tsing Hua University, CHIA-SENG CHANG, Institute of Physics, Academia Sinica — TSCs are characterized by a full superconducting gap in the bulk and topologically protected gapless surface or edge states. Within each vortex core of TSCs, there exist the zero energy Majorana bound states, which are predicted to exhibit non-Abelian statistics and to form the basis of the fault-tolerant quantum computation. So far, PbTaSe2 is the only stoichiometric bulk material exhibits the required topological surface states at $E_F$ combined with fully gapped bulk superconductivity [1]. Interestingly, two distinct and stable cleaved surfaces have been identified to be Pb- and Se-termination by using spectroscopic imaging-scanning tunneling microscope. Two terminations exhibit striking difference in both atomic and electronic structures above $T_c$. In the superconducting state, both exhibit a full superconducting gap and zero energy bound state in the superconducting vortex cores. Our results show PbTaSe2 is a great platform for the study of 2D TSC.

12:03PM F05.00003: Topological superconductors in the Pb-Sn-In-Te system*  
GENDA GU (Presenter), RUIDAN ZHONG, JOHN A. SCHNEELOCH, YANGMU LI, QIANG LI, TONICA VALLA, JOHN TRANQUADA, Condensed Matter Physics & Materials Science, Brookhaven National Laboratory — The discovery of 3D topological insulator materials and topological superconductor open up a new research field in the condensed matter physics. In order to search for the new topological superconductor, we have grown a large number of the single crystals of Pb-system (Pb-Sn-In-Te) topological crystalline insulator and their topological superconductor. We have measured the physical properties on these single crystals by various techniques. We have studied the effect of crystal growth condition, impurity and composition on the bulk electrical conductivity of these single crystals. We try to find out which composition and crystal growth condition is the best for the best topological superconductor. We have got the bulk topological superconductor with Tc=4.8K.

*The work is supported by DOE.

12:15PM F05.00004: Approaching the type 2 Dirac point in Co-doped PdTe2*  
WENKAI ZHENG (Presenter), RICO SCHONEMANN, National High Magnetic Field Laboratory, GREGORY T. MCCANDLESS, Department of Chemistry and Biochemistry, The University of Texas at Dallas, GRETA CHAPPELL, SHIRIN MOZAFFARI, YU-CHE CHIU, National High Magnetic Field Laboratory, JULIA Y. CHAN, Department of Chemistry and Biochemistry, The University of Texas at Dallas, RYAN BAUMBACH, LUIS BALICAS, National High Magnetic Field Laboratory — Topological states of quantum matter have been investigated intensively in recent few years. A combination of superconductivity and topological order is considered to be a potential platform for realizing Majorana fermions. PdTe2 was classified as a type 2 Dirac semimetal where the Dirac points are located 0.5 eV below the Fermi level. Furthermore, PdTe2 is a superconductor with Tc below 2K. In order to preserve the Dirac points and lower the Fermi level we substituted up to 50% of Pd with Co. While the magnetoresistance is strongly reduced compared to the pure Pd compound, our Co doped samples still show superconductivity with a Tc of 0.22 K at a Co concentration of 50%. So far however, all evidences still point towards PdCoTe2 being a conventional superconductor.

*This work was supported by DOE-BES through Award No. DE-SC0002613. The National High Magnetic Field Laboratory is supported by the National Science Foundation through NSF/DMR-1644779 and the State of Florida.

12:27PM F05.00005: Effects of point-like disorder on electronic properties of PdTe2 superconductor*  
ERIK TIMMONS (Presenter), MAKARY TANATAR, KYUIL CHO, SERAFIM TEKNOWIJOYO, NA HYUN JO, SERGEY BUDKO, PAUL CANFIELD, RUSLAN PROZOROV, Ames Laboratory and Department of Physics & Astronomy, Iowa State University, Ames, IA 50010, USA, MARCIN KONCZYKOWSKI, Ecole Polytechnique, Palaiseau, France — Electric and thermal conductivities were measured before and after the introduction of a controlled point-like disorder in single crystals of PdTe2 by 2.5 MeV electron irradiation. Superconducting transition temperature is suppressed, but not strong enough that together with the exponential variation of the low-temperature London penetration depth indicates nodeless superconductivity. The normal state resistivity perfectly follows the Matthiessen’s rule as seen in a parallel upwards shift after irradiation. Its temperature variation can be fitted well by the Bloch-Grüneisen formula with Debye temperature determined from the specific heat. Thermal conductivity measurements show a good agreement with the Wiedemann-Franz law.

*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract # DE-AC02-07CH11358. NHJ was funded by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4411.

12:39PM F05.00006: Enhanced Correlation Effects in Nodal-line Semimetal ZrSiSe  
YINMING SHAO (Presenter), Columbia University, ALEXANDER N. RUDENKO, Radboud University, JIN HU, University of Arkansas, YANGLIN ZHU, Tulane University, ALEXANDER I. LICHTENSTEIN, University of Hamburg, ZHIQIANG MAO, Pennsylvania State University, MIKHAIL KATSNELSON, Radboud University, DIMITRI BASOV, Columbia University — Three-dimensional (3D) Dirac fermions with highly-dispersive linear bands are usually considered weakly correlated, due to relatively large bandwidths (W) compared to Coulomb interactions (U). With the discovery of nodal-line semimetals, the Dirac dispersion has been extended to lines and loops, with reduced kinetic energy along the line [1]. However, experimental evidence for the predicted enhanced correlations in nodal-line semimetals has been rare. Here we show in ZrSiSe enhanced correlation effects through a combination of optical/magneto-optical spectroscopy and density-functional-theory (DFT) calculations. Near 40% kinetic energy reduction compared to DFT has been observed in ZrSiSe and the averaged Fermi velocity is also renormalized. ZrSiSe is therefore a novel candidate to study correlation-driven physics in Dirac systems as well as strong Berry curvature effects associated with spin-orbit-coupling.

12:51PM F05.00007: Possible valence skipping superconductivity in doped Dirac metal*  
TEPPEI UENO, Dept. of Physics, Okayama University, TAKANORI WAKITA, RII, Okayama University, TETSUYA FURUKAWA, TETSUAKI ITOU, Tokyo University of Science, TAKAYOSHI YOKOYA, JUN AKIMITSU, KAYA KOBAYASHI (Presenter), RII, Okayama University — We studied the superconductivity in NaCl-type structured AgSnSe2 (Tc~3-6 K). The material is perceived as Ag-doped to imaginary NaCl-type SnSe, a Dirac metal. By varying the ratio of Ag/Sn, i.e., changing the ratio of Sn valence states, 2+ and 4+, we found that the Sn 2+ state is crucial for the realization of superconductivity along with the lattice constant. This finding is supported by the XPS, showing the clear coexistence of Sn 2+ and Sn 4+ in the superconducting Ag-Sn-Se compounds, but not in non-superconducting Sn-Se. The NMR experiments on the same superconducting compounds, however, indicated the Sn state is almost 3+, as is expected from the neutrality. The disagreement on these experiments may come from the electronic states in the compound’s unique superconductivity.

*We thank MEXT Grand-in-Aid No. 18K03540 for support.

1:03PM F05.00008: Superconductivity and Nontrivial Band Topology in NbN Polytypes†  
KUNCHALA RAMESH BABU, GUANG-YU GUO (Presenter), National Taiwan University — Niobium nitride is a good superconductor in its cubic structure (d-NbN) with Tc = 17 K [1]. Recent experiments on hexagonal NbN (e-NbN) revealed the existence of superconductivity with a Tc of 12 K [2]. WC-type NbN possesses topological properties with three fold band crossings [3]. Here we study the electronic band structure and superconductivity in these NbN polytypes by performing density functional calculations. Interestingly, our results reveal that all three NbN polytypes are topological metals. Specifically, d-NbN and e-NbN are, respectively, type-II and type-I Dirac metals, while WC-NbN is a topological metal with triply degenerate nodes. Our results also show that the electron-phonon coupling in d-NbN is much stronger than in e-NbN and WC-NbN. This results in a much higher superconducting transition temperature (Tc = 18 K) than in e-NbN and WC-NbN. Our findings thus suggest that the NbN polytypes would provide valuable opportunities for studying exotic phenomena arising from the interplay between superconductivity and band topology.


†The authors acknowledge support from the MOST and NCTS of The R.O.C.

1:15PM F05.00009: Spontaneously polarized half-gapped superconductivity in UTe2*  
SHENG RAN (Presenter), University of Maryland, College Park & NIST, CHRIS ECKBERG, University of Maryland, College Park, QING-PING DING, YUJI FURUKAWA, Iowa State University & Ames Lab, TRISTIN E METZ, University of Maryland, College Park, SHANTA SAHA, I-LIN LIU, University of Maryland, College Park & NIST, MARK ZIC, University of Maryland, College Park, JOHNPIERRE PAGLIONE, NICHOLAS BUTCHE5, University of Maryland, College Park & NIST — We discovered novel nonunitary spin-triplet superconductivity in UTe2, with the highest Tc and Hc2 among all candidates. Superconducting state closely resembles that of ferromagnetic superconductors, but the normal state is paramagnetic and shows no indication of magnetic ordering. UTe2 exhibits an extremely large, anisotropic upper critical field Hc2, temperature independent NMR Knight shift in the superconducting state, and a large residual normal electronic density of states indicating that half of the electrons remain ungapped. All these results strongly indicate that the superconductivity in UTe2 is carried by nonunitary spin-triplet pairs. This discovery yields a new platform for encoding information using topological excitations and for manipulation of spin-polarized currents.

*Research at the University of Maryland was supported by the the National Science Foundation Division of Materials Research Award No. DMR-1610349, and the Gordon and Betty Moore Foundations EPiQS Initiative through Grant No. GBMF4419. Research at Ames Laboratory was supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Ames Laboratory is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358.
1:27PM F05.00010: Fermi-arc superconductivity in Dirac Semimetal $\text{Cd}_3\text{As}_2$  
CE HUANG (Presenter), Fudan University, TONG ZHOU, KAM TUEN LAW, The Hong Kong University of Science and Technology, FAXIAN XIU, Fudan University — $\text{Cd}_3\text{As}_2$ is a three-dimensional Dirac semimetal with separated Dirac points in momentum space which are connected by Fermi arcs. In spite of their extensive studies via transport and spectroscopic approaches, the coupling of Fermi-arc states to superconductivity remains elusive. Here, we report the observation of proximity-induced Fermi-arc superconductivity in SC/$\text{Cd}_3\text{As}_2$ hybrid structures. The proximity gap in Fermi arcs is comparable to the parent superconductor which exhibits a flat conductance plateau in differential conductance spectra. The proximity-induced pairing gap on bulk states, however, is small and manifests itself as a zero-bias broad peak (ZBBP). Corroborated with theory, we further unveil a systematic suppression of the ZBBP and an appearance of conductance plateau when the Fermi-arc states become gradually dominant.

1:39PM F05.00011: The spectral fingerprint of the enhanced surface superconducting gap in $\beta$–$\text{Bi}_2\text{Pd}$  
JIANYU GUAN (Presenter), LINGYUAN KONG, TIAN QIAN, YUJIE SUN, HONG DING, Chinese Academy of Sciences — Topological superconductors are attracting a majority of attentions and inspired community to investigate the candidate materials. The recent discovery of enhanced surface superconducting gap and zero bias conductance peak in $\beta$–$\text{Bi}_2\text{Pd}$ thin film by STM [1] provides a possibility to get higher $T_c$ topological superconductor. But the driving force behind the enhanced superconductivity is still under debate. We grown the $\beta$–$\text{Bi}_2\text{Pd}$ thin film by MBE system and detect using in-situ angle resolved photoemission spectroscopy. We observed quantum well bands due to the high quality of the grown thin film. More importantly, we clearly distinguished the bulk band and surface band in momentum space. In the surface band, we detected the spectral fingerprint of the enhance superconducting gap.

Reference  

1:51PM F05.00012: Topologically nontrivial phases in superconducting transition metal carbides  
RICHARD ZHAN (Presenter), XUAN LUO, National Graphene Research and Development Center — Topological superconductors have shown great potential in the search for unique quasiparticles such as Majorana fermions. Combining nontrivial band topology and superconductivity can lead to topological superconductivity due to the proximity effect. In this work, we used first principle calculations to predict that rocksalt phases of VC and CrC are superconducting with topologically nontrivial states. The phonon dispersions of these transition metal carbides displayed no imaginary frequencies, which suggests dynamic stability. Therefore, these transition metal carbides are practical candidates for studying topological superconductors and their associated Majorana bound states.

2:03PM F05.00013: Topological character of A15 superconductors*  
MINSUNG KIM (Presenter), CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory — A15 superconductors are type-II $s$-wave BCS superconductors that have been known for decades. However, the topological aspects of their electronic structures remain unnoticed so far. In this study, we perform first-principles band structure calculations to show that the band topology of the A15 superconductors $\text{Ta}_3\text{Sb}$, $\text{Ta}_3\text{Sn}$, and $\text{Ta}_3\text{Pb}$ is nontrivial. We also find that there appear topological surface states in accordance with the bulk-boundary correspondence. Due to the bulk superconductivity and the proximity effect, topological superconductivity will be induced at the surface, which can host Majorana zero modes at vortices. Our results show that the A15 superconductors are promising candidate materials to realize the $p_x + i p_y$ type topological superconductivity and the Majorana mode.

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Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F06 DCMP: Exotic Transport Properties: Magnetoresistance, Quantum Hall, and Others  
BCEC 109A - Dmitrii Maslov, University of Florida
**11:15AM F06.00001: Giant magnetoresistance in BaMn$_2$Pn$_2$ (Pn = As, Sb, Bi)**

KHUONG HUYNH (Presenter), WPI-AIMR, Tohoku University, TAKUMA OGASAWARA, STEPHANE YU MATSUSHITA, Department of Physics, Graduate School of Science, Tohoku University, TAIMU TAHARA, TAKANORI KIDA, MASAYUKI HAGIWARA, Center for Advanced High Magnetic Field Science, Graduate School Science, Osaka University, DENIS ARCON, Jozef Stefan Institute, KATSUMI TANIGAKI, WPI-AIMR, Tohoku University — We report our discovery of a new kind of giant magnetoresistance (GMR) in the family of BaMn$_2$Pn$_2$ antiferromagnets, where Pn stands for As, Sb, and Bi [1, 2]. BaMn$_2$Pn$_2$'s are intriguing materials hosting a magnetic hexadecapole ordering that preserves the parity-time symmetry even though both time and space inversion are broken [3]. The hexadecapole ordering microscopically stems from symmetry-preserved spin-dependent d-p hybridization that governs the low energetic excitations and therefore promises exotic transport properties. Here we describe a new GMR in BaMn$_2$Pn$_2$'s with the following features [1,2]: (1) the magnitudes of the unique negative GMR are larger than 98 %, being comparable with those of other exotic GMR systems, (2) GMR exhibits a very unusual angular under the rotation of magnetic fields, (3) GMR is band selective in sign, showing negative and positive signs for hole- and electron-like carriers, respectively. These properties are incompatible to any known mechanism of magnetoresistance and call for new explanations.


*This work was supported by World Premier International Research Center Initiative (WPI), MEXT, Japan.

**11:27AM F06.00002: Hall effects in giant magnetoresistance system BaMn$_2$Bi$_2$**

TAKUMA OGASAWARA (Presenter), Department of Physics, Graduate School of Science, Tohoku University, KHUONG HUYNH, WPI-AIMR, Tohoku University, STEPHANE YU MATSUSHITA, Department of Physics, Graduate School of Science, Tohoku University, TAIMU TAHARA, TAKANORI KIDA, MASAYUKI HAGIWARA, Center for Advanced High Magnetic Field Science, Graduate School Science, Osaka University, DENIS ARCON, Jozef Stefan Institute, KATSUMI TANIGAKI, WPI-AIMR, Tohoku University — A new kind of giant magnetoresistance (GMR) is observed in the family of G-type antiferromagnets BaMn$_2$Pn$_2$ 's, where Pn denotes pnictide elements of As, Sb, and Bi. The -98% GMR appears intriguingly with an unique angular dependence under rotating magnetic fields [1, 2] on the background of a complex magnetic hexadecapole ordering that preserves the parity-time symmetry even though the parity and time reversal symmetries are broken respectively[3]. Among the BaMn$_2$Pn$_2$ 's , BaMn$_2$Bi$_2$ shows the largest MR in the smallest magnetic field range and therefore is the key material of the BaMn$_2$Pn$_2$ family [1] for further detailed studies. We have measured the angular dependence of magnetoresistance and Hall effect of BaMn$_2$Bi$_2$ to investigate the effect of magnetic field on the electrical conductivity. The results of our analyses suggest that the observed GMR stems from a large enhancement in the mobility of hole-like carriers induced by magnetic fields.


*This work was supported by World Premier International Research Center Initiative (WPI), MEXT, Japan.

**11:39AM F06.00003: Effect of Chemical Substitutions on the Extreme Magnetoresistance and Topological State of PtSn$_4$**

ALANNAH HALLAS (Presenter), CHIEN-LUNG HUANG, EMILIA MOROSAN, Rice University — It has recently been discovered that the extreme magnetoresistive material PtSn$_4$ [1] has a novel topological state, with the observation of Dirac node arcs in ARPES measurements [2]. This material has a quasi-two dimensional crystal structure composed of an edge-sharing network of PtSn$_4$-square antiprisms. We study the effect of chemical substitutions on the electronic properties of PtSn$_4$ via two pathways: (i) we consider the effect of replacing platinum by gold, giving AuSn$_4$ and (ii) we consider the effect of substituting tin with lead, giving PtPb$_4$. In the first substitution the crystallographic properties are left unaltered (ABAB stacking, orthorhombic) but in the second there is a minor structural modification (AAA stacking, tetragonal). Both materials superconduct at low temperatures with $T_c = 2.5$ K for AuSn$_4$ and $T_c = 2.8$ K for PtPb$_4$. In this talk, we will present our studies of the electronic and topological properties of these compounds and comment on their relationship to PtSn$_4$.


*Supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative
11:51 AM F06.00004: Charge transport in doped SrTiO₃  
ABHISHEK KUMAR (Presenter), DMITRII MASLOV, University of Florida — Recent experiments identified an unusual T² dependence of the resistivity in doped strontium titanate (SrTiO₃). That this dependence is observed even at low doping, when umklapps are essentially impossible, and at temperatures far exceeding the Fermi energy eliminates electron-electron interaction as a possible source of the T² resistivity. The T² term may come from the interaction of electrons with two soft transverse optic (TO) phonons, characteristic for this material (the Epifanov-Levanyuk-Levanyuk mechanism). However, it is unclear within this model why the T² term would be observed at temperatures smaller than the TO phonon frequency. We show that this behavior can be understood within a model in which the TO frequency varies over the sample from a larger value, observed in neutron and Raman scattering experiments, to a smaller value. A microscopic justification of this model relies on the experimentally observed polar boundaries between antiphase domains. Within the same model, we showed that the next-order correction to T² term is T⁶ which is due to interaction of electrons with four TO phonons. Therefore, the TO phonon scattering is not able to explain the T³ behavior of the resistivity observed at higher temperatures.

12:03 PM F06.00005: Boundary layer theory for quantum Hall hydrodynamics  
SRIRAM GANESHAN (Presenter), Physics, City College of New York CUNY, ALEXANDER ABANOV, Stony Brook University, TANKUT CAN, ITS, CUNY Graduate Center, GUSTAVO M MONTEIRO, Physics, Universidade Estadual de Campinas-UNICAMP — In this talk, we consider non-dissipative two-dimensional broken parity fluids with odd viscosity and magnetic field with a free surface boundary condition. We show that for non-dissipative fluids, incompressibility must be violated at free surfaces to have a consistent hydrodynamic description of the dynamical boundary. Violation to incompressibility sources vorticity within the boundary layer which is an exclusive manifestation of odd viscosity. The thickness of the boundary layer is controlled by the velocity of sound. A non-dissipative boundary layer mechanism allows us to write the full variational principle for both bulk and boundary. In the limit of large sound velocity, we recover Quantum Hall like fluids where the bulk is incompressible but the thin boundary layer manifests compression modes. We discuss the applicability of our results to (fractional) quantum Hall fluids with a free surface.

12:15 PM F06.00006: Dynamics of the Phase Separated States in the Double Exchange Model  
JING LUO (Presenter), GIA-WEI CHERN, University of Virginia — We present large-scale simulations of spin dynamics in the phase-separated states of the one-orbital double-exchange model. These inhomogeneous electronic states consisting of ferromagnetic conducting clusters embedded in an antiferromagnetic insulating background play a crucial role in the colossal magnetoresistance phenomenon. We compute the dynamical structure factor of these nanoscale textures using an efficient real-space formulation of coupled spin and electron dynamics. Dynamical signatures of the various underlying magnetic correlations are identified. At small hole doping, the structure factor exhibits a dominating signal of magnons from the background Néel order and localized modes from small metallic clusters. A low-energy continuum due to large-size ferromagnetic clusters emerges at higher doping levels. Implications for experiments on magnetoresistive manganites are also discussed.

12:27 PM F06.00007: Detecting fractional Chern insulators through circular dichroism  
CECILE REPELLIN (Presenter), Massachusetts Institute of Technology, NATHAN GOLDMAN, Université Libre de Bruxelles — Great efforts are currently devoted to the engineering of topological Bloch bands in cold atomic gas. Recent achievements in this direction as well as the possibility of tuning inter-particle interactions suggests that strongly-correlated states reminiscent of fractional quantum Hall (FQH) liquids, could soon be generated in these atomic systems. In this context where transport measurements are limited, identifying unambiguous signatures of FQH-like states constitutes a challenge on its own. Here, we demonstrate that the fractional nature of the quantized Hall conductance, a fundamental characteristic of FQH states, could be finely detected in ultracold gases through a circular-dichroic measurement, namely by measuring the energy absorbed by the atomic cloud upon a circular drive. We discuss how such measurements, which were recently implemented in the integer-QH regime, could indeed be performed to distinguish FQH-type states from competing states (such as charge density waves). Our scheme offers a practical and powerful tool for the detection of topological order in quantum engineered systems.
12:39PM F06.00008: Bridging Hubbard Model Physics and Quantum Hall Physics in ABC Trilayer Graphene/h-BN moiré superlattice* YAHUI ZHANG (Presenter), SENTHIL TODADRI, Massachusetts Institute of Technology — Recently several phases resulting from electron correlations have been discovered in graphene moiré superlattice with narrow bands. In this talk I will focus on the moiré superlattice formed by ABC stacked trilayer graphene aligned with a hexagonal boron nitride substrate (TG/h-BN). Mott-like insulators in this system have already been observed experimentally by Feng Wang et.al. (Chen, Feng Wang et.al. arxiv: 1803.01985). Remarkably, in TG/h-BN, both the bandwidth and the topology can be tuned by an applied perpendicular electric field $D$. For $D<0$, the valence bands of the two valleys are trivial and the physics is governed by a spin-valley Hubbard model on triangular lattice. For $D>0$, the bands of the two valleys have non-zero Chern numbers $C=3,-3$. Therefore the TG/h-BN system can simulate both Hubbard model physics and nearly flat Chern band physics within one sample through a simple switch of the vertical displacement field. I am going to discuss several aspects of the resulting many body physics.

*The work was supported by NSF grant DMR-1608505, and partially by a Simons Investigator Award from the Simons Foundation to Senthil Todadri.

12:51PM F06.00009: Non-Abelian quasiholes in lattice Moore-Read states and parent Hamiltonians* JULIA WILDEBOER (Presenter), Department of Physics, Arizona State University, SOURAV MANNA, Max Planck Institute for the Physics of complex Systems, GERMAN SIERRA, Instituto de Fisica Teorica, UAM-CSIC, ANNE E. B. NIELSEN, Max Planck Institute for the Physics of complex Systems — A striking feature of fractional quantum Hall states is that they form an incompressible quantum state supporting emergent fractionally charged quasiparticle excitations with non trivial braiding properties. Excitations of non-Abelian nature command much attention from theorists and experimentalists due to their potential applications in quantum information especially topologically protected fault tolerant quantum computation. This talk will present Ising quasiholes in Moore-Read type lattice wave functions. We start by constructing Moore-Read type lattice states and then add quasiholes to them. By use of Metropolis Monte Carlo simulations, we analyze the features of the quasiholes, such as their size, shape, charge, and braiding properties. The braiding properties, which turn out to be the same as in the continuum Moore-Read state, demonstrate the topological attributes of the Moore-Read lattice states in a direct way. We also derive parent Hamiltonians for which the states with quasiholes included are ground states.

*JW thanks NSF DMR 1306897 and NSF DMR 1056536 for partial support.

1:03PM F06.00010: Theory of magnon transport in quantum Hall ferromagnet CHUNLI HUANG (Presenter), ALLAN MACDONALD, Physics, University of Texas at Austin — In two recent experiments, Stepanov et. al [Nat. Phys 14, 907–911 (2018)] and Wei. et al [Science 362, 6411, 229-233 (2018)] observed long distance, nonlocal magnon transport in quantum Hall magnetic states of graphene. In these experiments, bulk magnons are excited in close proximity to conducting spin polarized edge states that are under external voltage bias. While Stepanov et. al observed a nonlocal voltage linear in the bias voltage, Wei. et al observed a nonlocal voltage only when within a window of bias voltage that begins at Zeeman energy. Motivated by these observations, we present a simple theoretical model to study edge-current induced torque -- the coupled dynamics of itinerant spin-polarized edge states and insulating bulk magnons.

1:15PM F06.00011: Effective field theory of a vortex lattice in a bosonic superfluid* SERGEJ MOROZ (Presenter), Technical University of Munich, CARLOS HOYOS, Oviedo, CLAUDIO BENZONI, Technical University of Munich, DAM THANH SON, UChicago — Using boson-vortex duality, we formulate a low-energy effective theory of a two-dimensional vortex lattice in a bosonic Galilean-invariant compressible superfluid. The excitation spectrum contains a gapped Kohn mode and an elliptically polarized Tkachenko mode that has quadratic dispersion relation at low momenta. External rotation breaks parity and time-reversal symmetries and gives rise to Hall responses. We extract the particle number current and stress tensor linear responses and investigate the relations between them that follow from Galilean symmetry. We argue that elementary particles and vortices do not couple to the spin connection which suggests that the Hall viscosity at zero frequency and momentum vanishes in a vortex lattice.

*Our work is supported by the Emmy Noether Programme of German Research Foundation (DFG) under grant No. MO 3013/1-1. C. H. is supported by the Ramon y Cajal fellowship RYC2012-10370, the Spanish national grant MINECO-16-FPA2015-63667-P and the Asturian grant FC-15-GRUPIN14-108. D. T. S. is supported, in part, U.S. DOE Grant No. DEFG02-13ER41958, the ARO MURI Grant No. 63834-PH-MUR, and a Simons Investigator Grant from the Simons Foundation.
1:27PM F06.00012: Electronic Spectral functions, $\rho(T)$ and Raman response in the 2-d $t$-$J$ model* PEIZHI MAI
(Presenter), Oak Ridge National Lab and University of California, Santa Cruz, B SHASTRY, University of California, Santa Cruz — We study the two-dimensional $t$-$J$ model with a second neighbor hopping parameter $t'$, in a broad range of doping $\delta$ using a closed set of equations from the Extremely Correlated Fermi Liquid (ECFL) theory. The electronic spectral function is found to yield asymmetric energy distribution curves and symmetric momentum distribution curves. These are broadly consistent with experimental data. Using our spectral functions, we calculate the resistivity, whose curvature changes with varying $\delta$ is presented, and connect this change to the intensity loss in Angle-Resolved Photoemission Spectroscopy (ARPES) experiments. We also present results for a set of closely related dynamical response functions: the non-resonant Raman susceptibility for three principal geometries germane to the square lattice, and the optical conductivity. Where available, these results are in close correspondence to available high-resolution experimental results. Our results provide a set of testable predictions for future experiments.
*The work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences under Award # DE-FG02-06ER46319.

1:39PM F06.00013: Transport, multifractality and breakdown of single-parameter scaling in quasiperiodic systems. JAGANNATH SUTRADHAR (Presenter), SUBROTO MUKERJEE, RAHUL PANDIT, SUMILAN BANERJEE, Indian Institute of Science — We study the transport in 1d Aubry-Andre model, and its generalizations to 2d and 3d, which show significant deviations from single-parameter scaling theory providing a broad demarcation between QPS and RS. We study the conductance of open systems connected to leads as well as the Thouless conductance. Depending on dimension, the conductances show metal-insulator transition from localized to either ballistic, superdiffusive or diffusive transport typically through subdiffusive critical states. We show that, even though a beta function, $\beta(g) = d\ln(g)/d\ln(L)$, can be constructed separately for individual phases based on a overall length ($L$) dependence of typical dimensionless conductance $g$, in 1d and 2d, the single-parameter scaling is unable to describe the transition. Moreover, the conductances show strong non-monotonic variations (multifractal scaling in 1d) with system size and intricate resonant peak and subpeak structures of number theoretic origin, invalidating a strict definition of $\beta(g)$. We show that the non-monotonicity is very weak in 3d with a critical point having localization length exponent close to that of 3d Anderson transition and the single-parameter scaling is almost restored providing a good description of the metal-insulator transition.

1:51PM F06.00014: Pairing correlations in the incoherent phase of quantum Hall bilayers?* JAMES EISENSTEIN (Presenter), Physics, Caltech, LOREN PFEIFFER, KENNETH WEST, Electrical Engineering, Princeton — At sufficiently small layer separation, Coulomb interactions in bilayer 2D electron systems at high magnetic field can stabilize an excitonic phase in which electrons in one layer are bound to holes in the other. The excitonic phase is macroscopically phase coherent, exhibiting numerous remarkable transport properties analogous to those of superconductivity and superfluidity. While the excitonic phase is theoretically relatively well understood, the incoherent phase at layer separations slightly larger than the critical one is not. In this talk we will discuss recent transport and interlayer tunneling spectroscopy measurements which demonstrate the importance of interlayer Coulomb interactions in the incoherent phase. In addition to screening of the Coulombic repulsion between electrons in the same layer, our measurements suggest that interlayer electron-hole pairing correlations may persist into the incoherent phase at intermediate layer separations.

*This work was supported in part by the Institute for Quantum Information and Matter, a NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation via Grant No. GBMF1250. The work at Princeton University was funded by the Gordon and Betty Moore Foundation via Grant GBMF 4420, and by NSF MRSEC Grant 1420541.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F07 DCMP: One and Two Dimensional Correlated Electron Systems BCEC 109B - Konstantin Matveev, Argonne National Laboratory
11:15 AM F07.00001: Sound modes in one-dimensional quantum liquids

KONSTANTIN MATVEEV (Presenter), Argonne National Laboratory, ANTON ANDREEV, University of Washington — We study sound in one-dimensional Galilean invariant quantum liquids. In contrast to classical fluids, instead of a single sound mode we find a broad range of frequencies in which the system supports two sound modes. The nature of these modes depends on the type of particles forming the quantum liquid. In systems of spin-1/2 fermions, we find the first and second sound modes propagating at two different speeds. Similarly to superfluid $^4$He, the first sound is a wave of density, whereas the second one is a wave of entropy. In spinless quantum liquids we find two hybrid sound modes, which are simultaneous oscillations of both density and entropy, with relative phase shifts 0 or π. Their speeds are nearly equal, with the difference scaling linearly with the temperature.

*Work at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division. Work at the University of Washington was supported by the U.S. Department of Energy Office of Science, Basic Energy Sciences under Award No. DE-FG02-07ER46452.

11:27 AM F07.00002: The fate of shock waves in quantum one-dimensional fluids at late times

THOMAS VENESS (Presenter), LEONID GLAZMAN, Yale Univ — Classical hydrodynamics generically leads to the formation of shock waves which, at the most basic level, correspond to nonanalyticities in the fluid density as a function of spatial coordinates. At this classical level, small and smooth perturbations inevitably lead to such shocks. It is known that in free fermionic systems such classical nonanalyticities are rounded off at the shock points due to semi-classical corrections. We investigate how shock formation eventually crosses over to the established framework of generalised hydrodynamics at late times, as well as consider the rôle of interactions in the one-dimensional shock problem.

11:39 AM F07.00003: Numerical evidence for continuous transition between Ising ferromagnet and valence bond solid in one dimension

BRENDEN ROBERTS (Presenter), SHENGHAN JIANG, OLEXEI MOTRUNICH, Caltech — We perform a numerical study of a spin-1/2 model with $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry in one dimension which demonstrates an interesting similarity to the physics of two-dimensional deconfined quantum critical points (DQCP). Specifically, we investigate the quantum phase transition between Ising ferromagnetic and valence bond solid (VBS) symmetry-breaking phases. Working directly in the thermodynamic limit using uniform matrix product states, we find evidence for a direct continuous phase transition which lies outside of the Landau-Ginzburg paradigm. In our model, the continuous transition is found everywhere on the phase boundary. We find that the magnetic and VBS correlations show identical power law exponent, which is expected from the self-duality of the parton description of this DQCP. Critical exponents vary continuously along the phase boundary and are in agreement with predictions of the field theory for this transition. We also find a regime where the phase boundary splits with the appearance of an intermediate phase of coexisting ferromagnetic and VBS order parameters, as suggested by the theory.

11:51 AM F07.00004: Photoinduced enhancement of bond-order in the one-dimensional extended Hubbard model

CAN SHAO (Presenter), Beijing Computational Science Research Center, TAKAMI TOHYAMA, Tokyo Univ of Science, Katsushika, RUBEM MONDAINI, Beijing Computational Science Research Center, HONG-GANG LUO, HANTAO LU, Lanzhou University — Using the time-dependent Lanczos technique, we investigate the short-time evolution of the half-filled one-dimensional extended Hubbard model in the strong-coupling regime, when driven by a transient laser pulse. Starting from a phase displaying charge-density wave (CDW), a steady photoinduced in-gap state in the optical conductivity is found, depending on the parameters of the laser pulse. This potentially describes similar results of a recent experiment using organic salts [Nat. Phys. 7, 114 (2011)], also subjected to external drivings. On top of that, we parametrize the conditions of the pulse so as to maximize the overlap of the time-evolving wavefunction with excited states displaying the elusive bond-ordered wave of this model, with the focus on providing a protocol to experiments for its observation. Further, we try to make a connection between the emergence of this order and the formation of the aforementioned in-gap state, comparing with different types of excitations on the ground state.
12:03PM F07.00005: Competing orders in the one-dimensional Su-Schrieffer-Heeger model*  MANUEL WEBER
(Presenter), Department of Physics, Georgetown University, MARTIN HOHENADLER, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg — We study the phase diagram of the one-dimensional spinless Su-Schrieffer-Heeger (SSH) model at half filling as a function of phonon frequency and electron-phonon coupling. In the adiabatic limit of static phonons (vanishing phonon frequency), the ground state is well understood to be a bond-ordered Peierls state that supports topological excitations at domain walls. In the antiadiabatic limit (infinite phonon frequency), the model maps onto the t-V model with a Luttinger liquid phase below and charge-density-wave order above a critical coupling. Using a recently developed directed-loop quantum Monte Carlo method for retarded interactions [1], we study the competition between these orders at finite phonon frequencies.


*Manuel Weber is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award DE-FG02-08ER46542.

12:15PM F07.00006: Critical Entanglement for the Half-Filled One-Dimensional Extended Hubbard Model*  JON SPALDING (Presenter), SHAN-WEN TSAI, University of California, Riverside, DAVID K CAMPBELL, Physics, Boston University — A fundamental problem in many-body physics is the characterization and classification of the ground states for materials involving strongly correlated electrons. For the Extended Hubbard Model at half-filling in one dimension, this has historically required challenging Quantum Monte Carlo or DMRG calculations for large system sizes in order to extract phase diagram information. Within the last two decades, advances in quantum information theory, and in particular, conformal field theory results for entanglement entropy scaling, have enabled unprecedented accuracy in computing critical properties of ground states. In this talk, we present new techniques based on conformal field theory that enable rapid, cheap extraction of critical points and critical exponents at both 2nd order and BKT transitions for open-boundary DMRG wave functions. The results of our study of the Extended Hubbard Model point to the broad applicability of the approach.

*This research was supported in part by the NSF under grant DMR-1411345 and by UCR's GRMP fellowship (Winter 2016).
This work used the Extreme Science and Engineering Discovery Environment (XSEDE) COMET at the San Diego Supercomputer Center through allocation TG-DMR170082.

12:27PM F07.00007: Crossovers and critical scaling in the one-dimensional transverse-field Ising model*  JIANDA WU (Presenter), Tsung-Dao Lee Institute, LIJUN ZHU, University of California, Riverside, QIMIAO SI, Rice University — We consider the scaling behavior of thermodynamic quantities in the one-dimensional transverse field Ising model near its quantum critical point (QCP). We find that the crossovers obey a general scaling ansatz, and so does the critical scaling behavior of the specific heat and magnetic expansion coefficient. Furthermore, the Grüneisen ratio diverges in a power-law way when the QCP is accessed as a function of the transverse field at zero temperature. However, at the critical field, upon decreasing the temperature, the Grüneisen ratio approaches a constant instead of showing the expected divergence. This unusual result can be understood in terms of a peculiar form of the quantum critical scaling function for the free energy; the contribution to the Grüneisen ratio vanishes at the linear order in a suitable Taylor expansion of the scaling function. Our results establish the telltale thermodynamic signature of a transverse-field Ising chain, and will thus facilitate the experimental identification of this model quantum-critical system in real materials.

*This work was in part supported by the NSF Grant No.DMR-1611392 and the Robert A. Welch Foundation Grant No.C-1411. Q.S. acknowledges the hospitality of the Aspen Center for Physics (the NSF Grant No. PHY-1607611).
We describe the quantum phase transition in the N-state chiral clock model in spatial dimension $d=1$. With particular couplings, such a model is in the universality class of recent experimental studies of the ordering of pumped Rydberg states in a one-dimensional chain of trapped ultracold alkali atoms. For $N=3$, the model is expected to have a direct phase transition from a gapped phase with a broken global $Z_N$ symmetry, to a gapped phase with the $Z_N$ symmetry restored. The transition has dynamical critical exponent $z\neq1$, and so cannot be described by a relativistic quantum field theory. We map the transition onto that of a Bose gas in $d=1$, involving the onset of a single boson condensate in the background of a higher-dimensional N-boson condensate. We present a renormalization group analysis of the strongly coupled field theory for the Bose gas transition in an expansion in 2-d, with 4-N chosen to be of order 2-d. At two-loop order, we find a renormalization group fixed point which can describe a direct phase transition.

*NSF Grant No. DMR-1664842, the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Research and Innovation, SS: Cenovus Energy at Perimeter Institute, SW: NIST NRC Postdoctoral Associateship award.

We show unambiguous evidence for thermal and non-thermal mechanisms behind the insulator-to-metal transition in current-driven Mott materials. Distinguishing between these two mechanisms has proven difficult due to inhomogeneity of the current distribution in the device. By reducing the dimensionality of the devices to a one dimensional nanowire, inhomogeneity is avoided, thus allowing the two different mechanisms to be identified. The differences between the switching mechanisms in two prototypical Mott materials, VO$_2$ and V$_2$O$_3$, are discussed. Our results have direct implications for applications in neuromorphic technologies.

*We acknowledge support from the Vannevar Bush Faculty Fellowship program sponsored by the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering and funded by the Office of Naval Research through grant N00014-15-1-2848.

It is shown that Majorana edge modes appear in a strongly correlated phase of semiconducting nanowires with discrete rotational symmetry in the cross section. These modes exist in the absence of spin-orbit coupling, magnetic fields and superconductivity. They appear purely due to the combination of the three-dimensional Coulomb interaction and orbital physics, which generates a fermionic condensate exhibiting a topological ground state degeneracy in a sector of the spectrum which is gapped to continuum modes. The gap can be comparable in magnitude to the topological superconducting gap in other solid-state candidate systems for Majorana edge modes, and may similarly be probed via tunnel spectroscopy.

*Villum foundation
Danish National Research Foundation

A symmetry protected topological phase (SPT) is one which cannot be smoothly deformed into a trivial phase without breaking the symmetry. The symmetry which protects the phase acts “anomalously” on the edge of the SPT - for instance, in a non-onsite manner. Here, we examine the case when the anomaly is even more severe and the effective edge Hilbert space of the SPT does not admit a local tensor-product structure.

We begin with Fidkowski and Tarantino’s lattice model for the root SPT phase for the symmetry $G= Z_2 \times Z_2^f$ in 2d in the presence of an edge. Each site in the edge carries an Ising spin, and each domain wall hosts a Majorana fermion, so the size of the boundary Hilbert space does not scale simply with the number of sites. We introduce a description of this Hilbert space akin to the Jordan-Wigner bosonization of a fermion chain and find the action of the $Z_2$ symmetry on it. We construct a 3-site Hamiltonian which respects the $Z_2$ symmetry and find strong numerical evidence that it realizes an Ising CFT where the $Z_2$ symmetry acts as Kramers-Wannier duality.

*NSF GRFP
1:27PM F07.00012: Localization and Entanglement in Two-Dimensional Itinerant SYK Model† TZE TZEN ONG (Presenter), University of Tokyo — We study a two dimensional itinerant SYK model with a linear dispersion, and by an asymptotic power series solution of the large-N saddle point equations, we find that the random SYK interactions result in formation of localized bound states. We will also discuss localization and entanglement phenomenon from calculating the density-density correlation function and the out-of-time-correlation function.

†Japan Science and Technology Agency (JST) CREST

1:39PM F07.00013: Non-Linear transport in low density 2D hole systems‡ DMITRII KRUGLOV (Presenter), ANDREI KOGAN, Physics, University of Cincinnati, CHIEH-WEN LIU, XUAN GAO, Physics, Case Western Reserve University, LOREN PFEIFFER, KENNETH WEST, Princeton University — We report measurements of non-linear magnetotransport in 10 nm wide p-doped GaAs/Al0.1Ga0.9As quantum wells with low hole density (n ~ 10¹⁰ cm⁻²) and high mobility (m ≈ 5 x 10⁵ cm²/Vs). The Quantum Hall plateau-to-plateau transitions exhibit a universal dependence on bias voltage. We compare the results to theoretical predictions by assuming that the narrowing of the plateaus is caused by the temperature rise in the sample caused by the Joule heating. We find a good qualitative agreement with the predictions, but, surprisingly, the data show a stronger dependence on bias in the zero-bias limit than the theory suggests. We also discuss the high-frequency rectification spectroscopy as an approach for exploring dynamic effects in low-density hole systems and, in particular, the physics of insulating phases in two-dimensional transport at low carrier densities.

‡The work at CWRU was funded by the NSF (DMR-1607631). The work at UC was founded by the NSF (DMR-1206784). The work at Princeton University was funded by the Gordon and Betty Moore Foundation, and by the NSF MRSEC (Grant# 1420541).

1:51PM F07.00014: Magnetoresistance at the 2D MIT: Evidence of Micro-emulsion Phases§ SHIQI LI (Presenter), QING ZHANG, POUYAN GHAEMI, MYRIAM SARACHIK, Physics, City College of New York — Measurements of the in-plane magnetic field Bsat required to achieve full polarization of the electron spins in the strongly interacting two-dimensional electron system in a silicon MOSFET (Metal-Oxide-Semiconductor-Field-Effect Transistor) reveal the occurrence of a phase transition at a well-defined critical electron density for the metal-insulator transition determined from resistivity measurements. The behavior of Bsat as a function of electron density is consistent with the presence of a mixed, electronic micro-emulsion phase proposed by Spivak and Kivelson [1].

§Work supported by NSF grant DMR-1309008, BSF Grant 2012210. PG acknowledges support by NSF EFRI-1542863 and a PSC-CUNY Award.

2:03PM F07.00015: Phase diagrams of pi-flux quantum spin liquid in kagome lattice HYEOK-JUN YANG (Presenter), SUNGBIN LEE, Korea Adv Inst of Sci & Tech — We study possible phase transitions between spin liquids and magnetically ordered states of quantum spin ice in a pyrochlore lattice. Focusing on a Kagome layer in the presence of [111] magnetic field, the modified ice rule enables the effective action to be expressed in the language of compact U(1) gauge theory. While Ising interaction defines the ground-state manifold, the spin-flip term is mapped to hopping of gauge charge after perturbation. In particular, for frustrated J, the gauge charge experiences pi-flux around the hexagon built from the triangular plaquette. Analyzing the action, the phase diagram is developed which exhibits U(1) spin liquid and out of this phase. We will also compare our results with previous relevant experiments and quantum Monte-carlo simulations.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F08 DCMP: Superconductivity: Copper Oxide - Spectroscopy BCEC 150 - Ricardo Lobo, ESPCI ParisTech
11:15AM F08.00001: Terahertz spectroscopy of the cuprate superconductor La$_{2-x}$Sr$_x$CuO$_4$ in the photoexcited nonequilibrium state  
HIROAKI NIWA (Presenter), NAOTAKA YOSHIKAWA, Department of Physics, The University of Tokyo, 
DONGJOON SONG, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, 
RYO SHIMANO, Cryogenic Research Center and Department of Physics, The University of Tokyo — 

Ultrafast pump-probe spectroscopy has been a promising tool to study the interplay of complex orders and to reveal hidden states of condensed matter. In particular, the high-T$_c$ cuprate superconductors provide an interesting platform since they exhibit various electronic phases such as pseudogaps, charge/spin density-waves, stripe order, and superconductivity.

Here, we focused on an archetypal cuprate superconductor La$_{2-x}$Sr$_x$CuO$_4$ with the doping levels of $x = 0.125$ to $x = 0.15$, and investigated the dynamics after intense photoexcitation by utilizing near-infrared (800 nm) optical pump-terahertz probe spectroscopy. In the superconducting state, after photoexcitation we observed an emergence of a peak structure in the real-part conductivity accompanied by the destruction of the superconducting coherence indicated by the redshift of the Josephson plasma resonance. The peak structure sustains for several hundreds of picoseconds after the excitation and its height is strongly dependent on the excitation intensity. The doping dependence of the photoexcited state suggests the correlation between the peak structure and superconductivity.

11:27AM F08.00002: C-Axis Spectra of La$_{2-x}$Ba$_x$CuO$_4$ in the Normal and Superconducting State  
VLADIMIR MARTINEZ (Presenter), LUYI YAN, DAVID TANNER, Department of Physics, University of Florida, Gainesville, FL, USA, 32611, GENDA GU, Brookhaven National Labs, Long Island, NY, USA, 11973 — Reflectance spectra of superconducting La$_{2-x}$Ba$_x$CuO$_4$ have been studied for polarization parallel to the c-axis in a wide frequency range from 20-35,000 cm$^{-1}$, at doping from $0 \leq x \leq 0.155$ and temperatures above and below $T_c$. The samples are single crystals grown using the traveling solvent floating zone method. These samples were wet polished with alumina fine powder to make a good reflective surface. The c-axis spectra showed insulating behavior, with only lattice vibrations below the charge-transfer gap. We observed below $T_c$ no evidence for a Josephson plasma edge in the far infrared, despite seeing good superconducting behavior for the a-axis spectra. The results of annealing in an oxygen atmosphere will be discussed.

11:39AM F08.00003: Intrinsic electronic Raman spectrum and pairing symmetry in cuprate superconductors*  
HYUN-TAK KIM (Presenter), MIT & Quantum Lab., Electronics and Telecommunications Research Institute — Since the polarized electronic Raman scattering (ERS) measures the characteristics of the bulk rather than the surface, ERS data generate more accurate information. An ERS theory$^{1)$ is that, when $d_{x^2-y^2}$-wave symmetry is assumed, $I(\omega) \approx \omega$, linear behaviour in the $B_{2g}$ mode and $II(\omega) \approx \omega^3$ for the $B_{1g}$ mode were calculated below an energy gap. ERS experiments$^{1,2)$ showed the linear behaviour in the $B_{2g}$ mode of the node area below $T_c$ for underdoped cuprate crystals. This is evidence of $d$-wave symmetry. However, since the measured data in inhomogeneous crystals with at least two phases has an averaged effect of the two phases to the measurement region, the measured data should be decomposed to analyze the intrinsic property. The ERS data well decomposed in an electron-doped cuprate Pr$_{2-x}$Ce$_x$CuO$_{4+\delta}$ allow us to demonstrate the intrinsic effect. Here, we show the intrinsic nonlinear Raman spectrum obtained by subtracting the pseudogap characteristic of a nonlinear from the linear Raman spectrum measured in the $B_{2g}$ mode of the node area below $T_c$. The intrinsic nonlinear behaviour implies the existence of the nodal superconducting gap denying $d$-wave pairing symmetry. 1) PRL 72, 396 (1994). 2) PRB 72, 214510 (2005).

*Supported by principal project in ETRI and MS&ICT project (2018-0-00830).
Photoinduced phase transitions in cuprate superconductors: ordering vs. doping effects
RALPH EL HAGE (Presenter), VICTOR ROUCO, ANKE SANDER, Unité Mixte de Physique, CNRS Thales, Université Paris-Sud, Université Paris Saclay, 91767 Palaiseau, France, FABIAN CUELLAR, DAVID SANCHEZ MANZANO, JACOBO SANTAMARIA, Grupo de Física de Materiales Complejos, Dpt. Física de Materiales, Universidad Complutense de Madrid, 28040 Madrid, Spain, JAVIER VILLEGAS, Unité Mixte de Physique, CNRS Thales, Université Paris-Sud, Université Paris Saclay, 91767 Palaiseau, France — Complex oxides possess an extremely rich phase diagram, in which the transitions between different ground states are triggered by small changes of the carrier density or by disorder. Interestingly, the interplay between these two mechanisms —and the resulting phase— can be externally manipulated by illumination. Despite the amount of work performed on cuprate superconductors, a clear picture of the mechanisms governing photo-induced effects has not emerged. In particular, whether doping or ordering effects are dominant has not been settled. Here we investigate that through light illumination effects in oxygen deficient YBa$_2$Cu$_3$O$_{7-x}$ thin films in which different degrees of disorder are induced through i) changes in the growth conditions (“quenching”) and ii) ion irradiation. Generally, light induces an increase in the superconducting critical temperature and in the carrier density coupled to a decrease in the normal state resistivity. However differences in the response of quenched and irradiated samples have been observed, which suggests that light-induced ordering may play an important role in the photoinduced effects.

Infrared linear dichroism resonance in over-, under-, and optimally-doped cuprate superconductors
JUNGRYEOL SEO (Presenter), ALOK MUKHERJEE, MUMTAZ MURAT ARIK, DEEPU GEORGE, ANDREA MARKELZ, JOHN CERNE, University at Buffalo, The State University of New York, CHAO ZHANG, HAO ZHANG, JOHN Y.T. WEI, Department of Physics, University of Toronto, PETER ARMITAGE, Department of Physics and Astronomy, Johns Hopkins University, GAD KOREN, TAL KIRZHNER, Physics department, Technion - Israel Institute of Technology — We report systematic measurements on epitaxial thin films of high-temperature cuprate superconductors using polarization sensitive measurements. We measure the complex Faraday angle at zero magnetic field as a function of temperature (10-300K), energy (3 to 2330 meV), and doping. We observe a Faraday rotation signal, which shows sample orientation dependence that can be best associated with linear dichroism (LD) [1]. The LD signal may be due to nematic charge ordering in the cuprates, as has been observed in dc Hall transport measurements [2]. The Faraday rotation signal, as large as 22 mrad near 400 meV, is strongest in under-doped films even at 300K and it shows strong frequency dependence as well as doping dependence, which provides important clues for resolving the microscopic mechanism responsible for the anisotropy.


High temperature RIXS study of charge transfer excitations in cuprates
BIQIONG YU (Presenter), School of Physics and Astronomy, University of Minnesota, KENJI ISHII, Synchrotron Radiation Research Center, National Institutes for Quantum, SHUN ASANO, MASAKI FUJITA, Department of Physics, Tohoku University, DIEGO M CASA, Argonne National Laboratory, GUICHUAN YU, MARTIN GREVEN, School of Physics and Astronomy, University of Minnesota — Resonant inelastic X-ray scattering (RIXS) is a promising technique to study momentum-resolved electronic excitations in strongly correlated materials. Here we present results of a recent Cu K-edge RIXS study on the archetypal hole-doped cuprate La$_{2-x}$Sr$_x$CuO$_4$ and electron-doped cuprate Nd$_{2-y}$Ce$_y$CuO$_4$. Our measurements, which range from low temperature (15 K) to very high temperature (1200 K), indicate distinct spectral weight changes of charge-transfer excitations below ~ 2 eV. We will make a detailed comparison of the temperature dependent charge-transfer excitations in electron- and hole- doped cuprates.

Work at the University of Minnesota funded by the Department of Energy through the University of Minnesota Center for Quantum Materials under DE-SC0016371.
12:27PM F08.00007: Doping Dependence of Charge Density Wave in Bi-2212 Cuprate Superconductors*  
HAIYU LU (Presenter), MATTHIAS HEPTING, MAKOTO HASHIMOTO, YU HE, SUDI CHEN, KEJUN XU, SLAC National Accelerator Laboratory, SHIGEYUKI ISHIDA, YOSHIYUKI YOSHIDA, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, RICCARDO ARPAIA, Chalmers University of Technology, GIACOMO GHIRINGHELLI, LUCIO BRAICOVICH, Politecnico di Milano, BRIAN MORITZ, EDWIN HUANG, SLAC National Accelerator Laboratory, KURT KUMMER, NICHOLAS B BROOKES, European Synchrotron Radiation Facility, ZHI-XUN SHEN, THOMAS DEVEREAUX, WEI-SHENG LEE, SLAC National Accelerator Laboratory — The origin of the charge density wave (CDW) in high-temperature superconductor, its interplay with superconductivity, and more importantly, to which extent it influences lattice and charge degrees of freedom remain an active area of research. To gain further insights into these questions, it is necessary to characterize its doping and temperature dependence. We performed high energy resolution momentum-resolved resonant inelastic soft x-ray scattering (RIXS) experiments at the Cu L3-edge on the high-temperature superconductor Bi2Sr2CaCu2O8+x with the doping level across the entire phase diagram (Antiferromagnetic, underdoped, optimally doped, and overdoped). Doping dependence of the CDW, the associated phonon softening, and excitations will be discussed.

*This work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under contract DE-AC02-76SF00515

12:39PM F08.00008: Anisotropically damped magnetic excitations in La2-xSrxCuO4*  
HANNAH ROBARTS (Presenter), STEPHEN HAYDEN, University of Bristol, KEJIN ZHOU, Diamond Light Source — The collective magnetic excitations in cuprate materials have been the subject of significant research to unravel their potential role in the superconducting pairing mechanism [1]. We have performed resonant inelastic x-ray scattering (RIXS) measurements on these excitations on the model cuprate superconductor La2-xSrxCuO4 with doping x=0, x=0.12 and x=0.16. We find that the line-shape of the excitations is fairly-well described by a damped harmonic oscillator response model [2]. The damping parameter is strongly q-dependent. We perform measurements along high symmetry directions and, for the doped compounds, extend beyond this to map a full portion of the Brillouin zone revealing the anisotropy of the damping of excitation. The results are compared with high-energy inelastic neutron scattering.

References

*The authors acknowledge funding and support from the Engineering and Physical Sciences Research Council (EPSRC) Centre for Doctoral Training in Condensed Matter Physics (CDT-CMP), Grant No. EP/L015544/1

12:51PM F08.00009: Photo-enhanced metastable c-axis transport in stripe ordered cuprate La1.885Ba0.115CuO4*  
KEVIN CREMIN (Presenter), JINGDI ZHANG, University of California, San Diego, CHRISTOPHER HOMES, GENDA GU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, ZHIYUAN SUN, Department of Physics, Columbia University, MICHAEL FOGLER, University of California, San Diego, ANDREW MILLIS, DIMITRI N BASOV, Department of Physics, Columbia University, RICHARD DOUGLAS AVERITT, University of California, San Diego — Numerous cuprate-based superconductors exhibit a complex interplay between spin order, charge order and superconductivity. Light-matter interaction can provide alternate pathways to initiate phase transitions via non-linear drive or by readjusting the energy landscape between competing order parameters. THz time domain spectroscopy is performed on stripe ordered La2-xBa_xCuO4 (x = 0.115) to monitor the c-axis Josephson Plasma Resonance (JPR), which acts a direct probe of the superconducting dynamics following near-infrared excitation. After photo-excitation of the superconducting state with 1.55 eV pulses, we observe the emergence of a new long lived metastable state which displays a blue shifted plasma edge. This new phase is suggestive of enhanced c-axis transport not observed in equilibrium and has implications for superconducting fluctuations appearing above Tc in the charge ordered state. We also investigate the mechanism for how the electronic transition at 1.55 eV couples to c-axis vibrational modes which may aid in the superconducting fluctuations above Tc.

*Research supported by DOE-BES under DE-SC0018218
consistent with the results at Cu

ALEXEI E KOSHELEV, ULRICH WELP, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, KAZUO

implications for THz mesa source engineering.

We find that the optimal sidewall angle varies dramatically depending on the above parameters, and we discuss its sidewall angle as a function of device geometry, doping state, emission frequency, and intended operating temperature.

The drive voltage spread can be minimized by the correct choice of mesa sidewall angle. Here we calculate the optimal CO wave vector at O K-edge is consistent with the results at Cu L3-edge. Remarkably, the correlation length of CO at O K-edge is found to be longer than that from Cu L3-edge for all measured edges, indicating a stronger charge modulation associated with O sites than Cu sites. Different from one recent report on the existence of CO in heavily over-doped region, no CO is detected at both edges in slightly over-doped sample (p=0.18).

1:15PM F08.00011: Self-heating, phase coherence, and sidewall angle in stacked intrinsic Josephson junction Bi2Sr2CaCu2O8 terahertz sources

KAREN KIHSLSTROM (Presenter), TIMOTHY BENSEMAN, Physics, CUNY Queens College, ALEXEI E KOSHELEV, ULRICH WELP, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, KAZUO KADOWAKI, Institute for Materials Science, University of Tsukuba — The extremely anisotropic high-temperature superconductor Bi2Sr2CaCu2O8 contains stacked ‘intrinsic’ Josephson junctions with a large superconducting gap energy. Mesa-shaped devices constructed from this material are therefore a promising source of coherent, continuous-wave radiation in the ‘terahertz gap’ range.

To optimize the THz emission power and linewidth performance of these devices, it is essential to create a phase-coherent state among the stacked IJJs. This in turn requires minimizing the spread in their drive voltages, which is far from trivial when the IJJs are current-biased and shunted in series. This is further complicated by self-heating in the mesa, due to the poor c-axis thermal conductivity of Bi2Sr2CaCu2O8.

The drive voltage spread can be minimized by the correct choice of mesa sidewall angle. Here we calculate the optimal sidewall angle as a function of device geometry, doping state, emission frequency, and intended operating temperature. We find that the optimal sidewall angle varies dramatically depending on the above parameters, and we discuss its implications for THz mesa source engineering.

*This research is supported by PSC-CUNY Award 60792-00-48; and by the US Department of Energy, Office of Basic Energy Sciences, under Contract No. DEAC02-06CH11357.

1:27PM F08.00012: Evolution of charge order topology across a magnetic quantum phase transition in electron-doped cuprates

MIN GU KANG (Presenter), JONATHAN PELLICARI, Massachusetts Institute of Technology, ALEX FRANO, NICHOLAS BREZNAY, Physics, University of California, Berkeley, ENRICO SCHIERLE, EUGEN WESCHKE, BESSY, Helmholtz-Zentrum Berlin, RONNY SUTARTO, FEIZHOU HE, Canadian Light Source, PADRAIC SHAFER, ELKE ARENHOLZ, Advanced Light Source, MO CHEN, KETO ZHANG, ALEJANDRO RUIZ, ZEYU HAO, SYLVIA LEWIN, JAMES G. ANALYTIS, Physics, University of California, Berkeley, YOSHIIHARU KROCKENBERGER, HIDEKI YAMAMOTO, NTT Basic Research Laboratories, TANMOY DAS, Physics, Indian Institute of Science, RICCARDO COMIN, Massachusetts Institute of Technology — Charge order is now accepted as an integral constituent of the phase diagram of cuprate high-temperature superconductors. Unlike nesting-induced Peierls density waves, the charge correlations in the CuO2 planes have been predicted to display a rich momentum space topology depending on the detailed fermiology of the system. However, to date charge order has only been observed along the high-symmetry Cu-O bond directions. Here, using resonant soft X-ray scattering, we investigate the evolution of the full momentum space topology of charge correlations in 7T-Ln2CuO4 (Ln=Nd, Pr) as a function of intrinsic electron doping. We report that, upon electron doping the parent Mott insulator, charge correlations first emerge in a hitherto-unobserved form, with full (C4v) rotational symmetry in momentum-space. At higher doping levels, the orientation of charge correlations is sharply locked to the Cu-O bond high-symmetry directions, restoring a more conventional bidirectional charge order with enhanced correlation lengths. Our charge susceptibility calculations closely reproduce the drastic evolution in the topology of charge correlations across an antiferromagnetic quantum phase transition, highlighting the interplay between spin and charge degrees of freedom in electron-doped cuprates.
1:39PM F08.00013: Study of radiation spectrum of Bi$_2$Sr$_2$CaCu$_2$O$_{8+d}$ high-\(T_c\) superconducting terahertz emitters.  
TAKANARI KASHIWAGI (Presenter), GENKI KUWANO, TAKAYUKI IMAI, SHUNGO NAKAGAWA, YUUKI TANABE, RYUSEI OTA, KENTO NAKAMURA, YUKINO ONO, YOUTA KANEKO, SHINJI KUSUNOSE, MANABU TSUJIMOTO, University of Tsukuba, TAKASHI YAMAMOTO, QuTech Delft University of Technology, HIDETOSHI MINAMI, University of Tsukuba, RICHARD KLEMM, University of Central Florida, KAZUO KADOWAKI, University of Tsukuba — In order to understand the emission characteristics of Bi$_2$Sr$_2$CaCu$_2$O$_{8+d}$ (Bi2212) high-\(T_c\) superconducting THz emitters, it is very important to clarify the Joule heating characteristics of the devices. Recently, in order to reduce the self-heating from the Bi2212-THz emitters, we have proposed a stand-alone mesa structure of Bi2212 single crystals and its sandwich structures. The radiation characteristics obtained from these devices indicate clearly that the thermal management of the THz emitters is most important issue in order to obtain good radiation performance and reproducibility. 
In order to understand the details of the radiation characteristics of above thermal managed Bi2212-THz emitters, we have studied not only radiation frequency characteristics but also radiation linewidth characteristics. We measured the radiation spectrum ranging from 0.6 to 0.9 THz by using a sub-harmonic mixer. The observed radiation linewidths at low bias conditions seem to be broader than those at high bias conditions. The radiation spectrum at lower bias point have several peaks, however, the radiation spectrum at high bias condition seems to be single peak. The details of the these radiation characteristics will be discussed.

1:51PM F08.00014: Optical perturbation of the "hole-pockets" in the underdoped high \(T_c\) superconducting cuprates* 
SIMON FREUTEL, Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany, JONATHON RAMEAU, Brookhaven National Laboratory, LAURENZ RETTIG, ISABELLA AVIGO, MANUEL LIGGES, Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany, YOSHIYUKI YOSHIDA, HIROSHI EISAKI, National Inst. Adv. Industrial Science & Technology, Tsukuba, JOHN A. SCHNEELOCH, RUIDAN ZHONG, ZHIJUN XU, GENDA GU, Brookhaven National Laboratory, UWE BOVENSIEPEN, Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany, PETER JOHNSON (Presenter), Brookhaven National Laboratory — The high \(T_c\) superconducting cuprates are considered doped Mott insulators. As a function of doping and temperature there is a crossover from this regime into a phase characterized a Marginal Fermi Liquid. Several calculations of the doped Mott insulating phase indicate that the Fermi surface defines small pockets which at higher doping levels switch to a full closed Fermi surface, characteristic of a more metallic system. Here we use femtosecond laser based pump-probe techniques to investigate the structure of the Fermi surface in underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ and compare it with that associated with the optimally doped material. We confirm the concept of a small pocket in the underdoped system consistent with theoretical predictions in this strongly correlated state.

*This work was funded by the Deutsche Forschungsgemeinschaft through Sfb 616, Sfb 1242, and SPP 1458, from the Mercator Research Center Ruhr through Grant No. PR-2011-0003, and from the European Union within the seventh Framework Program under Grant No. 280555 (GO FAST). The work at Brookhaven Laboratory was supported in part by the Center for Emergent Superconductivity (CES), an EFRC funded by the US DOE, Office of Basic Energy Sciences and in part by the Office of Science, U.S. DOE under contract number DE-SC001274.

2:03PM F08.00015: Pressure tuning of competing orders and superconductivity in Bi$_2$Sr$_{1.6}$La$_{0.4}$CuO$_6$  
JIWEI HU, JIE XIN, XIAO-JIA CHEN (Presenter), Center for High-Pressure Science & Technology Advanced Research, VIKTOR V. STRUZHKIN, ALEXANDER GONCHAROV, Geophysical Laboratory, Carnegie Institution of Washington, HAI-QING LIN, Beijing Computational Science Research Center, CHENG-TIAN LIN, Max-Planck-Institut für Festkörperforschung — Systematic measurements of Raman scattering and magnetic susceptibility are performed on an optimally doped Bi$_2$Sr$_{1.6}$La$_{0.4}$CuO$_6$ with well characterized change density wave and pesudogap. A pressure-temperature phase diagram is obtained for this superconductor. The superconducting transition temperature \(T_c\) is found to initially increase with increasing pressure and then decreases upon heavy compression after passing a maximum at a critical pressure of 15 GPa. Meanwhile, either the charge-density-wave or the pesudogap is suppressed by the applied pressure with the disappearance of their lock-in or opening temperature at the critical pressure. The significant \(T_c\) enhancement in the low-pressure region benefits from the suppression of the competing orders. The phonon frequency of the oxygen atoms in the charge reservoir is observed to be closely correlated to the evolution of \(T_c\) with pressure. Meanwhile, the emergence of the charge disorder and its growth with pressure are detected after the critical pressure, indicating its unfavorable role to superconductivity. A complete picture for superconductivity with the competing orders, reservoir layer, and charge disorder for a cuprate superconductor is thus established.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM  
Session F09 DCMP: Superconductivity in Graphene etc.
11:15AM F09.00001: Nematic superconductivity stabilized by density wave fluctuations: Application to twisted bilayer graphene

VLADYSLAV KOZII (Presenter), HIROKI ISOBE, Massachusetts Institute of Technology, JORN VENDERBOS, Department of Physics and Astronomy, University of Pennsylvania, LIANG FU, Massachusetts Institute of Technology — Nematic superconductors possess unconventional superconducting order parameters that spontaneously break rotational symmetry of the underlying crystal. In this work we propose a mechanism for nematic superconductivity stabilized by strong density wave fluctuations in two dimensions. While the weak-coupling theory finds the fully gapped chiral state to be energetically stable, we show that strong density wave fluctuations result in an additional contribution to the free energy of a superconductor with multicomponent order parameters, which generally favors nematic superconductivity. Our theory shades light on the recent observation of rotational symmetry breaking in the superconducting state of twisted bilayer graphene.

*This work is supported by DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0018945. LF is partly supported by the David and Lucile Packard Foundation. JWFV was supported by the National Science Foundation MRSEC Program, under grant DMR-1720530.

11:27AM F09.00002: Antiferromagnetically ordered Mott insulator and d + id superconductivity in twisted bilayer graphene: A quantum Monte Carlo study

TONGYUN HUANG (Presenter), LUFENG ZHANG, TIANXING MA, Beijing Normal University — Using exact quantum Monte Carlo method, we examine the recent novel electronic states seen in magic-angle graphene superlattices. From the Hubbard model on a double-layer honeycomb lattice with a rotation angle \( \theta = 1.08^{\circ} \), we reveal that an antiferromagnetically ordered Mott insulator emerges beyond a critical \( U_c \) at half filling, and with a small doping, the pairing with \( d+id \) symmetry dominates over other pairings at low temperature. The effective \( d+id \) pairing interaction strongly increase as the on-site Coulomb interaction increases, indicating that the superconductivity is driven by electron electron correlation. Our non-biased numerical results demonstrate that the twisted bilayer graphene share the similar superconducting mechanism of high temperature superconductors, which is a new and ideal platform for further investigating the strongly correlated phenomena.

*This work were supported by NSFCs (Grant. Nos. 11374034 and 11334012). We acknowledge the support of HSFC of Beijing Normal University, and phase 2 of the Special Program for Applied Research on Super Computation of the NSFC-Guangdong Joint Fund.

11:39AM F09.00003: Possible superconductivity through the magnetic exchange in transition-metal intercalated bilayer graphene

KEVIN LUCHT, Department of Physics, Florida State University, ADITI D MAHABIR (Presenter), ALEXANDRIA ALCANTARA, Department of Physics, University of North Florida, ALEXANDER BALATSKY, Los Alamos National Laboratory, Institute for Materials Science, JOSE L. MENDOZA-CORTES, Department of Physics, Florida State University, JASON HARALDSEN, Department of Physics, University of North Florida — This study examines the possibility of superconductivity in transition-metal intercalated bilayer graphene. Using density functional theory, we determine electronic and magnetic properties through the electronic structure and density of states for all ten 3d transition-metal elements in a honeycomb configuration between two layers of graphene. Through an analysis of the electron density, we assess the induction of the magnetic moment in each case, where we estimate the exchange coupling through a comparison of the ferromagnetic and antiferromagnetic configurations. Furthermore, we show that the electronic band structure of the transition-metal intercalated layers have similar characteristics to those graphene layers intercalated with alkali and alkaline-earth metals, where superconductivity has been observed. Using a similar analysis, we find that the carbon \( \pi \) bands are below the Fermi, which is a possible indicator of superconductivity. More interestingly, the \( \pi \) bands seem to be degenerate to the transition-metal \( d \) bands, which could indicate hybridization and may lead to unconventional superconductivity.

*Energy and Materials Initiative, High-Performance Computer cluster at Florida State University. Institute for Materials Science at Los Alamos National Laboratory
11:51AM F09.00004: Pairing symmetry and spontaneous vortex-antivortex lattice in superconducting twisted bilayer graphene: A Bogoliubov-de Gennes approach*  SHIZENG LIN (Presenter), YING SU, Los Alamos National Laboratory — We study the superconducting pairing symmetry in twisted bilayer graphene by solving the Bogoliubov-de Gennes equation for all electrons in Moiré supercells. With increasing the pairing potential, the system evolves from the mixed non-topological $d + id$ and $p + ip$ phase to the $s + p + d$ phase via the first order phase transition. In the time-reversal symmetry breaking $d + id$ and $p + ip$ phase, vortex and antivortex lattice accompanying spontaneous supercurrent are induced by the twist. The superconducting order parameter is nonuniform in the Moiré unit cell. Nevertheless, the superconducting gap in the local density of states is identical in the unit cell. The twist induced vortices and non-topological nature of the mixed $d + id$ and $p + ip$ phase are not captured by the existing effective models. Our results suggest the importance of long-range pairing interaction for effective models.

*Computer resources for numerical calculations were supported by the Institutional Computing Program at LANL. This work was carried out under the auspices of the U.S. DOE Award No. DE-AC52-06NA25396 through the LDRD program, and was supported by the Center for Nonlinear Studies at LANL and the U.S. DOE Office of Basic Energy Sciences Program E3B5 (S.-Z. L.).

12:03PM F09.00005: Quantum Monte Carlo Study of Metal-Insulator Transitions on the Honeycomb Lattice  JINGYAO WANG (Presenter), TIANXING MA, Beijing Normal University — We investigate the band insulator-metal-Mott insulator transitions in the ionic Hubbard model on the 12*12 honeycomb lattice at half filling using determinant quantum Monte Carlo method. The phase diagram as a function of interaction U and staggered potential Δ indicates that the metallic state develops only if the interaction value varies in a moderate range. The Mott insulator state is antiferromagnetic. The conductivity decreases as the lattice size increases in metallic phase. A qualitative contrast to results obtained using the dynamical mean field theory is made at the end.

12:15PM F09.00006: Carbon-nanotube based highly flexible superconducting wire*  JEONG-GYUN KIM (Presenter), Sungkyunkwan University, HAEYONG KANG, Pusan University, DONGSEOK SUH, Sungkyunkwan University — In this work, we explored the feasibility of new fabrication of superconducting wire by using carbon nanotube (CNT) based yarn combined with superconducting materials. CNT yarn has been extensively studied due to its various outstanding mechanical properties. And it also could show multifunctional characteristics by combining with various guest materials. Here, we used a sputter-deposition process for niobium nitride (NbN) to make superconducting yarn. It shows superconducting property that is not much different from NbN film. And also we showed the superior mechanical flexibility of the sample by performing as knot tying and bending. In addition, we tested to reduce the resistance in the normal state for the practical necessity such as superconducting cable application.

*Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Department of Energy Science, Sungkyunkwan University, Suwon 16419, Korea.

12:27PM F09.00007: Theory of insulating phase and superconductivity in twisted bilayer graphene*  XINGYU GU (Presenter), EVAN LAKSONO, CHUAN CHEN, JIA NING LEAW, NIMISHA RAGHUJUVANSHI, SHAFFIQUE ADAM, Department of Physics, National University of Singapore — A correlated insulating phase and superconductivity have been recently observed in twisted bilayer graphene (tBG). We study theoretically these two phases in both the weak and strong coupling limit. We study theoretically these two phases in both the weak and strong coupling limit. In the weak coupling limit, using the random phase approximation, we find various possible combinations of density wave phases and pairing symmetries [1]. In the strong coupling limit, the insulating phase is anti-ferromagnetically (AFM) ordered, like in monolayer graphene [2]. However, we find there is no local magnetic moment in this AFM phase due to the special form of Wannier functions. Using the spin-fermion model, we find attractive electron-electron interaction mediated by the critical AFM fluctuations. This attractive interaction leads to chiral $d + id$ superconductivity. Using a finite size tight-binding model, we show explicitly the existence of edge Majorana modes.


*We acknowledge the Singapore Ministry of Education AcRF Tier 2 (MOE2017-T2-2-140) and National University of Singapore Department of Physics.
12:39PM F09.00008: Competing pairing propensities in twisted bilayer graphene

XIANXIN WU (Presenter), MARIO FINK, MICHAEL KLETT, Institut für Theoretische Physik und Astrophysik, Julius-Maximilians-Universität Würzburg, TIM WEHLING, Institute for Theoretical Physics, Bremen Center for Computational Material Science, University of Bremen, WERNER R HANKE, RONNY THOMALE, Institut für Theoretische Physik und Astrophysik, Julius-Maximilians-Universität Würzburg — We employ a synopsis of random phase approximation (RPA) and functional renormalization group (fRG) to investigate twisted bilayer graphene based on a two-orbital effective model on the honeycomb lattice. Exploiting the ability of N-patch fRG to resolve the harmonic composition of a given superconducting instability channel, we develop a detailed profile of electronically mediated unconventional superconducting instabilities in twisted bilayer graphene, and highlight experimental signatures to distinguish between the resulting possible scenarios.

12:51PM F09.00009: Magnetic and superconducting correlation in monolayer and twisted-bilayer graphene

TIANXING MA (Presenter), TONGYUN HUANG, LUFENG ZHANG, Beijing Normal University — Using exact quantum Monte Carlo method, we identify the phase diagram of the half filled, the lightly doped and heavily doped graphene, which shows a rather rich physical properties. At half filling, the system is driven to a Mott insulator with antiferromagnetic long range order by increasing interaction, and a transition from a d+id pairing to a p+ip pairing is revealed, depends on the next-nearest hoping and the electronic fillings. We also examine the recent novel electronic states seen in magic-angle graphene superlattices. From the Hubbard model on a double-layer honeycomb lattice with a rotation angle θ=1.08, we reveal that an antiferromagnetically ordered Mott insulator emerges beyond a critical U c at half filling, and with a small doping, the pairing with d+id symmetry dominates over other pairings at low temperature. The effective d+id pairing interaction strongly increase as the on-site Coulomb interaction increases, indicating that the superconductivity is driven by electron-electron correlation. Our non-biased numerical results demonstrate that the twisted bilayer graphene is a new and idea platform for further investigating the strongly correlated phenomena.

*This work was supported by the Natural Science Foundation of China (NSFC) (Nos. 11774033 and 11334012).

1:03PM F09.00010: Strain induced superconducting pair-density-wave states in graphene

CHUNG-YU MOU (Presenter), Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, FENG XU, School of Physics and Telecommunication Engineering, Shaanxi University of technology, Hanzhong, China, CHUNG-HOU CHUNG, Electrophysics Department, National Chiao-Tung University, Taiwan, TING-KUO LEE, Institute of Physics, Academia Sinica, Taiwan — Graphene is known to be non-superconducting. However, surprising superconductivity is recently discovered in a flat-band in a twisted bi-layer graphene. Here we show that superconductivity can be more easily realized in topological flat-bands induced by strain in graphene through periodic ripples. Specifically, it is shown that by including correlation effects, the chiral d-wave superconductivity can be stabilized under strain even for slightly doped graphene. The chiral d-wave superconductivity generally coexists with charge density waves (CDW) and pair density waves (PDW) of the same period. Remarkably, a pure PDW state with doubled period that coexists with the CDW state is found to emerge at a finite temperature region under reasonable strain strength. The emergent PDW state is shown to be superconducting with non-vanishing superfluid density, and it realizes the long searched superconducting states with non-vanishing center of mass momentum for Cooper pairs.

*We acknowledge support from the Ministry of Science and Technology (MoST), Taiwan. In addition, we also acknowledge support from Center for Quantum Technology, TCECM, and Academia Sinica Research Program on Nanoscience and Nanotechnology, Taiwan.

1:15PM F09.00011: Effective model for Majorana modes in graphene

ANTONIO MANESCO (Presenter), DURVAL RODRIGUES JUNIOR, GABRIEL WEBER, University of Sao Paulo — It was recently proposed that the interface between a graphene nanoribbon in the canted antiferromagnetic quantum Hall state and an s-wave superconductor may present topological superconductivity, resulting in the appearance of Majorana zero modes [1]. However, a description of the low-energy physics in terms of system parameters was still missing. Starting from a mean-field continuum model for graphene in proximity to a superconductor, we derive the low-energy effective Hamiltonian describing the interface of this heterojunction from first principles. A comparison between tight-binding simulations and analytical calculations with effective masses suggests that normal reflections at the interface must be considered in order to fully describe the low-energy physics.


*The work of ALRM was supported by FAPESP grant No. 2016/10167-8. DRJ is a CNPq researcher.
Bulk supercurrent at high magnetic field in Graphene Josephson junctions  
RUOYU CHEN (Presenter), YULU LIU, Ohio State University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, CHUN NING LAU, Ohio State University — Benefitted from its high mobility and gate-tunability, graphene could serve as an ideal platform hosting many innovative devices. Introducing superconductivity into graphene via proximity provides a path to complicated or large-scale graphene-based superconducting devices/circuits, and the combination of quantum Hall edge states and superconductivity may host Majorana Fermions which allows Fault-tolerant quantum computing. Here we report our efforts fabricating hBN-encapsulated graphene Josephson junctions in various geometries. While small supercurrent hosted by quantum Hall edge states has been reported in graphene before, we observed gate-tunable bulk supercurrent at moderate charge densities and magnetic fields up to 3 T. Latest data and comparison with theoretical models will be presented.

Andreev reflection in Graphene–superconductor junctions in the quantum Hall regime*  
JOSEPH CUOZZO (Presenter), STUART THOMAS, XIANG HU, ENRICO ROSSI, Physics, William & Mary — We investigate the Andreev reflection at an interface between a graphene layer in the quantum Hall regime and a superconductor. In graphene due to the spin and valley degrees of freedom there is an approximate SU(4) symmetry. The breaking of this symmetry due to interactions and the Zeeman effect leads to a splitting of the Landau levels. In this talk I will discuss the effect on the Andreev reflection of the breaking of the Landau levels' spin and valley degeneracy. I will then show results for the Andreev reflection amplitude, and the Andreev reflection contribution to the interface conductance, for various degrees of transparency of the interface.

*Work supported by ARO and ONR.

Coherent transport and electron interference in cuprate superconductor/graphene junctions*  
D PERCONTE, Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris Saclay, Palaiseau, France, CHRISTIAN ULYSSE, Centre de Nanosciences et de Nanotechnologies, CNRS, Université Paris-Saclay, Palaiseau, France, D BERCIOUX, Donostia International Physics Center, San Sebastian and IKERBASQUE, Bilbao, Spain, J TRASTOY, ANKE SANDER, SOPHIE D’AMBROSIO, Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris Saclay, Palaiseau, France, P. R. KIDAMBI, S HOFMANN, Department of Engineering, University of Cambridge, Cambridge, UK, BRUNO DLUBAK, PIERRE SENEOR, Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris Saclay, Palaiseau, France, F. SEBASTIAN BERGERET, Centro de Fisica de Materiales, CSIC-UPV/EHU, San Sebastian, Spain, JAVIER VILLEGAS (Presenter), Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris Saclay, Palaiseau, France — Proximity-induced superconductivity is particularly interesting in graphene. Among other reasons, because that effect can be externally controlled by tuning the Fermi energy (and vector) via electrical gating. For example, using high-temperature superconducting YBa2Cu3O7/graphene planar junctions, we recently demonstrated [1] gate-controlled superconducting electron interferences that allow modulating the Andreev reflection at the superconductor/graphene interface via Klein tunneling of electron/hole pairs. Here we will discuss new experiments in the same type of junctions, in which a different type of interferences –this time controlled by the bias voltage– are observed which are due to geometrical resonances and coherent propagation of electron/hole pairs across a graphene channel. This is substantiated by the relationship of the oscillations period and the graphene channel length (up to hundreds on nm), as well as by numerical simulations of the device conductance -which reproduce both the observed resonances and the background conductance. [1] D. Perconte et al. Nature Physics 14, 25 (2018)

*Work supported by the ERC grant 647100, ANR grants ANR-15-CE24-0008-01 and ANR-17-CE30-0018-04, and COST Action CA16218 “NanoCoHybri”

Tuesday, March 5, 2019 11:15 AM - 1:27 PM

Session F10 DMP GMAG: Fe-based Superconductors -- Magnetic properties  
BCEC 151B · Minjun Lee, Seoul National University
11:15AM F10.00001: Hedgehog spin-vortex crystal antiferromagnetic quantum criticality in \( \text{CaK(Fe}_{1-x}\text{Ni}_x\text{)}_4\text{As}_4 \) revealed by NMR

QING-PING DING (Presenter), WILLIAM MEIER, Ames Laboratory and Dept. of Phys. and Astro., Iowa State Univ., JINFANG CUI, Ames Laboratory and Dept. of Chem., Iowa State Univ., MINGYU XU, ANNA BOEHMER, SERGEY BUDKO, PAUL CANFIELD, YUJI FURUKAWA, Ames Laboratory and Dept. of Phys. and Astro., Iowa State Univ. — Two degrees of freedom, antiferromagnetism and nematicity, have been observed in most iron-based superconductors (SCs). In contrast to those compounds, the newly discovered SC \( \text{CaK(Fe}_{1-x}\text{Ni}_x\text{)}_4\text{As}_4 \) exhibits an antiferromagnetic (AFM) state, called hedgehog spin-vortex crystal (SVC) structure, without the orthorhombic distortion [1,2]. This system provides an opportunity to investigate the relationship between magnetic fluctuation and SC in a system that remains tetragonal. Here, we report an \(^{75}\text{As} \) nuclear magnetic resonance (NMR) study of \( \text{CaK(Fe}_{1-x}\text{Ni}_x\text{)}_4\text{As}_4 \) (0 \( \leq x \leq 0.049 \)). We will show the experimental evidence which suggests that, based on NMR data [3], a hedgehog SVC quantum-critical point (QCP) would exist around \( x = 0 \) in the normal state, but is avoided due to the onset of superconductivity. We will discuss the relationship of spin fluctuations and superconductivity in this system. Furthermore, the advantage of \( \text{CaKFe}_4\text{As}_4 \) over other iron-based SCs with QCP will also be discussed.


*This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

11:27AM F10.00002: Unusually stronger quantum fluctuation with larger spins: Novel phenomena revealed by emergent magnetism in pressurized high-temperature superconductor FeSe

WEI KU (Presenter), Tsung-Dao Lee Institute, YUTING TAN, School of Physics, Sun Yat-sen University, TIANYU ZHANG, School of Physics and Astronomy, Shanghai Jiao Tong University, TAO ZOU, Department of Physics and Astronomy, Michigan State University, ANTONIO M. DOS SANTOS, Quantum Condensed Matter Division, Oak Ridge National Laboratory, JIN HU, Department of Physics and Engineering Physics, Tulane University, DAO-XIN YAO, School of Physics, Sun Yat-sen University, ZHIQIANG MAO, Department of Physics and Engineering Physics, Tulane University, XIANGLIN KE, Department of Physics and Astronomy, Michigan State University — A counter-intuitive enhancement of quantum fluctuation with larger spins, together with a few novel physical phenomena, is discovered in studying the recently observed emergent magnetism in high-temperature superconductor FeSe under pressure. Starting with experimental crystalline structure from our high-pressure X-ray refinement, we analyze theoretically the stability of the magnetically ordered state with a realistic spin-fermion model. We find surprisingly that in comparison with the magnetically ordered Fe-pnictides, the larger spins in FeSe suffer even stronger long-range quantum fluctuation that diminishes their ordering at ambient pressure. This “fail-to-order” state then develops into an ordered state above 1GPa due to weakened fluctuation accompanying the reduction of anion height and carrier density. We further clarify the controversial nature of magnetism and its interplay with nematicity in FeSe in the same unified picture for all Fe-based superconductors. Our study establishes a generic exceptional paradigm of stronger quantum fluctuation with larger spins that complements the standard knowledge of insulating magnetism.

*Support from NSFC 11674220, 11474601, 11574404, 2015A030313176 and CMST 2016YFA0300500 and 2016YFA0300501

11:39AM F10.00003: Tuning the Magnetic and Superconducting Properties of Hole Doped BaFe\(_2\)As\(_2\): A Universal Scaled Phase Diagram

OMAR CHMAISSEM (Presenter), RYAN STADEL, Northern Illinois University, DANIEL BUGARIS, RAYMOND OSBORN, STEPHAN ROSENKRANZ, Argonne National Laboratory — Embarking on an extensive effort in which more than fifty hole-doped BaFe\(_2\)As\(_2\) samples have been produced and characterized by neutron diffraction allowed us to extract universal behaviors and properties of this rich system. All the measured magnetic and superconducting transitions values collapse into a single phase diagram. Strontium, calcium, and sodium substitutions at the barium site enabled the production of many samples in which both the re-entrant tetragonal double-Q magnetic C\(_4\) and the orthorhombic SDW magnetic C\(_2\) phases coexist and compete with superconductivity just before reaching the peak of the superconductivity-only region of the phase diagram. The evolution of \( T_N, T_c \) and the internal structural parameters are in agreement with recent theoretical models that correlate the stability of these observed phases with approaching a perfect tetrahedral FeAs\(_4\) angle and perfect Fermi surface nesting. Our results separate the individual roles played by either the As-Fe-As bond angles or the Fe-As bond lengths and demonstrate their combined effects in tuning the magnetic and superconducting properties.

*Work at the Materials Science Division at Argonne National Laboratory was supported by the US Department of Energy, Office of Science, Materials Sciences and Engineering Division.
11:51AM F10.00004: Possible multiple modes of neutron spin resonance in Ba$_{1-x}$K$_x$Fe$_2$As$_2$ and BaFe$_{2-x}$Ni$_x$As$_2^*$

HUIQIAN LUO, TAO XIE, SHILIANG LI, Institute of Physics, Chinese Academy of Sciences, UWE STUHR, TOM FENNELL, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, SERGEY DANILKIN (Presenter), Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organization — Motivated by the triple modes of neutron spin resonance with both odd and even L-symmetries in CaKFe$_4$As$_4$[1], we use inelastic neutron scattering to re-investigate the spin resonance in 122 system of iron-based superconductors. In the optimally hole doped Ba$_{1-x}$K$_x$Fe$_2$As$_2$, the spin resonance has very weak L-dependence both for intensity and center energy, while the H-dependence show a combination with an incommensurate mode at high energy and a commensurate mode at low energy. In the optimally electron doped BaFe$_{2-x}$Ni$_x$As$_2$, the spin resonance becomes L-dependent at low energy. A very weak even mode (L=2, 4, 6...) probably exist around 14 meV. Therefore, in contrast to the explanation based on weak L-dispersion on single spin resonance mode, we propose an alternative explanation based on the multiply Fermi surface nesting induced multi-modes with different symmetries, which give Q-dependent intensity either for out-of-plane or in-plane spin excitations.


*This work is supported by NSFC, MOST and CAS.

12:03PM F10.00005: Multiple Distinct Magnetic and Superconducting Phases in LaFeAs$_{1-x}$P$_x$O 1111 Characterized Via X-ray and Neutron Diffraction*

RYAN STADEL (Presenter), Northern Illinois University, MATTHEW KROGSTAD, STEPHAN ROSENKRANZ, RAYMOND OSBORN, Materials Science Division, Argonne National Laboratory, KEITH TADDEI, HFIR, Oak Ridge National Laboratory, DMITRY KHALYAVIN, ISIS, Rutherford Appleton Laboratory, JINKE BAO, DUCK YOUNG CHUNG, Materials Science Division, Argonne National Laboratory, OMAR CHMAISSEM, Northern Illinois University — Following the discovery of the microscopic co-existence of antiferromagnetic spin density waves and superconductivity in Ba$_{1-x}$K$_x$Fe$_2$As$_2$ and the low temperature structural re-entrance to the novel magnetic C$_4$ tetragonal phase in Ba$_{1-x}$Na$_x$Fe$_2$As$_2$, an effort was made to seek similar phases in the related LaFeAs$_{1-x}$P$_x$O 1111 system. Previous work had reported two superconducting domes as well as two distinct magnetic regions. While the low doping magnetic phase had been well characterized by neutron diffraction, the higher doped magnetic region had been deduced from short range $^{31}$P-NMR measurements. We present a detailed characterization of the nuclear and magnetic structures based on high resolution and high intensity x-ray and neutron powder and single crystal diffraction. Our work demonstrates distinct magnetic symmetries for the two magnetic regions of the phase diagram.

*Work at the Materials Science Division at Argonne National Laboratory was supported by the US Department of Energy, Office of Science, Materials Sciences and Engineering Division.

12:15PM F10.00006: Anisotropic spin excitations in detwinned parent iron pnictides

QIMIAO SI (Presenter), Rice University, CHANGLE LIU, Fudan University, XINGYE LU, Beijing Normal University, PENGCHENG DAI, Rice University, RONG YU, Renmin University of China — Motivated by recent inelastic neutron scattering measurement on the fully detwinned BaFe$_2$As$_2$, we study the spin excitations of a local-moment model in the (π,0) collinear antiferromagnetically ordered phase. We show that the spin quadrupole modes can provide significant contributions to the spin excitation spectrum at high energies, and demonstrate this effect in an S=1 frustrated spin model with bilinear-biquadratic interactions using a flavor wave approach in an SU(3) representation. As a combined effect of the magnons and quadrupole modes, the spin excitation anisotropy drops with increasing energy. Our results are in good agreement with the salient features of the experimental observation.
12:27PM F10.00007: Breaking of four-fold rotational symmetry driven by stripe-type magnetism in semiconducting KFe$_{0.8}$Ag$_{1.2}$Te$_2$  
YU SONG (Presenter), University of California, Berkeley, HUIBO CAO, BRYAN C. CHAKOUMAKOS, Oak Ridge National Laboratory, YANG ZHAO, NIST Center for Neutron Research, National Institute of Standards and Technology, AIFENG WANG, HECHANG LEI, CEDOMIR PETROVIC, Brookhaven National Laboratory, ROBERT J BIRGENEAU, University of California, Berkeley — Superconductivity in the iron pnictides and chalcogenides emerges in the vicinity of an electronic nematic state, whose driving force remains controversial. We use X-ray and neutron scattering to study the semiconducting alkaline metal iron chalcogenide KFe$_{0.8}$Ag$_{1.2}$Te$_2$, that is structurally analogous to the prototypical iron pnictide BaFe$_2$As$_2$. We find that KFe$_{0.8}$Ag$_{1.2}$Te$_2$ realizes isolated 2x2 Fe blocks, separated by nonmagnetic Ag atoms. Long-range magnetic order sets in below $T_N = 35$ K, with magnetic moments within each Fe block ordering into a stripe-type configuration. A structural transition that breaks four-fold rotational symmetry of the lattice accompanies the magnetic transition, resulting in different lattice spacings along the two orthogonal Fe-Fe bond directions. This difference in lattice spacings is similar to that in BaFe$_2$As$_2$ in magnitude, and like BaFe$_2$As$_2$, the lattice spacing is longer along the antiferromagnetically aligned Fe-Fe direction. Since KFe$_{0.8}$Ag$_{1.2}$Te$_2$ is a semiconductor, local-moment magnetism is likely responsible for driving the breaking of four-fold rotational symmetry, and similar magnetic interactions may play an important role in the superconducting alkaline metal iron chalcogenides.

12:39PM F10.00008: Study of the pressure on magnetism in spin-ladder superconductor BaFe$_2$Se$_3$  
SHAN WU (Presenter), ROBERT J BIRGENEAU, University of California, Berkeley, JUNJIE YIN, MENG WANG, Sun Yat-Sen University, BENJAMIN FRANDSEN, Brigham Young University, TOM FORREST, Diamond light source, CRAIG L. BULL, NICK FUNNELL, ISIS Facility, Rutherford Appleton Laboratory, GEDIMINAS SIMUTIS, RUSTEM KHASANOV, Paul Scherrer Institute, THOMAS SMART, University of California, Berkeley, MARTIN KUNZ, ANDREW DORAN, Advanced Light Source, Lawrence Berkeley — Magnetic fluctuations were proposed as important for the pairing glue to the unconventional superconductivity (SC). The proximity of an antiferromagnetic (AFM) ordered has been found ubiquitously, with the majority of the iron-based superconductors exhibiting the same two-dimensional square lattice structural motif. Optimal SC typically appears when the magnetic order is suppressed by applying pressure or doping carriers. Pressure-induced SC in the BaFe$_2$X$_3$ (X=Se,S) introduces a quasi-one-dimensional prototype for the studies of the unconventional SC\cite{1,2}. BaFe$_2$Se$_3$ shows a block-type AFM transition below $T_N = 256$ K. By applying pressure, the Mott insulating state is gradually suppressed and displays a SC dome above 10 Gpa similar to the BaFe$_2$S$_3$. In this talk, I will present a systematic study of the magnetic and structural properties under hydrostatic pressure in BaFe$_2$Se$_3$ using neutron diffraction, x-ray diffraction and muon spin relaxation techniques. These provide the information on how the magnetic phase evolves approaching the SC and compares to the case of BaFe$_2$S$_3$. \cite{1}H. Takahashi,et al.,Nat. Mater.(2018).\cite{2}J. Ying,et al.,PRB (2017).

12:51PM F10.00009: Quantum critical point in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ from London penetration depth measured by optical NV magnetometer  
KAMAL JOSHI (Presenter), NAUFER M NUSRAN, KYUIL CHO, MAKARIY TANATAR, SERGEY L. BUD'KO, PAUL CANFIELD, Ames Laboratory and Iowa State University, Ames, IA, USA, ALEX LEVCHENKO, University of Wisconsin, Madison, WI, USA, RUSLAN PROZOROV, Ames Laboratory and Iowa State University, Ames, IA, USA — Lower critical field, $H_{c1}$, allows direct access to London penetration depth, $\lambda$, which provides an insight into the normal-state electronic properties inside the dome of superconductivity in temperature-doping phase diagram. Using recently developed minimally invasive optical NV-centers magnetometry and the revised demagnetization corrections, $H_{c1}$ was measured in single crystals of electron-doped Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ for several $x$-values. The measurements reveal a sharp peak in $\lambda(x)$ near $x=0.057$, exactly the composition at which the long-range magnetic order becomes commensurate. Together with previous observation of quantum critical point (QCP) under the dome of superconductivity in isovalent AsP$_{122}$, our results provide strong evidence for a ubiquitous nature of QCP in iron pnictides at the disappearance of the long-range ordered magnetism at $T=0$.

*This work is funded by the U.S. DOE, Office of Basic Energy Sciences under Contract No. DE-AC02-05-CH11231

*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract # DE-AC02-07CH11358.
Effect of variable-energy electron irradiation on superconductivity in \(\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2\) crystals

KYUIL CHO (Presenter), MAKARIY A TANATAR, YONG LIU, THOMAS ANTONY LOGRASSO, RUSLAN PROZOROV, Ames Laboratory and Iowa state University, USA, MARCIN KONCZYKOWSKI, Ecole Polytechnique, Palaiseau, France — Point-like defects produced by MeV-range electron irradiation can be used as a phase-sensitive probe of the energy gap structure in superconductors. In complex compounds, the probability of knocking out an ion from a particular lattice site depends on the type of the ion and the incoming electron energy. Here we examine the effect of irradiation on superconducting \(T_c\) and electrical resistivity of in \(\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2\) single crystals using electrons of different energies, from 1.0 MeV to 2.5 MeV. From the resistivity measurements in-situ (during irradiation) and ex-situ (in a separate cryostat), the relation between the changes in \(T_c\) and residual resistivity as a function of electron energy was determined. The results will be discussed in a broader context of the connection between particular crystal structure and superconductivity.

*Work at the Ames Laboratory was supported by the Department of Energy- Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

Mapping the superfluid density in an Iron-based Superconductor

DOOHEE CHO (Presenter), KOEN BASTIAANS, DAMIANOS CHATZOPoulos, Leiden University, GENDA GU, Brookhaven National Laboratory, MILAN P ALLAN, Leiden University — Cooper pairs can tunnel through the vacuum barrier between two superconducting electrodes, known as a Josephson junction. Depending on the properties of the junction and the environment, one can extract the superconducting order parameter from the current-voltage spectra. Here, I will present the Josephson tunneling spectroscopic results of an unconventional Fe-based superconductor acquired with a superconducting STM tip. We demonstrate the Josephson tunneling induced characteristic current-voltage curves close to zero bias on a Pb(111) surface and a Fe-based superconductor. I will discuss the spatial variations of the superfluid density in this correlated superconductor and reveal their correlation with an inhomogeneous quasiparticle density of states.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F11 DMP DCOMP FIAP: Defects in Semiconductors -- Quantum Defects

High frequency electrometry and imaging with defects in silicon carbide

GARY WOLFOWICZ (Presenter), University of Chicago — Optically active defects in wide bandgap host materials are promising sensors of local properties such as magnetic fields, electric fields, temperature and mechanical strain [1]. While magnetometry has received considerable interest owing to the spin properties of these defects, electrometry and strain sensing have been significantly more challenging due to the weak sensitivity of the ground spin state.

Here we demonstrate that the charge state of defects in silicon carbide (SiC), including divacancies and silicon vacancies, can be used to sense high frequency (MHz – GHz) electric fields and acoustics [2]. Optical excitation can convert the defect from a bright (photoluminescent) charge state to a dark charge state, and vice-versa [3]. This conversion rate depends directly on local high frequency electric fields and mechanical strains, resulting in direct modulation of the photoluminescence intensity and enabling sensing protocols. We further develop methods for spectroscopy (phase and frequency resolution) and vector measurements.

We explore electric field and strain sensing using both this novel charge technique and spin measurements in various electromechanical devices. We map the electric fields from lithographically patterned capacitors and observe mechanical modes in a surface acoustic wave resonator and in clamped membranes. We obtain 3D spatial and high frequency information typically challenging to achieve with other sensing techniques. This demonstrates the potential of optically active defects for in-situ electrical and micromechanical systems characterization in commercial materials such as SiC.


*This work was supported by AFOSR, DOE, NSF GRFP and UChicago MRSEC.
11:51AM F11.00002: Optimizing Spin Readout of the Nitrogen-Vacancy Center in Diamond with Spin-to-Charge Conversion* DAVID HOPPER (Presenter), Physics, University of Pennsylvania, JOSEPH LAUIGAN, SADHANA MARIKUNTE, LEE BASSETT, Electrical and Systems Engineering, University of Pennsylvania — The nitrogen-vacancy center in diamond is a mature platform for quantum technology, enabling sophisticated quantum information protocols as well as versatile quantum sensors operating in previously unreachable size and field regimes. The standard photoluminescence-based spin readout is fast (300 ns) but typical measurements yield only a few hundredths of a photon on average, necessitating tens of thousands of repeats to overcome shot noise in detecting the spin state. Spin-to-charge conversion (SCC) offers an alternative readout with significantly improved single-shot information. However, this benefit comes at the expense of orders of magnitude longer readout durations. Here, we present a framework for optimizing the SCC readout parameters that leads to dramatic reductions in overall measurement acquisition times [1]. The improvements arise from the combination of an analytical charge readout model with numerical optimization of the overhead durations. We discuss relevant applications such as T1 relaxometry and control of nuclear registers and outline how other spin readout methods can benefit from this framework.


*This work was supported by NSF CAREER award EECS-1553511.

12:03PM F11.00003: Coupled defect centers for diamond quantum nodes* MAARTEN DEGEN (Presenter), SUZANNE VAN DAM, JOE RANDALL, ALETTA MEINSMA, RONALD HANSON, TIM HUGO TAMINIAU, Delft University of Technology — Nitrogen-vacancy (NV) defect centers in diamond are well-suited to realize quantum networks owing to a coherent spin ground state, nuclear quantum memories and an optical transition for remote entanglement. State-of-the-art experiments with single NV centers used 13C atoms as quantum memories to perform entanglement distillation and quantum error correction [Kalb et. al., Science, 2017, Cramer et al., Nat. Commun., 2015]. Such experiments involve an intrinsic trade-off: reducing the coupling to the NV center improves 13C quantum memories, but reduces gate speeds.

In this work, we aim to extend the possibilities of quantum networks by creating systems of two or more coupled defects centers in diamond. Such coupled defects, hold the promise to combine fast gates with well-isolated quantum nuclear memories. I will present recent progress towards this goal.

First, we realized a long coherence time, exceeding two seconds, of the host nitrogen spin of a single NV center, demonstrating its potential as a quantum memory. Second, I will discuss our recent progress using ion implantation and other techniques to realize coupled defects.

*We thank the NanoFront joined program, the Kavli Institute of Nanoscience and NWO for their support.

12:15PM F11.00004: Linewidth of NV-detected Electron Spin Resonance* BENJAMIN FORTMAN (Presenter), SUSUMU TAKAHASHI, University of Southern California — A nitrogen-vacancy (NV) center in diamond possesses unique electronic, magnetic and quantum properties enabling magnetic field sensing through optically detected magnetic resonance (ODMR). Due to the extreme sensitivity of an NV center to magnetic fields, the NV is a promising candidate for applications of electron spin resonance (ESR) with single spin sensitivity. In addition to the sensitivity, ESR using a single NV has a significant advantage in spatial resolution of the detection volume over conventional ESR because of the nanometer sensing distance on single NV-detected ESR. In this presentation, we discuss the linewidth of NV-detected ESR. In the experiment, we study NV-detected ESR on substitutional nitrogen centers in diamond and identify components partially contributing to the linewidth. We also discuss differences of the ESR linewidth between conventional and NV-based detection.

*This work was supported by the Searle Scholars Program and the National Science Foundation (DMR-1508661 and CHE-1611134).
12:27PM F11.00005: Ab-initio photoluminescence spectrum of NV⁻ centres by Time-Dependent Density Functional Theory  
AKIB KARIM (Presenter), Quantum Photonics Laboratory, RMIT University, IGOR LYSKOV, SALVY P. RUSSO, ARC Centre of Excellence in Exciton Science, RMIT University, ALBERTO PERUZZO, Quantum Photonics Laboratory, RMIT University — Quantum information and communication require single photons on demand, however current state of the art emitters are probabilistic. Defect centres in nanomaterials have shown promise as deterministic single photon sources. To investigate these materials, first principle models are required. Purely Density Functional Theory (DFT) models have met with much success, however, DFT is a ground state theory and excited states can only be calculated under strict assumptions. Here we demonstrate a method to calculate the ab-initio photoluminescence spectrum for NV⁻ centres using Time-Dependent Density Functional Theory (TD-DFT). Ground state properties are calculated using DFT. Excited state energies and transition dipole moments are calculated with Linear Response TD-DFT. Excited vibrational modes are given as normal modes the TD-DFT energy second derivatives. The emission rate is calculated from the transition dipole moment and Franck-Condon overlaps. Our technique can be extended to more general defects and is especially useful for edge effects like with small clusters or defects with Jahn-Teller distortions. The ability to recreate experimental photoluminescence spectra marks a step forward in understanding and controlling single photon emission for defect emitters.

12:39PM F11.00006: Simulation Driven Search for Promising Quantum Defects in Diamond  
ISAAC HARRIS (Presenter), EECS, MIT, CHRISTOPHER CICCARINO, BLAKE DUSCHATKO, SEAS, Harvard University, DIRK R. ENGLUND, EECS, MIT, PRINEHA NARANG, SEAS, Harvard University — Current research into quantum memories in diamond has mainly focused on the NV⁻ and SiV⁻ color centers, however both of these have clear limitations in spectral efficiency and spin coherence, respectively. More recent work has characterised the new group-IV centers GeV⁻, SnV⁻ and PbV⁻, as well as the neutral SiV, though other as yet unstudied defects in diamond are also possible. To efficiently screen these new defects, we use first-principles density-functional theory to predict important defect properties, including orbital structure, structural and charge stability, as well as vibrational effects on the emission profile. Promising defects are also investigated for possible Jahn-Teller distortions, and we discuss these implications. Overall, our results provide a roadmap toward the discovery of novel centers for quantum information.

12:51PM F11.00007: Optimizing the Production of Single Group IV Color Centers in Diamond*  
RODRICK KUATE DEFO (Presenter), EFTHIMIOS KAXIRAS, Harvard University, STEVEN L RICHARDSON, Howard University, Harvard University — The excitement of color centers, like the NV vacancy center in diamond, has been motivated by their use as single-photon emitters for applications in quantum information technology. Recent work has shown that a number of color centers in diamond using other Group IV elements (e.g. SiV, GeV, SnV and PbV)¹ may also be good candidates for quantum emitters. In this work we use density-functional theory (DFT) to study the thermodynamics and kinetics of these Group IV color centers in diamond. We find that for p-type diamond the production of isolated color centers will be enhanced. We further investigate the stability of complexes of these Group IV color centers in diamond with carbon vacancies which are present in diamond in abundance after implantation. We believe that this work may lead to optimal experimental conditions which lead to longer coherence times for color centers as previously discussed in the literature.²


*We are grateful for financial support from the NSF DMR-1231319, the Harvard Physics Graduate Prize Fellowship and the IACS Student Scholarship.
1:03PM F11.00008: Spin coherence properties of shallow donor-bound electrons in ZnO* [Invited]  KAI-MEI FU (Presenter), XIAYU LINPENG, MARIA L VIITANIEMI, University of Washington, ASWIN VISHNURADHAN, Applied Physics and QPEC, University of Tokyo, YUSUKE KOZUKA, National Institute for Materials Science, CAMERON W JOHNSON, University of Washington, MASASHI KAWASAKI, Applied Physics and QPEC, University of Tokyo — Defects in crystals are leading candidates for photon-based quantum technologies, but progress in developing practical devices critically depends on improving defect optical and spin properties. Motivated by this need, we study a new defect qubit candidate, the shallow donor in ZnO. We demonstrate all-optical control of the electron spin state of the donor qubits and measure the spin coherence properties. We find a longitudinal relaxation time $T_1$ exceeding 100 ms, an inhomogeneous dephasing time $T_2^*$ of 17 ns, and a Hahn spin-echo time $T_2$ of 50 us. The magnitude of $T_2^*$ is consistent with the inhomogeneity of the nuclear hyperfine field in natural ZnO. Possible mechanisms limiting $T_2$ include instantaneous diffusion and nuclear spin diffusion (spectral diffusion). These results are comparable to the phosphorous donor system in natural silicon, suggesting that with isotope and chemical purification long qubit coherence times can be obtained for donor spins in a direct band gap semiconductor.

*This material is based upon work supported by the National Science Foundation under Grant No. 1150647, 1820614.

1:39PM F11.00009: A first-principles study of the electronic structure of deterministically implanted donor arrays in silicon: multi-valley effects  WEI WU (Presenter), THORNTON GREENLAND, ANDREW JAMES FISHER, UCL Department of Physics and Astronomy and London Centre for Nanotechnology, University College London, WC1E 6BT, London, United Kingdom, H LE, STEVEN CHICK, BEN MURDIN, Advanced Technology Institute and Department of Physics, University of Surrey, Guildford, GU2 7XH, United Kingdom — Deterministically implanted donors in silicon provide an important route to develop quantum gates, analogue quantum simulators, and other atomic-scale devices [1]. We have computed the optical properties of a series of donor lines with up to 10 atoms in the spherical-band approximation (single isotropic valley) [2]. Our calculations show charge-transfer excitations play an important role, dominating the transition for separation $\sim$5nm and dropping down to 10 meV. We have also performed multi-valley calculations (with conduction-band anisotropy) for a donor pair and a three-donor linear cluster, which show distinct features in the excitation spectra arising from valley interaction. One consequence is to open up a gap between the ionic-state and the $1s\rightarrow2p$ intra-atom transition [3]. Single-valley calculations can be useful to understand the excited states of valley-polarized electrons [4]. Our calculations thus provide solid theoretical foundation to many promising applications for donor arrays, including valleytronics, quantum terahertz cascade laser devices, and quantum information technology.


1:51PM F11.00010: Creation and coherent control of Cr$^{4+}$ spin ensembles in commercial silicon carbide*  BERK DILER (Presenter), SAMUEL WHITELEY, CHRISTOPHER P ANDERSON, GARY WOLFOWICZ, University of Chicago, JOSEPH HEREMANS, Materials Science Division, Argonne National Laboratory, DAVID AWSCHALOM, University of Chicago — Optically active defect spins in solid-state materials, such as the nitrogen-vacancy center in diamond and vacancy complexes in silicon carbide (SiC), are an important resource for quantum technologies. Their electronic spins show promise as long-lived qubits with optical addressability. Recent work in 4H-SiC demonstrates the potential of transition metal defects [1]. In particular, Cr$^{4+}$ has a spin-1 electronic ground state with long $T_1$ times at cryogenic temperatures. High zero phonon line emission (73%), and narrow inhomogeneous optical ensemble linewidths (<7 GHz) of Cr$^{4+}$ enable optical spin initialization as well as readout using resonant near-infrared excitation. Here, we demonstrate that ion implantation followed by annealing at temperatures up to 1900 °C results in Cr$^{4+}$ ensembles with spectral-hole linewidths that are an order of magnitude narrower compared to as-grown samples. Improvements in material preparation and photon collection allow for coherent control and measurement of the spin properties of Cr$^{4+}$ defects, highlighting their potential for quantum information processing.


*ARO, AFOSR, NSF, UChicago MRSEC
Electric coupling and long dephasing times of single defect spins in commercial 4H-SiC

KEVIN MIAO (Presenter), ALEXANDRE BOURASSA, CHRISTOPHER P ANDERSON, SAMUEL WHITELEY, ALEXANDER CROOK, SAMUEL L BAYLISS, GARY WOLFOWICZ, University of Chicago, PETER UDVARHELYI, GERGO THIERING, VIKTOR IVADY, Hungarian Academy of Sciences, HIROSHI ABE, TAKESHI OHSHIMA, National Institutes for Quantum and Radiological Science and Technology, ADAM GALI, Hungarian Academy of Sciences, DAVID AWSCHALOM, University of Chicago — Divacancies (VV) in silicon carbide (SiC) are a promising platform for quantum communication owing to their long-lived spin coherence [1] and high-fidelity spin-to-photon interface [2] in a wafer-scale host material. Here, we investigate the properties of single basal $k\bar{h}$ VV in commercially available 4H-SiC. We report an electronic ground-state spin dephasing time ($T_2^*$) exceeding 60 µs for a single $k\bar{h}$ VV at 4 K, which is among the longest reported in a naturally abundant host. Furthermore, the $C_{1h}$ symmetry of $k\bar{h}$ VV quenches dynamic Jahn-Teller distortions, leading to long optical coherence and excited-state energy level coupling with ac electric fields. We observe optical Rabi oscillations with coherence times approaching the lifetime limit, permitting high-visibility quantum interference of emitted photons. We demonstrate coupling between excited-state energy levels and ac electric fields through the observation of a Floquet-dressed optical spectrum. These robust spin and optical properties make the $k\bar{h}$ VV a versatile candidate for quantum information processing and hybrid system applications.


*This work is supported by AFOSR, ARO, NDSEG, NSF, and UChicago MRSEC.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F12 DMP: Devices from 2D Materials -- Transport BCEC 153A - Fengnian Xia, Yale Univ - Tag(s): Focus

11:15AM F12.00001: Electronic properties of correlated two-dimensional materials [Invited] YUANBO ZHANG (Presenter), Dept. of Physics, Fudan University — Two-dimensional (2D) atomic crystals, best exemplified by graphene, have emerged as a new class of material that may impact future science and technology. So far semiconducting 2D materials attracted most attention. Meanwhile, vast opportunities exists in correlated 2D materials: the reduced dimensionality may lead to novel properties that are vastly different from that in the bulk, and the exposed surface makes these materials highly tunable. In this talk I will discuss the emerging opportunities in correlated 2D materials. In particular, I will talk about two correlated 2D materials that we found particularly interesting – metallic 2D ferromagnet Fe$_3$GeTe$_2$ and monolayer Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. We explore their electronic properties while the doping and dimensionality of the 2D systems are modulated.

11:51AM F12.00002: Studying Ambipolar Tellurene Field Effect Transistors using Microwave Near-Field Microscopy SAMUEL BERWEGER (Presenter), National Institute of Standards and Technology Boulder, GANG QIU, YIXIU WANG, Purdue University, BENJAMIN POLLARD, University of Colorado, KRISTEN L GENTER, ROBERT TYRELL-EAD, THOMAS M WALLIS, National Institute of Standards and Technology Boulder, WENZHUO WU, PEIDE (PETER) YE, Purdue University, PAVEL KABOS, National Institute of Standards and Technology Boulder — The successful development of nanoscale semiconducting devices requires precise control over adjoining regions of n- and p-type transport. Key challenges remain the development of new materials with bipolar transport as desired for homojunction devices as well as techniques capable of studying local variations in carrier type and associated conductivity with nanometer spatial resolution. Here we image local electronic variations in ambipolar field effect transistors made from 2D films (tellurene) of the 1D van der Waals material tellurium using near-field scanning microwave microscopy (SMM). We perform SMM imaging together with differential measurements to study spatial variations in both carrier type and the associated conductivity as a function of the applied global backgate voltage. We produce nanometer resolved maps of the local carrier equivalence backgate voltage and show that the apparent device conductivity minimum determined from transport measurements in fact arises from the local coexistence of p- and n-type regions.
12:03PM F12.00003: Effects of H$_2$ Interaction with MoS$_2$: Electronic Behavior and Sensing Applications* NATÁLIA REZENDE (Presenter), ALISSON RONIERI CADORE, ANDREJ DE CARVALHO GADELHA, CÍNTIA LIMA PEREIRA, VÍNICIUS ORNELAS DA SILVA, Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, 30123-970, Brasil, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Namiki, 305-0044, Japan, ANDRÉ SANTAROSA FERLAUTO, Centro de Engenharia, Modelagem e Ciências Sociais Aplicadas, Universidade Federal do ABC, 09210580, Brasil, ANGELO MALAQUIAS DE SOUZA, LEONARDO CRISTIANO CAMPOS, RODRIGO GRIBEL LACERDA, Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, 30123-970, Brasil — In this work, we probe the electronic properties of monolayer MoS$_2$ via interaction with H$_2$, aiming for sensing application. The MoS$_2$ FET exhibit a response to H$_2$ in a wide range of concentration (0.1-90 %) at relatively low temperatures (300-473 K). These H$_2$ sensor show desirable properties such absence of catalytic metal dopants (Pt or Pd) and full reversibility. Based in three experiments, we demonstrate that the conductivity of MoS$_2$ increases as a function of the H$_2$ concentration due to a reversible charge transferring process. Further, we propose that such process originates from the dissociative H$_2$ adsorption driven by interaction with sulfur vacancies in the MoS$_2$ surface ($V_S$). This proposal is in agreement with related DFT studies about H$_2$ adsorption on MoS$_2$. Finally, measurements on partially defect-passivated MoS$_2$ FETs using atomic layer deposited Al$_2$O$_3$ consisting of an experimental indication that the $V_S$ plays an important role in the H$_2$ interaction with the MoS$_2$. Our findings provide insights for futures applications in catalytic process between monolayer MoS$_2$ and H$_2$.

*We thank the financial support given by CAPES, Fapemig (Rede 2D), CNPq and INCT/Nanomaterials de Carbono.

12:15PM F12.00004: Anisotropic electron transport behaviors in few-layer ReSe$_2$* WEN-BIN JIAN (Presenter), PANG-CHIA CHANG, CHUN-YANG HO, ZHENG-JI OU, National Chiao Tung University, CHING-HWA HO, National Taiwan University of Science and Technology, Graduate Institute of Applied Science and Technology — The transition metal dichalcogenide of ReSe$_2$ had drawn much attention for decades since it is a layered semiconductor with strong anisotropy on the basal plane. The Re atoms are arranged to form clusters with the clusters aligned in a specified ‘b’-axis. After the improvement of material science, the anisotropy on the basal plane can be studied on single layer ReSe$_2$. In this talk, we will discuss the electrical exploration of the anisotropy on the basal plane of ReSe$_2$. We applied the mechanical exfoliation to make few-layer ReSe$_2$ flakes and the standard electron-beam lithography to make circularly oriented probing electrodes on the basal plane. We checked that the contact resistance is very small as compared with the ReSe$_2$ channel resistance. Using the circularly arranged electrodes, we studied electron transport in the direction parallel to the b-axis and in the direction making an angle with the b-axis. We studied angle dependence of electron mobility, the disorder parameter T0 of the Mott’s variable range hopping model, the metal-insulator transition, and the thermoelectric power. We observe an enhanced conductivity in the b-axis on the basal plane of the ReSe$_2$.

*This work was supported by Taiwan Ministry of Science and Technology under Grant Number MOST107-2119-M-009-011-MY3.

12:27PM F12.00005: Low-Frequency Noise Spectroscopy of the Charge-Density-Wave Phase Transitions in Vertical Tantalum Disulfide Devices* RUBEN SALGADO (Presenter), Electrical and Computer Engineering, University of California, Riverside, MATTHEW BLOODGOOD, TINA T. SALGUERO, Chemistry, University of Georgia, ALEXANDER A. BALANDIN, Electrical and Computer Engineering, University of California, Riverside — Noise spectroscopy has proven itself as an effective tool for investigating the phase transitions in two-dimensional (2D) charge density wave (CDW) materials [1]. Almost all studies of CDW effects in 2D systems focused on transport along the atomic planes. Here we report results of investigation of CDW transitions in vertical 1T-TaS$_2$ devices. We observed two jumps in electrical resistivity – at the temperature range from 150 K to 180 K, and another at 80 K to 85 K. The low-frequency noise spectral density, revealed strong peaks at these transition points, sometimes changing by as much as three orders-of-magnitude. The higher temperature feature can be associated with the transition between the commensurate and nearly commensurate CDW states. The lower temperature transition can indicate the debated “hidden” CDW phase. The obtained results are important for the proposed applications of vertical van der Waals heterostructures in memory and logic gates.


*This work was supported by NSF through the 2-DARE project: Novel Switching Phenomena in Atomic Heterostructures for Multifunctional Applications (NSF EFRI-1433395).
Type Control of MoOx/MoS2 Heterostructure Transistors by Oxidation Treatments

Presenter: PANG-CHIA CHANG
Co-authors: JIAN-JHONG LAI, PO-SHENG WANG, BING-SHIUAN SHIE, WEN-BIN JIAN, National Chiao Tung University, YEN-FU LIN, National Chung Hsing University

Molybdenum disulfide (MoS2) has attracted much attention due to great potential applications as electronics devices. By mechanical exfoliation, few-layer MoS2 can be obtained and made into field-effect transistors (FETs). In particular, we demonstrated that heating device under ozone exposure for several hours can change the device behaviors from natively n-type to either ambipolar or p-type. The treatments resulted in oxidation of MoS2 surfaces to molybdenum oxide (MoOx). Due to exhibiting high work function, MoOx was used as an efficient hole contact. By adjusting the time and temperature of oxidation treatments, the formation of MoOx and the work function of contact electrodes can be modulated. The MoS2 FETs after weak and strong oxidation treatments presented ambipolar and p-type feature, respectively. In MoOx/MoS2 heterostructure, the devices showed the Schottky contact behaviors. The effective Schottky barrier depended on both the gate voltage and source-drain voltage. Additionally, the electrical transport and transfer characteristics of ambipolar and p-type FETs were separately explored. In this report, the oxidation treatments not only simplify the complex fabrication but also improve the diversity of applications for nanoelectronic devices.

Reduction of Current-Voltage Hysteresis in Graphene Field Effect Transistor Achieved with Dry Transfer Using Flexible Tape Supporter

Authors: SUNGCHUL JUNG, HOON HAHN YOON, Ulsan National Institute of Science and Technology, HANBYUL JIN, National Institute of Standards and Technology, KINUHYUNG MO, GAHYUN CHOI, JUNGHYUN LEE, HYESUNG PARK, KIBOG PARK

In the conventional wet transfer method of Chemical Vapor Deposition (CVD) graphene, it is inevitable to have water molecules trapped between graphene and substrate. The trapped water molecules can cause the hysteretic behavior in current-voltage curves of graphene field effect transistor (GFET). Here, a new dry transfer method adopting the Kapton tape as an additional flexible supporting layer is demonstrated. The N2 blowing and heating processes are added to vaporize the water molecules adsorbed on graphene layer right before the transfer step. By comparing the I-V characteristics of wet- and dry-transferred GFET, the field effect mobility is found to be larger for the dry-transfer GFET in comparison with the wet-transferred one, possibly due to the more uniform Coulomb potential landscape. Also, the hysteretic behavior is found to be reduced substantially in accordance with the decrease of trapped water molecules. The obtained electron field effect mobilities are ~1118 cm²/Vs and ~415 cm²/Vs for dry- and wet-transferred graphene, respectively. Our dry transfer method can provide a simple and reliable way to transfer the CVD graphene onto an arbitrary substrate with its as-grown electrical properties being preserved, regardless of the substrate size.

High-Efficiency Thermoelectric 2D Tellurium Devices with Accumulation-type Metal-to-Semiconductor Contacts

Presenter: GANG QIU
Authors: YIXIU WANG, WENZHUO WU, PEIDE (PETER) YE

The paradigm of a good thermal electrical material is usually a heavily doped narrow bandgap semiconductor with good electrical conductivity and low thermal conductivity. Bulk Te has been theoretically predicted and experimentally demonstrated to be an outstanding thermoelectric material. Recent achievements in growing high quality 2D Te films allow us to explore the thermoelectric performance of 2D Te. Using nano-fabricated heater and thermometer, we were able to measure the room temperature Seebeck coefficient and power factor of 0.41 mV/K and 31.7 μW/cm•K. Using the thermal conductivity of bulk Te, we can estimate the lower bound of ZT value to be ~0.32 at 300 K, whereas the true ZT value should be much higher considering the suppression of thermal conductivity in thin films. The details of film thickness dependence are on-going and will be reported. Thermoelectrical current mapping was performed with a laser heater, and we found high work function metals such as Palladium can form rare accumulation type metal-to-semiconductor contacts to Te, which allows thermoelectrically generated carriers to be collected more efficiently. High-performance thermoelectric Te devices will have broad applications for energy harvesting or as a Peltier cooler in microsystems.
crystals by direct evaporations of high and low work-function metals platinum and gadolinium. Since metal-induced improvement of overall device performance in MoS2 transistors as the Schottky barrier height is lowered from ~100 meV to ~40 meV by inserting a WSe2 interlayer between the MoS2 channel and the metal electrodes. A significant advantage of using 2D semiconductors as a contact interlayer as opposed to previously reported insulator interlayers is that 2D semiconductor interlayers with appropriate band alignments are able to effectively reduce the Schottky barrier height without introducing a substantial tunneling barrier at the contacts.

1:27PM F12.00010: Strong Spin-Orbit Interaction in ultra clean graphene/transition-metal dichalcogenide heterostructures DONGYING WANG (Presenter), SHI CHE, Department of Physics, The Ohio State University, RUI LYU, Department of Physics, University of California, Riverside, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Tsukuba, Japan, CHUN NING LAU, MARC BOCKRATH, Department of Physics, The Ohio State University — Van der Waals heterostructures based on stacking two dimensional materials gives rise to new possibilities for designing tunable electronic systems. While combining the merits of individual layers, heterostructures provide a platform for studying interfacial interactions [1]. Among the many phenomena achieved by this proximity effect, inducing spin-orbit coupling (SOC) in graphene has attracted much attention for potential applications in topological physics. We study the enhancement of SOC in graphene induced by transition-metal dichalcogenides (TMDs). High carrier mobility at low temperature suggests that our devices have high quality graphene and very clean graphene/TMD interfaces. We measure magnetoresistance in these devices, which is large and positive, indicating the presence of ultra-strong weak antilocalization (WAL), as a signature of SOC induced in graphene. In contrast to previous works [2-3], our WAL strength is much higher, and we have explored the variation with carrier density more systematically. The WAL feature gradually decreases with increasing temperature and becomes unobservable above 60K.


1:39PM F12.00011: Ultimate Limit in Size and Performance of WSe2 Vertical Diodes SUYONG JUNG (Presenter), GHAZANFAR NAZIR, HAKSEONG KIM, Korea Research Institute of Standards and Science, JONGHWA EOM, Physics, Sejong University — Precise doping-profile engineering in van der Waals (vdW) heterostructures is a key element to promote optimal device performance in various electrical and optical applications with two-dimensional vdW materials. Here, we report tungsten diselenide-(WSe2) based pure vertical diodes with atomically defined p-i-n heterojunctions characterized by a series of quantum tunneling events, namely direct tunneling, Fowler–Nordheim (FN), and Schottky emission (SE). With optimally selected WSe2 thickness, where FN and SE tunneling events prevail, our vertical heterojunctions show superb diode characteristics of an unprecedentedly high current density (∼2 × 10^5 A/cm²) and low turn-on voltages while maintaining good current rectification.

1:51PM F12.00012: Direct observation of ballistic transport in vertical direction of Black Phosphorus ANYUAN GAO (Presenter), FENG MIAO, YI SHI, XIAOMU WANG, School of Physics, National Laboratory of Solid State Microstructures — Ballistic transport is the transport of carriers without scattering. In this regime, carriers travel freely and coherently in semiconductors and therefore the ballistic transport is highly desirable for the development of low power, high speed logic and quantum circuits. Due to its puckered lattice structure, the out-of-plane mobility of BP is comparable to in-plane mobility. Here, we report the direct observation of ballistic transport of BP in out-of-plane direction. The ballistic transport observed in vertical direction of BP is within a 3D framework which is different from 1D ballistic transport. Our results shed light on the development of efficiently facilitating carriers on the nanoscale.
The realization of stable and reliable molecular junctions taking advantage of graphene electrodes faces several issues. Nanoscale gaps with graphene electrodes can indeed exhibit signatures mimicking those of molecules, with gate-dependent resonance features [1,2]. Substrate effects can also play a role: Silicon dioxide has for instance been reported to yield feature-rich charge-transport characteristics in nanoscale graphene gaps, primarily due to switching within the oxide [3].

We report here on the realization of mechanically and electronically robust graphene-based multi-molecule junctions [4]. The mechanical stability is achieved by anchoring molecules directly to the substrate using silanization, rather than to graphene electrodes. The electronic stability is due to a large overlap between the electronic π-systems of neighboring head groups. The nature of the stacking leads to junctions less sensitive to the electrode properties. The junctions are reproducible throughout several devices and operate up to room temperature.

[4] M. El Abbassi et al., to be submitted
**11:27AM F13.00002: Synthesis and characterization of large-area single-crystal sheets of borophene on Cu(111) surface**

 RONGTING WU (Presenter), Department of Applied Physics, Yale University, New Haven, CT 06520, USA, ILYA K. DROZDOV, Brookhaven National Laboratory, Upton, NY 11973, USA, STEPHEN ELTINGE, Department of Physics, Yale University, New Haven, CT 06520, USA, PERCY ZAHL, Brookhaven National Laboratory, Upton, NY 11973, USA, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University, New Haven, CT 06520, USA, IVAN BOZOVIC, Brookhaven National Laboratory, Upton, NY 11973, USA, ADRIAN GOZAR, Department of Applied Physics, Yale University, New Haven, CT 06520, USA — Borophene, a theoretically proposed two-dimensional boron allotrope, has attracted attention as a candidate material platform for high-speed and flexible electronics. However, the single-crystal domains produced so far are too small for device fabrication. We report on synthesis of borophene on Cu(111) monitored in situ by low-energy electron microscopy (LEEM), diffraction and scanning tunneling microscopy, and ex-situ by X-ray photoelectron spectroscopy and atomic force microscopy. By growing borophene on Cu(111) surfaces, we obtain large single-crystal domains, up to 100 μm². We show that the crystal structure is a novel triangular network with h = 1/5 concentration of hexagonal vacancies. LEEM imaging capabilities provide detailed information about borophene growth, island faceting, evaporation and sub-surface dissolution. Data and calculations indicate charge-transfer coupling to substrate without significant covalent bonding. Our work sets the stage for fabricating borophene-based devices and substantiates the idea of borophene as a model for artificial 2D materials development.

R. Wu et al., “Large-area single-crystal sheets of borophene on Cu(111) surfaces”, Nature Nanotechnology 14, 44-49 (2019)

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**11:39AM F13.00003: Direct graphene growth on Anodic Aluminum Oxide (AAO) under different conditions using chemical vapor deposition**

 AAMNA ALSHEHHI (Presenter), IRFAN SAADAT, Electrical and Computer Engineering Department, Khalifa University Of Science and Technology, FAISAL ALMARZOQI, Chemical Engineering, Khalifa University Of Science and Technology, AMAL AL GHAFERI, Khalifa University of Science and Technology, KHADIJA AL DAGHAR, Abu Dhabi National Oil Company — Graphene is one of the promising 2D material due to their remarkable electrical, mechanical and chemical properties. In general growth conditions can be manipulated to synthesis graphene with different layer composition and properties. Direct synthesis of graphene is critical to establish new applications and come up with a manufacturing process for current applications. Recent studies started to focus on direct graphene growth on AAO and potential usage in new applications. The novelty of my study focusing on distinguishing between the quality of graphene growth with low pressure and ambient pressure. This paper will show the results of direct CVD graphene growth on AAO films with pore size ranging from 200 - 40(nm) under different conditions such as pressures (ambient & vacuum) and flow rates. (nm). These parameters play a critical role in the quality and various properties of graphene growth. The presence of graphene was confirmed via Raman spectroscopy with a laser wavelength of 532 nm. The D-mode, G-mode and 2-D mode appears at approximately 1348 cm⁻¹, 1616 cm⁻¹ and 2690 cm⁻¹ respectively. Additional characterization assessments such as SEM and AFM are ongoing and the results will be reported in the final paper.

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**11:51AM F13.00004: Wafer-scale Growth and Assembly of 2D Semiconductors [Invited]**

 KIBUM KANG (Presenter), Dept. of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (KAIST) — High-performance semiconducting films with precisely engineered thicknesses and compositions are essential for developing next generation electronic devices, which are becoming more integrated, complex, and multifunctional. My talk will introduce the novel processes that enable atomic-scale control of the thickness and spatial composition of semiconducting films on the wafer-scale. These processes include: (i) the wafer-scale generation of monolayer van der Waals semiconductors such as transition metal dichalcogenides (TMDCs) via metal-organic chemical vapor deposition (MOCVD), (ii) the atomic-level engineering of vertical thickness and composition through the layer-by-layer assembly of TMDC monolayers, and (iii) the transfer of atomically engineered films, using their van der Waals nature, onto arbitrary substrates. These capabilities provide a new material platform for both fundamental research and practical applications, including incorporation into existing integrated circuit technology to form hybrid materials (i.e. TMDC/CMOS) and boost electrical and optical functionality.
12:27PM F13.00005: Direct growth of mm-size twisted bilayer graphene (tBLG) by plasma enhanced chemical vapor deposition (PECVD)  
YEN-CHUN CHEN (Presenter), Physics, National Tsing-Hua University, Hsinchu, Taiwan, WEI-HSIANG LIN, Applied Physics, Caltech, Pasadena, CA 91125, USA, WEI-SHUAN TSENG, CHIEN-CHANG CHEN, Physics, Caltech, Pasadena, CA 91125, USA, GEORGE R ROSSMAN, Geological and Planetary Science, Caltech, Pasadena, CA 91125, USA, YU-SHU WU, Physics, National Tsing-Hua University, Hsinchu, Taiwan, CHIIDONG CHEN, Physics, Academia Sinica, Taiwan, NAI-CHANG YEH, Physics, Caltech, Pasadena, CA 91125, USA — PECVD techniques have been shown to be an efficient method to achieve single-step synthesis of high-quality monolayer graphene without the need of active heating. Here we report our progress in PECVD-growth of single-crystal hexagonal bilayer graphene (BLG) flakes and mm-size BLG films, both with the interlayer twisted angle controlled by the PECVD growth parameters. The twisted angle between stacked bilayer is determined by a combination of three experimental approaches, which include: 1) directly measuring the orientation of edges between two stacked layers by scanning electron microscopy, 2) evaluating the twisted angle-dependent Raman spectral characteristics of the G-, 2D- and R'-modes of graphene, and 3) analyzing the Moiré period captured by scanning tunneling microscopy. We find that the average twisted angle of BLG samples can be controlled from 0° (for perfect AB stacking) to ~ 20°, and the spread of twisted-angles for a given growth condition can be reduced to less than 7° over mm-size tBLG films. More comprehensive studies of various properties of PECVD grown-tBLG will be reported in this talk. 

The work at Caltech is supported by the National Science Foundation, and in Taiwan by the Ministry of Science and Technology.

12:39PM F13.00006: Synthesis of Artificial 2D Lattices of Monolayer Multi-junctions  
YI-CHENG CHIANG (Presenter), CHUN-AN CHEN, Materials Science and Engineering, National Tsing Hua University, KUAN-CHANG CHIU, Taiwan Semiconductor Manufacturing Company, Limited, KUAN-HUA HUANG, YING-YU LAI, XIN-QUAN ZHANG, ERH-CHEN LIN, MENG-HSI CHUANG, JENN-MING WU, YI-HSIEN LEE, Materials Science and Engineering, National Tsing Hua University — Recently, monolayers of transition metal dichalcogenides (TMDs) are ideal building blocks for constructing artificial 2D lattices. Heterostructures with multi-junctions of more than two monolayer TMDs are intriguing for exploring new physics. Here, the laterally stitched TMDs and the vertically stacked monolayers are constructed. A low growth temperature synthesis and a clean transfer method are developed for high quality hetero-interfaces. With optimized parameters, atomically sharp interfaces are successfully achieved in the synthesis of in-plane artificial lattices of the WS$_2$/WSe$_2$/MoS$_2$. Characterizations of the hetero-interfaces are presented.

12:51PM F13.00007: Boron and Nitrogen co-doping of Graphene by CVD  
TOMOTAROH GRANZIER-NAKAJIMA (Presenter), LAVISH PABBI, MAURICIO TERRONES, ERIC HUDSON, Pennsylvania State University — Substitutional doping of graphene offers a chance to modify its properties for various applications. Here using low pressure chemical vapor deposition we grow graphene doped simultaneously by both boron and nitrogen. Theoretical calculations have shown that in such systems boron and nitrogen dopants tend to segregate and form hexagonal boron-nitride like islands within the graphene sheet.\textsuperscript{1,2} Using STM we are able to observe these dopant structures with atomic resolution and show the results here.


1:03PM F13.00008: The Growth and Characterization of PECVD Silicene*  
BATTOGTOKH JUGDERSUREN (Presenter), KeyW Corporation, XIAO LIU, JAMES CLIFFORD CULBERTSON, NADEEM MAHADIK, US Naval Research Laboratory — Silicene, a two-dimensional nanoscale allotrope of silicon atoms with a buckled honeycomb structure, is predicted to have many interesting features. There is no evidence for the existence of natural silicene. Until recently, molecular-beam epitaxy (MBE) has been the only successful technique for silicene synthesis. Recently, we have found that plasma-enhanced chemical-vapor deposition (PECVD) has the potential to grow economically viable, large scale, high-quality mono- and multi-layer silicene comparable to that grown using MBE. In addition, we have shown that PECVD grown silicene is naturally hydrogenated and resistant to oxidation. In this work, we have grown PECVD silicene on polycrystalline and single crystalline silver thin films and characterized them using Raman spectroscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. The results show that we can grow nearly defect-free silicene on single crystalline Ag(111) films. We will discuss crystalline structure, hydrogenation, and oxidation-resistance properties of the PECVD silicene.

*Work supported by the Office of Naval Research
1:15PM F13.00009: Growth Physics of MoS2 Layer on the MoS2 Surface: A Monte Carlo Approach  KAMALIKA GHATAK, DIBAKAR DATTA, JATIN KASHYAP (Presenter), Mechanical and Industrial Engineering, New Jersey Institute of Technology — Layered Transition Metal Dichalcogenides (TMDs) are getting attention due to their layer-dependent tunable optoelectronic and mechanical behavior and the control over the experimental growth technique is required to synthesize desired stacked products. Alongside, a probabilistic computational approach is necessary to gain deeper insight into the in-situ growth physics. We, therefore, performed Grand Canonical Monte Carlo (GCMC) simulation as implemented in LAMMPS package with ReaxFF potential, and developed our in-house Kinetic Monte Carlo (KMC) code to model the growth physics of MoS2 layer on the substrate. We considered various pristine and defective growth surface to track the movement of the individual Mo and S. Non-periodic surface with various edge termination (such as chalcogen and metal termination) was also explored. Our Monte Carlo study captures the formation of the MoS2 on the perfect MoS2 surface starting with the individual Mo and S flux. We find that the growth temperature plays a crucial role in governing growth mechanisms. Further investigation is on-going on the growth physics of MoS2 and other TMDs (e.g., WS2) on pristine and defective substrates. Our modeling approach provides guidelines for the experimentalists for the optimal design of TMD bilayer growth.

1:27PM F13.00010: Cooling-mediated One-step Synthesis of Monolayer WSe2/WSe2xTe2-2x Lateral Heterostructures for High-Performance Spectral Photodetectors*  SANGMIN KANG (Presenter), Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, CHIA-HAO LEE, Department of Material Science and Engineering, University of Illinois at Urbana-Champaign, YIFEI LI, ZIJING ZHAO, KAI XIU, SHUSHAN XIA, HOJOON RYU, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, PINSHANE HUANG, WENJUAN ZHU, Department of Material Science and Engineering, University of Illinois at Urbana-Champaign — Tellurium (Te) based transition metal dichalcogenides (TMDCs), especially tungsten ditelluride (WTe2), have attracted intensively owing to their unique electrical and optical properties. However, the ternary alloy tungsten selenium telluride (WSe2xTe2-2x) and its lateral hetero-structure with other TMDCs remains largely unexplored due to the considerable challenge in synthesizing these materials, since WTe2 has very weak bonding and tends to decompose at high reaction temperature. Here, we demonstrate a successful one-step synthesis of monolayer WSe2/WSe2xTe2-2x lateral hetero-structures via cooling-mediated chemical vapor deposition. We find that the cooling rate and flow ratio between argon and hydrogen gas are crucial factors for the morphology. The Te incorporation in the alloy is studied by aberration-corrected scanning transmission electron microscopy. The correlation between Te composition and the bandgap of the alloy is simulated by density functional theory. Furthermore, through the study of the optical and electrical properties, we demonstrate the possibility of high-performance spectral photodetectors with spatially graded bandgap.

* The authors would like to acknowledge ONR support under Grant NAVY N00014-17-1-2973 and NSF support under grant no. ECCS 16-53241 CAR.

1:39PM F13.00011: Large homo pn junction using two type of atomic scale-thickness-MoS2  AHRUM SOHN (Presenter), JAEHWAN JUNG, SANG-WOO KIM, School of Advanced Materials Science & Engineering, Sungkyunkwan University — Molybdenum disulfide (MoS2) has attracted attention as a substitute material of Si for the next generation material due to its prominent physical properties. In order for MoS2 to replace Si, it must have not only such intrinsic properties but also be able to modulate the carrier type. Accordingly, several researchers have attempted to various doping methods for controlling the carrier type of MoS2, including coating physic or chemisorption of molecules, exposing plasma and substitutional doping process. In this study, we developed the layer-controllable and reproducible growth method of large scaled and Nb doped MoS2 films with reduction of growth time by 50 times as compared with previous method. To identify structural information of the films, atomic force microscopy (AFM), transmission electron microscopy (TEM), Raman spectroscopy, and X-ray spectroscopy (XPS) were conducted. p-type properties of Nb doped MoS2 was confirmed by STM and gate dependent transport measurement. Furthermore, we demonstrated ultra-thin homo p-n junction via vertical stacking and lateral stacking of n-type and p-type MoS2 grown by this method.
**1:51PM F13.00012: Synthesis of High Quality Monolayer Transition Metal Dichalcogenides using Direct Liquid Injection**

KATHLEEN MCCREARY (Presenter), ENRIQUE COBAS, AUBREY HANBICKI, BEREND JONKER, United States Naval Research Laboratory — In recent years, interest in monolayer transition metal dichalcogenides (TMDs) has rapidly increased, spurred by the possibility for integration into a variety of technologies such as photodetection, flexible electronics, and chemical sensing. While fundamental investigations can be performed on exfoliated flakes or chemical vapor deposition synthesized isolated islands, the limited size resulting from these techniques poses a significant barrier for implementation of TMDs in technological applications. To overcome these obstacles, new synthesis avenues should be explored. Here, we outline a novel technique that utilizes a commercially available Anneal Sys growth chamber equipped with direct liquid injection (DLI) heads for all precursors. The use of liquid, rather than solid precursors, provides fine control of both metal and chalcogen precursors leading to the synthesis of monolayer MoS$_2$ across cm$^2$ areas. Photoluminescence, Raman and XPS are used to evaluate DLI grown MoS$_2$, and indicate high quality material, with metrics comparable to or better than exfoliated and chemical vapor deposition grown MoS$_2$.

**2:03PM F13.00013: Controlled CVD growth of MoTe$_2$ and their use in near-infrared light detection**

ZHENG TANG LUO (Presenter), JIAWEN YOU, Department of Chemical and Biological Engineering, Hong Kong University of Science and Technology — Due to their low symmetry ultrathin structures and unconventional dielectric screening effects, 2D transition metal dichalcogenides (TMDs) have attracted significant research attention utilizing their tunable optical-electronic properties. We established general strategies for to synthesize high-quality graphene and TMDs layers with tailored properties using chemical vapor deposition (CVD). Here, we demonstrate a salt-induced CVD strategy to synthesize mono- and few-layer 1T’ and 2H phase MoTe$_2$, exploiting richer electronic properties of this materials derived from their tunable structures. The obtained materials has demonstrate exceptional performance when used for the near-infrared (NIR) light detection, arise from their reduced band gap of 2H phase MoTe$_2$. This study provides a new materials synthesis method aiming for the fabrication of for highly efficient, and broadband NIR photodetector.

*This project is supported by the Research Grant Council of Hong Kong SAR (Project number 16204518).

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**Tuesday, March 5, 2019 11:15 AM - 2:15 PM**

**Session F14 DCMP: Graphene: Light Matter Interactions**

**11:15AM F14.00001: Enhanced Raman scattering of graphene using double resonance in silicon photonic crystal nanocavities**

HIDENORI MACHIYA (Presenter), WIDIANTA GOMULYA, RIKEN, KOTARO KASHIWA, TAIKI INOUE, SHOHEI CHIAISHI, SHIGEO MARUYAMA, The University of Tokyo, YUICHIRO K. KATO, RIKEN — We demonstrate enhancements of Raman scattering from graphene on L3 photonic crystals using double resonances, which originate from simultaneous enhancements by a localized guided mode and a cavity mode [1]. By adjusting the photonic crystal cavity parameters, the double resonance [2] can be tuned to the G’ Raman scattering. Excitation wavelength dependence measurements show a large Raman peak enhancement when the excitation and emission wavelengths meet the double resonance condition. Furthermore, spatial imaging measurements are performed to confirm that the enhancement is localized at the cavity, and we find that the enhanced Raman intensity is 60 times larger compared to the on-substrate Raman signal. The observed cavity enhancement of Raman scattering opens up new possibilities for the development of graphene-based light sources for silicon photonics.

**References**


*Work supported by JSPS (KAKENHI JP16K13613, JP25107002) and MEXT (Photon Frontier Network Program, Nanotechnology Platform). W.G. is an International Research Fellow of JSPS. H.M. is supported by RIKEN Junior Research Associate Program.*
11:27AM F14.00002: Photonic Crystals for Nano-Light in Moiré Graphene Superlattices  SAI SUNKU (Presenter), GUANGXIN NI, Columbia University, BOR-YUAN JIANG, UC San Diego, HYOBIN YOO, Harvard University, AARON STERNBACH, MCLEOD SWINTON ALEXANDER, Columbia University, STAUBER TOBIAS, ICM, CSIC, Madrid, LIN XIONG, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, PHILIP KIM, Harvard University, MICHAEL FOGLER, UC San Diego, DIMITRI BASOV, Columbia University — Twisted bilayer graphene (TBG) consists of two layers of graphene rotated relative to each other. At very small twist angle, the atomic lattices relax and form a periodic array of Bernal-stacked domains separated by solitons. The solitons host topologically protected states and have previously been shown to efficiently scatter propagating surface plasmon polaritons (SPPs) [Jiang et al, Nano Lett, 17:7080 (2017)]. Therefore, an array of such solitons with a periodicity similar to the wavelength of SPPs should act as a photonic crystal for the SPPs. In this work, we use infrared nano-imaging to verify this proposition and demonstrate the interference of propagating SPPs in TBG. Furthermore, our calculations predict that a full plasmonic band gap is possible in this system.

11:39AM F14.00003: Fundamental Limits to graphene plasmonics  GUANGXIN NI (Presenter), MCLEOD SWINTON ALEXANDER, ZHIYUAN SUN, LEI WANG, LIN XIONG, Columbia University, KIRK W POST, University of California San Diego, SAI SUNKU, Columbia University, BOR-YUAN JIANG, University of California San Diego, JAMESHONE, CORY R DEAN, Columbia University, MICHAEL FOGLER, University of California San Diego, DIMITRI BASOV, Columbia University — Polaritons are hybrid excitations of light and matter that can confine the energy of long-wavelength radiation at the nano-scale. Plasmon polaritons may enable many enigmatic quantum effects including lasing, topological protection, and dipole-forbidden absorption. A necessary condition for realizing such phenomena is a long polariton lifetime, which is notoriously difficult to meet. Plasmon polaritons in graphene provide a platform for exploring light-matter interaction at the nano-scale. However, plasmonic dissipation in graphene has remained substantial and its fundamental limits remained undetermined. Here we use nanometre-scale infrared imaging to investigate propagating plasmon polaritons in high-mobility encapsulated graphene at cryogenic temperatures. In this regime, the propagation of plasmon polaritons is primarily restricted by the dielectric losses of the encapsulated layers, with a minor contribution from electron-phonon interactions. At liquid-nitrogen temperatures, the intrinsic plasmonic propagation length can exceed 50 plasmonic wavelengths, thus setting a record for highly confined and tunable polariton modes.

11:51AM F14.00004: Broadband mid-infrared graphene bolometer  SHAOFAN YUAN (Presenter), YALI QI, YAM INGO, YUAN RUIZ (Presenter), MARCIN MUCHA-KRUCZYNSKI, JOSHUA THOMPSON, Physics, University of Bath, VLADIMIR FALKO, National Graphene Institute — Using the continuum model, we study theoretically the purely electronic contributions to the Raman spectrum of twisted bilayer graphene (tBLG) for twist angles close to the magic angle [1]. We show that non-resonant excitations of electron-hole pairs between the first minibands above and below the neutrality point lead to a peak, the position of which is determined by the twist angle. We estimate the quantum efficiency of this Raman feature as $\sim 10^{-13}$, about two orders of magnitude less than the intensity of the G peak [2]. Because of its electronic origin, the new peak provides direct information about the flatness of the first minibands in tBLG.


*This contribution has been supported by the UK Engineering and Physical Sciences Research Council (EPSRC) through the Centre for Doctoral Training in Condensed Matter Physics (CDT-CMP), EPSRC Grant No. EP/L015544/1, as well as EPSRC Grant No. EP/N010345/1, the European Graphene Flagship project, and Lloyd's Register Foundation Nanotechnology Programme.
temperatures. High-mobility graphene is transferred to a periodically patterned SiO2 substrate with Si back-gate. This functionalities. We used near-field nano-imaging techniques to study graphene plasmonic crystals at cryogenic tunable parameters including gate voltage, twist angle, and superlattice potential enable efficient control of device quality graphene devices enable long-lived surface plasmon polaritons which propagate over several microns. Various doped graphene sheets due to third-order optical response.

demonstrate, for the first time, the angular dependency of s- and p- polarized light absorption in nanopatterned graphene. The wide-angle electronically tunable extraordinary light absorption promises graphene-based optoelectronic devices. The wide-angle tunable plasmonics in Dirac systems like graphene shows interesting characteristics because of massless electrons around the Dirac cone. Exciting surface plasmons on graphene is a distinct technique to increase the light absorption with low damping rate and provides the opportunity of electrical tunability of the resonance frequency and high degree of electric field confinement. Here, we demonstrate a novel design of an optical cavity-coupled hexagonal array of nanohole and nanodisk in monolayer CVD-grown graphene to excite Dirac plasmon. We study the surface plasmon lifetimes of the nanopatterns and their role in the enhanced light-matter interaction. By exploiting a high-k gate dielectric to dope the nanopatterned graphene electrostatically, the light absorption enhances to the record values of 60% on nanohole and 90% on nanodisk arrays in the 8-12 mm bandwidth with high spectral tunability. We theoretically and experimentally demonstrate, for the first time, the angular dependency of s- and p- polarized light absorption in nanopatterned graphene. The wide-angle electronically tunable extraordinary light absorption promises graphene-based optoelectronic devices.

*This work at the University of Central Florida was supported by DARPA under the WIRED program grant no. HR0011-16-1-0003.

12:15PM F14.00006: Photonic crystal for graphene plasmons LIN XIONG (Presenter), CARLOS FORSYTHE, ALEXANDER SWINTON MCLEOD, Columbia University, MINWOO JUNG, Cornell university, SAI SUNKU, GUANGXIN NI, Columbia University, SONG LIU, Kansas State University, MICHAEL FOGLER, University of California, San Diego, JAMES H. EDGAR, Kansas State University, GENNADY SHVETS, Cornell university, CORY DEAN, DIMITRI BASOV, Columbia University — Recent advancements in high-quality graphene devices enable long-lived surface plasmon polaritons which propagate over several microns. Various tunable parameters including gate voltage, twist angle, and superlattice potential enable efficient control of device functionalities. We used near-field nano-imaging techniques to study graphene plasmonic crystals at cryogenic temperatures. High-mobility graphene is transferred to a periodically patterned SiO2 substrate with Si back-gate. This heterostructure imprints the graphene with 80 nm-scale periodic variations in carrier density under application of a field effect, thus forming a gate-tunable photonic crystal for plasmons. We observed the formation of a selectively engineered full plasmonic bandgap where propagation of plasmons is strongly suppressed within the superlattice. Additionally, we implemented a designed domain wall within the superlattice which simultaneous supports strongly confined 1D plasmons within the plasmonic bandgap. These findings signify a new route towards designer-engineered band-structures to route and manipulate highly confined plasmons within high mobility graphene devices.

12:27PM F14.00007: Probing symmetry breaking in multilayer epitaxial graphene by circularly polarized magneto-infrared spectroscopy* YUXUAN JIANG (Presenter), ZHENGGUANG LU, National High Magnetic Field Laboratory, JAMES GIGLIOTTI, CLAIRE BERGER, WALTER DE HEER, Physics, Georgia Institute of Technology, DMITRY SMIRNOV, National High Magnetic Field Laboratory, ZHIGANG JIANG, Physics, Georgia Institute of Technology — Symmetry breaking in graphene in high magnetic fields has long been an intriguing problem. Here, we report a magneto-infrared transmission spectroscopy study of multilayer epitaxial graphene with circularly polarized light. A four-fold splitting of the zeroth Landau level is found in high magnetic fields and attributed to the lifting of the valley and spin degeneracies and the electron-hole asymmetry. We extract the magnetic field dependence of the splitting gaps and discuss their possible origins. We also observe a surprising electron-hole asymmetry reversal between the monolayer and bilayer graphene components of multilayer epitaxial graphene and propose a possible interpretation.

*This work is primarily supported by the DOE (Grant No. DDE-FG02-07ER46451). The IR measurement of this work was performed at the National High Magnetic Field Laboratory (NHMFL), which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490 and the State of Florida. Y.J. acknowledges support from the NHMFL Jack Crow fellowship.

12:39PM F14.00008: Wide Angle Electronically Tunable Enhanced Light Absorption in Nanopatterned Graphene* ALIREZA SAFAEI (Presenter), SAYAN CHANDRA, MICHAEL N. LEUENBERGER, DEBASHIS CHANDA, University of Central Florida — Plasmons in Dirac systems like graphene shows interesting characteristics because of massless electrons around the Dirac cone. Exciting surface plasmons on graphene is a distinct technique to increase the light absorption with low damping rate and provides the opportunity of electrical tunability of the resonance frequency and high degree of electric field confinement. Here, we demonstrate a novel design of an optical cavity-coupled hexagonal array of nanohole and nanodisk in monolayer CVD-grown graphene to excite Dirac plasmon. We study the surface plasmon lifetimes of the nanopatterns and their role in the enhanced light-matter interaction. By exploiting a high-k gate dielectric to dope the nanopatterned graphene electrostatically, the light absorption enhances to the record values of 60% on nanohole and 90% on nanodisk arrays in the 8-12 mm bandwidth with high spectral tunability. We theoretically and experimentally demonstrate, for the first time, the angular dependency of s- and p- polarized light absorption in nanopatterned graphene. The wide-angle electronically tunable extraordinary light absorption promises graphene-based optoelectronic devices.

*This work at the University of Central Florida was supported by DARPA under the WIRED program grant no. HR0011-16-1-0003.

12:51PM F14.00009: Theory of entangled-plasmon-pair generation in graphene* ZHIYUAN SUN, DIMITRI BASOV, Department of Physics, Columbia University, MICHAEL FOGLER (Presenter), University of California, San Diego — We study spontaneous parametric down conversion of terahertz photons into entangled plasmon pairs in graphene. This process is permitted by both symmetry and kinematics in a ribbon with an electron density gradient. We show that the conversion rate is maximized in ribbons containing lateral p-n junctions. We discuss how the quantum entanglement of the generated pairs can be measured by near-field optics techniques. We specify requirements for achieving plasmonic two-mode squeezed states and plasmonic instabilities in the presence of losses. We also study nonlinear plasmonic effects in a large-area uniformly doped graphene sheets due to third-order optical response.

*ONR Grant N00014-15-1-2671
1:03PM F14.00010: Pseudo-Euler equations from nonlinear optics: plasmon-assisted photodetection beyond hydrodynamics  
ALESSANDRO PRINCIPI (Presenter), DENIS BANDURIN, School of Physics and Astronomy, University of Manchester, HABIB ROSTAMI, Nordita, KTH Royal Institute of Technology and Stockholm University, MARCO CORRADO POLINI, Graphene Labs, Istituto Italiano di Tecnologia — A great deal of theoretical and experimental efforts have been devoted in the last decades to the study of long-wavelength photodetection mechanisms in field-effect transistors hosting two-dimensional electron systems. A particularly interesting subclass of these mechanisms is intrinsic and based on the conversion of the incoming electromagnetic radiation into plasmons of a two-dimensional electron system, which resonantly enhance the photoresponse, and subsequent rectification via hydrodynamic nonlinearities. Here we show that such conversion and subsequent rectification occur well beyond the frequency regime in which hydrodynamic theory applies. We consider the nonlinear optical response of generic 2D electron systems and derive pseudo-Euler equations of motion for suitable collective variables. These are solved in one- and two-dimensional geometries for the case of graphene and the results are compared with those of hydrodynamic theory. Significant qualitative differences are found, which are amenable to experimental studies. Our theory expands the knowledge of the fundamental physics behind long-wavelength photodetection.

1:15PM F14.00011: Strong Dirac Photoconductance in Charge Neutral Graphene-Boron Nitride-Graphene Heterostructures  
TREVOR ARP (Presenter), JACKY WAN, NATHANIEL MONROE GABOR, University of California, Riverside — Photoexcited hot charge carriers may shed light on the intriguing dynamics of electrons and holes near charge neutrality in very clean graphene. When two graphene layers are separated by thin hexagonal boron nitride (hBN), interlayer photocurrent can occur due to the exponential tail of the hot carrier distribution extending into the valence band of the hBN.[1] Using an ultrafast pulsed laser we excite a graphene-boron nitride-graphene (G-BN-G) heterostructure with photon energy less than the gap of the hBN and observe strong and highly nonlinear interlayer photocurrent as a function of the interlayer voltage. In a fully encapsulated heterostructure (BN-G-BN-G-BN), we find that the differential photocurrent can occur due to the exponential tail of the hot carrier distribution extending into the valence band of the hBN.

VASILI PEREBEINOS (Presenter), EE department, University at Buffalo — While graphene absorbs only 2.3% in the mid infra red (IR) spectral region, graphene plasmons have much stronger absorption in the far IR. Plasmons tunability by the external electric fields and by the spatial confinement offer a promising platform for opto-electronic and sensor applications. In this work [1], we demonstrate both theoretically and experimentally that the plasmon–plasmon and plasmon–radiation interactions modify strongly the plasmon resonance energy, radiative damping, and oscillator strength in graphene nanoribbon arrays. Even for the moderate filling factors of about 50%, plasmon radiative lifetime reduces to a ps time scale from a convetional ns time scale in the isolated graphene nanoribbon. We find scaling of plasmons with respect to the graphene doping level and filling factor, which both modify the strength of the long-range Coulomb and plamson-radiative interactions. The surprisingly large plasmon energy shift and radiative damping significantly affect the graphene-based plasmonic device performance.


1:39PM F14.00013: Optical Properties of Graphene/Al Hetero-film*  
HAOZHE WANG (Presenter), Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, SIDAN FU, Thayer School of Engineering, Dartmouth College, WEI SUN LEONG, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, JIFENG LIU, Thayer School of Engineering, Dartmouth College, JING KONG, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology — When two metal films stack together forming “hetero-film”, it has been generally accepted that the effective transparency is lower than the respective metal film as a result of the absorption accumulation. Here, we report a counterintuitive phenomenon where transparency of a hetero-film is significantly higher compared to the original metal film. Specifically, we found that by layering one-atom-thick graphene on an aluminum (Al) film, the transparency of the Al film is dramatically increased from ~60% to 80% under 550 nm wavelength light. More surprisingly, similar transparency enhancement is captured when Al film was deposited on the graphene film. Systematic characterizations and numerical simulations were conducted to understand this unusual phenomenon observed in the graphene/Al hetero-film, including Raman, XPS, SEM, AFM analyses. Furthermore, Hall measurements revealed that our graphene/Al hetero-film holds great promise to be used as flexible transparent electrodes.

*The authors acknowledge the support from NSF DMR/ECCS–1509197.
Resistively detected microwave absorption in highly twisted bilayer graphene

LIANGJI ZHANG (Presenter), JUSTIN LANE, Michigan State Univ, CHENYU ZHANG, J.I.A. LI, Brown University, CORY R DEAN, Columbia University, JOHANNES POLLANEN, Michigan State Univ — Resistively detected microwave absorption measurements of high-mobility two-dimensional (2D) electron systems are a powerful tool to explore the high-frequency spectroscopic and non-equilibrium response of correlated electron states in these systems. We have performed low-temperature magneto-transport experiments on a hexagonal boron nitride and dual graphite encapsulated twisted graphene bilayer while simultaneously irradiating the sample with microwave frequency photons. In this device the twist angle between the graphene flakes is relatively large, leading to a low-energy decoupling of the layers. Dual graphite gates allow us independent control of both the charge carrier density in the bilayer and a displacement electric field perpendicular to the 2D stack. We find that the differential magneto-conductance of the device, defined as the difference in conductance with and without microwave irradiation, shows well-defined oscillations in a large filling factor range down to the lowest Landau level. The dependence of these conductance oscillations on the magnetic field, displacement field, filling factor and microwave frequency will be discussed.

*This work was partially supported by the NSF (Grant no. DMR-1507788)

Resonant terahertz photoresponse and superlattice plasmons in graphene field-effect transistors

DENIS BANDURIN (Presenter), School of Physics, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom, DMITRY SVINTSOV, Moscow Institute of Physics and Technology (State University), Dolgoprudny 141700, Russia, IGOR GAYDUCHEKNO, Physics Department, Moscow State University of Education (MSPU), Moscow, 119435, Russian Federation, SHUIGANG XU, ALESSANDRO PRINCIPI, School of Physics, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom, MAKSIM MOSKOTIN, IVAN TRETYAKOV, Physics Department, Moscow State University of Education (MSPU), Moscow, 119435, Russian Federation, DENIS YAGODKIN, SERGEY ZHUKOV, Moscow Institute of Physics and Technology (State University), Dolgoprudny 141700, Russia, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044 Japan, IRINA GRIGORIEVA, School of Physics, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom, MARCO POLINI, Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, 16163 Genova, Italy, GREGORY GOLTSMAN, Physics Department, Moscow State University of Education (MSPU), Moscow, 119435, Russian Federation, ANDRE GEIM, School of Physics, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom, GEORGY FEDOROV, Moscow Institute of Physics and Technology (State University), Dolgoprudny 141700, Russia — Plasmons, collective oscillations of electron systems, can couple light and electric current, and thus can be used to create compact photodetectors, radiation mixers, and spectrometers. Despite the effort, it has proven challenging to implement plasmonic devices operating at THz frequencies. The material capable to meet this challenge is graphene as it supports long-lived electrically-tunable plasmons. In this talk, we will demonstrate plasmon-assisted resonant detection of THz radiation by antenna-coupled graphene FETs that act as both rectifying elements and plasmonic Fabry-Perot cavities amplifying the photoresponse. We will show that by varying the plasmon velocity using gate voltage, our detectors can be tuned between multiple resonant modes, a functionality that we apply to measure plasmons' wavelength and lifetime in graphene as well as to probe collective modes in its moire minibands. Our approach offers a convenient tool for further plasmonic research that is often difficult under non-ambient conditions and promises a viable route for various THz applications.


*We acknowledge Leverhulme Trust, Russian Science Foundation Grants N18-72-00234 and 17-72-30036, Russian Foundation for Basic Research No. 18-57-06001 and 16-29-03402.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F15 DMP: 2D Materials (Semiconductors) -- Optical Properties I

Northwestern - Tag(s): Focus
**11:15AM F15.00001: Optical excitations of transition-metal dichalcogenides with charged adsorbates**

MARTIK AGHAJANIAN (Presenter), ARASH A MOSTOFI, JOHANNES LISCHNER, Imperial College London — Direct band-gap semiconducting monolayer transition-metal dichalcogenides (TMDs) have been previously shown to demonstrate enhanced light absorption, which has promising applications in photovoltaic devices. This work explores the effects of charged adsorbates in MoS$_2$, MoTe$_2$, WS$_2$ and WTe$_2$ on their optical properties. Charged impurities on TMDs can give rise to bound states that extend over tens of nanometers due to weak screening in two-dimensional materials, hence it becomes difficult to capture their effects with conventional electronic structure calculations based on density-functional theory. In our approach, we first determine the electronic structure using large-scale tight-binding calculations which include a screened defect potential obtained from first-principles random-phase approximation calculations. Next, the Bethe-Salpeter equation is solved to include excitonic effects and obtain the optical absorption spectrum to compare with photoluminescence experiments. We indicate how trigonal symmetry present at the valleys of the band extrema results in deviation from simple hydrogenic behaviour of the bound states, and show dependence of excitonic resonances on the defect charge.

*Funded by EPSRC through the Centre for Doctoral Training in Theory and Simulation of Materials.

**11:27AM F15.00002: Nearly 90% circularly polarized emission in monolayer heterogeneous WS$_2$ single crystals by chemical vapor deposition (CVD)**

WEI-HSIANG LIN (Presenter), Dept. of Applied Physics, Caltech, WEI-SHIUAN TSENG, CORA WENT, Dept. of Physics, Caltech, GEORGE R ROSSMAN, Division of Geological and Planetary Science, Caltech, HARRY ATWATER, Dept. of Applied Physics, Caltech, NAI-CHANG YEH, Dept. of Physics, Caltech — Monolayer transition metal dichalcogenides (TMDCs) are promising materials for valleytronic applications because the two inequivalent valleys in the Brillouin zone. We report here novel optoelectronic properties of heterogeneous domains in CVD-grown monolayer WS$_2$ single crystals. Spatially resolved PL, Raman, X-ray photoelectron spectroscopy and Kelvin probe force microscopy images revealed the formation of homojunctions in these single crystals, which implied a direct correlation between the chemical stoichiometry and the optoelectronic heterostructure. Conductive atomic force microscopy (AFM) measurements revealed nanoscale distributions of electronically active defects in the heterogeneous WS$_2$, and the local defect density was found to be inversely proportional to the local PL intensity. Additionally, by optically pumping WS$_2$ with CPL and measuring the resulting spatially resolved CP emission ($P_{\text{circ}}$) at room temperature (RT) and low temperature (80K), we found significant $P_{\text{circ}}$ intensities even at RT, and $P_{\text{circ}}$ was inversely correlated with the defect density. At 80K, the degree of circularly polarized emission in low-defect domains was found to approach ~ 90%, suggesting nearly perfect valley polarization.

*This work is supported by the ARO and NSF.

**11:39AM F15.00003: Exciton regulation of resonant Raman scattering in monolayer MoS$_2$**

YUANXI WANG (Presenter), Pennsylvania State University, BRUNO R. CARVALHO, Universidade Federal do Rio Grande do Norte, VINCENT HENRY CRESPI, Pennsylvania State University — Strong excitonic effects in 2D semiconductors such as monolayer MoS$_2$ not only downshift its excitation spectrum from a single-particle one, but also redistribute excitation levels and wavefunction characters that profoundly affect exciton-phonon scattering processes, leaving strong signatures in resonant Raman measurements. We present a first-principles GW-Bethe-Salpeter equation (GW-BSE) approach based on perturbation theory to calculate resonant Raman intensities beyond the Placzek approximation. We show how excitonic effects in MoS$_2$ strongly regulate Raman scattering amplitudes and explain two puzzling experimental observations: the near absence of Raman response at the A and B band-edge excitons and the pronounced strength of Raman response near the C exciton. This perturbative approach reduces the number of GW-BSE calculations from two per Raman mode in finite displacement methods to one for all modes and allows a natural extension to higher-order resonant Raman processes [Phys. Rev. B 98, 161405 (2018)].

*This work is supported by computational time on the LSU-superMIC through the XSEDE allocation TG-DMR170050 and by the National Science Foundation Materials Innovation Platform under DMR-1539916. We acknowledge financial support from the Brazilian agencies CNPq and CAPES.
11:51 AM F15.00004: Optical tuning of magnetism with valley polarized excitation  
XIAO-XIAO ZHANG (Presenter), LIZHONG LI, ZEFANG WANG, JIE SHAN, KIN FAI MAK, Cornell University — Magnetic 2D materials hold great promises to allow a more active control of magnetism. By interfacing other 2D monolayers with the atomically flat magnet, we can create new functional materials that combines different features and properties. In this talk, I would present my work on the heterostructure of ferromagnetic CrBr$_3$ and monolayer transition metal dichalcogenide (TMDC) of WSe$_2$. I would show how the optical excitation within the WSe$_2$ would also affect the magnetism in CrBr$_3$. By employing circularly polarized light, valley and spin polarized carriers are created within the TMDC as a result of the valley optical selection rule. Sequential modification in the magnetic response in CrBr$_3$ indicates that there exists efficient spin transfer from the excited TMDC into the interfaced magnet. Further characterizations including temperature dependence, excitation detuning etc. would also be discussed. The efficient optical tuning of magnetism opens up promising directions to manipulate magnetic domains in an all-optical method.

12:03 PM F15.00005: Measuring Valley Susceptibility of Transition Metal Dichalcogenides with Second-harmonic Spectroscopy*  
YI WEI HO (Presenter), NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, HENRIQUE GUIMARAES ROSA, IVAN VERZHBITSKIY, Centre for Advanced 2D Materials, National University of Singapore, MANUEL JOSE FERREIRA DE LIMA RODIGUES, Center of Physics and Department of Physics, Universidade do Minho, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, GOKI EDA, VITOR PEREIRA, JOSÉ CARLOS VIANA-GOMES, Centre for Advanced 2D Materials, National University of Singapore — Polarization-resolved (PR) photoluminescence (PL) [1] and Kerr rotation (KR) [2] are commonly used to probe the degree of valley polarization (VP) of transition metal dichalcogenides (TMDs). Recently, second-harmonic (SH) generation was proposed to also probe VP [3], with the advantage over PL and KR of not requiring the material to have a bandgap or strong spin-orbital coupling, and thus extending VP measurements to other materials such as graphene.

In this work, we have develop a technique that uses a single laser beam prepared in a polarization state that simultaneously creates VP and pumps the SH process. By increasing the ellipticity of this pump beam, which translates into a larger VP in the sample, we observed an additional SH signal due to the VP, in good agreement with our theoretical model. Based on a transient analysis within the duration of the laser pulse, our model confirms SH susceptibility induced by VP to be directly proportional to the degree of VP, with the effect an order of magnitude higher for a quasi-resonant VP pump when compared to the off-resonant case.


*I thank scholarship support from NGS.

12:15 PM F15.00006: Light based control of Exciton Polaritons in Van der Waals Semiconductors  
AARON STERNBACH (Presenter), Physics, Columbia University, SIMONE LATINI, HANNES HUEBENER, UMBERTO DE GIOVANNINI, Max Planck Institute for the Structure and Dynamics of Matter, SANGHOON CHAE, Mechanical Engineering, Columbia University, LIN XIONG, YINMING SHAO, Physics, Columbia University, NORMAN SHI, Columbia University, GUANGXIN NI, Physics, Columbia University, NANFANG YU, Columbia University, MICHAEL FOGLER, Physics, University of California, San Diego, JAMES HONE, Mechanical Engineering, Columbia University, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter, DIMITRI BASOV, Physics, Columbia University — In this work we focus on exciton polaritons in the Van der Waals (vdW) Semiconductor, WS$_2$, under intense femto-second (fs) photo-excitation. Photo-excitation initiates a blueshift of the exciton polariton. This corresponds to an extremely large photo-induced change of the dielectric function. Detailed investigation of the dispersion and the fluence dependence indicate the observed effect arises from light-based control of excitons. The change to the dielectric function evolves over two distinct timescales. On the femtosecond timescale a large coherent contribution is observed. On the picosecond (ps) timescale part of the effect is found to persist. The equilibrium state is fully recovered approximately one hundred ps after the photo-excitation event. The information-rich data-sets available from interrogating the exciton-polariton allow us to explore the pathways toward active control of excitons. Additionally, our experimental approach allows us to access key quantities, such as the group velocity and real-space confinement of the exciton polariton, in the non-equilibrium state. Finally, our findings indicate that strong-light matter interactions in vdW semiconductors may be used to achieve all-optical control of significant magnitude.
Spin-Valley dependent optical response at monolayer transition metal dichalcogenide/ferrimagnet interface  TAKATOSHI AKAMATSU (Presenter), TOSHIYA IDEUE, MASARU ONGA, YUKI ITAHASHI, YUJI NAKAGAWA, YOSHIHIRO IWASA, Department of applied physics, University of Tokyo — Monolayer transition metal dichalcogenides (TMDs) is one of the potential candidates for valley-based electronics, since valley degree of freedom in TMDs couples with orbital and spin degree of freedoms, so that it can be manipulated by optical or magnetic method. So far, valley-optical responses related with orbital degree of freedom have been elucidated in monolayer TMDs. Recently, TMDs/magnet interfaces are widely studied as an ideal platform for studying the spin-valley related phenomena[1][2].

Here I report the characteristic optical responses at new interface of TMDs and ferrimagnetic Fe₃O₄. Valley-Zeeman effect and the probable spin-valley relaxation, which has been reported in previous works of TMDs/ferromagnet interfaces, have been also observed at the new interface. In the presentation, I also discuss the microscopic origin of the observed spin-valley relaxation.


Ultrafast Dynamics of Excitonic Rydberg Series in Single Layer WSe₂  MEHMET B YILMAZ (Presenter), EMRE ERGECEN, Department of Physics, Massachusetts Institute of Technology, NATHAN P WILSON, Department of Physics, University of Washington, JOSEPH VARGHESE, STEVEN VITALE, MIT Lincoln Laboratory, XIAODONG XU, Department of Physics, University of Washington, NUH GEDIK, Department of Physics, Massachusetts Institute of Technology — Single layer transition metal dichalcogenides (TMD) such as MoS₂ and WSe₂ have been the subject of intense attention for their optically accessible valley polarization. In these materials, circularly polarized light can be used to break the time-reversal symmetry and lift the degeneracy of the K and K’ valleys. Such optical control is of great importance for possible valleytronic applications. In this work, we will present broadband transient reflection microscopy results obtained from hBN capped single layer WSe₂ flakes. In these high quality samples, it is possible to observe the excitonic Rydberg states in the reflectivity data. We have studied the dynamics of these states after photo-excitation via pump-probe spectroscopy. When the excitation light energy is tuned below the band gap, high quality of these samples enable observation of novel valley selective coherent response in addition to the previously observed optical Stark shift.

*We acknowledge support from the US Department of Energy, BES DMSE and from the Gordon and Betty Moore Foundation's EPiQS Initiative grant GBMF4540.

Suspended Excitons in 2D Materials  OZGUR BURAK ASLAN, YAN JOE LEE (Presenter), Stanford University, YIFEI YU, LINYOU CAO, North Carolina State University, MARK BRONGERSMA, Stanford University — Excitons in atomically thin transition metal dichalcogenides (TMDCs, 2D materials) are strongly influenced by their environment. To eliminate that influence, we prepare suspended monolayer (1L) WSe₂ samples, enabling suspended excitons. We perform reflectance measurements and calculate the excitonic binding energies from the experimental observables: the energy differences between the 1s, 2s, and 3s states. We employ the recently developed quantum electrostatic heterostructure model for the calculations. We see that the binding energy of the ground state A exciton increases from about 0.3 eV (on substrate) to above 0.4 eV (suspended). A more striking feature of the suspended excitons is the ability to tune them even further by applying mechanical strain. By applying air pressure, we obtain reversible 0.15 eV redshift in the exciton resonance of a suspended 1L sample on a circular hole of 8 μm diameter under a pressure of 40 psi. Interestingly, the linewidth of the A exciton decreases more than half from about 45-50 meV to 20 meV at room temperature, due to the suppression of the intervalley exciton-phonon scattering. Our results show that suspended 2D materials are novel systems for fundamental studies as well as strong and dynamic tuning of the excitons.
The discovery of graphene marked the start of research in 2D electronic materials which was expanded in new directions with MoS₂ and other layered semiconducting materials. They have a wide range of interesting fundamental properties and potential applications. New opportunities are enabled by the band structure of transition metal dichalcogenides (TMDCs) in which we could harness the valley degree of freedom for valleytronics and next-generation photonics. Long-lived interlayer excitons in van der Waals heterostructures based on TMDCs have recently emerged as a promising platform for this, allowing control over exciton diffusion length, energy and polarization. I will show here how by using MoS₂/WSe₂ van der Waals heterostructures, we can realize excitonic transistors with switching action, confinement and control over diffusion length at room temperature in a reconfigurable potential landscape. Heterostructures with a long-range moiré potential such as in MoSe₂/WSe₂, on the other hand, offer the way to control polarization, emission and wavelength emitted by different optically active regions in the moiré.

*We acknowledge support by the Swiss National Science Foundation (Grant 153298), H2020 European Research Council (ERC, Grant 682332), Marie Curie-Sklodowska-Curie Actions (COFUND grant 665667), European Union's Horizon H2020 Future and Emerging Technologies under grant agreements No 696656 and 785219 (Graphene Flagship).

**1:03PM F15.00010: Exciton Manipulation in 2D TMDC Heterostructures** [Invited] ANDRAS KIS (Presenter), EPFL, Lausanne, Switzerland — The discovery of graphene marked the start of research in 2D electronic materials which was expanded in new directions with MoS₂ and other layered semiconducting materials. They have a wide range of interesting fundamental properties and potential applications. New opportunities are enabled by the band structure of transition metal dichalcogenides (TMDCs) in which we could harness the valley degree of freedom for valleytronics and next-generation photonics. Long-lived interlayer excitons in van der Waals heterostructures based on TMDCs have recently emerged as a promising platform for this, allowing control over exciton diffusion length, energy and polarization. I will show here how by using MoS₂/WSe₂ van der Waals heterostructures, we can realize excitonic transistors with switching action, confinement and control over diffusion length at room temperature in a reconfigurable potential landscape. Heterostructures with a long-range moiré potential such as in MoSe₂/WSe₂, on the other hand, offer the way to control polarization, emission and wavelength emitted by different optically active regions in the moiré.

1:39PM F15.00011: Optical spectroscopy of excited Rydberg excitons to 65 tesla in monolayer semiconductors

ANDREAS STIER (Presenter), MATEUSZ GORYCA, JING LI, SCOTT CROOKER, Los Alamos National Laboratory, NATHAN P WILSON, XIAODONG XU, University of Washington, EMMANUEL COURTADE, CEDRIC ROBERT, XAVIER MARIE, BERNHARD URBASZEK, INSA Toulouse — Monolayer transition-metal dichalcogenide (TMD) semiconductors, such as MoS₂, host very tightly-bound excitons due to reduced dielectric screening and relatively heavy electron / hole masses. Advances in the encapsulation of monolayer TMDs in atomically-flat hexagonal boron nitride (hBN) result in narrow neutral exciton resonances, as well as spectral features associated with excited Rydberg states. Optical spectroscopy in high magnetic fields was recently demonstrated to be a powerful way to uniquely identify these states in WSe₂ and to determine fundamental properties such as the exciton size, mass and binding energy [1]. Here, we report 65 T magneto-absorption spectroscopy of excited Rydberg excitons in hBN-encapsulated WS₂, MoS₂ and MoSe₂ monolayers. The distinct diamagnetic shifts of these excited states (2s, 3s, ..., ns) permits their unambiguous identification, and provide a direct measure of the reduced exciton masses. We compare our experimental results with numerical simulations of the non-hydrogenic Rytova-Keldysh potential for strictly 2D semiconductors, and more general models describing Coulomb interactions in thin-film semiconductors. [1]Stier et al., PRL 120, 057405 (2018).

1:51PM F15.00012: Berry Curvature Induces Exciton Fine-structure and Valley-dependent Autler-Townes Doublet in Molybdenum Diselenide Monolayer

CHAW KEONG YONG (Presenter), IQBAL B UTAMA, FENG WANG, University of California, Berkeley — The geometry phase of Bloch states in the momentum space, characterized by the Berry curvature, can strongly modify the electron dynamics and lead to novel transport phenomena, such as the anomalous Hall effect. Recently it was predicted that the nontrivial Bloch band geometry can also modify the collective optical excitations in transition metal dichalcogenide monolayers, and lift the energy degeneracy of exciton states with opposite angular momentum through an effective valley-orbital effect. Here we report the first experimental observation of the Berry curvature signature in the exciton spectrum of MoSe₂ monolayer using novel techniques based on intraexciton optical Stark spectroscopy. We demonstrate the time-reversal-symmetric analog of the orbital Zeeman effect resulting from the valley-dependent Berry curvature, which leads to energy difference of +14 (-14) meV between the 2p+ and 2p- exciton fine-structure in the K (K') valley. The coherent light-matter coupling between intraexciton states are remarkably strong, leading to a prominent valley-dependent Autler-Townes doublet. Our study opens up new pathways to manipulate the quantum states with infrared radiation and suggests the possibility to control the light-matter interaction via topological quantum phase engineering.

2:03PM F15.00013: Understanding thickness-dependent electronic and optical transitions of Ruddlesden-Popper halide perovskites

YEONGSU CHO (Presenter), TIMOTHY BERKELBACH, University of Chicago — Ruddlesden-Popper halide perovskites are layered heterostructures that are promising candidates for effective optoelectronic devices due to their photoefficiency and stability. Despite their high tunability through substitution and stoichiometry, the physics that control the resulting electronic and optical properties are still not fully understood. We investigate the dependence of the band gap and exciton binding energy on the inorganic layer thickness through the tight binding approximation and nonlocal screened Coulomb potential, making use of material properties of three-dimensional perovskites. Our theory provides an analysis of the optical gap measured by absorption and photoluminescence.

**Tuesday, March 5, 2019 11:15 AM - 1:51 PM**
**Session F16 DMP: Computational Materials Design and Discovery -- Semiconductors**

11:15AM F16.00001: Machine learned defect level predictor for semiconductors

ARUN KUMAR MANNODI, Kanakkithodi (Presenter), Center for Nanoscale Materials, Argonne National Laboratory, DUYEN H CAO, NARI JEON, Materials Science Division, Argonne National Laboratory, JI-SANG PARK, Department of Materials, Imperial College London, MICHAEL J DAVIS, Chemical Science Division, Argonne National Laboratory, ALEX MARTINSON, Materials Science Division, Argonne National Laboratory, MARIA CHAN, Center for Nanoscale Materials, Argonne National Laboratory — Electronic levels introduced by impurities and defects in the band gap are critically important in semiconductors for optoelectronic and photovoltaic (PV) applications. The energetics and energy levels of point defects can be reliably predicted using density functional theory (DFT) computations. However, the requirement of large supercells and inclusion of charged states make these computations very expensive, and trends and knowledge from previous calculations are not exploited in subsequent ones. In this work, we develop machine learned defect level predictors based on substantial DFT data for two classes of semiconductors: halide perovskites (MAPbX₃, MA = methylammonium, X = Cl/Br/I), and Cd-based chalcogenides (CdX, X=Te/Se/S). DFT data was generated for formation energies and transition levels of hundreds of vacancy, interstitial and substitutional defects, following which correlation analysis and random forest regression were used to map the properties to a set of unique numerical descriptors, resulting in cheap, accurate, quantitative prediction models. Such models can lead to accelerated prediction of defect states and allow efficient materials design of defect-tolerant semiconductors as well as semiconductors with suitably placed defect levels.

11:27AM F16.00002: Ternary semiconductors with tunable band gaps from machine-learning and crystal structure prediction

MAXIMILIAN AMSLER, (Presenter), Cornell University, CHRISTOPHER WOLVERTON, LOGAN WARD, VINAY I HEGDE, Northwestern University — Computational tools are being employed at an increasing rate to discover and design novel materials with tailored properties to tackle global environmental challenges. Besides the two most common approaches based on high-throughput density functional theory (DFT) calculations and crystal structure prediction schemes, novel methods based on materials informatics and machine learning (ML) models have recently emerged to assist the search for materials with improved properties in industrially relevant applications.

Here, we present a computational investigation of a series of ternary X₄Y₂Z compounds with X={Mg, Ca, Sr, Ba}, Y={P, As, Sb, Bi}, and Z={S, Se, Te}, which we identify by a combined search using a machine learning model and the minima hopping crystal structure prediction method. According to our ab initio results, these compounds are thermodynamically stable and semiconducting with band gaps in the range of 0.3 to 1.8 eV, well suited for various energy applications. We show that several candidate compounds exhibit good photo absorption in the visible range, and excellent thermoelectric performance due to high power factors and extremely low lattice thermal conductivities.

11:39AM F16.00003: Polarization engineering with novel nitride heterostructures from first principles*

NICHOLAS ADAMSKI, (Presenter), DARSHANA WICKRAMARATNE, CHRIS VAN DE WALLE, University of California, Santa Barbara — Novel heterostructures based on II-IV-nitride semiconductors in combination with the widely used III-nitrides are being explored due to the ability to access a wide range of band offsets and polarization charges at the interface. The polarization charges arise from contributions due to spontaneous and piezoelectric polarization. Exploiting polarization requires a systematic methodology for evaluating the polarization properties and band alignments for a variety of materials and their heterostructures. We study the spontaneous and piezoelectric polarization of the II-IV-nitrides using density functional theory with a hybrid functional. To determine band offsets we use surface calculations as well as alignments based on the electronic level of interstitial hydrogen. We use our results to explore II-IV-nitride/III-nitride heterostructures that give rise to low polarization fields, which is favorable for light emitters.

*This work is supported by ARO.
Dielectric screening plays an important role in preventing carrier scattering and trapping by point defects for many electronic semiconductors. We performed a material search study using the dielectric properties as a screen to identify new electronic semiconductors such as the halide perovskite solar materials. However, it was rarely considered as a screen to find new materials for deep UV LED design. We show that boron incorporation into AlGaN allows for improved lattice matching to AlN with only a small effect on the band gap. The a lattice parameter is more sensitive to boron incorporation than the c lattice parameter. We predict similar boron incorporation limits (~15% boron) as in BAIN, but with easier incorporation of low boron content than in BAIN due to increased configurational entropy.

*This work was supported by NSF DMREF program (1534221). Computational resources provided by DOE NERSC (DE-AC02-08CH11231).

12:03PM F16.00005: First-principle study of phosphors for white-LED applications: Stokes shift, emission linewidth and thermal quenching. [Invited] XAVIER GONZE (Presenter), YONGCHAO JIA, ANNA MIGLIO, IMCN, Université catholique de Louvain, SAMUEL PONCÉ, Department of Materials, Oxford University, MASAYOSHI MIKAMI, Yokohama R&D Center, Mitsubishi Chemical Corporation — Despite current impact of white-LED technology, available blue-to-red phosphors exhibit a too wide emission linewidth or some other drawback, such as strong thermal quenching behavior. In view of large-scale high-throughput search for better phosphors, an accurate but fast computational methodology is needed, not restricted to the ground state (formation energy), but covering excitation and emission energies, Stokes shift, emission linewidth, and emission intensity reduction through thermal quenching. We will present results from a constrained density functional theory methodology for about 30 Ce- and Eu-doped materials [1,2] with 4f → 5d transitions. It matches experimental data within 0.3 eV for both absorption and emission energies (ranging between 2.0 eV and 5.0 eV) and provides Stokes shifts usually within 30%. By contrast, the largely used semi-empirical Dorenbos approach [3] does not perform as well, although it provides physical insights to explain trends among the materials, including the different Stokes shifts. This first-principles approach also delivers emission linewidth and assessment of mechanisms for thermal quenching, based on a simple 1-dimensional configuration coordinate approach. For our representative set of Eu-doped materials, we find that the 4f-5d crossover model cannot be the dominant thermal quenching mechanism: the predicted barrier at the 4f-5d crossing is always higher than 1.5 eV. Also, it will be shown how to waive the one-dimensional restriction in the search for the lowest 4f-5d crossing energy barrier. [1] Y. Jia, S. Poncé, A. Miglio, M. Mikami & X. Gonze, Adv. Opt. Mat. 5, 1600997 (2017). [2] Y. Jia, A. Miglio, S. Poncé, M. Mikami & X. Gonze, Phys. Rev. B 96, 125132 (2017). [3] P. Dorenbos, J. Lumin. 91, 155 (2000); Phys. Rev. B 62, 15640 (2000).

*Work supported by FRS-FNRS Belgium through a postdoctoral researcher fellowship (YJ), and PdR Grant T.0238.13-AIXPHO. SP acknowledges funding from Leverhulme Trust (Grant RL-2012-001)

12:39PM F16.00006: Dielectric Behavior as a Screen in Rational Searches for Overlooked Electronic Materials: Metal Pnictide Sulfosalts. XIN HE (Presenter), School of Materials Science and Engineering, Jilin University, DAVID JOSEPH SINGH, Department of Physics and Astronomy, University of Missouri, PATSORN BOON-ON, MING-WAY LEE, Institute of Nanoscience and Department of Physics, National Chung Hsing University, LIJUN ZHANG, School of Materials Science and Engineering, Jilin University — Dielectric screening plays an important role in preventing carrier scattering and trapping by point defects for many semiconductors such as the halide perovskite solar materials. However, it was rarely considered as a screen to find new electronic semiconductors. We performed a material search study using the dielectric properties as a screen to identify potential electronic materials in the class of metal-pnictide ternary sulfosalts, containing Bi or Sb. We find significant cross-gap hybridization between the Sₚ derived valence bands and pnictogen pderived conduction bands in many of the materials. This leads to enhanced Born effective charges, and highly enhanced dielectric constants. We find a chemical rule for high dielectric constant in terms of the connectivity of the structure. Through first principles screening, we find a series of compounds with low effective mass, high dielectric constant and other properties that suggest good performance as electronic materials, and also several potential thermoelectric compounds. The results illustrate the utility of dielectric properties as a screen for identifying complex semiconductors.

*Work at Jilin University is supported by National Natural Science Foundation of China under Grant Nos. 61722403 and 11674121.
12:51 PM F16.00007: Sn(II)-containing phosphates as promising p-type optoelectronic semiconductors*  TIANSHU LI (Presenter), QIAOLING XU, Jilin University, HAOWEI PENG, Temple University, DAVID SINGH, University of Missouri-Columbia, LIJUN ZHANG, Jilin University — High-performance and stable p-type optoelectronic semiconductors, such as transparent conductors, have been searched for with decades of efforts. We herein proposed based on first-principles straightforward calculations and structure searches Sn(II)-containing phosphates Sn_nP_2O_{5+n} (n=2, 3, 4, 5, ...) as promising p-type semiconductors for optoelectronic applications. We found that these materials have large band gaps and can have moderate effective masses for both holes and electrons. Calculations of optical properties show that interband transitions in the visible are weak under hole doping. We also find an interesting inverse Burstein-Moss shift, which can be understood in terms of the Sn character of both the states at band edges. By investigating intrinsic defects properties, we identified dominant carrier traps and revealed ideal growth conditions for p-type Sn(II) phosphates. The results indicate that Sn_nP_2O_{5+n} with large n may be doped to p-type with promising attainable hole density. The unusual combinations of relatively high band gap, low carrier masses and high chemical stability suggest possible optoelectronic applications of Sn(II) phosphates.

*Work at Jilin University is supported by National Natural Science Foundation of China under Grant Nos. 61722403 and 11674121.

1:03 PM F16.00008: Computational design of new polymorphs of two-dimensional semiconductor InSe with enhanced interlayer interaction  YUANHUI SUN (Presenter), Jilin University, SONG-LIN LI, Nanjing University, KOUSHIK BISWAS, Arkansas State University, LIJUN ZHANG, Jilin University — Atomically thin, two-dimensional InSe has attracted considerable attention due to its widely tunable band gap and high electron mobility. The intriguingly high dependence of band gap on layer thickness remains poorly understood, and is generally attributed to quantum confinement effect. We demonstrated via systemic first-principles calculations in our previous work that strong interlayer coupling may be mainly responsible for this phenomenon, especially in the fewer-layer region. The interlayer coupling was also found to be an essential factor influencing other thickness-dependent material properties such as indirect-to-direct band gap transitions, fan-like phonon frequency diagrams, carrier mobilities, etc. In this work, by combining global structure search algorithm and first-principles calculations, we strikingly discovered two new polymorphs of InSe consisting of the monolayer in point group D_{3d}, distinct from the known one in point group D_{3h}. The new polymorphs show thermodynamic and lattice dynamical stability, and large transition barrier to the existing phases. One newly discovered polymorph exhibits the enhanced interlayer coupling, manifested by the most tunable band gap and the highest electron mobility among all the InSe phases.

1:15 PM F16.00009: A quantum-mechanical map for bonding and properties in materials*  JEAN-YVES RATY (Presenter), University of Liege, MATHIAS SCHUMACHER, RWTH Aachen, PAVLO GOLUB, National University of Singapore, VOLKER L DERINGER, University of Cambridge, CARLO GATTI, CNR-ISTM Università degli Studi di Milano, MATTHIAS WUTTIG, RWTH Aachen — Materials with rationally controlled properties play important parts in the development of new and advanced technologies. For instance, the properties of thermoelectric, phase-change, or topologically insulating materials can be traced back, to a significant extent, to the nature of bonding in materials. Here, we develop a two-dimensional map based on a quantum-topological description of electron sharing and electron transfer. This map intuitively identifies the fundamental nature of ionic, metallic, and covalent bonding in a range of elements and binary materials [1]. Furthermore, it highlights a distinct region for a mechanism recently termed “metavalent” bonding [2]. Extending this map into the third dimension by including physical properties of application interest, we show that bonding in metavalent compounds differs from the classical textbooks views of bonding. This map could be used to help designing new materials: by searching for desired properties in a 3D space and then mapping this back onto the 2D plane of bonding.

[2] Advanced Materials, accepted

*Work funded by F.R.S.-FNRS, RW, JARA-HPC, the Isaac Newton trust, the Danish Res. Found. the Deutsche Forschungsgemeinschaft and the EU FP7.
ABHIYAN PANDIT (Presenter), RAAD HALEOOT, BOTHINA HAMAD, University of Arkansas — Lead telluride (PbTe) and other lead-chalcogenides such as PbSe and PbS have been extensively investigated due to their potential applications in thermoelectric (TE) devices. Researchers previously reported good values of the figure-of-merit ($zT$) > 1.7 for PbTe – CdTe alloy at 775 K $^1$, and about 1.5 for doped PbTe with Thalium at 773 K $^2$. In addition, experiments showed that doping PbTe with Sn increases the figure of merit to 0.8 at 700 K $^3$. These promising experimental results were the motivation to carry out the electronic structure calculations of Pb$_{1-x}$Sn$_x$Te ($x = 0.25, 0.5, 0.75$) compounds using density functional theory $^4$ in this study. Based on the semi-classical Boltzmann theorem $^5$, the TE properties are computed and the results will be presented.

References:

This work was supported by Arkansas NASA EPSCOR Research Infrastructure Development (RID) grant number 002276-00001A. Calculations performed using High Performance Computer Center at the University of Arkansas.

HUJUN GU (Presenter), Fudan University — The band offset between different semiconductors is an important physical quantity determining carrier transport properties near the interface in heterostructure devices. Computation of the natural band offset is a longstanding challenge. We propose an intermediate-phase method to predict the natural band offset between two structures with different symmetry, for which the superlattice model cannot be directly constructed. With this method and the intermediate phases obtained by our searching algorithm, we successfully calculate the natural band offsets for two representative systems, (i) zinc-blende CdTe and wurtzite CdS and (ii) diamond and graphite. The calculation shows that the VBM of zinc-blende CdTe lies 0.71 eV above that of wurtzite CdS, close to the result 0.76 eV obtained by the three-step method. For the natural band offset between diamond and graphite which could not be computed reliably with any superlattice methods, our calculation shows that the Fermi level of graphite lies 1.51 eV above the VBM of diamond. This method, under the assumption that the transitivity rule is valid, can be used to calculate the band offsets between any semiconductors with different symmetry on condition that the intermediate phase is reasonably designed.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F17 DCOMP: Matter in Extreme Environments: Novel Materials BCEC 156A - Xiaolei Feng -

ANASTASIA NAUMOVA (Presenter), SERGEY LEPESHKIN, ARTEM OGANOV, Skolkovo Institute of Science and Technology — Understanding the high-pressure behavior of C-H system is of great importance due to its key role in organic, bio-, petroleum and planetary chemistry. We have performed a systematic investigation of the pressure-composition phase diagram of the C-H system at pressures up to 400 GPa using evolutionary structure prediction coupled with ab initio calculations and discovered that only saturated hydrocarbons are thermodynamically stable. Concluding our results, in C-H system only saturated hydrocarbons are thermodynamically stable. Several surprising stable methane-hydrogen co-crystals are predicted, some of them have potential energy storage purpose. We consider effects of temperature through the quasiharmonic approximation and report the pressure-temperature-composition phase diagram of the C-H system and pressure-temperature phase diagram of CH$_4$ (up to 2000 K).

We thank the Russian Science Foundation (grant 16-13-10459) for supporting this work. Calculations were performed on our Rurik supercomputer, the Arkuda supercomputer of Skolkovo Foundation, and at the supercomputer center of the University of Nizhny Novgorod.
**11:51AM F17.00002: Evolutionary prediction and experimental synthesis of SiOS at high pressure**

ONDREJ TÓTH, Department of Experimental Physics, Comenius University in Bratislava, Slovakia, MARIO SANTORO, FEDERICO GORELLI, GIANGAETANO PIETRAPERZIA, Istituto Nazionale di Ottica (CNR-INO) and European Laboratory for non Linear Spectroscopy (LENS), Sesto Fiorentino, Italy, MOHAMED MEZOUAR, GASTON GARBARINO, European Synchrotron Radiation Facility, Grenoble Cedex 9, France, ROMAN MARTONAK (Presenter), Department of Experimental Physics, Comenius University in Bratislava, Slovakia — SiOS represents a ternary generalization of the well-known and highly important family of binary AB2 compounds including CO2, SiO2, GeO2, CS2, SiS2, etc. The presence of two different bond lengths suggests that its crystal structures may be different from those found in SiO2 and SiS2. We applied evolutionary search based on DFT _ab initio_ calculations to determine crystal structures of SiOS for pressures up to 100 GPa. We predict the SiOS phase diagram at zero temperature and examined the structural, electronic and vibrational properties of the stable phases. At low pressure the stable phase is a tetrahedrally coordinated layered orthorhombic Cmc21 structure. This is predicted to transform at 14 GPa to an octahedrally coordinated layered monoclinic C2/m structure similar to the P-3m1 phase of SiS2. The system remains insulating up to 100 GPa with band gap above 1.8 eV. Following the theoretical prediction we synthesized SiOS by laser heating elemental Si, O and S in the diamond anvil cell at pressure of 8 GPa. The observed XRD pattern is in very good agreement with the theoretical prediction for the Cmc21 structure.

*Slovak Research & Development Agency APVV-15-0496; Slovak infrastr. high-perform. computing, ITMS 26230120002 and 26210120002, ERDF

**12:03PM F17.00003: Structure identification at extreme conditions**

JENNIFER NIEDZIELA (Presenter), ANDREW MISKOWIEC, ASHLEY SHIELDS, BIANCA HABERL, Oak Ridge National Laboratory — We are investigating a series of low-crystallinity, amorphous uranium oxides relevant for long term storage of spent nuclear fuel. One compound has stoichiometry of ~UO3.5 (a-UO3), which appears to be x-ray amorphous. To understand the a-UO3 structure, we couple density functional theory with a genetic algorithm structure prediction mechanism to identify stable structures of non-stoichiometric uranium oxides. The lowest energy predicted structure with stoichiometry UO3.5 contains a peroxide bridge, compatible with a study of comparable material using neutron pair-distribution function techniques. We attempted to crystallize a-UO3 using a diamond anvil cell and Raman spectroscopy up to 25 GPa and observed highly anharmonic responses to pressure, but no long range order. Computational studies on the low-energy structure from the genetic algorithm show commensurate responses to the dynamical observations, along with anomalous changes in local bonding character, suggesting an indirect pathway for material identification.

*This work was supported by the US Department of Energy. Postdoctoral research was funded by the US Department of Homeland Security.

**12:15PM F17.00004: Pressure-induced New Oxidation States for Gold Element**

JIANYAN LIN, SHOUTAO ZHANG, GUOCHUN YANG (Presenter), Department of Physics, Northeast Normal University, YANMING MA, State Key Lab of Superhard Materials, College of Physics, Jilin University — The formalism of the oxidation state of atoms in compounds is a key concept in chemistry. Finding novel compounds containing elements with unusually high oxidation states allows a deeper understanding of chemical behavior of elements. On the other hand, high oxidation state compounds usually bring new types of bonds with interesting physical and chemical properties. Thus, the preparation of compounds with unusual oxidation states becomes an attractive topic in chemistry and condensed-matter physics. Gold (Au) is a well-known fascinating element, but still hides interesting surprises to be discovered, especially for oxidation state. Here, we propose that high pressure becomes a controllable method for preparing high negative oxidation state of Au through its reaction with lithium. Au acts as a 6p-element in dense lithium aurides. Moreover, we identify two hitherto unknown stoichiometric compounds, AuF4 and AuF6, exhibiting typical molecular crystal character, in which Au demonstrates +4 and +6 oxidation states. Our work represents a significant step forward in a more complete understanding of the oxidation states of Au.
12:27PM F17.00005: Site-selective Mott insulator-metal transition in Fe$_2$O$_3$ under ultra-high pressures  
IGOR ABRIKOSOV (Presenter), Linköping University, Sweden and NUST "MISIS", Russia, IVAN LEONOV, Institute of Metal Physics, Yekaterinburg, Russia and NUST "MISIS", Russia, GREGORY KH. ROZENBERG, Tel Aviv University, Israel — The insulator-metal transition, induced by pressure, composition or by other means, represents perhaps the most profound transformation of the chemical bond in materials. Combining density functional plus dynamical mean-field theory (DFT+DMFT) calculations with experiment, we demonstrate that upon compression of Fe$_2$O$_3$ a novel type of Mott insulator-metal transition occurs, which is characterized by site-selective delocalization of the electrons [1]. Within the $P2_1/n$ crystal structure, which is stable in the pressure range 45-68 GPa, we observe equal abundances of ferric ions (Fe$^{3+}$) and ions having delocalized electrons (Fe$^M$). Thereby the transition is characterized by delocalization/metalization of the 3$d$ electrons on half the Fe sites, with a site-dependent collapse of local moments. Upon further compression above 75 GPa, we predict another phase transition, to a metal with a post-perovskite crystal structure and site-selective local moments [2]. Our results suggest that site-selective local moments in Fe$_2$O$_3$ persist up to ultra-high pressure of ~200-250 GPa, i.e. to pressure sufficiently above that at the core-mantle boundary.


12:39PM F17.00006: First-Principles Modeling and Evolutionary-Algorithm Prediction of Superhard B-C and B-N systems*  
WEI-CHIH CHEN (Presenter), CHENG-CHIEN CHEN, University of Alabama at Birmingham — Superhard materials with a Vickers hardness larger than ~40 GPa have a wide range of industrial applications such as cutting tools and protective coatings. Superhard boron-carbon (B-C) and boron-nitride (B-N) composites are especially important because of their superior high-temperature performance as compared to diamond and their low reactivity with ferrous metals. Here we employ evolutionary algorithm to predict the crystal structures of superhard B-C and B-N composites. We also apply density functional theory to study mechanical properties, electronic structures, phonon and Raman spectra of different B-C and B-N systems, including boron-doped cubic diamond and icosahedral boron subnitrides. Comparison of our calculations and recent experimental data will be discussed as well.

*This work is supported by the National Science Foundation EPSCoR RII-Track-1 Cooperative Agreement OIA-1655280. W.-C. Chen is also supported by the Blazer Graduate Research Fellowship from the University of Alabama at Birmingham.

12:51PM F17.00007: A First-Principles Study of Two High-Pressure Modifications of Fe$_3$N*  
MARIBEL NÚÑEZ VALDEZ (Presenter), Goethe Universität Frankfurt am Main — Most of the iron nitride compounds of the type Fe$_x$N are unstable at ambient pressure and temperature. However, Fe-rich nitrides can be synthesized in a high pressure confined environment. Using a large volume press and X-ray diffraction in combination with scanning electron microscopy techniques, two new high pressure phases of Fe$_3$N were observed with symmetries $P6_322$ and $P312$ [1]. In this work, we perform a first-principles study based on density functional theory (DFT) within the general gradient approximation (GGA) and the local density approximation (LDA), and report on the structural, electronic, and phase stability properties as a function of pressure of these two iron nitride modifications. The exploration and understanding of high-energy density nitride materials is important as many of them exhibit remarkable technological applications due to their hardness, superconductivity or mechanical traits.

* MNV is also at the Helmholtz Zentrum-Potsdam, Deutsches GeoForschungsZentrum (GFZ)

*MNV gratefully acknowledges the computing time granted by the John von Neumann Institute for Computing (NIC) and provided on the supercomputer JUWELS at Jülich Supercomputing Centre (JSC) under Project No. ID HPO24
1:03PM F17.00008: Study of peptides under simultaneous application of high pressure and shear*  
Samantha Clarke (Presenter), Brad A Steele, Lawrence Livermore Natl Lab, Jasmine Hinton, Department of Physics, University of Nevada, Las Vegas, Matthew Kroonblawd, Joseph Michael Zaug, I-Feng W. Kuo, Nir Goldman, Lawrence Livermore Natl Lab, Vitali Prukapanka, Eran Greenberg, Advanced Photon Source, Argonne National Laboratory, Elissaios Stavrou, Lawrence Livermore Natl Lab — There is a renewed interest in the role of non-hydrostatic mechanical stress, or shear stress, as a driver for reactions. Combining high pressure with mechanical shearing can significantly alter reaction mechanisms and lead to a decrease in the onset pressure of structural transformations. Such conditions can be achieved with a rotational diamond anvil cell (RDAC). We will discuss the study of simple amino acids and peptides subjected to high-pressure, high-shear conditions using an RDAC. Amino acids have been studied extensively under static compression due to their significance in the fields of chemistry and biology. We compare amino acid behavior under high shear to that in a conventional DAC. μ-Raman spectroscopy and X-ray diffraction are used to probe the phase transitions and amino acid condensation. Theoretical calculations are also performed using USPEX, metadynamics, and quantum molecular dynamics to predict novel phases and reaction barriers under compressive shear.

*This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344. Thanks to the Laboratory Directed Research and Development Program at LLNL for supporting this study under 18-LW-036.

1:15PM F17.00009: Effect of structure and composition on the electronic excitation-induced amorphization of La2Ti2-xZrxO7 ceramics  
Michel Sassi (Presenter), Tiffany Kaspar, Vaithiyalingam Shuttathanandan, Kevin Rossos, Steven Spurgeon, Pacific Northwest Natl Lab — An understanding of the response of ceramics (A2B2O7) operating in extreme environments is of interest for a broad range of applications, including potential nuclear wasteforms and in-core electronics. Here, ab initio molecular dynamic simulations have been used to investigate the effect of structure and B-site (=Ti, Zr) cation composition of lanthanum-based oxides on electronic-excitation-induced amorphization. We find that the amorphous transition in monoclinic layered perovskite La2Ti2O7 occurs for a lower degree of electronic excitation than for cubic pyrochlore La2Zr2O7. While in each case the formation of O2-like molecules drives the structure to an amorphous state, an analysis of the polyhedral connection network reveals that the rotation of TiO6 octahedra in the monoclinic perovskite phase facilitates the formation of O2-like molecules, while such octahedral rotation is not possible in the cubic pyrochlore phase. However, once the symmetry of the cubic structure is broken by substituting Ti for Zr, it becomes less resistant to amorphization. A compound made of 50% Ti and 50% Zr (La2TiZrO7) is found to be more resistant in the monoclinic perovskite than in the cubic pyrochlore phase, which may be related to the lower bandgap of the cubic phase.

1:27PM F17.00010: Structure and electrical properties of a single-crystal layered strontium manganese vanadate as a function of pressure*  
Victoria Soghomian (Presenter), Physics, Virginia Tech, Benjamin Medina, Mechanical Engineering, Virginia Tech, Qifan Yuan, Physics, Virginia Tech, Carla Slobodnick, Chemistry, Virginia Tech, Jing Zhao, Nancy Ross, Geosciences, Virginia Tech, C Stephen Hellberg, U.S. Naval Research Lab — We investigate the structural and electrical properties of a strontium manganese vanadate layered material, SrMn2(VO4)2(OH)(H2O), as a function of hydrostatic pressure. The material crystallizes in the space group C2/m. Variable temperature conductivity measurements, performed on single crystals, indicate semiconducting behavior, supported by DFT calculations. The manganese vanadate layers, consisting of chains of edge sharing MnO6 octahedra bridged by corner-sharing VO4 tetrahedra, are connected in the third dimension by octahedral Sr ions. Single-crystal x-ray diffraction under pressure up to 4 GPa indicates a reversible compression of the interlayer distance. The electrical conductivity of a single crystal as a function of pressure decreases at moderate pressures; beyond 0.4 GPa, the material is highly insulating. Interestingly, this change is not reversible. The same irreversible change in conductivity is also observed for the Ca and Ba analogs. Probing structural details at the lower pressure range by Raman spectroscopy, we observe a softening mode around 0.8 GPa related to the Mn octahedra.

*NSF DMR-1206338
Pressure-induced metallization and Superconductivity in PdSe₂

MOAZ ELGHAZALI (Presenter), PAVEL NAUMOV, HOSSEIN MIRHOSSEINI, VICKY SÜSS, Max Planck Institute for Chemical Physics of Solids, LUKAS MUECHLER, Princeton university, WALTER SCHNELLE, CLAUDIA FELSER, SERGEY MEDVEDEV, Max Planck Institute for Chemical Physics of Solids — Transition Metal Dichalcogenides (TMDs) continue to attract scientific interest due to their intriguing physical properties and potential technological applications. Here, we report the emergence of a pressure-induced dome-shaped superconductivity in PdSe₂ with a maximum critical temperature (T_c) of 13.1 K at 23 GPa, which is so far the highest T_c among TMDs family.

Lattice dynamics studies under pressure revealed a strong correlation between Se-Se dumbbells bonding and T_c. In addition, Ab initio calculations of the PdSe₂ electronic structure show the existence of topological non-trivial state with Dirac crossing and nodal lines in the vicinity of Fermi level. PdSe₂ provides therefore an exciting example to study the relationship between superconductivity and topologically non-trivial states, which can lead to discovery of novel superconducting states. We have revisited other TMD compounds to search for new superconductors. The related compounds NiSe₂ and PdS₂ have also been studied in comparison with PdSe₂. These compounds are not only interesting from the fundamental research perspective, but also for technological application as the electronically-driven insulator-metal transition at relatively low pressures could be promising in electronics applications such as memory devices.

High pressure synthesis of a new perovskite-type cuprate with doped Cu-O chains

MASAHARU ITO, HIDEFUMI TAKAHASHI, University of Tokyo, HIDEAKI SAKAI, Osaka University and JST-PRESTO, JUN FUJIOKA, University of Tokyo and JST-PRESTO, MASAYUKI OCHI, Osaka University, SHIRO SAKAI, RYOTARO ARITA, University of Tokyo and RIKEN CEMS, HAJIME SAGAYAMA, High Energy Accelerator Research Organization, YUICHI YAMASAKI, NIMS, YUICHI YOKOYAMA, HIROKI WADATI, University of Tokyo ISSP, YOSHIHIRO KUSANO, Okayama University of Science, YOSHINORI TOKURA, University of Tokyo and RIKEN CEMS, SHINTARO ISHIWATA (Presenter), University of Tokyo and JST-PRESTO — The discovery of high-temperature superconductivity in cuprates has spurred the search for novel low-dimensional cuprates such as spin-ladder compounds. On the other hand, less attention has been paid for the three-dimensional counterpart, the perovskite-type cuprates ACuO₃, presumably because of the difficulty in high-pressure synthesis. In this study, we have succeeded in the high-pressure synthesis of a novel GdFeO₃-type perovskite cuprate PrCuO₃ with quasi-one-dimensional Cu-O chains showing nearly metallic conductivity. Synchrotron x-ray diffraction and x-ray absorption spectroscopy reveal that the oxidation state can be described as Pr(4-δ)+Cu(2+δ)+O₃. The first principles calculations suggest that the formation of the Cu-O chain is caused by the A-B site charge transfer and the cooperative Jahn-Teller distortion of nearly divalent Cu ions. This system offers a unique opportunity to explore novel quantum phases of correlated electrons as the simplest one-dimensional counterpart of the high-temperature superconducting cuprates.

*This work is partly supported by Grant-in-Aid for Scientific Research, Japan Society for the Promotion of Science, Japan (Kakenhi No. 17H01195), JST PRESTO Hyper-nano-space design toward Innovative Functionality (Grant No. JPMJPR1412).
PETRU TIGHINEANU (Presenter), THOMAS FOESEL, Max Planck Institute for the Science of Light, TALITHA WEISS, Institute for Quantum Optics and Quantum Information, FLORIAN MARQUARDT, Max Planck Institute for the Science of Light — In our recent work [1] we showed how reinforcement learning with artificial neural networks (ANNs) can be a powerful tool to discover quantum-error-correction strategies fully adapted to the quantum hardware of a quantum memory. We employed a reinforcement-learning technique called natural policy gradient, in which the policy of the ANN is updated and improved according to the second-order gradient of the return (the cumulative sum of the reward) in the parameter space of the ANN.

The principal downsides of policy gradient are sample inefficiency and slow convergence, which can be critical in the case of a quantum system with an exponentially growing Hilbert space that is simulated classically. Here we conduct an in-depth study of the performance of more advanced reinforcement-learning techniques [2] applied to a noisy quantum memory. We find that the efficiency of training can be sped up by orders of magnitude via a careful choice of the technique and the corresponding hyperparameters, both of which are motivated by and related to the underlying physics.


VALENTIN STANEV (Presenter), JACK FLOWERS, ICHIRO TAKEUCHI, University of Maryland, College Park — Superconductivity in iron-based materials continues to be a focus of intense research effort a decade after its discovery. In particular, the interplay between structure and charge doping as drivers of superconductivity is still a matter of active debate. To address this question we use Machine Learning (ML) approach. Based on published data we created a database covering the available structural information of the 122 family of materials. Using the lattice parameters, pnictogen height and charge doping we trained several ML models designed to predict the critical temperature $T_c$ over the entire parameter space. The analysis of the models suggests that no single variable can fully explain and predict the evolution of $T_c$, and a combination of at least two parameters are needed. The ML predictions can be used to guide further exploration of the phase diagram of iron-based superconductors.

*This work was funded by ONR N00014-13-1-0635, ONR N00014-15-1-2222, AFSOR No. FA 9550-14-10332

PAVAO SANTAK (Presenter), GARETH CONDUIT, University of Cambridge — The physical properties of many alkanes are unknown, which prevents engineers from optimally deploying them in base oil lubricants. In order to address this issue, we train neural networks that can work with fragmented data, enabling us to exploit the property-property correlations and increase the accuracy of our models. We encode molecular structure into five nonnegative integers, which enables us to exploit the structure-property correlations. We establish correlations between branching and the boiling point, heat capacity and vapor pressure as a function of temperature. Furthermore, we explore the connection between the symmetry and the melting point and identify erroneous data entries in the flash point of linear alkanes. Finally, we predict linear alkanes' kinematic viscosity by exploiting the temperature and pressure dependence of shear viscosity and density.

AYANA GHOSH (Presenter), SERGE M NAKHMANSON, Materials Science and Engineering, University of Connecticut, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory — Actinide- and lanthanide-based materials constitute an important playground for exploring exotic properties stemming from the presence of itinerant or localized $f$-electrons. For example, uranium-based compounds have exhibited emergent phenomena, including magnetism, unconventional superconductivity, hidden order, and heavy fermion behavior. Among them, the magnetic properties with varying ordered states and moment size are sensitively dependent on pressure, chemical doping and magnetic field due to the strong-correlation effects on $5f$-electrons. So far, there have even been no reports of systematic studies to map out connections between structures and properties of these compounds. In order to investigate such links and bridge between theoretical and experimental learnings, we have constructed two databases combining results of high-throughput DFT simulations and experimental measurements, respectively, for a family of uranium-based binary compounds. We then utilized different machine learning models to identify related accessible attributes (features) and predict magnetic moments and ordering in these compounds.

*This work (LA-UR-18-30072) was supported by the U.S. DOE National Nuclear Security Agency through the LANL LDRD Program and the Institute for Materials Sciences at LANL.
12:39PM F18.00006: Machine learning-assisted search for high performance plasmonic metals* ETHAN SHAPERA (Presenter), Department of Physics, University of Illinois at Urbana-Champaign, ANDRE SCHLEIFE, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Plasmonics aims to manipulate light through choice of materials and nanoscale structure. Finding materials which exhibit low-loss responses to applied optical fields while remaining feasible for widespread use is an outstanding challenge. Online databases compiled computational data for numerous properties of tens of thousands of materials. Due to the large number of materials and high computational cost, it is not viable to compute optical properties for all materials from first principles. Geometry-dependent plasmonic quality factors for a training set of ~1,000 materials are computed using density functional theory and the Drude model. We train then apply random-forest regressors to rapidly screen Materials Project to identify potential new plasmonic metals. Descriptors are limited to symmetry and quantities obtained using the chemical formula and the Mendeleev database. The machine learning models filter through 7,445 metals in Materials Project. We iteratively improve the model with active learning by adding DFT results for predicted high quality factor metals into the training set. From this we predict Cu₃Au, MgAg₃, and CaN₂ as candidates and verify their quality factors with DFT.

*Blue Waters Sustained-Petascale Computing Project; NCSA Faculty Fellowship; NSF DMR-1555153

12:51PM F18.00007: Machine Learning and Crystal Structure Prediction of Molecular Crystals RUGGERO LOT, FRANCO PELLEGRINI, YUSUF SHAIDU, EMINE KUCUKBENLI (Presenter), International School for Advanced Studies — There is a natural synergy between data-hungry machine learning methods and crystal structure prediction of molecular crystals that requires a careful search in a vast potential energy landscape. In our previous study we demonstrated how taking advantage of machine learning methods can enable novel predictions even for well-studied molecular crystals [1]. In order to leverage this synergy further, we have been developing a deep neural network training tool, PANNA (Potentials from Artificial Neural Network Architectures), based on TensorFlow framework [2]. In creating transferable machine-learned potentials, the key step is the non-linear process of training the network model. We will demonstrate a variety of network training techniques that can be explored within PANNA, from ones that are commonly used in machine learning community to the ones that are specific to atomistic simulations. We will report the effect of data selection, input representation and training methods on the training dynamics and on the resulting potentials in the difficult case of molecular crystals.


1:03PM F18.00008: Fitting effective models using QMC parameter derivatives WILLIAM WHEELER (Presenter), SHIVESH PATHAK, LUCAS WAGNER, University of Illinois at Urbana-Champaign — Effective models are fundamental to our understanding of complex materials, but selecting the right model and parameters to accurately describe a particular material can be challenging. The recently developed density matrix downfolding method (DMD) [1] uses an ensemble of quantum Monte Carlo calculations to both select and fit parameters to effective models for materials. However, this method is computationally extremely demanding. In a similar spirit to force matching in classical model fitting [2], we improve the efficiency of DMD by computing derivatives of the energy and density matrix with respect to parameters of each trial wave function. We demonstrate the new technique by computing a band structure for silicon using first principles quantum Monte Carlo.


1:15PM F18.00009: Detection of Phase Transitions in Quantum Spin Chains via Unsupervised Machine Learning YUTAKA AKAGI (Presenter), NOBUYUKI YOSHIOKA, HOSHO KATSURA, Department of Physics, The University of Tokyo — In the field of machine learning, there has been an important breakthrough in recent years. What was at the center of it is the deep learning by artificial neural networks mimicking human brains. By deepening a process part which repeats extracting feature quantities through nonlinear transformations, so-called hidden layer, data/class separability and the discriminability have dramatically improved. Recently, the machine learning techniques have found a wide variety of applications in condensed matter and statistical physics. Examples include detection of phase transition and acceleration of Monte Carlo simulation. Meanwhile, most of these studies are based on supervised learning under well-known results, and there are only a few previous examples applying unsupervised learning. In this research, we investigate quantum phase transitions in various quantum spin chains by using an autoencoder which is one of unsupervised learning methods. In particular, we will show that the autoencoder whose input is only short-range correlators is capable of detecting even topological phase transition from the large-D phase to the Haldane phase without using either topological invariants or entanglement spectra.
1:27PM F18.00010: Supervised learning of phase transitions in classical and quantum systems* NICHOLAS WALKER (Presenter), KA-MING TAM, MARK JARRELL, Louisiana State University — Supervised machine learning methods are used to identify transitions in physical systems using the classical solid-liquid transition of a Lennard-Jones system as well as the strong coupling-local moment quantum transition in the soft-gap Anderson model as examples. Monte Carlo sampling was used to achieve a uniform sampling of configurational data across a large range of the relevant transition parameter for each system. Hyperbolic feature scaling is applied to the features followed by training a 1-dimensional convolutional neural network with the samples corresponding to the extreme parameters of each phase as training data. The rest of the configurational data is assigned phase classification probabilities by the neural network, allowing for the prediction of the transition point with respect to the chosen varied parameter. This is done by fitting the mean classification probabilities for each set of configurational data with respect to the varied parameter with a logistic function and taking the transition to be at the value of the parameter corresponding to the midpoint of the sigmoid. The results obtained are comparable to results using contemporary methods for each system.

*This work is funded by the NSF EPSCoR CIMM project under award OIA-1541079.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F19 DCOMP DCMP: Precision Many Body Physics V BCEC 156C - Luca Fausto Tocchio - Tag(s): Focus

11:15AM F19.00001: High-precision data for the unitary Fermi gas from diagrammatic series with zero convergence radius [Invited] RICCARDO ROSSI, CCQ, Flatiron Institute, TAKAHIRO OHGOE, University of Tokyo, KRIS VAN HOUCKE (Presenter), FELIX WERNER, Ecole Normale Superieure — In this talk I will mainly focus on the unitary Fermi gas (spin 1/2 fermions with contact interactions in 3D, which describes cold atomic gases at a Feshbach resonance) in the normal phase. Thanks to a diagrammatic Monte Carlo algorithm, we accurately sample all skeleton diagrams (built on dressed single-particle and pair propagators) up to order nine [1]. The diagrammatic series is divergent and there is no small parameter so that a resummation method is needed. We compute the large-order asymptotics of the diagrammatic series, based on a functional integral representation of the skeleton series and the saddle-point method. We show that the radius of convergence is actually zero, but the series is still resummable, by a generalised conformal-Borel transformation that incorporates the large-order asymptotics [2]. This yields new high-precision data, not only for the equation of state, but also for Tan's contact coefficient and for the momentum distribution [3]. I will also highlight some recent developments in (determinant) diagrammatic Monte Carlo and present new high-precision data for the Fermi polaron, which is a single impurity atom immersed in a Fermi sea.

References:

Understanding the metal-insulator transition in VO$_2$ from quantum Monte Carlo, DMFT, and experiment


JARON KROGEL (Presenter), ILKKA KYLANPAA, PANCHAPAKESAN GANESH, Oak Ridge National Laboratory, FRANK LECHERMANN, Universitat Hamburg, OLLE HEINONEN, Argonne National Laboratory, PAUL KENT, Oak Ridge National Laboratory — Vanadium dioxide displays the quintessential example of metal-insulator transition (MIT) physics in a strongly correlated material. Despite numerous studies, the nature of the MIT is still controversial and new perspectives are needed. Recent experiments view rutile VO$_2$ as an unconventional metal due to its anomalously low electronic thermal conductivity. Due to strong correlations in VO$_2$, beyond DFT approaches are required and here we study pristine and non-stoichiometric VO$_2$ with quantum Monte Carlo and DMFT. New perspective is provided by the momentum distribution, which contains no discontinuity in the metallic phase, indicating a non-Fermi liquid metal consistent with experimental findings. Quasi-1D back-scattering along the rutile c-axis is reminiscent of a Tomanaga-Luttinger liquid, where the scattering is induced by impurities. In non-stoichiometric VO$_2$ the calculated spectral function indicates a competition between $\alpha_{1g}$ and $\epsilon_{πg}$ orbitals which have a role in the formation of the insulating state. DMFT-VCA calculations show that the $\alpha_{1g}\epsilon_{πg}$ orbital dichroism falls below its pristine value at a doping concentration of $δ=0.07$, in near agreement with the experimentally determined critical doping threshold for the suppression of the insulating state.

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

Computable formulae for Hall and Nernst Coefficients of Strongly Correlated Metals

ASSA AUERBACH (Presenter), ILIA KHAIT, Technion - Israel Institute of Technology — Exact formulae for the temperature dependent Hall coefficient (published in Phys. Rev. Lett. 121, 066601 (2018)), and for a modified Nernst coefficient of metals are derived from the Kubo linear response functions. The formulae are valid for a large range of microscopic Hamiltonians of fermions and bosons, subject to arbitrary potentials and interactions. These DC transport coefficients (remarkably) depend solely on equilibrium susceptibilities, which are amenable to well controlled numerical algorithms - including Quantum Monte Carlo (in imaginary time), high temperature series expansions, and variational wavefunctions. Applications of these formulae are demonstrated for band electrons, the Bose Hubbard model, and for the t-J model.

This work is supported in part by the United States-Israel Binational Science Foundation, Grant No. 2016168, and the Israel Science Foundation, Grant No. 2022061.

Self Consistent Auxiliary Field Quantum Monte Carlo Method for Realistic Materials

SHIWEI ZHANG (Presenter), HAO SHI, Simons Foundation — The auxiliary field quantum Monte Carlo (QMC) calculations in interacting fermion systems require a constraint to control the sign and phase problem. The constraint involves an input trial wave function which restricts the random walks. We introduce a systematically improvable constraint for realistic materials. An independent-particle calculation is coupled to the phaseless auxiliary-field QMC calculation and the independent-particle solution is used as the constraint in QMC. The constraint is optimized by the self-consistency between the QMC and independent-particle calculations. We demonstrate this approach in transition metal oxides. Connection with other electronic structure methods will be discussed.

The Flatiron Institute is supported by the Simons Foundation.

Optimized multi-determinant trial wavefunctions for Constrained Path Monte Carlo

R. TORSTEN CLAY (Presenter), Mississippi State University — Two of the most successful types of methods for strongly-correlated models are quantum Monte Carlo and renormalization group methods. Both however suffer from limitations that make large calculations difficult except in special cases, for example one dimension (1D). The Density Matrix Renormalization Group method suffers from poor scaling beyond 1D. The Path Integral Renormalization Group (PIRG) method expands the wavefunction in Slater Determinants and is not limited by dimension, but by the strength of interactions. Quantum Monte Carlo calculations are severely limited by the Fermion sign problem. The Constrained Path Monte Carlo (CPMC) method prevents the exponential loss of precision from the sign problem through the use of a trial wavefunction. However, the trial wavefunction is an uncontrolled approximation with an unknown error. We demonstrate a way to combine the advantages of a renormalization method (PIRG) with those of a quantum Monte Carlo (CPMC), by using PIRG wavefunctions as CPMC trial wavefunctions. The advantage of PIRG wavefunctions as trial wavefunctions is that they can be systematically improved. We present results for PIRG-CPMC calculations on frustrated Hubbard models, comparing energies, spin correlations, and superconducting pair-pair correlations.
1:03PM F19.00006: Skeleton diagrammatic expansions with screened Hubbard interaction versus multivaluedness of the Luttinger-Ward functional  

AARAM JOO KIM (Presenter), EVGENY KOZIK, Department of Physics, King’s College London — We systematically study properties of high-order bold-diagrammatic expansions, which may converge to unphysical answers for the Hubbard interaction due to the multivaluedness of the Luttinger-Ward functional (LWF), by the prototypical example of the Hubbard atom. The diagrammatic Monte Carlo method with fully dressed propagator $G$ is adopted to generate the high-order series. By varying the level of screening in the interaction line; bare $U$, random-phase approximation $W_{rpa}$, and fully dressed $W_{exact}$, we present the convergence properties of the different bold series in connection with multiple branches of the LWF. In particular, we find that the bold-$GW_{exact}$ and bold-$GW_{rpa}$ series diverge well below the branching point of the LWF, but admit the analytic continuation beyond their convergence radius by standard techniques. We further explore the possibility of using the bold diagrammatic series in the strongly correlated regime to obtain precise results with controlled accuracy.

1:15PM F19.00007: Cluster Perturbation Theory Applied to Two-Particle Correlation Functions*  
PETER RAUM (Presenter), VITO SCAROLA, Virginia Tech, THOMAS MAIER, Oak Ridge National Lab — Developing techniques to solve Hubbard models is an active area of research due to their ability to capture the essential properties of many strongly correlated systems. Cluster Perturbation Theory (CPT) is an economic method to calculate the momentum and energy resolved single-particle Green's function that has been used extensively in direct comparisons with experiments. For example, the single-particle Green's Function can be observed with angle-resolved photoemission spectroscopy. However, many experimental observables are given by two-particle correlation functions. We extend CPT to compute these correlation functions and focus on a method to use CPT to calculate the transverse spin-susceptibility, measurable via inelastic neutron scattering on strongly correlated materials or with optical probes of atomic gases in optical lattices. We benchmark our method with the one-dimensional Fermi-Hubbard model at half-filling and compare with known results.

*V.W.S. and P.T.R. acknowledge support from AFOSR (FA9550-18-1-0505) and ARO (W911NF-16-1-0182). T.A.M. acknowledges support from the Scientific Discovery through Advanced Computing program, U.S. DOE Office of Science, Advanced Scientific Computing Research and BES, Division of Materials Sciences and Engineering.

1:27PM F19.00008: Optimized higher-order Lie-Trotter-Suzuki decompositions for two and more terms  
YIKANG ZHANG (Presenter), THOMAS BARTHEL, Duke University — Lie-Trotter-Suzuki decompositions of operator exponentials have a lot of applications in physics. For example, they are employed to sample equilibrium states in quantum Monte Carlo and to simulate the dynamics of quantum systems on quantum computers or on classical computers using tensor network state techniques. They also provide symplectic integrators for classical physics. Good higher-order decompositions for exponentials of $n=2$ non-commuting operators are well-known. These cover one-dimensional quantum systems with nearest-neighbor interactions. We present some optimized decompositions for $n=2$ and new higher-order decompositions for $n=3,4$ which are needed for one-dimensional systems with longer-ranged interactions or quantum systems in higher dimensions. The ordering of operators in the decompositions turns out to have substantial influence on the attainable approximation order and magnitudes of the leading error terms.

1:39PM F19.00009: Diagrammatic Monte Carlo approach to angular momentum in quantum many-body systems*  
GIACOMO BIGHIN (Presenter), Institute of Science and Technology Austria, TIMUR V TSCHERBUL, Department of Physics, University of Nevada, Reno, MIKHAIL LEMESHKO, Institute of Science and Technology Austria — We introduce a Diagrammatic Monte Carlo (DiagMC) approach to molecular impurities, possessing rotational degrees of freedom [1]. The technique is based on a diagrammatic expansion [2] that merges the usual Feynman diagrams with the angular momentum diagrams known from atomic and nuclear structure theory, thereby incorporating the non-Abelian algebra inherent to quantum rotations. Due to the peculiar way in which angular momenta couple, the configuration space is larger with respect to most DiagMC applications, and a new class of updates is needed in order to span it completely.

We exemplify the technique by obtaining an all-coupling solution of the angulon model - essentially a molecular impurity in a quantum many-body environment - showing that our approach correctly recovers the strong-coupling limit. However, the technique is general and can be applied to a broad variety of systems possessing angular momentum degrees of freedom, thereby establishing a far-reaching connection between DiagMC techniques and molecular simulations.


*This work was supported by the Austrian Science Fund (FWF), Project P29902-N27 and by NSF Grant No. PHY-1607610.
1:51PM F19.00010: Electronic structure of semiconductor nanoparticles from stochastic evaluation of imaginary-time path integral: nonrelativistic U(1) lattice gauge theory in the Kohn-Sham basis  

ANDREI KRYJEVSKI (Presenter), North Dakota State University, THOMAS LUU, Institute for Advanced Simulation, Jülich Center for Hadron Physics, Forschungszentrum Jülich GmbH — In the Kohn-Sham orbital basis imaginary-time path integral for electrons in a semiconductor nanoparticle has a mild fermion sign problem and is, therefore, amenable to evaluation by the standard stochastic methods. Utilizing output from the density functional theory simulations we compute imaginary-time electron propagators in several silicon hydrogen-passivated nanocrystals, such as Si_{35}H_{36}, Si_{87}H_{76} and Si_{147}H_{100}, and extract energies of low-lying electron and hole levels. Our qasiparticle gap predictions are in very good agreement with the results of recent G0W0 calculations.

2:03PM F19.00011: Insulating states from increased kinetic energy: counterintuitive physics in the basic model of organic conductors and superconductors*  

ADRIAN KANTIAN (Presenter), Uppsala University, THIERRY GIAMARCHI, DQMP, University of Geneva — The U-V model at quarter filling is the canonical model of the organic Bechgaard and Fabre salts, the first materials to exhibit a superconducting phase based on repulsive electron interactions, which is accompanied by competing magnetic phases just as for the cuprates of high-Tc superconductivity. However, just as for the doped 2D Hubbard model, the U-V model can exhibit very rich and complicated physics, which are a challenge to treat reliably. In the presented work, we show that the U-V model can give rise to surprising physics in which an insulating state emerges from increased transverse kinetic energy, by combining large-scale DMRG results with analytic RG of bosonized models of the 2-leg U-V Hubbard ladder.

*This work was supported in part by the Swiss NSF under MaNEP and Division II, as well as through support by the Swiss government for the MAQUIS collaboration under the HP2C Initiative.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F20 DCOMP: First-principles Modeling of Excited-state Phenomena in Materials V: Time-dependent Density Functional Theory


[Invited]  

NATHALIE VAST (Presenter), OLEKSANDR MOTORNYI, Laboratoire des Solides Irradiés, CEA-DRF-IRAMIS, Ecole Polytechnique, CNRS UMR 7642, ANDREA DAL CORSO, SISSA — Over a decade ago, a new type of surface plasmons has been both predicted theoretically for surfaces that support Shockley electronic surface states [1], and experimentally reported [2]. The so-called acoustic surface plasmon (ASP) exhibits a dispersion different from the behaviour of conventional surface plasmons. ASPs in gold have a twofold advantage for plasmonics applications: due to the linear dispersion, a signal consisting of several ASP waves can propagate without distortion; and vicinal Au surfaces have a step-terrace structure that provides the intrinsic grating on the atomic level, allowing, potentially, to couple the ASP to light.

I will present a new algorithm based on the Lanczos recursion within TDDFPT [3] that allows for accurate and efficient computations of the electron-energy loss spectra for arbitrary values of the transferred momentum \( \mathbf{q} \). The vicinal Au (455) surface could be modelled with 5 nm of gold (253 atoms) separated by 5 nm of vacuum. The effect of spin-orbit coupling on the ASP dispersion, as well as the role of intra- and inter-band transitions, have been examined. I show that the computation of plasmons on the quantum level is within reach for systems of unprecedented size.


*Supports from ANR-10-LABX-0039-PALM, DIM SIRTEQ, DGA, NEEDS-Matériaux and Chaire Énergie are gratefully acknowledged. Computer time was granted by École Polytechnique through the LLR-LSI project, by GENCI (Project No. 2210) and by the Partnership for Advanced Computing in Europe (PRACE Project No. 2010PA3750).
11:51AM F20.00002: Propagation of maximally localized Wannier functions in real-time TDDFT* DILLON C. YOST (Presenter), YI YAO, YOSUKE KANAI, Department of Chemistry, University of North Carolina at Chapel Hill — Real-time, time-dependent density functional theory (RT-TDDFT) has attracted much attention in recent years as an approach to study a variety of excited state phenomena ranging from optical excitations to electronic stopping. Many applications of RT-TDDFT involve the inclusion of a time-dependent applied electric field to perturb the system. In the length gauge representation, one can apply a scalar electric field to localized orbitals, such as maximally localized Wannier functions (MLWFs). We have implemented a method in the Q8@LL plane-wave pseudopotential RT-TDDFT code to transform the time-dependent Kohn-Sham (TDKS) states into MLWFs, allowing for simulations with time-dependent electric fields and for the calculation of absorption spectra and nonlinear optical responses for both isolated and periodic systems. The propagation of MLWFs in RT-TDDFT gives access to dynamic polarization and quantities such as the MLWF spread, allowing for detailed analysis of a wide range of excitation phenomena.

*This work is supported by the National Science Foundation under Grants No. CHE-1565714. Computer time was provided by the INCITE program with resources of the Argonne Leadership Computing Facility, a DOE Office of Science User Facility supported under Contract DE-AC02- 06CH11357.

12:03PM F20.00003: Maxwell+TDDFT multiscale simulation for optical response of nanomaterials* MITSUHARU UEMOTO (Presenter), KAZUHIRO YABANA, University of Tsukuba — We have been developing a novel multiscale simulation method which combines the time-dependent density functional theory (TDDFT)-based first principles electron dynamics and finite-difference-time-domain (FDTD)-based electromagnetic calculations. We apply this method to light propagation / scattering problem by semiconducting silicon nanoparticles and nanodimer structures with the length scale at a few hundred nanometer, which are often used as building block of optical devices. Under an irradiation of an intense femtosecond laser pulse (I > 10^{10} W/cm^{2}), carrier excitations by multiphoton processes take place due to the enhanced light field at the focal spot / hotspot. Thus, this method offers a useful tool to analyze optical nonlinearity at nanostructures in the first principles level.

*This work was supported in part by MEXT as a social and scientific priority issue (Creation of new functional devices and high-performance materials to support next-generation industries; CDMSI) to be tackled by using post-K computer.

12:15PM F20.00004: Maxwell + First-Principles TDDFT-MD Multi-Scale Simulation and Application to Impulsive Stimulated Raman Scattering Spectroscopy ATSUSHI YAMADA (Presenter), KAZUHIRO YABANA, Center for Computational Sciences, University of Tsukuba — Nonlinear optics in solids includes complex physics arising from coupled nonlinear dynamics of light electromagnetic fields, electrons, and phonons. We have developed a novel multi-scale simulation method to track coupled dynamics of electromagnetic field inside the material in macroscopic scale and electrons and atoms in solid in microscopic scale, where the Maxwell equations are solved to describe propagation of the light while first-principles Ehrenfest molecular dynamics (MD) calculation is performed based on time-dependent density functional theory (TDDFT), extending our previously developed multi-scale method. We have applied the method to impulsive stimulated Raman scattering spectroscopy of diamond. Simulations of pump and probe pulse propagations mimicking the experimental measurement process are performed using our developed open source free software, SALMON. We show detailed dynamical processes of generation of coherent phonon and amplification of Raman scattered wave as well as measured transmission signals.

12:27PM F20.00005: Microscopic and macroscopic Maxwell-TDDFT descriptions for light-matter interaction in thin materials SHUNSUKE YAMADA (Presenter), MASASHI NODA, Center for computational sciences, University of Tsukuba, KATSUYUKI NOBUSADA, Institute for Molecular Science, KAZUHIRO YABANA, Center for computational sciences, University of Tsukuba — We present a comprehensive theoretical framework for interaction of an ultrashort light pulse with a thin material based on the time-dependent density functional theory (TDDFT). We introduce a microscopic description solving the Maxwell equations for the light electromagnetic fields and the time-dependent Kohn-Sham equation for the electron dynamics simultaneously in the time domain on a common real-space grid. This scheme can simulate the light-matter interaction in thin films irrespective of the film thickness and the light intensity. For two limiting cases of extremely thin and sufficiently thick films, we develop approximate schemes. For the former, a 2D macroscopic description is developed: 2D response functions are introduced for a weak field, while time evolution equation is derived for an intense field. For the latter, the 3D macroscopic description coincides with the ordinary electromagnetism with the 3D bulk response functions for a weak field, or the multiscale Maxwell-TDDFT scheme for a strong field, which our group developed previously. In this talk, we show results for Si thin films and discuss the applicability of the microscopic and macroscopic descriptions.
12:39PM F20.00006: Magnetic Excitations in TDDFT with GGA kernel  NISHA SINGH (Presenter), PETER ELLIOTT, Theory, Max-Planck Institute of Microstructure Physics, TASHI NAUTIYAL, Physics, Indian Institute of Technology Roorkee, J. KAY DEWHURST, Theory, Max-Planck Institute of Microstructure Physics, SANGEETA SHARMA, Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy — In ordered magnets of all forms (ferromagnets, antiferromagnets, ferrimagnets, etc.) we encounter wave like excitations that propagate through the lattice of ordered spins. Correctly predicting these collective excitation modes is essential for understanding the thermodynamic properties of such materials. Theoretically, TDDFT within the linear regime, can successfully capture these low energy spin waves. However, it requires an approximation to the exchange-correlation (XC) kernel, which encapsulates the electron-electron interactions of the many-body systems. Despite the plethora of approximations for the XC energy functional, only the ALDA kernel has been implemented and applied to study these magnetic excitations. In the work presented here we climb up the Jacob's ladder of functional and derive the XC kernel for GGA functionals. This is then tested by calculating the magnon spectra for simple ferromagnets and Heusler ferrimagnets using the PBE GGA functional.

12:51PM F20.00007: Orbital magneto-optical response of periodic insulators from first principles  DAVID STRUBBE (Presenter), Department of Physics, University of California, Merced, IRINA LEBEDEVA, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, San Sebastián, ILYA V. TOKATLY, Universidad del País Vasco UPV/EHU, Donostia International Physics Center, and IKERBASQUE, ANGEL RUBIO, Universidad del País Vasco UPV/EHU and Max Planck Institute for the Structure and Dynamics of Matter — We present a reformulation of density matrix perturbation theory for time-dependent electromagnetic fields under periodic boundary conditions, which allows us to treat the orbital magneto-optical response of solids at the ab initio level. We use time-dependent density-functional theory (TDDFT) with the Sternheimer equation, implemented in the Octopus real-space code, to solve for the gauge-invariant part of the density matrix via the modern theory of polarization. Our computational scheme has an efficiency comparable to standard linear-response calculations of absorption spectra. Calculations of magnetic circular dichroism spectra for adenine, cyclopropane, and bulk silicon agree with the available experimental data. A clear signature of the valley Zeeman effect is revealed in the magneto-optical spectrum of a single layer of hexagonal boron nitride, with a g-factor similar to that observed in monolayer transition-metal dichalcogenides. The present formalism opens the path towards the study of magneto-optical effects in strongly driven low-dimensional systems.

1:03PM F20.00008: A General Model Order Reduction Scheme for the Evaluation of Spectroscopic Properties and Excited States  DAVID WILLIAMS-YOUNG (Presenter), ROEL VAN BEEUMEN, CHAO YANG, Computational Research Division, Lawrence Berkeley National Laboratory, XIAOSONG LI, Department of Chemistry, University of Washington — Due to the importance of spectroscopic methods in experimental physical chemistry, a primary directive in quantum chemistry is to be able to accurately and efficiently predict and interpret the response of molecular systems to external perturbations. Molecular response properties may be described in terms of propagators, such as the single particle Green's function and polarization propagator. Traditional methods to solve these problems, such as partial eigenvalue decompositions and direct linear system solves, become computationally intractable in cases where the spectral region of interest lies in the propagator's spectral interior. In this work is presented a novel model order reduction (MOR) technique for the rapid evaluation of molecular properties in arbitrary spectral regions. MOR accelerates the evaluation of these properties by constructing a rational Krylov subspace which spans the spectral region of interest. Numerical studies demonstrating the favorable computational cost and scaling of this method for linear response TDDFT are presented. Further, it will be demonstrated that bright eigenstates of the Hamiltonian may also be extracted from the same subspace. The proposed MOR algorithm will enable routine inquiry into previously intractable spectroscopic problems.

1:15PM F20.00009: Truncated methods applied to the direct calculation of exciton binding energies.  ARITZ LEONARDO (Presenter), University of the Basque Country, MIKEL ARRUBARRENA, centro de física de materiales (CFM), AI TOR BERGARA, University of the Basque Country, ANDRES AYUELA, centro de física de materiales (CFM) — Optical processes in insulators and semiconductors, including excitonic effects, can be described in principle exactly using time-dependent density-functional theory (TDDFT). Within this formalism, a family of exchange-correlation kernels known as long-range-corrected (LRC) kernels \((\text{fxc}=-\alpha/q^2)\) have shown to accurately reproduce optical spectra for several insulators and semiconductors. More recently, Ullrich and co-workers adapted the Casida equation formalism suitable for determining molecular excitations to periodic solids, this way the exciton binding energy may be calculated in a direct way without having to compute explicitly the response function. However, it appears that no LRC-type kernel is capable of simultaneously produce good optical spectra and quantitatively accurate exciton binding energies. In the present work we have adapted Casida's formalism following a different approach. The long range nature of the kernel, i.e. the \(q\to0\) singularity, is regularized employing a super-cell wigner-seitz truncation that clearly alters the previously calculated alpha values of the kernel. We will justify our calculation method and provide the alpha values for several insulating/semiconducting materials.
1:27PM F20.00010: Simulating valence and core excitons in solids within velocity-gauge real-time TDDFT.* SRI CHAITANYA DAS PEMMARAJU (Presenter), SLAC National Accelerator Laboratory — The application of real-time TDDFT (RT-TDDFT) to describe light-matter interactions in periodic solid-state systems has thus far been largely limited to situations where excitonic effects are not crucial primarily due to the inability of semi-local exchange-correlation (XC) functionals to describe exciton binding. In particular the simulation within TDDFT of accurate core-excitation spectra that are often strongly modulated by solid-state excitonic effects has been hindered. In this work, a recent atomic orbital basis implementation [1] of real-time TDDFT that exploits range-separated hybrid XC functionals within the generalized Kohn-Sham formulation [2] to simultaneously describe both valence and core excitonic effects in solids is presented. Optical properties and excitons in a number of representative solid-state systems are discussed from a time-domain perspective. Applications of the methodology to time-resolved core and valence spectroscopies are illustrated.


*This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515 through TIMES at SLAC.

1:39PM F20.00011: Relativistic real-time time-dependent density functional theory for molecular properties* LUKAS KONECNY (Presenter), MARIUS KADEK, KENNETH RUUD, MICHAL REPISKY, Hylleraas Centre for Quantum Molecular Sciences, University of Tromso — We present the development and applications of relativistic real-time time-dependent density functional theory. The method is based on the four-component Dirac–Coulomb Hamiltonian in the basis of restricted kinetically balanced Gaussian functions exploiting the noncollinear Kramers unrestricted formalism. A quasirelativistic two-component X2C Hamiltonian obtained from the original four-component Hamiltonian by an algebraic decoupling transformation is also considered. The equation of motion is formulated for the one-electron density matrix and solved in a series of discrete time steps utilizing the second order Magnus propagator corrected by a self-consistent extrapolation-interpolation procedure. Induced dipole moments recorded during simulations are transformed to the frequency domain to yield molecular spectra. Presented methodology includes scalar and spin-orbit relativistic effects variationally. It is demonstrated for valence and core electron molecular spectroscopies such as electron absorption and circular dichroism.

*Research Council of Norway Center of Excellence Grant No. 262695, Hylleraas Centre for Quantum Molecular Sciences Norwegian Supercomputer Program NOTUR Grant No. NN4654K

1:51PM F20.00012: Modes of Electron-Density Oscillation Corresponding to Absorption in Metal Clusters* RAJARSHI SINHA-ROY (Presenter), CINaM, Aix-Marseille University, CNRS, 13288 Marseille, France, PABLO GARcía-GONZÁLEz, Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidade Autónoma de Madrid, E-28049 Madrid, Spain, XÓCHITL LÓPEZ-LOZANO, ROBERT L WHETTEN, Department of Physics & Astronomy, The University of Texas at San Antonio, One UTSA circle, 78249-0697 San Antonio, TX., USA, HANS-CHRISTIAN WEISSKER, CINaM, Aix-Marseille University, CNRS, 13288 Marseille, France — Time-Dependent Density-Functional Theory (TDDFT) is widely used for calculating electron excitations in clusters and large molecules. For optical excitations, TDDFT is customarily applied in two distinct approaches: transition-based linear-response TDDFT (LR-TDDFT), and the real-time formalism (RT-TDDFT). The latter does not require the calculation of empty electron orbitals, which is specially advantageous when dealing with large systems. However, RT-TDDFT does not provide direct information on the nature of the excitations, unlike LR-TDDFT where the transition densities and the decomposition of the actual excitations in terms of independent-particle Kohn-Sham transitions are naturally obtained. In the present work, we show that the transition densities of the optically allowed transitions can be efficiently extracted from a single δ-kick time-evolution calculation. We assess the results by comparison with the corresponding LR-TDDFT ones and also with the induced densities arising from RT-TDDFT simulations of the excitation process using a quasi-monochromatic laser.

*We acknowledge support from french A*MIDEX grant (n. ANR-11-IDEX-0001-02), ANR grant (“FIT SPRINGS” ANR-14-CE08-0009), the Spanish MINECO grant (MAT2014-53432-CS-5-R), & HPC resources from GENCI-IDRIS (2016-096829).

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F21 DCOMP DCMP GSNP: Advances in Computational Methods for Statistical Physics and Their Applications II BCEC 157B - Danny Perez, Los Alamos National Laboratory - Tag(s): Focus
11:15AM F21.00001: Sampling large deviations of mobility and its application to glassy dynamics [Invited]
FRANCESCO TURCI, PADDY ROYALL, University of Bristol, THOMAS SPECK (Presenter), Johannes Gutenberg University Mainz — A major challenge in the computational sciences is the accurate sampling of events that are rare and have a low probability. Consequently, a wealth of advanced numerical methods devoted to this purpose has been developed. I will review the use of transition path sampling techniques to sample fluctuations of the single particle mobility in trajectories of a model glass former. In the supercooled regime, the dynamics is characterized by correlations that are trivial in space but highly non-trivial in time. There is numerical evidence for a dynamic phase transition from liquid to a jammed glass, which can be probed through a structural order parameter. I will present numerical and experimental results on the coexistence of the normal supercooled liquid with a phase that is rich in locally favored structures and dynamically arrested. Most strikingly, the coexistence region narrows as temperature is decreased, with the possibility that coexistence terminates at a finite temperature in a lower critical point. I will briefly discuss consequences for our understanding of the glass transition.

MARTIN MAGILL (Presenter), ANDREW NAGEL, HENDRICK W DE HAAN, University of Ontario Institute of Technology — Partial differential equations (PDEs) in nanobiophysics (NBP) often arise in complicated geometries. Typically, such problems would be solved with mesh-based numerical solvers. However, the stochastic many-body systems common to NBP are described by high-dimensional PDEs. Mesh-based solvers fail for such problems, so instead these PDEs are solved indirectly using particle simulations. Still, these particles are often subject to force fields, which are themselves described by similar PDEs. Furthermore, to establish how observables, like molecular mobility, depend on problem parameters, like molecular size, simulations must be repeated many times.

A new method for solving PDEs is to approximate solutions with deep neural networks (DNNs). DNNs can even learn solutions directly from the PDE problem statement, without using any external data. In this talk, I will illustrate some benefits of this method for solving PDEs in NBP. DNNs are memory-efficient, enabling complicated electric fields to be used in GPU-accelerated particle simulations. Surprisingly, DNNs can actually solve high-dimensional PDEs directly, as an alternative to particle simulations. Finally, this method can naturally be extended to express target observables as differentiable functions of problem parameters.

12:03PM F21.00003: Machine Learning Surrogate Models to Accelerate Monte-Carlo Calculation*
MARKUS EISENBACH (Presenter), JIAXIN ZHANG, ZONGRUI PEI, MASSIMILIANO LUPO PASINI, YING WAI LI, JUNQI YIN, Oak Ridge National Laboratory — While modern Monte-Carlo algorithms are highly efficient for computational statistical mechanics in many systems, it is desirable for many materials simulations to utilize energies that are evaluated using density functional theory to capture the complex interactions in multicomponent systems. In the past we have performed calculations by combining our LSMS first principles code with Wang-Landau Monte-Carlo calculations. The number of Monte-Carlo steps limits the applicability of this method even on high-performance computer systems. Thus, we are integrating a machine learning derived surrogate model with Monte-Carlo calculations. Here we present our results of deriving surrogate models from total energy calculations that replicate the behavior of first principles calculations of alloy ordering transitions. In addition to evaluating the attainable speedup, we explore strategies for reducing the dimensionality of the surrogate model as well as the impact of the model on the accuracy of the Monte-Carlo results.

*This work is supported in part by the Office of Science of the Department of Energy and by the LDRD Program of Oak Ridge National Laboratory. It used resources of the Oak Ridge Leadership Computing Facility, supported by the Office of Science of the U.S. Department of Energy.

12:15PM F21.00004: Reinforcement Learning and the Scientific Method
RORY COLES, University of Ontario Institute of Technology, ISAAC TAMBLYN (Presenter), University of Ontario Institute of Technology, National Research Council of Canada — Model-based reinforcement learning allows an agent to learn how their environment behaves around them, allowing for an optimal solution to be planned preemptively. In past reports, model-based reinforcement learning has been found to sample an environment more efficiently than model-free reinforcement learning, in which the agent is learning the best action to take given any one state.

In this work, we present an alternative to model-based reinforcement learning in which exploring and updating the model are separate actions. As a result, the agent must act in an environment when there is uncertainty in the state and learn to take detailed observations accordingly to update the model. To achieve success, the agent needs to extrapolate from the known model, conduct a test in order to obtain new data, and then base future decisions on those results. This is a well-known process: the scientific method. We then show how our newly developed method can be used to learn the dynamics of physics-based models and exploit the knowledge gained to achieve a given objective with a measurable confidence.
ZHENG FANG (Presenter), HENRY D. I. ABARBANEL, Department of Physics, University of California, San Diego — We formulate an equivalence between deep learning and state/parameter estimation problems in nonlinear dynamical systems. We also propose a general method (named Precision Annealing) inspired by this equivalence to perform learning tasks without backpropagation. Using the language of statistical physics, we then explain the novel optimization routine of the PA method and compare it with optimizations in conventional deep learning. Furthermore, we show up-to-date results of the PA method in various settings including standard deep learning tasks.

**12:39PM F21.00006: Training Classifiers With a Multi-Grid DMRG Algorithm**  
JUSTIN REYES (Presenter), University of Central Florida, EDWIN M STOUDENMIRE, Physics, University of California- Irvine — We introduce a novel machine learning architecture for the classification of large vector data. The architecture mimics the MERA architecture, with each layer providing a new renormalization "scale" to perform a DMRG-like optimization for the training of the network. We observe a dependence of the accuracy and generalization on the number of layers within the architecture, testing on audio classification datasets. We also modify the algorithm for the prediction of future data points in a time-dependent data set, characterizing its performance by the average absolute error in its prediction.

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**12:51PM F21.00007: Expanded Wang-Landau simulations: Towards a partition function-based prediction of properties for single component systems, mixtures and adsorbed phases**  
CAROLINE DESGRANGES, JEROME DELHOMMELLE (Presenter), University of North Dakota — Conventional simulation methods are carried out for a given set of thermodynamic conditions and they generally provide access to a few thermodynamic properties. However, the development of recent and powerful sampling methods, like the Wang-Landau sampling, has allowed for the direct evaluation of the density of states of a system. In recent work, we proposed an approach, known as Expanded Wang-Landau simulations, that yields highly accurate estimates of the grand-canonical partition function for a wide range of applications, ranging from the bulk to fluids confined in nanoporous materials. This, in turn, yields all thermodynamic properties. In particular, we show how this approach gives access to properties that are notoriously difficult to compute, including free energy and entropy, thereby shedding light on e.g. adsorption or assembly processes.

**1:03PM F21.00008: Relaxation Augmented Free Energy Perturbation**  
YING-CHIH CHIANG (Presenter), CHRISTOPHER CAVE-AYLAND, MARLEY SAMWAYS, University of Southampton, FRANK OTTO, Department of Chemistry, University College London, JONATHAN ESSEX, University of Southampton — We re-examine the concept of free energy calculation via a single-step free energy perturbation (sFEP) method, which frequently fails to converge due to the problem of insufficient sampling. We find a close resemblance between the operation in sFEP and the vertical transition between two different electronic states in quantum mechanics. The insufficient sampling problem then has a vivid physical interpretation as lacking the relaxation process after perturbation. Upon augmenting the traditional sFEP with the relaxation process, the new method agrees well with the exact solution, shedding new light on the underlying physics in free energy calculations.

*YCC thanks the Royal Society for funding this research (Newton International Fellowship NF171278).

**1:15PM F21.00009: Directed random walks and global updates for improved convergence in multicanonical Monte Carlo algorithms**  
YING WAI LI (Presenter), National Center for Computational Sciences, Oak Ridge National Laboratory, ALFRED FARRIS, Center for Simulational Physics, University of Georgia, MARKUS EISENBACH, National Center for Computational Sciences, Oak Ridge National Laboratory — Modern Monte Carlo algorithms such as multicanonical sampling and Wang-Landau sampling are robust methods to obtain the density of states for physical systems. However, they require a long time to converge, making them computationally expensive. We propose a novel scheme to achieve faster convergence and improve the efficiency of these algorithms. By performing a global update of the sampling weights across the phase space, the algorithm achieves uniform sampling quickly. Combining this global update scheme with the recently proposed histogram-free multicanonical method [1,2], we have observed three orders of magnitude of speedup compared to existing flat-histogram methods on Heisenberg models and a homopolymer model.


*This work used resources of the Oak Ridge Leadership Computing Facility, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
1:27PM F21.00010: Selecting initial distributions of states for efficient Monte Carlo sampling* THOMAS E BAKER (Presenter), Département de physique, Université de Sherbrooke, Institut quantique — A simple but massively parallel Monte Carlo method is demonstrated here [1]. Working with many different Monte Carlo samplers creates the opportunity to arrange the systems to partially cancel errors from insufficient relaxation. By averaging independent runs, auto-correlation is automatically canceled. This arrangement represents the idealized limit of parallel tempering. In order to determine an appropriate initial distribution, un-relaxed samples are randomly selected. Results from this method, called Genetic Tempering, for a variety of spin models are presented [2,3].


*This project was funded solely by Institut quantique. This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund (CFREF).

1:39PM F21.00011: Development of effective stochastic potential method using random matrix theory for calculation of ensemble-averaged quantum mechanical properties at non-zero temperatures* JEREMY SCHER (Presenter), ARINDAM CHAKRABORTY, Syracuse University — An ensemble-averaged description of quantum mechanical properties is computationally prohibitive because it requires performing many electronic structure calculations. In this work, the effective stochastic potential (ESP) method is presented for performing large-scale calculations of ensemble-averaged quantum mechanical properties, and alleviates the computational cost associated with the conformational sampling required to obtain these properties. The ESP method represents the thermal fluctuations in a chemical system as an effective stochastic potential, derived using random-matrix theory. We introduce the concept of a deformation potential and demonstrate its existence by the proof-by-construction approach. A statistical description of the deformation potential arising from non-zero temperature was obtained using an infinite-order central moment expansion of the distribution. The formal definition of the ESP was derived using a functional minimization approach to match the infinite-order expansion for the deformation potential. The ESP method was implemented using both HF and KS-DFT formalism, and ensemble-averaged ground and excited state energies will be presented.

*This material is based upon work supported by the National Science Foundation under Grant No. CHE-1349892.

1:51PM F21.00012: Constructing Generative Models via the Functional Renormalization Group NAHOM YIRGA (Presenter), DAVID K CAMPBELL, Boston University — Inference problems invert the traditional flow of statistical physics requiring the construction of a probability distribution given a limited set of observations. The fundamental challenge of inverse problems is separating the true couplings between variables from correlations that measure interactions between variables mediated by the entire system. We consider, for cases were additional measurements are possible, the functional renormalization group (fRG) as a tool for such a separation. Standard fRG flows start with a model Hamiltonian modified with a regulator that suppresses all interactions below a certain scale. As the flow proceeds the regulator slowly moves down through all scales until we converge to the fully interacting system. We invert this program and systematically freeze and remove long range correlations from a fully interacting system. We apply this inverted fRG scheme to the Ising and XY models. Finally, we address the required set of observables to make an fRG reconstruction a viable scheme.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F22 DCOMP: Education and Modern Computation BCEC 157C - Rubin Landau, Oregon State University - Tag(s): Invited
11:15 AM F22.00001: The Practical and Theoretical Future of Computation in Physics [Invited] STEPHEN WOLFRAM (Presenter), Wolfram Research — I started using computers for physics around 1972, and for the past 30+ years I've been building things like Mathematica and Wolfram|Alpha that have been used to do a lot of physics. Around 1980 realized that computation can be used not only for the practical doing of physics, but also as a framework for thinking about physics. Among other things that led to my book A New Kind of Science, and by now many new models in many fields (including physics) are getting made in terms of programs rather than traditional mathematical constructs.

In this talk, I'll discuss the framework I've been building for doing physics by computer, and its future implications—both in terms of theoretical modeling, data analysis and machine learning, as well as connections to the knowledgebase we've accumulated, and to real-time data taking. I'll also discuss what it means to think about the foundations of physics in computational terms—the implications of phenomena like undecidability and computational irreducibility, and what one can anticipate about the theoretical structure of physics in the future.

11:51 AM F22.00002: Computational Problems for Physics Courses Throughout the Curriculum* [Invited] RUBIN LANDAU (Presenter), Oregon State University — Physics courses too often include computation to illustrate physics, with little discussion of the underlying applied math and its commensurate level of precision and reliability. The authors have spent over two decades thinking up computational problems and demonstrations for their Computational Physics texts and for conference tutorials and institutional talks. A new book Computational Problems for Physics with Guided Solutions Using Python extends those problems and demos with the aim of having computation supplement a variety of existing courses. The text includes a large number of worked problems with fully guided solutions in Python, with other languages (Java, C, Fortran, Maple, and Mathematica) available on the Web.


*Funding over the last two decades has come from the National Science Foundation.

12:27 PM F22.00003: Hitting the ground running: Computational physics education that prepares students for research [Invited] AMY GRAVES (Presenter), ADAM D LIGHT, Swarthmore College — Integrating computation into the standard physics curriculum is becoming increasingly common for reasons of enhancing physics education. This begs the question of which elements of this type of teaching also feed into creating students ready to enter a computational physics research group, and come up to speed as contributing members. In this talk, we will review strategies currently being employed to train undergraduates to this task. We suggest that there is a need for the computational physics research community to collect and rank priorities for student skills. The issue of which computational tools and skills are needed (There are many!) will be rephrased as a question of which tools our incoming research students should (i) already know (ii) know exist in principle (iii) not know, but would be taught in the research lab setting. In other words: which skills and ideas are both natural and feasible to include in the classroom environment, and which are more suited to on-the-job training? We suggest resources within the domain of computational physics as well as in computer science, software engineering, and data science, for optimizing students' preparedness and productivity.
1:03PM F22.00004: Probing quantum mechanical energy on a local scale [invited] NITHAYA CHETTY (Presenter), Department of Physics, University of Pretoria — We explore the usefulness of using quantum mechanical energy densities, and investigate the computation of physically meaningful results despite the non-uniqueness of these quantities. In the case of the kinetic energy density, we define two different forms, the one form involving the \(-\hbar^2/2m \phi(x) \nabla^2 \phi(x)\), and the other involving \(+\hbar^2/2m |\phi(x)|^2\). Since the difference of these two approaches includes a boundary term, we specifically explore the kinetic energy current densities at the boundaries and demonstrate why the first form gives physically more meaningful results than the second form.

We carry these notions over to many electron systems, within the framework of density functional theory, where we consider the Coulomb energy. Once again, we note the non-uniqueness in defining the Coulomb energy density, the one form involving the square of the electric field vector, and the other involving the product of the Coulomb potential with the density. We demonstrate why the first form gives physically more meaningful results than the second form.

This sets the stage for extracting even more useful information from the computational studies of real material systems using standard methods.

1:39PM F22.00005: Developing the educational value of visualizations in physics [invited] JOAN ADLER (Presenter), Technion - Israel Institute of Technology — Many interesting physical phenomena occur at length scales that cannot be accessed with the naked eye. Some, especially those related to atoms and molecules, are too small. Astrophysical scales can be too large. Modern computations leading to computer visualizations enable access across all length scales. These types of calculations require a large amount of computer resources to carry out the basic computations with sufficient detail and elapsed time. One must think how to maximise the learning experience while minimising the student's technical effort. (Not to speak of minimizing the teachers' preparation effort so they can concentrate on pedagogy rather than developing theirs and their students' computer techniques.) If 3D material is simply presented as flat images its impact is curtailed. Thus interactivity, three dimensional images (stereo where possible) and some carefully curated student activity are needed. I will describe material prepared at the Technion that aids comprehension for not-too-great student effort, but at the same time allows for some ``hands-on'' interaction. Two approaches we use are: smoke visualization for electronic density of wavefunctions and fluid flow (3D, stereo) and WebGL for rotatable, zoomable images of lattices and molecules. The former require substantial running time and RAM memory to provide the raw data. All of the final visualizations are website based and accessible also on cellphones. The former have an analglyphic stereo option, the latter can be used with Oculus viewers.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F23 DLS: Laser Science BCEC 158 - Richard Averitt, Univ of California - San Diego

11:15AM F23.00001: High-resolution spectroscopy of whispering gallery mode optical microcavities in the evanescent field of tapered optical fibers.* NATHAN JORDAN (Presenter), ALEX KING, Physics, Gordon College, ADDISON OGOVOSKI, PRANAY SULTANIA, MARSHALL MA, Mechanical Engineering, Boston University, MUCHENG LI, YUNDONG REN, YUXIANG LIU, Mechanical Engineering, Worcester Polytechnic Institute, KAMIL EKINCI, SEAN ANDERSSON, Mechanical Engineering, Boston University, OLEKSIY SVITELSKI, Physics, Gordon College — Optical cavities with whispering gallery mode (WGM) resonances are interesting as building blocks for photonic devices, including fiber-integrated couplers and spectrometers, photonic crystals, and lasers. The high Q factors (10^3-10^5) along with their sensitivity to the surrounding environmental conditions allow the use of optical cavities as sensors of various physical quantities. We present results on polarized optical spectroscopy of spherical WGM resonant microcavities (D~5-50 micron) made of plastic, and silica and barium titanate glass, performed in air and water. The resonances were excited by evanescent light from optical fibers tapered either by chemical etching or by thermal pulling. The results of our experiments are consistent with theoretical predictions. We will discuss how to use these WGM resonances in order to apply forces to microparticles for microfluidic and biomedical applications.

*This work was partially supported by NSF CMMI awards # 1661700 and 1661586.
11:27AM F23.00002: Home-made Spectrometer to Study Whispering Gallery Mode Resonators* MARSHALL SHENDU MA (Presenter), ADDISON OGONOSKI, PRANAV SULTANIA, KAMIL EKINCI, SEAN ANDERSSON, Mechanical Engineering, Boston University, OLEKSIY SVITELSKYI, Department of Physics, Gordon College — Whispering gallery mode (WGM) resonances are promising phenomena for fiber-based photonic applications such as directional couplers, spectrometers, and light generators. These resonances can also be useful for applying forces to dielectric microbeads and sorting them. We designed and built a simple system to excite and detect the WGM resonances of microbeads in atmosphere and in a liquid environment. The system consists of a tunable laser, an optical fiber with a tapered region where the WGM resonators are placed, and a photo detector to monitor the power transmitted through the fiber. The tunable laser has a wavelength range of approximately 1500-1600 nm and a peak output power of 1.5 mW. The tapered region is produced by chemical etching with hydrofluoric acid of a standard SMF-28 optical fiber. The WGM resonances are excited in plastic or glass microbeads with diameters in the 10 to 45 micron range. The preliminary results were obtained at steps of 1 and 0.1 nm/s in a wavelength sweeping mode. The power transmission was more than 40% which is sufficient to overcome the substantial power loss occurred in a liquid environment.

*This work was partially supported by NSF CMMI awards 1661700 and 1661586.

11:39AM F23.00003: Efficient, phase-resolved polarization-dependent two-dimensional coherent spectroscopy JARED WAHLSTRAND (Presenter), GALAHAD WERNSING, LEON LU, Physical Measurement Laboratory, National Institute of Standards and Technology, ALAN D BRISTOW, Department of Physics and Astronomy, West Virginia University — Capturing spectra for multiple polarization configurations in two-dimensional coherent spectroscopy allows access to different quantum pathways in the light-matter interactions probed by the technique. This is typically done by manually rotating waveplates. We demonstrate a liquid crystal variable retarder-based control scheme to efficiently capture common polarization configurations of the rephasing four-wave mixing of a semiconductor microcavity, showing that the presence of biexcitons alters the nonlinear response of the exciton polaritons. We find the proper phase of the complex 2D spectrum for the collinear polarization configuration in the usual way, by comparing the four-wave mixing emission to the spectrally-resolved transient absorption. Importantly, because the phase shift induced by the variable retarders is known, spectra for all other polarization configurations can be correctly phased.

11:51AM F23.00004: Coupling length phase matching scenarios in dual-core silica fibers JING SU (Presenter), IVAN BIAGGIO, Lehigh University — We analyze optical dual core silica fiber configurations that can be achieved to obtain phase matched third-order nonlinear optical frequency conversion to obtain farther infrared laser sources from near-infrared lasers. The phase matching principle is based on the coupling length phase matching (CLPM) principle, which allows to tune the phase matching condition by tuning the distance between the two cores in the fiber. We describe the corresponding phase matching tuning curves for different choices of pump lasers and discuss the advantages and limitations of the technique.

12:03PM F23.00005: Floquet optical ring resonators* KATHLEEN MCGARVEY-LECHABLE (Presenter), PABLO BIANUCCI, Concordia University — This work discusses Floquet optical ring resonators (FORRs) on the silicon nitride photonics platform. A FORR builds upon the principles of a standard ring resonator with the addition of a small, periodic perturbation to the ring's dielectric material. Similar to a standard photonic crystal, this perturbation results in the formation of multiple photonic band gaps (PBGs) in the ring's optical spectrum. The size of the PBGs can be related to the degree of coupling between degenerate propagating and counter-propagating resonances of the ring. Through application of Bloch-Floquet theory, it is seen that the degree of spectral splitting between two degenerate modes can be precisely controlled by varying the strength of the l-th order Fourier coefficient of the ring's dielectric profile. Additionally, multiple Fourier coefficients may be added to the unperturbed ring's dielectric profile to split resonances across a broad spectrum of the ring. As a result, FORRs provide a new degree of freedom in manipulating the dispersion relation of a ring resonator, providing control over the spectral frequency and group velocity dispersion of a resonance. Potential applications of FORRs include dispersion engineering of optical frequency combs and integrated single photon sources.

*NSERC, FRQNT
12:15PM F23.00006: Exceptional points in microresonator Brillouin laser systems* YUKUN LU (Presenter), YU-HUNG LAI, MYOUR-GYUN SUH, KERRY VAHALA, Applied Physics, Caltech — We theoretically proposed and experimentally demonstrated the existence of exceptional points (EPs) in an on-chip microresonator Brillouin laser system. The coalescence of the eigenfrequencies as well as the eigenmodes is presented. When the laser system is operating near the EP, the boosted rotational sensitivity is confirmed, which enables on-chip optical gyroscopes with unprecedented sensitivity. Moreover, EPs also emerge below the lasing threshold, and the coherent perfect absorption (CPA) can be realized by tuning the pump power. EPs in on-chip microresonator Brillouin systems have applications in precise sensing and optical information manipulating.

*This work was supported by the Defense Advanced Research Projects Agency (DARPA) through SPAWAR (N66001-16-1-4046).

12:27PM F23.00007: Spontaneous symmetry breaking in an optical microcavity QI-TAO CAO (Presenter), YUN-FENG XIAO, School of Physics, Peking University, China — Spontaneous symmetry breaking is a ubiquitous property in diverse fields of modern physics, which is, however, elusive in optical domain. As a prominent photonic platform, the ultrahigh-Q whispering-gallery (WG) microcavity supports clockwise (CW) and counterclockwise (CCW) propagating waves with balanced amplitudes. Such chiral symmetry in a WG microcavity can be explicitly broken by removing the parity or time-reversal symmetry in previous works [1,2]. In this work, we report the experimental demonstration of the spontaneous chiral symmetry breaking in a single WG microcavity. The Kerr nonlinearity gives rise to an intensity-dependent CW-CCW coupling that becomes zero beyond a threshold, causing the original standing-wave mode to be unstable and spontaneously evolve into two chiral states with the unbalanced CW and CCW components [3,4]. Furthermore, we extended such the spontaneous symmetry breaking to the active regime and realized a unidirectional microlaser with the controllable chirality.


12:39PM F23.00008: Spatiotemporal Mode-Locking is Generalized Mode-Locking* LOGAN WRIGHT (Presenter), PAVEL SIDORENKO, ZACHARY M ZIEGLER, ANDREI ISICHENKO, Cornell University, BORS MALOMED, Department of Physical Electronics, School of Electrical Engineering, Faculty of Engineering, and the Center for Light-Matter Interaction, Tel Aviv University, CURTIS ROBERT MENYUK, Department of Computer Science and Electrical Engineering, University of Maryland Baltimore County, DEMETRIOS CHRISTODOULIDES, CREOL/College of Optics and Photonics, University of Central Florida, FRANK W WISE, Cornell University — In mode-locking, light in a resonator self-organizes into a nonlinear attractor, the dissipative soliton, often with rich dynamics. Mode-locking has enabled a myriad of applications through ultrashort duration pulses, high peak intensity, and broad frequency comb spectra. Virtually all work on the topic has considered light propagating on only one dimension, as in single-mode fiber. We recently demonstrated spatiotemporal mode-locking [1], the self-organized locking of many spatial and longitudinal modes into coherent pulses, i.e., three-dimensional mode-locking. Adding new dimensions to light's self-organization gives rise to new ways to control the light field. Here, we outline a general theory of spatiotemporal mode-locking, showing it to be a generalization of mode-locking, and present new experimental measurements of qualitatively new mode-locked states, comprising nearly 30 million locked modes. Additionally, we predict numerous other novel forms of mode-locking, and phenomena, such as spatiotemporal dissipative soliton competition. 1. L.G. Wright, D.N. Christodoulides, & F.W. Wise (2017). Spatiotemporal mode-locking in multimode fiber lasers. Science, 358(6359), 94-97.

*This work was supported by Office of Naval Research grant N00014-13-1-0649 and NSF grant ECCS-1609129

12:51PM F23.00009: Optically pumped lasing from Er-doped GaN epilayers in the infrared region YIZHOU WANG, HO VINH, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech, HONGXING JIANG (Presenter), JINGYU LIN, Department of Electrical and Computer Engineering, Texas Tech University, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — We report the realization of room-temperature, stimulated-emission in Er-doped GaN epilayers prepared by metal-organic chemical vapor deposition in the infrared region at room temperature. The lasing action of the Er doped GaN epilayers under optically pumped using an UV laser for the above bandgap excitation has been characterized. The observation of the amplified spontaneous emission has been presented through characteristic features of threshold behavior of emission intensity as functions of pump intensity, excitation length, and spectral linewidth narrowing by the variable stripe technique. Varying excitation length of the variable stripe setup, we have observed the optical gain of the GaN:Er epilayers is up to 75 cm-1. The generation of coherent radiation at 1.54 μm at room temperature paves the way for extended functionalities and integration capabilities for optoelectronic devices.
1:03PM F23.00010: A new high-efficiency regime for gas-phase terahertz lasers: Experiment and ab-initio theory*

FAN WANG (Presenter), Massachusetts Institute of Technology, PAUL CHEVALIER, ARMAN AMIRZHAN, MARCO PICCARDO, FEDERICO CAPASSO, Harvard University, STEVEN G JOHNSON, Massachusetts Institute of Technology, HENRY O EVERITT, Duke University — In this work, we present both a new theoretical description and experimental validations of molecular gas optically pumped far infrared (OPFIR) lasers that have much higher efficiency than traditional OPFIR lasers with much more compact volumes. First, we demonstrate a $^{13}$CH$_3$F OPFIR laser that achieves 10× greater efficiency and 1000× smaller volume than comparable commercial lasers. To fully understand this, we developed a new ab-initio theory that matches experiments quantitatively, within experimental uncertainties with no free parameters, by accurately capturing the interplay of millions of degrees of freedom in the laser—unlike previous OPFIR-laser models involving only a few energy levels that failed to even qualitatively match experiments at high pressures. Our model is general enough to capture the lasing behaviors of many other gases. By optically pumping N$_2$O with a QCL instead of a CO$_2$ laser, we predict a new regime of broad frequency-tunability for this traditionally narrow-band THz source. These results offer the possibility of a new generation of compact, frequency-tunable THz sources.

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2. MRSEC Program of the NSF under award number DMR-1419807

1:15PM F23.00011: A White Random Laser*

YUN-TZU HSU (Presenter), SHU-WEI CHANG, WEI-CHENG LIAO, YU-MING LIAO, CHENG-FU HOU, YING-HUAN CHEN, CHIA-TSE TAI, CHEN-YOU SU, Physics, National Taiwan University, TAI-YUAN LIN, Physics, National Taiwan Ocean University, YANG-FANG CHEN, Physics, National Taiwan University — Random laser with intrinsically uncomplicated fabrication processes, high spectral radiance, angle-free emission, and conformal onto freeform surfaces is in principle ideal for a variety of applications, ranging from lighting to identification systems. In this work, a white random laser (White-RL) with high-purity and high-stability is designed, fabricated, and demonstrated via the cost-effective materials (e.g., organic laser dyes) and simple methods (e.g., all-solution process and self-assembled structures). Notably, the wavelength, linewidth, and intensity of White-RL are nearly isotropic, nevertheless hard to be achieved in any conventional laser systems. Dynamically fine-tuning colour over a broad visible range is also feasible by on-chip integration of three free-standing monochromatic laser films with selective pumping scheme and appropriate colour balance. With these schematics, White-RL shows great potential and high application values in high-brightness illumination, full-field imaging, full-colour displays, visible-colour communications, and medical biosensing.

*This work was supported by the Ministry of Science and Technology and Ministry of Education of the Republic of China.

1:27PM F23.00012: High-order harmonic generation from hybrid lead halide perovskites*

HIDEKI HIRORI (Presenter), Kyoto Univ - Uji Campus, PEIYU XIA, Institute for Solid State Physics, University of Tokyo, YASUSHI SHINOHARA, Graduate School of Engineering, University of Tokyo, TOMOHITO OTOBE, Kansai Photon Science Institute, National Institutes for Quantum and Radiological Science and Technology, YASUYUKI SANARI, HIROKAZU TAHARA, Kyoto Univ - Uji Campus, NOBUHISA ISHI, JIRO ITATANI, Institute for Solid State Physics, University of Tokyo, KENICHI ISHIKAWA, Graduate School of Engineering, University of Tokyo, TOMOKO AHAREN, MASASHI OZAKI, ATSUSHI WAKAMIYA, YOSHIHIKO KANEMITSU, Kyoto Univ - Uji Campus — Nonlinear optical current induced by strong laser fields produces coherent radiation in spectral ranges inaccessible by lasers. Such high-harmonic generation (HHG) in solids is different from that in atomic gases; it has been shown that the intraband current caused by ultrafast acceleration of electron wave packets constitutes the nonlinear current [1,2]. However, how the concurrent field-driven population change in valence band contributes the nonlinear current remains unclear. Here, we studied the crystal orientation dependence of HHG intensity for hybrid organic-inorganic halide perovskites, which is well reproduced by the calculations based on an ab-initio approach. Our picture indicates that the virtual population change in the valence band is responsible for the HHG, which is of vital importance for achieving high generation efficiency and taking a full of information on bandstructure.


*This study was supported by CREST (No. JPMJCR16N3 and No. JPMJCR15N1), PRESTO (No. JPMJPR1427) grants, and the Center of Innovation Program from JST and KAKENHI (Nos. 18H03682, 18K14145, 17K05089, 18K13481, and No. 16H03881) grants from JSPS.
1:39PM F23.00013: Time- and angle-resolved photoemission spectroscopy using ultrafast XUV source at around 20 eV*  
YANGYANG LIU (Presenter), JOHN BEETAR, MD MOFAZZEL HOSEN, GYANENDRA DHAKAL, CHRISTOPHER SIMS, FIROZA KABIR, KLAUSS DIMITRI, SABIN REGMI, MICHAEL CHINI, MADHAB NEUPANE, Physics, University of Central Florida — Time- and angle-resolved photoemission spectroscopy (trARPES) has several advantages over conventional static ARPES measurements. Using trARPES, one can measure electronic states above the Fermi level, track femtosecond or picosecond dynamics in materials, and study transient laser-dressed band structures. We have developed a trARPES setup using high-order harmonic probe pulses produced using a commercial turn-key Yb:KGW laser. The laser, which emits 1030 nm, 290 fs laser pulses with average power of 20 W and tunable repetition rate between 50-200 kHz, is frequency-doubled using a BBO crystal, and focused into a krypton-filled gas cell to generate high-order harmonics. We eliminate low-order harmonic using an aluminum foil filter and optimize the harmonic cutoff using the laser intensity, thereby isolating the 9th harmonic at 21.7 eV. The 9th harmonic probe will be combined with a portion of the 1030 nm laser with a variable time delay for pump-probe experiments. Here, we will present the full characterization of the harmonic light source, as well as first time-resolved measurements in topological materials.

*This work is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415 and the startup fund from UCF (M.N.).

1:51PM F23.00014: Ultrafast relaxation of laser-excited flat nanoislands and nanoparticles investigated by ultrafast electron diffraction*  
AHMED ESMAIL, HUI XIONG, HANI ELSAYED-ALI (Presenter), Old Dominion Univ — Ultrafast electron diffraction is used to probe the electron-phonon energy relaxation and phonon dynamics in Bi flat nanoislands and nanoparticles. The sample was excited with 110-fs laser pulses. By controlling the temperature and laser fluence during the annealing of thin Bi films, we prepare polycrystalline flat nanoislands and nanoparticles and investigate their relaxation dynamics. The temporal development of the various relaxation pathways is probed with a temporal resolution up to ~1.5 ps. The results show dependence on direction and varies between the nanoislands and nanoparticles. The response of the (110) diffraction peak for the 5-nm thick flat nanoislands is found to be faster than ~16 nm diameter nanoparticles. The response of diffraction for both particle shapes is found to be anisotropic. We also investigate the superheating of flat nanomaterials and nanoparticles by monitoring the long-range order with excitation at various levels.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-000304287.

2:03PM F23.00015: Ultra-high speed laser-surgery with ultrafast bursts of pulses  
FATIH ILDAY (Presenter), Bilkent University — Ultrafast lasers allow thermal damage-free ablation irrespective of the material type. However, this process is slow and inefficient, with ablation volume having the remarkably poor logarithmic dependence on incident pulse energy. We recently demonstrated (Ilday et al., Nature 2016) ablation-cooled laser-material, whereby ultrafast pulses are sent in bursts, each containing hundreds of pulses separated by merely 100s of picoseconds, such that there is no time for heat to diffuse away from the processing region. The ablation rate increases by orders of magnitude and ablation becomes the dominant heat removal mechanism. Thus, the rest of the target material remains cool and without damage. We also reduced the required laser pulse energies by 1000 times and achieved record speeds in cutting biological tissue, metals and semiconductors (reaching 1 mm³/s). This new regime, where the ablation volume scales linearly with burst energy, has received much industrial interest, but there is also remarkable potential for extremely high-efficient and fast laser surgery. Is it possible to reach 1 mm³/s with biological tissue without thermal damage? As a more basic question, what the limitations to further decreasing the pulse separation time to less than the time it takes for ablation to occur.

Tuesday, March 5, 2019 11:15 AM - 1:51 PM

Session F24 DAMOP: Quantum Gases in Optical Lattices  
BCEC 159 - Ulrich Schneider, Cambridge University -

Tag(s): Focus
Microscopic studies of doped cold-atom Fermi-Hubbard antiferromagnets

CHRISTIE S CHIU (Presenter), GEOFFREY JI, Harvard University, ANNABELLE BOHRDT, Harvard University and Technical University of Munich, MUQING XU, Harvard University, JUSTUS BRÜGGENJÜRGEN, Harvard University and University of Hamburg, MICHAEL KNAP, Technical University of Munich, EUGENE DEMLER, FABIAN GRUSDT, MARKUS GREINER, DANIEL GREIF, Harvard University — The experimental platform of ultracold fermionic atoms in optical lattices offers new perspectives for studying the physics of strongly correlated materials. We use this platform to implement the Fermi-Hubbard model, a paradigmatic model thought to capture the physics of high-temperature superconductivity, the pseudogap, and other phenomena containing longstanding open questions. The additional tool of quantum gas microscopy enables site-resolved readout and access to projections of the many-body wavefunction in the Fock basis. I will report on our most recent studies of doped antiferromagnets, where there is no universally agreed-upon mechanism for the interplay between hole motion and antiferromagnetic order.

Toward low-entropy states in the Fermi-Hubbard model with quantum gas microscopy

MUQING XU (Presenter), CHRISTIE S CHIU, GEOFFREY JI, Harvard University, JUSTUS BRÜGGENJÜRGEN, University of Hamburg and Harvard University, ANTON MAZURENKO, MAXWELL F PARSONS, MARTON KANASZ-NAGY, RICHARD SCHMIDT, FABIAN GRUSDT, EUGENE DEMLER, DANIEL GREIF, MARKUS GREINER, Harvard University — Ultracold atoms in optical lattices are a powerful platform for studying strongly correlated quantum systems. We study the repulsive Fermi-Hubbard model through quantum gas microscopy with fermionic Lithium-6 atoms in a square lattice. This technique allows for single-site resolved readout and manipulation, and has enabled us to achieve long-range antiferromagnetic order across our entire sample by performing entropy redistribution. Accessing intriguing phases in the Fermi-Hubbard model, requires development of new techniques for low-entropy quantum state preparation. Here we report on our low-noise interfering optical lattice, which offers dynamically tunable lattice geometry and allows for studies of the Fermi-Hubbard model in dimerized, honeycomb, and triangular lattices. This tunability can alternatively facilitate an adiabatic ramp from an ultralow-entropy initial state, prepared through entropy redistribution, toward strongly-correlated quantum phases. Another possible application of this interfering lattice is to provide simultaneous readout of both spin species.

Photoemission spectroscopy of a Fermi-Hubbard system with a quantum gas microscope

PETER T. BROWN (Presenter), ELMER GUARDADO-SANCHEZ, WASEEM S BAKR, Princeton University — Strongly correlated systems with superconducting ground states, including the high-temperature superconducting cuprates and the unitary fermi gas, exhibit normal state precursors to the superconducting gap in their single-particle excitations. A quantitative understanding of these so called pseudogap regimes may elucidate details of the ground states, but developing this is difficult in real materials because the parameters of the microscopic Hamiltonian are not known. In cold atom experiments the development of fermionic quantum gas microscopes has enabled high-precision studies of fermions in optical lattices. The Hamiltonian parameters of these systems can be calculated from first principles, and good agreement between theory and experiment has been reported in recent studies of equal-time spin and density correlations. In this talk I will report on the development of angle-resolved photoemission spectroscopy (ARPES) compatible with quantum gas microscopy and its application to studying pseudogap physics in an attractive Fermi-Hubbard system across the BEC-BCS crossover, setting the stage for future studies of the pseudogap regime in repulsive Hubbard systems.

Progress toward a dipolar quantum gas microscope with an expandable lattice

ANNE HEBERT (Presenter), GREGORY PHELPS, AARON KRAHN, FURKAN OZTURK, MARKUS GREINER, Harvard University — Highly dipolar atoms present an exciting opportunity to extend previous experiments to more complex systems influenced by long range, anisotropic interactions. Erbium, with its large dipole moment, numerous isotopes, and rich Feshbach spectrum, is an excellent element for such research. We present on current progress toward the construction of a novel optical lattice expandable in all three dimensions. This expandable lattice gives us tunability of the lattice spacing by a factor of 20. This allows for short spacing lattice that maximizes the strength of the dipole-dipole interaction, and then allows for in situ imaging in a larger spacing lattice with higher fidelity.
12:03PM F24.00005: Progress toward an Erbium Dipolar Quantum Gas Microscope* GREGORY PHELPS (Presenter), ANNE HEBERT, AARON KRAHN, S. FURKAN OZTURK, MARKUS GREINER, Harvard University — Quantum gas microscopy provides an exciting platform for the study of in situ atom-atom interactions. Recent advances in quantum gas microscopy have allowed probing of the Bose-Hubbard and Fermi-Hubbard Hamiltonian. We are currently extending these platforms with the introduction of an Erbium Dipolar Quantum Gas Microscope allowing us to study dipole-dipole interactions in a lattice. Erbium has several exciting properties, which increase the control and flexibility of these systems. These include stable bosonic and fermionic isotopes, a large magnetic dipole moment (7μB), a large spin value (J=6 and F=19/2 for bosonic and fermionic isotopes), a rich Feshbach spectrum, and several broad and narrow atomic transitions. Here we are presenting our recent progress toward an Erbium Quantum Gas Microscope. This features the integration of several unique systems, such as a high-resolution reflective objective, an accordion lattice for imaging, and a low disorder optical lattice. These developments will allow us to benefit from the long-range interaction of Erbium and probe the Extended Bose-Hubbard and Extended Fermi-Hubbard Hamiltonian to an unprecedented degree.

*This work is supported by the ARO DURIP grant, MIT-Harvard CUA, and MIT MURI grant.

12:15PM F24.00006: Antiferromagnetic Order and Non-Equilibrium Distributions in the Floquet-Engineered Hubbard Model* NICKLAS WALLDORF, Department of Micro- and Nanotechnology, Technical University of Denmark, DANTE KENNES, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, JENS PAASKE (Presenter), Niels Bohr Institute, University of Copenhagen, ANDREW MILLIS, Department of Physics, Columbia University — The periodically driven half-filled two-dimensional Hubbard model is studied via a saddle point plus fluctuations analysis of the Keldysh action. The drive is implemented as an alternating electric field, and the system is coupled to a metallic substrate in thermal equilibrium to allow for a non-equilibrium steady state synchronized to the drive. For drive frequencies below the equilibrium gap, and strong enough drive amplitudes, the mean-field equation has multiple solutions with a substantial time-dependent component. Even for "Magnus" drive frequencies much larger than the equilibrium gap, a one-loop analysis around the mean-field solution shows that even if no real electron-hole pairs are excited, the ac drive produces a highly excited, generically non-thermal distribution of fluctuations, which can affect the physics significantly, for example destroying zero-temperature long-ranged antiferromagnetic order for large enough drive amplitudes.

*This research was funded by the Danish National Research Foundation (CNG and QDev), the Basic Energy Sciences Division of the U.S. Department of Energy (DE-SC0018218) and the Deutsche Forschungsgemeinschaft through the Emmy Noether program (KA 3360/2-1).

12:27PM F24.00007: Strong correlations in magic-angle semimetals JUSTIN WILSON (Presenter), YIXING FU, ELIO KOENIG, Department of Physics, Rutgers University, YANG-ZHI CHOU, Department of Physics, University of Colorado, Boulder, JED PIXLEY, Department of Physics, Rutgers University — In magic-angle graphene, Moiré patterns lead to an enlarged unit cell, mini-Brillouin zone, and strongly correlated phases (as shown experimentally). We generalize this behavior to a whole class of semimetallic models from one- to three-dimensions, and we show that the key ingredients are (1) an "untwisted" semimetallic band structure and (2) a spatially quasiperiodic structure (e.g., a "twist") [1]. As the quasiperiodic structure is enhanced, the velocity of the effective low-energy semimetal decreases until it vanishes at a quantum phase transition. The magic-angle phenomena are associated with this eigenstate phase transition which is a unique type of “Anderson delocalization” transition in momentum space. Further, it is accompanied with flat-bands and behaves universally across models. Lastly, we build effective Hubbard models on the new bands by computing Wannier states. The interactions in these Hubbard models are strongly enhanced at this transition, indicating the existence of strongly correlated phases. All ingredients to realize our proposal are available in present-day cold-atomic laboratories for which the magic-angle effect can be exploited to induce strong correlations in quantum degenerate gases.

**12:39PM F24.00008: Enhancement and destruction of superfluidity: Unusual effects of population imbalance of atomic Fermi gases on a 1D optical lattice**

QIJIN CHEN (Presenter), Department of Physics, Zhejiang University, JIBIAO WANG, School of Physics and Astronomy, Sun Yat-Sen University (Zhuhai Campus), China — We study the superfluid behavior of population imbalanced ultracold atomic Fermi gases with a short range attractive interaction on a 1D optical lattice, using a pairing fluctuation theory. Due to the lattice-continuum mixing in a 1D optical lattice, population imbalance now has highly unusual effects. While the transition $T_c$ in the balanced case decreases and scales as $k_F a$ in the BEC regime, it approaches a constant BEC asymptote in imbalanced case. Therefore, population imbalance may strongly enhance the superfluidity by raising $T_c$ to the constant BEC asymptote. In addition to the destruction of superfluidity in some range of intermediate pairing strengths, the BEC regime may also become inaccessible when the lattice spacing $d$ and the population imbalance $p$ become large, and/or the lattice hopping integral $t$ becomes small, in contrast to the 3D continuum or dilute 3D lattice case, for which the BEC regime is always accessible. Furthermore, even when the BEC regime is accessible, not all minority atoms are paired up in the BEC limit. Upon destruction of the superfluidity due to increasing $(d,p)$ or decreasing $t$, only 50% of the minority atoms form pairs.

*Supported by NSF of China (Grant No. 11774309) and the NSF of Zhejiang Province (Grant No.LZ13A040001).

**12:51PM F24.00009: Harmonic potential effect on the ground state of the “g-e” model**

JERESON SILVA VALENCIA (Presenter), RODRIGO CASTELLANOS CARO, ROBERTO FRANCO, National University of Colombia — Alkaline-earth fermionic atoms confined in one-dimensional optical lattices can be described by the so-called "g-e" model [Nat. Phys. 6, 289 (10)], which at half filling shows four interesting insulating phases (CDW, Orbital density wave (ODW), Spin Haldane (SH) and Spin-Peierls) [PRB 91, 075121(15)]. However, the confining potential has not been considered so far, for this reason we explore an extended "g-e" model where a harmonic potential for both $^1S_{0}$ (g) and $^3P_{0}$ (e) atoms was considered. Using the density-matrix renormalization group method, we found that diverse insulating phase coexist in the ground state and that the spin Haldane and the spin Peierls phases disappear with the confining potential, meaning that these phases will not be observed in the experiments. The evolution of the CDW and the ODW phases around the middle of the trap was studied for different parameters. This work is motivated by recent experimental results about $^{171}$Yb atoms confined in optical lattices [Arxiv:1810.00536v1].

*The authors are thankful for the support of DIEB-Universidad Nacional de Colombia.

**1:03PM F24.00010: Light-cone like spreading of correlations in the Bose Hubbard model at strong coupling**

MALCOLM KENNETT (Presenter), MATTHEW R FITZPATRICK, Simon Fraser University — We study the spreading of correlations in space and time after a quantum quench in the Bose Hubbard model. We derive equations of motion for the single-particle Green's function within the contour-time formalism, allowing us to study dynamics in the strong coupling regime. We discuss the numerical solutions of these equations and calculate the single-particle density matrix for quenches in the Mott phase. We demonstrate light-cone like spreading of correlations in the Mott phase in one, two, and three dimensions and calculate propagation velocities in each dimension. Our results show excellent agreement with existing results in one dimension and demonstrate the anisotropic spreading of correlations in higher dimensions.

*Supported by NSERC
Rigorous Results for the Ground States of the Spin-2 Bose-Hubbard Model

HONG YANG (Presenter), HOSHO KATSURA, Department of Physics, The University of Tokyo — In this work, we prove rigorous theorems for the ground states of the spin-2 Bose-Hubbard model, concerning the magnetic properties, degeneracies and forms of the wave functions. The theorems are highly universal in the sense that they do not depend on the lattice structure (including spatial dimension), particle number and spin-independent interaction.

The spin-2 Bose-Hubbard model is a model for ultracold \( f = 2 \) spinor bosonic atoms in optical lattices. We prove that, with \( c_1 \) and \( c_2 \) being the coefficients of the two spin-dependent interaction terms of the Hamiltonian, the ground state has a maximum total spin when \( c_1 < 0 \) and \( c_2 \geq 5c_1 \), while tends to be a singlet if \( c_1 = 0 \) and \( c_2 < 0 \). When \( c_1 = c_2 = 0 \), the model has SU(5) symmetry. Furthermore, the ground-state degeneracies and the forms of wave function are also exactly determined in each coefficient region. Our approach takes the advantage of the symmetry of the Hamiltonian and employs sophisticated mathematical tools including the Perron-Frobenius theorem and the min-max theorem, as well as the representation theory of so(5) Lie algebra.

References


Metal-Insulator-Superconductor Transition in Two-Channel Interacting Many-Body Systems*

THEJA DE SILVA (Presenter), Physics, Augusta University — Using a slave-rotor approach within a mean-field theory, we study two-channel interacting systems to investigate the competition of metallic, Mott-insulating, and superconducting phases. Considering spin-3/2 cold atoms on optical lattices as a model system and treating a spin-3/2 atom as a bound state of a charge and a spin, we uncover a novel form of matter due to the competition between metal and superconducting phase. This novel unconventional phase emerges as a result of the global U(1) broken symmetries with respect to both roton and spinon fields. Further, we argue that the emergence of this unconventional phase is a generic phenomenon associates with many body systems where there are competing interactions. As such, we show that this unconventional phase can exist in rubidium doped fullerides under pressure.

*The author acknowledges the support of Augusta University, ITAMP, and KITP. ITAMP is supported by a grant from the National Science Foundation to Harvard University and the Smithsonian Astrophysical Observatory. The KITP is supported in part by the National Science Foundation under Grant No. NSF PHY11-25915.

Quantum Joule expansions in one-dimensional lattices*

SHAN-WEN TSAI (Presenter), JIN ZHANG, University of California, Riverside, YANNICK MEURICE, University of Iowa — We discuss the expansion dynamics of nonintegrable systems that contain bosons or fermions in one-dimensional lattices. The particles are initially confined in half of the system with a thermal state described by the canonical ensemble. At short times after we remove the barrier before the front hits the other boundary of the lattice, the radial velocity of the expansion is a constant. The center of mass is accelerated with a constant acceleration. At long times, local observables can be approximated by a thermal expectation of another canonical ensemble with an effective temperature. The weights for the diagonal ensemble and the canonical ensemble match well for high initial temperatures that correspond to negative effective final temperature after the expansion. The negative effective temperature for finite systems goes to positive inverse temperatures in the thermodynamic limit for bosons but is a true thermodynamic effect for fermions. We also compare the thermal entanglement entropy and density distribution in momentum space for the canonical ensemble, diagonal ensemble and instantaneous long-time states calculated by exact diagonalization.

*Department of Energy Office of Science, Award Numbers: DE-SC0019139 and DE-SC0010113.
11:15 AM F25.00001: NV-Diamond Magnetometry in the NV-NV Interaction Limit

CONNOR HART (Presenter), ERIK BAUCH, Harvard University, JENNIFER SCHLOSS, MIT, RAISA TRUBKO, MATTHEW J TURNER, DIANA PRADO LOPES AUDE CRAIK, Harvard University, RONALD L WALSWORTH, Harvard-Smithsonian CfA — In nitrogen-vacancy (NV) ensembles in diamond, the magnetic sensitivity is commonly limited by a bath of other impurity spins, which decoheres the NV sensor spins. We demonstrate mitigation of NV-bath interactions by RF control of the spin bath or dynamical decoupling of the NV centers. In this regime, mutual NV-NV dipolar interactions dominate the ensemble spin properties ($T_2, T_2^*$). These techniques may yield improved DC and AC magnetic sensitivity up to a limit set by NV-NV dipolar interactions. For example, we show NV ensemble coherence times under XY8-n dynamical decoupling protocols limited by instantaneous diffusion. We present progress toward mitigating NV-NV interactions while preserving magnetic sensitivity, and conversely we outline ideas to leverage strong NV-NV interactions to further improve magnetic sensitivity.

11:27 AM F25.00002: A high-speed, strain-free NV-diamond magnetic imager for neuroscience

JENNIFER SCHLOSS (Presenter), Physics, Massachusetts Institute of Technology, CONNOR HART, MATTHEW J TURNER, Physics, Harvard University, PATRICK JAN SCHEIDEGGER, ETH Zurich, ERIK BAUCH, Physics, Harvard University, RONALD L WALSWORTH, Harvard-Smithsonian CfA — Real-time wide-field imaging of dynamic magnetic fields finds broad applications from condensed matter physics to neuroscience. We present a broadband, high-sensitivity magnetic imaging system designed to map magnetic fields from arrays of firing neurons. The imager employs pulsed Ramsey protocols on an ensemble of nitrogen-vacancy (NV) centers in diamond, and it achieves enhanced sensitivity, bandwidth, and uniformity compared to conventional continuous-wave optically detected magnetic resonance (CW-ODMR) imaging. We show further improvements through implementing double-quantum coherence imaging, which mitigates inhomogeneous crystal-lattice strain and microwave gradients over the field-of-view, and we demonstrate novel noise cancellation protocols. We present first images of nontrivial dynamic magnetic fields and steps toward real-time imaging of bio-magnetic fields from live, firing neurons.

11:39 AM F25.00003: Large-Scale Uniform Optical Focus Array Generation with a Phase Spatial Light Modulator

DONGGYU KIM (Presenter), Mechanical Engineering, MIT, ALEXANDER KEESLING, AHMED OMRAN, HARRY LEVINE, HANNES BERNIEN, MIKHAIL LUKIN, Physics, Harvard University, DIRK R. ENGLUND, Electrical Engineering and Computer Science, MIT — Uniform optical focus arrays are needed in a range of applications including multifocus multiphoton microscopy and multi-beam laser machining. Recently, such focus arrays were also developed as an essential tool for controlling ultra-cold atoms for quantum information processing. A challenge in these applications is to efficiently produce uniform large-scale optical focus arrays (LOFAs). Here, we present a new method for generating uniform LOFAs using a phase spatial light modulator. By identifying and removing undesired phase rotation in the iterative Fourier-transform algorithm, we demonstrate rapid and reliable generation of LOFAs containing O(10^3) optical foci with > 98% intensity uniformity.

11:51 AM F25.00004: Continuous frequency-domain multiplexing of heralded single-photon sources

THOMAS PARKER (Presenter), Physics, Imperial College London, THOMAS HIEMSTRA, PETER HUMPHREYS, ANDREAS ECKSTEIN, Physics, University of Oxford, BRIAN SMITH, University of Oregon, STEVE KOLTHAMMER, Physics, Imperial College London, IAN WALMSLEY, Physics, University of Oxford, MICHAL KARPINSKI, University of Warsaw, MARK BECK, Reed College, JOHANNES TIEDAU, Paderborn — Single-photon sources are an important tool for experiments in quantum optics and quantum information [1]. Heralded single-photon sources based on non-linear processes such as parametric down-conversion are ubiquitous. However, significant limitations arise due to the probabilistic nature of photon pair emission, as well as the possibility of generating more than one photon per pump pulse. In a technique known as multiplexing [2-3], the probability of generating a single photon can be increased by switching the output from multiple sources into a single channel.

We present a frequency-multiplexed single-photon source which increases the single-photon delivery probability without increasing multi-photon noise. This is accomplished by spectral detection and controlled frequency translation that both have a resolution greater than the single-photon bandwidth. In addition, we have measured the purity of the heralded photon by Hong-Ou-Mandel (HOM) interference showing a non-classical visibility of ~64%.


*EPSRC
Cooperative ultrastrong atom-light coupling from an effective mapping picture of single-photon superradiance. YAO ZHOU (Presenter), ZIHAO CHEN, JUNG-TSUNG SHEN, Electrical and System Engineering, Washington University in St Louis — As a manifestation of cooperative atom-light interaction from a cluster of atoms, single-photon superradiance has attracted considerable attention for its salient feature of a fast collective spontaneous emission rate and an enhanced coupling strength. It is found that when a cluster of atoms in a dense atom cloud or spatially distributed QED system obtains a largest collective spontaneous emission rate, which is the superadiant emission rate, their optical response is always indistinguishable with a single effective atom. From such effective mapping picture, one can obtain the superradiance conditions for a QED system. Specifically, we have analytically calculated the superradiance conditions for atoms trapped along a waveguide and for atoms coupled to whispering gallery mode resonators and computationally validated them. Based on strong coupling regime, an ultrastrong coupling strength proportional to atom number is accessible by exploiting the superradiance condition, and meanwhile the coherence between atoms remains without distorting the profile of optical response from a single atom. The ultrastrong coupling strength would benefit in the design of ultrafast optical devices, atomic mirror, and controllable optic add/drop filter.

X² Optical Frequency Comb by Cavity Phase Matching* NI XIN, ZHENDA XIE (Presenter), National Laboratory of Solid State Microstructures, School of Electronic Science and Engineering, School of Physics, and College of Engineering and Applied Sciences, Nanjing, SHUWEI HUANG, Department of Electrical, Computer, and Energy Engineering, University of Colorado Boulder, BAICHENG YAO, Key Laboratory of Optical Fiber Sensing and Communications (Education Ministry of China), University of Electronic Science and Technology of China, HUAYING LIU, NICOLÒ SERNICOLA, XINJIE LV, GANG ZHAO, ZHENLIN WANG, SHINING ZHU, National Laboratory of Solid State Microstructures, School of Electronic Science and Engineering, School of Physics, and College of Engineering and Applied Sciences, Nanjing — Micro-resonator-based optical frequency combs (OFC) are portable frequency standards with high beat note frequencies, which can be used for high precision spectroscopy, navigation, telecommunication and astronomy. Compared to the conventional micro-ring resonators, the resonators can benefit from much stronger nonlinearity for the comb generation from optical parametric down conversion processes, with new physics in these platforms. Here we report the optical frequency comb generation by cavity phase matching, where the large phase matching bandwidth enables broad comb span over 80 nm. The sheet cavity design allows high slope efficiency and peak output power, which exceed 22.6 % and 14.9 kW. Comb lines are measured to be equidistant within the instrument-limited accuracy. Therefore, we show that the sheet parametric oscillator is a promising candidate for portable integrated optical frequency comb generation.

Terahertz-optical intensity grating for creating high-charge, attosecond electron bunches JEREMY LIM (Presenter), Science and Maths cluster, Singapore University of Technology and Design, YIDONG CHONG, Nanyang Technological University, LIANG JIE WONG, Singapore Institute of Manufacturing Technology — Ultrashort electron bunches are useful for applications like ultrafast imaging, coherent radiation production, and compact sources of accelerated electrons. Currently, however, the shortest achievable bunches, at attosecond time scales, have only been realized in the single or very few electron regime, limited by Coulomb repulsion and electron energy spread. We will present ab initio simulation results and theoretical analysis which show that highly-charged bunches are achievable by subjecting moderately-relativistic (few MeV-scale) electrons to a superposition of terahertz and optical pulses. Using realistic electron bunches and laser pulse parameters which are within the reach of current compact setups, we provide two detailed examples: one with final bunches of ~1 fC contained within sub-400 as durations and 8 micron radii, and one with bunches of > 25 electrons contained within 20 as durations and 15 micron radii. Our results reveal a route to achieve such extreme combinations of high charge and attosecond pulse durations with existing technology.
12:39PM F25.00008: Investigating the nonlinear refraction index of Rb vapor by scanning the laser frequency through the atomic resonances.*
CLAUDIA PATRICIA MEJIA VILLAGRÁN (Presenter), Universidad Nacional de Colombia, ALEXANDRE ANDRADE CAVALCANTI DE ALMEIDA, SANDRA SAMPAIO VIANNA, Universidade Federal de Pernambuco (UFPE) —
We have observed self-focusing and defocusing in rubidium vapor by scanning the laser frequency through atomic resonances. These phenomena originate from the third order electric susceptibility, and have been used to measure the nonlinear refractive index of materials with the well-known technique Z-scan. However, few experimental measurements have been carried out near the resonances of atomic systems. In our experiment we scan the frequency of a diode laser through the resonances of rubidium vapor, contained in a fixed cell. The transmittance of the beam as a function of frequency detuning is detected after a small aperture, for different laser intensities and aperture radius. The theoretical model is a two-level system considering velocity distribution. A reasonably good fit of the experimental data is obtained, indicating that it is possible to measure the intensity-dependent term of the refractive index with this technique.
*Work supported by CNPq, FACEPE and CAPES (Brazilian Agencies).

12:51PM F25.00009: Revisiting the Photon-Drag Effect in Gold Films
JARED H STRAIT (Presenter), GLENN HOLLAND, WENQI ZHU, CHENG ZHANG, AMIT AGRAWAL, Physical Measurement Laboratory, National Institute of Standards and Technology, DOMENICO PACIFICI, School of Engineering and Department of Physics, Brown University, HENRI J LEZEC, Physical Measurement Laboratory, National Institute of Standards and Technology —
The photon-drag effect, the rectified current in a medium induced by conservation of momentum of absorbed or redirected light, is a unique probe of the detailed mechanisms underlying radiation pressure. We revisit this effect in gold, a canonical Drude metal for infrared frequencies. We discover that the signal for p-polarized illumination in ambient air is affected in both sign and magnitude by adsorbed molecules, opening previous measurements for reinterpretation. Further, we show that the intrinsic sign of the photon-drag effect is contrary to the prevailing intuitive model of direct momentum transfer to free electrons.

1:03PM F25.00010: Optical Forces between Coupled PT-symmetric Waveguides
MOHAMMAD-ALI MIRI (Presenter), Queens College, MICHELE COTRUFO, ANDREA ALU, Advanced Science Research Center, CUNY —
Evanescent wave coupling between two dielectric waveguides results in an optical force between the waveguides. This force is attractive (repulsive) when the coupled waveguide system is excited with the symmetric (anti-symmetric) mode and is transverse to the axis of wave propagation. Through energy conservation considerations, it is shown that the optical bonding force is proportional to the gradient of the propagation index of the symmetric and anti-symmetric supermodes with respect to the distance between the two guides. However, when gain or loss is involved in the waveguides, this derivative becomes undefined at an exceptional point singularity. In order to investigate forces at the exceptional point singularities, here we consider a PT-symmetric model of two coupled waveguides and calculate the force through Maxwell's stress tensor. Our results show that the optical bonding force is finite at the exceptional point. In addition, we find an extra force component which is directed along the axis of propagation.

1:15PM F25.00011: Floquet dynamics of classical and quantum cavity fields*
IVAR MARTIN (Presenter), Argonne National Laboratory —
We show that the time-dependence of electromagnetic field in a parametrically modulated cavity can be effectively analyzed using a Floquet map. The map relates the field states separated by one period of the drive; iterative application of the map allows to determine field configuration after arbitrary number of drive periods. For resonant and near-resonant drives, the map has stable and unstable fixed points, which are the loci of infinite energy concentration in the long time limit. The Floquet map method can be applied both to classical and quantum massless field problems, including the dynamical Casimir effect. The stroboscopic time evolution implemented by the map can be interpreted in terms of the wave propagation in a curved space, with the fixed points of the map corresponding to the black hole and white hole horizons. More practically, the map can be used to design protocols for signal compression/decompression, cavity cooling, and photon sensing.
*Work at Argonne National Laboratory was supported by the Department of Energy, Office of Science, Materials Science and Engineering Division.
1:27PM F25.00012: Reducing detrimental electrostatic effects in precision Casimir force measurements using argon ion bombardment and UV light  MINGYUE LIU (Presenter), JUN XU, ROBERT SCHAFTER, Department of Physics and Astronomy, University of California, Riverside, VLADIMIR MIKHAILOVICH MOSTEPANENKO, GALINA LEONIDOVNA KLIMCHITSKAYA, Institute of Physics, Nanotechnology and Telecommunications, Peter the Great Saint Petersburg Polytechnic University, UMAR MOHIDEEN, Department of Physics and Astronomy, University of California, Riverside — In precision Casimir force measurements between two neutral and grounded surfaces, the role and effect of electrostatic forces have to be fully understood in vacuum. The two Au coated surfaces can be contaminated with adsorbates leading to potential electrostatic patches. We have used 500 eV Ar ion bombardment of the surfaces and UV cleaning to remove the adsorbates prior to Casimir force measurements. The measurements were performed by means of dynamic atomic force microscopy operated in frequency shift mode. The force was measured between an Au coated hollow glass sphere attached to a Si cantilever and an Au coated silicon plate. To improve the sensitivity of the cantilever by reducing its spring constant, it was etched using concentrated KOH solution prior to attachment of the sphere. The residual potential difference between the Au sphere and the plate was reduced using Ar ion bombardment and UV light and checked to be independent of the sphere-plate separation. The measured Casimir force has been compared to theoretical prediction of the Lifshitz theory. For the distance ranges measured the experimental data are consistent with the electric permittivity of Au using the lossless plasma model behavior at zero frequency and tabulated optical data at all other frequencies.

1:39PM F25.00013: Casimir Force Measurement in the Cylinder-Plate Geometry  ROBERT SCHAFTER (Presenter), MINGYUE LIU, JUN XU, ROYA ZANDI, UMAR MOHIDEEN, University of California, Riverside — The Casimir effect has broad implications for the creation and operation of MEMS devices operating in the submicron regime. Experimental studies of the Casimir effect with smooth boundaries have primarily involved simple geometries such as the sphere-plate configuration. As Casimir forces are strongly dependent on the boundary shape, more complicated geometries will introduce modifications in the collective charge fluctuation anisotropy induced by the scattering of the zero point photons. In this work, we examine the Casimir forces between a cylinder and a sphere in a UHV environment, particularly examining the boundary effects of the 1-D role of the cylinders. To reduce the ellipticity of the cylinders involved, we have used an etched glass optical fiber, coated with Au to provide a conductive surface. Co-location of the sphere and cylinder was achieved using a piezoelectric stage with a capacitive sensor controlled PID loop. To eliminate residual electrostatic effects from surface adsorbates and resulting patches, we utilize in situ Ar ion bombardment and UV cleaning in the high vacuum environment prior to the measurement of the Casimir force. We compare the experimental results to theories using both the Proximity Force Approximation and the multiple scattering approach.

1:51PM F25.00014: Quantum sensing of large nuclear-spin clusters in diamond with atomic-scale resolution  MOHAMED ABOBEIH (Presenter), JOE RANDALL, CONOR BRADLEY, HANS BARTLING, MICHEL BAKKER, MAARTEN DEGEN, VIATCHESLAV DOBROVITSKI, TIM HUGO TAMINIAU, QuTech and Kavli Institute of Nanoscience Delft — The ability to resolve the 3D structure of large clusters of nuclear spins has the potential to be a revolutionary tool for NMR imaging of single molecules and solids. The nitrogen-vacancy (NV) center in diamond is a promising platform to achieve this goal. At the same time, its local nuclear spin environment already provides a model system to study, develop and test such new methods. Here we report on quantum sensing and atomic structure analysis of a 10+ nuclear-spin cluster in diamond with atomic-scale resolution. We develop pulse sequences to coherently control the nuclear spins forming the cluster, and directly measure the pairwise dipolar couplings between the nuclear spins with high precision. We then utilize the measured nuclear-nuclear couplings between the spins to determine their 3D structure with atomic-scale resolution. The methods developed in this work can be extended to samples outside the diamond, and mark an important step towards the ultimate goal of structural imaging of single molecules and proteins.


Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F27 DQI: Programming and Compilation -- the Quantum Computing Stack BCEC 160C

- Peter Groszkowski, University of Chicago - Tag(s): Focus

11:15AM F27.00001: The quantum computing stack: From quantum algorithms to optimized resource estimates  [Invited] THOMAS HAENER (Presenter), DAMIAN STEIGER, MATTHIAS TROYER, ETH Zurich — It is known that quantum computers offer up to exponential speedups over their classical counterparts for solving certain computational tasks. However, concrete comparisons of resource requirements for specific problem instances are still scarce. In this talk, I will discuss how software for quantum computing can support researchers in carrying out such analyses. Specifically, I will focus on automatic compiler optimizations and how these may offer great benefits even in the presence of hand-optimized libraries.
11:51AM F27.00002: Automatic Compilation for Portable and Scalable Quantum Software  ROBERT S SMITH (Presenter), ERIC C PETERSON, Rigetti Computing — Noisy intermediate-scale quantum (NISQ) processors are becoming larger (20–150 qubits) and more expressive (e.g., supporting a plurality of two-qubit interactions). However, since NISQ processors are error-prone, there is a great disparity between those programs which are desirable to write and those which execute reliably. Together, these aspects make it difficult to write quantum programs which are both portable (i.e., readily executable on different devices) and efficient (i.e., produce more accurate results using fewer resources). We discuss how automatic compilation helps achieve these simultaneous goals more consistently, and compare results of an open-source, extensible automatic compiler quilc to semi-manual counterparts.

12:03PM F27.00003: Compiler tools for hybrid quantum-classical algorithms  NIKOLAS TEZAK (Presenter), LAUREN CAPELLUTO, PETER KARALEKAS, ERIC C PETERSON, ROBERT S SMITH, MARK SUSKA, ADAM MOCARSKI, STEPHAN BROWN, CELENA TANGUY, RODNEY SINCLAIR, NIMA TAIE-NOBARIE, CHLOE SONG, STEFAN TURKOWSKI, MICHAEL RUST, GLENN JONES, SCHUYLER FRIED, DIEGO SCARABELLI, DEANNA ABRAMS, SHANE CALDWELL, COLM RYAN, PRASAHNT SIVARAJAH, WILLIAM J ZENG, BLAKE JOHNSON, CHAD RIGETTI, Rigetti Computing — We describe the Rigetti compilation toolchain and in particular how it supports optimized implementations of certain hybrid quantum-classical algorithms. Programs written in Quil are transpiled into a restricted subset of Quil instructions that are realizable on the available control hardware and target chip topology. These transpiled programs are further compiled into binary executables for custom FPGA pulse sequencers. The toolchain provides two key features that enable high performance hybrid computing: (1) gate parameters from the original input Quil program are translated to sequencer instructions that load from classical memory shared between the sequencer and classical host computer; (2) compiled programs can contain arbitrary control flow that branches off of single-qubit measurement results. The first feature enables the compilation of Quil into binaries that can be updated at run-time and the second, enables active reset of qubit states. Together these allow for rapid iteration in applications such as the optimization of a variational quantum algorithm, because these binaries can be re-executed many times for different input parameters without need for re-compiling or waiting for qubits to relax. We provide quantitative benchmarks of the improved wall-clock performance.

12:15PM F27.00004: Quantum Circuit Compilation to NISQ processors*  ELEANOR RIEFFEL (Presenter), DAVIDE VENTURELLI, NASA Ames Research Center — We describe automated reasoning approaches for QCC-NISQ, quantum circuit compilation to NISQ (noisy intermediate-scale quantum) processor architectures. We tested the approaches for different NISQ processor architectures and QAOA (quantum alternating operator ansatz) circuits. This approach is integrated into our software suite for automated, architecture aware, compilation for emerging gate-model quantum computers. We give an overview of the key components of this suite: a circuit synthesizer, a QCC-NISQ solver, and a visualizer.

*The authors would like to acknowledge support from the NASA Advanced Exploration Systems program, NASA Academic Mission Services (NNA16BD14C) and the NASA Ames Research Center.

12:27PM F27.00005: Less than a million CNOTs should be enough to solve a classically intractable instance of a scientific problem with a quantum circuit* [Invited]  DMITRI MASLOV (Presenter), IBM — The question I will try to answer in this talk is the following: what is the size of the smallest quantum computation capable of solving an instance of a scientifically interesting problem that is intractable for a classical computer? The problem I consider is Hamiltonian dynamics simulation, in the sense of the ability to sample probability distribution given by a state evolved under the target Hamiltonian for a specified time t and accurate to within a specified error epsilon. The core of the talk concerns the development and application of a range of algorithm design, circuit optimization, and hardware/software co-design techniques, the combination of which leads to the reduction in the quantum resource counts provided by pure algorithmic formulations by several orders of magnitude. Specifically, the best physical-level quantum circuit features under 650,000 CNOT gates, and the best fault-tolerant circuit features under 6.8x10^6 T gates. This illustrates that algorithmic and software-level optimizations will be indispensable for practical quantum computing.

*This material was based on work supported by the National Science Foundation, while DM working at the Foundation. Any opinion, finding, and conclusions or recommendations expressed in this material are those of the author and do not necessarily reflect the views of the National Science Foundation.
Overview and Comparison of Gate Level Quantum Software Platforms

RYAN LAROSE (Presenter), Michigan State University — Quantum computers are available to use over the cloud, but the recent explosion of quantum software platforms can be overwhelming for those deciding on which to use. In this paper, we provide a current picture of the rapidly evolving quantum computing landscape by comparing four software platforms—Forest (pyQuil), QISKit, ProjectQ, and the Quantum Developer Kit—that enable researchers to use real and simulated quantum devices. Our analysis covers requirements and installation, language syntax through example programs, library support, and quantum simulator capabilities for each platform. For platforms that have quantum computer support, we compare hardware, quantum assembly languages, and quantum compilers. We conclude by covering features of each and briefly mentioning other quantum computing software packages.

*Ryan LaRose acknowledges support from an Engineering Distinguished Fellowship through Michigan State University.

A case study for quantum software development: Linear systems solver

JAN GUKELBERGER (Presenter), MARTIN ROETTELER, MATTHIAS TROYER, Microsoft — As the power of quantum computing hardware is growing, software implementations and tools for accurate resource estimation that goes beyond simple asymptotic scaling become crucial for judging the feasibility of an application. Solving linear systems of equations is one of the prime applications for which quantum algorithms with an exponential advantage over the best known classical algorithms have been developed. In this talk, we report on the implementation of state-of-the-art quantum algorithms solving partial differential equations within the Microsoft Quantum Development Kit, which provides robust simulation, debugging, and resource estimation facilities. A key point in this work has been the handling of arithmetic functions: Gate synthesis facilitates accurate resource counts and is a requisite for deployment to quantum hardware, whereas emulation by the classical simulator allows for software testing on larger systems. To this end, we have equipped the Microsoft Quantum Development Kit with a generic and efficient emulation capability for quantum oracles defined by classical functions.

Two-step approach to scheduling quantum circuits

GIAN GIACOMO GUERRESCHI (Presenter), JONGSOO PARK, Intel Labs — As the effort to scale up existing quantum hardware proceeds, it becomes necessary to schedule quantum gates in a way that minimizes the number of operations. There are three constraints that have to be satisfied: the logical dependency of the quantum gates in the algorithm, the fact that any qubit may be involved in at most one gate at a time, and the restriction that two-qubit gates are implementable only between connected qubits. The last aspect implies that the compilation depends not only on the algorithm, but also on hardware properties like connectivity. Here we present a two-step approach in which logical gates are initially scheduled neglecting connectivity considerations and routing operations are added at a later step in ways that minimize their overhead. We rephrase the subtasks of gate scheduling in terms of graph problems like edge-coloring and maximum subgraph isomorphism. While this approach is general, we specialize to a one-dimensional array of qubits to propose a routing scheme that is minimal in the number of exchange operations. As a practical application, we schedule the quantum approximate optimization algorithm in a linear geometry and quantify the reduction in the number of gates and circuit depth that results from different scheduling strategies.

Real-time randomized compilation of quantum algorithms

GUILHEM RIBEILL (Presenter), MATTHEW WARE, BRIAN DONOVAN, LUKE GOVIA, BBN Technologies — Recent experiments have indicated the effectiveness of Pauli Frame Randomization (PFR) as a noise shaping technique. Not only does PFR tailor general noise into Pauli-stochastic noise, it also decouples qubits from their noise environment increasing system Markovianity. Presently, the randomization process requires extensive pre-compilation of pulse sequences. Here, we demonstrate an in hardware implementation of PFR on the BBN Arbitrary Pulse Sequencer II that generates randomized sequences in real-time. We first implement randomized benchmarking without pre-computing pulse sequences before using this capability to randomize a Gate Set Tomography experiment on a superconducting quantum processor.

*This material is based upon work supported by the U.S. Army Research Office under Contract No: W911NF-14-C-0048. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the U.S. Army Research Office.
1:51PM F27.00010: SKQuant-Opt: Optimizers for Noisy Intermediate-Scale Quantum Devices*  WIM LAVRIJSEN (Presenter), Computational Research Division, Lawrence Berkeley National Laboratory, ANA TUDOR, Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, JEFFREY LARSON, Mathematics and Computer Science Division, Argonne National Laboratory, KEVIN J. SUNG, Google Inc., LUCY LINDER, Institute of Complex Systems, Haute Ecole de Fribourg, JULIANE MUELLER, Computational Research Division, Lawrence Berkeley National Laboratory, JARROD R. MCCLEAN, RYAN BABBUSH, Google Inc., MIROSLAV URBANEK, COSTIN IANCU, WIBE A DE JONG, Computational Research Division, Lawrence Berkeley National Laboratory — Classical optimizers play an important role in quantum computing, e.g., in the hybrid Variational Quantum Eigensolver (VQE) and Quantum Approximate Optimization algorithms. They are used in hyperparameter tuning, calibration, machine learning, etc. Unfortunately, most of the easily accessible optimizers do not handle noise well, leaving them below threshold for use with Noisy Intermediate-Scale Quantum (NISQ) devices. We present skquant-opt, part of scikit-quant.org, a set of optimizers tuned for the needs of NISQ. We have taken the state-of-the-art optimizers and tested them on a range of VQE applications and on hyperparameter tuning for optimization on D-Wave. Mesh methods, including hybrids that add local models, yield the best results. We present these results as well as guidance on use. Collected in skquant-opt, we provide the best optimizers in Python, the most used language in quantum computing, through the standard channels. The interfaces are made consistent with default parameters attuned to quantum computing problems, allowing for easy application and fast evaluation.

*This work was supported by the Office of Advanced Scientific Computing Research, Quantum Algorithms Team Program, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F28 DQI: Quantum Computing with Open Quantum Systems BCEC 161 - Camille Lombard Latune, University of KwaZulu-Natal

11:15AM F28.00001: Dynamics of Quantum Photocells Driven by Periodic or Stochastic Photon Pulses  SANGCHUL OH (Presenter), Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University — We investigate the dynamics of a quantum photocell as a quantum heat engine, driven by external photon pulses. The photocell is assumed to be only in thermal contact with a cold reservoir, and the stream of work sources from a work or hot reservoir is represented by repeated photon pulses. The interaction between photon pulses and the photocell is described by the pumping term in a Lindblad master equation. By solving the Lindblad master equation, we study numerically the dynamics of a photocell driven by periodic, random, and Poisson photon pulses. We find that the fluctuations in power output of the photocell change dramatically, depending on the statistics of photon pulses and the parameters of the photocell. At low power output, the level occupation probabilities change somewhat smoothly over a long-period of time, even if the photocell is driven by random photon pulses. We analyze how the fluctuation in photon pulses affects the fluctuation in power output for various photon pulses and the parameters of the photocell.

11:27AM F28.00002: Coherent fluctuation relations: from the abstract to the concrete*  ZOE HOLMES (Presenter), Imperial College London, SEBASTIAN WEIDT, University of Sussex, DAVID JENNINGS, University of Leeds, JANET ANDERS, University of Exeter, FLORIAN MINTERT, Imperial College London — Recent studies using the quantum information theoretic approach to thermodynamics show that the presence of coherence in quantum systems generates corrections to classical fluctuation theorems. To explicate the physical origins and implications of such corrections, we here convert an abstract framework of an autonomous quantum Crooks relation into quantum Crooks equalities for well-known coherent, squeezed and cat states. We further provide a proposal for a concrete experimental scenario to test these equalities. Our scheme consists of the autonomous evolution of a trapped ion and uses a position dependent AC Stark shift.

*We acknowledge support from the Engineering and Physical Sciences Research Council, the U.K. Quantum Technology hub for Networked Quantum Information Technologies and the Royal Society.
KUN ZHANG (Presenter), JIN WANG, Stony Brook University — We study the macroscopic realism through Leggett-Garg inequality (LGI) for a two-qubit quantum system coupled with two environments characterized by either the bosonic (thermal and photonic) baths or fermionic (electronic) baths with different temperatures or chemical potentials respectively. Analytical form of LGI and the maximal values of LGI based on the quantum master equation beyond secular approximation are derived. We found that the nonequilibriumness quantified by the temperature difference or chemical potential difference can lead to the LGI violation or the increase of the maximal value of LGI, restoring the quantum nature from certain equilibrium cases where LGI is preserved giving classical realism. Our results shed light on the nature of the macroscopic realism and the relationship between the nonequilibriumness and quantum temporal correlation. Our finding of nonequilibrium promoted LGI violation suggests a new strategy for the design of quantum information processing and quantum computational devices to maintain the quantum nature and quantum correlations for long.

11:51AM F28.00004: Discord vs Distortion: Classical vs Quantum*  BARRY C SANDERS (Presenter), National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, WEI-WEI ZHANG, Physics, University of Sydney, YUVAL R SANDERS, Physics and Astronomy, Macquarie University, NIGUM ARSHED, National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China — Quantum discord is a popular quantum-resource measure but a nonzero value does not necessarily imply quantumness; nonzero classical discord arises if local measurements disturb the stochastic information state [V. Gheorghiu, M. C. de Oliveira and B. C. Sanders, Phys. Rev. Lett. 115, 030403 (2015)]. The classical interpretation of discord breaks down if and only if entanglement of formation for the informational state is nonzero, thereby creating a tight link between entanglement and genuine quantum discord. Here we present mathematical relations, and specifically monotonicity between discord and channel-distortion measures such as mean-squared distortion and Kullback-Leibler divergence. Whereas the previous result showed discord can be nonzero for stochastic information, our new results demonstrate a tight link between classical discord and other information-theoretic measures of noisy channels.

*Australian Research Council via the Centre of Excellence in Engineered Quantum Systems (EQuS) project number CE110001013; National Science Foundation of China Grant 11675164; CAS PIFI program (Grant No. 2016PT003; Natural Sciences and Engineering Research Council; Alberta Innovates.

12:03PM F28.00005: Information-theoretic aspects of the generalized amplitude damping channel  SUMEET KHATRI (Presenter), KUNAL SHARMA, MARK M WILDE, Louisiana State University — In this work, we provide an information-theoretic characterization and analysis of the generalized amplitude damping channel (GADC), which is the qubit analogue of the bosonic thermal loss channel. This channel can be used to model the dissipation in a qubit system in the presence of an environment at a finite temperature, and it arises in the study of spin chains. The purpose of our work is to provide bounds on the fundamental limits of the GADC for communicating classical, quantum, and private information. Using the notion of approximate degradability, we provide upper bounds on the quantum and private capacities of this channel. We also provide upper bounds based on data processing inequalities by exploiting the mathematical decomposition of the GADC into channels for which the quantum capacity is known exactly. Using a similar decomposition technique, we are able to provide upper and lower bounds on the classical capacity of the GADC.

12:15PM F28.00006: Superadditivity and boosting coherent information using useless channels  VIKESH SIDDHU (Presenter), Carnegie Mellon University — Superadditivity of the coherent information makes it hard to understand and compute the quantum capacity of a quantum channel, a central quantity in quantum information.

Recently, by using a qubit channel in parallel with itself, Leditzky, Leung and Smith [Phys. Rev. Lett. 121, 160501 (2018)] produced simple examples of superadditivity. We extend their results to a larger class of channels with qubit inputs and some channels with qutrit inputs. Some of these exhibit superadditivity in the sense that the coherent information of a channel is boosted when placed in parallel with a zero capacity channel, in particular a symmetric amplitude damping channel. Our superadditivity examples include limits of simple pcubed qubit and qutrit channels [Phys. Rev. A 94, 052331 (2016)].
Consequences of measurement back-action from quantum monitoring: non-standard speed limits and spontaneous symmetry breaking

LUIS PEDRO GARCIA-PINTOS (Presenter), university of massachusetts boston, DIEGO TIELAS, Universidad de la Plata, ADOLFO DEL CAMPO, university of massachusetts boston — The information acquired during the monitoring of a quantum system provides a state description that can differ greatly from the description given by agents ignorant of the outcomes. While the lack of information in the later results in a mixed density matrix following open system dynamics, the measurement back-action in the former case provides a more accurate description. We present consequences of such measurement back-action to two problems in quantum theory: the limits to the speed of evolution, and the process of spontaneous symmetry breaking.

For the problem of the speed of evolution, we show that there are trajectories for which standard quantum speed limits are violated, and determine the dispersion of the speed of evolution in an ensemble of realizations of continuous measurement records. Regarding the problem of spontaneous symmetry breaking, which is typically understood as a consequence of random fluctuations either in the Hamiltonian governing the evolution or in the state of the system, we present a novel alternative mechanism, induced by the measurement back-action. We show that, depending on the nature of the quantum monitoring, an observer can alter the topology and the pattern of symmetry breaking.

*John Templeton Foundation, UMass Boston, CONICET Argentina.

Characterizing Initial Correlations via Spectroscopy

PARTH JATAKIA (Presenter), SAI VINJANAMPATHY, KASTURI SAHA, Physics, Indian Institute of Technology Bombay — In the presence of initial correlations, quantum evolution cannot be described in terms of completely positive trace preserving maps. Such initial correlations can arise due to strong coupling between the system and environment and inform the applicability of important results in physics, such as the quantum regression formula. Therefore it is vital to characterize these correlations for a better understanding of the system and proper quantum control.

Taking inspiration from correlated spectroscopy, we demonstrate a method to determine the correlation between the system and the environment. Our spectroscopic method extracts information about the initial correlations from the system by benefiting from the system - environment interactions. We apply this formalism to Nitrogen-Vacancy centers in diamonds interacting with photonic modes of a cavity.

*IIT-SEED grant

Quantum Forking for Open Quantum Systems Simulation

JUNE-KOO(KEVIN) RHEE (Presenter), KAIST, ILYA SINAYSKIY, University of KwaZulu-Natal, DANIEL KYUNGDEOCK PARK, KAIST, FRANCESCO PETRUCCIONE, University of KwaZulu-Natal — Many quantum information processing tasks spend non-negligible computational costs for preparing an input quantum state. However, a quantum input state prepared for a specific algorithm cannot be reused for another task once measured by the postulate of the quantum measurement. Moreover, the quantum state cannot be cloned. Hence, in general, one is forced to repeat the state preparation routine per algorithm, even when individual algorithms receive the same input. Meanwhile, many quantum algorithms demand repetitions for sampling the answer. Thus while information processing tasks have the potential to benefit from laws of quantum mechanics, they also impose unavoidable redundancy. Here we introduce quantum information forking that allows an array of qubits to undergo independent processes in superposition to reduce the number of the state initialization procedure. As an example, we demonstrate the application of quantum forking to quantum Monte-Carlo sampling. In this case, quantum forking allows for the implementation of the independent propagation of the quantum trajectories, while maintaining the constant cost of initial state preparation.

*This work was supported in part by the Ministry of Science and ICT, Korea, under an ITRC Program, IITP-2018-2018-0-01402.
1:03PM F28.00010: Experimental Test of Decoherence Theory using Electron Matter Waves*  
PETER BEIERLE (Presenter), Physics, University of Cincinnati, LIYUN ZHANG, Physics, Xian Jiantong University, ZILIN CHEN, Physics, University Of Nebraska-Lincoln, HANS PETER WAGNER, Physics, University of Cincinnati, HERMAN BATELAAN, Physics, University Of Nebraska-Lincoln — A controlled decoherence environment is studied experimentally by free electron interaction as it travels over a [semi]conducting plates. The results are compared with physical models based on decoherence theory to investigate the quantum-classical transition. This first of its kind integrated approach may both further solidify previous claims that such matter-wave experiments are measuring the quantum-classical transition. 

Here we present these findings and progress towards monitoring the environment using space-time resolved optical methods [2], with the aim to study if we can also measure the loss of coherence of the environment induced by the free electron. This first of its kind integrated approach may both further solidify previous claims that such matter-wave experiments are measuring the quantum-classical transition. 


*We gratefully acknowledge support by the U.S. National Science Foundation under Grant No. 1602755.

1:15PM F28.00011: Using a Shot Noise Junction to Characterize a Josephson Travelling Wave Parametric Amplifier*  
JACOB EPSTEIN (Presenter), KYLE MCELROY, Johns Hopkins University Applied Physics Laboratory, LAFE SPIETZ, Spietz Applied Sciences, LLC, TIMOTHY M SWEENEY, Johns Hopkins University Applied Physics Laboratory, JOSE AUMENTADO, NIST Boulder, JOAN A HOFFMANN, Johns Hopkins University Applied Physics Laboratory — The Josephson Travelling Wave Parametric Amplifier (JTWPA) is a solution for a broad band amplifier with near quantum limited noise characteristics. Reported techniques using AC Stark shifts to characterize the noise of a JTWPA show excellent noise characteristics but are inherently narrow band. Using a shot noise tunnel junction (SNTJ) allows for broadband characterization of the noise temperature of the JTWPA. Techniques for optimizing the JTWPA for different measurement uses will also be discussed.

*The authors would like to acknowledge MIT Lincoln Laboratory for providing the JTWPA for this work.

1:27PM F28.00012: Stabilization of cavity Hilbert subspaces in cavity quantum electrodynamics by measurement-based quantum feedback*  
YVES BERUBE-LAUZIERE (Presenter), RÉMI AZOUIT, Electrical and Computer Engineering, Université de Sherbrooke — Measurement-based quantum feedback (MBQFB) for actively preparing and stabilizing Fock number states in a cavity quantum electrodynamics (CQED) set-up has been achieved by Haroche et al. The approach relies on injecting, after each weak dispersive measurement of the cavity state using Rydberg atoms flying through the cavity as sensors, a low average photon number classical coherent field to steer the cavity towards the targeted number state. Preparing and stabilizing a superposition of Fock states using MBQFB is more challenging since the superposition must be an eigenstate of the quantum measurement operators. This condition requires that each Fock state composing the superposition be an eigenstate with the same eigenvalue for each measurement operator. Owing to the special form of the measurement operators in the dispersive regime, this constrains the phase shift per photon to specific values and leads to the stabilization of subspaces. Results from realistic simulations taking into account decoherence and imperfections in a CQED set-up will be presented. These support the validity of the underlying theory that generalizes the previous theory for preparing Fock number states.

*Rémi Azouit acknowledges a Prized Postdoctoral Fellowship from Institut Quantique.

1:39PM F28.00013: Ground state cooling in the strong-coupling regime  
CHUNG KOW (Presenter), Physics and Applied Physics, University of Massachusetts Lowell, HAKAN TURECI, Electrical Engineering, Princeton University, ANJA METELMANN, Physics, Free University Berlin, ARCHANA KAMAL, Physics and Applied Physics, University of Massachusetts Lowell — Strong coupling between quantum systems, whereby the coupling strength greatly exceeds the decay rates, is a mainstay in quantum information platforms. Notably, this regime is explored in hybrid quantum systems involving entanglement between a microscopic and a macroscopic degree of freedom. Nonetheless, in certain instances it can be a liability; for instance, active cooling of a system to its ground state in the strong coupling regime leads to hybridization of the system and the bath modes. Here we present a novel approach using dissipation engineering that mitigates normal-mode splitting between the system and the bath, while preserving strong coupling between the two. Specifically, we employ an optomechanical setup where the mechanical mode is cooled without hybridizing with the optical bath. The connection of such dissipation-engineered cooling with the physics of exceptional points will also be discussed.
Engineered Dissipation as Your Side-kick: A Hybrid Scheme for Quantum Error Correction.

LASSE BJØRN KRISTENSEN (Presenter), Department of Physics and Astronomy, Aarhus University, MORTEN KJÆRGAARD, Research Laboratory of Electronics, Massachusetts Institute of Technology, CHRISTIAN KRAGLUND ANDERSEN, Department of Physics, ETH Zurich, NIKOLAJ T ZINNER, Department of Physics and Astronomy, Aarhus University — The main adversary when trying to harness the power of quantum computation is the ever-present occurrence of errors and decoherence. These effects constantly conspire to alter the state of the quantum bits of your quantum computer, thereby slowly corrupting the stored information and messing up the output of your beautiful quantum algorithms. Luckily, a plethora of quantum error correcting codes have been invented to help mitigate this problem. One interesting branch of this field is the study of autonomous error correction codes that attempt to fight fire with fire by engineering dynamics and dissipation of systems so that they become able to detect and correct errors on their own, without relying on an external experimenter doing costly measurement- and correction-steps. In this talk, we present a scheme that combine these ideas with traditional measurement-based error correction into a 6-qubit hybrid scheme capable of protecting qubits from photon-loss and dephasing errors, achieving 10-fold improvements in dephasing times and 5-fold improvements to relaxation times for realistic superconducting-qubit parameters and noise while employing only relatively simple local 2-qubit interactions.

Tuesday, March 5, 2019 11:15 AM - 1:51 PM

Session F29 DFD GSOFT GSNP: Flow of Complex Fluids, Polymers, and Particles BCEC 162A -
Marco G. Mazza, Max Planck Institute for Dynamics and Self-Organization

11:15AM F29.00001: Probing multiphase flows with x-ray near-field speckles*
JIN WANG (Presenter), QING ZHANG, YANG, QINGTENG ZHANG, MIAOQI CHU, Argonne National Laboratory — Multiphase flows of simple and complex fluids are of great fundamental and practical interests due to their multitude of applications. However, multiphase flows are also often difficult to study optically because of intense multiple light scattering from the phase boundaries in the flow, such as liquid/gas interfaces. X-rays are highly penetrable in a multiphase flow because of the weak interaction between x-rays and materials. X-ray near-field speckles can be generated readily when x-rays pass through the flow. The x-rays do not need to be completely coherent. A partial or local coherence is sufficient to produce significant intensity fluctuation in the transmitted beam that can used to probe both morphology and dynamics. Combined with ultrafast imaging, x-ray near-field speckles and their spatiotemporal correlations have been proven powerful to interrogate multiphase flows highly transient and far from equilibrium.

*This work and the use of Advanced Photon Source are supported by U.S. Department of Energy (DOE) Office of Science User Facility Division under Contract No. DE-AC02-06CH11357.

11:27AM F29.00002: Effects of passive hydrodynamics force on harmonic and chaotic oscillations in nonlinear chemical dynamics
JEAN BIO CHABI OROU (Presenter), Université d'Abomey-Calavi — This work studies the nonlinear dynamics and passive control of chemical oscillations governed by a forced modified Van der Pol–Duffing oscillator. We considered the dynamics of nonlinear chemical systems subjected to fluctuating hydrodynamic drag forces. The computation of fixed points of the nonlinear chemical system is made in detail by utilizing Cardan's method. The harmonic balance method is used to find the amplitudes of the oscillatory states. The Floquet theory and the Whittaker method are utilized to analyze and analytically determine the stability boundaries of oscillations. The influences of system parameters in general and in particular the effect of the parameter K and the constraint parameter ß which shows the difference between a nonlinear chemical dynamics order two differential equation and ordinary Van der Pol–Duffing equation are observed on the state of the second stability criterion. The effects of the control process on chaotic dynamics states are investigated through bifurcation structures, Lyapunov exponent, phase portraits and Poincaré section. The results obtained by the analytical methods are validated and complemented by the results of numerical simulations.
11:39AM F29.00003: HYDRODYNAMIC RESISTANCE DUE TO POLYMER-INDUCED ELASTIC TURBULENCE IN MICROFLUIDIC SERPENTINE FLOWS  SIDDHARTHA GUPTA (Presenter), RAJU NEELAMEGAM, SIVA A VANAPALLI, chemical engineering, texas tech university — It has been shown that viscoelastic curvilinear flows transition to turbulence in the limit of diminishing Reynolds numbers (Re → 0) with the onset determined by a critical Weissenberg number (Wic). Serpentine microfluidic geometries have been used to characterize such flows, however, the pressure drop-flow rate dynamics during elastic turbulence is still unexplored. To quantify the hydrodynamic resistance due to elastic turbulence, we map the pressure drop versus flow rate relationship due to elastic turbulence using the iCapillary technique. The instability was investigated for high molecular weight poly ethylene oxide in aqueous-glycerol solvents and a scaling relationship with a saturation plateau was observed for different solvent viscosities based on normalized solution driving pressure with respect to the solvent (ΔP/ΔP_{sol}) and plotting against the Weissenberg number. Additionally, Lagrangian representation of the flow was done with digital holography microscopy and CFD simulations were used to analyze deviations from simple shear thinning flows. Thus, we report the first known characterization of flow resistance due to elastic turbulence. The flow resistance relations may provide new insights for structural characterization of polymeric and biofluids.

11:51AM F29.00004: Heat Transfer Enhancement in Helically Micro-Coiled Tubes Using Nanoparticle-Viscoelastic Fluids by Elastic Turbulence  HAIE YANG (Presenter), Beihang University, GUICE YAO, Leeds University, HAICHUAN JIN, DONGSHENG WEN, Beihang University — In recent years, the application of micro-systems has received more and more attention. However, the microsystem scale is small, which greatly limits the flow Reynolds number. It’s difficult for the flow of Newtonian fluid to be turbulent flow at low Reynolds number, limiting the mixing and heat transfer in micro-systems. Nanoparticle-viscoelastic fluids (henceforth referred to as NPVE fluid) were utilized as the experimental group and water as the comparison group. Heat transfer performance of these two groups of fluids under different Reynolds numbers was tested, respectively. Heat transfer efficiency is approximately 35% stronger than water under the same conditions after using a viscoelastic suspension of nanoparticles.

12:03PM F29.00005: Turbulent Submerged Jets of Dilute Polymer Solutions  SAMI YAMANIDOUZISORKHABI (Presenter), GARETH MCKINLEY, IRMGARD BISCHOFBERGER, Massachusetts Institute of Technology — Dilute synthetic polymer solutions have been shown to reduce turbulent drag in pipelines and around marine vehicles. Water-soluble biopolymers such as flax seed mucilage extracts have the potential to serve as cheap and environmentally friendly alternatives to synthetic polymers. In this work, we employ Schlieren imaging to unveil the mixing dynamics and recirculating regions that develop in turbulent jets of dilute aqueous polymer solutions submerged in quiescent water. At the interface of the viscoelastic jet and water, a free shear boundary layer develops leading to momentum transfer between the two fluids. We demonstrate the impact of viscoelasticity on this momentum transfer and evaluate the performance of both synthetic polymers and biopolymers in damping turbulent vortical structures.

12:15PM F29.00006: Hydrodynamics around aggregating charged grains*  CHAMKOR SINGH (Presenter), MARCO G. MAZZA, Max Planck Institute for Dynamics and Self-Organization — The growth of protoplanetary dust from sub-millimeter sized particles to much larger scales is not well understood. There is considerable debate about the role of electrostatic charging of grains in the aggregation process. Additional complexity arises due to the presence of complex hydrodynamic flow that couples to the aggregating grains. We study this growth process using massively parallel molecular dynamics simulations for the granular particles in combination with the smoothed-particle hydrodynamics for the interstitial flow. The results from a detailed cluster analysis are presented. Finally we propose an effective kinetic model for the charged grain aggregation inside interstitial flow.

*Max-Planck Society

12:27PM F29.00007: Gravity-Driven Flow and Clogging in the Presence of an Obstacle*  ANNA BELLE HARADA (Presenter), KERSTIN NORDSTROM, Mount Holyoke College — We present experimental results of 2D gravity-driven flows of >10,000 monodisperse hard spheres (diameter = D) through an aperture (width = W). We introduce into the system a fixed obstacle of varying size (diameter = D_0) and distance above the aperture (L). We use a force sensor to measure the bulk flow rate, and high-speed, high-resolution video to track individual grains. We observe that obstacles tend to decrease the flow rate, but also decrease the clogging probability, and specifically measure the flow rate and clogging probability as a function of D_0 and L for different aperture widths. As our packing is crystalline, we can correlate these features with structural measurements in the material such as dislocations and the bond order parameter. We also present dynamical measurements such as nonaffine rearrangements and cooperative motion.

*Acknowledgement is made to the donors of The American Chemical Society Petroleum Research Fund (PRF# 56888-UNI9) for support of this research.
12:39PM F29.00008: Large-scale flow out of spatiotemporal chaos in electroconvection of cholesteric liquid crystal*
YOHSUKE FUKAI (Presenter), MASAKI SANO, Department of Physics, the University of Tokyo — Convection in a thin layer of liquid crystal driven by an electric field has long been studied as a model system to investigate pattern formation in out-of-equilibrium systems. In particular, it has been known that the flow typically shows spatiotemporal chaotic patterns called dynamic scattering mode with high voltage. In this presentation, we report our observation that this chaotic pattern organizes itself into a large-scale flow perpendicular to the electric field in the case where cholesteric liquid crystal with the negative dielectric constant difference is used. The typical scale of this flow pattern is more than 100 times larger than the distance between the electrodes, the characteristic length scale of the convection. We will discuss the effect of the anchoring and boundary conditions, and possible interpretation toward understanding the mechanism.

*This work is supported by Grant-in-Aid “KAKENHI” for JSPS Fellows (Grant No. 17J05559)

12:51PM F29.00009: Chemical and hydrodynamic instabilities produced by enzymatic surface reactions OLEG SHKLYAEV (Presenter), VICTOR V YASHIN, ANNA CHRISTINA BALAZS, Univ of Pittsburgh — Chemical oscillations are ubiquitous in nature and have a variety of promising applications. Here, we examine a linear stability of a multicomponent reactive fluid that contains two species, X and Y, which undergo transformations catalyzed by enzymes immobilized at two infinite horizontal plates confining the fluid. The surface reactions with the enzymes provide a negative feedback in the system. The first enzyme, localized on the first plate, promotes production of chemical X, while the second enzyme, immobilized on the second plate, promotes production of chemical Y, which inhibits the production of chemical X. Depending on the reaction rates and densities of the reactants, the monotonic and oscillatory instabilities could occur in the system. The first instability (similar to Rayleigh-Benard case) leads to roll-like convective structures that are periodically distributed along the layer. The second instability produces horizontally uniform temporal oscillations of concentrations of the chemicals X and Y. The findings provide guidance for designing micro-scale chemical reactors with improved functionalities.

1:03PM F29.00010: RMD2Kin: an automated, self-consistent, first-principles based approach to extract kinetic data from reactive molecular dynamics simulations* DANIIL ILYIN (Presenter), WILLIAM GODDARD, JULIUS OPPENHEIM, TAO CHENG, SERGEY ZYBIN, ROBERT NIENLEN, California Institute of Technology — Capturing intricate details of the chemistry of important technological processes such as combustion and chemical vapor deposition is a challenge in large-scale simulations. Conventionally, necessary kinetic data are obtained either empirically or from experiments in dilute conditions, and these data may not fully describe interactions that occur in realistic systems. We present here an automated, self-consistent, first-principles based approach to extract kinetic data and reaction mechanisms from reactive molecular dynamics simulations. This approach provides a detailed analytic description of the evolution of a complex chemical system from reactants through various intermediates to products, which can then be used to incorporate the correct reaction chemistry into computational fluid dynamics and/or continuum chemical dynamics simulations. This approach is self-consistent and does not require previous knowledge of the specific chemistry of the system. We refer to this approach as RMD2Kin.

*US Department of Energy Contract DE-AC07-05ID14517; Office of Naval Research Contract N00014-12-1-0538; National Science Foundation Grant ACI-1548562.

1:15PM F29.00011: Distribution of tracer particles around a catalytic Janus particle WILLIAM USPAL (Presenter), Department of Mechanical Engineering, University of Hawai'i at Manoa, JAIDEEP KATURI, Institute for Bioengineering of Catalonia (IBEC), The Barcelona Institute of Science and Technology (BIST), MIHAIL N. POPESCU, Theory of Inhomogeneous Condensed Matter, Max Planck Institute for Intelligent Systems, Stuttgart, SAMUEL SANCHEZ, Institute for Bioengineering of Catalonia (IBEC), The Barcelona Institute of Science and Technology (BIST) — Active Janus particles self-propel by catalyzing the decomposition of molecular “fuel” available in the surrounding solution. The resulting self-generated chemical gradients drive phoretic flow in an interfacial layer surrounding the particle, as well as chemi-osmotic interfacial flows along nearby container walls. Through experiments and theory, we consider the distribution of small tracer particles around a Janus particle in the vicinity of a planar wall. The Janus particle is either free to move or stuck to the wall, and its axis of symmetry is oriented in the plane of the wall. Experimentally, we observe that, under certain conditions, the catalytic cap of a particle is surrounded by a tracer-free exclusion zone. To understand this finding, we model the motion of tracer particles. In our model, the tracers are advected by fluid flows driven in the bulk solution by phoretic and/or chemi-osmotic interfacial flows. Additionally, the tracers can respond to chemical gradients through phoresis, providing a third contribution to tracer velocity. We find that these three ingredients can combine to create an exclusion zone. In particular, we highlight the essential role of chemi-osmotic flow, which is often neglected in modeling and interpretation of experiments.
Reducing Blood Viscosity and Suppressing Turbulence with Magnetic Field to Prevent Heart Attack and Stroke*

RONGJIA TAO (Presenter), Temple University — Heart attacks and strokes are the leading causes of death. High blood viscosity and turbulence in blood circulation are the keys to trigger these diseases, as they place much heavier workload on the heart, develop atherosclerotic plaque and may rapture blood vessels. Reducing blood viscosity and suppressing turbulence is thus the key to prevent cardiovascular diseases. Unfortunately, these two tasks conflict each other. Presently, the only method to reduce blood viscosity is to take medicine, but this method makes the turbulence worse because the Reynolds number goes up with viscosity reduction. Here we report our discovery with magnetorheology (MR): applying a strong magnetic field to blood along its flow direction, red blood cells are polarized and aggregated into short chains. The blood viscosity becomes anisotropic: it is significantly reduced along the flow direction, but is considerably increased in the directions perpendicular to the flow. The blood flow thus becomes laminar and turbulence is suppressed. Our lab and animal tests show that this technology can successfully prevent plaque development. The clinical trials further confirm that this MR technology can effectively cure hypertension and help people to prevent heart attack and stroke.

*American Heart Association.

Exploiting magnetocapillary interactions for swimming along liquid interfaces

NICOLAS VANDEWALLE (Presenter), GALIEN GROSJEAN, GRASP, Physics Dept, University of Liege, Belgium — When soft ferromagnetic particles are suspended at air-water interfaces in the presence of a vertical magnetic field, dipole-dipole repulsion competes with capillary attraction such that 2d structures self-assemble. The complex arrangements of such floating bodies are emphasized. The equilibrium distance between particles exhibits hysteresis when the applied magnetic field is modified. Irreversible processes are evidenced. By adding a horizontal and oscillating magnetic field, periodic deformations of the assembly are induced. We show herein that collective particle motions induce locomotion at low Reynolds number. The physical mechanisms and geometrical ingredients behind this cooperative locomotion are identified. These physical mechanisms can be exploited to much smaller scales, offering the possibility to create artificial and versatile microscopic swimmers. Moreover, we show that it is possible to generate complex structures that are able to capture particles, perform cargo transport, fluid mixing, etc...

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F30 DPOLY GSOFT DFD DBIO: Extreme Deformation II: Rate and Size Effects in Glasses, Networks, and Fibers

Deformation of Matrix-Free, Glassy Single Component Polymer NanoComposite at Extreme High Strain Rates

JINHO HYON (Presenter), EDWIN THOMAS, Rice University, JASON STREIT, RICHARD VAIA, Air Force Research Laboratory — Very thin, freestanding glassy polystyrene (PS) films show unexpectedly large energy absorption under rapid axisymmetric tensile loading at ballistic strain rates (~ 10^7/s). For supersonic microprojectile (3.7 μm diameter) impact (350~800 m/s), the more mobile and less entangled near-surface regions of the PS facilitate crazing and dramatically increase craze multiplication and subsequent growth with accompanying large adiabatic temperature rise of the highly deforming film. Here, we investigate the influence on the high rate deformation of grafting of the PS chains to nanoparticle (NP) surfaces. The covalent anchoring of several hundred polymer chains to individual silica NPs and the well-entangled coronal regions between NPs improve the stress transfer through the composite, yielding polymer nanocomposites with excellent energy absorption. The single component nanocomposite PS grafted nanoparticle (PSgNP) films (~ 1% v/v, 16nm diameter SiO2 NPs) show 25% enhanced high kinetic energy absorption per unit mass of the target film over the previous record specific energy absorption of the thin, freestanding homopolymer PS films.
EDWIN CHAN (Presenter), Materials Science and Engineering Division, National Institute of Standards and Technology, WANTING XIE, Department of Mechanical and Industrial Engineering, University of Massachusetts, CHRISTOPHER SOLES, Materials Science and Engineering Division, National Institute of Standards and Technology, JAE-HWANG LEE, Department of Mechanical and Industrial Engineering, University of Massachusetts — The fracture behavior of amorphous polymer glasses is strongly linked to the entanglement density. Traditionally, it is established that polymers exhibiting strain hardening, such as polycarbonate, tend to undergo ductile fracture rather than brittle fracture due to its high entanglement density. In this work, we use Laser-induced Projectile Impact Testing (LIPIT) to study the supersonic fracture behavior of polycarbonate films as a function of entanglement density. We show that the kinetic energy for microparticle penetration through the polymer film is affected by the molecular mass of the polymer or the plasticizer content. We show that this variation in the penetration energy to a change in the mechanism of fracture. Specifically, the fracture mechanism transitions from crazing to shear yielding due to changes in the entanglement density of polycarbonate film.

11:39AM F30.00003: Strain Rate Effects During Ultra-High Strain Rate Penetration of Polymeric Materials  
M. HUNTER BOWERING, Dave C Swalm School of Chemical Engineering, Mississippi State University, W. F. HEARD, U. S. Army ERDC, THOMAS E. LACY, JR, Department of Mechanical Engineering, Teaxs A&M University, CHARLES U. PITTMAN, JR., Department of Chemistry, Mississippi State University, SANTANU KUNDU (Presenter), Dave C Swalm School of Chemical Engineering, Mississippi State University — Energy dissipation during penetration of a material is an important consideration in designing lightweight armor to protect structures, equipment, and personnel from impact damage. A series of impact tests, with projectile velocities in the range 2-7 km/s, was performed on monolithic plates of ultra-high molecular weight polyethylene (UHMWPE), high density polyethylene (HDPE), and poly(methyl methacrylate) (PMMA). A relationship between back face debris cloud (BFDC) velocity and impact velocity was developed for each material. Damage zone sizes were compared, offering insights into the effects of molecular architecture on stress delocalization and energy dissipation during perforation. Monolithic plate thicknesses were varied in the UHMWPE and HDPE target populations to assess thickness effects on damage zone size and BFDC. Comparison of the apparent failure mechanisms and damage metrics, in conjunction with thermal analysis, were used to explain the relative performance of each material. PMMA demonstrated glass-like failure with finely particulated BFDCs, while perforation of HDPE resulted in fluid-like BFDCs. UHMWPE damage morphology possessed qualities of both PMMA and HDPE.

Permission to publish was granted by Director, Geotechnical & Structures Laboratory

11:51AM F30.00004: The Role of Fast Polymer Dynamics on the Mechanical Toughness of Polymeric Materials  
CHRISTOPHER SOLES (Presenter), KANAE ITO, ADAM B BURNS, Materials Science & Engineering Division, NIST, KEVIN A. MASSER, JOSEPH L. LENHART, Weapons and Materials Research Directorate, US Army Research Laboratory, MADHU SUDAN TYAGI, Center for Neutron Research, NIST — It is understood that there is a link between molecular relaxations in glassy polymers and mechanical toughness. The notion is that these relaxations dissipate the energy of impact and thereby enhance toughness. Decades of research have focused on correlating the mechanical toughness of a polymer with the relaxation processes quantified by relatively slow characterization techniques such as dynamic mechanical analysis, dielectric spectroscopy, or solid-state nuclear magnetic resonance. However, there is a disconnect because the time and length scale of the molecular mechanisms are typically several orders of magnitude faster and more localized than the experimental techniques used to characterize them. We revisit this by using quasielastic neutron scattering (QENS) to quantify both the collective excitation and molecular relaxations that occur on the time scale of ps to ns, and see how these motions correlate with mechanical toughness. We demonstrate a strong correlation between these fast polymer relaxations and toughness. We show that these fast polymer relaxations play a critical role in predicting the ability of a material mitigate impact under ballistic conditions where the strain rates can approach an inverse microsecond.
12:03PM F30.00005: A Quasi-mimetics Approach for Uncovering Starch-based Hybrid Materials* YIN FANG (Presenter), YUANWEN JIANG, ENDAO HAN, YILIANG LIN, James Franck Institute, University of Chicago, XIANGHUI XIAO, JIN WANG, Argonne National Laboratory, HEINRICH M JAEGGER, BOZHI TIAN, James Franck Institute, University of Chicago — Materials design through biomimetics aims to achieve functions similar to those found in nature. However, this requires a thorough understanding of the system used for mimicking (SuM), which would become a challenge when SuM is complex. Here, we propose a quasi-mimetics approach, which focuses on partial components in the SuM. Different from biomimetics, quasi-mimetics aims to probe the elusive behaviors in the complex SuM, as well as to uncover new functions not found in SuM. We illustrate this approach with a starch particle-embedded hydrogel composite where noodle dough serves as a SuM. The starch hybrid composite displays unprecedentedly high stretchability both in air and water, self-healing behavior, and strain-dependent mechanical training effect. Our mechanistic study showed that the unique mechanical features of the starch hybrid gel are related to the formation of covalent bonds between the interface of the starch particles and polymer network, as well as the dynamic hydrogen bonds in the hydrogel matrix. The new quasi-mimetics approach can be broadly applied to other material exploration and device applications.

*Office of Naval Research (ONR YIP, N000141612530; PECASE, N000141612958).

12:15PM F30.00006: Starch embedded hydrogels: Linking macroscopic mechanical properties with microscopic particle configurations* ENDAO HAN (Presenter), YIN FANG, James Franck Institute, University of Chicago, XIANGHUI XIAO, JIN WANG, Argonne National Laboratory, BOZHI TIAN, HEINRICH M JAEGGER, James Franck Institute, University of Chicago — When noodles are made, a flour dough can be stretched to an extremely long length without breaking. What can we learn from it in order to synthesize innovative hydrogels? Mimicking the microstructure of flour dough, we synthesized a hybrid hydrogel by embedding wheat starch granules in an alginate-PAA gel network. This hybrid hydrogel shows many amazing mechanical properties, such as substantially improved stiffness and toughness, extremely high stretchability (up to 8000% strain), and persistent memory that is rewritable with training. With the help of x-ray microtomography, we found direct links between the macroscopic stress-strain curves and the microscopic particle structures when such hybrid hydrogels are deformed under uniaxial extension. This quasi-mimetic process allows us to not only produce materials with novel properties, but also explore new physics with simple, highly controlled systems.

*Work supported by the University Chicago MRSEC, the Center for Hierarchical Materials Design, and DOE under Contract No. DE-AC02-06CH11357 and No. DE-SC0012704.

12:27PM F30.00007: The Thermoviscoelastic Behavior of a Main-Chain Liquid Crystal Elastomer* THAO NGUYEN (Presenter), Johns Hopkins University — Liquid crystal elastomers (LCEs) combine the anisotropic ordering of liquid crystals and viscoelastic behavior of an elastomeric network. This leads to remarkable mechanical properties, including reversible shape change in response to temperature or light, deformation induced soft elasticity and anisotropy, and extreme dissipation behavior. In this presentation, I will describe our efforts to characterize the rate-dependent and temperature-dependent large deformation behavior of an acrylate main-chain LCE networks to investigate the effects of mesogen order and chain alignment on the stress-strain response, soft elasticity behavior, and hysteresis. The experimental results showed that time-temperature superposition can be applied to the stress response of the LCEs in the nematic state throughout the soft elasticity plateau. All LCE networks, polydomains and monodomains stretched parallel and perpendicular to the director, exhibited the same rate-dependence for the modulus and hysteresis. However, the onset strain and duration of the soft elasticity plateau were relatively insensitive to the strain rate. These findings suggest that the rate-dependent stress response of the acrylate LCEs in the nematic state is insensitive to mesogen reorientation.

*Research was funded by the Army Research Office under the agreement W911NF-17-1-0165
Understanding failure processes of polymer gels is critical for numerous applications, ranging from adhesives to protective materials. We discuss the failure processes associated with the deep indentation and puncture of soft gels with an axisymmetric probe. We commonly observe that the first critical transition, associated with puncture, occurs at nominal stresses that can be as much as 100 to 1000 times the elastic modulus. To understand how soft gels can sustain such stress levels prior to initial failure, we have studied puncture as a function of size scale, velocity, and material network structure. Spherically-tipped indenters of radii, R=0.4-66 um were used to characterize puncture at length scales well above the network mesh size (nm), on the same order of magnitude as the elasto-capillary length (um), and significantly below the elasto-fracture length (mm). Critical energy release rate was found to be in agreement with the predicted scaling from the classical Lake-Thomas model modified for gel fracture via the failure mechanism of chain pull-out and plastic yielding of micelles. These experiments and proposed relationships provide new insight into how gels fail and how design paradigms may be shifted to more effectively engineer with soft gels.

*Funding: NSF 1609940.

Electrospun polymer nanofibers have garnered significant interest due to their strong size-dependent material properties, such as tensile moduli, strength, toughness, and glass transition temperatures. These properties are closely correlated with polymer chain dynamics. In most applications, polymers usually exhibit viscoelastic behaviors such as stress relaxation and creep, which are also determined by the motion of polymer chains. However, the size-dependent viscoelasticity has not been studied previously in polymer nanofibers. Here, we report the first experimental evidence of significant size-dependent stress relaxation in electrospun Nylon-11 nanofibers as well as size-dependent viscosity of the confined amorphous regions. In conjunction with the dramatically increasing stiffness of nano-scaled fibers, this strong relaxation enables size-tunable properties which break the traditional damping-stiffness tradeoff, qualifying electrospun nanofibers as a promising set of size-tunable materials with an unusual and highly desirable combination of simultaneously high stiffness and large mechanical energy dissipation.

*National Science Foundation, CMMI-1762560

The mechanical properties of semi-crystalline polymeric materials are largely determined by the architecture and amount of the crystalline domains. It is known for UHMWPE fibers that the toughest and stiffest fibers exhibit a structure consisting of extended chain crystals and lamella. This structure is produced via a post-drawing process where the fiber is deformed causing the re-organization of the polymer chains. There is a lack of understanding regarding how the crystalline structure develops during drawing and what role the various structural aspects play in the mechanical properties. We show, using SAXS/WAXS, that various crystalline structures can be produced during the manufacturing of PE fibers and that these architectures develop along unique pathways when drawn. Using a VADER1000 to perform post-drawing and tensile testing, understanding of the fibers mechanical response is found. We show that unique structures exhibit distinct relaxations and a critical stress at failure of PE fibers. This study provides a much deeper understanding of crystalline behavior in extension and allows for improved design of the post-drawing process.

*Research was sponsored by the Army Research Laboratory and was accomplished under Cooperative AgreementNumberW911NF-12-2-0022.

The buckling and twisting of slender, elastic fibers is a deep and well-studied field. Recently, there has been great interest in applying this knowledge to the development of miniature linear actuators (artificial muscle), but also to investigate linkages with the formation of helices in nature (e.g. tendrils) as well as DNA supercoiling. A slender rod that is twisted with respect to a fixed end will spontaneously form a hockle, or loop, to relieve the torsional stress that builds. Further twisting results in the formation of plectonemes — a helical excursion in the fiber that extends with additional twisting. Here we investigate the energy stored and subsequently released by hockles and plectonemes as they are pulled apart, in analogy with force spectroscopy studies of DNA and protein folding. Hysteresis loops in the snapping and unsnapping inform the stored energy in the twisted fiber structures.

*NSERC
Fiber networks with inter-fiber adhesion: role of adhesion in extreme network mechanics*

VINEET NEGI, AHMED SENGAB, CATALIN PICU (Presenter), Rensselaer Polytechnic Institute — Many soft materials of biological and industrial interest are composed from nanofibers. In such cases, inter-fiber adhesion may produce fiber bundling and organization on scales larger than that of individual components. We study both non-cross-linked [1] and cross-linked [2] networks with adhesive interactions between filaments. We determine the parametric range in which adhesion reorganizes the network and study the mechanical behavior of the resulting structures. We observe a broad range of tunable properties, including softening in tension, large strain range in which the structure responds linearly to applied strains, and adhesion-dependent elastic moduli. The results provide guidelines for material design and demonstrate that controlling inter-fiber adhesion may lead to fibrous materials with exceptional properties and behavior.


*This work was supported by the NSF through grant No. CMMI-1634328

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F31 DCP: Inspirations From Experiment (E) BCEC 203 - Cristina Puzzarini - Tag(s): Focus

Intrinsic Chiroptical Response: Can We Predict the Right Answer for the Right Reasons?*

PAUL M. LEMLER, CLAYTON L. CRAFT, PATRICK H. VACCARO (Presenter), Department of Chemistry, Yale University — The "intrinsic handedness" that distinguishes the mirror-image forms (enantiomers) of a chiral molecule gives rise to a variety of intriguing phenomena, perhaps none of which has had as profound and sustained an impact on the physical sciences as the characteristic interactions that take place with polarized light. Although the signatures of this optical activity have been recognized for over two centuries, their fruitful application for the determination of absolute stereochemical configuration has been revolutionized by the advent of computational paradigms capable of predicting such properties from first principles. Efforts to probe the dispersive circular birefringence (CB) of isolated chiral molecules at nonresonant wavelengths will be presented, with emphasis directed towards the marked influence that intramolecular dynamics and intermolecular forces can exert on intrinsic electronic response. Requisite isolated-molecule measurements have been made possible by ongoing development of cavity ring-down polarimetry (CRDP), an ultrasensitive chiroptical probe that has permitted the first quantitative studies of optical rotatory dispersion (ORD or wavelength-resolved CB) to be conducted in rarefied gaseous media. Quantum-chemical analyses have been enlisted to unravel the provenance of experimental findings and to elucidate the synergism among electronic and nuclear degrees of freedom that ultimately governs observed behavior. By alleviating the pronounced effects incurred from environmental perturbations (e.g., solvation), vapor-phase ORD benchmarks will be shown to afford a critical assessment of burgeoning optical-activity calculations, as well as an incisive means to expose the strengths and shortcomings inherent to various computational protocols.

*Support of the U.S. National Science Foundation under grant CHE-1464957 is gratefully acknowledged.

Probing electronic processes in large molecules

FRANCESCA CALLEGARI (Presenter), DESY — Attosecond science is nowadays a well-established research field, which offers formidable tools for the investigation and control of electronic processes [1,2]. The possibility to study molecules of increasing complexity with attosecond time resolution paves the way to disclosing the role of the electron dynamics in the photo-chemistry and photo-biology of complex systems. In this context, we have recently demonstrated that attosecond pulses can initiate charge migration between different functional groups of aromatic amino-acids [3]. In this talk I will first present a time-resolved study of photo-fragmentation of the nucleobase adenine, one of the key building blocks of DNA. Our most intriguing observation is that a stable dication of the parent molecule can be produced if (and only if) the probing NIR pulse is very briefly delayed from the XUV pulse. Our experimental and theoretical findings indicate that this short delay corresponds to the lifetime of the inner valence hole. The process also evidences the presence of a laser-assisted stabilization of the nucleobase.

In the second part of the talk I will show the results we have recently obtained for a very large polyatomic molecule, namely the C60 molecule. Here we have investigated delays in photoemission after exciting the Giant surface Plasmonic Resonance (GPR) around 20 eV. Clear signatures of the collective electron dynamics initiated by the XUV pulse can be extracted from the experimental data.

Designing Ligands to Control Molecular Nanomagnets: Strategies for 3d vs 4f

ANNIE POWELL (Presenter), Karlsruhe Institute of Technology — NA

Luminescence Measurements of the Hyperthermal Reactions of N⁺/N + NH₃

MICHAEL HAUSE (Presenter), Boston College Institute of Scientific Research, BENJAMIN PRINCE, RAYMOND BEMISH, Air Force Research Laboratory — Chemi-luminescence emitted in the ultraviolet, visible and near infrared from the collision of N⁺ or N with NH₃ at collision energies between 20-300 eV (center of mass) was measured and the energy dependence of the respective emissions quantified in the emission excitation cross sections. For both primary collision species, the strongest features are assigned to emissions from NH (A-X) and the hydrogen Balmer series. Additional features originating from N I and NH (c-a) emissions were also observed. Most of the transitions are consistent with short-range interactions resulting in collision induced dissociation of the NH₃ molecule. It has been found previously that the NH (A-X) cross sections are independent of collision partner in studies with Ar⁺, Kr⁺ and Xe⁺ with NH₃. Reaction with N⁺ largely agrees with these findings, but the cross sections from collisions with neutral N is much reduced.

Laser-Ionization of Energetic Compounds: Differences and Similarities between Structures and Energetics of Gaseous Monomers and Solid State

FATMA AKIN (Presenter), Bogazici University — As one of the processes following pulsed nanosecond or ultrafast laser ablation of solids, ionization is expected to direct molecular dissociation events. Ionization-induced effects on the RDX(s) and RDX (g) are computationally investigated using DFT methods and normal mode displacement calculations incorporating the Duschinsky effect. Structures, dissociation enthalpy and free energies of the resulting [(RDX)₂⁺] clusters show that ionization caused 75% of the conformers to be unstable in their neutral isomeric composition and orientation. Ionization causes charge-polarization, hydrogen-transfer, N-N dissociation and assisted HONO formation in solid RDX. The assisted HONO formation occurs via and suggests hydrogen mobility within the charged moieties, causing the greatest stabilization. The energy costs of ion-neutral dissociation are comparable to the hydrogen-transfer and NO₂ loss processes. The RDX conformational identity is a determining factor in the emerging dissociation pathways in both dimeric and monomeric forms. Ionization of the RDX surface is proposed as another source of NO₂ and HONO precursors of the NO⁺ ion observed previously.

Neural network - assisted analysis of X-ray spectra of bimetallic nanoparticles

NICHOLAS MARCELLA (Presenter), ANATOLY I FRENKEL, Stony Brook University — In X-ray absorption spectroscopy, it is problematic to analyze and interpret polyatomic systems consisting of elements that are neighbors in Periodic Table due to the overlapping edge regions and similar photoelectron scattering properties. This limits our ability to solve the local structure of interesting bimetallic nanocatalysts such as PtAu PdAg, IrPt, and RhAu. We have shown, recently, that X-ray absorption near edge structure (XANES) can be inverted to provide structural properties due the region's sensitivity to photoelectron scattering. Now, we take advantage of XANES sensitivity to electronic structure, specifically charge transfer. In this work, we demonstrate how our new Neural Network XANES (NN-XANES) method can be used to solve the structure of these difficult systems with better accuracy than existing methods. Our work suggests that NNs can yield distinct partial Pt-Au and Pt-Pt coordination numbers from Pt L3-edge XANES in PtAu, a feat impossible with EXAFS and other Z-contrast-limited techniques.

Raman enhancement effect using 2D materials as substrates: mechanism and application

HIKARI KITADAI, Department of Chemistry, Boston University, NANNAN MAO, Massachusetts Institute of Technology, SHENGXI HUANG, School of Electrical Engineering and Computer Science, Pennsylvania State University, XI LING (Presenter), Department of Chemistry, Boston University — Graphene enhanced Raman scattering (GERS) was first reported in our previous work in 2010, which opened the door of using 2D materials as substrates for Raman enhancement. Here, we will present a systematic study on the Raman enhancement effect on a variety of 2D materials. Raman enhancement effect at different levels is observed on different 2D materials, which is attributed to the chemical enhancement. The degree of charge transfer between molecule and 2D materials is obtained based on the selection rule of the enhancement to vibrational modes with distinct symmetries. A strong correlation is found between the Raman enhancement effect and the degree of charge transfer. Moreover, advantages of the Raman enhancement on 2D materials for practical applications will be discussed.

This work is supported by Boston University.
Probing the dynamics of small anions in optical cavities

ANDREA GRAFTON (Presenter), ADAM DUNKELBERGER, KENAN FEARS, RODERICK B. DAVIDSON, BLAKE SIMPKINS, JEFFREY OWRUTSKY, United States Naval Research Laboratory — Coupling vibrational modes to optical cavities offers a method to systematically and predictably modify the vibrational energy landscape of a molecule. A confined optical mode can couple to a resonant material transition and lead to enhanced absorption/emission rates, excited state population control, and the formation of new hybrid states. There is a rich history of coupling to electronic transitions, including quantum wells and J-aggregates, coupling to vibrational transitions has only been explored recently. We reported time resolved IR studies on strongly coupled vibration-cavity polaritons for W(CO)$_6$ in hexane. The result demonstrated that much of the response is due to uncoupled reservoir excited state absorption and there is evidence for an angle-tuning dependent decay time for the upper polariton (UP) to $\nu = 2$ transition. We have explored other solutes with shorter dephasing times vibration-cavity systems. Dicyanamide and thiocyanate have strong mid-IR absorptions and are capable of strong coupling to optical fields. However, in both anions, we do not observe the UP to $\nu = 2$ transition that was observed in the W(CO)$_6$ cavity. The results are discussed in terms of how they impact the prospects for observing polariton relaxation effects in vibration-cavity systems.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F33 FIAP: Energy Conversion and Storage Materials

11:15AM F33.00001: Shift current bulk photovoltaic effect influenced by quasiparticle and exciton* RUIXIANG FEI (Presenter), University of Pennsylvania, LIANG TAN, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, ANDREW RAPPE, University of Pennsylvania — We compute the shift current bulk photovoltaic effect (BPVE) in bulk BaTiO$_3$ and two dimensional monochalcogenide SnSe considering quasi-particle corrections and exciton effects. We explore changes in shift current peak position and magnitude reduction due to band renormalization. For BaTiO$_3$, we demonstrate that shift current is dramatically reduced near the band edge but enhanced at high energies due to exciton effect. Additionally, we reveal that the shift current is reduced in two dimensional monochalcogenide SnSe due to the enhancement of optical reflectivity from many-body corrections. Comparison of these results with experiments on BaTiO$_3$ indicate that mechanisms other than shift current may be contributing to BPVE. These results suggest that many-body corrections are important for accurate assessments of bulk photovoltaic materials and to understand the mechanisms behind the BPVE.

*R. F. was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Grant No. DE-FG02-07ER46431. L. Z. T. was supported by the U.S. Office of Naval Research, under Grant No. N00014-17-1-2574. A. M. R. was supported by the National Science Foundation, under Grant No. CHE-1808202. The authors acknowledge computational support from the NERSC of the DOE.

11:27AM F33.00002: Bulk photovoltaic effects in the presence of a static electric field* BENJAMIN M. FREGOSO (Presenter), Physics, Kent State University — Irradiated crystalline insulators in the presence of a static electric field exhibit three new types of nonlinear photocurrents. They represent physical singularities of the third order free electron polarization susceptibility and hence generalize the standard second order bulk photovoltaic effects. In the absence of momentum relaxation and saturation effects they grow as $t^n$ ($n=2,1,0$) with illumination time and are dubbed jerk, modified injection, and modified shift current, respectively. The presence of a static electric field gives rise to new processes which are described in detail. Experimental signatures and extensions to higher order susceptibilities are also discussed.

*NERSC-DOE contract No. DE-AC02-05CH11231

11:39AM F33.00003: Core-shell colloidal quantum dots for photovoltaics with improved open circuit voltage* YIJIN GUO (Presenter), SUE SHI, GILLIAN HAGEN, BENJAMIN A ZANK, ALEXI C ARANGO, Physics, Mount Holyoke College — High carrier recombination rates in lead sulfide (PbS) colloidal quantum dot (CQD) photovoltaics (PV) can result in a reduction in open circuit voltage (Voc). Surface states and sub-gap states are thought to increase recombination which leads to Voc loss. Here we present a method of forming an oxide shell on the CQD surface capped with native oleic acid ligands prior to the deposition of the CQD film and ligand swap. The core-shell QDs exhibit a narrowing in size distribution and the resulting devices yield improved Voc. In addition, films of core-shell QDs are more resilient to damage incurred during sputter deposition of overlying films. Because the thickness and uniformity of the oxide shell can be precisely controlled, a natural balance between trap passivation and charge transport can be achieved.

*NSF EAGER Award: 1744671
Mount Holyoke College Lynk Funding

1:51PM F31.00008: Probing the dynamics of small anions in optical cavities

ANDREA GRAFTON (Presenter), ADAM DUNKELBERGER, KENAN FEARS, RODERICK B. DAVIDSON, BLAKE SIMPKINS, JEFFREY OWRUTSKY, United States Naval Research Laboratory — Coupling vibrational modes to optical cavities offers a method to systematically and predictably modify the vibrational energy landscape of a molecule. A confined optical mode can couple to a resonant material transition and lead to enhanced absorption/emission rates, excited state population control, and the formation of new hybrid states. There is a rich history of coupling to electronic transitions, including quantum wells and J-aggregates, coupling to vibrational transitions has only been explored recently. We reported time resolved IR studies on strongly coupled vibration-cavity polaritons for W(CO)$_6$ in hexane. The result demonstrated that much of the response is due to uncoupled reservoir excited state absorption and there is evidence for an angle-tuning dependent decay time for the upper polariton (UP) to $\nu = 2$ transition. We have explored other solutes with shorter dephasing times vibration-cavity systems. Dicyanamide and thiocyanate have strong mid-IR absorptions and are capable of strong coupling to optical fields. However, in both anions, we do not observe the UP to $\nu = 2$ transition that was observed in the W(CO)$_6$ cavity. The results are discussed in terms of how they impact the prospects for observing polariton relaxation effects in vibration-cavity systems.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM
11:51AM F33.00004: Si24: a next-generation semiconductor with growing promise for future solar energy* MICHAEL GUERETTE (Presenter), Geophysical Laboratory, Carnegie Institution for Science — The recently discovered allotrope of silicon, Si24, is an exciting material for the future of solar energy due to a quasi-direct bandgap near 1.3 eV [1]. Synthesized via precursor Na4Si24 at high temperature and pressure (~850 °C, 9 GPa), free standing single crystals of on the 1 mm scale are now achievable [2]. An epitaxial relationship between Na4Si24 and diamond cubic silicon (DC-Si), observed through high-resolution transmission electron microscopy (HRTEM), is proposed to facilitate the growth of these high-quality Na4Si24 crystals from DC-Si wafers mixed with metallic Na. These observations illuminate a path toward scaling of Na4Si24 and Si24. Removal of Na from Na4Si24 on this length scale is shown to be effective, revealing intrinsic optical and electronic properties of Si24. Our results encourage the pursuit of Si24 for future solar energy conversion and efficient optoelectronics.


*Supported by Energy Frontier Research in Extreme Environments Center (EFree), award # DE-SC0001057.

12:03PM F33.00005: Tailoring the structure and defects of non-toxic nanocrystalline Bi2S3 solar cells MARYAM MASROOR SHALMANI (Presenter), PRATAP RAO, Worcester Polytechnic Institute — Solar cells can satisfy the increasing demand for energy worldwide, but the toxicity of semiconductors used in solar cells can overshadow their utility as a renewable source of energy. Bi2S3, with a desirable band gap of 1.3eV, and as a non-toxic n-type semiconductor can be a favorable replacement for toxic semiconductors containing Pb, Cd or Te. However, nanocrystalline Bi2S3 films synthesized by various techniques such as successive ionic layer adsorption and reaction (SILAR) have not reached high solar energy conversion efficiencies hitherto, and have primarily been studied as sensitizers for photoelectrochemical applications. Here, we report the synthesis and characterization of non-toxic all-inorganic solid-state Bi2S3 photovoltaic solar cells. We enhanced the solar energy conversion efficiency of the nanocrystalline Bi2S3 solar cells by optimizing the structure of the electron and hole transport layers, and by tailored annealing treatments that modify the size of the Bi2S3 nanocrystals and decrease their defect concentrations.

12:15PM F33.00006: The fluid-like nature of solid cubic halide perovskites* XINGANG ZHAO (Presenter), GUSTAVO DALPIAN, ALEX ZUNGER, University of Colorado, Boulder — X-ray diffraction ‘see’ in the high temperature phase of ABX3 halide perovskites a macroscopically averaged cubic structure with a single formula unit (FU) per cell. Yet DFT calculations on this structure reveal a number of anomalies: i) It has dynamically unstable phonons, ii) its band gap is lower than both experiment and molecular dynamics (MD) predictions, iii) the trends with A cation show inconsistency with experiment e.g., cubic FASnI3 has larger gap than the orthorhombic CsSnI3, and iv) it has higher total energy than the relaxed supercell with many repeated FUs. We find via DFT that the real microscopic structure of cubic halide perovskites is polymorphous, i.e., it contains a dynamic fluid-like distribution of different local motifs, each having differently tilted/rotated/B-atom displaced BX6 octahedra and differently oriented A molecules, the average of which is the fictitious monomorphous cubic structure. The polymorphous configurations have stable phonons and much larger band gaps, forming the correct description of trends in gaps and structures in the ABX3 group of materials. We will present the main effects that govern band gaps in perovskites, via carefully constructed static supercell approximants to the dynamic MD structure.

*Supported by DOE/EERE DE-EE-0008153
Due to the unique optical properties and high quantum efficiency, the lead halide perovskites have obtained great attentions in the recent years. Currently, the research focuses not only on their potential applications in solar cell, LED, and laser, but also on several unsolved fundamental issues, such as the origin of the luminescence of Cs$_4$PbBr$_6$. The mechanism of the luminescent Cs$_4$PbBr$_6$ perovskite is still under debate. Some people think that the pure Cs$_4$PbBr$_6$ crystals are non-emissive while the strong green PL (Photoluminescence) originates from the CsPbBr$_3$ nanocrystals encapsulated in the Cs$_4$PbBr$_6$ bulk crystals. The others claim that the strong emissive comes from the structural defects of the Cs$_4$PbBr$_6$ crystals. Despite the various reports to support each opinion, no final conclusion has been made up to now. In this work, we plan to controllably synthesize emissive and non-emissive Cs$_4$PbBr$_6$ crystals as well as CsPbBr$_3$ nanocrystals with a strong photoluminescence. By combining various techniques, such as Raman, XRD, (HR)TEM, PL, etc., we attempt to confirm the contribution of CsPbBr$_3$ dopants to the photoluminescence of Cs$_4$PbBr$_6$ crystals.
1:15PM F33.00011: Use of LIBS Technology for CO2 Leak Detection in Carbon Sequestration* CHET BHATT (Presenter), JINESH JAIN, DANIEL HARTZLER, AECOM, National Energy Technology Laboratory, DUSTIN MCINTYRE, National Energy Technology Laboratory — In this study, the in-situ measurement capability of Laser-Induced Breakdown Spectroscopy (LIBS) to detect CO2 leakage in geological carbon storage (GCS) was evaluated. As LIBS is an optics-based (contains no electronics) spectroscopic technique, it can perform contamination-free analysis in extreme conditions of underground environment. During the leakage, the interaction of CO2 with carbonate rocks at elevated pressures can release various metals which can potentially contaminate the drinking water sources above storage sites. Therefore, we evaluated the underwater LIBS technique for studying the carbonate dissolution with increased CO2 pressure. Dissolution experiments using four carbonates (CaCO3, SrCO3, MnCO3, and MgCO3) at the elevated CO2 pressure (ranging from ambient to 250 bars) were carried out by analyzing LIBS spectra obtained from aqueous solutions containing these carbonates. The results indicated the dissolution of all carbonates. However, the rate of dissolution varied from carbonate to carbonate. This study shows that in-situ monitoring of carbonate dissolution by underwater LIBS can be used for CO2 leak detection in GCS.

*National Energy Technology Laboratory

1:27PM F33.00012: Energy-Saving Meta-Glasses with Embedded Plasmonic Nanoparticles LUCAS VAZQUEZ BESTEIRO (Presenter), Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, XIANG-TIAN KONG, Department of Chemistry, University of Washington, ZHIMING M WANG, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, FEDERICO ROSEI, Énergie, Matériaux et Télécommunications, Institut National de la Recherche Scientifique, ALEXANDRE GOVOROV, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China — Plasmons are collective charge carrier excitations. Using different plasmonic materials to fabricate nanocrystals and controlling their size and geometry allows us to obtain sharp resonances from UV to near IR. By embedding ensembles of nanocrystals in dielectric materials, we can design metamaterials with specific transmission profiles that filter out a broad spectrum while remaining transparent to selected frequency bands.1 We discuss this idea in the specific context of its application in energy-saving windows.2 By blocking UV and IR radiation from the solar spectrum they reduce the energy expenditure of active cooling systems in warm climates, but they retain the desirable property of being transparent to visible light. In this talk we will present theoretical results for plasmonic glasses created with different nanoparticle geometries3 and materials, offering alternatives to current industrial fabrication standards, with comparable efficiencies and potentially lower costs.


1:39PM F33.00013: Unsteady State of a Solid State Device: Characteristic Cooling Length* PABLO EDUARDO RUIZ-ORTEGA (Presenter), MIGUEL OLIVARES ROBLES, SEPI ESIME Culhuacan, Instituto Politecnico Nacional — Thermoelectric modules (TEM) are solid state devices that can work as a Thermoelectric cooler (TEC). TECs can reach temperatures below that obtained with a steady-state current by applying an electrical current pulse which enables a transitory state in a Peltier couple. This phenomenon is known as supercooling. The objective of this work is to analyze characteristics parameters such as minimum cooling temperature, COP and temperature spatial profile in a TEC operated under current pulses and cooling load (Qc) pulses. We study a numerical model of a one-dimensional thermoelectric cooling system in the unsteady state. In this work, we propose a new parameter called characteristic cooling length to describe the distance in which occurs minimum cooling temperature in the elements of a TEM. Our results show the transient temperature spatial profile along the thermoelements of the TEM and the characteristic cooling length for different materials. We propose a general principle to make a judgment how the temperature profile will occur along the elements due to material properties under current pulse operation.

*This work was financially supported by Instituto Politecnico Nacional, México (grant 20180069). Pablo Eduardo Ruiz Ortega was financially supported by CONACyT-México (Grant 490910)
1:51PM F33.00014: Highly-Miscible and Bandgap-Tunable (Li\(_x\)Cu\(_{1-x}\))\(_2\)ZnSnS\(_4\) Alloys  HE LI (Presenter), XIAN ZHANG, TAO ZHANG, MENG LIN HUANG, SHIYOU CHEN, East China Normal University — Doping or alloying lithium into Cu\(_2\)ZnSnS\(_4\) (CZTS) has drawn extensive attention recently because it is crucial for fabricating high-performance Cu\(_2\)ZnSnS\(_4\) thin film solar cells. Experiments showed that lithium can be alloyed into CZTS with a high content and even completely substitute copper to form a new compound Li\(_2\)ZnSnS\(_4\) (LZTS). Using the first-principles calculations, we found that Li\(_2\)ZnSnS\(_4\) adopts wurtzite-kesterite as ground state structure with a band gap around 3.29 eV. The valence band offset between Li\(_2\)ZnSnS\(_4\) and Cu\(_2\)ZnSnS\(_4\) is 2.20 eV. As the Li content increases, the band gap of (Li\(_x\)Cu\(_{1-x}\))\(_2\)ZnSnS\(_4\) alloy increases rapidly with a big band gap bowing. The mixing enthalpies of (Li\(_x\)Cu\(_{1-x}\))\(_2\)ZnSnS\(_4\) alloys in the kersterite and wurtzite-kesterite structures are both small, suggesting that the (Li\(_x\)Cu\(_{1-x}\))\(_2\)ZnSnS\(_4\) alloys can easily form at a low growth temperature. These results demonstrate that the lithium alloying may be an effective way for adjusting the band structure and the optoelectronic properties of CZTS.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F34 DPOLY FIAP: Polymer Physics to Address the Dual Energy Challenge at Global Industrial Scale

11:15AM F34.00001: A New Carbon Ontology: Hydrocarbons as Benign Material Resource for Civilizational-Scale Building  MARK GOULTHORPE (Presenter), Massachusetts Institute of Technology — The talk will frame the macro scale of building and infrastructure development forecast for coming decades, especially in regions of population and economic growth, and highlight the startling environmental impact implicit in current building materials and methods as well as the in-use energy and maintenance footprints. Alternative materials that mitigate such impacts will be considered, such as mass timber, but the prime focus will be on emerging polymeric composite material-processing that has proved so successful in many other manufacturing sectors, especially in their remarkable structural capacity. A case will be made that adoption of polymeric composites offers potential for radical revision of building methods, with potential for civilizational-scale adoption in short timelines; and it will map out the environmental benefits that this might offer in both embodied and in-use impact. The challenges and impediments to broad uptake of hydrocarbon-derived buildings will be considered, and thoughts offered as to how these might be addressed effectively, with particular focus on fire retardancy and the economics of production. Emerging gas-deposition of carbon nanotube and graphene materials will be probed, which offer remarkable potential for poly-functional carbon dwellings that are suggestive of an elegant new carbon ontology: a carbon shroud for a carbon organism!

The talk will serve as a call for collaboration between upstream and downstream actors as vital to breaking into a highly entrenched and deeply conservative building “industry”. The need for radical new building technologies merits a purposeful mobilization (political, technical, logistical) that aims at nothing less than a massive re-orientation of hydrocarbon assets from prime use as fuel to prime use as building materials at a period of unprecedented urban development and against the backdrop of a mounting environmental crisis.
**11:51AM F34.00002: Tools for polymer design: predicting rheology from molecular weight distribution and branching topology** [Invited] DANIEL READ (Presenter), CHINMAY DAS, VICTOR BOUDARA, University of Leeds — Polymers make wonderful, useful materials! Yet, their success and ubiquity has itself caused problems, provoking examination of their sustainability and recyclability, and of the energy efficiency of their processing. In this context, the design and optimisation of new materials and processes requires tools with the ability to predict material properties and behaviour on the basis of their molecular structure. This talk will present our efforts to address the challenge of predicting the flow properties (rheology) of polymeric liquids, and discuss the physics underpinning the software we have developed. The potential design space is vast: practical polymers are polydisperse (broad and variable molecular weight distribution) and may contain branches (with potential to control the statistics of branch placement). These molecular variables affect the response of the polymers to flow: whether the strands align, or stretch, and by how much, in a given flow field. These dynamics in turn gives rise to relevant processing phenomena such as extension hardening, or shear thinning. We will focus on polydisperse linear polymers, for which we have developed a constitutive model ("Rolie-Double-Poly") embedded in software (https://reptate.readthedocs.io/) that quantitatively predicts non-linear rheology from molecular weight distribution. We will also discuss how chain branching affects the physics, as encoded within our "BoB" software (https://sourceforge.net/projects/bob-rheology/).

*EPSRC grant number EP/P005403/1

**12:27PM F34.00003: Micromechanics of oriented semi-crystalline polymers: from structure to properties** [Invited] HANS VAN DOMMELEN (Presenter), MOHSEN MIRKHALAF, Eindhoven University of Technology, JEVAN FURMANSKI, ExxonMobil Research and Engineering Company, LEON GOVAERT, Eindhoven University of Technology — The microstructure of semi-crystalline polymers, in terms of for example the degree of crystallinity, crystal type, size and orientation, may vary drastically depending on subtle details of the manner in which the polymer is shaped into the final product. For this material, often an oriented microstructure is formed, leading to anisotropic yield and failure kinetics.

To obtain a fundamental and quantitative understanding of how these anisotropic properties depend on the structure, a multiscale micromechanical model is developed. The modelling approach is based on a mean field framework, accounting for the crystalline phases, which are modelled by crystal plasticity and amorphous domains. The anisotropy of these amorphous regions is incorporated in the micromechanical model in the form of a pre-stretch of the amorphous network and anisotropic visco-plastic flow. Both aspects are found to be crucial for predicting the experimentally observed orientation dependence of the yield kinetics. With this combined experimental-modelling approach, new insight in the physical processes that govern the mechanics of semi-crystalline polymers are obtained.

*The authors gratefully acknowledge ExxonMobil corporation for financial support of this study.

**1:03PM F34.00004: A better future for fossil hydrocarbons and carbon nanomaterials** [Invited] MATTEO PASQUALI (Presenter), Rice University — Every year we extract over 4.2 GT of oil, 2.5 GT of natural gas, and 3.4 GT of coal to sustain our economy. That’s equivalent to 8.7 GT of carbon and 1.3 GT of Hydrogen. Almost all of these resources are burned to generate energy, causing over 30 GT of CO2 to enter the atmosphere which is unsustainable in view of climate change—the only significant exception is polymers, which fix 0.35 GT/yr of hydrocarbon resources (~3% of the total production) into valuable solid materials. At the same time, every year we use over 12% of the world energy production (over 60 EJ) towards primary metals; most of this energy goes into mining, refining, and processing ~3 GT/yr of metal ores into usable metals, chiefly 1.6 GT/yr of steel, 50 MT/yr of Aluminum, and 20 MT/yr of Copper; it is accompanied by the generation of 3.7 GT of CO2 emissions, equivalent to ~20% of the emissions caused by burning oil and gas. This is the extent of our “materials-energy nexus”.

Can we break this inefficient cycle and replace metals with materials made directly from hydrocarbons? Carbon Nanomaterials—primarily CNTs and graphene—offer an opportunity. They can be made via pyrolysis of methane and other hydrocarbons, with concurrent production of hydrogen. In the past decade, methods have been developed to convert CNTs and graphene into macroscopic materials (fibers, sheets, 3D structures) that could displace metals based on their properties—strength, electrical and thermal conductivity. In this talk, I will discuss why carbon nanomaterials could be great candidates to utilize natural gas on a very large scale (GT/yr) to make materials with zero CO2 footprint and positive hydrogen production. I will outline the scientific problems that need to be solved to realize highly-efficient synthesis and conversion of these materials and will present an estimate of the potential benefits of such a transition in our use of fossil hydrocarbons.

*This work is supported by AFOSR, DOE, and the Welch Foundation.
1:39PM F34.00005: Quantifying tie-chain fraction and its impact on charge transport in model conjugated polymers

[Invited] LYNN LOO (Presenter), Princeton University — The presence of tie chains that connect between crystallites can critically impact the electrical properties of conjugated polymers. Yet, the community has not yet been able to directly visualize them, let alone quantify their content in conjugated polymers. We applied the Huang-Brown model, a framework commonly used to elucidate the structural origins of mechanical properties in polyolefins, to quantify the tie-chain contribution to charge transport in a series of model poly(3-hexylthiophene), P3HT, and its blends. Plotting field-effect mobility as a function of tie-chain fraction, as extracted from the Huang-Brown model, collapses the data on a single curve not previously seen when the charge transport property is plotted against molar mass. We find a threshold tie-chain fraction of 10⁻³, below which intercrystallite connectivity limits macroscopic charge transport. Structural characterization via x-ray paracrystallinity analysis of these P3HT films suggests intracrystallite disorder to be the bottleneck that limits charge transport when crystallites are connected. Our study affirms the importance of connectivity between crystalline domains, with the Huang-Brown model implicating long polymer chains with rigid backbone to facilitate macroscopic charge transport.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F35 APS: Apker, Greene, Metropolis Award Session

BCEC 205B - Renata Wentzcovitch, Columbia

11:15AM F35.00001: LeRoy Apker Award Talk: Anyons in a Dynamical Toric Code Model* [Invited] NICHOLAS SHERMAN (Presenter), Physics, University of California, Berkeley, BRUNO NACHTERGALE, University of California, Davis — In 3+1 dimensions, all particles are classified as either bosons or fermions. However the story is different in 2+1 dimensions, where a new type of particle exists: anyons. Beyond the fundamental interest of anyons, they also harness the ability to implement fault-tolerant universal quantum computation. The use of anyons for the purposes of quantum computation was first proposed by Kitaev with the development of the toric code model. However, the anyons in this model are stationary states, and the dynamics of anyons are an essential ingredient in quantum computation. In this work, we introduce a dynamical toric code model by perturbing the toric code Hamiltonian. Anyons in this model have non-trivial dynamics while the anyon numbers are conserved. In this talk I will discuss the model, the dispersion relation of the low energy excitations, and the role symmetry plays in the features of the spectrum.

*Based upon work supported by the National Science Foundation under Grant DMS-1813149.

11:51AM F35.00002: Nicholas Metropolis Award for Outstanding Doctoral Thesis Work in Computational Physics

Talk: Astrophysical Simulations in the Era of Massively-Parallel Computation [Invited] EVAN E. SCHNEIDER (Presenter), Astrophysical Sciences, Princeton University — In this talk, I will describe my thesis work developing Cholla, a new hydrodynamics code for astrophysics that was designed to run natively on the graphics processing units (GPUs) that power the world’s fastest supercomputers. By harnessing the power of this new technology, Cholla is allowing us to run astrophysics simulations with unprecedented numerical resolution, leading to new insights regarding the physical structure of gas in galaxies. In addition to describing the design of the Cholla code (including details of both physical and numerical algorithms), I will also discuss the results of a recent project using Cholla to explore an interesting problem in galaxy evolution - the physics of galactic winds. Star-forming galaxies are commonly observed to be driving gas out at a variety of densities, temperatures, and velocities. These outflows are invoked to explain the discrepancy between the dark matter halo mass function and the stellar mass function of low-mass galaxies. Using petascale simulations run with Cholla on the Titan supercomputer, we can better resolve the hydrodynamic interactions between phases in these outflows, allowing us to constrain their origin and evolution. This combination of new software with new computer architectures has ushered in a new era of massively-parallel astrophysics simulations.
12:27PM F35.00003: LeRoy Apker Award Talk: The Aerodynamics of Ballistic Seed Dispersal in the Plant Family Acanthaceae* [Invited] ERIC COOPER (Presenter), Pomona College/ Stanford University — Plants in the Acanthaceae family ballistically launch seeds that rotate at up to 1660 Hz – one of the fastest rotation rates in the natural world. In numerous species, this high rate of backspin stabilizes seeds in a streamlined orientation, which we have analytically determined is a property of all ballistic spinning discs. Using high-speed video, we quantify the effect that this stability has on aerodynamic drag and dispersal range. Study of several species within the Ruellia genus shows plants reach the largest seed dispersal ranges (up to 10 m) when utilizing the aerodynamic benefits of stable backspin. This research opens the door to further comparative study across the 4000+ species of the Acanthaceae family. Combining systematic measurements of seed dispersal aerodynamics with existing phylogenetic data promises to shed light on open biological questions about the adaptive significance of seed dispersal.

* This work was done in collaboration with Molly Mosher, Carolyn Cross, Cole Becker and Professor Dwight Whitaker at Pomona College. We acknowledge the support of NSF MRI award 0722532, Pomona College, and the Pomona College SURP program.

1:03PM F35.00004: Richard L. Greene Dissertation Award Talk: Coherent Light-Matter Interactions in 2D Materials [Invited] EDBERT JARVIS SIE (Presenter), Stanford University — Monolayer transition-metal dichalcogenides are prime examples of 2D semiconductors that exhibit remarkable electronic properties. They have a pair of electronic valleys that can serve as a new degree of freedom to carry information. However, these valleys are normally locked in the same energy level, which limits their potential use for applications. Here, we discuss a direct optical method to tune the exciton energy levels of monolayer W52 in a valley-selective manner through the optical Stark effect [1] and the Bloch-Siegert shift [2], performed at MIT. The two effects are found to obey opposite selection rules, which enables us to separate the two effects at two different valleys. Finally, I will briefly discuss our recent experiments where the topological phases of semimetal WTe2 can be manipulated using light-induced atomic-scale lattice distortions [3], performed at SLAC/Stanford University.

References

1:39PM F35.00005: Richard L. Greene Dissertation Award in Experimental Condensed Matter or Materials Physics: Engineering Synthetic Quantum Operations [Invited] URI VOOL (Presenter), Harvard University — Coherent quantum effects are the hallmark of atomic systems. The field of circuit quantum electrodynamics also allows for the control of coherent quantum systems. However, these quantum states do not correspond to atomic degrees of freedom, but to the quantized behavior of the electromagnetic field in a macroscopic superconducting circuit. These “artificial atoms” simulate many of the effects in atomic systems, with the added benefits of tunability and fast control and measurement. In this talk we present the basic quantum objects accessible using superconducting circuits, and techniques we can use to create a richer variety of artificial atoms and quantum operations. One experiment focuses on selection rules in superconducting circuits. Using non-linear coupling, we are able to break the selection rules of a fluxonium artificial atom and drive forbidden transitions. We use this technique to construct a Λ system from the fluxonium coupled to a resonator at the fluxonium sweet spot. Another experiment focuses on the new artificial atoms and operations accessible by adding continuous external drives to the circuit. By taking the Jaynes-Cummings (JC) Hamiltonian of a qubit coupled to a cavity and adding two continuous tones, we are able to simulate an effective JC Hamiltonian in the transverse basis. The energies and interaction terms are completely governed by the drives, and the system can be tuned to any interaction regime in situ. This scheme also allows us to cool the qubit to the eigenstates of the transverse basis, and perform a continuous quantum non-demolition measurement of the transverse component of a qubit.

This talk presents work done during my Ph.D. in Michel Devoret's lab at Yale University.

**Tuesday, March 5, 2019 11:15 AM - 2:15 PM**

**Session F36 GMAG GMED: In-vivo Magnetic Measurements for Medical Diagnosis, Therapy and Discovery** BCEC 205C - Stephen Russek, National Institute of Standards and Technology Boulder - Tag(s): Invited
11:15AM F36.00001: Magnetic functional neuroimaging and transcranial magnetic stimulation [invited] AAPO NUMMENMAA (Presenter), Harvard Medical School — TBD

11:51AM F36.00002: MRI Magnetic Susceptibility Mapping In Vivo* [invited] KARIN SHMUELI (Presenter), Medical Physics & Biomedical Engineering, University College London — The magnetic susceptibility of living tissues depends on their composition and microstructure. Therefore, the emerging, non-invasive, magnetic resonance imaging (MRI) technique of quantitative susceptibility mapping (QSM) is beginning to yield clinically useful information on pathophysiology-related changes in tissue composition and microstructure. I will outline the physical principles underpinning QSM and describe QSM applications we have developed in sickle cell anaemia, healthy brain ageing and head-and-neck cancer.

Weak tissue susceptibilities (Schenck, Med Phys 1996) cause small magnetic field perturbations seen in phase of the complex MRI signal. In QSM we calculate susceptibility maps from MRI phase images. MRI phase is a 0 to 2π angle in the complex plane and must be unwrapped. The unwrapped images are dominated by large-scale background phase variations caused by the relatively large air-tissue susceptibility difference. Once the background field variations are removed the result is the input for susceptibility calculation. This is an ill-posed inverse problem for which many regularisation methods have been proposed. There is a plethora of algorithms available for each stage in the QSM pipeline and the MRI QSM community is working to achieve consensus on the best methods.

QSM has important advantages over phase images and a widespread precursor known as susceptibility weighted imaging (SWI): it overcomes the non-local and orientation-dependent phase contrast (Shmueli, MRM 2009) to improve visualisation of tissue structure and composition.

Clinical applications are emerging based on QSM's sensitivity to tissue calcifications, iron, myelin and deoxyhaemoglobin content. QSM highlights iron-rich brain structures in Parkinson's disease, microbleeds and haemorrhages and distinguishes these from calcifications. QSM allows quantification of venous oxygenation with functional QSM now able to detect brain activity.

*European Research Council Consolidator Grant

12:27PM F36.00003: Magnetoencephalography using optically-pumped magnetometers* [invited] SVENJA KNAPPE (Presenter), SEAN KRZYZEWSKI, NICHOLAS NARDELLI, BRANISLAV KORENKO, GLEB ROMANOV, ORANG ALEM, JERAMY HUGHES, Mechanical Engineering, University of Colorado — Current magnetoencephalography (MEG) uses a helmet-shaped array of low-temperature superconducting quantum interference devices (SQUIDs) to image the magnetic field produced by the neural currents inside the head with millisecond temporal resolution. Moving the sensors closer to the scalp holds the promise of simultaneously increasing the spatial resolution of MEG. Our optically-pumped magnetometers (OPMs) are room-temperature sensors that work on the principle of laser spectroscopy of alkali atoms in a vapor cell. They can be microfabricated and placed in close proximity to the scalp for MEG. The MEG test system we present consists of 48 microfabricated OPMs, that are integrated into pairs on small flying lead sensor heads, such that they form 24 first-order gradiometers with a baseline of 2 cm. The gradiometer and magnetometer data are read out simultaneously. The sensors are assembled on a conformal 3D printed helmet with spokes that can be adjusted in the radial direction through a ratchet system. The magnetic field in the radial direction to the head is recorded with the magnetometers and radial gradiometers. We present first standard MEG recordings of resting-state measurements and evoked responses.

*NIH R01 EB019440
NIH: R01 NS094604
NIH: R44 NS090894
1:03PM F36.00004: Smart magnetic probes for in-vivo metrology [Invited] GARY ZABOW (Presenter), Applied Physics, National Institute of Standards and Technology (NIST), STEPHEN DODD, ALAN KORETSKY, NINDS, National Institutes of Health (NIH) — Magnetic resonance imaging (MRI) represents one of the most outstanding examples of the successful application of something that began as fundamental physics research. Together with related NMR technologies, it now impacts many fields including food, pharmaceutical, chemical, energy, and of course medical industries, where it has rapidly become one of the most widely used medical imaging and diagnostic tools. Not requiring ionizing radiation, it can benignly probe deep within the body, offering excellent soft tissue contrast and, compared with other radiological methods, high resolution imaging.

But there remains much room to further develop the technologies. Specifically, this talk will discuss several recent examples [1,2] of how work in physics and engineering is enhancing the functionality of MRI through (i) new contrast agents 10-100x more powerful than existing alternatives that enable in vivo tracking of cells down to the single cell level, (ii) new micromagnetic structures that add "color" or multiplexing capabilities to traditionally black-and-white MRI, and (iii) smart polymer – magnetic composites that enable new radio-frequency (RF) addressable microsensors, or smart probes, for quantitative sensing. The talk will focus on the basic physics and engineering behind these imaging and sensing agents, including how they are made and some example first applications. Presentation will be at a general, introductory level; no prior knowledge of NMR/MRI required.

References:

1:39PM F36.00005: Ultra-low field and nonconventional MRI* [Invited] MATTHEW ROSEN (Presenter), Radiology, A.A. Martinos Center for Biomedical Imaging — A promising approach to portable MRI is operation at ultra-low magnetic field where cost-effective electromagnets become practical. MRI in the ultra-low field (ULF) regime — when the magnetic field used for signal detection is below 10 mT—is inherently challenging mainly due to intrinsically low Boltzmann polarization. We will discuss hardware methods to improve attainable SNR in the Johnston-noise-dominated regime of ULF using improved coils such as quadrature volume coils at 276 kHz (6.5 mT). We will also discuss our work to reduce noise and increase attainable information per unit time using compute-based approaches that leverage low-cost GPU. These include magnetic resonance fingerprinting (MRF) to enable multiple quantitative contrasts at ULF, and the use of our neural network deep learning approach, AUTOMAP (AUtomated TransfOrm by Manifold APproximation), to reconstruct highly-undersampled low SNR imaging data..

*We acknowledge funding from DOE/ARPA-E DE AR0000823 and DARPA N66001-17-C-4025.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F37 GMAG DMP: Pyrochlores I: Moment Fragmentation, Quantum Spin Liquids, and Beyond BCEC 206A - Bella Lake, Helmholtz-Zentrum Berlin - Tag(s): Focus

11:15AM F37.00001: Search for quantum phases in the rare earth zirconate and hafnate pyrochlore frustrated magnets [invited] MONICA CIOMAGA HATNEAN (Presenter), Department of Physics, The University of Warwick — Pyrochlores are interesting due to their versatile structure, frustrated magnetic lattice and their wide variety of exotic magnetic ground states (spin ices, spin frozen states, or long-range ordered states). The most studied pyrochlore oxides are the classical spin ices Dy2Ti2O7 and Ho2Ti2O7. One of the most interesting avenues of current research is into systems which exhibit novel magnetic ground states, such as quantum spin liquid (QSL) and quantum spin ice (QSI). Pr, Tb or Yb pyrochlores are good candidates for the realisation of quantum states. We have studied the zirconate and hafnate \(R_2M_2O_7\) (\(R=\) Rare Earth, \(M=\) Zr, Hf) oxides. Recent results show that they exhibit a variety of exciting magnetic behaviours and emergent properties, ranging from a disordered state with quadrupolar correlations and spin-ice-like excitations in \(Pr_2Zr_2O_7\), the fragmentation of magnetic moments into an ordered phase and a fluctuating state in \(Nd_2Zr_2O_7\), a disorder-induced QSL state in \(Tb_2Hf_2O_7\), to a potential QSI ground state with fractionalized excitations in \(Pr_2Hf_2O_7\). These investigations have been motivated by the availability of large high-quality single crystals of these materials. I will discuss the structural and magnetic characteristics of some of the zirconate and hafnate pyrochlores.
Antiferromagnet Ce₂Zr₂O₇

The pyrochlore antiferromagnet Ce₂Zr₂O₇ is sensitive to an instability of the Ce³⁺ oxidation state, whereby the 4f¹ electronic configuration of Ce³⁺ can be diluted via sample oxidation and the concomitant introduction of Ce⁴⁺ to the lattice.¹ For that reason, reduction of Ce₂Zr₂O₇ samples is required to enable a neutron scattering study of this material, the subject of this presentation. The spins in Ce₂Zr₂O₇ possess a local Ising anisotropy and interact via an antiferromagnetic coupling, which typically results in all-in all-out antiferromagnetic order. However the crystal electric field (CEF) wavefunctions of the Ce³⁺ ground state can have a dipole-octupole nature which is an ingredient for moment fragmentation and can allow for a disordered U(1) quantum spin liquid ground state.² High energy neutron spectroscopy confirms the dipole-octupole CEF ground state, and higher energy resolution inelastic neutron scattering shows a disordered ground state for Ce₂Zr₂O₇.

¹ S. Urban et al., Chem. Mater. 29 (21) (2017) 9218-9226
² Y.D. Li et al., Phys. Rev. B 95 (4) 041106(R) (2017)

Measurements at LANL were supported by the US DOE, Division of Materials Sciences and Engineering.

Neutron scattering study of breathing pyrochlore lattice material LiGaCr₄S₈

LiGaCr₄S₈ is a breathing pyrochlore lattice where the ordering of the Li⁺ and Ga³⁺ cations on the A-site of the spinel structure leads to the periodic expansion and contraction of Cr⁴⁺ tetrahedra. Strong magneto-elastic coupling drives negative thermal expansion in the temperature range 12-110 K. Neutron diffraction and inelastic neutron scattering experiments were carried out on polycrystalline samples of LiGaCr₄S₈ to investigate the spin configuration and spin-spin interactions. No long-range magnetic order is observed above 1.5 K. However, neutron diffraction shows the gradual appearance of a magnetic signal centered at |Q|~0.51 Å⁻¹ on cooling below ~100 K and a second contribution at |Q|~0.64 Å⁻¹ appears below 15 K. The inelastic neutron scattering data shows spin excitations with a zone boundary energy 12.6 meV at 4 K. The intensity of the inelastic signal weakens above 10 K though persists to nearly 100 K. At low energies the dynamic susceptibility can be described with a single temperature dependent relaxation.

*This research is funded by
1. Gordon and Betty Moore Foundation's EPIQS Initiative through Grant GBMF4416.
Non-spin-ice quantum spin liquid (QSL) with Ce-based dipole-octupole doublets Ce₂Zr₂O₇

Ce₂Zr₂O₇ is a high-quality single crystal grown by a floating zone method. We confirmed the Kramer doublet ground state in Ce³⁺ ions from crystal electric field measurements. We revealed that the quasi-elastic structure factor and Pauling entropy is totally suppressed in this system by carrying out diffuse neutron scattering and heat capacity measurements. Our AC magnetic susceptibility and muon-spin relaxation measurements suggest no spin freezing down to 0.02 K. Inelastic neutron scattering experiments display broad excitation continua along Brillouin zone boundaries, indicating fractional spin excitations, which is the key feature of QSL. This, together with the absence of features of spin ice and spin glass, suggest the system is a non-spin-ice QSL state at low temperature, where spins are highly correlated but fluctuate strongly.

Pyrochlore antiferromagnet CdYb₂Se₄ studied by neutron scattering

CdYb₂Se₄ is a geometrically frustrated pyrochlore lattice with exotic magnetic behavior. Our results give deeper insight into the CEF scheme and k=0 magnetic ground state. Additionally, we observed low energy spin excitations evolving with temperature and magnetic field. This grants a possibility to identify the exchange Hamiltonian of this frustrated antiferromagnet with strong quantum character.

Pyrochlore antiferromagnet CdYb₂Se₄

The pyrochlore lattice is well-established in titanates R₂Ti₂O₇ (R=rare earth) [1]. Spinel compounds AR₂X₄ with R-ions also residing on the pyrochlore lattice similarly exhibit unconventional magnetism [2, 3]. The basic distinction between the two families is the local environment of the rare earth ions [4, 5]. Here, we present a neutron scattering study of the crystal electric field (CEF), magnetic ground state, and spin dynamics of CdYb₂Se₄. Extending recent studies on CdYb₂Se₄ [2, 4], our results give deeper insight into the CEF scheme and k=0 magnetic ground state. Additionally, we observed low energy spin excitations evolving with temperature and magnetic field. This grants a possibility to identify the exchange Hamiltonian of this frustrated antiferromagnet with strong quantum character.


*SNF grant 200020_162626
12:39PM F37.00006: Ultrasound investigation of Ce$_2$Zr$_2$O$_7$ at low temperatures and in high magnetic fields.
ANDREA BIANCHI (Presenter), JÉRÉMIE DUDEMAIN, Université de Montréal, JONATHAN GAUDET, EVAN SMITH, BRUCE GAULIN, Department of Physics and Astronomy, McMaster University, YULIA GRITSENKO, SERGEI ZHERLITSYN, JOACHIM WOSNITZA, Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf — Through careful controlling the atmosphere during the growth of Ce$_2$Zr$_2$O$_7$ we have been able to stabilize Ce$^{3+}$ and prevent the formation of non-magnetic Ce$^{4+}$. This allows us to study the interesting case of doublet-octupole moment on a pyrochlore lattice. In the pyrochlore structure the Ce$^{3+}$ J = 5/2 multiplet is split by crystal field interactions resulting in wave functions for the ground state Kramers doublet which correspond to a linear combination of m$_J$ = ±3/2 states. A generic model for these unusual doublets supports two distinct symmetry enriched U(1) QSL ground states in the corresponding quantum spin ice regimes. We measured ultrasound down to 20 mK and in magnetic fields of up to 10 T with the field applied along the [111] direction for transversal and longitudinal modes. In zero field we observe a softening of the modes for temperatures below 0.8 K, which is an indication for quantum fluctuations. At 20 mK, an increase of the magnetic field leads to decrease of the sound velocity and the curves show hysteresis which is reminiscent of the behaviour observed in Dy$_2$Ti$_2$O$_7$ and Ho$_2$Ti$_2$O$_7$.


12:51PM F37.00007: Extended Coulomb Liquid of Paired Hardcore Boson Model on a Pyrochlore Lattice
CHUN-JIONG HUANG (Presenter), University of Science and Technology of China, CHANGLE LIU, Fudan University, ZI YANG MENG, Institute of Physics, CAS, YUE YU, Fudan University, YOUJIN DENG, University of Science and Technology of China, GANG CHEN, Fudan University — There is a growing interest in the U(1) Coulomb liquid in both quantum materials in pyrochlore ice and cluster Mott insulators and cold atom systems. We explore a paired hardcore boson model on a pyrochlore lattice. This model is equivalent to the XYZ spin model that was proposed for rare-earth pyrochlores with "dipole-octupole" doublets. Since this model has no sign problem for quantum Monte Carlo(QMC) simulations in a large parameter regime, we carry out both analytical and QMC calculations. We find that the U(1) Coulomb liquid is quite stable and spans a rather large portion of the phase diagram with boson pairing. Moreover, we numerically find thermodynamic evidence that the boson pairing could induce a possible Z$_2$ liquid in the vicinity of the phase boundary between Coulomb liquid and Z$_2$ symmetry-broken phase. Besides the materials' relevance with quantum spin ice, we point to quantum simulation with cold atoms on optical lattices.

1:03PM F37.00008: Magnetic phase diagram of dipolar-octupolar pyrochlores
OWEN BENTON (Presenter), RIKEN — Recent experiments have revealed intriguing magnetic properties in a variety of rare-earth pyrochlores R$_2$M$_2$O$_7$ with magnetic ions R=Nd, Sm, Ce. Common to these systems is a low energy crystal field doublet with so-called "dipolar-octupolar" character. This is associated with several interesting phenomena including magnetic moment fragmentation and possible quantum spin liquid ground states. Additionally, the application of a magnetic field in the (1,1,1) or (1,1,0) directions allows tuning from a fully 3-dimensional state in zero field to 2-dimensional or 1-dimensional states in high field. This rich set of phenomena calls for a unified description with which we can quantitatively understand and predict the properties of dipolar-octupolar pyrochlores. In this talk, we will explore the magnetic phase diagram of these materials in applied magnetic fields using a combination of analytical and numerical methods. Particular attention will be paid to the emergent low dimensional states induced by external fields along the (1,1,1) and (1,1,0) directions. This work will enable us to explain the behaviour of diverse dipolar-octupolar pyrochlores and the emergence of new quantum states in these systems.
1:15PM F37.00009: Dynamical structure factor of the three-dimensional quantum spin liquid candidate NaCaNi$_2$F$_7^*$

HITESH CHANGLANI (Presenter), Florida State University, SHU ZHANG, Johns Hopkins University, KEMP PLUMB, Brown University, OLEG TCHERNYSHYOV, Johns Hopkins University, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems — We study the spin-1 pyrochlore material NaCaNi$_2$F$_7$ [1] with a combination of molecular dynamics simulations, stochastic dynamical theory and linear spin wave theory. The dynamical structure factor from inelastic neutron scattering is well described by a near-ideal Heisenberg Hamiltonian incorporating small anisotropic terms and weak second-neighbor interactions [2]. We find that all three approaches reproduce remarkably well the momentum dependence of the scattering intensity and its energy dependence with the exception of the lowest energies. We find (i) a complete lack of sharp quasiparticle excitations in momentum space over much, if not all, of the energy range; (ii) linear spin-wave theory appears to apply in a regime where it would be expected to fail for a number of reasons. We elucidate what underpins these surprises, and note that basic questions about the nature of quantum spin liquidity in such systems pose themselves as a result [3].


*Supported by U.S. DOE grant DE-FG02-08ER46544, Deutsche Forschungsgemeinschaft grant SFB 1143 and Florida State University start-up funds.

1:27PM F37.00010: Intermultiplet transitions and long-range order in Sm-based pyrochlores

VIVIANE PECANHA-ANTONIO (Presenter), ERXI FENG, Jülich Centre for Neutron Science at MLZ, Forschungszentrum Jülich GmbH, D. T. ADROJA, FABIO ORLANDI, Rutherford Appleton Laboratory, ISIS Facility, THOMAS BRÜCKEL, Jülich Centre for Neutron Science and Peter Grünberg Institut, Forschungszentrum Jülich GmbH, YIXI SU, Jülich Centre for Neutron Science at MLZ, Forschungszentrum Jülich GmbH — We present bulk and neutron scattering measurements performed on the isotopically enriched $^{154}$Sm$_2$Ti$_2$O$_7$ (titanate) and $^{154}$Sm$_2$Sn$_2$O$_7$ (stannate) samples. Both compounds display sharp heat capacity anomalies, at 350 mK and 440 mK, respectively. Inelastic neutron scattering measurements are employed to solve the crystalline electric field (CEF) excitations scheme, which includes transitions between the ground and first excited $J$ multiplets of the Sm$^{3+}$ ion. In order to further validate those results, the single-ion magnetic susceptibility of the compounds is calculated and compared with the experimental static susceptibility measured in low applied magnetic fields. We show that the inclusion of intermultiplet transitions in the crystal field analysis is fundamental to the understanding of the intermediate and, more importantly, low temperature magnetic behaviour of the Sm-based pyrochlores. Finally, the heat capacity anomaly is shown to correspond to the onset of an all-in-all-out long-range order in the stannate sample, while in the titanate a dipolar long-range order can be only indirectly inferred.

1:39PM F37.00011: The magnetic structure of the antiferromagnetic pyrochlore Gd$_2$Ti$_2$O$_7$

JOSEPH PADDISON, University of Cambridge, GEORG EHLERS, SNS, Oak Ridge National Lab, JASON GARDNER, NSRRC Taiwan, ROSS STEWART (Presenter), ISIS neutron and muon source, STFC — Canonical examples of highly frustrated antiferromagnets are the gadolinium pyrochlores Gd$_2$Ti$_2$O$_7$ (GTO) and Gd$_2$Sn$_2$O$_7$ (GSO) both of which order at ~1 K with different structures. GSO forms the Palmer-Chalker structure with a $k = 0$ propagation vector while GTO is reported to form a more complicated - and still controversial - partially ordered state with a propagation vector of $k=(1/2, 1/2, 1/2)$, splitting the crystallographically equivalent Gd sites into non-equivalent magnetic sites [1]. Standard neutron diffraction techniques don't allow unambiguous determination of the k-state, (i.e. 1 or a combination of the 4 possible propagation vectors). However, using a combination of single crystal diffraction, diffuse and inelastic neutron scattering on both powder and single crystal samples of GTO, we have determined that the partially ordered magnetic structure is double-k with orthorhombic space group symmetry. This is in agreement with recent theoretical predictions of a double-k structure based on mean-field-theory with thermal fluctuations [2]

1:51PM F37.00012: Tuning Epitaxial Strain in XY Pyrochlore Er₂Ti₂O₇  CONNOR BUHARIWALLA (Presenter), EVAN SMITH, McMaster University, JONATHAN GAUDET, Johns Hopkins University, ADAM ACZEL, Oak Ridge National Laboratory, PATRICK FOURNIER, Université de Sherbrooke, BRUCE GAULIN, McMaster University — Tuning parameters in frustrated magnetism allow us to explore the complex landscape of magnetically fragile ground states. In epitaxial thin film samples, we can study the statespace of epitaxial strain (caused by the lattice mismatch between substrate and film) and the reduced dimensionality inherent to a thin film. Thin film works on frustrated titanate pyrochlores have focused on spin ice compounds (Ho₂Ti₂O₇ and Dy₂Ti₂O₇)[1-3] and the unconventional magnetic ground state of Tb₂Ti₂O₇[4]. This study examines the ordered magnetic ground state of Er₂Ti₂O₇. The ground state selection between the Ψ₂ and Ψ₃ basis states of the Γ₅ manifold and the relative stability of Γ₅ to Palmer-chalker configurations have been shown to be sensitive to a number of tuning parameters such as magnetic dilution and isovalent non-magnetic substitution. By fabricating films of different thicknesses using pulsed-laser deposition, we tune the epitaxial strain on the magnetic lattice, and examine the subsequent magnetic groundstate through bulk characterization and neutron scattering.


2:03PM F37.00013: Pyrochlore titanates RETi₂O₇ (RE = Ho & Er): Stoichiometry and Crystal Growth*  ALIREZA GHASEMI (Presenter), SEYED KOOPPAYEH, Johns Hopkins University — The pyrochlore cubic structure, with a corner sharing tetrahedra network, is the host for candidates of frustrated magnetic materials such as spin ices, spin liquids, and compounds with non-collinear XY orders [1–3]. Pyrochlore titanates, as a subgroup of the pyrochlore family, have been extensively studied; however, the reported physical properties have been shown to significantly vary from one sample to another. Here, we report a systematic study of synthesis and crystal growth by the float-zoning techniques. Structural quality, lattice parameters, stuffing defects and oxygen vacancies were found to depend on synthesis and growth conditions. A method to grow stoichiometric and high-quality single crystals of titanates is also reported [4].

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0019331.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F38 GMAG DMP: Molecular Nanomagnets  BCEC 206B - Stephen Hill, Florida State University - Tag(s): Focus

11:15AM F38.00001: Experimental Evidence for Non-Collinear Antiferro-toroidic Ground State in a Dy₉ Molecule*  QING ZHANG (Presenter), SHIQI LI, MYRIAM SARACHIK, City College of New York of CUNY, MICHAEL L BAKER, The University of Manchester, THEOCHARIS STAMATATOS, Brock University — The single molecular toroics are a class of coordination complexes that exhibit spin vortex chiral ground states due to non-collinear arrangements of local magnetic moments. While ab initio methods can predict local magnetic moments, unequivocal experimental determination has proven more challenging. Typically, angular dependent single crystal magnetization would be a good method to obtain anisotropy information. However, periodicity resultant from the cluster symmetry has hindered the use of this method for the study of many complexes including Dy₃ [1]. In this work, we consider a snub square molecule, Dy₈ [2]. Multiple orientation single crystal magnetization, measured at 0.3 K, reveal the orientation of moments. These measurements, with a simple Ising model, are used to identify a zero toroidal ground state in Dy₈, highlighting the robustness of vortex chirality within larger Dy based molecular lattices.


*Supported by ARO W911NF-13-1-1025 (CCNY); the synthesis of the Dy₈ cluster was supported by NSERC (Discovery grant to Th.C.S.).
11:27AM F38.00002: Calculation of Exchange Coupling Constants in Mn-Ce Molecular Magnets

DIANTENG CHEN
(Presenter), XIANGGUO LI, YUN-PENG WANG, Department of Physics and Quantum Theory Project, University of Florida, SAYAK DAS GUPTA, Department of Chemistry, University of Florida, XIAOGUANG ZHANG, Department of Physics and Quantum Theory Project, University of Florida, GEORGE CHRISTOU, Department of Chemistry, University of Florida, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — Recently several Mn-Ce molecular magnets have been synthesized, including Mn$_3$Ce$_2$ and Mn$_5$Ce$_3$ with three different ligands, but their magnetic properties are yet to be detailed. We calculate the energies of all the spin configurations of each of these molecules by density functional theory. From the calculations of each molecule, we determine a Heisenberg Hamiltonian with antiferromagnetic or ferromagnetic exchange coupling constants using both spin-projected and non-spin-projected energies of the broken symmetry solutions and compare the results to the coupling constants fitted from experimental susceptibility data.

*This work was supported by the US National Science Foundation DMREF program under Grant No. CHE-1534401.

11:39AM F38.00003: Spin Echo Measurements with a Customized Electron Spin Resonance Spectrometer of an Atomic-clock Transition in the Molecular Nanomagnet Cr$_7$Mn

KAI-ISAAK ELLERS (Presenter), GAJADHAR JOSHI, CHARLES COLLETT, JONATHAN FRIEDMAN, Physics and Astronomy, Amherst College, DANIEL SAVA, GRIGORE TIMCO, RICHARD WINPENNY, Chemistry, University of Manchester — Molecular nanomagnets are promising systems for quantum computation but such applications require sufficiently long coherence times ($T_2$) to permit quantum logic operations. We report on the development of low-cost, customized instrumentation for measuring $T_2$ in such molecules, as well as promising results from the spin-1 molecular nanomagnet Cr$_7$Mn. We dilute Cr$_7$Mn samples in toluene at concentrations between 0.00001% and 10% and perform spin echo measurements using our home-made electron-spin resonance spectrometer. This is achieved by coupling our samples to a loop-gap resonator with adjustable resonant frequency and irradiating with short (~100 ns) electromagnetic microwave pulses controlled by an FPGA. We observe spin echo and Rabi nutation from our sample and measure both $T_2$ and $T_1$, the spin-lattice relaxation time. Further, we find an enhancement of $T_2$ by a factor of three at the avoided level crossing that occurs at zero field, evidence of an atomic-clock transition, where the dependence of the transition frequency on magnetic field vanishes to first order.

*Work supported by U. S. National Science Foundation under Grant Nos. DMR-1310135 and DMR-1708692.

11:51AM F38.00004: Enhancing spin-spin coherence times in a Cr$_7$Mn molecular nanomagnet at a clock transition

GAJADHAR JOSHI (Presenter), KAI-ISAAK ELLERS, CHARLES COLLETT, Physics and Astronomy, Amherst College, DANIEL SAVA, RICHARD WINPENNY, GRIGORE TIMCO, Department of Chemistry, The University of Manchester, JONATHAN FRIEDMAN, Physics and Astronomy, Amherst College — The development of quantum computing based on the spin qubits is contingent on the synthesis of spin qubits with long spin coherence time. Molecular nanomagnets (MNMs) are unique systems that allow chemical engineering of physical parameters in order to enhance their spin relaxation times. Atomic-clock transitions afford a method to significantly increase the spin-spin relaxation times ($T_2$) for MNMs [1]. In dilute samples of Cr$_7$Mn MNM with effective spin $S=1$, we have measured $T_2$ values as high as 3 µs near a clock transition. We find that the effects of the clock transition are more pronounced with increased dilution and reduced temperature. We present the results of detailed studies of these effects and suggest ways to increase the coherence times further.

Reference:

*This work is supported by U. S. National Science Foundation under Grant Nos. DMR-1310135 and DMR-1708692.
Forming a Two-Qubit System from Dimers of Molecular Nanomagnets*

CHARLES COLLETT (Presenter), Department of Physics and Astronomy, Amherst College, Amherst, MA 01002, USA, PAOLO SANTINI, STEFANO CARRETTA, Dipartimento di Fisica e Scienze della Terra, Universita di Parma, Parma 43123, Italy, JONATHAN FRIEDMAN, Department of Physics and Astronomy, Amherst College, Amherst, MA 01002, USA — Molecular nanomagnets (MNMs) are a class of materials that can make good spin qubit candidates due to their chemical engineerability. We present a method for constructing two-qubit gates using dimers of Cr7Mn, a spin S=1 MNM that features a zero-field clock transition. Operating at this transition increases T2, allowing for more gates during the lifetime of the quantum state. We show that such a dimer system can be used to behave as a two-qubit system in which all of the transitions between states are clock transitions. One-qubit gates can be achieved using pulsed electron-spin resonance, and two-qubit gates can be implemented using an always-on exchange interaction between the molecules of the dimer. After truncating the Hamiltonian to its four lowest-energy states and transforming into the interaction picture, we simulated both a one-qubit gate as well as a CNOT gate sequence that has a duration of 85 ns, finding average fidelities of 99.5% for both gates. We will briefly discuss ongoing work to experimentally implement these protocols.

*Work supported by U. S. National Science Foundation under Grant Nos. DMR-1310135 and DMR-1708692.

Pulsed Electron-Spin Resonance Studies of Atomic Clock Transitions in a Dimer of the Molecular Nanomagnet Cr7Mn*

MICHAEL CHA (Presenter), JONATHAN FRIEDMAN, Department of Physics and Astronomy, Amherst College, Amherst, MA, USA, DANIEL SAVA, GRIGORE TIMCO, RICHARD WINPENNY, School of Chemistry, The University of Manchester, Manchester UK, CHARLES COLLETT, Department of Physics and Astronomy, Amherst College, Amherst, MA, USA — Qubits, or quantum bits, rely on a quantum system that can hold any superposition of two states as opposed to just 0 or 1 as with a classical bit. Various systems have been explored as qubit candidates, including photons, trapped atoms, and both nuclear and electron spins. Our research focuses on constructing two-qubit systems using dimers of molecular nanomagnets (MNMs), a class of magnetic material that can be chemically engineered to achieve various desired attributes. The focus of our current work, dimers of the MNM Cr7Mn, features such an attribute: clock transitions between multiple spin states that increase the lifetime of the quantum state. We present pulsed electron-spin resonance (ESR) studies of dilute Cr7Mn dimers in loop-gap resonators, including spectroscopic exploration of two clock transitions in the dimer as well as progress on implementing two-tone ESR for two-qubit gates.

*Work supported by U. S. National Science Foundation under Grant Nos. DMR-1310135 and DMR-1708692.

Entanglement in a molecular magnet dimer*

[Invited] TATIANA GUIDI (Presenter), ISIS, STFC, ISIS facility, Rutherford Appleton Laboratory, ELENA GARLATTI, STEFANO CARRETTA, PAOLO SANTINI, GIUSEPPE AMORETTI, Dipartimento di Science Matematiche, Fisiche e Informatiche, Universita’ di Parma, JACQUES OLLIVIER, HANNU MUTHA, Institut Laue-Langevin, GRIGORE TIMCO, RICHARD WINPENNY, School of Chemistry, The University of Manchester — Entanglement is a crucial resource for quantum information processing and its detection and quantification is of paramount importance in many areas of current research. Weakly coupled molecular nanomagnets provide an ideal test bed for investigating entanglement between complex spin systems. However, entanglement in these systems has only been experimentally demonstrated rather indirectly by macroscopic techniques or by fitting trial model Hamiltonians to experimental data. We have exploited the capabilities of four-dimensional inelastic neutron scattering (INS) to portray entanglement in weakly coupled molecular qubits and to quantify it [1]. The INS measurements on the prototype (Cr7Ni)2 supramolecular dimer has allowed us to demonstrate the potential of this approach, which allows one to extract the concurrence in eigenstates of a dimer of molecular qubits.

References

*Financial support from the FIRB Project No. RBFR12RPD1 of the Italian Ministry of Education and Research and from EPSRC(UK) grant number EP/K039547/1. We acknowledge the Institute Laue-Langevin and the ISIS Neutron and Muon Source for the neutron beamtime.
1:03PM F38.00008: Observation of Anisotropy-driven Quantum Dynamics of Single-Molecule Magnet Spins at 100mK* REBECCA CEBULKA (Presenter), ENRIQUE DEL BARCO, University of Central Florida — We will present the continuing results of the implementation of our novel experimental technique to allow pulse EPR studies (spin echo) of condensed samples of single-molecule magnets and single-atom magnets (non-diluted crystals) at temperatures at or below 100mK. The aim is to eliminate dephasing due to dipolar fluctuations by freezing the spin state of all molecules in the crystal in the ground state without the need of applying strong magnetic fields. We expect that these conditions would allow us to study the quantum dynamics of the spins as governed by the intrinsic molecular magnetic anisotropy, which should give rise to non-well defined Rabi oscillations of the spin state, including metastable precessional spin states.

*The authors acknowledge support from the U. S. National Science Foundation under Grants No.DMR-1503627 and No.DMR-1630174

1:15PM F38.00009: Combined THz and Pulsed EPR studies on a Yb(III) Single Ion Magnet JONATHAN MARBEY (Presenter), Florida State University, STERGIOS PILIGIKOS, Chemistry, University of Copenhagen, JOSCHA NEHRKORN, MYKHAYLO OZEROV, National High Magnetic Field Lab, STEPHEN HILL, Florida State University — Recently, the development of single molecule magnets has shifted rapidly away from the use of transition metals in favor of lanthanides due to their large single ion anisotropy. This is a direct consequence of the relatively strong spin-orbit coupling inherent to lanthanides, which, in the presence of the appropriate crystal field, gives rise to well separated spin-orbit projected states that can permit slow relaxation of the magnetization. The motivation for studying such systems presumes that the so-called Orbach process provides the primary pathway through which the magnetization relaxes. However, previous studies on Yb(trensal) (1) have shown that simply having a large zero field energy barrier is not a sufficient criterion to achieve a high blocking temperature. In doing so, it was demonstrated that 1 also has the additional potential for use as a molecular spin qubit. To further investigate these properties in 1, we employ both Fourier Transform Far Infrared spectroscopy and pulsed EPR measurements to: i) characterize the zero field splitting associated with the crystal field and ii) probe the interactions that limit both spin-lattice and spin-spin relaxation by measuring the dependence on temperature and magnetic field.

1:27PM F38.00010: Zero field stability of holmium single atom magnets* PATRICK FORRESTER (Presenter), FRANÇOIS PATTHEY, EDGAR FERNANDES, HARALD BRUNE, FABIAN NATTERER, Ecole polytechnique federale de Lausanne — Since their magnetic remanence was first measured in 2016, holmium single atom magnets on MgO/Ag(100) have garnered significant attention due to their hour long spin lifetimes, read and write-ability with spin-polarized scanning tunneling microscopy (SP-STM), and high coercive magnetic field [1-3]. Despite having been characterized with X-Ray absorption, STM, and electron spin-resonance STM, the system has not been measured at zero field. This has led to ambiguities concerning the electronic ground state of Ho/MgO and the stability of the system at zero field [3]. Here we present SP-STM measurements demonstrating the zero-field stability of Ho single atom magnets. Using antiferromagnetic Mn$_{88}$Ni$_{12}$ tips, we read the atom's magnetic state, allow it to evolve under zero field conditions, and read it again. We discuss how these measurements can be used to determine the electronic ground state of the system.


*P.R.F. appreciates support from the Fulbright U.S. Student Program. F.D.N. and P.R.F. thank the Swiss National Science Foundation for support under project numbers P200P2_167965 and 200020_176932.
In photo-excited Rb_xCo[Fe(CN)_y]_z@K_nNi[Cr(CN)_b]_d core@shell spin-transition nanoparticles, the rate of the relaxation in the core is accelerated by more than an order of magnitude due to the presence of the shell [1]. In addition, the relaxation rate continues accelerating with increasing shell thickness, which an electro-elastic model explains as a change in the mechanical properties of the core due to its interface with an increasingly rigid shell [1,2]. Here, nuclear inelastic scattering (NIS) was used to study a series of heterostructures with different shells and selectively determine the stiffness of the core, using the low-energy phonon modes and the partial phonon density of states. The results show a significant softening of the low-temperature state in the core with increasing shell thickness, providing a possible explanation for the observed relaxation rate increase. The bulk modulus for each sample was determined using PXRD, and interestingly, shells of different compositions appear to have dissimilar effects on the stiffness of the low-spin state of the core, expected to predominate at low temperatures.


Supported by NSF DMR-1708410 (MWM).

Detection of emergent magnetic states at molecular interfaces by LE-μSR

MATTHEW ROGERS (Presenter), University of Leeds, RHEA STEWART, STEPHEN LEE, University of St. Andrews, THOMAS PROKSCHA, Paul Scherrer Institute, OSCAR CESPEDES, University of Leeds — The interfacial states that form due to orbital hybridisation and charge transfer at molecular interfaces can lead to fascinating magnetic properties. Several approaches to the characterisation of these surface states have been taken in the recent past such as SQUID magnetometry and XMCD. However, the resolution of these methods is often tested due to the confinement of these effects to interfaces. In this study, we use low energy muon spin rotation (LE-μSR) to probe such phenomena. Probing the transition oscillations between hyperfine energy levels of C_60 that has been interfaced with non-magnetic copper layers. We observe an increase in the transition frequency due to Zeeman splitting of the hyperfine tensor. We may eliminate this state through demagnetisation of the interface allowing us to attribute this observation to the emergent magnetic states at the CuC_60 interface. In a second system comprised of a metal oxide-C_60 interface. We have shown that optical gating of this photovoltaic device leads to increases in local fields at the interface due to a spin-dependent trapping of charge, thereby acting as a ‘spin capacitor’. These measurements demonstrate the capability of the μSR technique for the characterisation of novel thin film molecular structures and devices.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F39 GMAG DMP: Magnetic Coupling and Exchange Bias

BCEC 207 - Nathan Satchell, Michigan State University - Tag(s): Focus
Although ferromagnetism (FM) is in general a long-range collective phenomenon, it is possible to induce local spatial variations of magnetic properties in FM materials. For example, systematic variation of the exchange coupling strength can be used to create systems that behave as if they are composed of virtually independent segments that exhibit "local" Curie temperatures (Tc). While it is obvious that such localization should be possible across some lengthscale, the magnitude of that lengthscale is not so intuitive, nor is the expected behavior of a material exhibiting a nearly continuous variation in exchange strength. We have explored these questions in real materials by using neutron scattering and mean-field simulations to study novel compositionally graded transition metal multilayer films as model systems [1-3].

Remarkably, we have found that non-local magnetic effects are significant only over distances less than 3 nm (possibly much less). Beyond that the structures behave as a continuum of decoupled layers with distinct Tc. This leads to fascinating functionality, including FM phase boundaries that can be reversibly moved up and down the thickness of a film with temperature, and modified with an applied magnetic field. Since we have demonstrated this for an itinerant metal, we assert that for virtually any modulated magnetic material system, collective effects should be suppressed to down to nanometer length scales, so that magnetic behavior overall can be well described in terms of local material properties.


*Basque Govt Project No. PI2015-1-19, the Spanish Ministry of Economy, Industry and Competitiveness under the Maria de Maeztu Units of Excellence Prog. MDM-2016-0618 and Project No. FIS2015-64519-R (MINECO/FEDER), and NSF Award No. 1609066.

11:51AM F39.00002: Magnetization Depth Profile in a Magnetic Insulating Film Under a Thermal Gradient*
TIMOTHY CHARLTON (Presenter), ERJIA GUO, ANDREAS HERKLOTZ, MICHAEL R. FITZSIMMONS, HO NYUNG LEE, Oak Ridge National Laboratory — By eliminating mobile electrons, insulator spintronics offer opportunities to reduce power loss and signal decay of metallic interconnects in complicated integrated circuits. As a consequence, there are no energy losses due to the heating by the conducting electrons or eddy currents. This strategy requires methods to generate, transport, and detect the spin and transfer them into a charge-based signal for further processing. A temperature gradient has been shown to generate a pure spin current inside a magnetic insulator that could be detected in an adjacent metallic film with a high spin-orbital angle (spin Seebeck effect, SSE). Little experimental evidence is known about the depth dependence of spin structure. Using a similar sample design, we have measured the polarized neutron reflectivity (PNR) from a YIG film with and without a temperature gradient. We will present the magnetization as a function of depth in the magnetic insulator extracted from the PNR along with structural, magnetic, and electric transport characterization. We have observed a larger than expected magnetization in the GGG substrate which may contribute to the size of the SSE in similar samples.

*This work is supported by U.S. Department of Energy, Office of Science and the Office of Basic Energy Sciences.

12:03PM F39.00003: Quantum Magnon Casimir effect  
RAN CHENG (Presenter), Electrical and Computer Engineering, University of California, Riverside — Magnons are the quanta of spin-wave excitations in magnetically ordered media. Spin-up and spin-down magnons coexist in antiferromagnets (AFs) where they act similarly as photons in many different phenomena. We find that the zero-point quantum fluctuation of magnons in AFs can play a significant role in determining the properties of magnetic thin films. When two ferromagnets are separated by an insulating AF, they can couple and exert spin torques on each other even at absolute zero temperature, thanks to the zero-point quantum fluctuation of magnons confined in the AF. This is in perfect analogy to the Casimir effect of photons confined between two plates. Moreover, we find that in a ferromagnet/AF bilayer, the magnonic Casimir effect leads to a counterintuitive temperature dependence of the overall magnetization.
We present results on an exchange biased spin valve whose interlayer undergoes a magnetic phase transition. The structure consisted of 3 variations of Py_xCu_{1-x}: Py_0.8Cu_0.2/Py_0.4Cu_0.6/Py_1.0Cu/IrMn. The IrMn serves to exchange bias the Py layer; the degree to which the rest of the sample exhibits exchange bias depends on ferromagnetic coupling between the Py_xCu_{1-x} layers. Magnetization and angle with respect to temperature (M v. T and $\phi_M$ v. T, respectively) measurements from polarized neutron reflectometry (PNR) indicate a sharp transition temperature at T = 160 K, which is the Curie temperature (TC) of the spacer layer. Below this, both the Py_0.8Cu_0.2 and Py layers exhibit exchange bias. As the temperature increases and the system approaches 160 K, the portion of the loop corresponding to the bottom free layer (Py_0.8Cu_0.2) shifts closer to zero, showing a Néel-like transition. When T > 160 K, the coupling between the top and bottom layers is broken, and EB is only observed for the Py layer in direct contact with IrMn. Additional measurements studying the dependence on layer thickness will be reported.

*This work is supported by NSF Grant #1609066.

We report on high stability and enhanced exchange bias (EB) of ultra-dense (Tb/inch^2) arrays of sub-100 nm Co/CoO nanodisks. Exchange-biased nanodisks are grown by electron beam deposition of Co (15nm) using nanoporous anodic aluminum oxide (AAO) templates as a mask [1]. The thickness of the CoO layer, and therefore the EB of the nanodisks, can be tuned by the oxidation time of the disks. We have found that an annealing time of 10 minutes at 250°C in air produces the maximum EB (800 Oe) at 50K. A comparative study with a reference Co thin film is presented, showing that the nanodisks develop larger EB and higher blocking temperatures at each oxidation time. Although magnetic dots suffer lateral oxidation, which is not possible in the film, a simple model that takes into account this effect demonstrates that the exchange energy density in dots must be higher than that in the Co/CoO film. This is an exciting example of how nanopatterning can improve the physical properties of thin film systems.


*Work Supported by, DOE Office of Basic Energy Science grant DE FG02 87ER-45332, and EU grant H2020-MSCA-RISE-2016-734801.
Effects of field annealing on MnN/CoFeB exchange bias systems

PATRICK QUARTERMAN (Presenter), National Institute of Standards and Technology, INGRID HALLSTEINSEN, Lawrence Berkeley National Laboratory, MAREIKE DUNZ, Center for Spinelectronic Materials and Devices, Faculty of Physics, Bielefeld University, D-33615 Bielefeld, Germany, ALEXANDER GRUTTER, National Institute of Standards and Technology, MARKUS MEINERT, Center for Spinelectronic Materials and Devices, Faculty of Physics, Bielefeld University, D-33615 Bielefeld, Germany, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, JULIE BORCHERS, National Institute of Standards and Technology — Antiferromagnets are commonly used in magnetic tunnel junction based spintronics to fix the ferromagnetic reference layer using the exchange bias effect. The antiferromagnetic MnN Θ-phase exhibits large exchange bias fields on CoFe films on order of 1800 Oe which can be enhanced with increased annealing temperature [1,2]. The exchange bias field in MnN/CoFeB systems is observed to be dependent on annealing temperature and MnN thickness. The effect of annealing temperature (as-deposited, 325 and 525 C) and MnN thickness (30 and 48 nm) on the magnetic and structural properties of MnN/CoFeB samples have been examined with polarized neutron reflectivity (PNR), x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD). PNR fits show that nitrogen increasingly diffuses from MnN to the underlying seed layer as the annealing temperature increases, which leads to a disappearance of the exchange bias effect when the MnN thickness is not sufficient. Intermixing of Mn, Fe, and Co at the MnN/CoFeB interface is also observed in PNR, XAS and XMCD measurements and is correlated to observed changes in magnetization.


EXCHANGE BIAS IN IrMn3/Py BILAYERS

JOSE HOLANDA DA SILVA JUNIOR (Presenter), JOHN E. PEARSON, MICHAEL VOGEL, AXEL F HOFFMANN, Materials Science Division, ARGANNE NATIONAL LABORATORY — Recently antiferromagnets have gained increased interest as active components for spintronics due to their intrinsic high frequency dynamics and resulting zero net magnetic moment. One such material is IrMn3 with the magnetic moments forming a triangular structure in the (111) planes and a giant magnetocrystalline anisotropy energy of 10 meV per formula unit. We prepared films of IrMn3 on different substrates ([001]MgO, [0001]Al2O3 and Si). Since spin-orbit torques are most pronounced for [100] oriented IrMn3 we investigated the temperature and cooling field dependence of exchange bias. X-ray diffraction shows predominantly [100] crystallographic orientations, with also a small contribution due to [111] oriented grains. Magnetometry measurements using a quantum design superconducting quantum interference device (SQUID) show that the exchange bias decreases with increasing temperature and an anisotropy of the coercivity with in-plane field direction.

*This work was supported by the U.S. Department of Energy, Office of Science, Materials Science and Engineering Division and CNPq, Conselho Nacional de Desenvolvimento Científico e Tecnológico - Brasil (Scholarship).

Exchange bias induced by molecular spinterface

JUNHYEON JO (Presenter), Ulsan National Institute of Science and Technology, JINHO BYUN, Pusan National University, INSEON OH, JUNGMIN PARK, MI-JIN JIN, Ulsan National Institute of Science and Technology, BYOUNG-CHUL MIN, Korea Institute of Science and Technology, JAEEKWANG LEE, Pusan National University, JUNG-WOO YOO, Ulsan National Institute of Science and Technology — Molecular spins as individual are promising quantum states for coming computation technology. The “on surface” configuration of molecules in proximity to a magnetic film allows control over the orientations of molecular spins and interfacial coupling between them. The stacking of planar molecular spins could favor antiferromagnetic interlayer coupling and lead to pinning of the magnetic underlayer via exchange bias, extensively utilized in magnetic devices. Here, we show tunable molecular exchange bias and its asymmetrical magnetotransport features by varying composition of metalloporphyrin/ferromagnet bilayers. The systems exhibit a wide range of interfacial coupling (ferromagnetic or antiferromagnetic) and exchange bias. Transport measurements of the bilayers reveal the molecular exchange bias effect on a fabricated device, representing asymmetric behaviors on anisotropic and angle-dependent magnetoresistance. Theoretical calculations demonstrate the orientation of spins and interfacial magnetic coupling, and further understanding to exchange bias. A study of interfacial coupling in molecule/ferromagnet systems and its impact on magnetic and magnetotransport behaviors will extend functionalities of molecular spinterface for emerging information technology.
1:27PM F39.00010: Effect of CoFe Dusting Layer and Annealing on the Magnetic Properties of Sputtered Ta/W/CoFeB/CoFe/MgO Layer Structures*  JUSTINE DROBITCH (Presenter), Electrical and Computer Engineering, Virginia Commonwealth University, YU-CHING HSIAO, HAO WU, KANG WANG, Electrical and Computer Engineering, University of California, Los Angeles, CHRISTOPHER S LYNCH, College of Engineering, University of California at Riverside, SUPRIYO BANDYOPADHYAY, Electrical and Computer Engineering, Virginia Commonwealth University, DANIEL B GOPMAN, Materials Science and Engineering Division, National Institute of Standards and Technology — Ultrathin CoFeB films are an essential building block of most emerging spintronic applications due to the tunable perpendicular magnetic anisotropy (PMA) energy, low Gilbert damping and high annealing stability. Improvements in these magnetic properties are being explored through interface engineering. We explored the effect of a CoFe wedge inserted as a dusting layer (0.1 nm – 0.3 nm thick) at the CoFeB/MgO interface of a sputtered Ta(2 nm)/W(3 nm)/CoFeB(0.9 nm)/MgO(3 nm) film – a typical structure for spin-orbit torque devices. Films were annealed in a Rapid Thermal Annealer (RTA) at temperatures varying between 300 °C and 400 °C in an Ar environment. Ferromagnetic resonance studies were carried out to estimate the effective PMA field and the Gilbert damping as a function of the CoFe thickness and across several annealing temperatures. While as-deposited films present only easy-plane anisotropy, a transition along the wedge from easy-plane to out-of-plane was observed across several annealing temperatures. Interlaying a CoFe dusting film between CoFeB and MgO provides an alternative approach for PMA in ultrathin films.

*Supported by NSF grant ECCS-1609303

1:39PM F39.00011: Hydrogen-driven switching of the magnetic surface anisotropy at the Co/Pd interface* GRACE CAUSER (Presenter), ANSTO, MIKHAIL KOSTYLEV, University of Western Australia, DAVID CORTIE, XIAOLIN WANG, University of Wollongong, FRANK KLOSE, Guangdong Technion-Israel Institute of Technology — Heterostructures exhibiting perpendicular magnetic anisotropy (PMA) have proven to be indispensable within the magnetic recording industry. By exploiting the hydrogen-induced modifications to PMA which occur exclusively at the ferromagnetic/Pd interface, an opportunity exists to expand the potential applications of PMA-based heterostructures into the realm of hydrogen sensing using ferromagnetic resonance (FMR) - an electron-spin based technology. Here, we present an interface-resolved in-operando study of a Co/Pd film which features tailorable PMA in the presence of hydrogen gas. We combine polarized neutron reflectometry with in-situ FMR to explore the nanoscopic interactions of hydrogen at the Co/Pd interface which affects the spin-resonance condition during hydrogen cycling. Key experimental data and theoretical modelling reveal that the interfacial PMA of the Co/Pd film suppresses non-reversibly upon primary exposure to hydrogen gas – highlighting a potential avenue for spintronics-based hydrogen sensing.

*The Australian Government Research Training Program Award and the Australian Institute of Nuclear Science and Engineering Postgraduate Research Award.

1:51PM F39.00012: Perpendicular Magnetocrystalline Anisotropy on 3d Transition-Metals Multilayers – A First-principles Study  THI PHUONG THAO NGUYEN (Presenter), Institute of Scientific and Industrial Research, KOHJI NAKAMURA, Department of Physics Engineering, Mie University, TAMIO OGUCHI, Institute of Scientific and Industrial Research — Magnetic tunnel junctions (MTJ) with perpendicular magnetocrystalline anisotropy (MCA) have much attention for applications to high-density, high-thermal stability, nonvolatile memories. Strong perpendicular MCA appears in transition-metal films such as Co/Pt, Co/Pd and CoFeB/Pd due to the strong hybridization between the 3d and 5d orbitals at the interfaces. The remaining challenge in these systems is to understand the role of the hcp-fcc phase transition that occurs in cobalt, which leads to the change of the easy magnetization direction. To address this challenge, the mechanisms of MCA in hcp-like and fcc-like stacking of Co-based 3d transition-metal multilayers are systematically investigated by using full-potential linearized augmented plane wave calculations. The MCA energy of possible atomic-layer alignments of Co-based films including Mn, Fe, and Ni layers is presented. The results predict that large perpendicular MCA can be achieved in Co/Ni multilayers for both hcp-like and fcc-like stackings. The large perpendicular MCA arises from a second-order effect of spin-orbit coupling between occupied and unoccupied Ni $d_{yz,xz}$ states near the Fermi level. A promising transition-metal film for MTJ with giant perpendicular MCA and the preferred stacking stability is demonstrated.
Ab initio calculations of structural, optical and magnetic properties of ordered MxPt1-x, (M= Co, Ni, Fe and Mn) binary alloys — Ab initio calculations of the structural, optical and magnetic properties of ordered M x Pt 1-x, (M= Co, Ni, Fe and Mn) binary alloys have been performed. The optimized parameters of L10 CoPt, FePt and MnPt systems have been calculated and found to be (a o = 3.805, c o = 3.707 )Å, (a o = 3.88 , c o = 3.73 )Å and (a o = 4.03 , c o = 3.69 )Å, respectively. In addition, we found that L12 Ni 3 Pt exhibits a o = 3.64 Å. Our calculations of electronic band structure, density of states (DOS) and partial density of states of M x Pt 1-x binary alloys indicate that the contributions to total DOS of M x Pt 1-x come mainly from M-3d and Pt-5d electronic states, in CoPt, Ni 3 Pt, FePt and MnPt. Furthermore, magneto-crystalline Anisotropy Energy (MAE) of CoPt, FePt and MnPt systems have been calculated using The Force theorem and the slap approach and found to be (5 × 10 7 erg/cm 3 ), (6.5× 10 7 erg/cm 3 ) and (1.2 × 10 7 erg/cm 3 ) respectively. Our results reveal that ordered M x Pt 1-x exhibit attractive optical and magnetic properties that make them potential candidates for optical-electronic and magneto-optical devices.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F40 GMAG DMP: Transport in Magnetic Materials — Qiming Shao, University of California, Los Angeles — Tag(s): Focus

Current polarity-dependent manipulation of antiferromagnetic domains (Invited) — PETER WADLEY (Presenter), SONKA REIMERS, STUART POOLE, OLIVER AMIN, MU WANG, School of Physics and Astronomy, University of Nottingham, JOAO GODINHO, Department of Spintronics and Nanoelectronics, Institute of Physic, ASCR, Prague, KEVIN EDMONDS, RICHARD CHAMPION, School of Physics and Astronomy, University of Nottingham, VÍT NOVÁK, JOERG WUNDERLICH, TOMAS JUNGWIRTH, Department of Spintronics and Nanoelectronics, Institute of Physic, ASCR, Prague, BRYAN GALLAGHER, School of Physics and Astronomy, University of Nottingham — Antiferromagnetic spintronics offers the potential for ultrahigh speed dynamics, stability against strong magnetic field perturbations, higher component packing density owing to the lack of stray fringing fields, as well as a wider material base and qualitatively new physical phenomena. Tetragonal CuMnAs is a testbed system in which the antiferromagnetic order parameter can be switched reversibly using electrical currents (1). Previously, orthogonal in-plane current pulses were used to induce 90 degree rotations of antiferromagnetic domains in a multi-terminal geometry(2). This type of switching has now also been demonstrated in another antiferromagnet system with similar symmetry properties (4,5).
Here, we demonstrate a new mechanism by which antiferromagnetic domain walls in CuMnAs can be manipulated to realize stable and reproducible domain changes using only two electrical contacts. In this geometry, current polarity is reversed changing the sign of the current-induced fields. The resulting Néel spin orbit torque acts primarily on the domain wall. The reconfigurations are imaged using x-ray magnetic linear dichroism microscopy, and detected electrically. The switching by domain wall motion can occur at much lower current densities than coherent domain switching.

5)Meinert et al arXiv:1706.06983
**11:51AM F40.00002: Dynamic Spin Transport in Antiferromagnetic Insulators: Non-sinusoidal Angular Dependent Spin Pumping in Y\textsubscript{3}Fe\textsubscript{5}O\textsubscript{12}(YIG)/NiO/Pt Trilayers**  
YANG CHENG (Presenter), Ohio State University, RICARDO ZARZUELA, Physics, University of California, Los Angeles, JACK T BRANGHAM, AIDAN J LEE, SHANE WHITE, P CHRIS HAMMEL, Ohio State University, YAROSLAV TSERKOVNYAK, Physics, University of California, Los Angeles, FENGYUAN YANG, Ohio State University — Antiferromagnets (AF), which usually serve as the passive layer in spintronics research, have recently been found as effective spin transport media in the FMR driven spin pumping measurement. For example, a YIG/Pt bilayer shows that with the insertion of a 1 nm NiO interlayer could enhance the inverse spin Hall voltage ($V_{\text{ISHE}}$), which scratches the surface of the promising antiferromagnetic spintronics. Recently, we studied the out-of-plane angular dependence of $V_{\text{ISHE}}$ in YIG/NiO/Pt heterostructures with different thicknesses of NiO under a large range of temperatures. The appearance of plateaux for $V_{\text{ISHE}}$ over the out-of-plane field angle is very different from the YIG/Pt bilayer, which should have a sinusoidal dependence. A maximum is even found at around 30° from the surface normal for specific values of NiO thickness and temperature. By modeling the spin structure of NiO under an out-of-plane magnetic field after considering the interplay among the interfacial exchange coupling, the AF easy-plane anisotropy, and the field-induced hard-axis anisotropy in NiO, the main features of the experimental data in the nontrivial angular dependence of the spin pumping in YIG/NiO/Pt trilayers have been reproduced.

*This work was supported by OSU MRSEC (DMR-1420451) and DOE (DE-SC0001304).

**12:03PM F40.00003: Spin-Orbit Torque Switching in a Nearly Compensated Heusler Ferrimagnet**  
JOSEPH FINLEY (Presenter), Massachusetts Institute of Technology, CHIA-HAO LEE, PINSHANE HUANG, Materials Science and Engineering, University of Illinois Urbana-Champaign, LUQIAO LIU, Massachusetts Institute of Technology — Ferrimagnetic materials combine the advantages of the low magnetic moment of an antiferromagnet and the easiness of realizing magnetic reading of a ferromagnet. Recently, it was demonstrated that compensated ferrimagnetic half metals can be realized in Heusler alloys, where high spin polarization, zero magnetic moment, and low magnetic damping can be achieved at the same time. In this work, by studying the spin-orbit torque induced switching in the Heusler alloy Mn$_2$Ru$_{1-x}$Ga, we found that efficient current-induced magnetic switching can be achieved in a nearly compensated sample with strong perpendicular anisotropy and large film thickness. Our work demonstrates the possibility of employing compensated Heusler alloys for fast, energy-efficient spintronic devices.

**12:15PM F40.00004: Magnetism and Magneto-Electric Transport in Amorphous Cobalt- and Iron-Germanium Thin Films**  
DINAH SIMONE BOUMA (Presenter), Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, FRANK BRUNI, Department of Physics, University of California, Berkeley, ROBERT STREUBEL, Materials Sciences Division, Lawrence Berkeley National Laboratory, XIAOQIAN M CHEN, Materials Sciences Division, Lawrence Berkeley National Laboratory, and University of Kentucky, SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Laboratory, NOAH KENT, Materials Sciences Division, Lawrence Berkeley National Laboratory, and Department of Physics, University of California, Santa Cruz, ZHANGHUI CHEN, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, PETER FISCHER, Materials Sciences Division, Lawrence Berkeley National Laboratory, and Department of Physics, University of California, Santa Cruz, STEPHEN DOUGLAS KEVAN, Advanced Light Source, Lawrence Berkeley National Laboratory, FRANCES HELLMAN, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — Thin films (65 < t < 100nm) of amorphous cobalt- and iron-germanium (a-Co$_x$Ge$_{1-x}$ and a-Fe$_x$Ge$_{1-x}$) with 0.40 < x < 0.61 exhibit similar electrical resistivity but remarkably different magnetization for a fixed transition metal concentration x. For all compositions investigated, the resistivity depends weakly on temperature but strongly on x, with only slight differentiation between the Fe and Co transition metal species. However, a low-temperature upturn in resistivity associated with resonant impurity scattering is observed in a-Fe$_x$Ge$_{1-x}$ but absent in a-Co$_x$Ge$_{1-x}$ due to their different magnetic properties: where all measured compositions of a-Fe$_x$Ge$_{1-x}$ are itinerant ferromagnets with a Curie temperature that increases with x, a-Co$_x$Ge$_{1-x}$ is paramagnetic down to $T = 2$ K in the same composition range. This behavior parallels these materials' crystalline cousins: B20 FeGe hosts a rich magnetic phase diagram, while B20 CoGe is paramagnetic thanks to a pseudogap just above the Fermi level in its density of states. The long-range order that enables this explanation in those materials is absent in our amorphous films, leading us to ascribe the magnetic behavior of these alloys to more localized, short-range physics.

*Work supported by DOE BES MSD DE-AC02-05-CH11231, Magnetic Materials Program*
Parametric resonance is a versatile tool for excitation of spin waves in nano-magnonic devices. Here we present a joint theoretical and experimental study of parametric resonance of magnetization in nanowires made from bilayers of Pt and Permalloy (Py). In this system, damping of spin waves in Py can be tuned via antidamping spin Hall torque arising from electric current in the Pt layer. We report parametric excitation of spin waves driven by microwave current applied to the nanowire, and tuning of the resonance properties by direct current. Under magnetic field applied perpendicular to the wire axis, we observe parameter excitation of two types of spin wave eigenmodes: bulk and edge modes. Comparison of our theoretical description of parametric resonance of these modes to the experimental data reveals important role played by the Oersted field produced by ac and dc currents for the excitation process. Theoretical analysis of the data allows us to extract information on the spin Hall efficiency in the Pt/Py device as well as on damping parameters of the excited spin wave modes.

*Fondescyt Project 1170781 (Chile), Basal Program for Centers of Excellence, Grant FB0807 CEDENNA, CONICYT.

Reciprocity relations between the entries of the conductance matrix of a multi-terminal linear device, comprising normal metallic and strong ferromagnetic elements with spin-inactive interfaces between them. In particular, reciprocity equates the spin transmissions through a two-terminal element in the opposite directions. When applied to “geometric spin ratchets”, reciprocity shows that certain effects, announced for such devices, are, in fact, impossible. Finally, we discuss the relation between our work and the spintronic circuit theory formalism.

Ya. B. is grateful to CNRS for financial support of the visits to the Laboratoire de Physique Theorique, Toulouse.

Spin current-driven transitions of magnetic domain patterns in a prototypical multilayer stack of Ta/CoFeB/MgO. The transition processes are demonstrated to be greatly related to responses of topological defects to the spin orbit torque. A moderate perpendicular magnetic field favors stripe domains in the ferromagnetic layer; however, the stripes are cut into dense skyrmions with applying current pulses, where half-skyrmions at the ends of stripes have been proposed to be important. More types of topological excitations are observed in labyrinthine domain patterns at a zero magnetic field. The topological defects can be deleted/generated by spin current with lower/higher current densities. The current-induced deletion/generation of topological defects leads labyrinthine domains to transform into phases with a strong/weak orientational order. We conclude from a derived Thiele equation and micromagnetic simulations that both the current-driven motion of topological defects and magnetization manipulations at domain walls are of significance in current-induced transitions.

We acknowledge the financial support by the National Key R&D Program of China through Grant No. 2017YFA0303202 and by US National Science Foundation through Grants No. DMR-1307056.
1:03PM F40.00008: Activation barriers for creation and annihilation of magnetic droplet solitons  GABRIEL CHAVES-O’FLYNN (Presenter), Department of Thin Films, Institute of Molecular Physics Polish Academy of Sciences, DANIEL L STEIN, ANDREW D KENT, Department of Physics, New York University — Droplet solitons are magnetization fluctuations that preserve their shape as they precess with uniform frequency $\omega=0$. They satisfy a delicate balance between anisotropy and exchange interactions, and decay in the presence of dissipation. To prevent this, a spin polarized current $\sigma$ can be applied via a nanocontact of radius $\rho^*$. The magnitude of the current can be increased to induce switching between uniform precession at the ferromagnetic resonance frequency ($\omega=1$), and a stable precession at a frequency larger than the Zeeman frequency ($\omega=0$, in zero applied field).

In the absence of dissipation, conservative solitons of frequency $\omega_0$ are described by a function $\Theta(\rho;\omega_0)$ where $\Theta$ is the angle of the magnetization with the easy axis ($z$) and $\rho$ is the distance to the center of the nano contact [1].

We introduce an effective energy $\xi$ that quantifies the work done (against damping and spin torque) to create a fluctuation of arbitrary shape $\Theta(\rho)$. We show that, for specific values of $\sigma$, some conservative soliton solutions are saddles of $\xi$. This allows us to calculate activation barriers $\Delta\xi$ between uniform precession at the ferromagnetic resonance and stable solitons. We present results of $\Delta\xi$ as a function of $\sigma$ for a variety of nanocontact radii $\rho^*$ and spin-torque anisotropy parameters $\nu$.

1:15PM F40.00009: Effect of magnetic tunneling layer in van der Waals Josephson Junction  HIROSHI IDZUCHI (Presenter), Tohoku University(IMRAM) and RIKEN(CEMS), KEN HARADA, CEMS, RIKEN, KO-FAN HUANG, Physics department, Harvard University, NA HYUN JO, Iowa State University and Ames Laboratory, DAISUKE SHINDO, Tohoku University(IMRAM) and RIKEN(CEMS), PAUL CANFIELD, Iowa State University and Ames Laboratory, PHILIP KIM, Physics department, Harvard University — Van der Waals (vdW) material has been attracted much attention recently because of their unique features including the accessibility to atomically thin and flat single-crystalline heterostructure. The two-dimensional (2D) nature of these heterointerfaces often enhances the quantum effect. Here, we report vdW ferromagnet can provide a unique opportunity to study the interplay of superconductivity and magnetism. We fabricated a ferromagnetic tunneling device consisting of vdW ferromagnet and superconductor. We observed that the devices exhibit Josephson coupling through magnetic tunneling across 1-6 atomic unit cell thick ferromagnetic insulating layers. Our observation is in contrast with the lack of Josephson coupling reported across traditional ferromagnetic insulating materials such as EuS. We also observed that our superconductor/ferromagnet hybrid devices show the hysteretic critical current against magnetic field sweep. The observed hysteresis differs from the one expected from the coercive field of the ferromagnet. Further study on magnetic structure and switching current distribution indicates the observed phenomena arisen from the interplay between magnetic domain and superconducting vortex structures.

1:27PM F40.00010: Noncollinear Spin Torque Effect in Magnetic Heterojunctions: Combined First-Principles Calculation and TB-NEGF Method*  BAO-HUEI HUANG (Presenter), CHIA-CHIA CHAO, YU-HUI TANG, Department of Physics, National Central University, CHAO-CHENG KAUN, Academia Sinica, Research Center for Applied Sciences — In this study, our newly developed “JunPy” [1] package has successfully combined the self-consistent Hamiltonian by using the first-principles calculation [2], including multi-band dispersion relation and complicated interfacial coupling, with the TB model and the non-equilibrium Green's function (NEGF) method to investigate the noncollinear magnetotransport properties in nm-scale magnetic heterojunctions. This program is first testified by the spin-polarized currents and the noncollinear spin torque effect in conventional Fe/MgO/Fe MTJ. We further employed it to predict the giant field-like spin torque (FLST) effect in the amine-ended single-molecule magnetic junction [3], which may open a new avenue for multifunctional manipulation in next-generation organic FLST-MRAMs with lower power consumption.


*This work is supported by the Ministry of Science and Technology (MOST 106-2112-M-008-011- and 106-2633-M-008-002-) and the National Center for Theoretical Sciences, Republic of China.
1:39PM F40.00011: Double Tunnel Junction Experiments With Asymmetric Barriers* LEONARDO RIÓS E (Presenter), EDGAR PATINO, University of the Andes, DENIS CHEVALLIER, University of Basel — Magnetic tunnel junctions constitute a research area of great promise due to its potential application in faster and non-volatile memories. Current studies on Magnetic Tunnel Junctions (MTJ) are abundant for different magnetic and insulator materials. Nevertheless, available references for Double Magnetic Tunnel Junctions (DMTJ) are scarce. Previous studies on Tunneling Magnetoresistance (TMR) Oscillations in DMTJ indicate that asymmetry in the potential barriers is a significant aspect for controlling the TMR. In the present work we show the fabrication of Al/Al₂O₃/Al/Al₂O₃/Al double tunnel junctions with asymmetric barriers by e-beam evaporation and oxygen plasma processes in UHV chamber. The experimental process allows us to characterize each of the junctions separately. This way the parameters, width and thickness, were easily extracted for each of the junctions, prior to be used in a model for double tunnel junctions.

*Convocatoria 2018-2 Para la financiación de proyectos de investigación y presentación de resultados en eventos académicos categoría: estudiantes de doctorado candidatos, proyecto código INV-2018-33-1268

1:51PM F40.00012: Low frequency noise in MgO magnetic tunnel junctions with magnetic flux concentrator* YIOU ZHANG (Presenter), GUANYANG HE, GANG XIAO, Brown University — Magnetic tunnel junctions (MTJ) have been widely studied as ultra-sensitive magnetic sensors, due to their high sensitivity, low power consumption, and small size. Field detectability of MTJ sensor, particularly at low frequency, is primarily limited by its intrinsic 1/f noise. Hence understanding in the noise performance of MTJ sensor is important for its application. Also, magnetic flux concentrator can enhance signal level of MTJ sensor, yet its role in the noise performance of the sensor system is not fully investigated. In this work, we have measured sensitivity and low-frequency noise spectrum (1 Hz – 10 kHz) of MgO-based MTJ sensor incorporated with an on-chip magnetic flux concentrator. We have found that 1/f noise strongly depends on the bias magnetic field, and a linear relationship between 1/f noise and sensitivity is observed. This result indicates that 1/f noise in highly-sensitive MTJ sensor is dominated by magnetic noise, originated from thermal magnetic fluctuations. Role of magnetic flux concentrator in noise performance will also be discussed.

*The work was supported by National Science Foundation through Grants No. DMR-1307056, and by King Abdullah University of Science and Technology (KAUST).

2:03PM F40.00013: All-electrical control of spin transport in a three-terminal yttrium iron garnet/platinum nanostructure* MATTHIAS ALTHAMMER (Presenter), TOBIAS WIMMER, STEPHAN GEPRÄGS, MATHIAS WEILER, RUDOLF GROSS, HANS HUEBL, Walther-Meißner-Institut, Bavarian Academy of Sciences and Humanities — Pure spin currents, i.e. the flow of angular momentum without an accompanying charge current represents a new paradigm in the field of spintronics. Most importantly, pure spin currents can be transported by fermions, i.e. by electrons, in electrical conductors as well as by bosons, i.e. by quantized magnetic excitations, in magnetically ordered insulators. Interestingly, heterostructures consisting of spin-orbit coupled metals with magnetically ordered insulators allow to investigate pure spin current transport in both regimes and their interconversion at the interface [1]. We here report on the control of magnon spin currents via a DC charge current injected pure spin current. To this end, we utilize three electrically isolated platinum (Pt) electrodes deposited on an ultrathin yttrium iron garnet (YIG) film. Employing all-electrical injection and detection mechanisms, we provide evidence for efficient spin transport manipulation by a DC charge current in these devices. Moreover, we discuss the physical origin of non-linear effects in such structures.


*Financial support by the DFG via project AL 2110/2-1 is gratefully acknowledged.
Observation of magnetic vortex pairs at room temperature in a planar α-Fe₂O₃/Co heterostructure

PAOLO G. RADAELLI (Presenter), FRANCIS CHMIEL, NOAH WATERFIELD PRICE, ROGER JOHNSON, Clarendon Laboratory, University of Oxford, ANNE D LAMIRAND, Diamond Light Source, Didcot, UK, JONATHON L SCHAD, Department of Materials Science and Engineering, University of Wisconsin-Madison, GERRIT VAN DER LAAN, Diamond Light Source, Didcot, UK, DAVID T HARRIS, Department of Materials Science and Engineering, University of Wisconsin-Madison, JULIAN J IRWIN, MARK S RZCHOWSKI, Department of Physics, University of Wisconsin-Madison, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison — Vortices, occurring whenever a flow field 'whirls' around a one-dimensional core, are among the simplest topological structures, ubiquitous to many branches of physics. In the crystalline state, vortex formation is rare, since it is generally hampered by long-range interactions: in ferroic materials (ferromagnetic and ferroelectric), vortices are observed only when the effects of the dipole–dipole interaction are modified by confinement at the nanoscale, or when the parameter associated with the vorticity does not couple directly with strain. We observed an unprecedented form of vortices in antiferromagnetic haematite (α-Fe₂O₃) epitaxial films, in which the primary whirling parameter is the staggered magnetization [1]. Remarkably, ferromagnetic topological objects with the same vorticity and winding number as the α-Fe₂O₃ vortices are imprinted onto an ultra-thin Co ferromagnetic over-layer by interfacial exchange. Our data, supported by micro-magnetic modelling, suggest that the ferromagnetic vortices may be merons (half-skyrmions, carrying an out-of-plane core magnetization), and indicate that the vortex/meron pairs can be manipulated by the application of an in-plane magnetic field, giving rise to large-scale vortex–antivortex annihilation.


Collinear Anomalous Hall Antiferromagnets

HUA CHEN (Presenter), Colorado State University, ALLAN MACDONALD, The University of Texas at Austin — It is now well established both theoretically and experimentally that the anomalous Hall effect (AHE) can exist in certain noncollinear antiferromagnets with vanishing total magnetization. Using similar symmetry arguments we propose that the AHE and the related properties such as magneto-optical Kerr effect, anomalous Nernst effect, orbital magnetization, etc., can also exist in many collinear antiferromagnets with symmetry-allowed spin canting. Similar to the noncollinear case, these AHE-related effects will still be finite when the net spin magnetization vanishes. We give two classic examples, NiF₂ and α-Fe₂O₃, corresponding to different mechanisms for spin canting, i.e. single-ion anisotropy and Dzyaloshinskii-Moriya interaction. Although these two materials are good insulators and may not be easily doped in order to measure the AHE, the discussion is general and can be applied to many other canted antiferromagnets. We construct minimal models with spin-orbit coupling terms compatible with these canting mechanisms, and discuss the similarities and differences between the collinear and the noncollinear cases.

Nonlocal Spin Transport Mediated by a Vortex Liquid in Superconductors

SE KWON KIM (Presenter), Department of Physics and Astronomy, University of Missouri - Columbia, ROBERTO MYERS, Department of Materials Science and Engineering, The Ohio State University, YAROSLAV TSERKOVNYAK, Department of Physics and Astronomy, University of California, Los Angeles — Departing from the conventional view on superconducting vortices as a parasitic source of dissipation for charge transport, we propose to use mobile vortices as topologically-stable information carriers [1]. To this end, we start by constructing a phenomenological theory for the interconversion between spin and vorticity, a topological charge carried by vortices, at the interface between a magnetic insulator and a superconductor, by invoking the interfacial spin Hall effect therein. We then show that a vortex liquid in superconductors can serve as a spin-transport channel between two magnetic insulators by encoding spin information in the vorticity. The vortex-mediated nonlocal signal between the two magnetic insulators is shown to decay algebraically as a function of their separation, contrasting with the exponential decay of the quasiparticle-mediated spin transport.


This work was supported by the Army Research Office under Contract No. W911NF-14-1-0016 and the NSF-funded MRSEC under Grant No. DMR-1420451.
12:15PM F41.00004: Detecting spin current fluctuations in quantum magnets via microwave resonators

JOSHUA AFTERGOOD (Presenter), SO TAKEI, Physics, Queens College — We theoretically examine spin transport across coupled quantum spin chains that are further coupled to a microwave cavity in series with a transmission line. Spins in the quantum magnet couple inductively to the microwave field and imprint spin transport signatures into the output photon field detected on the transmission line. We first show that in the non-invasive coupling limit the total output photon power is directly proportional to spin current noise at the cavity resonance frequency, and thus that spin current noise is detectable without recourse to destructive techniques. We also discuss the possibility of photon feedback effects on the spin conductivity and noise for the invasive coupling limit.

12:27PM F41.00005: Development of a System for Low Temperature Optical Measurement of Three-Dimensional Magnon, Plasmon and Spin Torque Transfer Dynamics

YU-SHENG OU (Presenter), XINRAN ZHOU, HARSHA KANNAN, HANG CHEN, RASOUL BARRI, STEPHANIE ANN LAW, JOHN Q XIAO, MATTHEW F DOTY, University of Delaware — Spin-dependent phenomena in magnetic heterostructures and topological insulators (TIs) have attracted lots of attention from the perspective of both fundamental science and device development. For example, the spin orbital interaction in ferromagnet (FM)/heavy metal (HM) bilayers allows for all-electrical manipulation of magnetization. Moreover, the protected and linear-dispersed surface states of TIs leads to the unique spin-momentum locking. Despite extensive studies of these novel phenomena, there remain important questions about their underlying mechanisms. For example, the dynamics of these phenomena, which are critical for device applications, remain poorly understood. To address these important questions in the field, we have developed an experimental apparatus allowing ultrafast and quasi-DC optical study of magnon, plasmon, and spin orbit torque (SOT) in a wide variety of magnetic systems at low temperature and in the presence of a two-dimensional magnetic field. To benchmark the capability of this instrument, we present data demonstrating time-resolved Magneto-Optical Kerr Effect (TRMOKE) study of the SOT-driven magnetization dynamics in both Py/Pt and CoFeB/Ta bilayers.

*NSF (DMR-1624976)

12:39PM F41.00006: Time-resolved Magneto-optical Kerr Effect Studies on Permalloy/Ru/Permendur Trilayers

HENGZHOU LIU (Presenter), CHRISTOPHER E STEVENS, Department of Physics, University of South Florida, MOJTABA RANJBAR, Department of Physics and Astronomy, Uppsala University, JOHAN AKERMAN, Department of Physics, University of Gothenburg, YEVDGEN POGORYELOV, OLOF KARIS, Department of Physics and Astronomy, Uppsala University, DARIO A ARENA, DENIS KARAISKAJ, Department of Physics, University of South Florida — We investigate a series of magnetic trilayer samples consisting of Ni_{20}Fe_{80}(Py)/Ru [x]/Fe_{49}Co_{49}V_{2}(Pmd), where the Ru spacer thickness [x] is varied from 0.7 nm to 17 nm to change the indirect exchange coupling (IEC) between the two magnetic layers. We study the dynamics of these structures by using time-resolved magneto-optical Kerr effect (TR-MOKE) to observe the initial demagnetization and subsequent precession of the magnetic moments as the system returns to equilibrium. Even though the TR-MOKE signal is generated primarily from the top Pmd layer, we observe an unusual beating pattern in the TR-MOKE signal indicative of two coupled oscillators with different precession frequencies. The coupling between the two oscillators depends on the thickness of the Ru spacer layer and hence the strength of the IEC. The results point to the usefulness of TR-MOKE in investigating dynamic coupling effects, including spin pumping, in layered magnetic films.

12:51PM F41.00007: Structural, Magnetic, and Transport Properties of Fe(1-x)Rh(x)/MgO(001) Films Grown by Molecular-Beam Epitaxy

ANTONIO MEI (Presenter), DARRELL G. SCHLOM, Materials Science & Engineering, Cornell University — Fe(1-x)Rh(x) layers are grown with varying rhodium fraction x on (001)-oriented MgO substrates by molecular-beam epitaxy. Film structural, morphological, magnetic, and transport properties are investigated. At room temperature, layers are ferromagnetic (FM) for x ≤ 0.48 and antiferromagnetic (AF) for x > 0.48. Separating the two magnetically ordered phases at x = 0.48 is an abrupt change in the Fe(1-x)Rh(x) lattice parameter of Δa = 0.0028 nm (Δa/a = −0.9%). For AF layers, the FM state is recovered by heating across a first-order phase transition. The transition leads to a large resistivity modulation, Δρ/ρ = 80%, over a narrow temperature range, ΔT = 3 K, in stoichiometric Fe(0.50)Rh(0.50)/MgO(001). The resistivity change is explained using a model based on independent spin conduction channels. For samples with compositions deviating from x = 0.50, fluctuations broaden ΔT and defect scattering reduces Δρ/ρ.
Recent discoveries in antiferromagnets (AFs) such as spin-orbit torques, spin Seebeck effects and inverse spin Hall effects have opened up new possibilities for spintronics devices.[1] Of particular interest is the equiatomic FeRh, which undergoes a temperature driven antiferromagnet-to-ferromagnet magnetic phase transition. This metallic AF is also promising for spintronics applications due to its relatively large spin-orbit coupling arising from Rh. We have grown epitaxial FeRh films on MgO (100) and patterned them into measurement devices using photolithography and ion milling. We performed anomalous Hall effect (AHE) and anomalous Nernst effect (ANE) measurements on 20-nm-thick FeRh films at various temperatures. Our findings show a drastic suppression of both AHE and ANE signals in the AF phase. Interestingly, these non-vanishing signals are opposite in sign compared to their ferromagnetic counterparts, which may suggest changes of inherent symmetries in the electronic structure of FeRh across its magnetic phase transition.


The spin-reorientation transition occurring in perpendicularly-magnetized films as a function of film thickness is well known. Long-range dipole interactions act to form antiparallel domains in the perpendicular phase that precedes the reorientation to in-plane magnetization via a canted phase. In equilibrium, the domains walls move freely to minimize the global energy and form a uniform striped pattern. This spatial averaging causes the reorientation to occur at a non-integer number of monolayers (ML). When the domain walls are pinned in thinner films, the system minimizes energy locally, and a metastable reorientation transition occurs on isolated islands that are 1 ML thicker than the surrounding film. These two versions of the same transition produce two separate peaks in the susceptibility $\chi_\perp$ (in a perpendicular field), if it is measured as the film is grown. We report here observation of a dynamical version of the reorientation transition as the domain walls depin and the system moves from locally to globally determined energetics. The measured susceptibility $\chi_{001}$ (in an in-plane field) exhibits a divergence. These observations provide insight to the role of dipole interactions in the transitions from the perpendicular phase to the paramagnetic and canted phases.

Relaxation effects are of primary importance in the description of magnetic excitations, leading to a myriad of methods addressing the phenomenological damping parameter. In this work [1], we compare several well-established forms of calculating the intrinsic Gilbert damping within a unified theoretical framework, mapping out their connections and approximations required to derive each formula. Most methods lead to similar results for the bulk ferromagnets Fe, Co and Ni, due to the low spin-orbit interaction strength and the absence of the spin pumping mechanism. Starting from simulated ferromagnetic resonance spectra based on the underlying electronic structure, we unambiguously demonstrate that the damping parameter obtained within the constant broadening approximation diverges for three-dimensional bulk magnets in the clean limit, while it remains finite for monolayers. Our work puts into perspective the several methods to compute the Gilbert damping, building a solid foundation for future investigations of magnetic relaxation effects in any kind of material.


Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 -- DYNASORE)
1:39PM F41.00011: Quantum spin-transfer torque induced nonclassical magnetization dynamics and electron-magnetization entanglement  PRIYANKA MONDAL (Presenter), Dept. of Physics & Astronomy, University Of Delaware, MARKO PETROVIĆ, PETR PETR PLECHAC, Department of Mathematical Sciences, University Of Delaware, BRANISLAV NIKOLIC, Dept. of Physics & Astronomy, University Of Delaware — Spin transfer torque (STT) is usually known to appear from non-collinearity of two spins but recent experiments [A. Zholud et al., Phys. Rev. Lett. 119, 257201 (2017)] have shown change in magnetization in spin valves at cryogenic temperature even when electron spin is collinear to magnetization, pointing at overlooked quantum effects in STT (which can lead to highly nonclassical magnetization states). Using fully quantum many-body treatment, we showed that change in magnetization below cryogenic temperature come from entanglement between injected electron subsystem and anisotropic quantum Heisenberg ferromagnetic chain, caused by STT coming from non-collinearity of the two subsystems (which explains the experiment). Furthermore, the same processes—entanglement and thereby induced decoherence—are present also in standard noncollinear geometry, together with the usual magnetization rotation. This is because STT in quantum many-body picture is caused only by electron spin-down factor state, and the only difference between collinear and noncollinear geometries is in relative size of the contribution of the initial separable state containing such factor state to superpositions of separable many-body quantum states generated during time evolution.

1:51PM F41.00012: Time-retarded damping and magnetic inertia in the Landau-Lifshitz-Gilbert equation self-consistently coupled to electronic time-dependent nonequilibrium Green functions*  UTKARSH BAJPAI (Presenter), BRANISLAV NIKOLIC, University of Delaware — The conventional LLG equation is a widely used tool to describe dynamics of local magnetic moments, viewed as classical vectors. Here we demonstrate that recently developed [M. D. Petrovic et al., arXiv:1802.05682] self-consistent coupling of the LLG equation to time-dependent quantum electrons using time-dependent nonequilibrium Green function (TDNEGF) microscopically generates time-retarded damping in the LLG equation described by a memory kernel. For sufficiently slow dynamics, the memory kernel can be expanded to extract a time dependent Gilbert damping and magnetic inertia terms. Using examples of precessing single or multiple magnetic moments, as well as field-driven motion of a magnetic domain wall, we quantify the difference in their time evolution computed from conventional LLG equation vs. our TDNEGF+LLG approach. The faster DW motion predicted by TDNEGF+LLG approach reveals that important quantum effects are missing from conventional classical micromagnetics simulations. We also demonstrate large discrepancy between TDNEGF+LLG-computed nonperturbative result for charge current pumped by a moving DW and the same quantity computed by perturbative spin motive force formula combined with the conventional LLG equation.

*This work was supported by NSF Grant No. ECCS 150909.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F42 DQI: Applications of Noisy Intermediate Scale Quantum Computers III  BCEC

210A - Kristan Temme - Tag(s): Focus

11:15AM F42.00001: Gate-efficient simulation of molecular eigenstates on a superconducting qubit quantum computer  MARC GANZHORN, DANIEL EGGER, PAULINE OLLITRAULT, PANAGIOTIS BARKOUTSOS, GIAN SALIS, NIKOLAJ MOLL, ANDREAS FUHRER, PETER MUELLER, IBM Research - Zurich, MARCO ROTH, Forschungszentrum Juelich, STEFAN WOERNER, IVANO TAVERNELLI, STEFAN FILIPP (Presenter), IBM Research - Zurich — A key requirement to perform simulations of large quantum systems on current quantum processors is the design of quantum algorithms with short circuit depth. To achieve this, it is essential to realize a gate set that is tailored to the problem at hand and which can be directly implemented in hardware [P. Barkoutsos et al., Phys. Rev. A 98, 022322 (2018)]. Here, we experimentally demonstrate that exchange-type gates are ideally suited for calculations in quantum chemistry [M. Ganzhorn et al., arXiv:1809.05057]. We determine the energy spectrum of molecular hydrogen using a variational quantum eigensolver algorithm based on exchange-type gates in combination with a method from computational chemistry to compute the excited states. We utilize a parametrically driven tunable coupler to realize exchange-type gates that are configurable in amplitude and phase on two fixed-frequency superconducting qubits. With gate fidelities around 95% we are able to compute the eigenstates within an accuracy of 50 mHartree on average, a limit set by the coherence time of the tunable coupler.
11:27AM F42.00002: Improved variational algorithms for optimization problems in a quantum computer

PANAGIOTIS BARKOUTSOS (Presenter), ANTON ROBERT, IBM Research - Zurich Research Laboratory, GIACOMO NANNICINI, IBM Research - Thomas J. Watson Research Center, IVANO TAVERNELLI, STEFAN WOERNER, IBM Research - Zurich Research Laboratory

— Recent advances in Noisy Intermediate-Scale Quantum (NISQ) computers allow us to solve combinatorial optimization problems encoded in Hamiltonians via hybrid quantum/classical variational algorithms. Current approaches minimize the expectation of the problem Hamiltonian for a parameterized trial state generated in the quantum circuit. The expectation is obtained by sampling the full outcome of an ensemble of measurements of the corresponding matrix element, while the trial wavefunction parameters are optimized classically. This procedure is fully justified for quantum mechanical observables (i.e. molecular energy). However, in the case of the simulation of classical optimization problems, which yield diagonal Hamiltonians, we argue that it is more natural to aggregate the samples using a different aggregation function than the expected value. In this talk, we present results of the aforementioned scheme for a plethora of interesting optimization problems where we demonstrate faster convergence towards more accurate solutions.

11:39AM F42.00003: Variational Approaches for Quantum Simulation

TIMOTHY HSIEH (Presenter), Perimeter Institute for Theoretical Physics, WEN WEI HO, Harvard, CHERYNE JONAY, Perimeter Institute for Theoretical Physics

— Many non-trivial quantum states, such as quantum critical points or topological phases, can potentially be realized in synthetic quantum systems, such as trapped ions or superconducting circuits. However, finding efficient and realizable approaches for such state preparation is challenging. I will show how a variant of the Quantum Approximate Optimization Algorithm (QAOA), originally introduced as a variational approach for solving classical optimization problems, serves as an efficient and general approach for realizing non-trivial quantum states. I will then show how long-range interactions, for example those in trapped ions systems, can further facilitate quantum state preparation.

11:51AM F42.00004: Quantum gate-model approaches to exact and approximate optimization [Invited]

STUART HADFIELD (Presenter), USRA / NASA Quantum Artificial Intelligence Laboratory

— Many of the most challenging computational problems arising in practical applications are tackled by heuristic algorithms which have not been rigorously proven to outperform other approaches but rather have been empirically demonstrated to be effective. While quantum heuristics have been proposed since the early days of quantum computing, true empirical evaluation of the real-world performance of these algorithms is only becoming possible now as increasingly powerful quantum gate-model devices continue to come online.

In this talk, I will give an overview of the NASA QuAIL team's ongoing investigation into quantum gate-model heuristic algorithms for exact and approximate optimization. In particular, we consider the performance of the Quantum Approximate Optimization Algorithm on NP-hard optimization problems, and describe algorithm parameter setting strategies for real-world quantum hardware. We then show a generalization of QAOA circuits, the Quantum Alternating Operator Ansatz, especially suitable for low-resource implementations of QAOA for problems with hard (feasibility) constraints. The talk will conclude with a discussion of research challenges, particularly for optimization and sampling applications of QAOA, and the potential of more general quantum heuristics to give advantages over classical computers.

12:27PM F42.00005: Simulating Transmon Lattices for Analysing System Constraints in the Noisy Intermediate Quantum Scale

JONATHON MILLER (Presenter), University of Houston, Clear Lake

— Thermal noise from electrical circuit components and noise due to fluctuations in energy levels of Transmon circuits have the cumulative effect of decreasing the coherence time of these systems. As coupled Transmon systems scale to the noisy intermediate quantum scale, accurate characterization of noise accumulation and its effects on coherence time and quantum logic gate fidelity is vital. The answer this work aims to provide is the limitations on the coherence time imposed by the noise as the system scales from a few to many (50-100) qubits. The noise analysis is being carried out by a computational simulation of a linear Transmon chain forced into a confinement and surrounded by a bath of thermal photons characteristic of the circuit component radiation. A Generative Artificial Intelligence is used to explore the space of superconducting circuits to develop an understanding of the thermal constraints of a Noisy Intermediate Scale Quantum Computer.
12:39PM F42.00006: Characterizing quantum circuits by short-cutting quantum errors and a unitary-dissipative "polar" decomposition for quantum channels*  ARNAUD CARIGNAN-DUGAS (Presenter), Applied Mathematics, University of Waterloo, MATTHEW ALEXANDER, JOSEPH EMERSON, University of Waterloo — The richness of quantum dynamics allows for a plethora of noise models which, given only a partial knowledge of a device's components can result in widely different conclusions regarding the quality of larger circuits. In fact, the sole formulation of an assessment regarding the overall operational performance is demanding in that it typically requires invoking a broad range of quantum dynamical scenarios. In this work, we pave the way between partially characterized elementary operations and circuits thereof. Our paving stone consists of a simplified picture of quantum processes that we refer to as the leading Kraus (LK) approximation. This incomplete dynamical representation closely prescribes the evolution of celebrated characterization figures of merit, namely the average gate fidelity, which captures the overlap between an implemented operations and their targets, and the unitarity, which captures the level of coherence in the noise. Moreover, the transparency in the LK parametrization allows the derivation of a quantum unitary-dissipative (polar) factorization for quantum channels.

*This research was supported by the U.S. Army Research Office, TQT, CIFAR, the Government of Ontario, and the Government of Canada through CFREF, NSERC and Industry Canada.

12:51PM F42.00007: Quantum Feedback Protocol for Approximating Single-Body Green's Functions at Finite Temperature*  JEFFREY COHN (Presenter), KHADIJEH NAJAFI, JAMES FREERICKS, BARBARA JONES, Georgetown University — We present a quantum feedback algorithm that aims to approximate single-body Green's functions at finite temperature. Extracting a single particle Green's function from a quantum computer is a well known process, but if one is interested in thermal properties the challenges and resources necessary for full Gibbs state preparation are generally too expensive for these machines in the near future. Here, we examine how sampling from more easily preparable states can yield precise approximations to single-particle Green's functions at finite temperature. We also show, through a feedback mechanism, that one can test for convergence and extract the effective temperature of the system being simulated. Further, we compare the trade-offs of different approaches to make these techniques applicable on near term devices. We draw on the ideas of the Eigenstate Thermalization Hypothesis as well as specific properties of Green's functions and use a family of 1-D Fermi-Hubbard models as our test case.

*This work was supported by the National Science Foundation under grants numbered PHY-1620555. JKF was also supported by the McDevitt bequest at Georgetown University.

1:03PM F42.00008: Quantum simulation and Time-Dependent Density Functional Theory*  JAMES WHITFIELD (Presenter), JAMES BROWN, JUN YANG, Dartmouth College — Time evolution of quantum systems is of interest in physics, in chemistry, and, more recently, in computer science. One route to numerically propagating quantum systems is time dependent density functional theory. The application of TDDFT to a particular system's time evolution is predicated on V-representability which we've analyzed in previous work. Here we consider the application of quantum simulation to the problem of characterizing time-dependent Kohn-Sham potentials. We consider both the V-representability of some simple 1D examples numerically and their implementation using quantum computation. The measurement of the one-body electronic probability density on quantum hardware given various qubit encodings is also discussed.

*This material is based upon work supported by the U.S. Department of Energy, by both the Office of Science, Office of Advanced Scientific Computing Research, under the Quantum Computing Application Teams program and the Office of Basic under topic area Quantum Computing in Chemical and Materials Sciences.

1:15PM F42.00009: Digital quantum simulation of a two-dimensional electron gas pierced by a strong magnetic field  MICHAEL KAICHER (Presenter), SIMON BALTHASAR JÄGER, FRANK K WILHELM, Univ des Saarlandes, RYAN BABBUISH, Google Inc., PIERRE-LUC DALLAIRE-DEMERS, Xanadu — A two dimensional electron gas, confined to a finite disk geometry and pierced by a strong transversal magnetic field at zero temperature describes the physical setting of the fractional quantum Hall effect. We give an ab-initio roadmap on how this system may be simulated on a quantum processor. We show how the approximate ground state could be extracted through a hybrid quantum-classical variational algorithm and how to extract ground state properties. This heuristic method can be extended to incorporate more physical effects, such as impurity models, to ultimately test theoretical models against experimental data beyond the limits of classical computational power.
1:27PM F42.00010: Linear Depth Circuit Unitary Coupled Cluster Wavefunctions for Quantum Computation*
WILLIAM HUGGINS (Presenter), JOONHO LEE, MARTIN HEAD-GORDON, BIRGITTA K WHALEY, University of California, Berkeley
— Motivated by the rapid development of quantum computing hardware we introduce a new unitary coupled cluster wavefunction ansatz for quantum chemistry which we call k-UpCCGSD. k-UpCCGSD employs k products of the exponential of a sparse generalized doubles excitation operator, together with generalized single excitation operators, resulting in a wavefunction which can be approximated by a linear-depth circuit. We compare its performance with that of the generalized unitary coupled cluster ansatz employing the full generalized singles and doubles excitation operators (UCCGSD), as well as with the standard ansatz containing only excitations between occupied and virtual orbitals (UCCSD). We find that k-UpCCGSD offers an appealing tradeoff between accuracy and cost, and dramatically outperforms the standard UCCSD, particularly for the calculation of low-lying excited states.

*This work was supported by the U.S. Department of Energy, Office of Advanced Scientific Computing Research, Quantum Algorithm Teams Program, and Basic Energy Sciences Division.

1:39PM F42.00011: Quantum digital simulation of three toy models using IBM quantum hardware.*  PEDRO CRUZ, Departamento de Fisica, Universidade de Porto, RONAN GAUTIER, CentraleSupélec, GONÇALO CATARINA, JOAQUIN FERNANDEZ-ROSSIER (Presenter), QuantaLab & Quantum Materials and Energy, International Iberian Nanotechnology Laboratory — Using the phase estimation algorithm it is possible, in principle, to obtain the eigenstates of a large family of many-body Hamiltonians. In this talk we will present the results of our attempts to implement phase estimation algorithms to obtain the eigenvalues of 3 simple model Hamiltonians, using IBM quantum hardware. For that matter, we have considered a two level system, a two site Ising model with longitudinal magnetic field, and a two site Hubbard model at half filling. We have made use of both the phase estimation and iterative phase estimation algorithms. We have explored to which point the unwanted hardware noise compromises the accuracy of the algorithm. In the case of the Hubbard model, for which a Trotterization procedure is required, we study the optimal number of Trotter steps. Our results illustrate the limits of the phase estimation approach for quantum digital simulation in state of the art hardware.

*We acknowledge funding from FCT Portugal projects, UTAP-EXPL/NTec/0046/2017 and PTDC/FIS-NAN/4662/2014

1:51PM F42.00012: Implementing the Variational Quantum Eigensolver with native 2-qubit interaction and error mitigation*  TAKAHIRO TSUNODA (Presenter), ANDREW D PATTERSON, Condensed Matter Physics, University of Oxford, XIAO YUAN, SUGURU ENDO, Materials, University of Oxford, JOSEPH RAHAMIM, PETER A SPRING, MARTINA ESPOSITO, SALHA JEBARI, KITTI RATTER, SOPHIA SOSNINA, GIOVANNA TANCREDI, BRIAN VLASTAKIS, Condensed Matter Physics, University of Oxford, SIMON BENJAMIN, Materials, University of Oxford, PETER LEEK, Condensed Matter Physics, University of Oxford — The variational quantum eigensolver (VQE) is an algorithm that may provide near-term applications of small-scale quantum computers, in quantum chemistry and optimisation problems. In order for the VQE to provide accurate solutions to problems on real devices, methods have been proposed recently to mitigate the errors caused by imperfect gates. In this presentation, we report a quantum chemistry simulation using the VQE on a 2-qubit superconducting device in which we use fixed frequency qubits and build the algorithm using the native 2-qubit interaction resulting from a static capacitive coupling. The hardware ansatz of the VQE is constructed by varying the timings of echo pulses to manipulate the native ZZ coupling. This method allows us to implement a VQE algorithm without needing repeated 2-qubit-gate tune-up, and enables simple and understandable implementation of error mitigation.

*We acknowledge financial support from the EPSRC, Oxford Instruments Nanoscience, Oxford Quantum Circuits Ltd, the Oxford Centre for Applied Superconductivity, the Nakajima Foundation and the Masason Foundation.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F43 DCMP GMAG: Topological Spintronics  BCEC 210B - Nitin Samarth, Pennsylvania State University - Tag(s): Invited
11:15AM F43.00001: Topological Insulator Surface States for Spintronics* [Invited] ALLAN MACDONALD (Presenter), University of Texas at Austin — Spintronics is the study of the mutual influence between charge transport in conductors and charge neutral spin degrees of freedom, especially the collective spin degrees of freedom of magnetically ordered systems. The effects of spintronics all require coupling between spin and orbital degrees of freedom. Systems containing thin-films of three dimensional topological insulators (TIs) are in many cases ideal hosts for spintronics studies because of the strong spin-orbit coupling present in the protected TI surface states, which can also serve as an isolated two-dimensional charge transport channel. I will discuss theories of the closely related anomalous Hall, spin Hall, spin-orbit torque, magneto-resistance, and spin-pumping effects in isolated TI thin films, and in TI thin films proximity coupled to conducting and insulating ferromagnets and antiferromagnets. My talk will focus on discussing possible applications of topological insulators in thin-film devices for electrically controlled magnetism, and emphasize the separate roles played by top and bottom TI surfaces.

*This work is supported by the DOE office of Basic Energy Sciences under grant DE-FG02-02ER45958 and by the Army Research Office MURI program under Grant Number W911NF-16-1-0472.

11:51AM F43.00002: Magnetic Topological Insulator Heterostructures: From Axion Physics to the Topological Hall Effect* [Invited] CUI-ZU CHANG (Presenter), Pennsylvania State University — Topological insulator is a material in which the interior is insulating but wherein the electrons travel without resistance along surface/edge conducting channels. The nontrivial Dirac surface/edge states of a TI are induced by intrinsic strong spin-orbit coupling and protected by time-reversal symmetry (TRS). Breaking the TRS of a TI with magnetic doping can lead to many exotic topological quantum phenomena such as the quantum anomalous Hall (QAH) effect [1]. The QAH effect has been experimentally demonstrated in magnetic TI thin films, specifically Cr- and/or V- doped (Bi,Sb)Te [2]. Recently, we fabricated magnetic TI based sandwich heterostructures wherein two TI films doped with the same or different magnetic ions are sandwiched by an undoped TI layer. The undoped TI layer serves as a spacer to decouple the exchange interaction between the two magnetic TI layers, thus the magnetization in each magnetic TI layer can be treated independently. In heterostructures with different magnetic TI layers, we realized a zero Hall conductance plateau in the antiparallel magnetization alignment region, which is a realization of the axion insulator state. This observation provides a promising platform for the exploration of axion electrodynamic physics [3]. In heterostructures with the same magnetic doping, we observed a crossover from the QAH to topological Hall (TH) effects. The combination of QAH and TH effects in a single sample facilitates the study of the interplay of momentum-space and real-space Berry curvatures in magneto-transport phenomena [4].


*This work is supported by the ARO Young Investigator Program Award (W911NF1810198), the U.S. DOE Award # DE-SC0019064 and the Alfred P. Sloan Research Fellowship.

12:27PM F43.00003: Dirac-Surface-State Modulated Spin Dynamics in a Ferrimagnetic Insulator at Room Temperature* [Invited] JING SHI (Presenter), University of California, Riverside — In heterostructures of magnetic insulator/topological insulator or MI/TI, a large enhanced spin Seebeck effect was attributed to the spin-momentum locking of the TI surface. In this work, we demonstrate dramatically modified spin dynamics of MI by the spin-momentum locked Dirac surface states of the adjacent TI. As the Bi-concentration $x$ is systematically tuned in 5 nm thick (Bi$_x$Sb$_{1-x}$)$_2$Te$_3$ TI film, the weight of the surface relative to bulk states peaks at $x = 0.32$ when the chemical potential approaches the Dirac point. At this concentration, the Gilbert damping constant of the precessing magnetization in 10 nm thick Y$_2$Fe$_5$O$_{12}$ MI film in the MI/TI heterostructures is enhanced by an order of magnitude, the largest among all concentrations. In addition, the MI acquires additional strong magnetic anisotropy that favors the in-plane orientation with similar Bi-concentration dependence. These extraordinary effects of the Dirac surface states along with the enhanced spin Seebeck effect distinguish TI from other materials such as heavy metals in modulating spin dynamics of the neighboring magnetic layer, which can be harnessed for spintronic applications.

*This work was supported as part of the SHINES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. SCO012670, NSF Grants No. DMR-1207469, ONR Grant No. N00014-16-1-2657, and the STC Center for Integrated Quantum Materials under NSF Grant No. DMR-1231319.
1:03PM F43.00004: Discovery of quantum confinement effect in sputtered topological insulator films and observation of room-temperature high spin–orbit torque* [Invited] MAHENDRA DC, ROBERTO GRASS, JUNYANG CHEN, MAHDI JAMALI, DANIELLE HICKEY, DELIN ZHANG, ZHENGYANG ZHAO, HONGSHI LI, PATRICK QUARTERMAN, YANG LV, MO LI, University of Minnesota, AURELIEN MANCHON, King Abdullah University of Science and Technology, K. ANDRE MKHOYAN, TONY LOW, JIANPING WANG (Presenter), University of Minnesota — In this talk, we will report and discuss the experimental demonstration and first-principles calculation of quantum confinement in topological insulator. First, we report Bi$_{x}$Se$_{(1-x)}$ films with high SOT at RT grown onto thermally oxidized silicon substrates by magnetron sputtering, which is a semiconductor industry compatible process. The dc planar Hall and ST-FMR methods were used for the characterization of SOT in Bi$_{x}$Se$_{(1-x)}$/CoFeB heterostructures with in-plane CoFeB. At RT, the of the sputtered Bi$_{x}$Se$_{(1-x)}$ film is up to two orders of magnitude larger than that of HMs. Notably, we developed perpendicular CoFeB multilayers on Bi$_{x}$Se$_{(1-x)}$ films, and we demonstrated switching of the magnetization using SOT arising from the Bi$_{x}$Se$_{(1-x)}$ with very low switching current density in bilayers at RT. Second, we will report our discovery of the quantum confinement effect in topological insulators. The sputter deposited Bi$_{x}$Se$_{(1-x)}$ has granular structure with grain size as small as approximately 6 nm. Electronic band-structure analysis indicates that the reduced dimensionality and quantum confinement strongly influences the spintronic properties of the TI. Our theory identifies the presence of lowly dispersive surface bands with large charge-to-spin conversion efficiency in nanoscale grains, which might explain the experimentally observed enhancement in the figure-of-merit. The demonstrated ease of growth of the films on a silicon substrate, and successful growth and switching of perpendicular CoFeB multilayers on Bi$_{x}$Se$_{(1-x)}$ film provide an avenue for the use of Bi$_{x}$Se$_{(1-x)}$ as a spin-density generator in SOT-based memory and logic devices.

Mahendra DC, et al, “Room-temperature high spin–orbit torque due to quantum confinement in sputtered Bi$_{x}$Se$_{(1-x)}$ films” Nature Materials. 17, 800-807 (2018); DOI: 10.1038/s41563-018-0136-z

*This work was supported by C-SPIN, one of six STARnet program research centers.

1:39PM F43.00005: Exploring Non-Trivial Nature of Topological Surface States in SmB6 [Invited] MINGZHONG WU (Presenter), TAO LIU, Colorado State Univ, YUFAN LI, Johns Hopkins University, LEI GU, University of California, Irvine, JUNJIA DING, Argonne National Laboratory, HOUCHEN CHANG, PRAVEEN JANANTHA, Colorado State Univ, BORIS KALINIKOS, St. Petersburg Electrotechnical University, VALENTYN NOVOSAD, AXEL F HOFFMANN, Argonne National Laboratory, RUQIAN WU, University of California, Irvine, CHIA-LING CHIEN, Johns Hopkins University — Being the first rare earth mixed valence system and the first Kondo insulator, SmB6 may very likely be the first topological Kondo insulator too. Recent studies have confirmed the existence of topological surface states (TSS) and surface chiral spin textures in single-crystal SmB6 bulk materials, but the non-trivial nature and depth scale of the TSS remain unresolved. In this talk I will report our recent work on the use of spin pumping to study the non-trivial feature of the TSS in SmB6 [1]. Our experiments used SmB6 thin films grown on magnetic insulator Y$_3$Fe$_5$O$_{12}$ (YIG) bulk materials. Upon the excitation of magnetization precession in the YIG, a pure spin current is generated that flows from the YIG into the SmB6 film and produces, via spin-orbit coupling, a lateral electrical voltage in the SmB6 film. The spin-pumping voltage signal becomes considerably stronger as the temperature decreases from 150 K to 10 K. Such an enhancement most likely originates from the spin-momentum locking feature of the TSS of the SmB6 film and may thereby serve as a strong evidence for the nontrivial nature of the TSS. The voltage data also show a unique film thickness dependence that suggests a TSS depth of about 32 nm for the TSS. The data also indicate a spin diffusion length of about 39 nm in the SmB6 film. The spin-pumping results are supported by temperature-dependent transport measurements and theoretical analyses using a tight binding model.


Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F44 DCMP: Manifestations of Phonon Hydrodynamics in Thermal Transport BCEC

21OC - Andrea Cepellotti, University of California, Berkeley - Tag(s): Invited
11:15AM F44.00001: Novel Vistas in Thermal Transport: Relaxons, Frictions, Viscosities, and Coherences* [Invited]  
NICOLA MARZARI (Presenter), Ecole polytechnique federale de Lausanne — We examine the emergence of correlated transport phenomena in systems described by the linearized Boltzmann transport equation (LBTE), with examples then centered around heat transport. First, we show how phonons, traditionally considered the carriers of heat, are only a high-temperature approximation to the exact carriers, that we term relaxons, showing how thermal conductivity can be mapped exactly into a kinetic theory of the relaxon gas, and where the effect of boundaries can be understood in terms of frictions. Second, we show how the LBTE admits coherent propagating solutions with well defined wavevectors and lifetimes, of which second sound is a special case. Last, we discuss generalizations towards the Navier-Stokes continuum, and towards disordered materials. Work performed in collaboration with Andrea Cepellotti (UC Berkeley), Michele Simoncelli (EPFL), and Francesco Mauri (Sapienza U. of Rome).

*This research was supported by the Swiss National Science Foundation through Project ID 200021_143636 and the National Centre of Competence in Research MARVEL.

11:51AM F44.00002: Observation of the Poiseuille flow of phonons in black phosphorus [Invited]  
YO MACHIDA (Presenter), Department of Physics, Gakushuin University — The travel of heat in an insulating solid is commonly pictured as a flow of phonon quasi-particles. In such a picture, phonons are decelerated by scattering with each other. However, in rare circumstances, momentum-conserving scattering between phonons dominate, and phonons can enter a hydrodynamic regime, where they flow like fluids inside a crystalline lattice and retard only by hitting the sample boundaries. This phenomenon dubbed “phonon Poiseuille flow”, which is a phononic counterpart of the Poiseuille flow in classical hydrodynamics, was thought to occur only in ultrapure solids.

In the presentation, we report on a study of heat flow in bulk black phosphorus, a material attracting renewed attention for a variety of fundamental and technological reasons. We show that the thermal conductivity of this material exhibits a faster than cubic temperature dependence just below the peak temperature of thermal conductivity. Consequently, the effective phonon mean free path shows a nonmonotonic temperature dependence at the onset of the ballistic regime, with a size-dependent Knudsen minimum. These are hallmarks of Poiseuille flow previously observed in a handful of solids. Comparing the phonon dispersion in black phosphorus and silicon, the low-energy phonon density of states in black phosphorus is found to be much larger, favoring normal momentum-conserving scattering events. Contrary to the previous belief, our results imply that the most important requirement for the emergence of Poiseuille flow is the facility of momentum exchange between acoustic phonon branches [1].


12:27PM F44.00003: Phonon Hydrodynamics in Graphene and Graphite [Invited]  
GANG CHEN (Presenter), ZHIWEI DING, SAMUEL HUBERMAN, RYAN DUNCAN, VAZRIK CHILOYAN, KEITH ADAM NELSON, ALEXEI MAZNEV, Massachusetts Institute of Technology — In the hydrodynamic regime, phonons drift with a nonzero collective velocity under a temperature gradient, reminiscent of viscous gas and fluid flow. The study of hydrodynamic phonon transport has spanned over half a century but has been mostly limited to cryogenic temperatures (<20 K). Recently, we predict based on first principles calculations that hydrodynamic phonon transport can occur in suspended graphene at significantly higher temperatures and wider temperature ranges compared to bulk materials. Furthermore, we identified graphite as a three-dimensional material that supports phonon hydrodynamics at significantly higher temperatures (~100 K). The significant hydrodynamic nature of phonon transport in graphite is attributed to its strong intralayer sp² hybrid bonding and weak van der Waals interlayer interactions. The hydrodynamic transport is manifested through drift motion of phonons, phonon Poiseuille flow, and second sound. Recent experiments demonstrating second sound up to 100K will be discussed.

1:03PM F44.00004: Thermal conductivity of strontium titanate: signatures of phonon hydrodynamics* [Invited]  
KAMRAN BEHNIA (Presenter), ESPCI ParisTech — Temperature dependence of thermal conductivity in strontium titanate reveals four different regimes of heat flow between 2K and 400 K. At high temperature, in the kinetic regime, phonons are scattered off each other by Umklapp processes and thermal conductivity is inversely proportional to temperature. At low temperature, their mean-free-path is set by domain boundaries. This is the ballistic regime. Between these two limits, one can detect the Ziman regime where Umklapp events are rare. The hybridization of soft optical phonon with acoustic phonons enhance Normal (momentum-conserving) collisions and leads to a faster-than cubic temperature dependence of thermal conductivity in a narrow tempearture window. This is a hallmark of Poiseuille flow of phonons previously observed in a handful of solids.

*Science Without Borders program of CNPq/MCTI-Brazil, FAPERJ fellowships, Fonds ESPCI and QuantEmX Grant (No. GBMF5305) from ICAM and the Gordon and Betty Moore Foundation.
Hydrodynamic heat transport in semiconductors at the nanoscale* [Invited] XAVIER ALVAREZ (Presenter), JAVIER BAFALUY, JUAN CAMACHO, Physics Department, Universitat Autònoma de Barcelona, XAVIER CARTOIXA, Electrical Engineering Department, Universitat Autònoma de Barcelona, POL TORRES, ALBERT BEARDO, LLUC SENDRA, Physics Department, Universitat Autònoma de Barcelona — Recent experiments in heat transport on silicon using ultrafast laser heating techniques have shown significant discrepancies with Fourier like behaviour[1-3]. The interpretations of these results using only a ballistic to diffusive transition of the carriers have shown to be unfruitful. The consequence is that heat transport at the nanoscale is still an incompletely described topic.

Phonon hydrodynamics has emerged in the last years as a candidate to cover this gap. The appearance of this regime has been associated to the dominance of normal collisions. Its presence has been proven in 2D materials or at low temperatures[4-5], when N-collisions are dominant and in consequence collective effects can be observed easily. But recent works have shown that hydrodynamic effects can still have an important impact when resistive collisions are dominant[6-7]. In this case its presence has to be noticed through indirect evidences. Hydrodynamics has been used to understand the lack of validity of the Mathiessen rule in silicon or the dependence of the Thermal Boundary Resistance on the size of the contact.

Kinetic Collective Model (KCM) has been developed to describe heat transport using two key concepts. On one side, the splitting in collective regime (when normal scattering is dominant) and kinetic regime (when it is not important). On the other side, the inclusion of nonlocal and memory effects that introduce hydrodynamic behavior in the description. From the combination of both concepts it can be shown that hydrodynamic phenomena can emerge in both, collective and kinetic regimes, with different particularities in each case.


We acknowledge Spanish Ministry of Economy and Competitiveness under Grant TEC2015-67462-C2-2-R, TEC2015-67462-C2-1-R (MINECO/FEDER).

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F45 DCMP: Surface Physics BCEC 211 - Steven Erwin, United States Naval Research Laboratory

11:15AM F45.00001: Atomic and Electronic Structures in Intermetallic CaBi₂ Thin Films YANFENG LYU (Presenter), HANMINING YUAN, SAMIRA DANESHMANDI, SHUYUAN HUYAN, PAUL C. W. CHU, Texas Center for Superconductivity, University of Houston — Bismuth-based alloys and compounds are promising candidates for novel topological nontrivial materials due to the strong spin-orbit coupling effect in the heavy bismuth element. The search for topological superconductivity and Majorana fermions in these materials have attracted significant interest. Recently, intermetallic CaBi₂ single crystal was reported to be superconducting, while the atomic, electronic, and topological properties have never been investigated. Using molecular beam epitaxy, we have successfully grown CaBi₂ thin film on TiO₂-terminated SrTiO₃(100) substrate. The lattice and electronic structures were probed by using in-situ reflection high-energy electron diffraction, scanning tunneling microscopy and ex-situ X-ray diffraction. We found the epitaxial CaBi₂ thin film has a Volmer-Weber growth mode and the surface has four totally different terminations: two are non-reconstructed, and the others are reconstructed to 1×2 and c(5×5), respectively. The different electronic density of states and physical properties relevant to these different surface terminations were also investigated.
Tellurium has a curious crystal structure where one dimensional covalently bound chains are held together by van der Waals interactions in a hexagonal pattern. Additionally, theory predicts that the (0001) surface (perpendicular to the chains) of tellurium is a candidate to host a zero-energy bound state. Since evaporated thin films tend to grow in the (1000) direction, we use a Te single crystal to examine the (0001) surface by low temperature scanning tunneling microscopy/spectroscopy. The samples were cut from a larger single crystal and chemo-mechanically polished. After introduction into the ultra-high vacuum system the samples were carefully cleaned by Ar ion sputtering and annealing cycles. We found two surface structures as candidates for the native (0001) surface. The first is a row structure with a period of twice the lattice constant hinting at dimerization of the dangling bonds. The second is more complicated with rows separated by terraces of variable width. This might be a higher-index surface or induced by residual contamination. Initial spectroscopy measurements will also be discussed.

**Quantum saturation of capacitance in metals**

There are two contributions to the electronic capacitance in between two electrodes. First, there is the classical capacitive effect as an electric field is being developed in between these. Another contribution, which has often been neglected for metals, is related to the Pauli exclusion principle for the difficulty to accumulate charges on the electrode surface, the so-called quantum capacitance [T. Christen and M. Büttiker. Phys. Rev. Letters 77 (1996), 1]. Here we report the use of a Scanning Tunneling Microscope at low temperatures to study the variations of the capacitance as we approach two metallic electrodes made of Pt or Au. Three regimes are clearly visible in this process: A classical increase of capacitance which at short distances turn to saturation to the quantum capacitance limit, and finally, a leak of capacitance due to quantum tunneling.

**Comparison of Features for Au and Ir Adsorbed on the Ge (110) Surface**

The surface is modeled by a slab consisting of 108 Ge atoms with a 10 Å vacuum region. Hydrogen atoms are used to saturate the dangling orbitals at the other side of the vacuum region. The relaxed surface with the Au or Ir adatom shows the following distinct features: (1) Au is located at the top of the surface while Ir is located below the top layer of the Ge atoms, as a result of the smaller 1.423Å atomic radius of Ir vs. 1.503Å for Au. (2) No bond formation occurs between the metallic adatoms and the Ge atoms because the more tightly bound nature of the d-states in the metal elements do not allow hybridization to form sp³-type directional orbitals, as seen in charge density plots. (3) The Ir charge density is more deformed than Au, because the partially filled d-shell in Ir can be more easily polarized than the completely filled d-states of Au. Comparisons will be made to Ir/Ge(111) and Au/Ge(110) data measured by STM and LEEM.

**References**

*Spanish government: MAT2016-78625
Comunidad Valenciana: PROMETEO/2017/139

*NSF DMR-1710748 (SC, CYF); NSF DMR-1710306 (TSR); National Natural Science Foundation of China Grants 61376102, 11174048 computational support from Shanghai Supercomputer Center (RKX, HZX).
12:03PM F45.00005: Step-Spacing Distributions Revisited: Curved Crystals Bring Many Opportunities and Challenges to Analysis* THEODORE L. EINSTEIN (Presenter), University of Maryland, College Park, J. ENRIQUE ORTEGA, FREDERIK SCHILLER, MARTINA CORSO, IGNACIO PIQUERO-ZULAICA, CSIC and U. Basque Country, San Sebastian (Spain), JORGE LOBO-CHECA, CSIC and U. Zaragoza (Spain), AITOR MUGARZA, ICN2 Barcelona (Spain) — While the properties of vicinal surfaces with close-packed steps are long well understood, recent experiments using curved crystals invite examination of many orientations under the same temperature and other conditions [1]. In addition to having simultaneously a range of geometries, each of which may be preferred for specific epitaxial growth and chemical reactions, one can now test scaling theories of terrace-width distributions (TWDs) based on fundamental theories and the existence of a single characteristic length, the mean terrace width. For close-packed steps, TWDs are well described by a single-parameter Wigner distribution. For fully-kinked steps, the stiffness tends to vanish, and some of the underlying assumptions of that analysis fail [2]. Hence, TWDs typically do not scale. Furthermore, surface states introduce a new length, λF, which can confound the scaling analysis. For large terrace widths, a description in terms of quantum well states offers a novel accounting of the TWD. Other subtleties and open questions are discussed.


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12:15PM F45.00006: Tunneling Spectroscopy of the excitonic insulator phase in Ta₂NiSe₅* JINWON LEE (Presenter), Department of Physics, Pohang University of Science and Technology (POSTECH), CHANG-JONG KANG, Department of Physics and Astronomy, Rutgers University, MANJIN EOM, Department of Physics, Pohang University of Science and Technology (POSTECH), JUN SUNG KIM, Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science (IBS), BYUNG IL MIN, Department of Physics, Pohang University of Science and Technology (POSTECH), HAN WOONG YEOM, Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science (IBS) — The excitonic insulator phase is one of the novel electronic ground states driven by many-body interactions. Despite its theoretical proposal about 60 years ago, its material realization is still unclear. Ta₂NiSe₅ is a strong candidate, exhibiting a temperature-driven phase transition without any other competing phase such as the charge-density-wave. Experimental evidence so far includes an anomalous increase of the electric resistivity, the flat valence band maximum, and optical gap measurements. We provide further evidence of the excitonic insulator phase in Ta₂NiSe₅ using scanning tunneling microscopy/spectroscopy. At 78 K, the single-particle gap is measured as 300 meV and the orbital characters at the valence band maximum (-175 meV) are inverted from the high-temperature phase. These results indicate the strong interband (or electron-hole band) interaction in the gap opening, which is in a good agreement with the excitonic scenario. Moreover, our model calculation reveals that the non-interacting phase in Ta₂NiSe₅ has a semimetallic band structure, implying the excitonic condensation in Ta₂NiSe₅ is close to the Bardeen-Cooper-Schrieffer (BCS) regime.

*This work was supported by the Institute for Basic Science (Grant No. IBS-R014-D1).

12:27PM F45.00007: STM investigation of oxygen dissociation on Ag/Cu(111) near surface alloy* LAURA CRAMER (Presenter), CHARLIE EMILE SYKES, Tufts University — Both experiment and theory have demonstrated the ability of near surface alloys (NSAs) to desirably tune catalyst properties. These alloys consist of a solute metal confined to the first few atomic layers and present in lower concentrations than the host metal. This alters the electronic and thus catalytic properties of the alloy. Deposition of Ag on Cu(111) leads to a well-characterized NSA with Ag confined to the uppermost layer. The presence of Ag in the topmost layer forms a dislocation loop in the underlying Cu(111) due to strain from lattice mismatch. Ag-based catalysts are the current industrial standard for many partial oxidation reactions, guiding our interest in oxidation dissociation on Ag/Cu(111). Herein, we report on the observation of oxygen dissociation on extended Ag ensembles on Cu(111) via room-temperature scanning tunneling microscopy (STM). Atomic oxygen coverage was observed to scale with increasing oxygen exposure. Through time-lapse STM images, we observed localized diffusion of oxygen on Ag ensembles. These results hint at the potential for this surface to perform partial oxidation reactions with enhanced selectivity and activity.

*US Department of Energy
Phase Transitions of Condensates Investigated in an Atom by Atom Way

AISHA AHSAN
(Presenter), S. FATEMEH MOUSAVI, THOMAS NIJS, SYLVIA NOWAKOWSKA, OLHA POPOVA, ANELIIA WÄCKERLIN, Department of Physics, University of Basel, JONAS BJORK, Department of Physics, Chemistry and Biology, IFM, Linköping University, LUTZ H GADE, Anorganisch-Chemisches Institut, Universität Heidelberg, THOMAS JUNG, Paul Scherrer Institute — Condensation processes and phase transitions are investigated in an atom-by-atom way in on-surface nanosized confinements. Structural transformations are induced thermally and by local probe excitation. The pores of a metal-organic network occupied with 1 up to 9 Xe atoms have been investigated in their propensity to undergo ‘condensed solid’ to ‘confined fluid’ transitions. Different transition temperatures are identified, which depend on the number of Xe atoms in the condensate and relate to the stability of the Xe clustering in the condensed ‘phase’. This work is of fundamental interest and reveals the feature-rich behaviour of transitions of confined planar condensates which provide a showcase towards future ‘phase-transition’ storage media patterned by self-assembly.


Macroscopic Transport Signatures of Alkali Metal Surface Doping in Quantum Materials

CHRISTOPHER PARZYCK (Presenter), BRENDAN FAETH, KYLE M SHEN, Cornell University — Carrier injection by surface deposition of alkali metals has become a staple technique in the investigation of doping effects in many materials. Owing to their extremely low ionization potentials, alkali metals act readily as electron donors and since the resulting free carriers are localized to the material surface this technique has traditionally been used in conjunction with surface sensitive probes of the electronic structure, namely ARPES and STM. Here we present the use of macroscopic electrical transport measurements, in conjunction with potassium surface dosing, to examine doping effects in bulk single crystals of Ba(Fe1-xCox)2As2 and MoS2 as well as thin film FeSe. This technique allows measurement of the effects of doping on macroscopic electrical properties while maintaining a high level of crystalline order in the doped structure. Additionally, it provides a promising route to studying the evolution of electronic properties with carrier concentration in materials less amenable to electrostatic gating techniques, namely superconductors with a metallic parent state.

A Comprehensive Computational Study of Adatom Diffusion on the Aluminum (1 0 0) Surface

JAMES CHAPMAN (Presenter), Materials Science and Engineering, Georgia Institute of Technology, ROHIT BATRA, Materials Science and Engineering, University of Connecticut, BLAS PEDRO UBERUAGA, GHANSHYAM PILANIA, Materials Science and Technology Division, Los Alamos National Lab, RAMAMURTHY RAMPRASAD, Materials Science and Engineering, Georgia Institute of Technology — The complexity of adatom diffusion on the Al (100) surface is reflected by the existence of several low-energy non-trivial atomic exchange or vacancy formation mechanisms. Interestingly, these mechanisms have energy barriers lower than or comparable to that of the simple (and intuitive) hopping mechanism. While prior studies mainly used classical potentials to understand diffusion processes active on Al (100) surface, here we use accurate (and expensive) density functional theory (DFT) computations to estimate barriers associated with nine low-energy adatom diffusion mechanisms. We find that there exist several exchange mechanisms with energy barriers less than or equal to that of the trivial hop mechanism, thereby highlighting mechanisms that can be relevant during surface/crystal growth. Our results paint a highly complex picture of the diffusion landscape on Al (100) and provide insights into how such mechanisms may contribute toward large length- and time-scale surface phenomena. Further, we show that some of the commonly used interatomic potentials fail to accurately capture the details of adatom diffusion on Al (100).

*This work was supported by the NSF, and the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
which are relatively inert on their own. Density-functional-theory calculations demonstrate that, when a H₂ molecule enters the channel between the jaws, it splits into two H atoms by quantum interactions and a gentle mechanical squeeze.

Indirect experimental evidence is consistent with the present predictions. Au-based nutcrackers are predicted to operate at room-temperature, while less-expensive Cu-based ones are predicted to be active at a slightly elevated temperature. Indirect experimental evidence is consistent with the present predictions. Such in silico design holds promise for inexpensive, high-performance heterogeneous catalysts for H₂ dissociation and may inspire new approaches to other complex reactions.
2:03PM F45.00015: Structural stability and electronic properties of the chiral topological superconductor Pb$_3$Bi/Ge(111): A first-principles study

LEIQIANG LI (Presenter), WEI QIN, SHANG REN, PING CUI, ZHENYU ZHANG, University of Science and Technology of China — In a separate study, we have shown that a hole-doped Pb$_3$Bi monolayer can serve as a highly appealing new platform for realizing two-dimensional (2D) intrinsic chiral topological superconductivity. Using first-principles calculations, here we systematically investigate the structural stability of Pb$_3$Bi grown on Ge(111) substrate, and find two nearly degenerate lattice configurations labeled as T$_1$ and H$_3$. For the T$_1$ structure, the appearance of type-II van Hove singularity in the density of states arises from the Bi doping, where the $p$ orbit of Bi hybridizes with that of Pb, leading to the emergence of saddle-like band structures. Moreover, for both the T$_1$ and H$_3$ structures, Bi doping gives rise to larger Rashba-type splittings of the energy bands. We also find a sizable energy barrier of $\sim$0.30 eV per formula unit from the T$_1$ to H$_3$ structure. These findings are expected to stimulate new research activities in searching for 2D intrinsic topological superconductors.

*Supported by NSF of China

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F46 DMP GMAG: 4d/5d Transition Metal Systems -- Perovskite Iridates

BCEC 212 - Gang Cao, University of Colorado, Boulder - Tag(s): Focus

11:15AM F46.00001: “Molecules” in solids against magnetism in 4d and 5d compounds

[Invited] DANIEL KHOMSKII (Presenter), University of Cologne — Close to Mott transition several novel states can appear [1]. In particular, “molecular clusters” can be formed in the solid, such as dimers, trimers, etc. [2]. Especially important for these phenomena is the role of different d-orbitals, which leads to different orbital-selective effects. In my talk I will formulate the main ideas and will illustrate such phenomena, especially dimer formation, on many examples, especially for systems with 4d and 5d electrons. The concept of orbital-selective Peierls transitions will be proposed and justified [3, 4]. In systems containing structural metal dimers there may exist in the presence of different orbitals a special state with partial formation of singlets by electrons on one orbital, while others are effectively decoupled and may give e.g. long-range magnetic order or stay paramagnetic. Similar situation can be realized in dimers spontaneously formed at structural phase transitions, which can be called orbital-selective Peierls transition [5]. Yet another consequence of this picture is that for odd number of electrons per dimer there exist competition between double exchange mechanism of ferromagnetism and the formation of singlet dimer by electron on one orbital. Such molecular states can strongly reduce and effectively suppress double exchange ferromagnetism [6]. I will discuss some implications of these phenomena, and consider examples of real systems, in which orbital-selective phase are realized.

11:51AM F46.00002: Mott transition and collective charge pinning in electron doped Sr$_2$IrO$_4^*$  KAI WANG, NIMROD BACHAR (Presenter), JEREMIE TEYSSIER, WEIWEI LUO, WILLEM RISCHAU, GERNOT SCHEERER, ALBERTO DE LA TORRE, Department of Quantum Matter Physics, University of Geneva, ROBIN S. PERRY, London Centre for Nanotechnology and UCL Centre for Materials Discovery, University College London, FELIX BAUMBERGER, DIRK VAN DER MAREL, Department of Quantum Matter Physics, University of Geneva — We studied the in-plane dynamic and static charge conductivity of electron doped Sr$_2$IrO$_4$ using optical spectroscopy and DC transport measurements. The optical conductivity indicates that the pristine material is an indirect semiconductor with a direct Mott gap of 0.55 eV. Upon substitution of 2% La per formula unit the Mott gap is suppressed except in a small fraction of the material (15%) where the gap survives, and overall the material remains insulating. Instead of a zero energy mode (or Drude peak) we observe a soft collective mode (SCM) with a broad maximum at 40 meV. Doping to 10% increases the strength of the SCM, and a zero-energy mode occurs together with metallic DC conductivity. Further increase of the La substitution doesn’t change the spectral weight integral up to 3 eV. It does however result in a transfer of the SCM spectral weight to the zero-energy mode, with a corresponding reduction of the DC resistivity for all temperatures from 4 to 300 K. The presence of a zero-energy mode signals that at least part of the Fermi surface remains ungapped at low temperatures, whereas the SCM appears to be caused by pinning a collective frozen state involving part of the doped electrons.

*Swiss National Science Foundation (projects 200021-153405 and 200021-162628.)

12:03PM F46.00003: electric control of the structural properties of spin-orbit coupled 5$d$ iridate Sr$_2$IrO$_4^*$  FENG YE (Presenter), CHRISTINA HOFFMANN, WEI TIAN, Oak Ridge National Laboratory, JIEMING SHENG, Physics Department, Renmin University of China, HENGDI ZHAO, HAO ZHENG, GANG CAO, Department of Physics, University of Colorado at Boulder — The unique competition between spin-orbit interactions (SOI) and Coulomb correlation in 5$d$ elements compounds drives unusual physical behaviors. Due to the entanglement of spin and orbital degrees of freedom, the form of magnetic interactions depends on the underlying lattice geometry. In the case square-lattice Sr$_2$IrO$_4$, the Hamiltonian is governed by an isotropic Heisenberg plus a dipolar-like anisotropy term and leads to a weak canted antiferromagnetic order. Recent bulk measurement identified a novel coupling between the applied electric current and the canted IrO$_6$ octahedra. This drives a large nonlinear structural response closely tracking the magnetization. Neutron diffraction study on the structural evolution reveals an anomalous response of local IrO$_6$ distortion with respect to the applied electric current in the basal plane. Our results indicate the combination of SOI and the canted antiferromagnetic order provides a new paradigm for simultaneous electric control of the physics properties.

*Research at ORNL’s SNS was sponsored by the Scientific User Facilities Division, Basic Energy Sciences, U.S. Department of Energy (DOE). The work at U Colorado was supported by the National Science Foundation via grant DMR-1712101.

12:15PM F46.00004: Fracturing the inter-plane magnetic correlation in Sr$_2$IrO$_4$ with single laser pulse*  RUITANG WANG (Presenter), JIAQI LIN, Institute of Physics, Chinese Academy of Sciences, HAIDAN WEN, Argonne National Laboratory, DEREK MEYERS, Brookhaven National Laboratory, JIAN LIU, University of Tennesse, XUERONG LIU, ShanghaiTech University — Pump and probe type experiments have been generally performed to study the non-equilibrium dynamics of the charge, spin and lattice. Besides the generally expected full recovery to the ground states after long enough time, meta-stable states, which are not available from thermal equilibrium evolution, can emerge. We show that, upon single laser pulse pumping, the 3D AFM ordering in Sr$_2$IrO$_4$ is fractured into lower dimension and the system enters a meta-stable state. Such effect was studied as function of laser fluence. Our results show that the in-plane spin ordering correlation length is macroscopic (micron size), and the same before and after the pumping. While the out-of-plane correlation in the meta-stable state is quickly suppressed with the increasing of laser fluence, and saturates to be about ~1 unit cell without further reduction.

*Work at ShanghaiTech U. was partially supported by MOST of China under the grand No. 2016YFA0401000. R. W. was supported by international partnership program of Chinese Academy of Sciences under the grand No.112111KYSB20170059. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.
12:27PM F46.00005: Relativistic Quasi-particle Nature Emerging in semi-metallic Sr$_2$IrO$_4$. JEONG WOO HAN (Presenter), Physics and photon science, GIST, SUN WOO KIM, Physics, Hanyang University, WONSHIK KYUNG, Lawrence Berkeley National Laboratory, CHANGYOUNG KIM, Physics and astronomy, Seoul National University, GANG CAO, Physics and Astronomy, University of Kentucky, JINCHEN WANG, Physics, Renmin University of China, SANGMO CHEON, Physics, Hanyang University, JONGSEOK LEE, Physics and photon science, GIST — Whereas Dirac carrier responses have been extensively investigated in weakly-correlated-systems, it is rare to observe the Dirac physics in strongly-correlated-materials. Here, we provide experimental and theoretical evidences of an emergence of a Dirac dispersion in Tb-doped Sr$_2$IrO$_4$ which exhibits a semi-metallic and paramagnetic ground state. From the symmetry analyses, we find that the multiple crystal symmetries including nonsymmorphic symmetry play a pivotal role in the development of the Dirac dispersion, and furthermore, an intrinsic d-wave gap order collapse the line-nodal Dirac dispersion into the point-nodal dispersion. Linear dispersion of the energy band near the Fermi level is confirmed by angle-resolved photoemission spectroscopy, and the Dirac carrier responses are further manifested by an extremely low-scattering rate (~6 cm$^{-1}$) of free carriers.

12:39PM F46.00006: Evidence of resistive switching into a dynamical state in antiferromagnetic iridates* MORGAN WILLIAMSON (Presenter), SHIDA SHEN, Physics Department and Texas Materials Institute, University of Texas at Austin, GANG CAO, Department of Physics, University of Colorado-Boulder, JIANSHE ZHOU, Texas Materials Institute, University of Texas at Austin, MAXIM TSOI, Physics Department and Texas Materials Institute, University of Texas at Austin — Resistive switching, which is targeted for antiferromagnetic (AFM) memory applications [1], has recently been observed in the AFM iridates Sr$_2$IrO$_4$ [2] and Sr$_3$Ir$_2$O$_7$ [3, 4]. Here we demonstrate that the switching state at high electrical biases displays an increased noise pattern, which is indicative of a dynamical state at high biases. We employ a spectrum analyzer to characterize the noise pattern associated with the high-bias switching state and investigate the dependence of the noise spectrum on the magnitude of applied bias and magnetic field. The emergence of the noise was found to be strongly correlated with the onset of resistive switching. The noise power density displayed a 1/f$^2$ frequency dependence with an amplitude mimicking the hysteretic behavior of the resistance switching. We argue that the observed noise spectrum could be associated with a random switching between different states and discuss various interpretations of its origin.


*This work was supported in part by NSF grants DMR-1712101 and DMR-1122603, and by KAUST Award No. OSR-2015-CRG4-2626.

12:51PM F46.00007: Magnetic frustration revealed by the two-magnon Raman scattering in Sr$_2$IrO$_4$ and Sr$_3$Ir$_2$O$_7$ EKATERINA PÄRSCHKE (Presenter), Department of Physics, University of Alabama at Birmingham, YAO WANG, Department of Physics, Harvard University, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory and Stanford University, Stanford Institute for Materials and Energy Sciences, CHENG-CHIEN CHEN, Department of Physics, University of Alabama at Birmingham — Exploring the physics of spin-orbit Mott insulators such as iridates is expected to shed light onto high-temperature superconductivity as well as provide valuable insights into the interplay of spin-orbit coupling, Hund’s and Coulomb interactions. Of particular interest are low-energy magnetic excitations in one- and two-layer perovskites Sr$_2$IrO$_4$ and Sr$_3$Ir$_2$O$_7$. While one-magnon excitations in these materials are fairly well understood, their two-magnon Raman energies have been reported to vary greatly and lack simple correlation with single-magnon bandwidth. Here, we employ exact diagonalization to compute the Raman response of both systems and show that magnetic frustration and finite spin gap are responsible for the unexpectedly low two-magnon peak in Sr$_3$Ir$_2$O$_7$. We also present a modified spin wave approach for an intuitive explanation of the numeric results. Our analysis highlights magnetic frustration as one of the important differences between single- and double-layer perovskites iridates and emphasizes its impact on the two-magnon Raman response in general.

1:03PM F46.00008: Angle-resolved photoemission spectroscopy studies on Rh-doped Sr2IrO4 JIMIN KIM (Presenter), CALDES, Institute for Basic Science, SUNWOOK PARK, Department of Physics, POSTECH, JONATHAN DENLINGER, Lawrence Berkeley Natl Lab, BUMJOON KIM, Department of Physics, POSTECH — Doped Mott insulator feature a plethora of rich physics, most of which remain unclear, owing to strong correlation between electrons therein. Sr$_2$IrO$_4$, a spin-orbit coupled Mott insulator, is a prominent candidate to host such emergent phenomena, especially, similar to those in cuprate high-temperature superconductors. Therefore, it is worthwhile to study a phase diagram of Sr$_2$IrO$_4$ as a function of dopant density to unveil possible instabilities or exotic phases. To this end, we performed angle-resolved photoemission spectroscopy (ARPES) studies on hole-doped Sr$_2$IrO$_4$, achieved by ionic substitution of Rh for Ir, due to the relatively weak spin-orbit coupling of Rh. Obtained ARPES spectra and related phenomena will be discussed in terms of the phase diagram.
Correlation Effects and Hidden Spin-Orbit Entangled Electronic Order in Parent and Electron-Doped Iridates Sr$_2$IrO$_4$*  

SEN ZHOU (Presenter), Institute of Theoretical Physics, Chinese Academy of Sciences, KUN JIANG, Physics, Boston College, HUA CHEN, Physics, Zhejiang Normal University, ZIQIANG WANG, Physics, Boston College — Recent experiments discovered hidden order in the parent and electron-doped iridates Sr$_2$IrO$_4$, some with striking analogies to the cuprates, including Fermi surface pockets, Fermi arcs, and pseudogap. Here, we study the correlation and disorder effects in a five-orbital model derived from the band theory. We find that the experimental observations are consistent with a d-wave spin-orbit density wave order that breaks the symmetry of a joint twofold spin-orbital rotation followed by a lattice translation. The associated staggered circulating Jeff = 1/2 spin current can be probed by advanced techniques of spin-current detection in spintronics. This electronic order can emerge spontaneously from the intersite Coulomb interactions between the spatially extended iridium 5d orbitals, turning the metallic state into an electron-doped quasi-2D Dirac semimetal with important implications on the possible superconducting state suggested by recent experiments.

*This work is supported by the U.S. Department of Energy, Basic Energy Sciences Grant No. DE-FG02-99ER45747 (Z.W. and K. J.) and the Key Research Program of Frontier Sciences, CAS, Grant No. QYZDB-SSW-SYS012 (S. Z.).

Pseudogap and electronic structure of electron-doped Sr$_2$IrO$_4$*  

ALICE MOUTENET (Presenter), CPhT, Ecole Polytechnique, ANTOINE GEORGES, Collège de France, MICHEL FERRERO, CPhT, Ecole Polytechnique — We present a theoretical investigation of the effects of correlations on the electronic structure of the Mott insulator Sr$_2$IrO$_4$ upon electron doping. A rapid collapse of the Mott gap upon doping is found, and the electronic structure displays a strong momentum-space differentiation at low doping level: The Fermi surface consists of pockets centered around (π/2,π/2), while a pseudogap opens near (π,0). Its physical origin is shown to be related to short-range spin correlations. The pseudogap closes upon increasing doping, but a differentiated regime characterized by a modulation of the spectral intensity along the Fermi surface persists to higher doping levels. These results, obtained within the cellular dynamical mean-field-theory framework, are discussed in comparison to recent photoemission experiments and an overall good agreement is found.


*This work has been supported by the European Research Council grant ERC-319286-QMAC and the Swiss National Science Foundation (NCCR MARVEL). The Flatiron Institute is supported by the Simons Foundation.

Magnetic excitations in Sr$_2$IrO$_4$ measured with inelastic neutron scattering  

STUART CALDER (Presenter), DANIEL PAJEROWSKI, MATTHEW BRANDON STONE, ANDREW MAY, Oak Ridge National Laboratory — The widespread current interest in 5d materials stemmed from the observation that relativistic spin-orbit coupling drives a Mott-like insulating ground state with pseudospin $J_{\text{eff}}=1/2$ magnetic moments in the iridate compound Sr$_2$IrO$_4$. One surprising and enduring aspect of the physics of Sr$_2$IrO$_4$ is the observation of similarities to the parent unconventional cuprate La$_2$CuO$_4$. The degree to which this analogy holds, and if this suggests a proximate unconventional superconducting regime in Sr$_2$IrO$_4$, stands as an important outstanding question. In particular, a central issue in Sr$_2$IrO$_4$ is to understand how the strong spin-orbit coupling affects the magnetic excitations. Inelastic neutron scattering (INS) allows direct access to the magnetic excitations, but measurements have so far been lacking due to several hurdles posed by iridates. Utilizing time-of-flight INS with a gram sized single crystal array we successfully overcame these challenges. The results reveal direct evidence for two-dimensional in-plane magnetic interactions in Sr$_2$IrO$_4$ and allows a definition of the spin-gap. Modelling of the INS results with an isotropic 2D Hamiltonian supports a robust analogy with the physics of unconventional cuprates.
1:51PM F46.00012: Ferroelectric field and magnetic field effect on the spin-orbit coupled Mott insulator Sr$_2$IrO$_4$

ARNOUD EVERHARDT (Presenter), Materials Sciences Division, Lawrence Berkeley National Laboratory, YUN-LONG TANG, XIAOXI HUANG, Department of Materials Science and Engineering, University of California, Berkeley, JAY LEFEBVRE, SHANE CYBART, University of California, Riverside, R RAMESH, Department of Materials Science and Engineering, University of California, Berkeley — The 4d and 5d transition metals are commonly characterized by a decreased Hubbard repulsion $U$ which diminishes correlation effects, but simultaneously by an increased spin orbit coupling to create a new type of correlation effects which have been leading to such as spin-orbit coupled Mott insulators, Weyl semimetals, axion insulators and spin liquids. This rich physics allows small perturbations to create large effects in these strongly correlated materials. The Ruddlesden-Popper series of Sr$_{x+1}$Ir$_x$O$_{3x+1}$ shows large differences in conductive behavior, where the $n=\infty$ perovskite SrIrO$_3$ is metallic while the $n=1$ Sr$_2$IrO$_4$ is an insulator due to a spin-orbit coupling band splitting to a $J_{\text{eff}}=1/2$ state. This state has many similarities to the high $T_C$ cuprate superconductors which show an $S=1/2$ state, which loses its antiferromagnetism and becomes superconducting upon hole doping. Likewise, theoretically it is argued that under electron doping it is possible to drive Sr$_2$IrO$_4$ superconducting. Here a ferroelectric field effect is used on ultrathin Sr$_2$IrO$_4$ films to drive it to a more metallic state, by playing on the competition between electron doping and the canted antiferromagnetic transition at $\sim$200K.

2:03PM F46.00013: Effects of spin-orbit coupling on the metal-insulator transition in Sr$_2$Ir(1-x)T(x)O$_4$ (T = Rh,Ru)

BEREND ZWARTSENBERG (Presenter), RYAN P DAY, ELIA RAZZOLI, MATTEO MICHARDI, Quantum Matter Institute, University of British Columbia, NAN XU, MING SHI, Swiss Light Source, Paul Scherrer Institute, JONATHAN DENLINGER, Advanced Light Source, Lawrence Berkeley National Laboratory, STUART CALDER, Oak Ridge National Laboratory, BUMJOON KIM, Physics, Pohang University of Science and Technology, HIDENORI TAKAGI, Max Planck Institute for Solid State Research, ILYA ELFIMOV, ANDREA DAMASCELLI, Quantum Matter Institute, University of British Columbia — We study the role of spin-orbit coupling (SOC) in the metal-insulator transition of Rh- and Ru-substituted Sr$_2$IrO$_4$. Although similar, Rh and Ru have significantly different effects in driving the insulator to metal transition. Whereas Rh substitution realizes a Fermi surface at concentrations of 0.16 and higher, Ru substituted samples are insulating for similar values. We study the progression of effective SOC in the Rh substituted samples through a method based on photoemission matrix elements. We find that Rh reduces the effective SOC. This interpretation is substantiated by cluster models which show that SOC mixes into an average of the two subspecies. This mixing however, is strongly dependent on orbitals having similar energies. We argue that this quantitatively explains the difference between Ru and Rh substitution: since Ru has one less electron, the orbital energies are different from Ir, hence SOC mixing is ineffective. The model thus does not only explain the observed reduction of SOC in the Rh doped samples, it also shows why this reduction does not occur in Ru doped samples, thereby demonstrating that SOC is a key parameter in describing the MIT in Rh substituted Sr$_2$IrO$_4$.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F47 GERA: Energy Storage: Li Ion Batteries BCEC 213 - Sarbajit Banerjee, Texas A&M Univ

11:15AM F47.00001: The Hierarchical Structure of Nanoporous Carbon Electrode Materials Elucidated by Water Sorption: a Comparison of Multiple Structural Models

JOSE ESPITIA (Presenter), JOSE L BANUELOS, University of Texas, El Paso — The total amount of energy that an electrical double layer capacitor (EDLC) can store depends on the voltage and the accessible surface area for ion electrosorption. Nanoporous carbon materials with a high specific surface area, such as carbide derived carbon (CDC), make ideal electrodes for EDLC devices. Recent reports of water’s diffusional dynamics dependence on CDC pore size indicate confinement effects similar to that observed in pores of 16 Å. Small-angle neutron scattering (SANS) was used to find to what degree pores are filled with water (D2O) at intermediate stages of loading for four TiC-CDC powders, each with different pore size distributions. We present models to reproduce the SANS data, consisting of subnanometer pores as well as mesopores. In addition, the structure of the room temperature ionic liquid (RTIL) [C4mim]+[Tf2N]- and water confined inside the micropores (< 2 nm) of carbide derived carbon (CDC) were investigated using small angle x-ray scattering (SAXS). This study provides information on the length scales of the CDC porosity, the extent to which RTIL enters micropores, and how confinement affects the charge-ordered structure of the RTIL.
11:27 AM F47.00002: Achieving Fast kinetics and enhanced Li storage capacity for Ti$_3$C$_2$O$_2$ by intercalation of quinone molecules.

EDIRISURIYA SIRIWARDANE (Presenter), Department of Physics and Astrophysics, University of North Dakota, ILKER DEMIROGLU, CEM SEVIK, Department of Mechanical Engineering, Anadolu University, DENIZ ÇAKIR, Department of Physics and Astrophysics, University of North Dakota — In this work, we demonstrated that high Li storage capacity and fast kinetics are achieved for Ti$_3$C$_2$O$_2$ by preintercalating organic molecules C$_6$H$_4$O$_2$ and C$_6$F$_4$O$_2$. As compared to Ti$_3$C$_2$O$_2$ bilayer without linkers, considered pillared structures facilitate a much faster transport and higher charge/discharge rate for Li. For example, while the diffusion barrier of a Li ion within pristine Ti$_3$C$_2$O$_2$ bilayer is around 1.0 eV, it becomes 0.3 eV in pillared structures. Although we can only intercalate one monolayer of Li within pristine Ti$_3$C$_2$O$_2$ bilayer, our calculations showed that at least two layers of Li can be stored between Ti$_3$C$_2$O$_2$ layers of pillared structures, without forming bulk Li and losing the pillared structure upon Li loading/unloading. A small change in the in-plane lattice parameters (<1%) and interatomic bond lengths, and ab-initio molecular dynamics simulations prove the stability of the pillared structures against Li intercalation and thermal effects.

*Computer resources are provided by Computational Research Center at University of North Dakota. A part of this work was supported by UND Early Career Award (20622-4000-02624) and ND EPSCoR through NSF grant #OIA-1355466.

11:39 AM F47.00003: Direct-write Lithiation of Silicon Using a Focused Ion Beam of Li.

WILLIAM MCGEHEE (Presenter), EVGHENI STRELCOV, VLADIMIR OLESHKO, CHRISTOPHER SOLES, NIKOLAI BORISOVICH ZHITENEV, JABEZ J MCCLELLAND, National Institute of Standards and Technology — We report progress in developing Li$^+$ focused ion beams (FIB) as a novel probe for exploring nanoscale electrochemistry in battery-relevant materials. Electrochemical processes involve numerous parallel reactions that complicate our microscopic understanding of these systems, and new tools are needed to probe ionic transport at the level of grain boundaries, interfaces, and single defects. Here, we demonstrate the use of Li$^+$ FIB to direct-write controlled quantities of Li into 35 nm thick crystalline silicon membranes in vacuo at doses from $10^{15}$ cm$^{-2}$ to $10^{18}$ cm$^{-2}$. The concomitant morphological, structural, and functional changes in the implanted silicon are characterized using a combination of electron and scanning probe microscopy. We observe saturation of interstitial lithium in μm-scale implanted regions as well as spill-over of excess lithium on the membrane's surface. Prospects for future work exploring transport across grain boundaries and implantation at higher resolution are discussed.


RAJENDRA JOSHI (Presenter), VERONICA BARONE, Department of Physics and Science of Advanced Materials, Central Michigan University, Mt. Pleasant, MI, 48858, JESSE EICKHOLT, Department of Computer Science, Central Michigan University, Mt. Pleasant, MI, 48858, JUAN ERNESTO PERALTA, Department of Physics and Science of Advanced Materials, Central Michigan University, Mt. Pleasant, MI, 48858 — Data driven machine learning approaches have been increasingly adopted in the materials science community as an efficient alternative to density functional theory calculations to predict the properties of materials. In this work, we show how machine learning can be applied to energy storage materials. In addition, we compare the performance of different machine learning approaches for predicting the future energy storage materials.

12:03 PM F47.00005: Structure-Property of Li-S Nanoparticles via Molecular Dynamics Simulation.

KAH CHUN LAU (Presenter), Physics and Astronomy, California State University, Northridge, CA 91330, USA., YING LI, NICHOLS ANTHONY ROMERO, Computational Science Division and Leadership Computing Facility, Argonne National Laboratory, Lemont, IL 60439, USA. — Lithium-sulfur (Li-S) batteries offer higher energy densities than most reported lithium-ion batteries. However, our understanding of Li-S battery is still largely unknown at the level of the nanoscale. The structural properties of Li-S materials were investigated via molecular dynamics (MD) simulations using the ReaxFF force field. Several Li-S nanoparticles with different Li:S composition ratios and various structures are studied. Our MD simulations show that, among the four structures we constructed for Li$_2$S$_8$ nanoparticles, the core-shell structure is the most thermodynamically stable one during the charging (delithiation) process. In contrast to bulk crystal Li$_2$S, we find the presence of mixed lithium sulfide and polysulfide species are common features for these Li-S nanoparticles. The complex distribution of these sulfide and polysulfide speciation are dictated by both stoichiometry and local atomic structures in the nanoparticle. These findings will provide insight into further development of functionalized lithium-sulfur cathodes.

*Supports from the Margaret Butler Postdoctoral Fellowship at Argonne National Laboratory, and California State University Northridge Faculty start-up fund are acknowledged.
12:15PM F47.00006: Chemo-mechanical modeling of defective graphene for energy storage in Lithium-Ion Battery
VIDUSHI SHARMA (Presenter), DIBAKAR DATTA, Department of Mechanical and Industrial Engineering, New Jersey Institute of Technology — The process of Li insertion and extraction imparts repeated mechanical loading and unloading of anode materials which ultimately leads to mechanical degradation and battery failure. With the persistent need to model efficient anode materials that can withstand repeated mechanical loading, we have looked into the potential of defective graphene(DG) based 2D materials which have enhanced Li adsorption and good mechanical strength to undergo several cycles of charge-discharge. In this work, we have primarily used grand canonical Monte Carlo and molecular dynamics (GCMC-MD hybrid) to model complete charge and discharge profiles of DG varying from single layer to multilayered systems. Stress distribution upon charge and discharging have been analyzed to predict crack nucleation and propagation. Density Functional Theory (DFT) was used to benchmark our GCMC-MD results. Enhanced adsorption of Li resulted in incomplete desorption during discharging which resulted in decreased over-all charge-discharge cycle stability of the system. Further, inherently having low shear strength, it was determined that the presence of Li atoms significantly affects the overall slippage of one DG over another along with their load-bearing capacity.

12:27PM F47.00007: First-Principles Study of Lithiation of Type I Ba-Doped Silicon and Germanium Clathrates
XIHONG PENG (Presenter), ANDREW DOPILKA, QUN WEI, CANDACE K CHAN, Arizona State University — Si and Ge clathrate materials have recently been investigated for their electrochemical properties as anodes for Li-ion batteries due to their unique cage structures and ability to incorporate extrinsic guest atoms. First-principles calculations were used to investigate the type I clathrate compounds Si_{46}, Li_{x}Ba_{x}Si_{46}, Li_{x}Ba_{x}Al_{6}Si_{40} and Li_{x}Ba_{x}Ge_{43}, for understanding the preferred structures of small degrees of lithiation and Li diffusion paths. The results showed that Li insertion into framework or Ba vacancies could stabilize the clathrate structure. Si substitution by Al lowered the formation energies of the lithiated compounds. For Ba-doped Ge clathrates, it was found that Li insertion into the three framework vacancies in Ba_{9}Ge_{43} is energetically favorable. However, the high energy barrier (1.6 eV) for Li diffusion between vacancies and around Ba guest atoms suggests that framework vacancies are unlikely to significantly contribute to lithiation processes unless the Ba guest atoms are absent. The study elucidated the preferred structural configurations for Li in type I, Ba-doped Si/Ge clathrates and also be informative for efforts related to understanding the structures obtained after electrochemical insertion of lithium into the clathrates.

*NSF DMR-1710017

12:39PM F47.00008: Linear stability analysis of time-dependent electrodeposition in charged porous media
EDWIN KHOO (Presenter), HONGBO ZHAO, MARTIN BAZANT, Massachusetts Institute of Technology — We study the linear stability analysis of time-dependent electrodeposition in a charged porous medium flanked by a pair of planar metal electrodes. Discretization of the linear stability problem results in a generalized eigenvalue problem that is solved numerically. Analytical approximations obtained from a boundary layer analysis valid at high wavenumbers agree well with the full numerical solutions. Under galvanostatic conditions, in the classical case of zero pore surface charges, the voltage and electric field at the cathode diverge when the cation concentration there vanishes at Sand's time. The same phenomenon happens for positive surface charges but at a time earlier than Sand's time. In contrast, negative surface charges allow the electrochemical system to sustain an overlimiting current via surface conduction past Sand's time, keeping the voltage and electric field bounded. Therefore, at Sand's time, negative surface charges greatly reduce the electrode surface instabilities while zero and positive surface charges magnify them. We also use the stability analysis to analyze how using a pulse current in electroplating and metal battery charging reduces diffusion limitations and electrode surface instabilities at high currents in the presence of negative surface charges.

12:51PM F47.00009: Developments in X-ray full-field nano-tomography at the Advanced Photon Source for in situ characterization of battery and fuel cells
VINCENT DE ANDRADE (Presenter), SUNIL BEAN, MICHAEL WOJCIC, FRANCESCO DE CARLO, ALEX DERIY, Advanced Photon Source, Argonne National Laboratory — The Transmission X-ray Microscope (TXM) at beamline 32-ID of the Advanced Photon Source beamline at Argonne National Laboratory has been tailored for high throughput and high spatial resolution in operando nano-tomography experiments. Over the first 5 years of operations, it imposed as a very productive instrument, particularly in the domain of battery research. It benefits from the in-house development of cutting-edge X-ray optics, complex opto-mechanical components and a suite of software including Tomopy and other based on machine learning to push the limit of 3D nano-imaging while reducing total X-ray dose. It operates either with a moderate spatial resolution (40-50 nm) and large field of view (~50 µm) or at very high spatial resolution (16 nm) at a smaller field of view (~10 µm). This presentation will give an overview of in situ experiments on batteries with different kind of cells, as well as our efforts for characterizing low-Z material like Li oxide, black carbon or polymers.
1:03PM F47.00010: Tailoring storage capacity and ion kinetics in Ti2CO2/graphene heterostructures by functionalization of graphene  
DENIZ CAKIR (Presenter), University of North Dakota, CEM SEVIK, Eskisehir Technical University  
— Using first-principles calculations, we evaluated the electrochemical performance of heterostructures made of Ti2CO2 and chemically modified graphene for Li batteries. We found that heteroatom doping and molecule intercalation have a large impact on storage capacity and Li migration barrier energies. While N and S doping do not improve the storage capacity, B doping together with molecule interaction make it possible to intercalate two layers of Li which stick separately to the surface of Ti2CO2 and B-doped graphene. The calculated diffusion barrier energies (E_diff), which are between 0.3 and 0.4 eV depending on Li concentration, are quite promising for fast charge/discharge rates. In addition, the predicted E_diff as much as 2 eV for the diffusion of Li from Ti2CO2 surface to B-doped graphene surface significantly suppress the interlayer Li migration, which diminishes the charge/discharge rates. The calculated volume and lattice parameter changes indicate that Ti2CO2/graphene hybrid structures exhibit cyclic stability against Li loading/unloading. Consequently, the performed first-principles calculations evidently highlight the favorable effect of molecular intercalation on the capacity improvement of ion batteries.

1:15PM F47.00011: Lithium Interaction with Graphene Materials at Finite Temperature  
YUSUF SHAIDU (Presenter), EMINE KUCUKBENLI, STEFANO DE GIRONCOLI, Condensed Matter Physics, International School for Advanced Studies  
— The increasing demand for high energy density lithium ion batteries motivates a search for alternative electrode materials. Experimentally obtained graphene based structures have been suggested to replace the state-of-the-art graphitic anode [1]. We characterized the Li adsorption on graphene both at zero and finite temperatures. The zero temperature study was carried out by means of density functional theory (DFT) accounting for van der Waals interactions while the finite temperature behavior was studied by Monte Carlo techniques with DFT-derived Li-graphene interaction potential constructed via cluster expansion method. At zero temperature, the dispersed Li configurations are unstable with respect to metallic Li. At higher temperatures, entropic effects stabilize lower concentrations with respect to bulk Li while below 400\,K, the formation of 2D Li-clusters is stable over a random distribution of Li. In order to understand the nature of Li interactions with all carbon materials rather than single layer graphene, we are developing an artificial-neural-network based lithium-carbon interaction potential employing Behler and Parrinello symmetry functions[2] as structural descriptors. This will allow a detailed investigation and characterization of Li interaction with these materials.

1:27PM F47.00012: Simulated studies of Li-Mn-O heterostructured nanoparticles on lithiation*  
PHUTI NGOEPE (Presenter), DONALD HLUNGWANI, RAESIBE LEDWABA, Materials Modelling Centre, University of Limpopo, Sovenga, 0727, South Africa  
— Simulated amorphisation and recrystallization (A+R) technique is employed to synthesise Li-Mn-O nanoparticles, particularly those in the range of 3000 atoms, which are amenable to linear scaling DFT methods. The A+R method has been previously successfully used to study nanostructures of MnO2 [1], with composite structures. The discharge cycling process of the nanoparticle was simulated by lithiating the Li-Mn-O composite nanoparticle at different lithium concentrations. Each nanoparticle was characterized by interrogating their radial distribution functions (RDFs) and simulated X-ray diffraction patterns (XRDs). Furthermore, the structural changes with lithiation were visualised and details of various defects, including grain boundaries could be observed from microstructures. The presence of layered and spinel components were also noted and validated by XRDs. In the future, the simulated structures will be used to voltage profiles using linear scaling DFT methods.


*We acknowledge support of the SARCHI of the National Research Foundation, Department of Science and Technology in Pretorua and the Centre for High Performance Computing in Cape Town.
1:39PM F47.00013: Probing Electrical Degradation of Lithium Ion Battery Electrodes with Nanoscale Resolution
SEONG HEON KIM (Presenter), SEONG YOUNG PARK, HEECHUL JUNG, Samsung Advanced Institute of Technology —
The investigation of the electrical conductivity evolution during cycling can lead to a better understanding of the
degradation in electrode materials for Li-ion batteries (LIBs). In this study, we probed the electrical degradation of LIB
electrodes with nanoscale resolution via quantitative and comparative scanning spreading resistance microscopy (SSRM).
First, the electrical degradation of cathode materials, LiNi_{0.8}Co_{0.15}Al_{0.05}O_2 (NCA), was studied [1]. After 300
charge/discharge cycles, stepwise-increasing resistance distributions toward the centers of the secondary particles were
observed. Second, the electrical degradation of LIB anodes, the blended Si-C composites with graphite (Gr) particles, was
investigated using SSRM [2]. From the SSRM measurements, it was obviously demonstrated that the electrical conductivity
of the Si-C composite particles is considerably degraded by 300 cycles of charging and discharging, although the Gr
particles maintain their conductivity. Our approach using SSRM technique can be an effective method to study the
nanoscale electrical properties of various LIB electrode materials.


1:51PM F47.00014: TiSe2 as a Cathode for Multivalent Ion Batteries*
MANUEL SMEU, TAYLOR JURAN (Presenter), Binghamton University — To drive large scale energy storage, it is imperative to investigate the properties of multivalent ion batteries (MVIBs). TiSe_2 cathodes experience electron delocalization in metal-ligand units, a trait shown to improve battery performance. Both TiSe_2 and the Chevrel phase (CP) experience d-p orbital hybridization, suggesting TiSe_2 may demonstrate similar MVIB performance to the CP, an established MVIB cathode. TiSe_2 has been previously studied with a Mg anode, though it was not studied with other multivalent metals, in particular Ca, which has demonstrated superior performance to Mg in some respects. In this computational study, we investigate the intercalation of TiSe_2 with several mono/multivalent ions from the following metal anodes: Li, Na, Mg, Ca, Zn, and Al (with a particular focus on Ca-ion). We used density functional theory methods, including the SCAN functional, to calculate the average voltages for the aforementioned metals paired with TiSe_2. We consider other crucial battery properties, including volume change, diffusion kinetics, material characterization, and stability.

*Supported as part of the Multidisciplinary GAANN fellowship in Smart Energy Materials, a Graduate Areas of National Need, funded by the U.S. Department of Education, Award P200A150135.

2:03PM F47.00015: Infrared Imaging of Batteries During Charging by Magnetic Augmented Rotational System (MARS)
LAILA ALQARNI, VISHWAS DANTHI SHIVARAM, NAVJOT S PANCHHI, SHUANG DUE, New Jersey Institute of Technology, TIEN SEE CHOW, ETD Inc., RAVINDRA NUGGEHALLI M (Presenter), New Jersey Institute of Technology —
Modern-day rechargeable batteries such as lithium-ion based batteries exhibit major benefits over previous iterations. Their longer-useful & higher-cycle life without significant loss of capacity makes them suitable for the current market. Downside, Li-ion batteries require sophisticated voltage management systems to prolong their life and stop thermal runaway. Safety is a major concern for large-scale Li-ion batteries.

In our study, we use Infrared Thermography (IT) to monitor, map and interpret the thermal behavior of batteries during charging/discharging with the electromagnetic contactless gear system that charges the batteries (Magnetic Augmented Rotation System-MARS). Data relating to heat generation and the internal and external heat transfer obtained from IT will be utilized for a detailed analysis of the heat distribution in the system, as well as to identify and locate areas of excess heat.

As increased heating is a signal of non-uniform distribution of charge/failure, infrared is the best diagnostic tool to identify these hot spots in the early stages of degeneration. Experimental and analytical techniques will be used to construct a model for charge transfer and the associated thermal map.
Tuesday, March 5, 2019 11:15 AM - 1:27 PM

Session F48 DFD GSNP: Fluid Mechanics -- General BCEC 251 - Michael Allshouse, Northeastern University

11:15AM F48.00001: Strain rate effects on front propagation in advection reaction diffusion systems*  THOMAS NEVINS (Presenter), DOUGLAS H KELLEY, University of Rochester — The growth of a reactive scalar in a flowing fluid is known as an advection-reaction-diffusion (ARD) system. In this talk I will focus on effects of flow strain rate (deformation) within ARD systems - specifically chemical systems - through experiments measuring front propagation. Fronts in this context are the borders of reacted regions. Fronts are often modelled as moving with velocity equal to the sum of flow and chemical front speed in stagnant fluid. We find strain rate to have profound effects in multiple contexts. For example, I will present how reactive mixing in a two-dimensional (2D) experimental flow does not behave like a 2D ARD system due to strain rate. We also perform experiments on reactions in the presence of straining flows to demonstrate how chemical front speed is altered, how bulk reaction is changed in turn, and how in special situations stirring can actually inhibit reaction. We identify various processes by which shear strain changes front speed, and make predictions about the size of these changes. These results may explain part of why mixing changes reactions and how flow sometimes creates reaction barriers.

*Funded through the Department of Defense National Defense Science and Engineering Graduate Fellowship (NDSEG).

11:27AM F48.00002: Front induced feedback in convective flowfields*  SAIKAT MUKHERJEE (Presenter), Biomedical Engineering and Mechanics, Virginia Tech, MARK RICHARD PAUL, Mechanical Engineering, Virginia Tech — We numerically study the feedback between a propagating front and the underlying flowfield for a range of different parameters. The flowfields are generated by a modified form of the Boussinesq equation, which generates counter rotating convection rolls in a long shallow layer of fluid. The strength of the convection rolls is quantified by the Rayleigh number. In many reaction-advection-diffusion systems, a difference in buoyancy between the products and the reactants creates secondary fluid rolls which interact with the existing convection rolls and affect the velocity and geometry of the propagating front and the underlying flowfield. This roll formed due to the backaction of the front on the flowfield also affects the geometry of the front interface, noticeably making it more tilted and stretched. We quantify the strength of this backaction roll by a quantity called the solutal Rayleigh number, which is related to the ratio of the buoyancy difference between the products and the reactants to the diffusion coefficient of the products. We investigate the interaction of this front induced backaction roll and the convection rolls in two dimensional cellular flow and for three dimensional spatiotemporally chaotic flow.

*Partial support by DARPA Grant No. HR0011-16-2-0033.

11:39AM F48.00003: Coherent Structure Detection using Topological Tools and a Graph Theoretic Approach  CALEDONIA WILSON (Presenter), SPENCER SMITH, Mount Holyoke College — For general aperiodic fluid flows, coherent structures help organize the dynamics, much as invariant manifolds and periodic orbits do for autonomous or periodic systems. The prevalence of such flows in nature and industry has motivated many successful techniques for defining and detecting coherent structures. However, these approaches often require very fine trajectory data to reconstruct velocity fields. Instead, we use topological techniques to help detect coherent trajectory sets in relatively sparse 2D fluid advection problems. More specifically, we use a homotopy-based algorithm, the ensemble-based topological entropy calculation (ETEC), which evolves fluid material curves forward in time as minimal length bands stretched about the moving data points. These bands are represented as the weighted edges of a triangulation, which allows us to analyze flows using graph theoretic tools. In this way, highly connected components of appropriately constructed graphs can be used to partition the fluid particles into coherent trajectory sets.

11:51AM F48.00004: The Phase Diagram of Leaking Flows  HEATHER KURTZ (Presenter), CAROLINE TALLY, KATHARINE JENSEN, Williams College — When a pipe springs a leak, the exiting fluid can either jet away cleanly, dribble down along the surface, or not flow out at all. Past investigations of this “teapot effect” have focused on jetting and dribbling liquid flows separately as functions of initial flow velocity, wetting, and viscosity, but there has been little focus on the transition between flow regimes. In this work, we characterize a liquid leaking from a small hole as the flow transitions from jetting to dribbling, and dribbling to no flow. We map the phase diagram of these leaking flow transitions as a function of hydrostatic pressure and pipe tipping angle, and investigate the contributions of fluid viscosity, hole size, and surface wetting to the boundaries on this phase diagram.
12:03PM F48.00005: Ensemble-based Topological Entropy Calculation in Three Dimensions  ERIC ROBERTS (Presenter), SUZANNE SINDI, University of California, Merced, SPENCER SMITH, Mount Holyoke, KEVIN MITCHELL, University of California, Merced — Topological entropy measures the number of distinguishable orbits in a dynamical system, thereby quantifying the complexity of chaotic dynamics. Such knowledge aids greatly in a wide variety of natural and industrial fluid systems, including the rapidly developing field of microfluidics and the large-scale dispersion of pollutants in the Earth's atmosphere and oceans. We introduce a computational geometry framework for estimating a three dimensional flow's topological entropy from the collective motion of an ensemble of system trajectories. This work is analogous to the entropy calculation extracted from the "braiding" of system trajectories in two dimensions and is a first step towards building a triangulation-based method for computing topological entropy from an ensemble of trajectory data in three dimensions and higher. In it, we consider a two-dimensional rubber sheet stretched around a collection of points in a three-dimensional flow. A 3D triangulation may be used to track point-face or edge-edge collisions and the rubber sheet may be chosen as one of the faces in the initial triangulation. As the points evolve in time, they carry the sheet along with them, stretching and folding it so that its growth reflects the flow complexity.

12:15PM F48.00006: Uncertainty quantification in Lagrangian clustering analysis  GUILHERME SALVADOR VIEIRA (Presenter), MICHAEL ALLSHOUSE, Mechanical Engineering, Northeastern University — Partitioning ocean flows into regions that minimally mix with their surroundings can identify materially coherent vortices and assist in search and rescue planning by reducing the search domain. One method for such partitioning is the Lagrangian clustering analysis, which identifies sets of trajectories that move as a compact set. This method has been applied to deterministic, chaotic systems, revealing underlying transport barriers. For ocean models, however, in addition to the complex dynamics, there are several sources of uncertainty, such as model initialization and parameters, limited knowledge of oceanographic processes, and ocean boundary conditions and forcing. Therefore, the Lagrangian clustering analysis, when applied to ocean forecasts, should incorporate uncertain parameters and the resulting coherent structures should be robust to model uncertainty. Through application to a geostrophic flow, we present an investigation of the sensitivity of the spectral clustering method to uncertain parameters and an approach for applying this method to an ensemble of simulations.

12:27PM F48.00007: Lubricated motion in an elastic tube*  MARIE TANI, Tokyo Metropolitan University, THOMAS CAMBAU, JOSE BICO, ESPCI, PMMH, ETIENNE REYSSAT (Presenter), CNRS-ESPCI, PMMH — The motion of objects through elastic constrictions is relevant to various problems in physiology and biology. We describe a model experiment where a rigid sphere is displaced through a narrower elastic tube. Lubricating the contact with a fluid significantly reduces friction on the wall of the tube. The friction force increases as the sliding velocity to the power 1/3 and depends on the fluid viscosity, mechanical properties of the tube and geometric mismatch. We derive a scaling law and a minimal numerical model to account for our experimental data.

*We thank JSPS for funding Marie Tani.

12:39PM F48.00008: A Random Choice SPH Scheme with Adaptive Viscosity*  ZHIXUAN CAO (Presenter), FBU (Fluids Business Unit), ANSYS Inc., ABANI K PATRA, Department of Mechanical and Aerospace Engineering, State University of New York at Buffalo, E. BRUCE PITMAN, Department of Materials Design and Innovation, The State University of New York at Buffalo — Classical smoothed particle hydrodynamics (SPH) method employs explicit artificial viscosity, which typically produce more dissipation than need, incorrectly smears contact discontinuities and overwhelms fluid turbulence. Several studies have proposed highly tuned versions of artificial viscosity, turning on and off near shocks or other troublesome wave features. A different scheme adapts Godunov's idea of solving local Riemann problems as building blocks for SPH solver. However, these methods still introduce an effective numerical diffusion that can infect the entire numerical solution. We propose a new SPH scheme that combines an approximate version of Glimm's Random Choice method (RCM) with SPH. Our version approximately resolves hydrodynamic waves, and samples the approximate solution without explicit artificial viscosity. Several attractive features of this method is demonstrated by 1D shock tube tests. First, this method introduces adaptive artificial viscosity, assigning larger dissipation near discontinuities and smaller elsewhere. Secondly, it is less dissipative than classical SPH and GSPH resulting in less smearing of shock. Thirdly, this method also ameliorates pressure ``wiggle" around contact discontinuity.

*The wrok is supported by Grants No. NSF ACI/1131074.
12:51PM F48.00009: Dimensionality reduction of convection-dominated flows on an optimally morphing grid
RAMBOD MOJGANI (Presenter), MACIEJ BALAJEWICZ, University of Illinois at Urbana-Champaign — Foundations and preliminary results of a new projection-based model order reduction approach are summarized. The method is specifically designed for convection dominated nonlinear fluid flows. In this method, the evolution of the flow is approximated on an optimally morphing grid. The low-rank grid deformation, a solution of an optimization problem, is generated in such a way that the low-dimensional representation of the states on this morphing grid has lower error when compared to traditional POD on an Eulerian grid. Global basis functions are used to approximate the state variables on the low-rank grid. It is demonstrated that in this framework, certain wave-like solutions exhibit low-rank structure and thus, can be efficiently compressed using relatively few global bases. The proposed approach is successfully demonstrated for the reduction of several representative 1D and 2D problems, featuring nonlinearities, and bi-directional waves with different boundary conditions and is compared with the traditional method on the Eulerian grid.

1:03PM F48.00010: An Exact Simple Solution of the Compressible Navier-Stokes Equation*
AMADOR MURIEL (Presenter), Natural Science Research Institute —
We display a simple exact solution of the compressible Navier-Stokes equation without an external field. The field velocities and density are:

\[ v_x = n_0 v_{x_0} \exp[-a((x-v_{x_0} t)^2+(y-v_{y_0} t)^2+(z-v_{z_0} t)^2)] \]
\[ v_y = n_0 v_{y_0} \exp[-a((x-v_{x_0} t)^2+(y-v_{y_0} t)^2+(z-v_{z_0} t)^2)] \]
\[ v_z = n_0 v_{z_0} \exp[-a((x-v_{x_0} t)^2+(y-v_{y_0} t)^2+(z-v_{z_0} t)^2)] \]
\[ n = n_0 \exp[-a((x-v_{x_0} t)^2+(y-v_{y_0} t)^2+(z-v_{z_0} t)^2)] \]

where all variables are defined and explained in A. Muriel, Results in Physics 6, 461 (2016) or ResearchGate, amadormuriel@gmail.com. The pressure tensors are calculable from the above field velocities using the Navier-Stokes equation itself. The density, the field velocities and the derivable pressure tensors constitute the simplest exact solution to date of the Navier-Stokes equation. We invite readers to check the self-consistency of the solution. The origin of this solution, as well as others, will be explained and illustrated. Surprisingly, this simple solution meets all stipulations of the problem definition by the Clay Institute of Mathematics. This solution is valid for a compressible fluid instead of an incompressible fluid required by the Institute.

*We acknowledge the Balik Scientist Program of DOST, Philippines for its support.

1:15PM F48.00011: Bottom up lattice Boltzmann: the path from Molecular Dynamics to lattice Boltzmann methods
ALEXANDER WAGNER (Presenter), M. REZA PARSA, North Dakota State University, ALEKSANDRA PACHALIEVA, Mechanical Engineering, TU Munich — We show how lattice Boltzmann simulations can be understood as a coarsegraining and averaging of Molecular Dynamics simulations. Typically lattice Boltzmann methods are verified by analyzing the hydrodynamic limit of the method. It is known that this approach is not sufficient for several kinds of application. In contrast, our approach allows to bottom up derivation of lattice Boltzmann methods, and gives guidance for the design of lattice Boltzmann (or lattice gas) methods for fluctuating and/or non-ideal systems and gives an alternative path to compare competing collision operators and equilibrium distributions as well as forcing terms currently used and gives a fundamental test of what the correct form of these terms is.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F49 DPOLY: Advanced Morphological Characterization of Polymer III: Anomalous Soft X-ray Scattering BCEC 252A - Cheng Wang, Lawrence Berkeley Natl Lab - Tag(s): Focus
11:15AM F49.00001: Critical-Dimension Grazing-Incidence Small Angle X-Ray Scattering: Applications using Soft, Tender and Hard X-Rays*  GUILLAUME FREYCHET (Presenter), DINESH KUMAR, ISVAR CORDOVA, RONALD J PANDOLFI, PATRICK NAULLEAU, CHENG WANG, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Laboratory — As the lithographically manufactured nanostructures are shrinking in size, conventional techniques, such as microscopies (SEM, AFM) reach their resolution limits. We have developed a high performance Grazing Incidence SAXS simulation tool to reconstruct the in-depth profile highly ordered material such as line gratings [1]. Here, we will present the latest development and applications of the technique using hard x-rays on line gratings and contact holes. Moreover, the CD-GISAXS approach was extended to study line edge roughness, latent images [2] and lamellae structure of diblock copolymers, taking advantage of the full energy range provided at the advanced light source and more specifically of the chemical sensitivity provided by soft and tender x-rays scattering.


*Acknowledgement:
This work was supported by the Center for Advanced Mathematics for Energy Research Applications (CAMERA), by the Office of Science, Office of Basic Energy Sciences and US DoE.

11:27AM F49.00002: Label-free measurement of core-shell Pluronic F127 Micelle nanostructure determined using in-situ Resonant Soft x-ray Scattering*  TERRY MCAFEE (Presenter), ISVAR CORDOVA, Advanced Light Source, Lawrence Berkeley National Laboratory, THOMAS FERRON, Physics & Astronomy, Washington State University, CHENG WANG, Advanced Light Source, Lawrence Berkeley National Laboratory, BRIAN COLLINS, Physics & Astronomy, Washington State University — Micelles are key to many applications such as drug delivery, and their size, shape and internal molecular conformation are of critical importance to their performance. By having both hydrophobic and hydrophilic monomer groups, polymers like Pluronic F127 self-assemble into spherical core-shell structures called Micelles. However, confirming the structural parameters, in particular conformation, is difficult if not impossible to date. Here we demonstrate a novel technique capable of such measurements based on Resonant Soft X-ray Scattering (RSoXS), which is uniquely sensitive to bond orientation and capable of probing organic materials using their intrinsic chemical structure for contrast manipulation rather than laborious and potentially disruptive isotopic labeling that is required in techniques such as neutron scattering. Like electron microscopy, RSoXS requires a high vacuum environment. By adapting a Poseidon Protochips TEM holder for use at BL11.0.1.2 of the Advance Light Source, we show that RSoXS can now be performed in in-situ/operando environments, allowing sample structure and interactions to be measured in the same conditions/environment as the intended application.

*This work may have been supported by DOE and was supported by NSF MRI under Grant #1626566.

11:39AM F49.00003: Correlating anisotropy in polarized resonant soft X-ray scattering of block copolymer active layers with organic photovoltaic device performance  JOSHUA LITOFSKY (Presenter), ENRIQUE D GOMEZ, Pennsylvania State University — The use of Resonant Soft X-ray Scattering (RSoXS) allows the study of domain spacing and molecular orientation of conjugated polymers in the active layer of organic photovoltaics through tuning of the X-ray energy and polarization. Using the conjugated block copolymer system of poly(3-hexylthiophene) with acceptor blocks poly(fluorene-alt-dithienylbenzothiadiazole), (PFTBT), poly(carbazole-alt-dithienylbenzothiadiazole) (PCDTBT), and poly(phenylene-alt-dithienylbenzothiadiazole) (PPDTBT), along with alkyl side chain-added analogs PFT6BT, PCT6BT, and PPT6BT, we can examine the effects that morphological changes have on electronic device performance. The addition of hexyl side chains to the acceptor blocks decrease the degree of molecular order, as measured by the scattering anisotropy from RSoXS. This anisotropy has been shown to define the strength of alignment of chains with respect to the block copolymer interface within nematic domains, and can be used to directly compare long-range order between polymers. Based on our early findings, we believe that suppression of the long-range order is directly related to lower fill factors and lower device efficiencies. Studies into the charge carrier mobilities and crystallinity support these findings across the polymer systems.
11:51AM F49.00004: Advanced characterization of molecular nanostructures and interfaces with resonant X-ray scattering* [invited] BRIAN COLLINS (Presenter), Washington State University — Emergent properties within molecular materials are determined by their nanoscale ordering, in particular at interfaces. This has revealed a potential for their use in drug delivery, printable electronics, and bottom-up nano-assembly if their ordering can be controlled. A major roadblock is the lack of nanoprobes that can precisely characterize ordering within these delicate materials that contain light elements, 3D structures, and low crystallinity. I will discuss recent progress in developing a new class of measurements based on X-rays resonant with molecular transitions to enable quantitative characterization of molecular order. Resonant soft X-ray scattering (RSoXS) combines polarized spectroscopy with scattering, enabling sensitivity to bond type and orientation — similar to ellipsometry and Raman spectroscopy but with higher spatial resolution. Contrast variation can be achieved by tuning the photon energy — similar to deuteration in neutron scattering but without the need of laborious and disruptive chemical labelling. I will highlight our recent progress in developing quantitative RSoXS analyses for characterizing molecular interfaces as well as ordering within and between nanostructures. In particular, the ability of polarized RSoXS to measure local molecular orientation even in polydisperse 3D matrices is not possible with any other technique. I will also touch on our work in developing a new instrument to measure structural evolution of solvated nanoparticles and operando electrochemical processes. As RSoXS continues to mature, it will enable increased understanding and control of molecular and hybrid nanostructures resulting in revolutionary new technologies based on these novel materials.

*DOE Early Career Award, NSF Major Research Instrumentation

12:27PM F49.00005: Probing Molecular Orientation using Polarized Resonant Soft X-ray Reflectivity* JACOB THELEN (Presenter), National Institute of Standards and Technology, CAMILLE BISHOP, University of Wisconsin - Madison, DANIEL SUNDAY, ELIOT H GANN, National Institute of Standards and Technology, MARK EDIGER, University of Wisconsin - Madison, DEAN DELONGCHAMP, National Institute of Standards and Technology — Charge transport in organic semiconducting films is inherently anisotropic: it depends on the orientation and packing of the molecules, which in turn are influenced by molecular structure and film processing conditions. A technique capable of non-destructively depth-profiling molecular orientation with (sub)nanometer-level depth resolution would enable a significant improvement in the understanding of structure-property-processing relationships in organic semiconductor devices. We explore the feasibility of using polarized resonant soft X-ray reflectivity (p-RSoXR) as a tool to profile molecular orientation by studying a model set of glassy small molecule (posaconazole) films with different net orientations. By comparison with variable angle spectroscopic ellipsometry (VASE) and near edge X-ray absorption fine structure (NEXAFS) data, we show that p-RSoXR is sensitive to both surface and bulk molecular orientation in the films. We conclude by demonstrating our approach to extracting orientation profiles from p-RSoXR data, as well as discussing the current strengths and limitations of the technique.

*J.L.T. was supported by a National Research Council (NRC) postdoctoral fellowship at the National Institute of Standards and Technology (NIST).

12:39PM F49.00006: Effects of Confinement on the Structure of Bottlebrush Polymers in Thin Films DANIEL SUNDAY (Presenter), National Institute of Standards and Technology, ALICE CHANG, Chemistry and Chemical Engineering, California Institute of Technology, MOSHE DOLEJSI, PAUL F NEALEY, Institute for Molecular Engineering, University of Chicago, ROBERT H GRUBBS, Chemistry and Chemical Engineering, California Institute of Technology, R. JOSEPH KLINE, National Institute of Standards and Technology — Bottlebrush block copolymers (BCPs) have intriguing potential in nanopatterning and photonics applications as they lack entanglements and can rapidly assemble. As a result, bottlebrush BCPs can self-assemble with periodicities over 100 nm, a length scale which is challenging to achieve with linear BCPs. Nanopatterning applications will require confinement of bottlebrush BCPs in thin films, where their behavior is still poorly understood. The assembly of bottlebrush BCPs of polystyrene-b-poly(lactic acid) (PS-b-PLA) in thin films was studied using a combination of techniques. Blade coating was used to produce a controlled thickness gradient so that the impact of the thickness/periodicity ratio can be studied. The resulting structures were evaluated using a combination of atomic force microscopy (AFM), grazing incidence X-ray scattering (GISAXS) and resonant soft X-ray scattering (RSoXS). The effects of solvent and annealing conditions on the resulting morphologies was also explored.
Improving Optical Models of Polarized R-SoXS for Quantitative Measurement of Molecular Orientation within Polymer Nanostructures

VICTOR MURCIA (Presenter), Materials Science and Engineering, Washington State University, BRIAN COLLINS, Physics and Astronomy, Washington State University — Resonant soft X-ray scattering (RSoXS) with polarized X-rays is sensitive to local molecular orientation within nanostructures but it is difficult to interpret the scattering patterns due to a lack of appropriate optical models. Uniaxial optical tensors have been used successfully to measure average global molecular orientation in X-ray absorption spectroscopy (XAS) and ellipsometry. The model reduces into diagonal tensors whose elements correspond to parallel and perpendicular alignments of the incident electric field with respect to the transition dipole moment. It is uncertain, however, if such a model will work in polarized RSoXS as it assesses differences in local ordering. We show how to create such a model using XAS measurements and test it against polarized RSoXS measurements on pure films of a semicrystalline conjugated polymer. We show the model works for the pi* resonances but breaks down in regions that include other transitions. DFT calculations demonstrate how not all transitions follow uniaxial symmetry and require a lower symmetry model to reproduce measurements. Combining XAS and DFT into such a new model may enable further details of local molecular orientation to be extracted by pol-RSoXS that remove current limitations of XAS.

*DOE Career Award DE-SC0017923

Characterization of ion distribution around the surface of micelles under high salt conditions using small angle neutron scattering and resonant soft x-ray scattering

HANQIU JIANG (Presenter), GREG BEAUCAGE, KARSTEN VOGTT, University of Cincinnati — Surfactants can self-assemble into micelles once reaching critical micellar concentration. Industrially, high concentration of inorganic salts are frequently employed as additives for surfactant systems to depress the CMC of the system, enhance further growth of micelle and eventually alter the rheological behavior of targeted systems. Although frequently employed in commercial surfactant products and in biological systems, little was known about how ions behave around these aggregates under high salt condition. An ion cloud model was recently developed based on the screening effect observed in small angle neutron scattering for the high salt condition. To verify this model, resonant soft x-ray scattering was performed by setting the energy of the incident x-ray close to the absorption edge of Cl atom, which allows the manipulation of the scattering length density. The scattering contribution of the ion cloud layer can thus be obtained through the subtraction of scattering curves measured at different energies. This also allows verification of the forcefield and other protocols applied in micelle simulations and enhance the predictability of micelle behavior.

*P&G
DOE NSLS II DE-SC0012704

Elucidating microphase separation in perfluoropolyether triblock copolymers using scattering techniques

DEEP SHAH (Presenter), University of California, Berkeley, KEVIN OLSON, University of North Carolina, Chapel Hill, XIUHONG LI, BRUCE ALLEN GARETZ, New York University, SUE MECHAM, JOSEPH M. DESIMONE, University of North Carolina, Chapel Hill, NITASH BALSARA, University of California, Berkeley — Short chain perfluoropolyether (PFPE) polymers have recently been shown to conduct and solvate lithium salts, and thus can be used as homopolymer electrolytes for battery applications. In an attempt to improve the transport characteristics, poly(ethylene oxide) (PEO) has been covalently bonded to the ends of PFPEs to form triblock copolymers of type A-B-A. By increasing the lengths of the PEO segments, the segregation strength of the copolymers increases; at the highest PEO molecular weight, the copolymers microphase separate. While phase separation was not immediately apparent using small angle X-ray scattering (SAXS), measuring birefringence with depolarized light scattering (DPLS) allows for the conclusion of phase separation. The Flory-Huggins interaction parameter between PEO and PFPE was calculated to determine the segregation strength as a function of salt concentration. This work provides thermodynamic data on the interactions between non-fluorinated end-groups and fluorinated backbones.
1:27PM F49.00010: Stability of Complex Spherical Packing Phases in Low-Molecular-Weight Diblock Copolymers
JIAYU XIE (Presenter), CHI TO LAI, ANCHANG SHI, McMaster University — Block copolymers are known for their ability to self-assemble into an array of ordered structures. Of special interest are the spherical packing phases due to their similarity to the atomic crystals. Until the past decade, the packing arrangement was believed to be primarily body-centered cubic for diblock copolymers. However, recent experimental and theoretical studies have revealed the emergence of various complex spherical phases including the Frank-Kasper phases. Qualitatively, the agreement between experimental and theoretical phase behaviour of diblocks is remarkable. On the other hand, quantitative differences still exist. These discrepancies could be due to numerous factors, such as polydispersity and the non-Gaussian nature of low-molecular-weight polymers used in experiments. In this work, we examine the formation of complex spherical phases for low-molecular-weight polymers with conformational asymmetry. Using the self-consistent field theory applied to freely-joint polymer chains, we model the conformational asymmetry by a difference in the bond lengths of the A and B blocks. Our results indicate that, consistent with the experiments, the inclusion of polydispersity and short-chain statistics leads to a shift of the phase boundaries between different ordered phases.

1:39PM F49.00011: Effect of Free-Volume Holes on Dynamic Mechanical Properties of Epoxy Resins for Carbon-Fiber-Reinforced Polymers Studied by Positron Annihilation* HONGJUN ZHANG (Presenter), SELVAKUMA SELLAIYAN, T. KAKIZAKI, AKIRA UEDONO, Division of Applied Physics, Faculty of Pure and Applied Science, University of Tsukuba, Y. TANIGUCHI, K. HAYASHI, Epoxy Resin Materials Center, Nippon Steel & Sumikin Chemical Co. Ltd. — We studied the effect of free-volume holes on dynamic mechanical properties (storage modulus $E'$, loss modulus $E''$, damping factor $\tan \delta$, and complex viscosity $|\eta^*(T)|$) for six types of amine-cured epoxy resins with different chemical structures. Positron annihilation lifetime (PAL) experiments were applied to determine the free-volume hole properties of each sample. The correlations between hole fraction and dynamic mechanical parameters were studied by Williams-Landel-Ferry equation. In the temperature range of $T_g(PAL) < T < T_g(PAL)+100$ °C ($T_g$ given by PAL experiments), regular variations of dynamic mechanical parameters with increasing relative hole fraction $(1-h_{PAL}@T)/h_{PAL}$, where $h_{PAL}$ is the hole fraction from PAL experiments, and $h_{PAL}@T_{ref}$ is the $h_{PAL}$ at reference temperature $T_r$ are revealed: (1) $\log[E'(T)]$ and $\log[|\eta^*(T)|]$ initially decrease linearly and then remain nearly unchanged; (2) $\log[E''(T)]$ and $\log[\tan \delta(T)]$ initially increases linearly and then decreases linearly. In this work, PAL spectroscopy provided precious quantitative information of free-volume holes in polymers [1].


*Financially supported by SIP-IMASM operated by the Cabinet Office of Japan

1:51PM F49.00012: Effect of temperature on thermal conductivity of aligned amorphous polyethylene - Molecular Dynamics study RAJMOHAN MUTHAIAH (Presenter), JIVTESH GARG, University of Oklahoma — The effects of temperature dependence of the thermal conductivity ($k$) of chain-oriented amorphous polyethylene (PE) using Molecular Dynamics Simulation. We found that the temperature corresponding to a peak $k$ progressively decreases by increasing the levels of orientation. Un-oriented PE exhibits the peak $k$ at 350K, while aligned PE under an applied strain of 400% shows a maximum at 100K. This transition of peak $k$ to lower temperatures with increasing alignment is explained in terms of a crossover from disorder to anharmonicity dominated phonon transport in aligned polymers. The disorder in the polymer chain is manipulated to support this crossover corresponding to peak $k$. Disorder is controlled through a change in the dihedral parameters of the potential function, allowing a change in the relative fraction of trans and gauche transformations. The results shed light on the underlying thermal transport processes in aligned polymers and hold importance for low temperature applications of polymer materials in thermal management technologies.
**11:15AM F50.00001: Emergence of large-scale chirality in photonic crystals in insects and butterflies** [Invited] GERD SCHROEDER-TURK (Presenter), School of Engineering and IT, Murdoch University — The biological world is filled with chiral structures, formed from a soup of building blocks that usually include both achiral and chiral molecules. In this talk, I will focus on chiral structures that emerge at the scale of hundreds of nanometers in solid insect nanostructures, and that then act as biophotonic crystals. Of particular interest in this context are the Gyroid nanosolids that form in several butterflies, as highly ordered 3D network-like porous materials, and which then contribute in particular to green coloration. I will review in particular what we understand (and not understand) about the formation of these structures; in this context, the fortuitous discovery of a butterfly nanostructure in Thecla Opisena is noteworthy. It appears to show a time-frozen snapshot of various stages of the formation which allows us to infer properties of the formation from high-resolution electron and X-ray tomography images.


**11:51AM F50.00002: Chiral Gyroidal Thin Films from Block Copolymer Self-Assembly as Structural Directing Templates for Fabrication of Mesostructured Crystalline Inorganic Materials** QI ZHANG, FEI YU (Presenter), ULRICH WIESNER, Cornell University — It has always been a challenge to fabricate crystalline materials with well-defined mesopores, which could find applications in microelectronics and catalysis. Block copolymer self-assembly offers a scalable, facile pathway to intricate mesostructures. We present on the use of amphiphilic triblock terpolymer co-assembly with additives to prepare high-temperature stable, mesoporous thin-film templates with chiral alternating gyroid structures (G^A). This mesoscale chirality emerges from the calcination and preservation of only one of the interpenetrating G^A domains and is inaccessible via conventional top-down approach. The resulting mesoporous molds can be backfilled with a wide range of inorganic materials to direct their mesostructures. Upon melting via transient laser heating on the nanosecond time scale, crystallized materials conformally fill the 3D continuous mesopores and inherit the chirality, without destroying the underlying template. Template removal yields mesoporous, crystalline inorganic materials, with optional epitaxy on the substrate.

*We thank the National Science Foundation (DMR-1707836) for funding support. This work made use of the Cornell Center for Materials Research Shared Facilities, Cornell NanoScale Facility, and the Cornell High Energy Synchrotron Source.

**12:03PM F50.00003: New Spontaneously Chiral 3D Network Structures in Thermotropic Liquid Crystals** GORAN UNGAR (Presenter), Xian Jiaotong University, HUANJUN LU, YAXIN LI, XIANG-BING ZENG, Materials Science and Engineering, University of Sheffield — Spontaneous mirror symmetry breaking has been discovered recently in bicontinuous cubic phases [1], as well as in a special isotropic melt phase [2] of achiral rod-like mesogens. While the double gyroid Ia-3d phase is always achiral, the triple network cubic, previously given the Im-3m spacegroup, is always chiral. More recently in such compounds another chiral phase was found [3], turning out to be the so-called “SmQ”. This phase has previously been found only in enantiopure chiral compounds, and its structure was unclear. Now we find that it is also bicontinuous, with two isochiral networks of orthogonal twisted columns [3]. We have also re-examined the triple-network phase; due to its now recognised chirality, a new lower-symmetry spacegroup is assigned, resulting in a new structural model, still a triple network. It thus turns out that all known bicontinuous phases formed by transverse-lying rods in networks segments feature induced chirality, which is cancelled only in the racemic double gyroid.


*Financial support from EPSRC (EP-P002250) is acknowledged.

**12:15PM F50.00004: Self-assembly of chiral networks in achiral block copolymer systems using coarse-grained simulations** POORNIMA PADMANABHAN (Presenter), NATALIE BUCHANAN, KRYSSIA BROWKA, Rochester Institute of Technology — Ordered network materials, such as the double gyroid, are comprised of two interwoven networks embedded in a matrix and can be formed via the self-assembly of block copolymers. Using a triblock copolymer, one can form an alternating gyroid thereby breaking network symmetry and resulting in a structurally chiral morphology. In this talk, we investigate the self-assembly of model achiral block copolymers into gyroid morphologies using coarse-grained molecular simulation. By co-assembling with a selective homopolymer, the thermodynamic stability of the morphology is further improved. The geometric topology is quantified, and the effect of varying volume fraction on net chirality is explored.

*Kate Gleason College Fund
**12:27PM F50.00005: Chirality from segments to domain shapes in ordered block copolymer networks**  
ABHIRAM REDDY (Presenter), ISHAN PRASAD, GREGORY GRASON, University of Massachusetts Amherst — Multi-continuous structures offer an attractive route to devise functional materials where three dimensional microphase geometry can influence transport, mechanical, and optical properties. BCPs, assemble into a variety of such network phases, provide the ability to tune the properties of the network structures. Recently, it has been shown that underlying the inhomogeneous spatial density profiles of BCP domains, are intra-domain segment orientation textures that couple to the domain geometry. Here, we will quantify chirality at different length scales in these self-assembled systems and ask specifically what is the coupling of domain geometry on local segment twist. To this effect, we define two measures of chirality at global (inter-node dihedral rotation at the network scale) and local (cholesteric ordering at segment scale) and study their correlation in network morphologies self-assembled from ABC terpolymers. We use SCFT to show how these chiral order parameters change upon varying volume fraction, interblock repulsion and network symmetry. This study forms the basis to understand the thermodynamics of chirality transfer from chiral interactions at the segment scale to controllable chiral network symmetries at the mesodomain scale.

*Work supported by the Brandeis NSF MRSEC

**12:39PM F50.00006: Lyotropic Liquid Crystals: The Emergence of Chiral Structures**  
MOHAN SRINIVASARAO (Presenter), School of Materials Science and Engineering, and School of Chemistry and Biochemistry, Georgia Institute of Technology, KATHIK NAYANI, JUNG OK PARK, JINXIN FU, RUI CHANG, School of Materials Science and Engineering, Georgia Institute of Technology — Crystallization of tartrates by Pasteur provided the first glimpse of spontaneous mirror-symmetry breaking, and that led to the foundation of stereochemistry as a discipline. A consequence of mirror-symmetry breaking is optical activity, and since the time of its discovery by Biot in the early 1800s, has fascinated scientist. Since those early studies, the appearance of macroscopic chirality from both chiral and achiral molecules has been of interest. In this talk, we discuss the appearance of macroscopic chiral structures from a class of liquid crystals, referred to as lyotropic liquid crystals under various conditions.

**12:51PM F50.00007: A different kind of Lyotropic Liquid Crystalline Phase: The case of Orange-II and gamma-Cyclodextrin**  
GERMANO IANNACCHIONE (Presenter), Physics, Worcester Polytechnic Institute, JUNG OK PARK, MOHAN SRINIVASARAO, School of Materials Science and Engineering, Georgia Institute of Technology — Liquid crystallinity, either thermotropic or lyotropic, arises from species which are either rod or disk shaped. Lyotropic systems occur when an asymmetrically shaped species is dissolved in a solvent at a concentration high enough to force the formation of an anisotropic phase. For either case, the asymmetrically shaped species can be built solely from covalent bonds, where no additional assembling process is required for the species to have an appropriate aspect ratio. Here, we report on the formation of a different kind of lyotropic liquid crystal formed by the non-covalent association of two species, g-cyclodextrin and a dye molecule, Orange II, in water as the solvent. This system is different in that it requires two different compounds that self-assemble to build a larger species with geometrical asymmetry. In an effort to understand the complexation and the formation of the liquid crystalline phase, we present data on UV-Visible spectra, conductometric titrations, fluorescence spectroscopy as well as heat capacity measurements on the formation of the anisotropic structure in water solutions. The studies point to a stoichiometry of 2 dye molecules per g-cyclodextrin, that eventually form a rodlike entity, giving rise to the formation of a liquid crystalline phase.

**1:03PM F50.00008: Microdomain morphology, curvature and twist in colloidal membranes of bidisperse rod mixtures**  
DOUGLAS HALL (Presenter), University of Massachusetts Amherst, JOIA MILLER, Brandeis University, JOANNA ROBASZEWSKI, University of California, Santa Barbara, MICHAEL F HAGAN, Brandeis University, ZVONIMIR DOGIC, University of California, Santa Barbara, GREGORY GRASON, University of Massachusetts Amherst — Long and short rod-like viral particles condense into a single-layer membrane driven by a dextran depletant. The organization of the micron-sized rods is more easily probed experimentally than nanometer scale structures in phospholipid membranes, yet both systems are described by liquid crystalline models. In the colloidal membrane system, rods microphase separate and form circular raft domains with self-limiting domain size in equilibrium, much larger than the range of rod-rod interactions. Recent experimental evidence shows that the intra-membrane domain boundaries discriminate between long-rod and short-rod sides, so that short-rod rafts twist significantly more than long-rod rafts. Also, long-rod rafts are unstable to asymmetric and concave morphologies. We develop a model to describe the microstructure and thermodynamic effects of the intra-rod domain edge, and we predict a thermodynamic coupling between domain edge curvature and rod-tilt. This coupling is achiral and distinct from the aspects of raft formation previously captured by a chirality driven model. We argue that this curvature/tilt coupling should exist in any model of phase-separating membranes as a coupling between in-plane tilt and second-derivatives of composition.

*Work supported by the Brandeis NSF MRSEC
**1:15PM F50.00009: Microphase Separation and Stability of Chiral Rafts in Colloidal Membranes**
CHAITANYA JOSHI (Presenter), JOIA MILLER, ARVIND BASKARAN, Physics, Brandeis University, GREGORY GRASON, Polymer Science and Engineering, University of Massachusetts Amherst, ZVONIMIR DOGIC, Physics, University of California, Santa Barbara, MICHAEL F HAGAN, APARNA BASKARAN, Physics, Brandeis University — Colloidal membranes are an experimental system composed of rod-like chiral particles that are driven by depletion interactions to self-assemble into one-rod-length thick monolayers. Their large size enables the study of behaviors that cannot be visualized in lipid bilayers, as they are described by the same continuum theory. Membranes formed from a mixture of short right-handed rods and long left-handed rods exhibit microphase separation, wherein one rod species forms finite-sized rafts floating in a background membrane of the other rod species. This system exhibits complex membrane-mediated interactions between rafts, which depend on the depletant concentration and the chirality of the rods. In this talk I will present a Ginzburg-Landau theory that explains the existence and interactions of rafts. Consistent with recent experiments, we find that decreasing the background chirality allows rafts to form with either right-handed (in the direction preferred by chirality) or left-handed (counter to the preferred direction) twist. Further, pairs of like-twisted rafts have repulsive interactions, while pairs of oppositely-twisted rafts have attractive interactions. The theory allows for a mechanistic understanding of these behaviors.

*This work is funded by the NSF MRSEC DMR-1420382*

**1:27PM F50.00010: Light-Matter Interactions of Chiral Inorganic Nanomaterials**
NICHOLAS KOTOV (Presenter), University of Michigan — The studies of photonics phenomena in chiral inorganic nanoparticles (NPs) encompass sophisticated nanoscale constructs from metals, semiconductors, ceramics, and nanocarbons with multiple chiral geometries with characteristic scales from Ångströms to microns. What drives the rapid development of this field are the uniquely high values of optical anisotropy are attributed to resonances of incident electromagnetic radiation with plasmonic and excitonic states typical for metals and semiconductors as well as resonant states. Distinct similarities between the geometries and light-matter interactions involving chiral supramolecular and biological systems can also be traced. The analysis of these similarities with known biological, supramolecular, and liquid crystalline materials help us understand in greater depth the role of chiral asymmetry in Nature and accelerate the development of technologies based on chiroplasmonic, chiroexcitonic, and chirmagnetic effects. Technological prospects of chiral inorganic materials with current front-runners being biosensing, chiral catalysis, polarization optics and chiral photonics will be discussed in this talk.

*National Science Foundation; DoD Vannevar Bush Fellowship*

**1:39PM F50.00011: Exploiting shape to control percolation of grain boundaries in packings of ellipsoids on curved surfaces**
ZHAOYU XIE (Presenter), TIM ATHERTON, Tufts University — Packings of hard objects provide insights into the properties of crystals, glasses and granular media. When the packing occurs on a curved surface, it requires defects to accommodate the curvature. For identical spheres packed on a spherical surface, the packings are largely crystalline with grain boundaries or “scars”, while for sufficiently polydisperse spheres the packings typically form an amorphous state. We recently showed that these regimes can be connected by a percolation transition on the neighbor graph, whereby the scars grow as a function of particle size anisotropy. Here we show that manipulating particle shape can cause a similar transition. Ellipsoids of varying aspect ratio are packed on a spherical surface with scars at low aspect ratio; these scars elongate and disconnect the crystalline regions with increasing aspect ratio. The cluster growth and scaling are shown to agree with percolation theory. The influence on the cluster growth of interactions between the particle shape and the surface on which they are packed will also be presented, as well as prospects for the exploitation of other particle shapes, such as chiral particles, to control the transition.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1654283.*

**1:51PM F50.00012: Formation of Twisted Bundles from Small Regular Arrays of Polymer Nanopillars**
CHENG ZENG (Presenter), ISAAC BRUSS, MOHAMMAD SHAHJAMALI, EDVIN MEMET, VINOTHAN N MANOHARAN, Harvard University — Elastocapillary assembly has been used to form twisted bundles in large arrays of nanopillars, often placed in square lattices. We study how the emergence of twisting can be controlled by both the dimensions of individual pillars and the local bundle geometry. Using direct laser writing, we fabricate nanopillars with high spatial resolution in arbitrary lattices. The bundles are composed of a central pillar surrounded by 4 to 7 outer pillars that are evenly spaced from one another. Although no chirality is programmed into the design, we find that twisted bundles form under certain combinations of pillar spacing (D) and pillar height (H). Interestingly, we find that achiral bundles always form when D/H is small, even with long and flexible pillars. We find a transition from achiral to chiral bundles when D/H is 0.2 to 0.3. To understand this transition, we use a scaling model and numerical simulations.

*This work was supported by DARPA under grant no. FA8650-15-C-7543.*
MOHAMMAD SHAHJAMALI (Presenter), School of Engineering and Applied Sciences, Harvard University — We present experimental self-assembly of high aspect ratio nanopillars into chiral clusters in response to capillary force. We take advantage of pillars with an aspect ratio of up to 500 with adjustable dimension, shape, porosity and two-dimensional arrangement fabricated by two-photon lithography and oxygen plasma etching. Using such freedom of design in combination with the kinetically controlled evaporation of a liquid, we devise systems where we can externally introduce five-fold disclination defects on the surface of clustered pillars due to geometrical frustration. In addition, we can kinetically control the number of assembled clusters per array and adjust the handedness of the twists in asymmetrical arrays of nanopillars.

Tuesday, March 5, 2019 11:15 AM - 1:51 PM

Session F52 DPOLY: Padden Award Symposium BCEC 253B - Amalie Frischknecht, Sandia National Laboratories - Tag(s): Focus

11:15AM F52.00001: 24 MINUTE DELAYED START TIME —

11:39AM F52.00002: Dynamic Heterogeneity in Entangled Linear and Ring Polymers: Single Molecule Studies Reveal Surprises due to Molecular Architecture YUECHENG ZHOU (Presenter), Materials Science and Engineering, University of Illinois at Urbana-Champaign, CHARLES SCHROEDER, Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign — We directly observe the non-equilibrium dynamics of single ring polymers suspended in semi-dilute solutions of linear chains. Our results show that ring polymers fluctuate drastically in chain extension even at steady-state, yet ring polymers exhibit markedly less molecular individualism during transient stretching compared to linear chains. We hypothesize that ring polymer extension fluctuations arise due to threading of linear polymers through open ring polymer chains in flow. The fluctuation frequency as a function of strain rate and concentration is quantified, and trends are consistent with increasing concentration. We further study the relaxation of linear polymers in entangled solutions of purely linear chains. Our results show dynamic heterogeneity in relaxation such that single polymer relaxation trajectories exhibit either a single-mode or double-mode exponential decay, which starkly contrasts relaxation behaviors from dilute and semi-dilute unentangled solutions. We interpret the power law scalings of these relaxation times as a function of concentration, and our single molecule results are discussed in the context of the classic tube model and reptation theory. Our results show that molecular behavior is markedly heterogeneous in non-dilute polymer solutions.

11:51AM F52.00003: Leveraging conductivity-enhancing pathways in homopolymer-blended block polymer electrolytes MELODY MORRIS (Presenter), Department of Chemical and Biomolecular Engineering, University of Delaware, RYAN NIEUWENDAAL, Materials Science and Engineering Division, National Institute of Standards and Technology, JOSEPH DURA, Center for Neutron Science, National Institute of Standards and Technology, THOMAS H EPPS, Department of Chemical and Biomolecular Engineering, Department of Materials Science and Engineering, University of Delaware — Block polymer (BP) electrolytes are appealing alternatives to liquid, gel, or homopolymer systems because the mechanical, thermal, and conductive properties are decoupled such that enhanced stability and performance are achievable. As a method to increase conductivity, polystyrene-b-poly(oligo-oxyethylene methacrylate) [PS-b-POEM] BPs were blended with a more mobile, ion-conducting POEM homopolymer; the blends then were doped with lithium salts. By adding homopolymers of different molecular weights, wet brush or dry brush regimes were achieved, as confirmed via neutron reflectometry. The wet brush polymer blends increased the mobility of both the polymer and lithium as suggested by the reduction of T_g,POEM and via line narrowing in variable temperature Li-7 solid-state nuclear magnetic resonance measurements, respectively. However, the dry brush blend demonstrated an overall higher ionic conductivity, likely due to the presence of homopolymer-rich ion channels. The results of this study provide key design parameters to promote enhanced conductivity via homopolymer-rich pathways in BP-based electrolytes.

*United States Department of Energy (Basic Energy Sciences, DE-SC0014458), Samsung (17A01588), Thomas & Kipp Gutshall Professorship
12:03PM F52.00004: Designing Coacervate-forming Systems Using Charge Sequence    TYLER LYTLE (Presenter), CHARLES SING, University of Illinois at Urbana-Champaign — Oppositely-charged polyelectrolytes can associatively phase separate in a salt solution via a process known as ‘complex coacervation’. Coacervation is driven in part by a large entropic gain due to counterion condensation and release. This drives coacervation by replacing condensed counterions with the oppositely-charged polyelectrolyte, leading to a significant increase in the counterion translational entropy. The magnitude of this entropy change can be tuned by altering the sequence of charged and neutral monomers, which leads to significant changes in phase behavior. We have developed a theoretical model to understand this connection between sequence and phase behavior by mapping the coacervate molecular structure to a 1D adsorption model that can be evaluated using the transfer matrix method. This transfer matrix theory uses inputs from Monte Carlo simulations to determine the phase separation and is able to determine the phase separation of sequence-defined polyelectrolytes. Theoretical results exhibit qualitative agreement with experimental and simulation results. These sequenced systems provide insights into the phase separation of intrinsically-disordered proteins and a method to use sequence specificity to tune the phase behavior of coacervate-based materials.

12:15PM F52.00005: Interaction parameters governing self-assembly of ion-containing block copolymers    WHITNEY LOO (Presenter), NITASH BALSARA, University of California, Berkeley — Block copolymers have been studied for use in lithium metal solid-state batteries due to their ability to decouple ion transport and mechanical properties. It is not surprising that several theoretical models have been developed to describe the effect of salt on self-assembly including the counter-ion entropy model of Rabin, the Born solvation approach of Wang, the ionic self-consistent field theory (SCFT) of Sing and de la Cruz, the polarizable field theory of Fredrickson, and the free ion SCFT of Qin. In order to discriminate between theories, we have determined the morphology of a series of block copolymer/salt mixtures as a function of composition, chain length, salt concentration and temperature. The effect of salt on chain dimensions is determined independently from neutron scattering experiments on homopolymer/salt mixtures. The effective interactions between the blocks are determined by two methods: from characterization of disordered concentration fluctuations and from the locations of phase boundaries. Comparisons between experiment and theory will be presented. The experiments show the presence of coexisting phases at some phase boundaries (e.g. two BCC phases with different lattice constants) that have not been seen in salt-free systems nor captured by any theory.

12:27PM F52.00006: Spontaneous degrafting of polyelectrolyte brushes from solid substrates    YEONGUN KO (Presenter), JAN GENZER, North Carolina State University — Polymer brushes grafted covalently to solid substrates may degraft in some instances. We study the stability of strongly and weakly charged polymeric grafts derived from poly(2-dimethylaminoethyl methacrylate) (PDMAEMA). We employ surface-initiated atom transfer radical polymerization to prepare polymer assemblies featuring gradients of grafting density and molecular weight. The degree of permanent charge in strong electrolytes is adjusted by reacting PDMAEMA with methyl iodide to a given extent. We interrogate the stability of those surface-grafted polymers under various pH at ionic strength values in solution. Swelling of the brush due to electrostatic charging in aqueous media (adjusted by varying pH and degree of quaternization) generates tension along the grafted macromolecular backbone. Such tension focuses at the bottom-most section of the polymer brush close to the substrate. This lowers the activation energy for breaking labile chemical bonds either in the initiator itself or the head-group chemistry of the initiator that links the initiator to the underlying substrate. Weak polyelectrolyte brushes are more stable than strong polyelectrolyte grafts. The stability of brushes decreases with increasing pH and decreasing ionic strength of surrounding solution.

12:39PM F52.00007: Crystallization Modes of Poly(3-dodecylthiophene)-based Block Copolymers Depend on Regioregularity    JIN-SEONG KIM (Presenter), KAIST, JONATHAN P COOTE, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, JUNGHUN HAN, KAIST, GILA E STEIN, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, BUMJOON KIM, KAIST — Conjugated block copolymers (BCPs) can self-assemble into highly ordered nanostructures in a melt state. However, when cooled below the melting temperature, crystal growth can disrupt the self-assembled structure and produce a poorly-ordered fibrillar texture. Here, we demonstrate that crystallization modes of poly(3-dodecylthiophene) (P3DDT)-based BCPs can be tuned through regioregularity (RR) and morphology. When cylindrical BCP structure is formed, crystal growth tends to break through the morphology even with low RR, showing both “break-out” and “template” crystallization modes. In contrast, when lamellar structure is formed, crystal growth remains confined by the second block domain with high RR. This morphology-dependent behavior is attributed to geometric compatibility of P3DDT crystal growth and the self-assembled symmetry: in a lamellar phase, the P3DDT chain orientations at the block interface are compatible with crystal growth, and both the alkyl-stacking and π-π growth directions are unrestricted within a lamellar sheet. In a cylindrical phase, the radial orientation of P3DDT chains at the block interface is not compatible with crystal growth, and the hexagonal close-packed symmetry only allows for one direction of unrestricted crystal growth.
Manipulating chain architecture has long been explored as a strategy to tailor the properties of polymer melts and solutions; as such, there is a rich body of literature probing the physics of nonlinear polymer architectures. Herein, we examine the chain scaling exponent ($\nu$) and effective polymer-solvent and polymer-polymer interactions as a function of architecture, solvent quality, and polymer concentration. We find striking quantitative agreement between our coarse grained (CG) molecular dynamics (MD) simulations, Polymer Reference Interaction Site Model (PRISM) theory, and small-angle neutron scattering (SANS) experiments to study linear and cyclic polymer solutions. Specifically, we examine the chain scaling exponent ($\nu$) and effective polymer-solvent and polymer-polymer interactions as a function of architecture, solvent quality, and polymer concentration. We find striking quantitative agreement between our computational and experimental results, and we show that the linear and cyclic $\nu$ and effective interactions are similar in good solvents but significantly depart from one another as solvent quality decreases. These surprising trends are most pronounced at low polymer concentrations due to the balance between available intra- vs. inter-chain contacts in the linear and cyclic architectures. We also discuss the benefits and drawbacks of varying CG model resolution, providing guidance for others to make the correct choice of model when studying the polymer physics of similar systems.

Self-consistent field theory (SCFT) provides impressive predictive capabilities for the equilibrium phases of a variety of block copolymer systems. When solved to high accuracy, qualitative as well as quantitative results can be compared to experiments. In this work, we exploit neural networks (NN) unique capability as a universal function approximator to evolve the fields in SCFT for several iterations during free energy minimization. To fully evolve the system, we use a hybrid algorithm mixing a proper PDE solver with the trained NN. The hybrid approach is verified on a diblock copolymer system. Convergence is achieved in all cases, independent of computational cell size, and molecular characteristics (volume fraction, and degree of block incompatibility). The lessons drawn from the NN-SCFT implementation can be extended to other energy minimization problems such as density functional theory (DFT).

Assembly of soft matter into three-dimensional structures at the nanoscale holds promise in fields including microfluidics and photonics, and transfer molding offers a low-cost, large-area approach to patterning such structures. In transfer molding, an ink is coated into a nano-patterned stamp, cured, and transferred to a substrate in a layer-by-layer fashion. We studied wetting, surface treatment, and adhesion in the context of continuous processing techniques with a focus on selective filling of stamps, a size scale dependence on adhesion following plasma exposure, and comparison of batch and continuous surface treatments. Residual-layer-free transfer molding was achieved through identification of wetting regimes related to the coating process combined with plasma doses orders of magnitude lower than the optimal dose suggested in prior literature on plasma bonding. Comparison of plasma treatment and corona discharge treatment for multi-layer adhesion further underscored the importance of brief surface treatments for both process throughput and stamp lifetime. This work brings transfer molding to new size scales, opening new opportunities for research in low-cost, multi-layer nano-patterning.
LIWEN CHEN (Presenter), SANGWOO LEE, Rensselaer Polytechnic Institute, HAN SEUNG LEE, Characterization Facility, University of Minnesota — Block copolymer micelles are versatile model spherical particles in the investigation of self-assembling structures of spherical particles and associated phase transformation phenomena. We investigated the close-packed structures of spherical poly(butadiene-b-ethylene oxide) (PB-PEO) diblock copolymer micelles dispersed in water using synchrotron X-ray scattering measurements. Remarkably, rapid thermal quenching of disordered PB-PEO micelle solutions to different temperatures induced three representative close-packed structures: face-centered cubic (fcc), random stacking of 2-dimensional hexagonal close-packing (rhcp), and hexagonal close-packing (hcp). Careful examination of the 2-dimensional scattering patterns revealed that the clear correlation between the type of close-packed structures and the size of crystallites controlled by the depth of thermal quenching: the smallest crystallites stabilize hcp, and as the size of crystallites increases, the hcp transforms to rhcp and eventually settled to fcc. This observation shows the interfacial tension effect is crucial for the selection of the metastable crystal structures confined in small crystallites.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F53 GSNP: Marginal Stability in Amorphous Materials and Beyond BCEC 253C - Patrick Charbonneau, Duke University - Tag(s): Invited

11:15AM F53.00001: Aging, Jamming and the Mechanisms of Marginal Stability in Amorphous Solids [Invited] PETER WOLYNES (Presenter), Rice University — The random first order transition theory of glasses provides a route to understanding not only the dynamics of the supercooled liquid state, but also the history dependent properties of nonequilibrium amorphous states, i.e., glasses. I will review its implications for preparing marginally stable amorphous packings as well as the dynamic implications of the competing existence of thermodynamically stable periodic crystals for obtaining such amorphous assemblies.

11:51AM F53.00002: Jamming of particles and machine learning models* [Invited] PIERFRANCESCO URBANI (Presenter), Institut de physique théorique, Université Paris Saclay, CNRS, CEA, F-91191 Gif-sur-Yvette — In this talk I will describe the analogy between hard spheres in high dimension and some machine learning problems focusing on the properties of their landscape and their jamming transition. I will highlight how marginal stability emerges in both cases and what are its consequences.

*This work is supported by “Investissements d’Avenir” LabEx PALM (ANR-10-LABX-0039-PALM).

12:27PM F53.00003: Marginally stable phases in structural glasses* [Invited] CAMILLE SCALLIET (Presenter), LUDOVIC BERTHIER, Laboratoire Charles Coulomb, Universite de Montpellier, FRANCESCO ZAMPONI, Laboratoire de Physique Theorique, ENS — A novel form of amorphous matter characterized by marginal stability was recently discovered in the mean-field theory of structural glasses. In the marginally stable phase, structural glasses inherit the richness of spin-glass physics characterized by ergodicity breaking transitions, complex free energy landscapes, rejuvenation and memory effects. We study analytically and numerically Weeks-Chandler-Andersen glasses. By changing external parameters, we continuously explore physical regimes relevant to granular matter, foams, emulsions, hard and soft colloids, and molecular glasses. Our results suggest that marginal phases should be observable for colloidal and non-Brownian particles near jamming. In this regime, we numerically observe rejuvenation and memory effects. By contrast, we find that molecular glasses do not present marginally stable phases, but our study reveals instead the presence of localised excitations presumably relevant for mechanical and vibrational properties of structural glasses.

1:03PM F53.00004: A jamming transition controls the landscape in deep learning* [Invited] MATHIEU WYART
(Presenter), Physics, EPFL — Deep learning has been immensely successful at a variety of tasks, ranging from classification to
AI. Learning corresponds to fitting training data, which is implemented by descending a very high-dimensional loss
function. Understanding under which conditions neural networks do not get stuck in poor minima of the loss, and how the
landscape of that loss evolves as depth is increased remains a challenge. Here we predict, and test empirically, an analogy
between this landscape and the energy landscape of repulsive ellipses. We argue that fully-connected networks a phase
transition delimits the over- and under-parametrized regimes where fitting can or cannot be achieved. In the vicinity of this
transition, properties of the curvature of the minima of the loss are critical. This transition shares direct similarities with
the jamming transition by which particles form a disordered solid as the density is increased, which also occurs in certain
classes of computational optimization and learning problems such as the perceptron. Our analysis gives a simple
explanation as to why poor minima of the loss cannot be encountered in the overparametrized regime, and puts forward
the surprising result that the ability of fully connected networks to fit random data is independent of their depth. Our
observations suggests that this independence also holds for real data. We also study a quantity Δ which characterizes how
well (Δ<0) or badly (Δ>0) a datum is learned. At the critical point it appears to be power-law distributed, suggesting that
near the transition the loss landscape has a hierarchical structure and that the learning dynamics is prone to avalanche-
like dynamics, with abrupt changes in the set of patterns that are learned.

*This work was partially supported by the grant from the Simons Foundation (#454935 Giulio Biroli, #454953 Matthieu
Wyart). M.W. thanks the Swiss National Science Foundation for support under Grant No. 200021-165509.

1:39PM F53.00005: Marginal stability in finite dimensions [Invited] SHO YAIDA (Presenter), Facebook AI Research, Facebook
Inc. — Glassy materials are omnipresent in everyday life from windows to plastics to piles of sand. Yet our understanding
of both their (equilibrium) liquid and (out-of-equilibrium) solid phases lags far behind that of crystalline counterparts.
Recent advances are rapidly changing the ways in which we understand these common-yet-physically-enigmatic materials.
This talk overviews one such advance -- the discovery of the Gardner phase transition from normal to marginally-stable
glasses. Our work in particular indicates that such a transition, first found in abstract infinite-dimensional models, can
survive down to the three-dimensional world. This transition reinforces the overriding role of rugged free-energy
landscapes that dictate physics of glassy systems, with tangible consequences on jamming, yielding, and beyond.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F54 DPOLY GSOFT GSNP: Confined Polymer Glasses I: Modeling, Aging, and Local
Connectivity BCEC 254A - Reika Katsumata, University of Massachusetts, Amherst - Tag(s): Focus

11:15AM F54.00001: Relaxation-Function-Dependent Two-Barrier Model for Nanoconfinement Effects on the Glass
Transition* DAVID SIMMONS (Presenter), DANIEL MAURICIO DIAZ VELA, Chemical and Biomedical Engineering, University of
South Florida — One of the central challenges in the study of nanoconfined systems has been the fact that distinct
measures of these systems can report quantitative and qualitative differences in perturbations from bulk. This scenario
has been further complicated by the recent observation in experiment of an apparent onset condition of
nanoconfinement effects at temperatures only modestly above Tg. This observation has raised additional questions
regarding the interpretation of large observed nanoconfinement effects in simulated systems at temperatures relatively
much further above Tg. Here, using simulations and scaling theory, we show that this rich phenomenology can be unified
via the combination of a two-barrier model of the glass transition with a barrier-truncation scenario for nanoconfinement
effects. We discuss strong implications of these results for the viability of existing theories of the glass transition.

*This material is based upon work supported by the National Science Foundation under Grant No. CBET 1705738. The
authors acknowledge the W. M. Keck Foundation for generous support enabling development of simulation
methodologies employed in this work.
11:27AM F54.00002: Modeling the Depth-dependent Dynamics of Confined Systems*  JANE E LIPSON (Presenter), RONALD WHITE, Dartmouth College — This talk will focus on our recent results modeling dynamics and glassiness in confined systems. One technique is the Limited Mobility model (LM), a coarse-grained kinetic simulation approach where mobility at a site depends on facilitation through mobility at nearby sites. LM results include mobile layer depths in freestanding films, as well as the effect of nanoparticles on the surrounding matrix. Our Cooperative Free Volume model (CFV) is a different approach. This is a rate model in which the system’s free volume ($V_{\text{free}}$), predicted through our Locally Correlated Lattice (LCL) equation of state analysis of bulk thermodynamic data, plays the key role in determining the local molecular cooperativity. The CFV model describes independent $T$- and $V_{\text{free}}$-contributions to the pressure-dependent segmental relaxation times, $\tau(T,V)$. This talk will focus on our ability to describe the dynamics of confined systems, where the local density (and thus the $V_{\text{free}}$-contribution) is altered by the presence of an interface. For example, our recent CFV work reveals the point at which film samples lose the contribution from regions of bulk-like dynamics, which will lead to insight on the position-dependent mobility across an interfacial region.

*This work is supported by NSF DMR-1708542

11:39AM F54.00003: The Important Roles of Topological Constraints on Interfacial Effects of Nanoconfined Polymers*  BIAO ZUO (Presenter), Department of Chemistry, Zhejiang Sci-Tech University, Princeton University, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University, XINPING WANG, Department of Chemistry, Zhejiang Sci-Tech University — Interfaces play a significant role in determining the dynamics of nanoconfined polymers. Recent experiments and simulations have revealed the long-range nature over which interfacial effects originating at the polymer-substrate interface can propagate within a thin film. Here, we show that topological constraints, that is, the interpenetration and entanglement between chains directly adsorbed to the substrate and neighboring non-adsorbed chains, play a major role in the suppression of thin film dynamics. This is because such constraints increase motional coupling of free and adsorbed chains, thus giving rise to a mechanism for the propagation of substrate effects. In addition, we demonstrate that the propagation of the suppressed interfacial dynamics can be tuned by controlling the local conformation of chains adsorbed to the substrate surface.

*Natural Science Foundation of China (Grants 21504081 and 21674100)
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11:51AM F54.00004: Surprising Impact of Chain Connectivity in Altering Local Glass Transition Temperature Near Interfaces [invited]  CONNIE ROTH (Presenter), XINRU HUANG, ROMAN R BAGLAY, MICHAEL THEES, YANNIC GAGNON, JENNIFER A MCGUIRE, Physics Dept, Emory University, Atlanta, Georgia USA — Our group has recently investigated how the local glass transition temperature $T_g(z)$ changes across interfaces between two polymers with widely different bulk glass transition temperatures $T_{gbulk}$. Starting with a single interface between two semi-infinite domains ($\Delta T_{gbulk} \approx 80$ K), we used a localized fluorescence method to demonstrate broad profiles in $T_g(z)$ across dissimilar polymer-polymer interfaces spanning hundreds of nanometers and observed to be asymmetric relative to the composition profile. A key finding of these results is the observation that the broad coupling of dynamics across the dissimilar polymer-polymer interface only occurs if this interface is annealed to equilibrium. Efforts to understand what factors during polymer interface formation cause these broad profiles in $T_g(z)$ find that chain connectivity appears to be surprisingly important. This is confirmed by measurements near silica substrates with tethered chains where low grafting densities (~10 vol% tethered chains) are observed to cause large +50 K increases in local $T_g$. We now explore what property changes take place in multilayer systems during interface annealing using different experimental techniques with the goal of understanding how interfaces mediate dynamical coupling across dissimilar polymer domains. Advanced materials design is headed towards increasing amounts of interfaces with progressively smaller domain sizes where the geometrical arrangement of these interfaces can be utilized to alter local material properties for desired applications.
12:27PM F54.00005: Comparison of Physical Aging and Local Glass Transition in Glassy-Rubbery Bilayer Films

JENNIFER A MCGUIRE (Presenter), MICHAEL THEES, CONNIE ROTH, Physics Dept, Emory University — Block copolymers consisting of glassy and rubbery polymers in direct contact with each other are common in many industrial applications, with the stability of the glassy domains critical to the material’s function. Recent fluorescence measurements by our group have shown large changes in local glass transition temperature $T_g(z)$ across glassy-rubbery polystyrene (PS) / poly(n-butyl methacrylate) (PnBMA) multilayer films. Previously we have demonstrated a correlation between reduced physical aging rates in thin single layer PS films with local $T_g$ reductions near the free surface. Here we explore if a similar correlation between physical aging and local $T_g$ exists near glassy-rubbery polymer interfaces. Physical aging of PS films capped with rubbery PnBMA layers are measured using ellipsometry, avoiding the competing effects of the free surface and allowing us to isolate the impact of a single glassy-rubbery interface. Reductions in physical aging rate with decreasing PS layer thickness are observed, but the reduced layer thicknesses needed to make the ellipsometry measurements viable induce finite size effects altering the local $T_g(z)$ profile relative to previous profiles on semi-infinite bilayers, necessitating direct comparisons on equivalent systems with both techniques.

12:39PM F54.00006: Role of hydrophilic support on the physical aging and stress development in thin polynorbornene films

ELIZABETH LEWIS (Presenter), Polymer Engineering, The University of Akron, CHRISTOPHER M STAFFORD, NIST - Natl Inst of Stds & Tech, BRYAN VOGT, Polymer Engineering, The University of Akron — Thin film properties can be impacted by their local environment, especially when in contact with other polymers. Here physical aging of poly(butylnorbornene-ran-hydroxyhexafluoroisopropyl norbornene), BuNB-r-HFANB, thin films coated on ultra-thin (2nm) layers of poly(acrylic acid), PAA, or poly(styrene sulfonate), PSS, is examined along with residual stress evolution in BuNB-r-HFANB during aging. Decreasing BuNB-r-HFANB film thickness tends to decrease the physical aging rate ($\beta$), but this quantitatively is altered by PSS or PAA. Even for thick films (>500nm), aging rate at 100°C is accelerated on PAA compared to silicon, while thickness dependence of BuNB-r-HFANB aging is enhanced (compared to silicon) when in contact with PSS with apparent aging rate decreasing by a factor of 2 as film thickness decreases from 1000 nm to 250 nm. Removal of BuNB-r-HFANB from substrate enables mechanical properties (elastic modulus and residual stress, $\sigma_R$) to be resolved via wrinkling. Elastic modulus is effectively invariant of substrate (polymer layer), while there is a small effect of physical aging on the modulus. The stress in the films is compressive and evolves non-monotonically during aging. $\beta$ can be mostly collapsed when scaled as $h\sigma_R^{-1/3}$.

*This work was funded by NSF grant no. CMMI-1462284

12:51PM F54.00007: Effect of Substrate on the Stability of Ultra-thin Vapor Deposited Molecular Glasses

YI JIN (Presenter), YUE ZHANG, CONNOR WOODS, ZAHRA FAKHRAAI, University of Pennsylvania — We have recently demonstrated the existence of long-range correlation between the free surface and substrate dynamics in ultrathin supported molecular glass films such that when the substrate interactions are changed from weakly interacting to neutral, the extent of $T_g$ reduction and enhanced film dynamics is reduced and the stability against dewetting is increased for films as thick as 30 nm. The stability of vapor-deposited glasses is strongly influenced by the surface mobility and its gradients. Since the surface dynamics are affected by the substrate for ultra-thin films one would expect the stability to follow. Here, we show that ultra-thin films of TPD ($N,N'$-diphenyl-$N,N'$-bis(3-methylphenyl)-1,1' -biphenyl-4,4'-diamine) vapor-deposited on a neutral substrate have higher stability (higher density change and lower fictive temperatures) compared to those deposited on a weakly-interacting substrate. The density change is also found to be higher in ultrathin films (<50 nm) compared to the bulk films (>200 nm, steady state condition). These results suggest a possibility that film/substrate interactions could speed up effective aging rates, or deter dewetting during deposition, giving rise to more efficient amorphous packings.

*NSF-DMREF DMR-1628407
NSF-MRSEC DMR-1720530
Role of Solvent Washing Conditions on the Creation of Adsorbed Layers from Melt Films

MICHAEL THEES (Presenter), JENNIFER A MCGUIRE, XINRU HUANG, CONNIE ROTH, Physics Dept, Emory University — Recent reports have proposed the presence of adsorbed layers may strongly affect dynamics in thin supported films. Often assumptions are made about the presence of adsorbed layers within melt films based on annealing time and temperature, where subsequent washing of films with solvent is interpreted as “revealing” the structure of the adsorbed layer within the melt (so-called Guiselin experiment). However, this interpretation is contrary to extensive literature studies from the 1980-90s on displacement experiments of adsorbed chains in solution measuring exchange kinetics with a third component called the “displacer”, either another polymer or second solvent, that displaces the initially adsorbed polymer due to its preference for the substrate interface. These studies, along with direct surface diffusion measurements by Granick’s group in the regime of strong adsorption, suggest adsorbed polymer chains are extremely mobile during solvent washing. We test this interpretation by demonstrating the measured residual adsorbed layer strongly depends on solvent washing conditions. Consistent with work by Cohen Stuart’s group, we show acetone as a displacer removes nearly all of the initially adsorbed chains, even after melt films were extensively annealed at elevated temperatures.

Substrate Effect on $T_g$ of Random Copolymers of 4-tert-butylstyrene and 4-acetoxy styrene

TONG WANG (Presenter), JINSONG YAN, HAILIN YUAN, Department of Physics, Hong Kong University of Science and Technology, HO YI LAM, Department of Chemical and Biological Engineering, Hong Kong University of Science and Technology, CHAO LV, BINYANG DU, Department of Polymer Science and Engineering, Zhejiang University, OPHELIA TSUI, Department of Physics, Hong Kong University of Science and Technology — Confinement effect on the dynamics of polymers in nanoscale films is known to cause variations in the glass transition temperature, $T_g$, of the films with film thickness. We studied the $T_g$ of random copolymers of 4-tert-butylstyrene (4TBS) and 4-acetoxy styrene (4AS). Our result indicates that the component with a stronger substrate confinement effect dominates the $T_g$ of the copolymer films. We have also explored the influence of pre-annealing time on the $T_g$'s. According to a previous study, by shortening the pre-annealing time, the $T_g$ reductions of thin 4TBS films were enhanced. In our copolymer films, we found that that adjusting the pre-annealing time only affected the $T_g$ of the copolymer films in which 4TBS is the majority component.

Theory of interface-nucleated changes of dynamical constraints and their spatial transfer in glass-forming films

KENNETH SCHWEIZER (Presenter), ANH D. PHAN, University of Illinois at Urbana-Champaign — We formulate a new force-based microscopic theory for how dynamic caging constraints in glass-forming liquids at an interface are modified and spatially transferred into the film interior in the context of the dynamic free energy concept of the Nonlinear Langevin Equation (NLE) approach. The caging constraints vary exponentially with distance from the interface with a correlation length of modest size and weak sensitivity to thermodynamic state. This imparts a roughly exponential spatial variation of all key features of the dynamic free energy, and a double exponential form for the alpha time gradient. Results have been obtained for vapor, rough pinned particle solid, vibrating (softened) particle solid, and smooth hard wall interfaces, with the crucial dynamical differences arising from the first layer where caging constraints can be weaken, softened or hardly changed. Comparison of the predictions for the dynamic localization length and glassy modulus with simulations and experiments for vapor interface films reveals good agreement. Using the new ideas in Elastically Collective NLE theory yields quantitative results for the relaxation time gradient, decoupling phenomena, $T_g$ gradient and other properties of colloidal, molecular and polymeric films.
1:39PM F54.00011: Heterogenous dynamics, connectivity and domain formation in polymer glasses: a fractal dimension analysis approach* ANNA LAPPALA (Presenter), Los Alamos National Laboratory, DOMINIC PHILLIPS, Physics, University of Cambridge, JAKOB JAZBEC, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, TURAB LOOKMAN, KARISSA SANBONMATSU, Los Alamos National Laboratory — Dynamical heterogeneity in glassy systems was first proposed in order to explain non-exponential relaxation patterns in single-component glassy systems, with different relaxation times contributing to produce the observed relaxation. It has been suggested that due to the influence of intramolecular interactions and chain connectivity, there is a fundamental difference between the nature of the glass transition in polymers and in standard glass-formers. Here, we study polymer collapse using fractal dimension (Df) analysis, demonstrating that dynamical arrest upon glass transition affects the evolution of Df in a non-trivial manner. We identify heterogenous dynamics both in bulk and near the free surface, showing characteristic domain patterns in local displacement and connectivity. We demonstrate that although covalent bonding promotes glass formation and caged dynamics, bonding sequentiality that defines a polymer chain is not critical in bulk: glassy dynamics is purely a result of the number of connections per particle, independently of how these connections are formed. However, bonding sequentiality does play an important role in the surface effects of the glass, highlighting a major difference between polymeric and colloidal glasses.

*This work was supported by LDRD, CNLS & NIH

1:51PM F54.00012: Novel calculation method for the work of adhesion of polymer-grafted surface MASAYUKI URANAGASE (Presenter), SHUJI OGATA, Nagoya Institute of Technology — Molecular simulations are often used to elucidate solid-liquid interfacial properties. In the problem of adhesion, several methods to calculate the work of adhesion, which enables quantitative evaluation of the strength of the adhesion between two materials, have already been proposed. However, application of these methods is restricted to the flat solid surface. It is necessary to improve existing methods for efficient calculation of the work of adhesion for the complex solid surfaces such as polymer-grafted surfaces. We developed the novel method to calculate the work of adhesion using molecular simulation. In this method, we introduced two techniques to perform efficient calculation for complex solid surfaces. First, liquid molecules contacted with the solid surface are separated from it using spherical potentials around atoms grafted to the surface. This enables separation of liquid molecules according to the surface structure. Second, appropriate update scheme of parameters contained in the potential is found to suppress the variation in the free energy gradient, which reduces the error of numerical integration. Using this method, we studied the dependence of hydrophilicity of the gold surface modified by poly(ethylene oxide) on the ratio of poly(ethylene oxide).

2:03PM F54.00013: Slip Length in Deeply Supercooled Molecular Glass Formers* CONNOR WOODS (Presenter), GUI GAO, PATRICK J WALSH, Chemistry, University of Pennsylvania, ROBERT RIGGLEMAN, Chemical and Biological Engineering, University of Pennsylvania, ZAHRA FAKHRAAI, Chemistry, University of Pennsylvania — In polymer melts, the hydrodynamic boundary condition at the substrate interface can deviate from the normally assumed no-slip boundary condition such that fluid velocity at the substrate is non-zero in supported high-molecular weight polymer thin films. Depending on the substrate/polymer interactions, the measured slip lengths can be on the order of the film thickness or larger, greatly influencing film dynamics during dewetting. De Gennes’ original theory for slip in polymers predicts that the slip length should approach the monomer size in molecular liquids. We show that for deeply supercooled molecular glass formers near their Tg, in which chain dynamics cannot play a role in slip, the slip lengths can be surprisingly large and still on the order of the film thickness on a weakly interacting substrate. To better understand the origin of slip in these systems, we investigate the role of molecular shape and orientation near the substrate using a series of molecules that range from rod-like to nearly spherical. We also employ coarse-grained molecular dynamics simulations to gain insight into the origins of the observed slip.

*Funded by NSF-DMREF-1628407, NSF career award (DMR-1350044), NSF-PIRE (OISE 154884) and XSEDE allocation TG-DMR150034.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F55 DPOLY DCOMP DBIO GSNP: Advancing Polymer and Biopolymer Physics though Simulation and Theory II: Functional Polymers and Gels BCEC 254B - Yaroslava Yingling, North Carolina State University - Tag(s): Focus
11:15AM F55.00001: Effects of Ion Group Distribution on the Structure and Dynamics of Amorphous Ionomers^*  
GARY GREST (Presenter), Sandia National Laboratories, DIPAK ARYAL, University of Texas, Austin, DVORA PERAHIA, Clemson University — Ionic clusters control the structure, dynamics, and transport in ionic polymers. These ionic groups associate into random clusters in melts, where the distribution and morphology of the clusters impact the transport in these materials. Using fully atomistic molecular dynamics simulations we study melts of polystyrene sulfonate with 10% sulfonation with random, precise and blocky distributions of of the SiO₃⁻ sulfonate groups along the backbone. We find that for random distribution, the clusters in average are elongated, whereas the clusters are more globular when the sulfonate groups are equally spaced along the backbone. Elongated and globular coexists for blocks of sulfonate groups. The average ionic cluster size is comparable for the random and precise distributions and larger for the blocky distribution. We show that the low wavevector peak in the structure factor S(q) is much more well-defined for the precise and block cases compared to the random one. Interestingly, over the time scales of 1000 ns studied, the mobility of the block chains is higher than the random and precise, even though the ionic clusters are larger. The Na⁺ counterions are condensed and move at the same rate as the sulfonate groups.

^*Funded in part by DOE DE-SC0019284

11:27AM F55.00002: Modeling Explicit-Ion Effects in Weak Polyelectrolyte Complexes  
VIKRAMJIT RATHEE (Presenter), HYTEM SIDKY, BEN J SIKORA, JONATHAN WHITMER, University of Notre Dame — Polyelectrolytes may be classified into two primary categories (strong and weak) depending on how their charge state responds to the local environment. Both of these find use in many applications, including drug delivery, gene therapy, layer-by-layer films, and fabrication of ion filtration membranes. The mechanism of polyelectrolyte complexation is, however, still not completely understood. Here we detail computer simulations aimed at providing a comprehensive picture of the titration and complexation behaviour of these weak polyelectrolytes and perform thermodynamic investigation through coarse-grained molecular simulations permitting us to calculate the free energy of complex formation and its dissection into energetic and entropic contributions. Our investigations indicate that entropic contributions indeed dominate the free energy of complex formation for strong polyelectrolytes, which is in agreement with experiments, but are less important than energetic contributions when weak electrostatic coupling or weak polyelectrolytes are present.

11:39AM F55.00003: Polyelectrolytes under spatial and dielectric confinement  
TRUNG NGUYEN (Presenter), Chemical and Biological Engineering, Northwestern University, MONICA OLVERA DE LA CRUZ, Materials Science and Engineering, Northwestern University — Understanding the conformational behavior of polyelectrolytes inside viral capsids and lipid vesicles is crucial for gene delivery and drug loading applications. In this talk, we focus on the collective effects of dielectric mismatch and spatial confinement on the conformational behavior of a model polyelectrolyte chain and counterions confined in a spherical cavity. We show that surface polarization due to dielectric mismatch between the media inside and outside the cavity influences the chain conformational behavior. Specifically, it is found that surface polarization increases the work required to change the equilibrium (unconfined) chain conformation and favors the collapsed conformations with smaller size. The roles of surface charge density, electrostatic strength between the monomers and counterions and multivalent counterions are also discussed. The findings therein offer insights into the effects of dielectric mismatch, which were often overlooked in previous studies on confined polyelectrolytes.

11:51AM F55.00004: Electronic Structure of Polymer Dielectrics: The Role of Chemical and Morphological Complexity  
LIHUH CHEN (Presenter), ROHIT BATRA, School of Materials Science and Engineering, Georgia Institute of Technology, RAGHAVAN RANGANATHAN, School of Materials Science and Engineering, Georgia Institute of Technology, GREGORY SOTZING, YANG CAO, University of Connecticut, RAMAMURTHY RAMPRASAD, School of Materials Science and Engineering, Georgia Institute of Technology — The electronic structure of polymers contains signatures that correlate with their short-term and long-term integrity when subjected to large electric stresses. A detailed picture of the electronic structure of realistic models of polymers has been difficult to obtain, mainly due to the chemical and morphological complexity encountered in polymers. In this work, we have undertaken a comprehensive analysis of the electronic structure of six model polymers displaying chemical and morphological diversity, namely, polyethylene (PE), polypropylene (PP), polystyrene (PS), poly(methyl methacrylate) (PMMA), polyethylene terephthalate (PET) and polybutylene terephthalate (PBT), using first-principles density functional theory computations and classical molecular dynamics simulations. In particular, we have studied the role of monomer chemistry, tacticity and large-scale morphological disorders in shaping the electronic structure of these polymers. Appropriate connections and comparisons between the computed results and the available experimental data have also been provided. Critical insights on physico-chemical and electronic structures relationships are revealed, providing a pathway for understanding the factors that control electrical conduction and degradation of polymers.
12:03PM F55.00005: Microscopic origin of the morphotropic-like phase boundary in P(VDF-TrFE)  BING ZHANG (Presenter), WENCHANG LU, Department of Physics, North Carolina State University, YANG LIU, HAIBIBU AZIGULI, WENHAN XU, QING WANG, Department of Materials Science and Engineering, The Pennsylvania State University, JERRY BERNHOLC, Department of Physics, North Carolina State University — Ferroelectric materials with compositions near a morphotropic phase boundary (MPB) exhibit dramatically enhanced electromechanical properties, which could be utilized in advanced actuators, transducers, sensors and energy-harvesting applications. We have recently observed [1] a morphotropic-like phase boundary for the first time in an organic material, poly(vinylidenefluoride-co-trifluoroethylene) [P(VDF-TrFE)], which makes it possible to develop high-performance electroactive polymers. This talk describes the results of our extensive first-principles calculations for this class of polymers. We find that chirality introduced by the TrFE monomers plays the central part in the structural competition that leads to a phase boundary between the trans-planar and the 3/1-helical chain conformations, explaining and supporting the experimental results.


12:15PM F55.00006: Molecular Modeling of Polyetherimides* CHENGYUAN WEN (Presenter), SHENGFENG CHENG, Virginia Tech — Molecular modeling plays an increasingly important role in quantifying properties of polymeric materials and clarifying molecular mechanisms underlying material behavior. We use both atomistic and coarse-grained molecular dynamics (MD) and Monte Carlo (MC) simulations to investigate polyetherimides (PEIs), which are widely used for automotive industry, aircrafts, medical instruments, and chemical devices. We have developed a transferrable coarse-grained MD model of PEIs that is able to capture their thermal expansion properties and mechanical moduli, and demonstrated the importance of including entropic correction terms in the calculation of potentials of mean force when the coarse-grained force field is trained with atomistic MD simulations. To understand the dispersity of branched PEIs, we have developed a MC simulation tool based on the Gillespie algorithm for their polymerization reaction including branching. The comparison between MC simulations, the Stockmayer theory, and experiments on the molecular weight distributions of branched PEIs will be discussed. We use simulations to clarify the application range of the Stockmayer theory and to investigate the branching behavior of PEIs when the theory is not applicable.

*Supported by SABIC Global Technologies BV.

12:27PM F55.00007: A unifying perspective on rigidity in under-constrained materials* MATTHIAS MERKEL (Presenter), Syracuse University & Université Aix-Marseille, KARSTEN BAUMGARTEN, BRIAN P TIGHE, Delft Univ of Tech, M. LISA MANNING, Department of Physics, Syracuse University — We present a novel approach to understand rigidity in under-constrained materials, including sub-isostatic spring networks as well as 2D and 3D vertex models for dense biological tissues. We show that the onset of rigidity is determined by a purely geometric criterion. This allows us to analytically predict the elastic material properties close to the transition, which depend only on few geometric coefficients. We obtain exact expressions for the magnitudes of bulk modulus and shear modulus discontinuities at the rigidity transition, several scaling relations of the shear modulus, and the magnitude of the anomalous Poynting effect. Moreover, we show that the ratio of the excess shear modulus to the shear stress is inversely proportional to the critical shear strain with a prefactor of three, which we expect to be a general hallmark of rigidity in under-constrained materials induced by geometric incompatibility.

Quantum Chemistry Simulations for Dynamic Network Polymers*  
MICHAEL BUCHE (Presenter), Theoretical and Applied Mechanics, Cornell University, ZACHARY SPARROW, Chemistry and Chemical Biology, Cornell University, YUVAL VIDAVSKY, Mechanical and Aerospace Engineering, Cornell University, ROBERT DISTASIO, Chemistry and Chemical Biology, Cornell University, MEREDITH SILBERSTEIN, Mechanical and Aerospace Engineering, Cornell University — Conventional elastomers are crosslinked by covalent bonds. These covalent crosslinks create a permanent network, substantially increasing stiffness but decreasing stretchability. Alternatively, if polymers can be made with crosslinks that are strong, but able to break and reform, they will have similar stiffness benefits as the covalently crosslinked material without sacrificing stretchability, resulting in a high toughness material. Additionally, properties such as self-healing and solid-liquid transitions are also possible through this mechanism. In this talk, I will discuss a dynamic network polymer synthesized using organometallic coordination compounds as crosslinks, focusing on the behavior of the crosslinks as investigated using density functional theory. The potential energy surface of these crosslinking structures is reshaped as force is applied. The reaction paths of the structures are discovered using the growing string method, and are studied under increasing force. These studies yield force-dependent kinetics information that can be used to create a physics-based constitutive model of the material to compare with experimental mechanical tests.

*This research is funded by the National Science Foundation (CMMI-1653059) and the Office of Naval Research (N00014-17-1-2989).

Molecular Simulation Study of Orientational Dynamics in a Cross-linked Epoxy Network*  
KETAN S KHARE, FREDERICK PHELAN JR. (Presenter), National Institute of Standards and Technology — Subtle changes in the chemistry of cross-linked epoxy networks have a drastic impact on the thermomechanical properties of cross-linked epoxy, which indicates the strong connection between chemical topology and polymer physics in these materials. Here, we study the orientational dynamics of cross-linked epoxy using atomistic molecular dynamics simulations. Specifically, we characterize the reorientation of vectors defined at atomic and molecular length-scales using first and second order Legendre polynomials (C1 and C2, respectively) at temperatures across the glass transition. For atomic length scales, we use the bond vectors of selected groups of atoms. For molecular length scales, we use end-to-end vectors of the epoxy monomer and the cross-linker that comprise the network. We then use the time—temperature superposition (TTS) principle to create master curves of C1 and C2. We find that while TTS can be successfully applied at molecular length scales, the topological location of the atoms can cause a distinct signature in the orientational dynamics of the bond vectors, which can be teased out using TTS. We are interested in using atomistic simulations to connect molecular insight with macroscopic properties.

*U.S. NIST grant number 70NANB16H005

Soft Nanoparticles as Adhesives for Gel-like Materials*  
RYAN SAYKO (Presenter), ZHEN CAO, HEYI LIANG, ANDREY DOBRYNIN, The University of Akron — It is known that nanoparticles can act as effective adhesives for soft polymeric materials. Using a combination of molecular dynamics simulations and theoretical calculations, we study the ability of soft nanoparticles to glue together gel-like surfaces. In particular, we have shown that at the interface between two gel-like surfaces nanoparticles can be in a bridging state, Pickering state, or engulfed state. The depth of indentations produced by nanoparticles into soft substrates is controlled by nanoparticle size, nanoparticle and substrate Young's modulus, and their surface properties. Using molecular dynamics simulations, we have elucidated relationships between deformations of the nanoparticles and substrates and their elastic and surface properties. By varying moduli of nanoparticles and gel-like substrates, we find that it is possible to observe a coexistence of both bridging state and Pickering state. Furthermore, we use the Weighted Histogram Analysis Method to calculate the work required for separation of two gels which interface is reinforced by nanoparticles. To explain our simulation results, we have developed a model relating the work of substrate separation with the physical parameters describing contact phenomena in nanoparticle/substrate systems.

*NSF DMR-1624569
1:15PM F55.00011: Modeling mechanics of large colloidal microgel suspensions*  
SVETOSLAV V NIKOLOV (Presenter), Mechanical Engineering, Georgia Institute of Technology, ALBERTO FERNANDEZ-NIEVES, School of Physics, Georgia Institute of Technology, ALEXANDER ALEXEEV, Mechanical Engineering, Georgia Institute of Technology — Large colloidal suspensions, comprised of soft and deformable microgel particles, exhibit a rich mechanical and phase behavior. As the particle density increases above close packing, individual particles start to deform and interpenetrate. Experimentally, these systems exhibit a high energy storage capacity and fast response times which makes them particularly attractive as self-healing and reconfigurable materials. The soft nature of the particles and their responsiveness to stimuli, such as temperature and pH, allows for external control of the emergence of liquid, liquid-crystal, and glassy phases. In our work, we utilize dissipative particle dynamics to construct large colloidal suspensions and study how the mechanical behavior of these suspensions changes with packing fraction and solvency. The colloidal suspensions are represented by an array of soft and deformable polymeric gels which are comprised of interconnected of polymer chains. We seek to determine how the behavior of individual chain parameters affects the underlying mechanical behavior of the suspensions in this multiscale system.

*Project supported by the National Science Foundation of U. S. A. (DMR-1255288, DMR-1609841, DGE-1650044, and TG-DMR-180038)

1:27PM F55.00012: Tuning microscopic interactions in dry (co-)polymer systems for improved thermal conductivity  
DEBASHISH MUKHERJI (Presenter), Stewart Blusson Quantum Matter Institute, University of British Columbia, JOERG ROTTLER, Department of Physics and Astronomy, University of British Columbia — Polymers are an important class of soft matter whose properties are dictated by large fluctuations. Because of this reason commodity polymers are perfect candidates for the fully flexible design of advanced functional materials. However, while polymers are highly useful in a wide range of everyday materials, one of the greatest drawbacks of polymeric materials is their poor thermal conductivity in an amorphous state (i.e., between 0.1 - 0.5 W/m/K). Using molecular dynamics simulations of an all atom model, we propose new (co-)polymer systems in their dry state that are otherwise water soluble in dilute solutions and thus dictated by strong hydrogen bonding. These results may serve as a design principle for the dry polymer systems with improved thermal properties.

1:39PM F55.00013: Advancing Polymer and Biopolymer Physics through Simulations and Theory: a few examples  
[Invited]  ALEXANDER GROSBERG (Presenter), New York University — In the talk, a few examples of successfull theoretical developments in biopolymer physics will be given.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F56 GSNP: Granular Materials and Flows  
BCEC 255 - Mark Shattuck, City College of New York

11:15AM F56.00001: The influence of pressure on segregation and diffusion in a shear flow*  
PAUL UMBANHOWAR (Presenter), ALEXANDER M FRY, JULIO MARIO OTTINO, RICHARD LUEPTOW, Northwestern University — The effect of confining pressure on segregation and diffusion of granular material is studied in Discrete Element Method (DEM) simulations of horizontal planar shear flow, where a feedback scheme maintains a constant shear rate for varying pressure. Both the segregation rate and the ultimate degree of segregation in initially mixed size-bidisperse and density-bidisperse beds decrease with increasing pressure. In contrast, the collisional diffusion is pressure independent. Consequently, segregation is reduced relative to diffusive mixing with increasing pressure. To test these findings, we compare DEM results to predictions of a continuum model that includes a pressure dependent segregation velocity and a pressure independent diffusion term. The model accurately predicts the steady-state segregation for both size and density bidisperse mixtures over a wide range of flow conditions. Additional simulations with segregated initial conditions demonstrate that a high enough overburden pressure reduces segregation sufficiently that significant mixing occurs, implying that manipulation of the shear-pressure state in granular flows could be used to drive particle mixtures to either mixed or segregated states as desired.

*Funded by the Procter & Gamble Company and NSF Grant No. CBET-1511450.
11:27AM F56.00002: Kinetic Theory Approach for Modeling Granular Segregation  RICHARD LUEPTOW (Presenter), YIFEI DUAN, PAUL B UMBANHOWAR, Northwestern University — Momentum conservation equations for individual constituents have been used to derive expressions for the percolation velocities of bidisperse segregating species in a granular flow. Many gravity-driven segregation models assume that the inter-species drag takes the form of Darcy's law, which gives a linear relation between the drag forces and the percolation velocities. However, a simple linear drag law is not sufficient to describe the segregation behavior. To address this, we propose a relation based on the kinetic theory of granular flow that includes terms to account for the effects of the particle surface friction, the coefficient of restitution, and the local inertial number. The percolation velocity derived from the momentum balance equation with this drag model agrees well with DEM simulations of uniform shear flows of density bidisperse particles, accurately predicting the difference between upward species velocity and downward species velocity through the depth of the flowing layer for different density ratios and relative constituent concentrations.

11:39AM F56.00003: Size segregation in driven granular media*  PHILIP WANG (Presenter), Mechanical Engineering and Materials Science, Yale University, ABE CLARK, Physics, Naval Postgraduate School, NICHOLAS OUELLETTE, Civil and Environmental Engineering, Stanford University, MARK SHATTUCK, Physics, The City College of the City University of New York, COREY SHANE O’HERN, Mechanical Engineering and Materials Science, Yale University — Granular flows involve grains of different sizes and mass densities, which either remain well-mixed or segregate. We perform discrete element simulations of model granular systems composed of frictionless, bidisperse disks (with diameter $D_l$ and $D_s$, mass density $\rho_l$ and $\rho_s$, for large and small disks) under gravity and driven by either simple shear or vibration to understand parameters that control mixing and segregation. We have shown that sheared granular system possess 1) a geometrically-segregated regime, where the system becomes increasingly segregated with decreasing $D_s/D_l$, 2) a weight-segregated regime, where the system becomes less segregated as $D_s/D_l$ decreases further, and 3) well-mixed states. We identified the boundaries between these three regimes as a function of $D_s/D_l$ and $\rho_s/\rho_l$. We performed similar studies of vibrated systems to determine if the boundaries between mixed and segregated states depend on the driving method. We show that the large particles rise to the top only if $\rho_l<\rho_s$, i.e. we only find weight-segregation in vibrated systems. We also show that by driving only large particles in vibrated systems, large particles will rise for intermediate packing fractions (0.7>$\phi$>0.5).

*P.W. and C.S.O. acknowledge support from ARO Grant No. W911NF-17-0164.

11:51AM F56.00004: Lift force in size and density segregation  LU JING (Presenter), ADITHYA SHANKAR, PAUL UMBANHOWAR, RICHARD LUEPTOW, Northwestern University — We computationally study the forces experienced by a large intruder in a sheared particle bed. The intruder is attached to a virtual spring, which allows measurement of segregation forces when the intruder reaches an equilibrium position. By subtracting a buoyancy-like contribution from the overall segregation force, the lift force on the intruder is measured for a variety of size and density ratios, and local shear rates. We find that lift force depends only on size ratio and shear rate, but not on density ratio. At a given shear rate, the lift force scales with the square of the size ratio. We propose a lift force model that successfully predicts the combination of size and density ratios at which the intruder rises or sinks. In the future, the lift force model will be used to predict segregation velocity in size and density disperse mixtures.

12:03PM F56.00005: Mesoscopic features of a granular dynamics under cyclic compression*  ZACKERY BENSON (Presenter), ANTON PESHKOV, MICHELLE GIRVAN, IREAP, IPST, University of Maryland, College Park, DEREK C. RICHARDSON, Department of Astronomy, University of Maryland, College Park, WOLFGANG LOSERT, IREAP, IPST, University of Maryland, College Park — We study the reversibility of rotational motion of spherical grains via molecular dynamics simulations. From the simulations, we are able to capture the motion, position, and force distribution of grains during cyclical compression and dilation and find excellent agreement with our experimental data. Additionally, we analyze the network structure formed from the contact forces between individual grains and show how the network dynamics are affected by compression amplitude as well as the evolution of the network from a transient to a steady state. Further, we use a simple machine learning approach combined with experimental data to characterize different states of our granular system.

*This work was supported by National Science Foundation grant #5244620 as well as the National Science Foundation Graduate Research Fellowship Program.
12:15PM F56.00006: Avalanche precursors in a frictional model  

AXELLE AMON (Presenter), IPR, University of Rennes, 
BAPTISTE BLANC, JEAN-CHRISTOPHE GEMINARD, Physics Department, ENS Lyon — An experimental approach to study precursors to avalanches is to progressively tilt a box filled with sand and to monitor the events that take place below the avalanche angle. Such experiments have shown the existence of two types of events: localized rearrangements implying only a few grains and large coherent events implying an increasing part of the sample. Those micro-ruptures occur with an angular periodicity, starting from about half of the avalanche angle until the avalanche takes place.

We will present a numerical and theoretical study of a simple one-dimensional model which captures most of those experimental features. The model consists in elastically coupled sliders on a frictional incline of variable tilt. This simplified model allows a statistical approach leading to master equations describing the state of the system as a function of the angle of inclination. Our central results are the possibility of incomplete stick-slip events under the threshold and the existence of an internal threshold for the outbreak of rearrangements well below the avalanche.

12:27PM F56.00007: Modeling avalanches in granular matter  

PIERRE SOULARD (Presenter), ESPCI ParisTech, DENIS DUMONT, PAUL RAMBACH, Université Mons, THOMAS SALEZ, LOMA, University of Bordeaux, ELIE RAPHAEL, ESPCI ParisTech, PASCAL DAMMAN, Université Mons — Sand is a complex material. At rest, a sand pile is a solid. But as soon as the external stress exceeds a certain threshold, it starts flowing like a liquid. During an avalanche, the two states coexist: a liquid phase rolls on the top of a solid phase, the latter is the result of the sedimentation of the liquid phase. The global description of the rheology of the granular material is still an open question and an active field of research.

In 1994, Bouchaud et al. developed a phenomenological description of the complex interactions between the two phases for starting avalanches. Inspired by this approach, we build a new description of the physics of an avalanche, and applied it to the collapse of a granular column. We compare our theoretical predictions to 3D DEM numerical simulations and experiments for various granular materials.

12:39PM F56.00008: Collapse of Granular Column: an Adequate Tool to Characterize Granular Matter  

DENIS DUMONT (Presenter), University of Mons, PIERRE SOULARD, ESPCI, PAUL RAMBACH, University of Mons, THOMAS SALEZ, University of Bordeaux, ELIE RAPHAEL, ESPCI, PASCAL DAMMAN, University of Mons — In spite of a large effort of the scientific community, a global description of the rheology of granular assembly remains largely elusive. To gain a better insight into the mechanical behavior of granular matter, we focus on a canonical set-up: the collapse of columns under gravity. We carried on 3D DEM numerical simulations and experiments for various granular columns on a frictional plane.

Interestingly, this flow configuration is dictated by only two parameters: the aspect ratio of the initial column, a, and the friction. The dynamics and final shape of the pile can be rationalized through a modified BCRE scheme. The model only includes two parameters, the aspect ratio of the initial column and the dynamic or neutral angle. Interestingly, all the friction coefficients, grain-grain and grain-wall, are encoded in this single value.

12:51PM F56.00009: Inertial Phenomena and Resistive Force Theory in Wheeled Locomotion on Dry Granular Media*  

ANDRAS KARSAI (Presenter), Physics, Georgia Institute of Technology, SHASHANK AGARWAL, KEN KAMRIN, Mechanical Engineering, Massachusetts Institute of Technology, DANIEL GOLDMAN, Physics, Georgia Institute of Technology — We use an automated testbed to systematically conduct single-wheel (20 cm diam.) locomotion experiments in dry granular media (~1 mm poppy seeds) at angular velocities \( \omega \) (0.7-6.4 rad/s) where substrate-based inertial effects emerge. In contrast to Resistive Force Theory based predictions for which translation speed is proportional to angular velocity, as \( \omega \) increases, the translation speed plateaus to a speed dependent on wheel geometry and the system's force distributions. A frictional plasticity model shows similar phenomena despite lacking a rate-dependent constitutive model. This effect can be explained through a force-momentum balance which accounts for the inertial effects caused by changes in substrate inflow/outflow in the system's local volume. This force balance creates a net force loss that increases with translational velocity, creating a material-enforced speed limit for wheeled locomotion. Current RFT models describe quasistatic kinematic bodies, but an inertial correction to the RFT forces shows promise in extending RFT into capturing speed-dependent scenarios as well.

*This work was funded by the Army Research Office, Triangle Park.
1:03PM F56.00010: Understanding slipping of wheels in granular media locomotion

SHASHANK AGARWAL (Presenter), Massachusetts Institute of Technology, ANDRAS KARSAI, DANIEL GOLDMAN, Georgia Institute of Technology, Atlanta, KEN KAMRIN, Massachusetts Institute of Technology

Slipping of circular wheels at high rotation rates on granular media like sand is a commonly experienced phenomenon. At the same time, granular materials themselves are known to be rate-insensitive for a fairly large range of strain rates. In order to identify the fundamental phenomena responsible for the sudden increase in the slipping of wheels above a certain rotational velocity, a plasticity-based continuum modelling study is performed. Lugged wheel locomotion simulations, validated against experimental findings, are performed for a wide range of rotation rates. A momentum conservation-based argument is proposed to explain and predict the onset of increased slipping. An empirical form of optimal rotation rates for wheel locomotion in terms of various associated system parameters is also suggested.

1:15PM F56.00011: Clogging of soft particles in vibrating 2D hoppers

MIA MORRELL (Presenter), ERIC WEEKS, Emory University

We study the outflow of soft, low-friction hydrogel beads from a quasi-2D hopper, examining the probability of clog formation as a function of hopper exit width. By tilting the hopper chamber, we vary the force of gravity driving the flowing bead system. We find that clogging of soft beads requires the hopper aperture to be only slightly larger than the bead diameter, and increasing the force driving the beads towards the exit results in a decreased probability of clogging, holding exit width constant. We then investigate the effects of vibration of the entire hopper system, working in a high frequency limit. Vertical vibrations decrease the clogging probability, due to a disruption of clogging arches. Horizontal vibrations increase the clogging probability, due to an effectively smaller slit size.

*This work is supported by NSF Grant No. DMR-1609763.

1:27PM F56.00012: Measuring the yield stress of charged granular media: how a net charge leads to cohesive powders

C. MARK LEWIS, JEREMY M. LAPRADE, BRANDON M. HOOVER, ABDOUN R. AYOUBA, FREEMAN S. DONG, OSCAR S. HERNANDEZ-DAGUER, ANTHONY DINSMORE (Presenter), University of Massachusetts Amherst

Charged powders are common in nature and industry yet still exhibit many surprising behaviors that are poorly understood. Here we report that piles of grains that all carry the same sign of net charge can, surprisingly, behave like a brittle, cohesive solid. Our experiments probe slab-shaped piles placed on an insulating substrate atop a grounded plate. Sample were irradiated with ions from a corona discharge device and the final surface voltage, $V_S$, was measured. For ordinary sand, removing the pile from the ground plate caused the charged grains to fly off. By contrast, sand grains with hydrophobic coating formed piles that were stable, cohesive and rigid. We measured the rigidity of these piles in two ways: the minimum tilt angle $\theta$ that led to failure, and the yield shear stress, $\sigma_Y$. We found that both quantities increased as $V_S^2$. $\theta$ can exceed 90° and $\sigma_Y$ can reach three times its zero-charge value. We also measured the decay of $V_S$ over time and found that a stretched exponential function fit the data over timescales of many days. These results may lead to new ways to manipulate charged granular materials and provide new insights into the properties of lunar or Martian soils.

*This work is funded by a gift from the Xerox University Affairs Committee.

1:39PM F56.00013: Jamming and Tiling in Aggregation of Rectangles

ELI BEN-NAIM (Presenter), Theoretical Division, Los Alamos National Laboratory, DANIEL BEN-NAIM, Department of Computer Science, University of California, Santa Barbara, PAUL KRAPIVSKY, Department of Physics, Boston University

We study a random aggregation process involving rectangular clusters. In each aggregation event, two rectangles are chosen at random and if they have a compatible side, either vertical or horizontal, they merge along that side to form a larger rectangle. Starting with $N$ identical squares, this elementary event is repeated until the system reaches a jammed state where each rectangle has two unique sides. The average number of frozen rectangles scales as $N^2$ in the large-$N$ limit. The growth exponent $\alpha=0.229\pm0.002$ characterizes statistical properties of the jammed state and the time-dependent evolution. We also study an aggregation process where rectangles are embedded in a plane and interact only with nearest neighbors. In the jammed state, neighboring rectangles are incompatible, and these frozen rectangles form a tiling of the two-dimensional domain. In this case, the final number of rectangles scales linearly with system size.
1:51PM F56.00014: Analyzing The Flow of a System of Spheres Using Shape-Anisotropic Particles  JUSTIN ROBERTS (Presenter), SHUBHA TEWAR, University of Massachusetts Amherst — We report here on a simulation conducted using LAMMPS [https://lammps.sandia.gov] of a small concentration of dimers in a gravity-driven flow of spheres. The simulation box is a quasi-2D vertical hopper with a rectangular outlet containing a 1% concentration of dimers in an equal mixture of frictional spheres of diameter ratio 1.2. Each dimer consists of two contacting spheres glued together, and all spheres undergo the same Hertzian contact interactions. We track the positions, velocities and orientations of the dimers relative to the flowing spheres and find that while the flow is collisional, the dimers do not reorient significantly except near the walls and near the outlet, where the fluctuations in the sphere velocities are higher. However, as outlet size changes, the region with the largest reorientation per dimer moves from near the edges for large openings, to near the center for small openings, thus appearing to track where velocity fluctuations are large.

2:03PM F56.00015: Confined Packing of Granular Rods* JULIAN FREEMAN (Presenter), CONG CAO, Emory University, SEAN F PETERSON, School of Physics & Astronomy, Rochester Institute of Technology, YUJIE WANG, Department of Physics, Shanghai Jiao Tong University, SCOTT FRANKLIN, School of Physics & Astronomy, Rochester Institute of Technology, ERIC WEEKS, Emory University — We conduct a series of experiments and simulations to observe the effects surfaces have on the packing structure of randomly packed rods. Our experiments use cylindrical containers of different diameters, and rods of aspect ratios ranging from 4 to 32. We find that the rods packed into smaller cylindrical containers yielded lower volume fractions than in larger containers. Our results are extrapolated to an infinite container size, and the subsequent volume fraction decreases with increasing aspect ratios, in agreement with previous simulations. We also do x-ray tomography experiments and study simulated rod packings, which reveal boundary layers where the packing differs from the bulk. At the bottom, rods form layers, although their average volume fraction is similar to that of the bulk. The sides and top layers are both packed with lower volume fractions than the bulk. In particular, the top boundary layer has the strongest perturbation to the overall volume fraction.

*NSF (DMR-1609763)

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F57 GSNP: Systems Far from Equilibrium, including Fluctuation Theorems and Fluctuation-Dissipation Relations BSEC 256 - Martin Bazant, Massachusetts Inst of Tech-MIT

11:15AM F57.00001: Numerical Measurement of the Anomalous Dimension in a Two-Species Reaction-Diffusion Model  BENJAMIN VOLLAMAYR-LEE (Presenter), JOSHUA D. HELLERICK, Bucknell University, ROBERT C. RHOADES, Center for Communications Research, Princeton, NJ — We consider a two-species reaction-diffusion model that consists of the trapping reaction $A + B \rightarrow A$ with traps that either annihilate $A + A \rightarrow \emptyset$ or coalesce $A + A \rightarrow A$. Both species undergo diffusion with distinct diffusion constants $D_A$ and $D_B$. We introduce a simulation technique that provides the full probability distribution of $B$ particles for a given realization of the trap dynamics, greatly improving statistical accuracy. We measure in one dimension the $\beta$ particle density decay exponent and the recently predicted anomalous dimension $\varphi$ that appears in the asymptotic $B$ particle correlation function $C_B(r, t) \sim r^\varphi f(r/t^{1/2})$. These exponents are predicted via renormalization group calculations to be universal for dimensions $d \leq 2$, depending only on the diffusion constant ratio and the trap reaction type. We compare our measured values to the renormalization group predictions, and to various exact solutions based on 3-walker and 4-walker problems.

11:27AM F57.00002: Towards a bolometric measurement of the heat of erasure in superconducting logic* OLLI SAIRA (Presenter), MATTHEW MATHENY, RAJ KATTI, Caltech, GREGORY WIMSATT, UC Davis, SIYUAN HAN, U Kansas, JAMES CRUTCHFIELD, UC Davis, MICHAEL ROUKES, Caltech — In his seminal 1961 paper, Landauer derived a lower bound on the heat dissipation by any computing device per irreversible logical operation, such as erasing (resetting) a bit. I will outline a new approach for an unencumbered measurement of the heat of bit erasure using a superconducting flux qubit and an ultrasensitive bolometer. First, using a gradiometric flux qubit as the physical bit subsytem, I will revisit a classical trajectory-tracking demonstration of efficient bit erasure. Owing to the high intrinsic speed of superconducting flux logic, we are able to extract a high-resolution histogram of the work exerted on the system during an erasure cycle. The experimental work histogram display universal features expected for a generic efficient implementation of bit erasure. In addition, the experimental work distributions enable us to test recently-discovered Fractional Fluctuation Theorems, generalizing Landauer’s erasure bound. Second, I will argue that a combination of superconducting logic cell and a bolometer is an ideal way to measure the heat of erasure through its effect on the dissipative environment.

*This work was supported by the U. S. Army Research Office under contract W911NF-13-1-0390.
11:39AM F57.00003: Collective Power: Minimal Model for Thermodynamics of Nonequilibrium Phase Transitions
TIM HERPICH, JUZAR THINGNA, MASSIMILIANO ESPOSITO (Presenter), University of Luxembourg — We propose a thermodynamically consistent minimal model to study synchronization which is made of driven and globally interacting three-state units. This system exhibits at the mean-field level two bifurcations separating three dynamical phases: a single stable fixed point, a stable limit cycle indicative of synchronization, and multiple stable fixed points. These complex emergent dynamical behaviors are understood at the level of the underlying linear Markovian dynamics in terms of metastability. Stochastic thermodynamics is used to study the dissipated work across dynamical phases as well as across scales. This dissipated work is found to be reduced by the attractive interactions between the units and to nontrivially depend on the system size.


*This research was supported by the National Research Fund, Luxembourg (AFR PhDGrant No. 11271777) and by the European Research Council project NanoThermo (ERC-2015-CoG Agreement No. 681456).

11:51AM F57.00004: Number of hidden states needed to physically implement a given conditional distribution
JEREMY OWEN (Presenter), Physics, Massachusetts Institute of Technology, ARTEMY KOLCHINSKY, DAVID WOLPERT, Santa Fe Institute — We consider the problem of constructing a physical process over a state space X that applies some desired conditional distribution P to initial states to produce final states. This problem arises in various scenarios in the thermodynamics of computation and nonequilibrium statistical physics (e.g., when designing processes to implement some desired computation, feedback-control protocol, etc.). It is known that there are conditional distributions that cannot be implemented using any master equation involving just the states in X. Here we show that any conditional distribution P can be implemented if additional “hidden” states are available, and provide an upper bound on how many such states are required to implement any P in a thermodynamically reversible manner. Our results imply that for certain P that can be implemented without hidden states, having additional states available permits an implementation that generates less heat. These results can be seen as uncovering a novel type of cost of the physical resources needed to perform information processing—the size of a system’s hidden state space.

*Grant No. FQXi-RFP-1622 from the FQXi foundation, and Grant No. CHE-1648973 from the U.S. National Science Foundation

12:03PM F57.00005: The thermodynamics of computing with circuits
DAVID WOLPERT (Presenter), ARTEMY KOLCHINSKY, Santa Fe Institute — As Landauer showed, any physical process that implements a given computation must generate a minimal amount of heat. Common engineered systems implement computations using circuits, as do many biological systems (e.g., gene regulatory networks). The topology of such circuits introduces additional constraints on the physical system implementing the computation. One might expect that this increases the minimal amount of heat needed to implement that computation, beyond the minimal amount needed if there are no constraints on how the computation can be implemented. We derive exact equations for the minimal amount of heat that is generated by any physical process that implements a given computation using a specified circuit. We also quantify how that minimal amount of heat compares to the minimal amount when the constraint of implementing the computation with the specified circuit is removed. These results provide a rich, new set of optimization problems that must be addressed by any designer of a circuit, if they wish to minimize thermodynamic costs.

*We would like to acknowledge the Santa Fe institute, and Grant No. CHE-1648973 from the U.S. National Science Foundation.
12:15PM F57.00006: Population dynamics of driven autocatalytic reactive mixture* HONGBO ZHAO (Presenter), MARTIN BAZANT, Massachusetts Institute of Technology — A reactive mixture undergoes thermal fluctuation and reacts with the reservoir when chemically driven. We apply the Fokker-Planck equation consistent with statistical physics to describe the ensemble dynamics. We illustrate the effect of autocatalysis on the ensemble dynamics by comparing systems with identical thermodynamics yet different reaction kinetics. Fictitious phase separation may occur in autocatalytic systems. Reversely, autoinhibition may suppress phase separation, leading to dynamic phase behavior entirely different from thermodynamic equilibrium.

We also present examples found in electrochemical systems such as lithium iron phosphate and LiNi1/3Mn1/3Co1/3O2 (NMC). XRD, STXM and other analytical techniques have revealed intriguing asymmetric autocatalytic or autoinhibitory reaction kinetics and the corresponding phase transition behavior during charge and discharge. As an application, we obtain the inherent reaction kinetics from XRD and electrochemical experiments performed on NMC and demonstrate the agreement between experiments and simulation.

*This work is supported by Toyota Research Institute.

12:27PM F57.00007: Information Thermodynamics of Turing Patterns GIANMARIA FALASCO (Presenter), RICCARDO RAO, MASSIMILIANO ESPOSITO, University of Luxembourg — We set up a rigorous thermodynamic description of reaction-diffusion systems driven out of equilibrium by time-dependent space-distributed chemostats. Building on the assumption of local equilibrium, nonequilibrium thermodynamic potentials are constructed exploiting the symmetries of the chemical network topology. It is shown that the canonical (resp. semigrand canonical) nonequilibrium free energy works as a Lyapunov function in the relaxation to equilibrium of a closed (resp. open) system and its variation provides the minimum amount of work needed to manipulate the species concentrations. The theory is used to study analytically the Turing pattern formation in a prototypical reaction-diffusion system, the one-dimensional Brusselator model, and to classify it as a genuine thermodynamic nonequilibrium phase transition. The framework paves the way to study the energy cost of pattern manipulation and information transmission in complex biochemical systems.

12:39PM F57.00008: Thermolubricity and the Jarzynski equality* ERIOS TOSATTI (Presenter), SISSA and ICTP, Trieste, Italy, FRANCO PELLEGRINI, EMANUELE PANIZON, SISSA, Trieste, Italy, GIUSEPPE SANTORO, SISSA and ICTP, Trieste, Italy — Two different pieces of physics in nanoscale sliding friction are thermolubricity and the Jarzynski identity. The first: a dry slider can at high temperature and low velocity exhibit thermolubric friction \( f \propto v \) replacing ordinary stick-slip friction \( f \propto \log v \) in opposite conditions. The second: satisfaction (violation) of Jarzynski's identity is tied to the abundance (scarcity) of negative work events ("free lunches"). Thermolubricity and Jarzynski are general in nature and separately met in experiments including sliding emulations in optical lattices, and protein force spectroscopy. We prove analytically and demonstrate numerically in the classical Prandtl-Tomlinson point slider model that the presence or absence of thermolubricity is exactly equivalent to satisfaction or violation of the Jarzynski equality. The divide between the two regimes simply coincides with the total frictional work per cycle falling below or above \( kT \) respectively. This concept can, with due caution, be extended to more complex sliders, and invites crosscheck experiments, such as searching for free lunches in cold ion sliding as well as in forced protein unwinding, and alternatively checking for a thermolubric regime in dragged colloid monolayers.

*Supported by ERC MODPHYSFRICT Contract no. 320796

12:51PM F57.00009: Dynamic critical properties of non-equilibrium Potts models with absorbing states* JAMES STIDHAM (Presenter), AHMADREZA AZIZI, MICHEL PLEIMLING, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — We present the results of numerical simulations of non-equilibrium Potts models with absorbing states that allow for different scenarios, depending on the range of the spin-spin interactions [1]. These scenarios encompass a voter critical point, as well as the presence of both a symmetry-breaking phase transition, and an absorbing phase transition. We investigate time-dependent quantities that provide insights into the transient properties of the models.


*Research was sponsored by the US Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.
1:03PM F57.00010: Stability of dynamical quantum phase transitions in disordered systems  
CHRISTIAN MENDL (Presenter), JAN CARL BUDICH, TU Dresden — Dynamical quantum phase transitions (DQPTs) appear at critical times (so-called Fisher zeros) of the Loschmidt amplitude \( G(t) = \langle \psi | e^{-iHt} | \psi \rangle \), where \( | \psi \rangle \) denotes the initial quantum state and \( H \) the Hamiltonian governing the nonequilibrium time evolution. So far DQPTs have mostly been investigated for systems with momentum conservation, but the fate of DQPTs in the presence of spatially uncorrelated disorder remains a largely open question. In this work we address this question by resorting to a supercell representation, which allows us to maintain a generalized version of the momentum space framework. Specifically, Fisher zeros appear as vortices of the complex phase of \( G(t) \) in the momentum-time plane; these vortices can only continuously change with the onset of disorder. Thus we hope to shed light on the dynamical behavior of disordered systems out of equilibrium.

1:15PM F57.00011: Femtosecond imaging of nonequilibrium phase transitions: Symmetry breaking and prethermalization in interacting CDW systems*  
JOSEPH WILLIAMS (Presenter), FARAN ZHOU, TIANYIN SUN, Michigan State Univ, MERCOURI KANATZIDIS, CHRISTOS MALLIAKAS, Northwestern University, CHONG-YU RUAN, Michigan State Univ — In correlated many-body systems, the fundamental processes of spontaneous symmetry breaking (SSB) to form long-range order may be intercepted by competing interactions between particles. In such cases, the transition becomes sharp over the control parameters, and surprising synchronicity develops to manifest macroscopic switching between two stable long-range orders. This departure from SSB behavior has been the hallmark of macroscopic switching of quantum materials, but never before have the microscopic processes been captured with atomic detail. Here we demonstrate a surprising post-laser-quench self-organization of an interacting CDW system exhibiting critical slowdown near thermal and interaction driven critical points. Unlike in SSB system, such photoinduced criticalities primarily emerged in the time domain and manifested in the prethermalization and dynamical phase transition. Using femtosecond (fs) imaging, we capture these highly tunable, nonequilibrium processes and the emerging unconventional symmetry-broken intermediate state, opening up an entirely new dimension in studying and controlling phase transitions far from equilibrium.

*We acknowledge support by NSF MRI facility grant: DMR1625181 and DOE grant: DE-FG02-06ER46309

1:27PM F57.00012: Nanoscale virtual potentials using optical tweezers*  
JOHN BECHHOEFER (Presenter), AVINASH KUMAR, Simon Fraser University — We combine optical tweezers with feedback to impose arbitrary time-dependent potentials on a colloidal particle. The feedback trap detects a particle’s position, calculates a force based on an imposed “virtual potential,” and shifts the trap center to generate the desired force. This kind of feedback trap can both extend the capabilities of optical tweezers and test fundamental ideas in stochastic thermodynamics. For the former, we have controlled trap stiffness to make tweezer response truly isotropic in three dimensions, allowing unbiased measurement of dynamics. For the latter, we have created virtual double-well potentials with well separations of 11 nm and dwell times of a few ms, scales that approach those of protein-folding dynamics. Such a speed-up of dynamics will allow measurement of stochastic trajectory-based quantities for systems far from equilibrium.

*Work funded by NSERC (Canada).

1:39PM F57.00013: Disordered Kitaev chain with long-range pairing: Loschmidt echo revivals and dynamical quantum phase transitions  
UTKARSH MISHRA (Presenter), Asia Pacific Center for Theoretical Physics (APCTP), Pohang, Gyeongbuk, 790-784, Korea, ROUHOLLAH JAFARI, Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45137-66731, Iran, ALIREZA AKBARI, Asia Pacific Center for Theoretical Physics (APCTP), Pohang, Gyeongbuk, 790-784, Korea — We explore the dynamics of long-range Kitaev chain by varying pairing interaction exponent, \( \alpha \). In a finite size system, it is known that Loschmidt echo has periodic revivals for quenching to the critical point. We find that the revivals in the Loschmidt echo are connected to the energy gap at finite size system, regardless of the initial state. Moreover, and contrary to expectations, for the long-range pairing case, \( \alpha < 1 \), the first revival time (periodicity) scales inversely with the group velocity at the gap closing point, instead of the maximum group velocity. Analyzing the effect of quenched averaging disorder shows the robustness of the first revival time against disorder. For the dynamical phase transition, the presence of disorder washes out the non-analyticities in the rate function of return probability.
The Boltzmann distribution predicts the collective behavior of systems at thermodynamic equilibrium as a function of their constituent parts. Yet most systems in nature—especially living systems—are not at equilibrium, and a unified theory of their behavior does not currently exist. I will show that the Boltzmann distribution is a special case of a general probability flow equation (PFE) that governs stochastic systems, even if far from equilibrium. The PFE is an analog of the voltage equation governing electronic circuits, where resistors, batteries, node voltages, and path currents correspond to equilibrium rate constants, driven rate constants, probabilities, and probability flows, respectively. I will discuss how this new approach can be used to recapitulate known properties of weakly driven systems as well as derive new relations applicable to strongly-driven systems. These relations include general limits on performance and efficiency which are independent of system details; experimental data are used to show that living systems often operate at those limits.

*Leland Fikes Foundation
Heising-Simons Foundation

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F58 GSOFT: Colloids II BCEC 257A - Urs Gasser, Paul Scherrer Institute

11:15AM F58.00001: Synthesis and Assembly of Janus Particles  MENEKA BANIK (Presenter), RABIBRATA MUKHERJEE, Indian Institute of Technology Kharagpur — Over the years, a wide variety of Janus particles with anisotropy in terms of size, shape and chemical functionality have been explored. Synthesis and self-assembly of such particles has been an area of active research. Owing to their anisotropic nature Janus particles experience highly directional interaction. However, assembly of Janus particles on a surface driven by attractive interaction is an area not yet properly explored. One of the probable reasons for this is that most of the synthesized Janus particles are surface immobilized and suffer from significant damage during dislodgement. Also, the anisotropic particles synthesized by chemical route lack uniformity and monodispersity.

Here we have developed a technique for dislodging surface bound Gold-PS Janus particles by UV induced degradation of a PMMA layer. By this method of dislodging Janus particles no damage to the particles occur. Also, an adhesion promoting layer is not required and PS particles with very thin gold coating (~5 nm) can be dislodged. We have also studied the assembly of the dislodged Janus particles on different surfaces and observed that on such surfaces the particles orient in a preferred fashion depending on the particle-substrate interaction.

11:27AM F58.00002: Adsorption and denaturation of structured polymeric nanoparticles at an interface  JIE FENG (Presenter), Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, CHANG TIAN, H. JEREMY CHO, SUJIT DATTA, ROBERT K PRUD'HOMME, Chemical and Biological Engineering, Princeton University — Nanoparticles (NPs) have been widely applied in fields as diverse as energy, environment, and human health. However, the adsorption and trapping of NPs at interfaces is still poorly understood. In many applications, such as drug delivery, understanding NP interactions at an interface is essential to determine and control adsorption onto targeted areas. Therapeutic NPs are especially interesting because their structures involve somewhat hydrophilic surface coronas, to prevent protein adsorption, and much more hydrophobic core phases. Here, we investigate the evolution of NP attachment and structural evolution at the air–liquid interface over time scales from 100 ms to 10s of seconds. We document three distinct stages in NP adsorption. In addition to an early stage of free diffusion and a later one with steric adsorption barriers, we find a hitherto unrealized region where the interfacial energy changes due to surface "denaturation" or restructuring of the NPs at the interface. We adopt a quantitative model to calculate the diffusion coefficient, adsorption rate and barrier, and extent of NP hydrophobic core exposure at different stages. Our results deepen the fundamental understanding of adsorption of structured NPs at an interface.
Phase Separation of Ferromagnetic Nematic and Isotropic Colloidal Suspensions*

MIN SHUAI (Presenter), XI CHEN, CHEOL SOO PARK, JOSEPH E MACLENNAN, MATT GLASER, NOEL ANTHONY CLARK, Department of Physics, University of Colorado Boulder — Suspensions of disk-shaped ferromagnetic barium hexaferrite nanoplates in isotropic solvent spontaneously form a ferromagnetic nematic phase for nanoplate concentrations higher than the Onsager isotropic–nematic phase transition point for hard disks [Nat Comm, 7: 10394, 2016]. At an overall concentration below this value and within the coexistence region, such suspensions phase separate into ferromagnetic nematic and isotropic domains. Under these conditions, the suspension can be driven into a uniform state by mechanical or magnetic stirring, and undergoes a dynamic process of phase separation immediately after the removal of stirring forces, which we have investigated by polarized optical microscopy. Starting from a diffuse, birefringent mesh, nematic regions rapidly coalesce into a three-dimensional network of fine, short, straight filaments. If left undisturbed, these filaments coarsen, combining with each other until the isotropic phase between them is eliminated. In the presence of a weak external magnetic field, filaments along the field direction tend to grow most quickly. We also observe ferromagnetic nematic domains with exotic topological structures, particularly under sudden changes in external field.

*This work is supported by NSF MRSEC DMR-1420736 and NASA NNX17AC74G.

Topological Protection in Densely Packed Anisotropic Colloids*

WILLIAM ZYGMUNT (Presenter), Chemical Engineering, University of Michigan, ERIN TEICH, Applied Physics, University of Michigan, GREG VAN ANDERS, Physics, Engineering Physics & Astronomy, Queen's University, SHARON GLOTZER, Chemical Engineering, University of Michigan — It has been long known that there exist topologically protected phases in strongly coupled systems dominated by quantum effects. Recently, analogous phases have been discovered in classical systems of mechanical metamaterials. Here, we demonstrate the existence of topologically protected phases in systems of densely-packed, hard, anisotropic colloids. Previously reported transitions in dense packings as a function of the constituent particle shape lead to the existence of topologically protected thermodynamic phases in such systems, which are shown to be stable away from the limit of densest packing, down to packing fractions of about 75%. Our discovery expands the library of topological phases, and realizing these phases in experiment could provide a new means of producing complex soft materials that are resistant to thermal fluctuations, with applications in robust information storage and processing, and plasmonic materials.


Pitch-dependent behavior of colloids in confined cholesteric liquid crystals*

GIUSEPPE BONIELLO (Presenter), Chemical and Biomolecular Engineering, University of Pennsylvania, FRANCESCA SERRA, Physics and Astronomy, Johns Hopkins University, KATHLEEN STEBE, Chemical and Biomolecular Engineering, University of Pennsylvania — Confined soft matter provides unique opportunities to impose energy landscapes to address and control colloid dynamics. In this context, the geometry of bounding surfaces can be employed to mold an energy landscape. Within this landscape, colloids assemble into reconfigurable, hierarchically organized structures, a leading challenge in material science. Example soft matter systems include liquid crystals. For instance, when nematic liquid crystals (NLCs) are confined in a vessel, bend and splay distortions can be used to position particles. Here we study cholesteric liquid crystals (ChLCs) in a vessel with undulated boundaries. ChLCs have an “intrinsic” twist distortion which adds to the ones imposed by the solid boundaries. The cholesteric pitch competes with the other length scales in the system (colloid radius, vessel thickness, wavelength of boundaries undulations), enriching the possible configurations. Depending on the pitch-to-radius and pitch-to-thickness ratios the interaction can be attractive or repulsive, alternatively. By tuning the pitch (i.e. changing the concentration of the chiral dopant), it is possible to selectively promote or inhibit particle trapping at the docking sites.

*Army Research Office
12:15PM F58.00006: Microstructure and stress propagation in the nematic glass phase of colloidal cellulose nanocrystals  MATTHEW SARTUCCI (Presenter), Georgetown University, BHARATH NATARAJAN, JEFFREY GILMAN, NIST, JEFFREY S URBACH, Georgetown University — Suspensions of cellulose nanocrystals (CNC's) in low ionic strength aqueous solutions can undergo an isotropic-nematic phase transition due to the anisotropic nature of CNC's. At concentrations above a certain threshold, when the system is well into the nematic regime but far below the maximum stable concentration, these suspensions can form a soft solid with a modulus of approximately 500 Pa. The nematic phase is not homogeneous throughout this system but instead forms many domains, each consisting of collectively aligned CNC's with an average orientation that differs from neighboring domains. This work seeks to understand the mechanical contribution of the domain structure, as observed through cross polarization and boundary stress microscopy, to the macroscopic properties measured through bulk rheology.

12:27PM F58.00007: Modulated colloidal deposition and accumulation in model porous media  GAETAN GERBER (Presenter), IFSTTAR / SEAS, Université Paris-Est / Harvard University, PHILIPPE COUSSOT, Université Paris-Est — Suspended colloids flowing through porous structures are subject to various events, including size-exclusion clogging [1], surface adsorption, or interactions with previously attached bodies. Current models [2,3] qualitatively describe those local mechanisms, while observations are mostly limited to break-through analysis and 2D geometries.

Here, we observe and quantify the local adsorption mechanisms on the internal surface of a 3D porous structure. We consider the accumulation of charged colloids (1µm) in model packs of silica grains and vary the intercolloidal interactions to modulate colloidal aggregation. Deposition is followed by confocal microscopy to identify the precise deposition mechanisms (grain scale) and estimate the spatiotemporal distributions of deposited particles (cm scale). We observe and model two main regimes: (i) deposition of a Langmuirian single-layer of particles due to repulsive intercolloidal interactions, and (ii) multi-layer deposits reaching a critical size (cohesion to drag equilibrium; including potential clogging), when screening those interactions. This provides new tools to predict the transport of suspensions, e.g. for soils remediation or filtration processes.

[1] Gerber, PRL 2018

12:39PM F58.00008: Size Control and Monodispersity of Silica Nanospheres and Applications in Nanofiltration*  RYAN VINCENT (Presenter), SEAN MCBRIDE, Physics, Marshall University — Due to their low reactivity and high thermostability, amorphous silicon dioxide nanoparticles have drawn much attention in the field of nanotechnology. This work reports on the synthesis methods and reaction parameters used to produce monodispersed silica nanospheres of systematically varied sizes using modified Stöber methods. Employing W/O microemulsion systems assisted by amino acid monomers and more traditional Stöber systems, nanosphere diameters were well controlled from single-digit nanometers to several micrometers. Effects of chemical compositions and other reaction parameters effecting TEOS hydrolysis were optimized for each Stöber system. Additionally, the monodispersed spheres were assembled into close-packed systems where the porosity and volumetric flowrates were controlled by the nanoparticle radii. Detailed characterization of the particles and arrays was performed using atomic force microscopy and scanning electron microscopy. Developing a porous system with a tunable effective pore size is a fundamental interest in the field of filtration.

*This work is partially supported by the National Science Foundation under Award No. OIA-1458952. The authors also acknowledge support from Marshall University.

12:51PM F58.00009: Non-Stokes drag of electrophoresis: a new insight into an old problem  MAIJIA LIAO (Presenter), Yale University, MING-TZO WEI, Chemical and Bio-molecular engineering, Princeton University, H DANIEL OU-YANG, Physics Department, Lehigh University, PING SHENG, Physics Department, Hong Kong University of Science and Technology — Mobility, the ratio of a charged-particle drift speed in a DC electric field to the magnitude of the field is typically used to quantify electrophoresis. Drag coefficient cannot be measured in a DC field because application of an external force to measure force alters the flow pattern, yielding an apparent drag force that is Stokes-like. The intrinsic electrophoretic drag can be determined, however, by optically trapping a charged particle and placing it in a low-frequency AC field. Using the frequency-dependent phase shift of the particle motion relative to that of the AC field and the magnitude of the particle displacement, this approach yields drag coefficient, effective charge and also a mobility that is the same as that measured using a DC field. The drag coefficient is markedly different from that of the Stokes. Using the drag coefficient and the mobility as input for numerical calculations based on the Planck-Nernst-Poisson equation and the Stokes equation reveals a well-defined transition between an inner and outer flow in the vicinity of the particle. This study provides a new insight into an old problem by providing experimentally measurable quantities, i.e., effective charge, electric force and drag coefficient a microscopic definition.
1:03PM F58.00010: Gradient expansions to capture the nonlocal physics of the electrical double layer* PEDRO DE SOUZA (Presenter), MARTIN BAZANT, Chemical engineering, MIT — A hallmark of highly charged surfaces or concentrated electrolytes is strong, nonlocal electrostatic and density correlations. In these regimes, the classical Poisson-Boltzmann (PB) mean-field theory for dilute electrolytes breaks down, and the predictions using PB can be qualitatively and quantitatively incorrect. For example, the influence of nonlocal electrostatic correlations lead to charge reversal and like-charge attraction, even though PB theory predicts an exclusively repulsive interaction between like-charged surfaces. Size correlations can lead to oscillatory density profiles that are not captured by PB theory. Here, we explore using a nonlocal Landau-Ginzburg-like free energy functional to describe the structure of an electrical double layer at a charged surface, as well as overlapping electrical double layers, at high charge density and concentration. We show that the correct boundary conditions of such a nonlocal model are given by a force balance at the interface, where the nonlocal effects must vanish. We apply the model to calculate surface forces, interactions between biological molecules, and electrokinetic flows.

*National Science Foundation Graduate Research Fellowship
Professor Amar G. Bose Research Grant

1:15PM F58.00011: Computer Simulations of Packed Soft Colloids* TOM RIDLEY, DANIEL READ (Presenter), OLIVER G HARLEN, JOHAN MATTSSON, University of Leeds — Soft colloids are micron-scale structured objects such as polymer microgels, that are compressible and deformable. Even at high packing ratios, a soft colloid may still be able to undergo cage-breaking due to particle deformation. The link between the detailed elastic properties of soft colloids and the resulting dynamics are presently not well understood. Soft colloids show rich rheological behaviour we wish to understand the links between the single particle elastic properties and the resulting rheology. We use a recently developed algorithm, Fluctuating Finite Element Analysis, for simulating viscoelastic objects undergoing thermal excitation. While symmetric soft particle potentials have been much studied, our approach captures the detailed shape deformations of the colloidal particles so that the structure and anisotropic deformation of the particles are taken into account. We investigate varying effective volume fraction and find evidence of cage-breaking events even where the effective volume fraction exceeds the close packed limit. Additionally, we present results of varying modulus and steady shear rates for a constant effective volume fraction.

*Supported by EPSRC CDT in Soft Matter and Functional Interfaces, EP/L015536/1

1:27PM F58.00012: Diffusion of DNA-coated colloids on DNA coated surface JEANA(AOJIE) ZHENG (Presenter), DAVID J PINE, New York University — In order for DNA-coated colloids to anneal and form crystals, they must roll and diffuse while attached to each other. Here we report on the diffusion of DNA-coated colloidal spheres on a flat DNA-coated substrate. Near the DNA-melting temperature, the mean square displacement is linear in time as expected for normal diffusion, but the diffusion coefficient is much smaller than for free diffusion. As the temperature is lowered, the motion becomes subdiffusive, which suggests the presence of random free energy barriers in the DNA-mediated interactions.

1:39PM F58.00013: Microscopic dynamics of stress relaxation in a nanocolloidal soft glass YIHAO CHEN (Presenter), Johns Hopkins University, SIMON ROGERS, UIUC, SURESH NARAYANAN, Argonne, JAMES HARDEN, U. Ottawa, ROBERT LEHENY, Johns Hopkins University — Following the cessation of flow-inducing shear, soft disordered solids often display a protracted recovery during which the stress slowly decreases to a finite value known as the residual stress. While numerous rheology studies have characterized the macroscopic nature of this stress relaxation, little is known about the underlying microscopic structural dynamics. We report x-ray photon correlation spectroscopy (XPCS) experiments with in situ rheometry performed on a soft glass composed of a dense suspension of charged silica nanoparticles subject to step strains that induce yielding. The XPCS measurements characterize the particle-scale and mesoscale motions within the glass that underlie the subsequent slow decay of the stress. The XPCS correlation functions indicate these dynamics are anisotropic, with slow, convective-like particle motion along the direction of the preceding shear that persists for surprisingly large times after flow cessation and that is accompanied by highly intermittent motion in the perpendicular (vorticity) direction. The close correspondence between these dynamics and the stress relaxation is demonstrated by power-law scaling between the characteristic velocity of the convective motion and the rate of stress decay.
1:51PM F58.00014: Particle anisotropy tunes emergent behavior in active colloidal systems  
SHANNON MORAN (Presenter), University of Michigan, ISAAC BRUSS, Harvard University, SHARON GLOTZER, University of Michigan — Since early studies of active systems, investigators have sought to understand the role of particle interactions on a system's emergent collective behavior. Particle anisotropy has been shown to impact the collective behavior of active systems, but studies to date have been qualified demonstrations of concept rather than systematic treatments. In this computational work, we investigate the role of particle anisotropy in shape and driving force director on the phase behavior of an active colloidal system. We find that these anisotropic interactions can combine to enable critical densities lower than those found in systems of isotropic particles, while in some cases actually elevating the critical density. Specifically, we find that tailoring particle anisotropy can enable more "effective" inter-particle collisions to tune the critical system density for phase separation. Additionally, we observe nucleation of multiple clusters in the phase separation regime, similar to those observed in biological systems. In designing programmable active colloidal systems, steric interactions such as those described here may offer a simple route for tailoring emergent behaviors in active materials.

*NSF GRFP (No. DGE 1256260)

2:03PM F58.00015: Reversible cluster formation and dynamical arrest in colloidal dispersions  
RAMON CASTANEDA PRIEGO (Presenter), Physical Engineering, University of Guanajuato — Combining molecular simulations, experimental characterizations and theoretical calculations: 1) we conclusively demonstrate that the cluster morphology in short-ranged attractive colloidal systems (SRACS) at equilibrium conditions can be uniquely determined by the reduced second virial coefficient; our findings link the reversible colloidal aggregation with the extended law of corresponding states, 2) we show that gelation in adhesive hard-sphere dispersions is the result of the rigidity percolation with coordination number equal to 2.4; these results connect the concept of critical gel formation in SRACS to the universal concept of the rigidity percolation and, finally, 3) we provide a unified description and a general overview of the different aspects of the glass transition in largely asymmetric binary mixtures of hard-spheres; we highlight the fundamental relevance in considering explicitly the dynamics of both large and small particles to properly account for the glassy scenario.

*1. Conacyt (Grant. Nos. 237425, 287067)
2. Marcos Moshinsky Foundation.
3. Alexander von Humboldt Foundation.

Tuesday, March 5, 2019 11:15 AM - 2:03 PM

Session F59 GSOFT DPOLY DBIO: Rheology of Gels I
BCEC 257B - Jacinta Conrad, University of Houston - Tag(s): Focus

11:15AM F59.00001: Failure precursors in colloidal and biopolymer gels  
[Invited] LAURENCE RAMOS (Presenter), STEFANO AIME, ANGELO POMMELLA, LUCA CIPELLETTI, CNRS/University Montpellier, Laboratoire Charles Coulomb — Material failure is widespread and occurs on vastly different lengthscales, from earthquakes to the atomic level. It often involves sudden and unpredictable events, with little or no macroscopically detectable precursors. A better understanding of the mechanisms leading to failure is however highly desirable and would have deep implications, possibly paving the way to predicting failure.
We will present experiments probing failure precursors in two types of gel: colloidal and biopolymer gels. Colloidal gels can be regarded as model network forming materials, are brittle and exhibit a power law linear viscoelasticity, whereas biopolymer gels are more complex, show strain-hardening and develop negative normal stresses under shear. We use original set-ups that simultaneously probe the macroscopic rheological response and the microscopic structure and dynamics of a gel submitted to a constant shear stress. We show that the failure is systematically preceded by qualitative and quantitative change of the dynamics, from reversible particle displacement to a burst of irreversible plastic rearrangements with a complex spatial evolution in the sample. Those plastic events are failure precursors of the materials and may be regarded as a novel tool to understand the sudden failure of solids.

* This work was funded by ANR (grant n. ANR-14-CE32-0005-01), CNES, and the EU (Marie Sklodowska-Curie ITN Supolens, Grant No. 607937).
minimum at a characteristic temperature (characteristic temperature (characteristic
well as the volume fraction of microgels. In the range of
even when
emerge, the suspensions show solid-like properties due to the network-like flocculation of microgels (colloidal gelation),
We discuss the contributions of packing degree effect and interparticle interaction effect to viscoelasticity. [1]
and poly(N-isopropylacrylamide) core-shell particles of largely different attraction strengths, 5kT and 30kT. We show that we can
systematically tune the viscoelastic moduli of the binary mixtures by two orders of magnitude, and the spectra of the
relaxation time by seven orders of magnitude, simply by altering their mixing proportions. Using confocal fluorescence
microscopy and differential dynamic microscopy, we link these changes in the mechanical properties to the microscopic
characteristics of the structure and dynamics of the gel networks.

*This work was partly supported by MEXT KAKENHI Grant Number JP18K19113.

**12:27PM F59.00005: Tunable viscoelasticity of binary colloidal gels** JAE HYUNG CHO (Presenter), IRMGARD BISCHOFFBERGER, Mechanical Engineering, Massachusetts Institute of Technology — The mechanical properties of colloidal gels depend strongly on the inter-particle interactions. We investigate the potential to engineer the linear viscoelastic properties of colloidal gels at low volume fractions by mixing two types of home-made polystyrene-poly(N-isopropylacrylamide) core-shell particles of largely different attraction strengths, 5kT and 30kT. We show that we can systematically tune the viscoelastic moduli of the binary mixtures by two orders of magnitude, and the spectra of the relaxation time by seven orders of magnitude, simply by altering their mixing proportions. Using confocal fluorescence microscopy and differential dynamic microscopy, we link these changes in the mechanical properties to the microscopic characteristics of the structure and dynamics of the gel networks.
12:39PM F59.00006: Enhanced gelation in binary mixtures of nanoparticles with tunable short-range attraction
JAMES HARDEN (Presenter), University of Ottawa, HONGYU GUO, NIST, MARTINE BERTRAND, University of Ottawa, TYLER SHENDRUK, Loughborough University, SUBRAMANIAN RAMAKRISHNAN, Florida State University, ROBERT LEHENY, Johns Hopkins University — We report a combined experimental, theoretical, and simulation study of the phase behavior and microstructural dynamics of concentrated binary mixtures of spherical nanoparticles with a size ratio near two and with a tunable, intrinsic short-range attraction [1]. In the absence of the attraction, the suspensions behave as well mixed, hard-sphere liquids. For sufficiently strong attraction, the suspensions undergo a gel transition. Rheometry measurements show that the fluid-gel boundary of the mixtures does not follow an ideal mixing law, but rather the gel state is stable at weaker interparticle attraction in the mixtures than in the corresponding monodisperse suspensions. X-ray photon correlation spectroscopy measurements reveal that, in contrast with depletion-driven gelation at larger size ratio, gel formation in the mixtures coincides with dynamic arrest of the smaller nanoparticles while the larger nanoparticles remain mobile. Molecular dynamics simulations indicate the arrest results from microphase separation that is caused by a subtle interplay of entropic and enthalpic effects and that drives the smaller particles to form dense regions.


12:51PM F59.00007: Rheology of Colloid Gels with Depletion and Bridging Attractions*
NA PARK (Presenter), JACINTA CONRAD, Chemical and Biomolecular Engineering, University of Houston — Polymers are often added to suspensions as viscosity modifiers or stabilizers, but they can induce attractive interactions between particles that alter the suspension phase behavior and, in turn, the rheology. These attractions may be depletion attractions or bridging attractions, depending on whether the polymers adsorb on the surface of the particles. Here, we developed a model attractive colloidal suspension with depletion and bridging attractions. Co-polymer particles of 2,2,2-trifluoroethyl methacrylate and tert-butyl methacrylate were suspended in a refractive index- and density-matched mixture of glycerol and water. To these suspensions, we added poly(acrylamide) or poly(acrylic acid) to induce depletion or bridging attractions, respectively. The rheology was measured and analyzed for each set of samples with increasing concentration of polymer, corresponding to stronger attraction strengths. Significantly different rheology resulted by simply changing the polymer additive in these suspensions, suggesting that processability of suspensions may be tuned by changing the type and interactions of polymer additives in formulations.

*NSF (CBET-1803728) and the Welch Foundation (E-1869)

1:03PM F59.00008: Analyzing Onset of Non-Linearity of a Fractal Colloidal Gel in the Neighborhood of Critical Point
KHUSHBOO SUMAN (Presenter), YOGESH M JOSHI, Department of Chemical Engineering, Indian Institute of Technology Kanpur India — A colloidal dispersion of Laponite exhibits all the rheological features of a sol-gel transition. While undergoing gelation, Laponite dispersion passes through the critical state stress characterized by a percolated space-spanning fractal network for which the relaxation modulus shows a time dependent power law decay in the linear regime. When subjected to step strain in the non-linear regime, relaxation modulus shifts vertically to the lower values such that the deviation from linearity can be accommodated by use of a strain dependent damping function. We also perform creep-recovery, startup shear and large amplitude oscillatory shear (LAOS) experiments on the Laponite dispersion at the critical gel state and record deviation in the response as flow becomes nonlinear. We also develop a quasi-linear integral model with relaxation modulus weighted by damping function to account for the effect of non-linear strain. Remarkably the proposed quasi-linear integral model predicts the deviation from linearity in the creep-recovery, startup shear and LAOS very well, leading to a simple formulation to analyze the nonlinear rheological behavior of fractal gels.

1:15PM F59.00009: Singular dynamics in the failure of soft adhesive contacts
JUSTIN BERMAN (Presenter), KATHARINE JENSEN, Williams College — We use optical microscopy and high-speed imaging to characterize the rapid recoil of soft, silicone gels after an extreme deformation and release from a point contact during the failure of a soft adhesive contact. The gel immediately recoils away from the final contact point with a self-similar surface profile that evolves as a power law in time, suggesting that adhesive detachment is a space-time singularity. The singular dynamics we observe are consistent with a relaxation process driven by surface stress and hindered by viscous flow of the gel's free fluid phase through its porous, elastic network. Our results emphasize the importance of accounting for both the liquid and solid phases of gels in understanding their mechanics, especially in extreme deformation.
**States of self stress in disordered solids: memory, heterogeneity, and yielding**

SHANG ZHANG (Presenter), University of Michigan, Ann Arbor; VISHWAS VASISHT, University of Grenobles Alpes (France); LEYOU ZHANG, University of Michigan, Ann Arbor; EMANUELA DEL GADO, Georgetown University; XIAOMING MAO, University of Michigan, Ann Arbor —

States of self stress (SSSs), equilibrium stress distributions in a mechanical network with zero net force on any component, govern load-bearing abilities of this network. SSSs are determined by the geometry of the network (because they span the null space of the network's equilibrium matrix), and thus encode the memory of how the mechanical network is prepared. We present our results on SSSs in disordered solids generated by molecular dynamics simulations, and discuss how SSSs are affected by the preparation history of these solids (e.g., cooling rate, compression, shear), and explore the relation between SSSs in a disordered solid and its yielding under stress.

*SZ, LZ, and XM thank the support from the National Science Foundation (Grant No. DMR-1609051).

VV and EDG thank the Impact Program of the Georgetown Environmental Initiative and Georgetown University, Kavli Institute for Theoretical Physics at the University of California Santa Barbara and National Science Foundation (Grant No. NSF PHY17-48958).

**Scaling theory for mechanical critical behavior in fiber networks**

JORDAN SHIVERS (Presenter), SADJAD ARZASH, Department of Chemical and Biomolecular Engineering, Rice University; ABHINAV SHARMA, Leibniz Institute for Polymer Research; FRED C. MACKINTOSH, Department of Chemical and Biomolecular Engineering, Rice University —

As a function of connectivity, spring networks exhibit a critical transition between floppy and rigid phases at an isostatic threshold. For connectivity below this threshold, fiber networks were recently shown theoretically to exhibit a rigidity transition with corresponding critical signatures as a function of strain. Experimental collagen networks were also shown to be consistent with these predictions. We develop a scaling theory for this strain-controlled transition. Using a real-space renormalization approach, we determine relations between the critical exponents governing the transition, which we verify for the strain-controlled transition using numerical simulations of both triangular lattice based and packing-derived fiber networks.

*This work was supported in part by the National Science Foundation (DMR-1826623 and PHY-1427654).

**Structure and Dynamics of Hydrogen Bonds in the Deep Eutectic Solvent Choline Chloride/Urea: from Molecular Dynamics Simulation with Ab-Initio Polarizable Force Field**

KYEONG-JUN JEONG (Presenter), HYUNTAE JUNG, Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin - Madison; JESSE MCDANIEL, School of Chemistry and Biochemistry, Georgia Institute of Technology; ARUN YETHIRAJ, Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin - Madison; CHANG YUN SON, Division of Chemistry and Chemical Engineering, California Institute of Technology; —

Deep Eutectic Solvents (DESs) are a novel class of chemical solvents with beneficial properties. DESs consist of an ionic compound and a neutral hydrogen bond donor (HBD) species, where intermediate compositions of these result in large melting point depression. Although the hydrogen bond of HBD with anions is now known as a key factor in this eutectic phase behavior, the relation between microscopic details and bulk properties is not fully understood. In this study, we develop and import a first-principle-based polarizable force field for choline chloride/urea DES in molecular dynamics simulation. The bulk liquid properties are reproduced without applying charge scaling on the ions. The pair correlation and lifetime of hydrogen bond between HBD and ions exhibit strong character only when the model is polarizable, while its non-polarizable counterpart loses such specificity. Our study implies that the essential rebalancing of molecular interactions in DESs is contingent on polarizability of the model.

*This work is supported by US Department of Energy, Basic Energy Sciences Contract DE-SC0017877. Computational resources are provided by Oak Ridge Leadership Computing Facility (OLCF) and National Energy Research Scientific Computing Center (NERSC).
11:15AM F60.00001: Herbert P. Broida Prize Talk: Spectroscopic and dynamical probes of atmospheric reaction pathways* [Invited] MARSHA LESTER (Presenter), University of Pennsylvania — Alkene ozonolysis is a primary oxidation pathway for alkenes, the most abundant organic compounds in the Earth's troposphere after methane, and also an important source of atmospheric hydroxyl radicals (OH). Alkene ozonolysis takes place through a complicated reaction pathway with multiple intermediates and barriers on the way to OH products. A carbonyl oxide species, known as the Criegee intermediate (RR’COO), represents a critical branching point on the pathway that controls the products formed in this important class of reactions. In this laboratory, the simplest Criegee intermediate CH2OO and methyl-, dimethyl-, ethyl-, and vinyl-substituted Criegee intermediates are generated by alternative synthetic schemes. Recent studies have focused on characterizing the Criegee intermediates utilizing infrared and ultraviolet spectroscopic methods, and examining their unimolecular and bimolecular reactions under laboratory and atmospheric conditions. Infrared 'fingerprint' and electronic spectra reflecting π-conjugation of the Criegee intermediates are obtained, along with time-resolved studies of their unimolecular decay to OH radical products. Remarkably, the conformation and nature of the substituents (R, R’) of the Criegee intermediates are found to have a profound effect on their reaction dynamics and subsequent chemistry in the atmosphere.

*Research supported by the National Science Foundation, Division of Chemistry under grant CHE-1664572 and U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences under grant DE-FG02-87ER13792.

11:51AM F60.00002: Irving Langmuir Prize in Chemical Physics Talk: Interphase Human Chromosome Exhibits Glassy Dynamics [Invited] DAVE THIRUMALAI (Presenter), University of Texas at Austin — The structural organization of the condensed chromosomes is being revealed using chromosome conformation capture experiments and super-resolution imaging techniques. Fingerprints of their three-dimensional organization on length scale from about hundred kilo base pairs to millions of base pairs have emerged using advances in Hi-C and super-resolution microscopy. I will describe using a minimal Chromosome Copolymer Model (CCM) with two loci types corresponding to euchromatin and heterochromatin that the dynamics is similar to that observed in glasses. Chromosome organization is hierarchical involving the formation of chromosome droplets (CDs) on short genomic scale followed by coalescence of the CDs, reminiscent of Ostwald ripening. Glassy landscapes for the condensed active chromosomes might provide a balance between genomic conformational stability and biological functions.

12:27PM F60.00003: Earle K. Plyler Prize for Molecular Spectroscopy & Dynamics Talk: Energy transfer and conversion in molecular junctions* [Invited] ABRAHAM NITZAN (Presenter), University of Pennsylvania and Tel Aviv University — In molecular conductance spectroscopy, the current through a molecule (or molecules) connecting two metal or semiconductors electrodes is measured as a function of the applied voltage. With eye on potential applications, the main issues facing researchers are fabrication, characterization, stability, functionality and control. These considerations bring into focus the need to study systems comprising molecules and metal nanostructures not only for their electrical transport properties but also for their optical, thermal and mechanical response and for their function as energy conversion devices. This talk will review our work on these subjects, and present recent results on current induced light emission, photovoltaic response and electron transfer induced heat conduction in such systems.

*This research has been supported by the NSF (Grant No. CHE1665291) and by the US-Israel Binational Science Foundation.

1:03PM F60.00004: Nonadiabatic dynamics at metal surfaces: Surface hopping and electronic friction WENJIE DOU (Presenter), University of California, Berkeley, JOSEPH E SUBOTNIK, University of Pennsylvania — The coupled electron-nuclear dynamics at molecule-metal interfaces that involve electrons transfer as well as nuclear motions are intrinsically nonadiabatic and difficult to model. Here we present two approaches to treat such nonadiabatic dynamics. In the weak molecule-metal interaction regime, we propose a surface-hopping scheme, where nuclei evolve on diabatic potential energy surfaces with stochastic hopping between them. We demonstrate that such a surface-hopping scheme gives correct detailed balance and recovers Marcus electron transfer rate at molecule-metal interfaces. In the strong molecule-metal interaction regime, we derive a Langevin equation, where classical nuclear degrees of freedom evolve on an adiabatic potential energy surface, while experiencing electronic friction and random force from electronic response. Our form of electronic friction is completely general, but does reduce to previously published expressions without electron-electron interaction. When electron-electron correlations are included, we show electronic friction exhibits Kondo resonance, whereas a mean-field treatment is completely inadequate.
**1:27PM F60.00005: A molecular perspective on the structure and thermodynamics of ice interfaces in atmospherically relevant systems**  
ARPA HUDAIT (Presenter), University of Utah — The processes at the surface of ice modulate crystal growth, adsorption of solutes and atmospherically relevant chemical reactions. These processes are not well characterized, in part, due to lack of spatial and temporal resolution of the existing experimental techniques. Despite decades of investigation, how ice interface modulate the structure of ice grown in atmospheric conditions is yet to be elucidated. In this presentation I will discuss my work using molecular simulations and theory to elucidate the role of thermodynamics of ice interfaces in modulating the structure of atmospheric ices, and the behavior of solutes at the ice interface.

References
3. Hudait et al. Sink or Swim: Ions and Organics at the Ice–Air Interface. JACS 2017, 139 (29), 10095-10103.

*This work was supported by the National Science Foundation through Award CHE-1305427 “Center for Aerosol Impacts on Climate and the Environment”.

**1:51PM F60.00006: Cavity-Enhanced Ultrafast Spectroscopy**  
[Invited] YUNING CHEN (Presenter), Chemistry, Stony Brook University, MYLES C SILFIES, THOMAS ALLISON, Physics, Stony Brook University — Using the general pump-probe concept, there are various spectroscopy techniques, such as transient absorption spectroscopy and 2D spectroscopy, for studying ultrafast dynamics. These methods are typically restricted to optically thick samples, such as solids and liquid solutions. In these systems, the dynamics often have broad spectral features due to the collisions between the sample molecules and the solvent molecules.

In a molecular beam, the molecules are cold and isolated from the disturbance of solvent molecules. Measurements taken in these gas-phase molecules can be more directly compared to theoretical predictions. Using frequency comb lasers and optical cavities, we have developed an all-optical technique, Cavity-Enhanced Ultrafast Spectroscopy, to study dynamics in molecular beams with femtosecond temporal resolution. The narrow-linewidth frequency comb laser is coupled into two optical cavities that overlap at the focus. The sample molecules under study are introduced to the overlap by a molecular beam with a noble gas carrier. We have carried out a series of transient absorption measurements in I₂ and I₂-Ar clusters in a molecular beam and have demonstrated ultrafast transient absorption measurements with a detection limit of ΔOD = 2×10⁻¹⁰(1×10⁻⁹/√Hz). Such a high sensitivity enables one to take all-optical ultrafast spectroscopy measurements in samples with column densities less than 10¹⁰ molecules/cm² and overall, this represents a nearly 4 orders of magnitude improvement over the previous state of the art. In this talk, I will discuss the technical details of this spectrometer and the experiment in I₂. I will also present a widely tunable version of this spectrometer operating at probe wavelengths between 450 and 700 nm using only one set of dispersion-managed cavity mirrors.

*Funding: National Science Foundation 1708743

**Tuesday, March 5, 2019 11:15 AM - 2:15 PM**

**Session F61 GSOFT DBIO GSNP: Active Matter III**  
BCEC 258B - Karsten Kruse, Max Planck Institute for Chemical Physics of Solids - Tag(s): Focus

**11:15AM F61.00001: Self-Organizing Microtubule Spindles**  
[Invited] JENNIFER ROSS (Presenter), University of Massachusetts Amherst — The cell is a complex autonomous machine taking in information, performing computations, and responding to the environment. Many of the internal structures and architecture is transient and created through active processes. Recent advances in active matter physics with biological elements are opening new insights into the physics behind how cellular organizations are generated, maintained, and destroyed. I will present several stories about how microtubules can be self-organized into cellular structures using molecular motors (kinesin-1), crosslinking proteins (MAP65), and the inherent microtubule polymerization. These works illustrate the importance of fundamental physics to build the structures inside living cells while informing on new physics we can learn from biological elements and materials.

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Alignment and controlled formation of topological defects in living fibroblast cells by liquid crystals

TARAS TURIV (Presenter), Advanced Materials and Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, JESS KRIEGER, School of Biomedical Sciences, Kent State University, HAO YU, Advanced Materials and Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, IRAKLI CHAGANAVA, Institute of Cybernetics, Georgian Technical University, 0186 Tbilisi, Georgia, QI-HUO WEI, Advanced Materials and Liquid Crystal Institute and Chemical Physics Interdisciplinary Program and Physics Department, Kent State University, MIN-HO KIM, School of Biomedical Sciences, Kent State University, O D LAVRENTOVICH, Advanced Materials and Liquid Crystal Institute and Chemical Physics Interdisciplinary Program and Physics Department, Kent State University — Arrays of living tissue-forming cells behave as orientationally ordered active nematics and create topological defects of strength +1/2 and -1/2. These defects play an important role in compressive-dilative stresses in tissues and facilitate effects such as apoptosis and cell migration. The challenge is to design orientational patterns of cells with predetermined spatial locations of topological defects in them. We propose an approach to control the alignment of human dermal fibroblast (HDF) cells by substrates with photoaligned liquid crystal polymers (LCPs). With a plasmonic metamask alignment method, we patterned the director orientation of the LCPs with topological defects of integer (+1, -1) and semi-integer (+1/2, -1/2) strength. Combination of polarized, phase contrast and fluorescent microscopies proves that the HDF cells align along the patterned director of the LCP substrate. The patterns cause a modulation of cell density, as the cells accumulate near the cores of the defects with positive topological charge. The approach could be used to control the locations of defect formation in tissues of living cells and potentially control the extrusion of undesirable cells.

The work is supported by NSF DMREF grant DMS-1729509 and by Office of Sciences, DOE, grant DE-SC0019105.

Bioenergetics of cell jamming

STEPHEN J DECAMP (Presenter), NICOLAS CHIU OGASSAVARA, JENNIFER MITCHEL, JEFFREY FREDBERG, Harvard University — Cellular jamming is a ubiquitous phenomenon in epithelial biology that has been shown to govern processes ranging from development in the drosophila gastrulation and zebrafish embryo vertebrate axis elongation, to disease pathophysiology including carcinoma metastasis and asthmatic airway remodeling. A jammed epithelial monolayer remains quiescent and solid-like, whereas unjamming of the monolayer leads to a solid-to-fluid transition in which the cellular collective gains a migratory phenotype, elongated cell shapes, and accompanying mechanical softening. Although jamming has been demonstrated to play a fundamental role in the dynamics of confluent epithelial tissues, the metabolic requirements that fuel the jamming transition and its associated far-from-equilibrium cellular mechanics remain unexplored. Here we measure the metabolic state of individual cells within a confluent monolayer using the cytosolic redox ratio (NAD+/NADH), a reporter of overall cellular bioenergetic potential. Surprisingly, we find that jammed cells near a PDMS barrier have a significantly increased metabolic demand. After barrier removal, and subsequent unjamming, the redox potential of cells near the leading edge of an advancing monolayer decreases to a baseline value consistent with the jammed bulk.

Spatial heterogeneity of cilia contributes to directed flow generation

GUILLERMINA RAMIREZ-SAN JUAN (Presenter), Bioengineering, Stanford University, MU HE, Physiology, University of California San Francisco, ARNOLD MATHIJSSEN, Bioengineering, Stanford University, LILY JAN, Physiology, University of California San Francisco, WALLACE MARSHALL, Biophysics and Biochemistry, University of California San Francisco, MANU PRAKASH, Bioengineering, Stanford University — In living organisms arrays of thousands of micrometer-scale motile cilia coordinate over centimeters to transport fluid. Tissues need to accommodate a variety of specialized cell types, thus cilia do not cover surfaces uniformly. However, how the density and localization of cilia impact flow generation is unknown. Here we combine measurements of cilia organization in the mouse airway with a reduced order hydrodynamic model, to study how spatial organization of cilia integrates across scales to produce long-range flows. Our measurements show that ciliated cells are uniformly distributed but occupy only a fraction of the total surface of the tissue. Furthermore, we measure basal body alignment and tissue-scale cilia orientation (from nm to cm) and find large variations in the local and global orientation of cilia. Despite this spatial heterogeneity, flow measurements show that ciliated cells produce large-scale directed steady flows. Using our model we explore the robustness of the flow to changes in density and orientation of cilia. We find that a fractional coverage of the area by ciliated cells allows the flow to be robust to changes in cilia orientation. Altogether our results highlight the importance of collective cilia properties for flow generation by cilia arrays.
12:27PM F61.00005: Cellular herding: learning from swarming dynamics to experimentally control collective cell migration  DANIEL COHEN (Presenter), Princeton University — Multicellular life is driven by collective cell migration spanning morphogenesis, growth, wound healing, and even cancer invasion. Our lab works to interactively manipulate collective cell migration in living tissues, akin to how a shepherd herds sheep. Our first approach relies on ‘Outside-In’ perturbations to direct epithelial collective migration in real-time by exposing cells to programmable electric fields (electrotaxis). Crucially, we have shown that collective migration patterns within a tissue will track even complex 2D field commands (e.g. diverging fields)—a fact that we are exploiting to interactively ‘sculpt’ living tissues via collective migration control. In parallel, we have developed an ‘Inside-Out’ swarm control approach based on introducing ‘cellular mimics’—3D microstructures mimicking the geometry and cadherin presentation of native cell-cell junctions—to tissues in order to recapitulate cell-cell recognition and adhesion between a living tissue and a cellular mimic. By linking into the endogenous coupling network (cell-cell adhesion), these cellular mimics are allowing us to manipulate and program collective cell migration from within a tissue. Together, our swarm control approaches offer new tools to interactively control the behavior of living tissues.

*This research was sponsored by the Army Research Laboratory and accomplished under grant no. W911NF-16-1-0185. The views and conclusions in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Army Research Laboratory or the U.S. government. K.v.d.V. acknowledges support from an Early Postdoc.Mobility fellowship from the Swiss National Science Foundation, and M.S. acknowledges support from the Deutsche Forschungsgemeinschaft under grant no. 396632606.

12:39PM F61.00006: Collective mechanical properties of insect swarms† KASPER VAN DER VAART (Presenter), MICHAEL SINHUBER, NICHOLAS QUELETTE, Stanford University — Social animals routinely form groups, which are thought to display emergent, collective behavior. This suggests that animal groups should have properties at the group scale that are not directly linked to the individuals, much as bulk materials have properties distinct from those of their constituent atoms. We show that laboratory insect swarms possess emergent mechanical properties, displaying a collective viscoelastic response to applied oscillatory visual stimuli. We find that the swarms strongly damp perturbations. Thus, unlike bird flocks, which appear to use collective behavior to promote lossless information flow through the group, our results suggest that insect swarms use it to stabilize themselves against environmental perturbations.

†This research was jointly funded by the Federal Ministry of Education and Research of Germany and the Max Planck Society.

12:51PM F61.00007: Adhesion Strategies of Chlamydomonas in Heterogeneous Habitats  CHRISTIAN TITUS KREIS, ALEXANDROS FRAGKOPOULOS, MARINE LE BLAY, CHRISTINE LINNE, ALICE GRANGIER, MARCIN M MAKOWSKI, OLIVER BAEUMCHEN (Presenter), Max Planck Institute for Dynamics and Self-organization (MPIDS), Göttingen, Germany — In contrast to marine phytoplankton, many photoactive microbes live in complex environments, such as liquid-infused soil and moist rocks, where they encounter and colonize a plethora of surfaces. We discovered that the adhesion of Chlamydomonas to surfaces can be reversibly switched on and off by light [1]. Our in vivo single-cell micropipette force spectroscopy experiments suggest that light-switchable adhesiveness is a natural functionality to actively regulate the transition between freely-swimming (planktonic) and surface-associated state, which yields an adhesive adaptation to optimize the photosynthetic efficiency of the cells in variable and inhomogeneous light conditions. Probing the adhesion forces on model substrates with tailored properties and dissecting the contributions from different intermolecular interactions reveal a universal protein-mediated adhesion mechanism that allows the cells to effectively colonize any type of abiotic surface in their heterogeneous natural habitats. Complementary to our single-cell force measurements, we characterize the surface colonization by cell adsorption assays from which we extract population level morphological and dynamical characteristics.


1:03PM F61.00008: Out-of-plane beating components of active axonemes isolated from Chlamydomonas reinhardtii‡ AZAM GHOLAMI (Presenter), Max-Planck Institute for Dynamics and Self-organization, Göttingen, Germany, SOHEIL MOJIRI, Göttingen University, ALBERT JOHANN BAE, Department of Biomedical Engineering, University of Rochester, JÖRG ENDERLEIN, Göttingen University, EBERHARD BODENSCHATZ, Max-Planck Institute for Dynamics and Self-organization, Göttingen, Germany — Cilia and flagella are ubiquitous in the living world. They are essential for micro-scale driven transport of fluids or cells by cilia/flagellar beating. Their slender bodies are composed of a microtubule/molecular motor structure that when taken independently are called an axoneme. Axonemes move by bending waves that emerge from the interplay between internal stresses generated by dynein motor proteins. Here we use the novel multi-plane phase contrast imaging technique to record the three dimensional beating pattern of isolated axonemes from Chlamydomonas reinhardtii that beat in the vicinity of a substrate. We measure the torsion of the axoneme along the contour length with high spatiotemporal resolution. High precision information on out-of-plane beating component of axonemes allows us to check the validity of the resistive-force theory.

‡We acknowledge MaxSyBio consorsium, which is jointly funded by the Federal Ministry of Education and Research of Germany and the Max Planck Society.
OLGA SHISHKOV (Presenter), MICHAEL MACALINO, DAVID L HU, Georgia Institute of Technology — Black soldier fly larvae are a non-pest insect under consideration as a method of recycling food waste to sustainable protein. These larvae live in large groups in rotting food waste, where they experience hydrostatic forces from the dirt they are in and active forces from their bodies colliding. We investigate how larvae react to these forces by compressing larva aggregations and measuring their response. Larvae align in a container as they follow their instinct to dig downwards, and thus increase their packing fraction and elastic modulus. This study will benefit how larvae are raised in industry by ensuring that larvae are comfortable with their environment and level of substrate, do not expend energy on hiding, and eat and grow quickly.

MICHAEL SINHUBER (Presenter), KASPER VAN DER VAART, NICHOLAS OUELLETTE, Stanford University — In the wild, many animal species form aggregations that behave collectively. Unavoidably, these systems are subject to ubiquitous environmental perturbations such as wind, acoustic and visual stimuli. The way these environmental perturbations influence the animals’ collective behavior, however, is poorly understood, in part because conducting controlled quantitative perturbation experiments in the wild is challenging. To circumvent the need for controlling environmental conditions in the field, we study collective swarms of the midge *Chironomus riparius* in a laboratory experiment where we have control over external perturbations. In this talk, we consider the effect of laboratory-generated perturbations like air flow or variable light exposure on the swarming behavior.

We find that not only do individuals in the swarm respond to these perturbations by changing their kinematics, but also the swarm as a whole can respond by changing its global properties such as its volume, attraction of individual midges to its center or its pressure, indicative of a collective reaction.

*This research was sponsored by the ARL under grant no. W911NF-16-1-0185. M.S. was supported by the DFG under grant no. 396632606. K.v.d.V. received support from an Early Postdoc Mobility fellowship from the SNF.

HANGJIAN LING (Presenter), Civil and Environmental Engineering, Stanford University, GUILLAM E MCIVOR, Center for Ecology and Conservation, University of Exeter, KASPER VAN DER VAART, Civil and Environmental Engineering, Stanford University, RICHARD T VAUGHAN, School of Computing Science, Simon Fraser University, ALEX THORNTON, Center for Ecology and Conservation, University of Exeter, NICHOLAS OUELLETTE, Civil and Environmental Engineering, Stanford University — Collective animal motion has long been modeled using self-propelled particles that are assumed to be identical and to follow same interaction rules. In nature, however, group members can be quite different, and such differences may shape the group behavior. Here, we study how social relationships in bird flocks affect the local interactions and group dynamics. We used 3D optical tracking to study flocks of jackdaws (*Corvus monedula*), a highly social corvid species that forms lifelong, monogamous pair bonds. We show that jackdaw flocks contain discrete pairs that are likely to reflect the pair bonds. We find that paired birds interact with fewer neighbors than unpaired birds and use less energy when flying. Pairing thus appears to grant energetic benefits. However, we also find that flocks with more pairs have shorter velocity correlation lengths, in agreement with a generic self-propelled particle model, indicating that social relationships may inhibit efficient information transfer through the group. Our results reveal a critical tension between individual- and group-level benefits during collective behavior in species with differentiated social relationships, and have many evolutionary and cognitive implications.

*Human Frontier Science Program*
Active flow of low density pedestrian crowds

ALESSANDRO CORBETTA (Presenter), Eindhoven University of Technology, CHUNG-MIN LEE, California State University Long Beach, JORIS WILLEMS, Eindhoven University of Technology, ROBERTO BENZI, University of Rome Tor Vergata, FEDERICO TOSCHI, Eindhoven University of Technology — The dynamics of pedestrian crowds share deep connections with the statistical physics of active matter. Pedestrians move following own will and objectives: this amounts in huge variability in the motion, observable even in diluted conditions. Despite such individual unpredictability, ensemble-level universal physical features emerge and encompass common and rare fluctuations of both the solo and the interacting dynamics. Reaching a quantitative understanding of these features is a major scientific challenge with deep societal impact, e.g. in the design of civil infrastructures or of crowd management measures.

We investigate from observational experiments held in real-life settings (stations, festivals, museums) and in diluted conditions statistical features of pedestrian motion. We leverage on datasets including millions of trajectories acquired with and without external influencing stimuli (i.e., crowd control measures, like signage or visual cues), via home-made high-fidelity tracking systems. On this basis, we quantify the PDFs of individual velocity, position, body rotation and mutual-contact-avoidance "social" forces - possibly in dependence on stimuli. We propose an active-Brownian particle model of the dynamics based on Langevin-like equations statistically quantitative.

WITHDRAWN ABSTRACT

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F62 DQI: New Avenues for Quantum Error Correction

Fault-tolerant quantum computation with few qubits [Invited] BEN REICHARDT (Presenter), University of Southern California — Reliable qubits are difficult to engineer, but standard fault-tolerance schemes use seven or more physical qubits to encode each logical qubit, with still more qubits required for error correction. We give space-efficient methods for fault-tolerant error correction and computation.

For example, with the Steane seven-qubit code, we give a scheme that uses three extra qubits, arranged in two dimensions, to fault-tolerantly extract three syndromes in parallel. With a 19-qubit system, we show that one can protect and compute fault tolerantly on seven encoded qubits. The procedures could enable testing more sophisticated protected circuits in small-scale quantum devices.

New prospects for fault-tolerant quantum error correction with biased-noise cat-qubits [Invited] SHRUTI PURI (Presenter), Yale Univ — Exploiting the structure of noise or "noise-bias" in physical qubits could improve the threshold and overhead requirements for fault-tolerant quantum error correction. The challenge however is to be able to maintain the noise bias while performing elementary operations such as a CNOT gate. I will show how this challenge can be overcome by using the so called stabilized cat-qubits in a parametrically driven non-linear oscillators. In such a qubit, the bit-flip errors increase linearly with the size of the cat, while phase-flips are exponentially suppressed with the cat-size. The stabilized cat-qubit, therefore, exhibits a strongly biased-noise channel. In fact, the phase of the drive determines a continuous family of biased noise cat-states. I will discuss how a bias-preserving CNOT gate can be implemented with these cat-qubits by rotating them through the continuous family of the cat-states in the phase space. I will also present a set of other bias-preserving operations that can be performed with the stabilized cat-qubit. These results provide a new direction for designing error correction codes with high thresholds and reduced overheads.
Experimental quantum error correction with binomial bosonic codes

 LSU acknowledges the support from National Key Research and Development Program of China No.2017YFA0304303 and National Natural Science Foundation of China Grant No.11474177. SMG acknowledges grants from ARO W911NF1410011 and NSF DMR-1609326.

Scalable quantum error correction with the bosonic GKP code

We review the bosonic GKP (Gottesman-Kitaev-Preskill) code which encodes a qubit into an oscillator and its possible implementation in a microwave mode in circuit-QED hardware. We discuss how GKP code states can be created from Schroedinger cat states or from a dispersive interaction with a qubit. We propose a scalable architecture which uses a surface code on top of the GKP qubits. For a noise model of Gaussian stochastic displacement errors, we discuss how to decode such toric-GKP code and give estimates for the threshold standard deviation, corresponding to a low (4 or more) number of average photons in the GKP code states.

Encoding and controlling a GKP logical qubit in a trapped-ion oscillator

We describe trapped-ion experiments in which we encode a logical qubit using the motion of a single trapped ion. One powerful code of this type is constructed from a set of logical and error-check operators which are displacements in the oscillator phase space [1,2]. We create, measure and manipulate logical information stored in such a code, including teleportation of non-Clifford rotations onto the code space [3]. Alongside the direct focus on quantum computation, the techniques developed for this work also provide new perspectives for quantum control and measurement.

We acknowledge support for this research from the Swiss National Fund, the NCCR QSIT, ETH Zürich, and IARPA.
11:15AM F63.00001: Observing the interplay between bacterial behaviors and the physical landscape inside the zebrafish gut* [Invited] RAGHUVEER PARTHASARATHY (Presenter), University of Oregon — In any ecosystem, the structure of the landscape and the activities of its organisms influence one another. This is true in the vertebrate gut as well, where vast numbers of microbes cooperate, compete, and influence both normal and disease-related functions of their hosts. In gut ecosystems, however, we know little about spatial structure, bacterial behaviors, and physical forces. Most of our knowledge comes from sequencing-based studies lacking spatial or temporal information, severely limiting our ability to understand, let alone manipulate, the gut microbiome. To address this, my lab applies light sheet fluorescence microscopy to a model system that combines an in vivo environment with a high degree of experimental control: larval zebrafish with defined sets of bacterial species. I will describe this approach and experiments that have revealed how a species can manipulate intestinal mechanics to facilitate invasion; how differences in bacterial behaviors across species correlate with differences in spatial distributions; and how genetic switches and antibiotics can reveal the roles of individual behaviors such as motility in governing community outcomes. In all of these cases, the physical structure of the microbiome emerges as a major determinant of its population dynamics.

*This research was supported by the National Science Foundation under Award 1427957, and the National Institutes of Health under Awards P50GM09891, P01 GM125576-01, F32AI112094, and T32GM007759. Work was also supported by an award from the Kavli Microbiome Ideas Challenge, a project led by the American Society for Microbiology in partnership with the American Chemical Society and the American Physical Society and supported by The Kavli Foundation.

11:51AM F63.00002: Growth strategy of microbes on mixed carbon sources XIN WANG (Presenter), Harvard Medical School, KANG XIA, XIAQJING YANG, CHAO TANG, Center for Quantitative Biology, School of Physics and Peking-Tsinghua Center for Life Sciences, Peking University — A classic problem in microbiology is that bacteria display two types of growth behavior when cultured on a mixture of two carbon sources: in certain mixtures the bacteria consume the two carbon sources sequentially (diauxie) and in other mixtures the bacteria consume both sources simultaneously (co-utilization). The search for the molecular mechanism of diauxie led to the discovery of the lac operon and gene regulation in general. However, questions remain as why microbes would bother to have different strategies of taking up nutrients and in the case of co-utilization what determines the partition and distribution of carbon sources in the cell. Here we show that diauxie versus co-utilization can be understood from the topological features of the metabolic network. A model of optimal allocation of protein resources quantitatively explains why and how the cell makes the choice when facing multiple carbon sources. When two carbon sources are being co-utilized, the model predicts the percentage of each carbon source in supplying the synthesis of every type of amino acid, which is quantitatively verified by experiments. Our work solves a long-standing puzzle and provides a quantitative framework for the carbon source utilization of microbes.

12:03PM F63.00003: A quorum sensing-controlled program of aggregation in V. cholerae* MATTHEW JEMIELITA (Presenter), NED WINGREEN, BONNIE BASSLER, Princeton University — Bacteria communicate and collectively regulate gene expression using the process called quorum sensing (QS). QS relies on population-wide responses to extracellular signal molecules called autoinducers. We demonstrate that, in Vibrio cholerae, QS activates a novel program of multicellularity, which we call aggregation. Aggregation is distinct from the canonical surface-biofilm formation program, which QS represses. Specifically, aggregation is induced by autoinducers, rapidly occurs in cell suspensions, and does not require cell-division, features distinct from those characteristic of V. cholerae biofilm formation. A genetic screen identifies components required for aggregation, revealing proteins involved in V. cholerae intestinal colonization, stress response, as well as a protein that distinguishes the current V. cholerae pandemic strain from earlier pandemic strains. We propose that aggregate formation is important for V. cholerae to transit between the marine niche and the human host. Further exploration of the aggregation process may yield insight into principles that allow bacteria to rapidly build multicellular communities and collectively defend against environmental insults or withstand starvation.

*Funded by the HHMI, NIH, NSF, and the Alexander von Humboldt Foundation.
12:15PM F63.00004: Verticalization of bacterial biofilms* FARZAN BEROZ (Presenter), Physics, University of Michigan, Ann Arbor, JING YAN, BENEDIKT SABASS, Princeton University, YIGAL MEIR, Ben-Gurion University of the Negev, HOWARD A STONE, BONNIE BASSSLER, NED WINGREEN, Princeton University — Biofilms are communities of bacteria adhered to surfaces. Recently, biofilms of rod-shaped bacteria were observed at single-cell resolution and shown to develop from a disordered, two-dimensional layer of founder cells into a three-dimensional structure with a vertically-aligned core. In this talk, I will discuss how verticalization is driven by a series of localized mechanical instabilities on the cellular scale. For short cells, these instabilities are primarily triggered by cell division, whereas long cells are more likely to be peeled off the surface by nearby vertical cells, creating an "inverse domino effect". The interplay between cell growth and cell verticalization gives rise to an exotic mechanical state in which the effective surface pressure becomes constant throughout the growing core of the biofilm surface layer. This dynamical isobaricity determines the expansion speed of a biofilm cluster and thereby governs how cells access the third dimension. In particular, theory predicts that a longer average cell length yields more rapidly expanding, flatter biofilms. We experimentally show that such changes in biofilm development occur by exploiting chemicals that modulate cell length.

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12:27PM F63.00005: Light dependent motility of microalgae induces pattern formation in confinement ALEXANDROS FRAGKOPOULOS (Presenter), JOHANNES FREY, FLORA-MAUD LE MENN, JEREMY VACHIER, Dynamics of Complex Fluids, Max Planck Institute for Dynamics and Self-Organization, MARCO G. MAZZA, Department of Mathematical Science, Loughborough University, OLIVER BAEUMCHEN, Dynamics of Complex Fluids, Max Planck Institute for Dynamics and Self-Organization — A collection of self-propelled particles can undergo complex dynamics due to hydrodynamic and steric interactions. In highly concentrated suspensions, it is possible for such particles to form large-scale concentration patterns, where the active suspension separates into regions of high and low particle concentrations. Here we present that suspensions of Chlamydomonas reinhardtii cells, a unicellular soil-dwelling microalgae and a model organism of puller-type microswimmers, may form patterns of high and low cell density regions in confinement under specific light conditions. We find that there are significant deviations in the motility of the cells under different light intensities and cell densities, which regulate patron formation in such active suspensions. Finally, by performing active Brownian simulations of such active particles with the observed motility characteristics, we show that we can re-create the pattern observed in our experiments.

12:39PM F63.00006: The universal dynamics of the human microbiome AMIR BASHAN (Presenter), Bar-Ilan University, TRAVIS GIBSON, HMS, JONATHAN FRIEDMAN, Hebrew University, VINCENT CAREY, SCOTT WEISS, HMS, ELIZABETH HOHMANN, MGH, YANG-YU LIU, HMS — In this talk I will address a simple but fundamental question: are the microbial ecosystems in different people governed by the same host-independent (i.e. "universal") ecological dynamics? Answering this question determines the feasibility of general therapies and control strategies for the human microbiome. I will introduce our novel methodology that distinguishes between two scenarios: host-independent and host-specific underlying dynamics. This methodology has been applied to study different body sites across healthy subjects. We also analyzed the gut microbial dynamics of subjects with recurrent Clostridium difficile infection and the same set of subjects after fecal microbiota transplantation. The results can fundamentally improve our understanding of forces and processes shaping human microbial ecosystems, paving the way to design general microbiome-based therapies.

12:51PM F63.00007: Deciphering Functional Redundancy in the Human Microbiome LIANG TIAN (Presenter), Department of Physics, Hong Kong Baptist University, XUWEN WANG, ANGKUN WU, YUHANG FAN, Channing Division of Network Medicine, Brigham and Women's Hospital and Harvard Medical School, JONATHAN FRIEDMAN, Department of Plant Pathology and Microbiology, Faculty of Agriculture, Food and Environment, The Hebrew University of Jerusalem, AMBER DAHLIN, Channing Division of Network Medicine, Brigham and Women's Hospital and Harvard Medical School, MATTHEW WALDOR, Division of Infectious Diseases, Brigham and Women's Hospital and Harvard Medical School, GEORGE WEINSTOCK, The Jackson Laboratory for Genomic Medicine, SCOTT WEISS, YANG-YU LIU, Channing Division of Network Medicine, Brigham and Women's Hospital and Harvard Medical School — Although the taxonomic composition of the human microbiome varies tremendously across individuals, its gene composition or functional capacity is highly conserved. The striking conservation of functional capacity implies an ecological property known as functional redundancy. Although this redundancy is thought to underlie the stability and resilience of the human microbiome, its origin is elusive. Here, we decipher the basis for functional redundancy in the human microbiome by analyzing its genomic content network --- a bipartite graph that links microbes to the genes in their genomes. We show that this network exhibits special topological features that favor high functional redundancy. Moreover, we find that the assemblage of microbes plays a more important role than their abundances in determining the high functional redundancy of the human microbiome. We propose a simple genome evolution model to explain the key topological features observed in the real genomic content network. These observations deepen our understanding of species-function relationships, a critical step for developing function-based diagnostics and therapeutics.
1:03PM F63.00008: A numerical model of Vibrio fischeri growth and intraspecific competition* YUEXIA LIN (Presenter), Paulson School of Engineering and Applied Sciences, Harvard University, STEPHANIE NICOLE SMITH, ALECIA SEPTER, Marine Sciences, The University of North Carolina at Chapel Hill, CHRISTOPHER RYCROFT, Paulson School of Engineering and Applied Sciences, Harvard University, EVA KANSO, Aerospace and Mechanical Engineering, University of Southern California — E. scolopes squid are colonized with V. fischeri bacteria, and this symbiosis serves as a model system for studying host-microbe interactions. Wild-caught adult squids harbor multiple strains of V. fischeri that engage in intraspecific competition during initial host colonization. However, little is known about how competing strains interact at the single-cell level to influence their spatial structure as they coexist. When grown on agar surfaces, two competing strains form segregated spatial patterns that is dependent on their ability to kill one another. We developed an experimentally informed, multi-agent numerical model of cell growth, division, and death in 2D that can simulate intercellular interactions and environmental factors. In particular, the model accounts for intraspecific competition via mutual killing and differences in growth. This computational model is used to explore conditions that allow a diversity of strains to coexist, as well as investigate the spatiotemporal properties of this coexistence. We present results that demonstrate the method's ability to capture the segregated patterns and their length scales, and explore parameter space that is hard to access in experiments.

*Y. L. is supported by DOE CSGF.
E. K. acknowledges NSF INSPIRE grant 1608744.

1:15PM F63.00009: Machine learning the space-time phase diagram of bacterial swarm expansion* HANNAH JECKEL (Presenter), ERIC JELLI, RAIMO HARTMANN, PRAVEEN SINGH, Max Planck Institute for Terrestrial Microbiology, RACHEL MOK, Department of Applied Mathematics, Massachusetts Institute of Technology, JAN FREDERIK TOTZ, Department of Theoretical Physics, Technische Universität Berlin, LUCIA VIDAKOVIC, Max Planck Institute for Terrestrial Microbiology, BRUNO ECKHARDT, Department of Physics, Philips-University Marburg, JORN DUNKEL, Department of Applied Mathematics, Massachusetts Institute of Technology, KNUT DRESCHER, Max Planck Institute for Terrestrial Microbiology — Coordinated dynamics of individual components in active matter are an essential aspect of life. Establishing a comprehensive, causal connection between intercellular and macroscopic behaviors has remained a major challenge due to limitations in data acquisition and analysis techniques suitable for multi-scale dynamics. Here, we combine a high-throughput adaptive microscopy approach with machine learning, to identify key biological and physical mechanisms that determine distinct microscopic and macroscopic collective behavior phases which develop as Bacillus subtilis swarms expand over five orders of magnitude in space. Our experiments and particle-based simulations reveal that the microscopic swarming motility phases are dominated by physical cell-cell interactions. These results provide a unified understanding of bacterial multi-scale behavioral complexity in swarms.

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1:27PM F63.00010: Switching and Torque Generation in Swarming Bacteria* KATIE FORD, JYOT ANTANI (Presenter), ARAVINDH NAGARAJAN, Texas A&M University, MADELINE JOHNSON, Chemical and Biomolecular Engineering, Vanderbilt University, PUSHKAR LELE, Texas A&M University — Escherichia coli swarm on semi-solid surfaces with the aid of flagella. It has been hypothesized that swarmer cells overcome the increased viscous drag near surfaces by developing higher flagellar thrust and by promoting surface wetness with the aid of a flagellar switch. The switch enables reversals between clockwise (CW) and counterclockwise (CCW) directions of rotation of the flagellar motor. Here, we measured the behavior of flagellar motors in swarmer cells. Results indicated that although the torque was similar to that in planktonic cells, the tendency to rotate CCW was higher in swarmer cells, surprisingly. Consistent with earlier reports, moisture added to the swarm surface restored swimming in a CCW-only mutant, but not in a FliG mutant that rotated motors CW-only (FliGCW). Fluorescence assays revealed that FliG<sub>CW</sub> cells grown on agar surfaces carried fewer flagella than planktonic FliG<sub>CW</sub> cells. The surface-dependent reduction in flagella correlated with a reduction in the number of putative flagellar preassemblies. These results suggest that the conformational dynamics of switch proteins play a role in the proper assembly of flagellar complexes and flagellar export, thereby aiding bacterial swimming.

*R01GM123085
1:39PM F63.00011: Geometric control of bacterial surface accumulation\*  RACHEL MOK (Presenter), JORN DUNKEL, Massachusetts Institute of Technology, VASILY KANTSLER, University of Warwick — Controlling and suppressing bacterial accumulation at solid surfaces is essential for preventing biofilm formation and biofouling. Whereas various chemical surface treatments are known to reduce cell accumulation and attachment, the role of complex surface geometries remains less well understood. Here, we report experiments and simulations that explore the effects of locally varying boundary curvature on the scattering and accumulation dynamics of swimming Escherichia coli bacteria in quasi-two-dimensional microfluidic channels. Our experimental and numerical results show that a non-convex periodic boundary geometry can decrease the average cell concentration at the boundary by more than 50% relative to a flat surface.

\*MIT OGE Chyn Duog Shiah Memorial Fellowship (R.M.), James S. McDonnell Complex Systems Scholar grant (J.D.), Royal Society Research Grant RG150072 (V.K.)

1:51PM F63.00012: Atomistic modeling of molecule-lipid interactions to understand small-molecule induced outer membrane vesicle biogenesis in Gram-negative bacteria  AO LI (Presenter), JEFFREY W SCHERTZER, XIN YONG, Binghamton University — With the role of packing biochemical cargos, outer membrane vesicles (OMVs) of Gram-negative bacteria have great importance in many disease-related processes. Recent studies have shown a strong link between a self-produced small molecule, Pseudomonas Quinolone Signal (PQS), and OMV biogenesis in Pseudomonas aeruginosa. We conducted all-atom molecular dynamics simulations to elucidate the interactions between PQS and a model outer membrane. We discovered two characteristic states of PQS, namely attachment on the membrane surface and insertion into the Lipid A leaflet. The time-resolved position of PQS and the angle between its heterocyclic ring and alkyl side chain reveal a four-staged dynamical process: flotation, attachment, folding, and insertion. Remarkably, PQS bends its hydrophobic chain into a closed conformation to lower the energy barrier for penetration through the hydrophilic Lipid A head-group zone, which was confirmed by the potential of mean force (PMF) measurements. Simulation with multiple PQS exhibit significant aggregation of these amphiphilic molecules in the surrounding aqueous phase. Yet, both attached and inserted states were simultaneously observed even in the presence of PQS aggregation. These findings provide critical insight into OMV biogenesis.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F64 DBIO GSOFT: Physics of the Cytoskeleton Across Scales II  BCEC 259B - Loren Hough -

11:15AM F64.00001: Physical Guidance of Cytoskeletal Dynamics* [Invited]  WOLFGANG LOSERT (Presenter), University of Maryland, College Park — The guided migration of cells is a complex dynamical process involving carefully regulated polymerization and depolymerization of the elements of the cellular scaffolding, in particular actin. Recent work has shown that polymerizing and depolymerizing actin can be described as an excitable system which exhibits natural waves or oscillations on scales of hundreds of nm, and that wave-like dynamics can be seen in a wide range of natural contexts. I will show that surface nanotopography on scales observed in vivo nucleates and guides the wave-like dynamics of actin polymerization, and that such guided actin waves control cell migration for a broad range of cell types. Furthermore controlled actin waves provide a simple framework to understand seemingly complex aspects of cell migration including the response to chemical and electrical guidance cues, and the ability of cells to follow each other precisely in streams. Thus the excitable systems character of the cellular scaffolding provides a simple, universal framework for analyzing guided migration in living systems.

*Supported by the Air Force Office of Scientific Research grant FA9550-16-1-0052

11:51AM F64.00002: Fluctuation-driven contractility without motors*  SIHAN CHEN (Presenter), TOMER MARKOVICH, FREDERICK MACKINTOSH, Rice University — Contractility in cells is usually due to molecular motor activity, such as in the case of the contractile ring, in which actin and myosin generate during cytokinesis. Recent experiments, however, have suggested non-motor-based contraction in some cells. Here, we present a model for contraction based on stochastic binding of actin filaments that are known to have an asymmetric force response. This leads to continuous net contraction via a Brownian ratchet-like mechanism, provided that the crosslinking is active and violates detailed balance. Using this model, we calculate the force-velocity relation and find a stall force for the system, which could be used to test this model.

*This work was supported in part by the National Science Foundation (Grants DMR-1826623 and PHY-1427654).
12:03PM F64.00003: Regulation of Pulsed Contraction of Actomyosin Networks  JING LI (Presenter), QILIN YU, Purdue University, MICHAEL MURRELL, Yale University, TAEOYON KIM, Purdue University — Actomyosin contractility regulates various biological processes including cell migration and cytokinesis. Cell cortex underlying a membrane, which is a representative actomyosin network in eukaryote cells, exhibits dynamic contractile behaviors. Interestingly, the cell cortex shows reversible aggregation of actin and myosin called pulsed contraction in diverse cellular phenomena. While contractile behaviors of actomyosin machinery have been studied extensively in several in vitro and computational studies, none of them successfully reproduced pulsed contraction observed in vivo. In this study, we first reproduced the pulsed contraction only with the mechanical and dynamic behaviors of cytoskeletal components. We found that clusters with physiologically relevant size and duration can appear in the presence of both F-actin turnover and angle-dependent F-actin severing resulting from buckling induced by motor activities. In addition, we showed that RhoA signaling regulating the dynamics of F-actin and myosin can enhance the stability and durability of pulsed clusters. Our study sheds light on the underestimated significance of F-actin dynamics for the pulsed contraction and on the cooperative mechanism between mechanical and biochemical factors.

12:15PM F64.00004: Regulation of Motions of Myosin Motors in the Actin Cortex  WONYEONG JUNG (Presenter), Purdue University, ALI TABEI, University of Northern Iowa, TAEOYON KIM, Purdue University — Active transport driven by molecular motors in the cytoskeleton plays an important role in various cellular processes. It has been hypothesized that motions of myosin motors in the cortex are determined by the architecture of the cortex. However, the effects of dynamic, force-dependent behaviors of cytoskeletal components on myosin motors remain elusive despite their potential importance. In this study, we employed an agent-based computational model to study motions of myosin in the cell cortex. The model accounts for possible governing factors, including force-dependent walking of motors and the turnover of cross-linkers and F-actin. We found that motions of motors can be suppressed due to three reasons. Motors can slow down significantly either by local force generation or global force transmission between motors. It is also possible F-actin aggregation prevents motors from consistently walking. However, F-actin turnover can recover motor motility in all three cases by inducing force relaxation on motors and cross-linkers. Our results shed light on how myosin motions are regulated by many factors in vivo.

12:27PM F64.00005: Dynamics of focal adhesion orientation in response to time varying stretch  RUMI DE (Presenter), Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India — Mechanical forces play a central role in determining cell function and fate. The effect of time varying stretch is particularly striking which affects many cellular processes such as adhesion, orientation, migration, wound healing to name a few. Focal adhesions act as mechanosensors and in turn regulate the response of cells in tissues. It is not yet well understood how the stretch induces cytoskeletal organization, or how it affects the assembly of focal adhesions. We present a simple theoretical model based on a novel approach in the understanding of stretch sensitive bond association and dissociation processes together with the elasticity of the cell-substrate system to predict the growth, stability and the orientation of focal adhesions in the presence of static as well as cyclic stretches. Our model agrees well with several experimental observations; most importantly, it explains the puzzling observations of parallel orientation of focal adhesions under static stretch and nearly perpendicular orientation in response to fast varying cyclic stretch. Moreover, it also elucidates the existence of threshold frequency and stretch magnitude for orientational response that have been found to vary across cell types.

12:39PM F64.00006: Mechanism of Generating Pulling Force via Actin Polymerization*  FOWAD MOTAHARI (Presenter), ANDERS CARLSSON, Department of Physics and Center for Engineering Mechanobiology, Washington University in St. Louis — Actin polymerization is the primary mechanism for overcoming the large turgor pressure that opposes endocytosis in yeast. Actin-based pulling forces are less well understood than pushing forces. We stochastically simulate a system of 144 semiflexible actin filaments in a square network, treating all subunits explicitly. Each filament interacts with the membrane via a potential having both attractive and repulsive components. The protein Sla2, which binds actin filaments to the membrane, is assumed to slow the growth of the filaments near the array center by having a strongly attractive potential. The (de)polymerization rates depend on the filament-membrane gap. We include both actin network elasticity and filament-tip bending. We find that the outer filaments push on the membrane, while the inner filaments pull on it. We calculate the force distribution for various model parameters, including the potential depths, the free filament on- and off-rates, the numbers of fast- and slow-growing filaments, and the network rigidity. Under the most favorable conditions, the total pulling force is the sum of the stall forces of all the pushing filaments.

*Supported by NIGMS R01 GM107667 to AEC and NSF CMMI:15-458571 to AEC.
The role of the actin filament brancher Arp2/3 in the dynamics and structures of actomyosin networks

JAMES LIMAN (Presenter), Bioengineering, Rice University, CARLOS A. BUENO, Systems, Synthetic, and Physical Biology, Rice University, YOSSI ELIAZ, Department of Physics, University of Houston, PETER WOLYNES, HERBERT LEVINE, MARGARET CHEUNG, Center for Theoretical Biological Physics, Rice University — Actomyosin network contractility underlies the motility and division of a cell, involving contraction and expansion that are driven by active protein motors and actin treadmilling. In this work, we present novel computational and theoretical approaches to model contractility and growth in actomyosin networks and evaluate the spatiotemporal patterns of actin reorganization. We consider two different actomyosin network morphologies, unbranched and branched. For the unbranched case, the system includes motor proteins (non-muscle myosin IIA (NMIIA)) and cross-linker proteins (α-actinin). For the branched case, the system includes a third component—Arp2/3 complexes—that allows us to investigate the role of branching in actomyosin contractility. We observe that linkers modulate contraction in the unbranched and the branched actomyosin networks. The branched actomyosin networks relax more slowly than their unbranched counterparts. However, the branched networks show pronounced convulsive contractions. We expect our results to give an insight into the importance of the branched morphological formation in enhancing contractility of the actomyosin networks.

Actin Dynamics Measured and Characterized by Optical Flow

LEONARD CAMPANELLO (Presenter), RACHEL LEE, MATT J. HOURWITZ, JOHN T FOURKAS, WOLFGANG LOSERT, University of Maryland, College Park — Actin dynamics are an important component of critical functions such as cell migration and immune response. Specifically, waves of actin are present in a wide range of conditions such as cell-cell adhesion formation and immune cell activation. We utilize periodic surface topographies comparable in size to in vivo collagen fiber networks to generate actin dynamics consistent with what would be observed in real cell microenvironments. We show that, when in contact with such textured surfaces, many cell types exhibit esotaxis — guidance of the actin waves by the surface texture. The one-dimensional waves of actin are very reproducible, which allows us to quantify these actin dynamics in cell types with dissimilar migratory modes and physiological purposes — slowly migrating epithelial MCF10A cells and fast migrating neutrophil-like HL60 cells. Using a computer vision algorithm called Optical Flow, we designed and employed an automated analysis program to characterize the pixel scale guidance of actin waves, as well as their mesoscale characteristics.

Epithelial Wound Healing Coordinates Distinct Actin Network Architectures to Conserve Mechanical Work and Balance Power

ALAN TABATABAI, VISAR AJETI, ANDREW FLESZAR, Yale Univ, MICHAEL F STADDON, Physics, University College London, DANIEL S. SEARA, Yale Univ, CHRISTIAN SUAREZ, Molecular Genetics and Cell Biology, University of Chicago, MUHAMMAD YOUSAFZAI, Yale Univ, DAPENG BI, Physics, Northeastern University, DAVE KOVAR, Molecular Genetics and Cell Biology, University of Chicago, SHILADITYA BANERJEE, Physics, University College London, MICHAEL MURRELL (Presenter), Yale Univ — How cells with diverse morphologies and cytoskeletal architectures modulate their mechanical behaviors to drive robust collective motion within tissues is poorly understood. During wound repair within epithelial monolayers in vitro, cells coordinate the assembly of branched and bundled actin networks to regulate the total mechanical work produced by collective cell motion. Using traction force microscopy, we show that the balance of actin network architectures optimizes the wound closure rate and the magnitude of the mechanical work. These values are constrained by the effective power exerted by the monolayer, which is conserved and independent of actin architectures. Using a cell-based physical model, we show that the rate at which mechanical work is done by the monolayer is limited by the transformation between actin network architectures and differential regulation of cell-substrate friction. These results and our proposed mechanisms provide a robust quantitative model for how cells collectively coordinate their non-equilibrium behaviors to dynamically regulate tissue-scale mechanical output.

We acknowledge funding ARO MURI W911NF-14-1-0403, NSF CMMI-1525316, NIH RO1 GM126256 and NIH U54 CA209992.
Molecular crowding modulates actin filament mechanics and structure* NICHOLAS CASTANEDA, MYEONGSANG LEE, HECTOR RIVERA-JACQUEZ, RYAN MARRACINO, THERESA MERLINO, Nanoscience Technology Center, University of Central Florida, HYERAN KANG (Presenter), Department of Physics, Nanoscience Technology Center, University of Central Florida — The cellular environment is crowded with macromolecules that reduce accessible volume for biomolecule interactions and protein assembly. Actin filament assembly and mechanics play critical roles in many cellular functions including structural support, cell movement, and force generation. Although the effects of molecular crowding on actin assembly have been shown, how crowded environments affect filament conformations and mechanical properties remain unclear. Here, we investigate the effects of molecular crowding on actin filament mechanics and structure both in vitro and in silico. Direct visualization of filaments in the presence of crowders allows for the quantification of filament thermal bending dynamics and mechanics. Biophysical analysis show that molecular crowding enhances filament’s effective bending stiffness and reduces average filament lengths. Utilizing molecular dynamics simulations, we demonstrate that molecular crowding leads to changes in filament conformations and inter-subunit contacts affecting filament mechanics. This work suggests that the interplay between excluded volume effects and non-specific interactions induced by molecular crowding may modulate actin filament mechanics and structure.

*We thank NSF for support of this work through REU site EEC 1560007.

How multivalent crosslinker proteins affect the self-assembly of actomyosin networks* YOSSI ELIAZ (Presenter), MARGARET CHEUNG, University of Houston; Center for Theoretical Biological Physics (Rice University) — Actomyosin networks are nonequilibrium active matter systems with millions of nanometer-scale proteins that self-assemble to form complex biomechanical structures 10,000 times larger than its constituent proteins. These networks play a key role in the morphology of neuronal dendritic spines whose plasticity regulates long-term memory formation and retention. We use a coarse-grained model to simulate actomyosin networks with both active and passive multivalent crosslinker proteins. Passive crosslinkers bind filaments statically while active crosslinkers (motor proteins) exert force and walk along the polarized filaments. So far, only systems with divalent crosslinkers have been simulated in large scales. Our computational simulations allow us to understand how and when active and passive multivalent crosslinkers promote bundled, scaffolded, isotropic, or clustered phases of the networks. More specifically, our model reveals the dependencies between the network structure and the multivalent crosslinker’s type, concentration, and properties.

*This work was supported by the National Science Foundation under Grants No. NSF CHE-1743392, No. NSF PHY-1427654, and No. NSF OAC-1531814.

Tug-of-war by active gel shapes positioning symmetry in cell-sized compartment RYOTA SAKAMOTO (Presenter), Department of Physics, Kyushu University, MASATOSHI TANABE, Department of Physics, Waseda University, TETSUYA HIRAIWA, Department of Physics, The University of Tokyo, KAZUYA SUZUKI, SHIN’ICHI ISHIWATA, Department of Physics, Waseda University, YUSUKE T. MAEDA, Department of Physics, Kyushu University, MAKITO MIYAZAKI, Department of Physics & The Hakubi Center for Advanced Research, Kyoto University — Force generation powered by actin cytoskeleton is underlying a wide range of phenomena from heart beating to cell migration [1]. To understand the underlying physical principles, in vitro reconstruction of actin cytoskeleton in water-in-oil droplet has been developed as a cell model, in which spontaneous F-actin flow and actomyosin clusters were self-organized [2]. However, it remains unclear how the spatial positioning of these structure is determined. To understand actomyosin-mediated geometric positioning, we confined actomyosin droplets in quasi two-dimensional chamber. We find that periodic actomyosin waves move the cluster to center, while the cluster is towed to edge by percolation of radial actomyosin network. By considering time-lag between maturation of actomyosin cortex and that of percolated network, active gel model recovers size-dependent two-state cluster positioning, which will give insights into the nucleus and spindle positioning in vivo [3]. We revealed active role of physical confinement to control intracellular positioning through actin cytoskeleton.

Dynamic stiffening and softening of a system of colloids cross-linked via polymers

ELISABETH RENNERT (Presenter), Rochester Institute of Technology, GASTON MOORHEAD, University of San Diego, JENNIFER ROSS, University of Massachusetts, Amherst, MICHAEL RUST, University of Chicago, RAE ROBERTSON-ANDERSON, University of San Diego, MOUMITA DAS, Rochester Institute of Technology — With the goal of deciphering the design principles for biomimetic materials that can autonomously stiffen and soften, we investigate colloids as a model system that can dynamically transition between fluid-like and gel-like states when crosslinked with polymers. The model is first developed with a system of colloids interacting via Lennard Jones potential, a fraction of which are further connected via passive crosslinkers. We study this system using Brownian Dynamics simulations and obtain collective properties, such as the time needed to form system spanning networks and elastic moduli, for various colloid volume fractions, interaction strengths, and cross-linker concentrations. Using experimental parameters for polystyrene spheres and Bovine Serum Albumin (BSA) crosslinkers, we predict the behavior of real systems. Next, we replace the passive, one-shot crosslinkers in our model by active cross-linkers that can dynamically attach and detach, and characterize the degree of order and the mechanical response of the system as a function of time. Our results provide insights into the design of self-sustaining soft materials that can dynamically stiffen and soften, and how the properties of such materials can be tuned.

*This work was funded by a W.M. Keck Foundation Research Grant.

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F65 DBIO: Biomaterials: Structure, Function, Design II

BCEC 260 - Pupa Gilbert, University of Wisconsin - Madison - Tag(s): Focus

Molecular Mechanics of Mussel Inspired Copolymers and Coatings [Invited] PEYMAN DELPARASTAN, KATERINA MALOLLARI, University of California, Berkeley, HAESHIN LEE, KAIST, PHILLIP MESSERSMITH (Presenter), University of California, Berkeley — A number of marine organisms rely on adhesive secretions for attachment to substrates in wet, turbulent environments. In the case of mussels, adhesion is mediated by the byssus- a remarkably strong and tough tissue comprised of collagenous protein threads terminally anchored by an adhesive pad. Byssal proteins have very specialized amino acid compositions, likely related to the specific challenges of achieving adhesion in the wet marine environment. Several byssal proteins contain high levels of 3,4-dihydroxy-L-alanine (DOPA), and there is a growing interest in developing mussel-inspired materials that contain catechols and other functional groups such as primary amine. Mussel inspired coatings derived from the spontaneous polymerization of dopamine, so-called ‘polydopamine’ coatings, have been widely reported in the literature for their ability to be deposited on a variety of substrates. However, the composition of polydopamine remains unknown. In this talk, we will describe our recent results on the molecular mechanics of polydopamine and related coatings using single molecule force spectroscopy. The results favor a ‘polymer’ model of polydopamine structure, casting doubt on models suggesting polydopamine is a supramolecular aggregate of small molecules and oligomers.
Adhesion Strategies of Dictyostelium discoideum - a Force Spectroscopy Study

MARCO TARANTOLA (Presenter), NADINE KAMPRAD, Max Planck Institute for Dynamics and Self-Organization, HANNES WITT, Physical Chemistry, University of Goettingen, MARCEL SCHROEDER, CHRISTIAN TITUS KREIS, OLIVER BAEUMCHEN, Max Planck Institute for Dynamics and Self-Organization, ANDREAS JANSCHOFF, Physical Chemistry, University of Goettingen — Biological adhesion is essential for all motile cells and limits locomotion to substrates displaying a compatible surface chemistry. However, organisms that face vastly varying environmental challenges require a different strategy. Dictyostelium discoideum (D.d.), a soil-living slime mould, faces the challenge of overcoming variable chemistry by employing fundamental forces of colloid science. To understand the origin of D.d. adhesion, we realized and modified a variety of conditions comprising specific adhesion proteins, glycolytic degradation, ionic strength, surface hydrophobicity and van der Waals interactions by generating tailored model substrates. Employing AFM-based single cell force spectroscopy we show that experimental force curves upon retraction exhibit two regimes. The first part up to the critical adhesion force can be described in terms of a continuum model, while a second regime of the curve beyond the critical adhesion force is governed by stochastic unbinding of individual binding partners and bond clusters. This versatile mechanism allows D.d. to adhere to a large variety of natural surfaces.

*We thank the Max Planck Society (fellow program), the SFB 937 ‘Collective behaviour of soft and biological matter’ (Project A8) and the Volkswagen Foundation (Living Foam) for funding.

In-vivo study of Yielding and Post-yielding behavior of Cytoplasm and its linkage with the cytoskeleton

SIJIE SUN (Presenter), JING XIA, DAVID A WEITZ, Harvard University — We study the yielding and post yielding behavior of cytoplasm in vivo. Cytoplasm, as an omnipresent component of the cells, is known to have finite Young's modulus and resists deformation, while intracellular cargo transports as fast as micron per second is observed in cytoplasm. In this study, the 3T3 cell line is adapted as a template to investigate the yielding and post yielding behavior of the cytoplasm. We find that cytoplasm yields at $10^2$ Pascal scale. The post yielding behavior may be modelled as Bingham fluid. Further control experiment illustrates that both heterogeneity and microtubules significantly contribute to the yielding behavior: The resistance of cytoplasm has multiple resources, and the dynamic assembling and dissembling of the microtubules are essential for yielding. Also, the cytoplasm close to microtubule-organizing centre (MTOC) has higher resistance towards yielding. Our experiment demonstrates the solid to fluid transform of cytoplasm under finite force.

Load-dependent bond kinetics have varied effects on the dynamics and mechanics of actomyosin contractility

PASHA TABATABAI (Presenter), DANIEL S. SEARA, IAN LINSMEIER, MICHAEL MURRELL, Yale Univ — Within the cytoskeleton, myosin motor proteins consume chemical energy and generate mechanical work within the filamentous actin network essential for diverse cell functions like migration, division, and shape change. Myosin unbinding kinetics are force dependent- exhibiting "catch-bond" behavior which decreases the probability of unbinding under load. Altering the binding kinetics of proteins is prohibitively difficult, thus the impact of load dependent binding kinetics on the dynamics and mechanics of actomyosin contractility are unclear. To this end, we use coarse grained molecular dynamics simulations to explore the effect of catch bonds on the accumulation and dissipation of mechanical energy in the actomyosin cytoskeleton. We find that motor binding that increases under load sensitizes the network to myosin motor concentration, increasing the rate of contractility while simultaneously increasing network toughness, or the storage of mechanical energy.

*We acknowledge funding ARO MURI W911NF-14-1-0403.
12:27PM F65.00005: High stretchability, strength and toughness of living cells enabled by hyperelastic vimentin network*  JILIANG HU (Presenter), YIWEI LI, MING GUO, Department of Mechanical Engineering, Massachusetts Institute of Technology — In many normal and abnormal physiological processes, including cellular migration during normal development and invasion in cancer metastasis, cells are required to withstand severe deformations. The structural integrity of eukaryotic cells under small deformations has been known to depend on the cytoskeleton including actin filaments (F-actin), microtubules and intermediate filaments (IFs). However, it remains unclear how cells resist severe deformations since both F-actin and microtubules fluidize or disassemble under moderate strains. Here, we demonstrate that vimentin intermediate filaments (VIFs), a marker of mesenchymal cells, dominate cytoplasmic mechanics at large deformations. Our results show that cytoskeletal VIFs form a stretchable, hyperelastic network. This network works synergistically with other dissipative cytoplasmic components, substantially enhancing the strength, stretchability, resilience and toughness of the living cytoplasm.

* M. G. would like to acknowledge the support from the Department of Mechanical Engineering at MIT

12:39PM F65.00006: Fibril formation kinetics of insulin solutions in an interfacial shearing flow  NICHOLAS DEBONO (Presenter), ADITYA RAGHUNANDAN, HANNAH R. MIDDLESTEAD, A HIRSA, Rensselaer Polytechnic Institute — The formation of amyloid fibril plaques and the accumulation of such structures in vivo is the hallmark of disorders such as Alzheimer's and type-II diabetes. Fibril formation can be accelerated by several factors including changes to pH and temperature conditions. However, the role of the dominant and most varying in vivo factors of fluid flow and shear at hydrophobic interfaces in protein aggregation pathways remain poorly understood. Proteins adsorbed at the air/fluid interface are also subjected to significant hydrodynamic stresses during bioprocessing and drug handling, which leads to unwarranted denaturation/aggregation and subsequent loss in drug efficacy. Here, we study the kinetics of fibril formation for human recombinant insulin solutions in an interfacial shearing flow using fixed time-point ThT fluorescence and native-protein absorbance assays across a wide range of rotation rates. We identify differences in the morphology of the fibril structures formed at the air/fluid interface and in bulk solution at different stages of fibril seeding and growth. This is key to elucidating the aggregation pathway and toxicity of shear-induced denaturation and protein fibril formation.

12:51PM F65.00007: MULTI-SCALE MICRORHEOLOGY USING FLUCTUATING SEMIFLEXIBLE FILAMENTS AS STEALTH PROBES  KENGO NISHI (Presenter), University of Gottingen, CHRISTOPH F. SCHMIDT, Duke University, FREDERICK MACKINTOSH, Rice University — Microrheology is commonly performed using micron-sized beads embedded in the (soft) medium to be studied. Inserting beads can be problematic in confined or hard to access places and can cause artifacts. Here, we introduce the use of single-walled carbon nanotubes (SWNTs), which are model semi-flexible polymers with non-photobleaching fluorescence, as “stealth probes”. We embedded SWNTs in viscoelastic media and analyzed thermally driven shape fluctuations. We show that the bending dynamics of SWNTs embedded in soft media can be used to probe the viscoelastic properties of such media at multiple scales, corresponding to the wavelengths of the modes analyzed. We found that the viscoelastic moduli of polymer solutions measured by SWNTs are in excellent agreement with those by measured by conventional micro/macrorheology, which validates the method.

1:03PM F65.00008: In situ imaging of strained collagen fibrils*  CHRIS PEACOCK (Presenter), LAURENT KREPLAK, Department of Physics and Atmospheric Science, Dalhousie University — Damage to collagenous tissues remain difficult to treat due to uncertainty of how their constituents operate under tension. The smallest of these constituents is the collagen fibril, a rope-like aggregate of collagen molecules with a structure comparable to man-made fibres. While the force-elongation curve of collagen fibrils is fairly well characterized, structural changes due to elongation remain poorly understood. In this talk I will present an in situ atomic force microscopy approach to probe the morphology and cohesiveness of strained fibrils.

*C.P. and L.K. acknowledge funding from the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Canada Foundation for Innovation (CFI)
1:15PM F65.00009: Collagen-inspired self-assembly of twisted filaments  MARTIN FALK (Presenter), Massachusetts Institute of Technology, LUCY COLWELL, University of Cambridge, AMY DUWEL, Draper Labs, MICHAEL PHILLIP BRENNER, Harvard University — There have been dramatic developments in our ability to functionalize submicron scale objects with molecules enabling specific interactions between building blocks, opening up an enormous design space for solutions of particular engineering problems. Here, we explore the physics of collagen self-assembly in order to deduce design rules for the self-assembly of twisted filaments. Despite the well-known structure of collagen, identifying which aspects of its design are required for reproducing collagen-like features in synthetic analogues is unknown. Using computer simulations, we propose a scheme mediated by specific interactions to self-assemble collagen-like triple helices. The assembly nucleates chiral defects, in which two of the filaments switch orientations. Such defects can be eliminated with a modest energetic bias, or nucleated by introducing mechanical weak spots. By inducing spatial variation of the enthalpy of helix formation, we can localize another type of defect where the helix becomes locally unbound. Local unbinding slows assembly, evoking kinetic pathologies previously ascribed to mutations in the primary collagen amino acid sequence. In analogy to collagen, controlled formation of defects could enable hierarchical self-assembly of bundles of twisted filaments.

1:27PM F65.00010: Mechanism of metal-like conductivity in bacterial protein nanowires*  SOPHIA YI, YANGQI GU, JENS NEU, J. PATRICK O’BRIEN, SIBEL EBRU YALCIN, DENNIS VU, WINSTON HUYNH, VICTOR BATISTA, CHARLES A SCHMUTTENMAER, NIKHIL MALVANKAR (Presenter), Yale Univ — Proteins are considered electronically insulators. However, nanofilaments produced by Geobacter sulfurreducens exhibit metal-like conductivity. To elucidate the mechanism of electron transport, we measured the electrical and optical conductivity of filaments from multiple mutant strains as a function of molecular length, temperature, frequency, pH and π-stacking. We demonstrate that intrinsic conductivity of individual filaments can be described by theoretical model for quasi-one-dimensional materials. To determine the molecular architecture responsible for conductivity, we are using a suite of complementary experimental and computational methods. Our studies show that filaments show π-stacking, that can cause intermolecular electron delocalization, conferring metallic conductivity to filaments. Furthermore, increasing π-stacking improves their crystallinity, yielding a longer mean free path for electrons, and stronger electronic coupling which yields 1000 times lower electron attenuation than other proteins. These studies will help development of genetically programmable biomolecular materials with tunable functionality through precise control of their electronic and protein structure.

*Funded by NIH New Innovator and NSF CAREER Awards.

1:39PM F65.00011: Cancer, p53, and non-classical self-assembly of amyloids and their first order phase transitions*  [Invited]  MOHAMMAD SAFARI, Biochemistry, Princeton University, ANATOLY BORIS KOLOMEISKY, Chemistry, Rice University, JACINTA CONRAD, PETER VEKILOV (Presenter), University of Houston — About half of human cancers are associated with mutations of the tumor suppressor p53. Gained oncogenic functions of the mutants have been related to aggregation behaviors of wild-type and mutant p53. The thermodynamic and kinetic mechanisms of p53 aggregation are poorly understood. Here we find that wild-type p53 forms an anomalous liquid phase. The liquid condensates exhibit several behaviors beyond the scope of classical phase transition theories: their size, ca. 100 nm, is independent of the p53 concentration and decoupled from the protein mass held in the liquid phase. Thermodynamic analyses elucidate another unusual property of this liquid phase: lack of constant solubility. The nucleation of p53 fibrils deviates from the accepted mechanism of sequential association of single solute molecules. We find the liquid condensates serve as pre-assembled precursors of high p53 concentration that facilitate fibril assembly. Fibril nucleation hosted by precursors represents a novel biological pathway, which opens avenues to suppress protein fibrillation in aggregation diseases.

*This work was supported by grants from NASA (NNX14AD68G and NNX14AE79G), NSF (MCB-1518204, DMR-1710354, and DMR-1131155), and the Welch Foundation (E-1869)

Tuesday, March 5, 2019 11:15 AM - 2:15 PM

Session F66 DBIO GSNP: Inference, Information, and Learning in Biophysics I  BCEC 261 - David Schwab, Princeton Univ - Tag(s): Focus
11:15AM F66.00001: Bounding Information flow in E. Coli chemotaxis

HENRY H MATTINGLY, Dept. of Molecular Cellular and Developmental Biology, Yale University, THIERRY EMONET, Dept. of Physics and Dept. of Molecular Cellular and Developmental Biology, Yale University, BENJAMIN MACHTA (Presenter), Dept. of Physics and Systems Biology Institute, Yale University —

The bacteria *Escherichia coli* climbs shallow gradients by tumbling - randomly reorienting their directed runs - when they sense they are moving away from chemical attractants. In the absence of any information from their receptors *E. coli* would be unable to move in a directed fashion, moving stochastically by runs and tumbles with an effective long-scale diffusion constant D. Here we show that to climb a gradient with average speed V requires a transfer entropy rate, I, from direction of motion, through receptor activity, and ultimately to tumbling behavior of at least I = V^2/2D. This provides a lower bound on the requirements of the signaling cascade that can be inferred from single bacteria trajectories. We discuss how this bound constrains the design of the receptor and signaling system.

*HM and TE were supported by NIH R01 GM106189

11:51AM F66.00002: Towards a New Theory of Biological Information

DANIEL INAFUKU (Presenter), Physics, University of Illinois at Urbana-Champaign, KAY KIRKPATRICK, Mathematics, University of Illinois at Urbana-Champaign — Many attempts have been made to understand biomolecular machines, such as the ribosome, from a computational and information-theoretic perspective. However, it is well-understood that current information theory is limited to symbolic (i.e., syntactic) manipulations only and is not equipped to deal with objects that possess functions beyond such manipulations. In this study, we present a quantitative analysis of the information-processing abilities of several classes of biomolecular machines that demonstrates their capacities for biological information. Furthermore, we argue that such machines possess functions that lie beyond the scope of traditional Shannon information theory and require a new description to completely characterize them. Finally, we propose new ways to extend current models by rigorously abstracting the structure and dynamics of these machines.

*National Science Foundation Graduate Research Fellowship
National Science Foundation CAREER Award DMS-1254791

12:03PM F66.00003: Information transmission and evolution of crosstalk in noisy signal transduction networks

AMMAR TAREEN, Cold Spring Harbor Laboratory, NED WINGREEN, Department of Molecular Biology, Princeton University, RANJAN MUKHOPADHYAY (Presenter), Clark University — Reliable transmission of information about the environment along cellular signaling pathways is crucial for accurate regulation of cellular function. However, signaling pathways are often highly interconnected, creating signal transduction networks consisting of multiple pathways. How did such complex, interconnected networks evolve and what constraints did the dynamics of evolution place on their architecture? Does crosstalk between pathways necessarily lead to reduction in the amount of information that can be reliably transmitted? In this talk, we will study information transmission and the evolution of cross-talk between noisy signaling pathways with the aim of addressing these and related questions. For this purpose, we develop a sequence-based evolutionary algorithm and evolve networks consisting of more than one pathway based on physically motivated fitness functions. We show how two fitness functions, both related to measures of information transmission, lead to very different evolutionary outcomes, one with a high degree of crosstalk and the other without. We relate the evolutionary outcomes to the fitness landscapes, and discuss the biological implications of our results.

12:15PM F66.00004: Information loss under coarse graining: A geometric approach

ARCHISHMAN RAJU (Presenter), Centre for Studies in Physics and Biology, Rockefeller University, JAMES PATARASP SETHNA, Cornell University, BENJAMIN MACHTA, Yale University — We use information geometry, in which the local distance between models measures their distinguishability from data, to quantify the flow of information under the renormalization group. We show that information about relevant parameters is preserved, with distances along relevant directions maintained under flow. By contrast, irrelevant parameters become less distinguishable under the flow, with distances along irrelevant directions contracting according to renormalization group exponents. We develop a covariant formalism to understand the contraction of the model manifold. We then apply our tools to understand the emergence of the diffusion equation and more general statistical systems described by a free energy. Our results give an information-theoretic justification of universality in terms of the flow of the model manifold under coarse-graining.

*AR and JPS were supported by NSF DMR 1312160 and DMR 1719490. BBM was supported by NSF PHY 0957573 and a Lewis-Sigler Fellowship.
12:27PM F66.00005: The strength of protein-protein interactions controls the information capacity and dynamical response of signaling networks*  CHING-HAO WANG (Presenter), Physics, Boston University, CALEB BASHOR, Bioengineering, Rice University, PANKAJ MEHTA, Physics, Boston University — Eukaryotic cells transmit information by signaling through complex networks of interacting proteins. Here we develop a theoretical and computational framework that relates the biophysics of protein-protein interactions (PPIs) within a signaling network to its information processing properties. We formulate a statistical physics-inspired model and combine it with information-theoretic methods to find that PPIs are a key determinant of information transmission within a signaling network, with weak interactions giving rise to “noise” that diminishes information transmission. While noise can be mitigated by increasing interaction strength, the accompanying increase in transmission comes at the expense of a slower dynamical response. This suggests that the biophysics of signaling protein interactions give rise to a fundamental “speed-information” trade-off. We further use this framework to interrogate the relationship between pathway cross-talks and information capacity, as well as its implications in synthetic biology.

*This work was also supported by NIH NIGMS grant 1R35GM119461, and by Simons Investigator in the Mathematical Modeling of Living Systems (MMLS) awards to PM.

12:39PM F66.00006: Random input expansion improves classifier accuracy  JULIA STEINBERG (Presenter), MADHU ADVANI, HAIM SOMPOLINSKY, Harvard University — We have discovered a surprising phenomena in the problem of inference with noisy high dimensional data: that adding random input dimensions (completely uncorrelated to the data) can lead to lower generalization error when training max-margin classifiers. When applied appropriately, we prove that this expansion of the network can yield equivalent solutions to the addition of slack variables in support vector machine learning. We also consider two layer networks and demonstrate that this phenomenon can allow wide random neural networks with sparse activity to handle output noise more effectively than networks exactly matched to the structure of the teacher network. This finding has implications for the design of neural networks and in understanding the role of neurogenesis and short-lived synapses in biological neural network structures.

12:51PM F66.00007: The renormalization group and information bottleneck: a unified framework  ANDREW TAN (Presenter), University of Toronto, LEENOY MESHULAM, Massachusetts Institute of Technology, WILLIAM BIALEK, Princeton University, DAVID SCHWAB, City University of New York — Achieving useful simplified descriptions of high-dimensional systems is a fundamental problem in statistical physics. A central issue is formalizing which details should be retained and which discarded, such that we are left with only “relevant” information. In statistical physics, the outcome of the renormalization group is a reduced description where we are left with an accurate description of the macroscopic behavior of the system. In information theory, we use the information bottleneck to determine the optimal balance between features we accurately convey and those that are irrelevant complexity. Here we present an approach that unifies the concepts of the renormalization group and the information bottleneck. We achieve a coarse-graining procedure where we can control what “relevant” information we choose to keep, e.g. retaining information about long-distance features while removing local information. Studying the method in the information plane allows us to automatically select the best representation at each size. Variational approaches allow us to scale up our implementation, so that this approach can be successfully applied to large systems. We test our method on a variety of datasets from both physics and machine learning.

1:03PM F66.00008: Optimal visual motion estimation in a natural environment*  WILLIAM BIALEK (Presenter), Physics, Princeton University and The CUNY Graduate Center, SHIVA SINHA, ROBERT DERUYTER VAN STEVENINCK, Physics, Indiana University — Many organisms, from flies to humans, use visual signals to estimate their motion through the world. In flies we know that the precision of motion estimation is close to the limits set by photon shot noise and diffraction blur, yet the actual estimates suffer from systematic errors, some of which are shared by human perception. To explore the structure of the motion estimation problem, we have constructed a camera/gyroscope system that allows us to sample, at high temporal resolution, the joint distribution of input images and rotational motions during a long walk in the woods. From these data we construct the optimal estimator of velocity based on spatial and temporal derivatives of image intensity in small patches of the visual world. Over the bulk of the naturally occurring dynamic range, the optimal estimator exhibits the same systematic errors seen in neural and behavioral responses, including the confounding of velocity and contrast. These results suggest that apparent errors of sensory processing may reflect an optimal response to the physical signals in the environment.

*Supported in part by the NSF through the Center for the Physics of Biological Function (PHY-1734030), the Center for the Science of Information (CCF--0939370), and grant PHY-1607612
1:15PM F66.00009: The Stochastic Complexity of Spin Models: Are Pairwise Models Really Simple?  ALBERTO BERETTA, Quantitative Life Sciences, The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, I-34014 Trieste, Italy, CLAUDIA BATTISTIN, Kavli Institute for Systems Neuroscience and Centre for Neural Computation, Norges Tekniske-Naturvitenskapelige Universitet (NTNU), Olav Kyrres Gate 9, 7030 Trondheim, Norway, CLÉLIA DE MULATIER (Presenter), Department of Physics and Astronomy, University of Pennsylvania, 209 South 33rd Street, Philadelphia, PA 19104-6396, USA, IACOPO MASTROMATTEO MASTROMATTEO, Capital Fund Management, 23 rue de l'Université, 75007 Paris, France, MATTEO MARCELLI, Quantitative Life Sciences, The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, I-34014 Trieste, Italy — Models can be simple for different reasons: because they yield a simple and computationally efficient interpretation of a dataset (e.g. in terms of pairwise dependencies)--as in statistical learning--or because they capture the laws of a specific phenomenon--as in physics--leading to non-trivial falsifiable predictions. In information theory, the simplicity of a model is quantified by the stochastic complexity, which measures the number of bits needed to encode its parameters. In order to understand how simple models look like, we study the stochastic complexity of spin models with interactions of arbitrary order. We show that bijections within the space of possible interactions preserve the stochastic complexity, which allows to partition the space of all models into equivalence classes. We thus found that the simplicity of a model is not determined by the order of the interactions, but rather by their mutual arrangements. Models where statistical dependencies are localized on non-overlapping groups of few variables are simple, affording predictions on independencies that are easy to falsify. On the contrary, fully connected pairwise models, often used in statistical learning, appear to be highly complex, because of their extended set of interactions, and are hard to falsify.

1:27PM F66.00010: Who is your neighbor? Inferring locality from pairwise correlations  MAHAJABIN RAHMAN (Presenter), ILYA NEMENMAN, Emory University — Modeling multivariate biological systems, such as multielectrode neural recordings, genetic sequences, or gene expression patterns, requires identification of combinatorial interaction coefficients coupling the measured variables. This is impossible to do from data sets of realistic sizes. One could hope to regularize the inference by imposing the constraint that interactions must be local. However, whether two variables are neighbors and thus can interact is unknown for many biological data sets. Here we explore the possibility that neighborhood relations can be inferred from the pairwise correlation matrix, even in the undersampled data limit. Our toy model consists of a set of images whose pixels are shuffled randomly, but in the same way for all images, such that spatial information is lost, but pixel-to-pixel correlations are preserved. We use t-SNE, a dimensionality reduction and visualization technique, to embed the shuffled pixels in space, such that strongly correlated pixels end up next to each other. We observe that embedding the data in 2D space produces images nearly identical to the originals, save for global transformations. This shows that analysis of the covariance matrix correctly identifies local neighborhoods, as well as the global dimensionality of the data.

1:39PM F66.00011: Mean Field Analysis of Batch Normalization  MINGWEI WEI (Presenter), Department of Physics and Astronomy, Northwestern University, JAMES STOKES, Tunnel Technologies, DAVID SCHWAB, The Graduate Center, City University of New York — Batch Normalization (BatchNorm) is an extremely useful component of modern neural network architectures, enabling optimization using higher learning rates and achieving faster convergence. In this paper, we use mean-field theory to analytically quantify the impact of BatchNorm on the geometry of the loss landscape for multi-layer networks consisting of fully-connected and convolutional layers. We show that it has a flattening effect on the loss landscape, as quantified by the maximum eigenvalue of the Fisher Information Matrix. These findings are then used to justify the use of larger learning rates for networks that use BatchNorm, and we provide quantitative characterization of the maximal allowable learning rate to ensure convergence. Experiments support our theoretically predicted maximum learning rate, and furthermore suggest that networks with smaller values of the BatchNorm parameter achieve lower loss after the same number of epochs of training.

1:51PM F66.00012: Nonequilibrium cooperative sensing  VUDTIWAT NGAMPRUETIKORN (Presenter), Northwestern University, DAVID J. SCHWAB, The Graduate Center, CUNY, GREG STEPHENS, Vrije Universiteit (Amsterdam) & OIST Graduate University (Okinawa) — While cellular sensing relies on both cooperation between receptors and energy consumption to suppress noise, their combined effect is not well understood. Here we introduce a minimal model of interacting sensors which allows for the detailed exploration of signal statistics and cooperation strategies in the context of optimal sensing. For two sensors we show that the sensing strategy which maximizes the mutual information between the signal and the sensors depends both on the noise level and the statistics of the signals. For signals on a single sensor, nonequilibrium, asymmetric couplings result in maximum information gain in the noise-dominated limit while for joint, correlated signals, the improvement is greatest in the low-noise limit. In particular we show that optimal sensing does not always require energy consumption. We detail the difference in mechanism behind nonequilibrium improvement for univariate and correlated signals and our results provide insight into the principles of optimal sensor design.
A Novel Algorithm for Unsupervised Behavioral Classification

ADAM FINE (Presenter), NIRAG KADAKIA, THIERRY EMONET, Yale Univ — I present a novel software package used for extraction of behavioral patterns from a data matrix with no a priori assumptions about the form of the data. The underlying algorithm transforms a data matrix into the time-frequency domain using a wavelet transform, which is analogous to taking a Fourier transform at each time step. This equalizes the power between frequency components, to ensure repeated high frequency motions do not dominate. The transformed matrix is then decomposed into behavioral patterns and their relative activity over time using an algorithm called seqNMF [1]. Though the algorithm was originally developed for positional data from an assay of Drosophila, it has been used to extract behavioral patterns from other organisms (e.g. E. coli) as well. The algorithm is robust with respect to both the number of underlying patterns in the data as well as the length of the patterns. In addition, the lack of any input other than the data itself makes the software package a powerful unsupervised classification tool with broad potential applications.


Tuesday, March 5, 2019 11:15 AM - 1:27 PM

Session F67 APS/SPS: Undergraduate Research VI

11:15AM F67.00001: Fabrication of Sensitive MEMS-based Magnetometer for Biomagnetic Applications* ZAINAB BATOOL (Presenter), RALITSA MIHAYLOVA, ANDY CLARK, Department of Physics, Bryn Mawr College, JOSH JAVOR, Department of Mechanical Engineering, Boston University, XUEMEI CHENG, Department of Physics, Bryn Mawr College, DAVID JOHN BISHOP, Department of Mechanical Engineering, Boston University — The electrocardiogram (ECG) is the standard method of heart disease detection but is inconveniently sized and susceptible to conductive tissue noise and signal attenuation by filtering. Additionally, the superconducting quantum interference device (SQUID) systems operate in vacuum, are expensive and large, and are rivaled by atomic magnetometers (AMs), which are compact and sensitive but limited by spin relaxation. Here we report the development and fabrication of a MEMS-based, 100pT/cm sensitive, inexpensive magnetometer device, which may overcome the mentioned limitations. The device measures gradient fields by detecting magnetic force exerted on a commercial MEMS capacitive accelerometer through the coupled micro-sized, permanent magnet. Present limitations of this device are fabrication throughput and magnet characterization. Here we discuss characterization by a vibrating sample magnetometer (VSM) and obstacles in a custom micro-gluing technique.

*This work was jointly supported by CELL-MET, an NSF Engineering Research Center, under award number 1647837 and by the Center for Engineering Mechanobiology (CEMB), an NSF Science and Technology Center, under grant agreement CMMI: 15-48571

11:27AM F67.00002: Low-Frequency Vibration Isolation for Atom Interferometry* NINA INMAN (Presenter), Physics, Bryn Mawr College, FONG EN OON, RAINER DUMKE, Physics and Applied Physics, Nanyang Technological University, MICHAEL LIM, Rowan University — The isolation of low-frequency vibrational noise must be applied in most gravimeters to allow for accurate measurement of Earth's local gravitational acceleration. Optimal performance of a gravimeter can be achieved by mitigating the effects of vibration on inertial acceleration measurement. A seismometer is used to detect vibrational noise and produce a voltage signal from which the magnitude and frequency of vibrations can be calculated. A system was constructed to record vibrational noise and compute its Fourier Transform. The output is low-pass filtered and can be fed back to a voice coil to correct residual noise detected on a vibration isolation platform. The next steps include determining the appropriate cut-off frequency range and benchmarking the performance in various environments.

*The authors acknowledge support from NSF-IRES 1559410.

11:39AM F67.00003: Quantization of the Vibrations of a Thin Elastic Plate ELIOT HEINRICH (Presenter), DENNIS CLOUGHERTY, University of Vermont — Suspended thin films have been successfully used as high-Q mechanical oscillators in hybrid optomechanical systems to study fundamental quantum mechanical effects. Motivated by these experiments, we consider a Hamiltonian description of the vibrations of a clamped, elastic circular plate. The Hamiltonian of this system features a potential energy with two distinct contributions: one that depends on the local mean curvature of the plate, and a second one that depends on its Gaussian curvature. We quantize this model using a complete, orthonormal set of eigenfunctions for the clamped, vibrating plate. The resulting quanta are the flexural phonons of the thin circular plate. As an application, we use this quantized description to calculate the rms displacement of the plate's center for arbitrary temperature.
**11:51AM F67.00004: Measuring Viscosity with A Damped Harmonic Oscillator**

DONAVAN EBERSOLE (Presenter), TY NAQUIN, JAMES SANDERS, Physics and Chemistry Department, Troy University — The damped harmonic oscillator is a staple of undergraduate physics education, and the Stokes' Law drag is often used as an example of such damping. This force has the required form of $F = -bv$; however, the coefficient $b$ is dependent on the fluid viscosity, which is itself a function of the fluid's temperature. We attached a spherical mass to the end of spring that was suspended in the liquid; the other end of the spring was attached to a force sensor. After slightly displacing the mass, we used Pasco software to record the Hooke's Law force during the motion. A graph of force versus time yields the damping coefficient, from which we could measure the fluid's viscosity. By comparing the viscosity to a table of known values, we could then determine the fluid's temperature.

*This work was funded by an NSF grant through a program called Louis Stokes Alliances for Minority Participation (LSAMP).*

**12:03PM F67.00005: Nonlinear resonance for a generalized parametric oscillator**

YAO LUO (Presenter), Nanjing University — Multiple discrete stationary solutions, namely "amplitude quantization", found in kick-excited pendulums have not been well understood over decades. We show that these discrete solutions are subharmonic resonance originated from the nonlinear periodic driving force. From theoretical analysis, we reveal the relationship between subharmonic resonance frequency and symmetry of the driving force: odd subharmonic resonance occurs under even symmetric driving force and vice versa. We also show that multiple periodic solutions coexist near subharmonic resonance frequencies, in particular dual solutions are discovered. While the usual parametric oscillator has periodic driving force proportional to displacement and experience subharmonic resonance at even multiples of the pendulum's frequency, our mathematical model can be viewed as generalized parametric resonance which has nonlinear periodic driving force and experience subharmonic resonance at integral multiples of the pendulum's frequency. In order to investigate the stability conditions and evolution of the solutions, we calculate the frequency response curves, bifurcation diagram, phase diagrams, Poincare maps and the stability diagrams.

**12:15PM F67.00006: Exploring Resonance Effects on Ferromagnetic Microwire Solenoid Sensitivity for Motion Tracking Applications**

JAKE POLER (Presenter), VALERY J ORTIZ, TATIANA M EGGERS, MANH-HUONG PHAN, University of South Florida — The high frequency GMI effect is a sensitive phenomenon found in amorphous, soft ferromagnetic materials. The GMI effect has potential to introduce a new class of long range, contact-free small field magnetic sensing[1]. GMI sensors allow for low-cost, robust systems capable of a wide range of motion tracking applications. A challenge these sensors present to applications comes from the quick decay of magnetic field lines, restricting their sensing distance. In an attempt to achieve better sensitivity and longer ranges, Cobalt-based microwires have been wound into solenoids around Plexiglas molds with various lengths of wire. Further, the number of turns used, affects the magnitude and frequency of transmission line resonance. GMI responses were measured around resonance to determine the optimal operating frequency for each sensor and to observe the relation to the circuit's current nodes. Of the solenoids constructed, the 12 turn, 203 mm solenoid had the highest sensitivity. The optimal operating frequency was 32.4 MHz, which allowed for a range of 250 mm. For comparison, GMR sensors have a detection range of 190 mm[2].


*NSF REU #1560090*

**12:27PM F67.00007: Building time-dependent temperature field in a multi-field coupling system**

JIAHAO DONG (Presenter), Nanjing University — Solving time-dependent field remains challenging in most situations due to convergence difficulty. In this paper, we systematically research the solving method of the time-dependent temperature field in case of a multi-field coupling system, including mesh partition methods, decoupling strategies, iterative algorithms, etc. We apply our method to an apparatus called “Curie Point Engine”. In the example, a nickel disc located in an inhomogeneous magnetic field is heated asymmetrically, and then is driven to rotate around the axle by the asymmetrical magnetic force. In this case, the temperature field, magnetic field and the motion of the disc are all time-dependent and coupled. We apply the dynamic mesh method due to the motion of the disk. The validity of our method is confirmed by comparing the simulation results to our experimental images of a Curie Point Engine recorded by a thermal imager.
12:39PM F67.00008: A statistical comparison of OAR doses between Helical Tomotherapy and VMAT plans*  
Micheal Taylor (Presenter), Physics, University of South Florida, Dawn Gintz, Jimmy Caudell, Vladimir Feygelman, Kujtim Latifi, Eduardo Moros, Radiation Oncology, Moffitt Cancer Center — Head & neck cancer patients have a high risk of nutritional problems caused by their cancer and the toxic side effects of radiotherapy. The feasibility dose-volume histogram (fDVH) algorithm available in the PlanIQ software (Sun Nuclear Corporation, Melbourne, FL) has been validated to optimally aid in the sparing of certain organs-at-risk (OAR's) in head & neck volumetric modulated arc therapy (VMAT) plans. This study evaluates the met or missed opportunities for limiting dose to OAR's by applying the fDVH tool to head & neck Helical Tomotherapy plans and compare them to VMAT plans of similar dose and staging. Head & neck cancer patients treated in 2014 were selected. All patients had the following OAR's reviewed in an imaging handling software (Mirada Medical, Oxford, UK): larynx, inferior pharyngeal constrictor, submandibular glands, and parotids. Any missing or inadequate contours were edited. Only patients treated with a 70 Gray Simultaneous Integrated Boost Tomotherapy/VMAT plan with a bilateral elective neck were analyzed. Patients with the same or a similar cancer stage as defined by the American Joint Committee on Cancer were grouped, and the differences in areas under the fDVH's and actual DVH's were statistically compared.

*Funded by NSF REU grant #1560090

12:51PM F67.00009: Symmetry Breaking and Iterated-Map Networks  
Houssemeddine Mhiri (Presenter), Moyi Tian, Lars Q English, Dickinson College — The logistic map is a simple mathematical model commonly used to explore discrete-time systems. L’Her, et al. [1] implemented an electronic circuit that mimics the behavior of coupled logistic maps to great precision. While L’Her’s circuit provides the basis for our experimental exploration of logistic map networks, it lacks practical control of initial conditions. We reproduced L’Her’s circuit and introduced automated manipulation of the initial conditions and of the coupling voltage through an Arduino Uno Microcontroller. This additional control allows for a close exploration of symmetric states and symmetry-broken states that the coupled logistic maps exhibit under specific conditions. Indeed, for fixed values of the growth rate, the manipulation of initial conditions produces an array of symmetric and symmetry-broken states. We will use this data to generate basins of attraction for the corresponding growth parameters. Conversely, if we fix the growth rate and iteratively increment the coupling strength, we experimentally observe interesting bifurcation behavior involving the symmetric, symmetry-broken, as well as phase-shifted solutions.


1:03PM F67.00010: Comparing Classical And Quantum Finite Automata*  
Kaitlin Gili (Presenter), Department of Physics and Engineering Physics, Stevens Institute of Technology, Rudy Raymond, Rodney Van Meter, IBM Q Hub, Keio University, Kohei M Itoh, Department of Applied Physics and Physico-Informatics, Keio University — Quantum computers offer advantages that motivate the exploration of quantum algorithms and models with the expectation that they can solve many more complex problems than classical computers. Here, we are exploring one of the simplest models of computation by comparing Deterministic Finite Automata and Quantum Finite Automata (Ambainis and Freivalds, 1998). This research focuses on applying quantum principles to the following problem: Consider a string $a^i$ with $i$ letters. We want to determine whether the string is in the language $L$ where $L = \{a^i \mid i \text{ divides } p\}$ and $p$ is a given prime number. If $i$ divides $p$, we accept the string into the language with a 0 qubit state, and if not, we reject it with a qubit state of 1. Classically, using the highest known prime integer, this algorithm requires a minimum of 77,232,917 bits, whereas the quantum finite automata only requires 27 qubits. Using Python's Quantum Information Software Kit (Qiskit), I have implemented a program [1] that can determine if the length of a string is divisible by a large prime number with exponentially fewer qubits.


*This work was supported by the Nakatani Foundation and Keio University.
A code was generated in MATLAB to model the temperature of plant (Arabidopsis) leaves ($T$) during 25 s periods of hypo- ($\mu g$) and hyper- ($2g$) gravity ($g$) produced by parabolic flights. Temporal data $T(t)$ vary inversely with $g(t)$ and are reproduced by a model that accounts for heat transfer across the boundary layer (BL) between the leaf and air [1,2], conduction through the stem into the growth media, and heat from the plant metabolism. While the BL and stem conduction terms are analytically known, the metabolic power is approximated as a function of $T$ to simulate the $T(t)$ data. Extending the metabolic power term to include time dependent dose-response mechanisms requires comparison of model predictions to $T(t)$ data from longer periods of low-$g$. Thus, analysis of $T(t)$ data from parabolic flights simulating lunar gravity over longer times will check the fully adaptive $T(t)$ at low-$g$. Sub-orbital flights with 5 min periods of $\mu g$ will test further extensions of the model.


*Supported by UF CCMS Undergraduate Fellowship (JJK-P), NSF DMR-1708410 (MWM) and DMR-1156737 (UF REU), and NASA NNX15AB12G (RJF and ALP).
11:39AM F68.00003: Tailoring machine learning for tackling the Large Hadron Collider problems  ANTONY HALIM (Presenter), Minerva University — Machine learning has proven its vitality in devising complex systems. The wide range of tasking techniques allowed machine learning to be a qualified tool for analyzing the vast amount of data obtained from the Large Hadron Collider. These tasks can range from tracking pattern recognition, particle identification, to search for rare decays. As a new tool starts to spread, the need for modifying increases to adapt to the new users' tasks. One approach is the design of packages. Here I present a machine learning package in R, designed for analyzing the Large Hadron Collider data, focusing mainly on particle identification through the measured particle parameters and the detector system, and also spotting rare decays using the supervised learning based classification techniques of machine learning. Machine learning does not only focus on easing the data analysis process that is already taking place, but it offers an opportunity for implementing new search strategies for rare phenomena through novel techniques. This step aims to assist physicists and researchers, and it also takes a further step ahead of enabling users to personalize more the tool through having an open source of the package accessible to users.

11:51AM F68.00004: Heavy Graviton Search at the Large Hadron Collider*  YUHAN GUO (Presenter), ALFREDO GURROLA, SAVANNA R STARKO, PAUL DOUGLAS SHELDON, WILL JOHNS, OISHIK RAY, Vanderbilt University, ANDRES FLOREZ, Universidad de los Andes — The Standard Model (SM) of particle physics, aimed to relate particles and forces, fails to build such relation for gravitation. Certain theories predicting “Graviton,” mediator for gravitation, to be a massive (hence potentially detectable) spin-2 particle have raised high experimental interest. Yet so far no search has discovered such particle at the Large Hadron Collider (LHC). This research develops a search methodology for a massive spin-2 particle using Vector Boson Fusion (VBF) processes at the LHC. We consider potential reasons the current searches, mainly relying on Drell-Yan (DY) production mechanisms, have observed no graviton, including potentially low coupling strength between the graviton, quarks, and gluons. The VBF topology, with no reliance upon the QCD coupling strength, offers an alternative and complementary search strategy. We further combine the VBF topology with the diphoton decay channel, a novel search for the LHC. We show that the requirement of a high mass diphoton pair combined with two high pT forward jets with large dijet mass and with large separation in pseudorapidity can significantly reduce the SM backgrounds. We expect discovery potential for TeV scale graviton masses.

*This work is supported by NSF Award PHY-1506406.

12:03PM F68.00005: Survey of Tensor Networks*  SAMUEL DESROSIERS (Presenter), GLEN EVENBLY, THOMAS E BAKER, Département de physique & Institut quantique, Université de Sherbrooke — Tensor networks have become a robust method over the past few decades to represent quantum systems and solve them efficiently. These numerical methods can optimize a system by keeping the most important degrees of freedom, allowing us to solve large systems more efficiently. We review the fundamentals of this field, including a deep connection with entanglement. Basic aspects of tensor networks and common algorithms are presented. Specifically, algorithms for classical spin systems are compared to study their effectiveness.

*S.D. graciously thanks the 2018 Institut Transdisciplinaire d'Information Quantique (INTRIQ) undergraduate internship project scholarship. T.E.B. thanks Institut quantique for funding through the postdoctoral fellowship program. G.E. thanks Institut quantique and the Département de physique. This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund (CFREF).

12:15PM F68.00006: Clifford Algebraic Representations of SU(n)  DAVID KELLEY (Presenter), Rochester Institute of Technology — The SU(n) groups are Lie groups defined as the set of all unitary n-by-n matrices with determinant 1, whose operation is multiplication. Although defined in terms of matrices, these groups are abstract mathematical structures, and are thus independent of their representation. One representation of SU(n), often used in the standard model of particle theory, constructs the elements using Clifford Algebra. This representation has been shown to be valid for SU(3), but higher dimensions remain unexplored. We investigate such representations of the SU(n) groups.
Enhanced Global Symmetry of N = 4 Gauge Theories in 3d

ZHAOZHEN TONG (Presenter), Department of Physics, Imperial College London — Moduli spaces of some 3d N = 4 quiver gauge theories are studied by computing the Hilbert series of their Coulomb branch. Although this had been recognized as the traditionally difficult branch to study due to quantum correction, development of monopole formula has provided a simple approach to solving the problem. Our work focuses on obtaining the global symmetry of a quiver gauge theory from its Hilbert series. Many of the quivers being studied are A, D, B Dynkin diagrams with a minimally unbalanced gauge node and the results show that their global symmetries have been enhanced to symplectic groups, corresponding to freely generated Coulomb branches. We have made an argument that simplifies the process of identifying symplectic global symmetries. A potential class of quivers is also proposed as a generalisation of some obtained results, and the quiver is compared with some previous work that takes different approaches to the problem, such as brane construction etc. B type quivers are not included in the proposed generalisation, and its symplectic global symmetry may indicate an extension of previous work to non-simply laced quivers.

This work was supported by Department of Physics, Imperial College for undergraduate student research.

Numerical analysis of nonlinear localized modes in vibrational and magnetic lattices

HIEU LE (Presenter), LARS Q ENGLISH, Dickinson College — We numerically investigate the existence of nonlinear, spatially localized modes for various lattice Hamiltonians using Newton-Raphson method to obtain numerically exact solutions. We start by examining the well-known one-dimensional Fermi-Pasta-Ulam lattice with quadratic and quartic potentials and obtain solution branches in both frequency and nonlinear coefficient via continuation. We continue by propagating the solution in time with Runge-Kutta degree 4 (RK4) method. We then turn to two-dimensional ferromagnetic and antiferromagnetic lattices: here intrinsic localized modes were demonstrated in previous research, and more recently the topological magnetic skyrmions has stimulated intense interest. We again apply the Newton-Raphson method to obtain nontrivial solutions for certain spin-lattice Hamiltonians, and then propagate the solution in time with RK4method.

Cosmic Ray Detector Array Project

ANDREW REYES (Presenter), CHRISTIAN HERNANDEZ, ARAM NINO CANIZAL, Hartnell College — Supernovae across the universe eject cosmic rays that impact atomic nuclei in Earth's atmosphere to create secondary particles like muons. In order to measure the cosmic rays and the secondary radiation, we used light sensitive Photomultiplier detectors connected to scintillator sheets by optical fibers enclosed in a light tight box. We assembled multiple detector boxes to measure the high speed muon particles and using 3 different detector boxes we formed an array. The properties of the cosmic ray muons were studied by using a four fold coincidence experimental setup. The detector signals were converted using the DRS4 digitizer and analyzed using CERN PAW package. In this conference, our results of the cosmic ray array would be presented. In addition, we would discuss how the pressure and temperature of the Earth's atmosphere may cause variations in the collected counts of cosmic rays.

Using Eclipses to Probe Physical Conditions Along the Jet in the X-Ray Binary SS433

XINYI LIU (Presenter), Wheaton College, HERMAN MARSHALL, MIT Kavli Institute, DIPANKAR MAITRA, Wheaton College, MICHAEL NOWAK, NOBERT SCHULZ, MIT Kavli Institute, DIEGO ALTAMIRANO, University of Southampton, JACK STEINER, MIT Kavli Institute, THE Galactic X-ray binary SS 433 is the only known astrophysical object to exhibit strong, relativistically red- and blue-shifted emission lines from elements such as S, Si, Fe, Ni. The X-ray emission lines originate in a jet outflow that is launched somewhere very close to the compact accretor (a black hole or a neutron star). Between 2018 August 10-14, SS 433 was observed using the High Energy Transmission Grating Spectrometer system on the Chandra X-ray Observatory, and also using the Neutron star Interior Composition Explorer (NICER) mission aboard the International Space Station. The observations were designed to take advantage of the eclipse and carry out time-resolved spectroscopy and timing studies to infer spatial variation of physical properties such as composition, temperature, and density at different distances along the jet. Preliminary analysis of the Chandra data reveals a plethora of emission lines due to various ionization states of different elements such as Fe XXV, Si XIV, and others. In addition to phenomenological fits to determine properties of the observed emission lines, we will present results from fitting collisionally ionized plasma models, and timing results from NICER.

*We gratefully acknowledge funding from the Chandra Guest Observers Program.

Tuesday, March 5, 2019 11:15 AM - 1:39 PM

Session F69 FGSA FHP: How Physicists Communicate

BCEC 052A - Rachael Mansbach, University of Illinois at Urbana-Champaign - Tag(s): Invited, Undergraduate
11:15AM F69.00001: Whisper Networks in Astrophysics [Invited] CHANDA PRESCOD-WEINSTEIN (Presenter), University of New Hampshire — I will discuss how social media (like Twitter and Facebook) and communications mediums that are social (like Slack) have transformed how physics and astronomy are done. I will specifically discuss whisper networks that circulate rumors about new scientific discoveries as well as information about chronic harassers in our field.

11:51AM F69.00002: Capture Communication of Physicists Through the Archive [Invited] MICHELLE BAILDON (Presenter), Massachusetts Institute of Technology — TBD

12:27PM F69.00003: Sociological Perspectives on the Confirmation, Analysis and Communication of Results in the Physical Sciences [Invited] HARRY COLLINS (Presenter), Cardiff University — TBD

Tuesday, March 5, 2019 12:30 PM - 2:00 PM

Session G71 APS/SPS: Students Lunch with the Experts BCEC Ballroom East/West

12:30PM G71.00001: Students Lunch with the Experts — Students may sign up to enjoy a complimentary box lunch while participating in an informal and stimulating discussion with an expert on a topic of interest to them.

Tuesday, March 5, 2019 2:00 PM - 2:00 PM

Session G70: Poster Session I (2:00pm-5:00pm) BCEC Exhibit Hall - Tag(s): Poster, Undergraduate

G70.00001: UNDERGRADUATE RESEARCH —

G70.00002: Machine Learning Applied to Mult-Electron Events in Scintillator* HARRISON LABOLLITA (Presenter), Mathematics and Physics, Piedmont College, MORTEN HJORTH-JENSEN, SEAN LIDDICK, National Superconducting Cyclotron Laboratory — Conversion electron spectroscopy is a viable tool when studying the nuclear phenomenon, shape coexistence. When a neutron-rich nucleus beta decays, a neutron transforms into a proton and emits an electron. Due to electromagnetic interactions, this can result in the ejection of an electron from the atom, a process called internal conversion. Because this process is essentially simultaneous in time, it is pivotal to differentiate between the electron emitted from the nucleus and the internal conversion electron emitted from the atom. Here we apply supervised machine learning algorithms to distinguish between one and two electron events, as well as determine the origin of the electron. With simulated data, we were able to successfully train a convolutional neural network (CNN) to distinguish between a one and two electron event with 96.79% accuracy. Furthermore, we successfully trained a CNN to predict the origin of the electron for one electron events. Our results show promise that our models’ performance will generalize to experimental data. Once our models are complete, machine learning will be an important data analysis tool for conversion electron spectroscopy.

*Funded by the NSF through Research Experience for Undergraduates at Michigan State University.

G70.00003: Radio Emission of Supernova Remnants in the Large Magellanic Cloud* KAUALANI MANEAFAGE (Presenter), California Lutheran University, JOHN R. DICKEL, Physics & Astronomy, University of New Mexico — A supernova remnant (SNR) is an expanding shell of gas that results from the explosive death of a star. When observing a SNR at radio wavelengths, the object appears fainter in the higher frequencies and brighter in the lower frequencies due to synchrotron radiation. There has not been a complete catalog of SNRs in the Large Magellanic Cloud (LMC), shown in Figure 1. As a result, in May 2017, Luke M. Bozzetto and Miroslav D. Filipović et. al published an article with a catalog of 59 SNRs, using their own measurements and references of other data. Their paper also proposed 15 SNR candidates, all located in the LMC. Their measurements focused on the radio properties of these objects. One of these properties is the spectral index, which is the brightness as a function of frequency, and is shown in Figures 4 and 5. However, some of the objects cataloged and proposed have missing radio data. Using the Astronomical Image Processing System (AIPS) and data previously collected by John R. Dickel, we analyzed the missing radio data for these objects cataloged in the 3-, 6-, and 20-cm radio wavelength bands.

*I would like to thank the National Science Foundation (NSF) for funding the internship and University of New Mexico for allowing me the opportunity to participate in the research.
**G70.00004: Mössbauer Investigation of Hafnium Oxide-Hematite Nanoparticles**

MONICA SORESCU, ABIGAIL FERRIS (Presenter), Duquesne University — Hafnium-oxide-doped hematite, $x\text{HfO}_2(1-x)\alpha\text{-Fe}_2\text{O}_3$, with molar concentrations $x=0.1, 0.3, 0.5,$ and $0.7$ was prepared by high-energy ball milling at sample times of BMT=$0, 2, 4, 8$ and $12$ hours. The Mössbauer spectra of the nanoparticle systems were parameterized using NORMOS-90. It can be said that concentrations of $x=0.1, 0.3$ and $0.5$ show general trends, but once concentration rose to $x=0.7$ the sample had more subspectra, allowing new phases to be identified. Each concentration at BMT=$0$ had one sextet, pertaining to hematite. As the BMT and the concentration of the sample increased, the splitting increased, denoting a greater substitution of the hafnium ions into the hematite lattice. Concentration $x=0.1$ did not show additional splitting until reaching BMT=$4$ hours, where the data split from one sextet to two sextets then split further by BMT=$12$ hours resulting in four sextets and a doublet. Concentration $x=0.3$ was similar, with BMT=$0$ displaying only one sextet but BMT=$12$ hours resulted in five sextets and a doublet necessary for an accurate fit. Concentrations higher than $x = 0.3$ at BMT=$0$ required one sextet and one doublet, but no other time had such a pattern aligned with it.

*This work was supported by the National Science Foundation under grants DMR-0854794 and DMR-1002627.

**G70.00005: Experimental Multi-Photon Quantum Walk on a Directed Graph**

TONG WU, School of Physics, Nanjing University, JOSH IZAAC, School of Physics, The University of Western Australia, ZIXI LI (Presenter), KAI WANG, ZHAOZHONG CHEN, SHINING ZHU, School of Physics, Nanjing University, JINGBO WANG, School of Physics, The University of Western Australia, XIAOSONG MA, School of Physics, Nanjing University — Quantum walks are of crucial importance in the development of quantum information processing algorithms. Recently, another potential application has been proposed, where one could efficiently perform network analysis with quantum walks, especially on vertex centrality ranking. However, it is challenging to rank the centrality of a directed network via quantum walks, since it corresponds to a non-Hermitian Hamiltonian, which leads to non-unitary dynamics and thus cannot be simulated by conventional quantum walks. In this presentation, we solve the non-unitary challenge by introducing pseudo-Hermitian evolutions. We report the first experimental realization of centrality ranking of a directed graph on a photonic platform with multi-photon parity-time-symmetric quantum walks. The experimental results agree well with theoretical predictions.

**G70.00006: Making a Video to Teach a General Audience about Memristors**

EMMA RHODENIZER (Presenter), NADINE GERGEL-HACKETT, Mary Baldwin University — Memristors are a novel nanotechnology with the potential to enable faster and smarter computing. Because of the impact that these nanoelectronic devices could have on our everyday technology, it is important to educate the general public about memristor physics, including their applications and advantages. My research involved learning about the memristor-related work performed by previous Mary Baldwin University undergraduate physics students and then creating a video describing this work to a general audience. The video was made using a combination of Blender animation software and VideoPro video production software, along with still images and audio. My final product is a YouTube video that explains the Mary Baldwin University memristor research and highlights potential future applications of that research.

**G70.00007: Mössbauer Investigation of Molybdenum Trioxide-Hematite Nanoparticles**

MATTHEW KNAUSS (Presenter), MONICA SORESCU, Physics, Duquesne — Molybdenum trioxide-doped hematite, $x\text{MoO}_3(1-x)\alpha\text{-Fe}_2\text{O}_3$ with molar concentrations $x=0.1, 0.3, 0.5,$ and $0.7$ was prepared using high-energy ball milling, taking samples at $0, 2, 4, 8,$ and $12$ hours. The resulting Mössbauer spectra of nanoparticle systems were parametrized using NORMOS-90. At ball milling time (BMT) $0$ hours, each concentration produced a spectrum consisting of $1$ sextet since no lattice substitutions occurred. For all concentrations, a doublet subspectrum emerges from the initial sextet as the BMT increases. For each sample, this appears around BMT $= 4$ hours and is more intense as the BMT increases, indicating the substitution of Fe$^{3+}$ into the MoO$_3$ lattice. Most fits only had $1$ sextet except for concentration $x = 0.1$, BMT 4, 8, and 12 hours, and concentration $x=0.3$, BMT 12 hours. This additional sextet indicates Mo was substituted into the Fe$_2$O$_3$ lattice. The absence of this Mo substitution is due to the difference in ionic radii of Mo$^{6+}$ to Fe$^{3+}$ since the ionic radius of Mo$^{6+}$ is over twice the ionic radius of Fe$^{3+}$. Since the substitution of Fe$^{3+}$ into the MoO$_3$ was more present than the substitution of Mo$^{6+}$ into Fe$_2$O$_3$, the solid solution has a limited mutual solubility.

*This work was supported by the National Science Foundation under grants DMR-0854794 and DMR-1002627.

**G70.00008: ABSTRACT WITHDRAWN**
G70.00009: Investigation of correlation of chemical structure and electronic band structure of Fe-Ga system*  
JEAN ALVAREZ (Presenter), Bergen Community College, KALANI HETTIARACHCHILAGE, The Collage of New Jersey, NEEL HALDOLAAARACHCHIGE, Bergen Community College — Fe-Ga phase diagram is studied in detail to investigate the correlation of chemical structure and electronic band structure. There were 6 different phases reported on this system only one of them studied in detail experimentally and theoretically. We investigated chemical structure and electronic band structure of all other phases. Electronic band structure revealed an interesting detail of Ga rich non-magnetic semiconducting phase transforms into a series of magnetic phases towards the Fe rich side. It also revealed that the physical properties of the materials are very sensitive to the stoichiometry and structural deviations of the phases. This study will provide the groundwork to further studies of this materials and also provide an interesting avenue to investigate verity of new materials with potentially interesting physical properties.

*Department of Education, STEMatics grant, Bergen Comunity College.

G70.00010: Detection and Classification of High Energy Beta Radiation induced Damage of Raspberry Pi Zero intended for OPAL CubeSat*  
JONH MOJICA DECENA (Presenter), JOHN R DENNISON, BRIAN D WOOD, Physics, Utah State University, RYAN MARTINEAU, Space Dynamics Laboratory, MICHAEL J TAYLOR, Physics, Utah State University — Radiation survivability of a Raspberry Pi Zero was studied with extended exposures from 0.2 to 2.5 MeV beta radiation of >200krad of total ionizing dose (TID) while undergoing continuous diagnostic cycles. Determining the threshold for radiation damage of inexpensive commercial-off-the-shelf (COTS) components is critical as a cost-saving method in the construction of spacecraft. Characterizing radiation induced damage of COTS with TID allows for proper precautionary measures to maintain spacecraft functionality over the duration of their mission. The specific point and type of failure due to TID is determined to mitigate deleterious effects through enhanced shielding and software or hardware redundancy. TID in the memory and processor units before system failure was measured, along with type, frequency of error, and possibility of system recovery. Careful determination of heat conduction in vacuo of IC’s was conducted to avoid overheating due to delivered battery power and radiation energy deposition. The results will facilitate construction and design of the USU-led OPAL CubeSat, to determine if this COTS can survive >200krad TID received during its 1-2yr mission in LEO orbit.

*Supported through partial funding from a USU Office of Research and Graduate Studies URCO grant.

G70.00011: Reconstruction of HIPPO Supersonic Gas Jet Target*  
XIANFENG WANG (Presenter), Xi'an Jiaotong University, SHANE MOYLAN, CHRISTOPHER J SEYMOUR, LUIS A MORALES, GWENAELLE GILARDY, DANIEL J ROBERTSON, EDWARD STECH, MANOEL COUDER, Univ of Notre Dame — HIPPO, a supersonic windowless helium gas jet target, is designed and reconstructed as the target for the beam from the 5 MeV 5U electrostatic accelerator located at the Nuclear Science Laboratory (NSL) of the University of Notre Dame. Connected to the target area, St. George recoil separator has been developed to perform, in inverse kinematic, radiative capture experiments of interest to nucleosynthesis. Inverse kinematics, here, means that a heavy ion beam is bombarding a lighter nuclear target. The nozzle-catcher system and chamber have been designed and prepared. A differential pumping system is set up to lower the pressure in the target chamber down to $10^{-7}$ torr in the beamline. The advantages of the windowless design and advantages that gas target compared with the solid target will be discussed. An Arduino based system is set up and now we are able to control the pumps with the touch screen. We have performed the pressure measurement and got the thickness data. Initial experiments are discussed along with plans for future use at the NSL.

*This work is supported by the National Science Foundation and the University of Notre Dame.
G70.00012: Training Neural Networks for Object Recognition Using Blurred Images* AZHAR HUSSEIN (Presenter), Department of Chemical and Physical Sciences, University of the Virgin Islands, XAVIER BOIX, TOMASO POGGIO, Department of Brain and Cognitive Sciences, Massachusetts Institute of Technology — A shortcoming of deep neural networks is that they require a vast amount of data to train. An example of this is object recognition, a computer vision technique for identifying objects in images or videos. We hypothesized that, when training with few data examples, blurring the input images would cause the neural network to perform better compared to non-blurred images, because of the removal of unnecessary details. In this study, we trained a convolutional neural network on the blurred images, varying the amounts of blur in order to determine how the validation accuracy changes. Our preliminary results suggest that blurring the images does not help when learning from few examples; however, we cannot fully disprove the hypothesis because it requires further experimentation with other data sets and convolutional neural network models. In the future, we can use image blurring to study eccentricity dependence, a property of the human visual system that standard convolutional neural networks do not currently replicate. This research will ultimately bring us closer to understanding and replicating how the human brain processes vision.

*This material is based upon work supported by the Center for Brains, Minds and Machines (CBMM), funded by NSF STC award CCF-1231216.

G70.00013: Response of Photoreceptors, Dynamic Modeling of Adaptation and Saturation ANNA SMITH (Presenter), KENNEDI L TURNER, TIRTHABIR BISWAS, Loyola University New Orleans — Photoreceptors have the ability to generate biological responses as a result of stimulation via light. The purpose of this research project is to mathematically model the photoreceptor responses such that we are able to quantitatively capture its key aspects, like the observed adaptation over time and saturation under extreme stimulus. Past photoreceptor models were examined and modified to yield a new dynamic model that was able to provide excellent fits to response of the retinal cells under a variety of stimulus conditions, such as bright and “dark” flashes of light on top of some given initial “background” lighting. Our analysis strongly suggests that just a direct coupling of membrane potential to light is not sufficient to capture the behavior of photoreceptors. Nonlinear coupling between the membrane potential and some “internal” variable that controls adaptation in the cell is necessary to accurately predict the photoreceptor response. On one hand our research may provide insight into the microphysical processes inside the cell, and on the other, help improve exploring the complexities of neural networks.

G70.00014: Electrospun PEDOT:PSS nanoribbon field effect transistor with a ferroelectric polymer gate insulator* ALONDRA ROSARIO (Presenter), NICHOLAS PINTO, University of Puerto Rico at Humacao — Poly(3,4-ethylenedioxythiophene) doped with poly(styrene sulfonic acid) – PEDOT:PSS was electro-spun to produce high aspect ratio nanoribbons. The ribbons of varying thicknesses were electrically characterized in a field effect transistor (FET) configuration with ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a ferroelectric (FE) poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET.

뉴스-RUI-DMR-1800262, NSF-PREM-DMR-1523463

G70.00015: A Schottky diode fabricated by crossing MoS2 with an electro-spun PEDOT-PSS nano-ribbon* KELOTCHI FIGUEROA (Presenter), JOSÉ PEREZ, AHMAD MATAR ABED, IDALIA RAMOS, NICHOLAS PINTO, Physics and Electronics, University of Puerto Rico at Humacao, MENGQIANG ZHAO, ALAN T JOHNSON, Physics and Astronomy, Univ. of Pennsylvania — Monolayer MoS2 was grown via chemical vapor deposition while PEDOT-PSS nanoribbons were fabricated via electrospinning. Each of these materials was electrically characterized separately in a field effect transistor configuration using SiO2 as the gate dielectric. MoS2 exhibited n-type behavior while PEDOT-PSS showed an Ohmic response. By crossing MoS2 with a PEDOT-PSS nanoribbon, the current-voltage curve across the junction was non-linear and similar to that of a diode. When a positive (negative) voltage was applied to PEDOT-PSS (MoS2), the device turned on in the first quadrant of the I-V curve. Reversing the external connections resulted in the diode turning on in the third quadrant. The rectification ratio was 625 and the turn-on voltage was 0.1V. The device output data was analyzed using the standard thermionic emission model of a Schottky junction yielding an ideality parameter of 1.9 and a barrier height of 0.18eV. A low turn voltage from our diode makes it better for small signal detection and has the advantages of having a higher ac rectification efficiency and a lower power loss compared to standard Si or Ge p-n diodes.

*NSF-DMR-PREM1523463 and NSF-DMR-RUI 1800262
G70.00016: Investigation into the Interface Between Salt Solutions and Hydrophobic Surfaces  
ANTHONY FLORIMBIO (Presenter), CAYTON HORNBERGER, ZACHARY ZOLL, ADELE POYNOR, Allegheny College — When water is forced into contact with a hydrophobic surface a depletion layer, a region of low density water, is formed at the interface. In nature surfaces do not deal with pure water, rather instead they interact with various aqueous salt solutions. We study octadecanethiol, a hydrophobic self-assembled monolayer, and mercaptoundecanoic, a hydrophilic self-assembled monolayer, in various aqueous salt solutions. We use contact angle measurements, scanning electron microscopy, and surface plasmon resonance to study the interfacial properties of these surfaces.

G70.00017: Exploring how protamine folds DNA in sperm*  
YUXING MA (Presenter), ADAM D. D. SMITH, ASHLEY CARTER, Amherst College — DNA compaction is crucial for the transmission of genetic information. In sperm, the protein protamine binds to the major groove of DNA and compacts the DNA more tightly than histones. The more highly folded the DNA, the more hydrodynamic the sperm and the more likely it will reach the oocyte without UV damage. To understand the mechanism by which protamine packs DNA, we used an in vitro tethered particle motion assay and video microscopy to visualize the folding of 25 nm DNA. Because this length is shorter than the diameter of a DNA-protamine loop, we did not expect the DNA to fold. However, when we graphed the standard deviation of beads’ motion over time, we found that the standard deviation decreases as protamine concentration increases. Our results suggest that protamine can fold short-length DNA molecules. Understanding the process by which this interaction occurs has applications in male infertility, epigenetics, and nanoengineering.

*Dean of the Faculty Funding from Amherst College, the Cottrell Science Award from the Research Corporation (ARC, Award #23239) and the CAREER award from the National Science Foundation (ARC, Project #1653501).

G70.00018: AFM analysis of protamine-induced compaction in short-length DNA fragments*  
RYAN MCMILLAN (Presenter), LUKA DEVENICA, ASHLEY CARTER, Amherst College — During spermatogenesis, small, positively charged protamine proteins dramatically condense the DNA in the nucleus. This tight compaction both minimizes hydrodynamic drag on the sperm and protects the DNA from ultraviolet radiation. Protamine also is an excellent candidate for use in nanoengineering as a way to self-assemble DNA nanostructures. Here our goal is elucidate the physical mechanism for how protamine causes DNA to fold into a ring of ~50 nm in diameter. To study this question, we used an atomic force microscope (AFM) to image protamine-DNA complexes. By varying the concentration of protamine in the assay, we are able to image the intermediate steps in the folding pathway. We find that short-length (50 nm or less) DNA fragments form half loops that become increasingly more folded as the protamine concentration is increased. Future work will investigate whether this looping is induced by enthalpic or entropic forces.

*This research was supported through the Amherst College SURF Program, the Amherst College Dean of the Faculty, and NSF CAREER Award #1653501.

G70.00019: Simulation of long range ordering in an ionic liquid using molecular dynamics*  
ALEXIS PUYLEART (Presenter), St. Norbert College, EMILY DALBEY, RALPH WHEELER, Northern Illinois University — In the last few years, a startling amount of electronic devices have been recalled due to issues regarding the safety of the battery. This is because the current electrolytes in batteries are volatile and flammable. Ionic liquids are currently being explored as possible alternatives to current electrolytes in lithium ion batteries. As a result, it is important to understand the structure of ionic liquids when lithium is added. Experimental structure factors of N-alkyl-N-methylpyrrolidinium and bis(trifluoromethylsulfonyl)imide (TFSI) from x-ray diffraction data show three peaks at low wavenumber values: a prepeak, a second peak due to charge alternation, and a third peak due to charge adjacency. Molecular dynamics computer simulations were used to calculate structure factors and investigate why the charge alternation peak disappears after adding LiTFSI.

*National Science Foundation REU Grant CHE -1659548
**G70.00020: Electronic Band Structure Studies of Binary Iridates in Ir-Ga Phase Diagram**

DAVID GORDON (Presenter), Bergen Community College, KALANI HETTIARACHCHILE, The Collage of New Jersey, NEEL HALDOLAARACHCHIGE, Bergen Community College — Binary iridates in Ir-Ga system is studied in detail by using the computational method. Correlation of chemical structure and electronic band structure of Ir-Ga are investigated in detail. There were several different phases reported on this systems but none of them were studied in detail experimentally or computationally. Electronic band structure studies revealed an interesting detail of the phases of Ir-Ga systems. This study also suggested that the physical properties of these materials can be tuned by using the stoichiometry and structural deviations of the phases. We also propose that some of the phases could be interesting to search for novel physical properties. This result will generate the enthusiasm of experimentalist to further studies these iridate materials and also open a new avenue to broaden the search for new materials with potentially important novel physical properties.

*Department of Education, STEMatics grant, Bergen Community College.

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**G70.00021: Computational Modelling of the Photo-Field Effect**

WILLIAM SCHENKEN (Presenter), REUBEN T COLLINS, IDEMUDIA AIRUOYO, Colorado Sch of Mines — The photoresponse of a thin film transistor depends on the mode of operation the transistor is in, in an effect known as the photo-field effect. The extent of this effect then depends on the properties of material composing the transistor. This intensity and state dependent photosresponse is explored in amorphous silicon (a-Si) thin film transistors (TFTs) with computational modelling. Results of the numerical simulation agree with observed experimental results. Possible sources of the effect are analyzed and related to parameters in the model. The results from a-Si TFTs are then related to experimental results of TFTs consisting of a-Si embedded with nanocrystalline silicon (nc-Si) quantum dots (the composite material denoted as a/nc-Si), and future work involving a more explicit relationship between the parameters in the model and the properties of a/nc-Si is discussed.

*This research was supported in part by the NSF through award number DMR-1810463.

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**G70.00022: Optimization of Serpentine Micromixers with Non-Rectangular Cross-Sections**

JOSHUA CLARK (Presenter), PETRU STEFAN FODOR, CHANDRASEKHAR KOTHAPALLI, Cleveland State University — Serpentine or spiral-shaped microchannels have been popular choices for microfluidic mixers due to their relatively easy fabrication and possibility for re-use. The technique used in these types of microchannels aims to utilize the cross-sectional transversal (Dean) flows experienced by the fluids as they round a curved channel. Because of the reliance on centrifugal forces the mixing quality is strongly Reynolds number-dependent, with quality mixing occurring only at Re>100. It has been shown that the use of channels with non-rectangular cross-sections can be used as an effective strategy in this type of design to induce mixing at much lower flow rates. In this work, we seek to optimize the geometrical parameters of these channels to maximize their overall mixing performance. The results of the optimization process were obtained numerically through computational solutions of the flow fields and fluid concentration. Experimental results are also included showcasing the increase in mixing quality. We found that our optimized designs substantially outperformed standard serpentine geometries with rapid mixing being achievable down to Re~20.

*This work was supported by the National Science Foundation under Grant No. 1659541 and by Cleveland State University under the 2018 USRA office.

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**G70.00023: Measurement of Adhesion between Nanoparticles and Model Calcite Interfaces**

TAYLOR TROTTIER (Presenter), NANCY BURNHAM, Worcester Polytechnic Institute — The extractive efficiency of primary and secondary oil extraction techniques is generally limited to ~30% of total volume. The most popular and cost-effective secondary recovery techniques are based on the premise of waterflooding, which uses water injection wells to increase subsurface pressure and improve oil yield. Some of the water utilized in these methods is seawater adulterated with surfactants and nanoparticles.[1] In order to accurately predict diffusion of this solution underground it is necessary to understand how modifying seawater chemistries affect the nanoparticles used to tag injection wells. Previous research has shown an inverse correlation between calcium concentration and adhesive forces measured by an Atomic Force Microscope.[2] Adhesion rates between various nanoparticles and a calcite interface were determined using Total Internal Reflection Fluorescence microscopy and single particle tracking techniques.

2. S. L. Eichmann, N. A. Burnham, Calcium-Mediated Adhesion of Nanomaterials in Reservoir Fluids. Scientific Reports. 7 (2017)
**G70.00024: Evidence of Particles During Electrochemical Pd-D Co-deposition**

MICAH KARAHADIAN (Presenter), HEIDE M DOSS, Point Loma Nazarene University — Palladium deuterium co-deposition is used to explore condensed matter reactions. CR-39, a thermoset resin is a well characterized integrative detector that, when etched, shows tracks created by energetic charged particles produced in nuclear reactions. Analysis of tracks provides particle minimum energy and insights into identification (e.g. alpha versus proton). Certain tracks infer neutrons interacting with carbon atoms within the detector, resulting primarily in three alphas (e.g. triple tracks). We report our findings of Pd/D co-deposition on Au wire in an electrolytic cell, and our controls. Our findings imply the presence of nuclear reactions.

**G70.00025: Probing a Mixed Dark Matter Scenario with the CLASS Code**

ADDY EVANS (Presenter), Physics, Oklahoma State University-Stillwater, ROUZBEH ALLAHVERDI, Physics, University of New Mexico — The purpose of our research is to further understand the physical properties of dark matter. We present the physical constraints of a mixed dark matter scenario in which there is a mixture of both warm and cold dark matter. The warm dark matter in our model arises from a non-thermal decay of a heavy particle that occurs when the Universe is \( \sim 0.1-1 \) second old. By using the CLASS code, we have plotted the linear matter power spectrum of these scenarios and compared them to the observed matter power spectrum of Lyman-alpha forests. We find that warm dark matter with a mass of 50 GeV to 450 GeV can exist in fractional amounts, while warm dark matter with a mass of 460 GeV to 1 TeV can potentially comprise the entire dark matter population.

*This work was supported by the National Science Foundation, award number 1659618.

**G70.00026: Room Temperature Field Effect Investigation in SrIrO3/SrTiO3 Thin Films**

ALEJANDRO ZAFRA (Presenter), Department of Physics, California State University, San Marcos, JIAN LIU, Department of Physics, University of Tennessee, Knoxville, STEPHEN A TSUI, Department of Physics, California State University, San Marcos, LIN HAO, Department of Physics, University of Tennessee, Knoxville — Insulating thin films of layered SrIrO3/SrTiO3 (SISTO) have been chosen as a candidate system in which to explore field effect resistance switching, where the application of an electric field induces a reversible change in the electrical resistance. This allows for the possibility of creating a new field effect transistor (FET). The SISTO films were synthesized via pulsed laser deposition. The resistance was measured at room temperature using the 4-wire method. The field effect gate was created by placing an ion gel droplet on the film covered by a sheet of Pt foil. Preliminary data demonstrates the change of electrical resistance of the film upon application of voltage across the ion gel. Future work will include improving the experimental setup to reduce the likely temperature-dependent drift in the resistance measurements and investigating the effects of altering the voltage.

*APS; McNair Scholars Program; Office for Training, Research, and Education in the Sciences (OTRES); Louis Stokes Alliance for Minority Participation (LSAMP)

**G70.00027: Temperature Dependent Self-Assembly of 9,10-dibromo-anthracene on Ag(111)**

CORY F. ASHWORTH (Presenter), TRISTAN D. BLACKWELL, Physics, Radford University, TIMOTHY J. FUHRER, Chemistry, Radford University, THOMAS P PEARL, Physics, North Carolina State University, SHAWN HUSTON, Physics, Radford University — Thin film growth of 9,10-dibromo-anthracene (DBA) on Ag(111) up to a full monolayer has been studied via UHV scanning tunneling microscopy (STM). Prior studies of thin film growth for deposition of this molecule on the same substrate while at room temperature has demonstrated debromination of the molecule followed by self-assembly of a chain-like structure mediated by Ag adatoms [1]. However, our results show no debromination and instead a honeycomb network is formed. The reason for this discrepancy is still under investigation, with present studies focused on accurately cataloguing substrate temperature during film growth. We note that other STM studies of brominated organic molecules grown at reduced substrate temperatures have shown debromination of those molecules only upon subsequent annealing of the film [2]. A molecular model of our film growth will be presented, with the organization of the film most likely driven by weak bromine-bromine bonding between adjacent molecules.

References:


G70.00028: Systems-level Transcriptomic Analyses for Comprehensive Characterization of the IgG3 B Cell Subclass
ANUSH DEVADHASAN (Presenter), Ragon Institute of MGH, MIT and Harvard — Prior studies have suggested that HIV antiviral control may be achieved via the induction of highly polyfunctional IgG3 antibodies (Abs). Here we employ a systems approach to characterize the IgG3 transcriptional profile by identifying intrinsic differences between IgG3 B cells vs IgG1 and IgM B cells that might suggest mechanisms by which B cell molecular circuitry can be programmed to induce and preserve IgG3 Abs. Strikingly, differentially expressed genes between isotype pairs reveal IgG3 is substantially different from other subclasses independent of patent phenotype and time point and subsequently observe clustering by subclass, as opposed to phenotype/time point. Significantly enriched KEGG and Hallmark pathways and GSEA immunological signatures in differentially expressed genes indicate increased activation of basic cellular processes and restriction of transient signaling in IgG3. Therefore this study 1) demonstrates transcriptomic analyses are an effective strategy for characterization of highly homogenous cell subpopulations and 2) offers critical insight into systems level transcriptional signatures of the IgG3 subclass, paving the path for future downstream experiments.

G70.00029: Robust laser frequency drift tracking and data sharing platform to perform qubit calibration for an ion trap quantum computer
SHUQI XU (Presenter), ELI MEGIDISH, WEI-TING CHEN, JOSEPH BROZ, CLEMENS MATTHIESEN, HARTMUT HAEFFNER, Physics, Univ of California - Berkeley — One of the fundamental requirements for using optical transitions as qubits is an accurate control of the phase of the electric field of the laser field driving the qubit transition. For this it is necessary to calibrate the laser frequency accurately. The calibration can be achieved by simple spectroscopy scan of the optical transition. Alternatively, one can use Ramsey spectroscopy achieving a higher signal-to-noise ratio in a given time. However, if the laser frequency jumps significantly with respect to the atomic transition, one may switch by one Ramsey fringe. Here we implement a laser frequency drift tracker for the Ca⁺ quadrupole transition at 729 nm based on the Ramsey method. An algorithm adjusts automatically the Ramsey wait time to stay in tracking range while maintaining the accuracy. In addition, we develop a platform such that different ion trap experiments can share and use tracking results from other ion trap experiments.

G70.00030: Measurements with Position-Momentum Entangled Photons*
ZEENAT BAIG (Presenter), ZOYA SHAFIQUE, SEAN JAMES BENTLEY, Adelphi University — We constructed a system to generate position-momentum entangled photons. These particles interact non locally therefore anything done to one photon affects the other. We produce 405 nm photons that become two entangled 810 nm photons through the process of spontaneous parametric down conversion. We are able to extract data about the position and momentum properties such as joint uncertainties of these photons. The spatial uncertainty was found through near-field detection, a process where we imaged our crystal onto a single slit. Through far-field detection, we were able to get the momentum uncertainty. This involved focusing the beam onto slits which resulted in a fourier transform. Once optimized, we used our system as the basis for a high-sensitivity magnetic field sensor.

*We would like to thank Adelphi University

G70.00031: The Dynamics of Polymeric Microgels with Varying Crosslinker Concentration*
SAMANTHA TIETJEN (Presenter), JACOB ADAMCZYK, KIRIL STRELETZKY, Cleveland State University — Polymeric microgels synthesized by crosslinking amphiphilic polymer chains exhibit a reversible volume phase transition under the effect of environmental conditions such as temperature of a solution. The common behavior of these microgels is to deswell from a large to small size with an increase in temperature above the transition. Microgels in this study were synthesized by crosslinking a polysaccharide in a surfactant solution. When varying the amount of crosslinker by a factor of a hundred, three apparent behavioral regimes emerged from light scattering measurements: at low crosslinker concentrations, microgels deswelled and became more diffusive with temperature increase, at mid-range crosslinker concentrations they didn’t significantly change their size with temperature, and, at high concentrations, microgels showed a reversed behavior, where they grew and became less diffusive with increase in temperature. These apparent regimes are possibly due to nonuniform crosslinker distribution in the polymer microgel, which becomes more prevalent at large concentrations of the crosslinker.

*Special thanks to CSU's Undergraduate Summer Research Award program, and NSF REU Award #1659541 for support.
G70.00032: Models for diffusion and Island growth of hydrogen on graphene  SKY SEMONE (Presenter), University of Pittsburgh, MAJID KARIMI, CARL LEBLOND, Indiana University of Pennsylvania, GIAN FRANCO VIDALI, Syracuse University — A Hydrogen atom can either physisorb or chemisorb on a graphene surface. A model for the diffusion of a hydrogen atom, between nearest neighbor chemisorption sites on graphene surface, is presented. The parameters of the model are optimized against a full set of barriers obtained from the first principles. The energy barrier of the hopping hydrogen is related to the local environment of the hopping hydrogen. In model I, the local environment of the migrating hydrogen include four sites (or 24 configurations). Depending on whether these sites are occupied or empty a total of sixteen configurations (barriers) are required to be calculated. Due to symmetry, only 10 of these configurations are independent. In model II, the local environment of the migrating hydrogen include eight sites (28 configurations). Out of these 256 configurations, a little more than half of them are independent. Models I and II have three and four parameters, respectively. The parameters of the two models are obtained by fitting the barriers to the corresponding ones from the Quantum Espresso code. The comparisons between the models and the first principles would serve as a gauge as to whether extension to a larger local environment is warranted.

G70.00033: Modeling Superconducting Resonators for Astronomical Photon Detection*  DANIEL MORALES (Presenter), Physics, Texas Lutheran University, KARWAN ROSTEM, EDWARD J WOLLACK, NASA GSFC — The current generation of Cosmic Microwave Background (CMB) polarization experiments demand high-performance background-limited sensor arrays to achieve the desired levels of instrument sensitivity. One particularly promising approach, known as MKIDs (Microwave Kinetic Inductance Detector), is based on monitoring the response of a resonator in the presence of radiation with sufficient energy to influence the device's superconducting properties. This sensor architecture is amendable to realizing high focal plane density while maintaining readout with low parasitic thermal loads in a sub –kelvin cryogenic environment. We explore the use of a finite element analysis method solver to carry out electromagnetic simulations of representative sensor geometries.

*Society of Physics Students 2018 Internship Program

G70.00034: Investigation of Nanoparticles Using QCM  CELESTE CISNEROS (Presenter), CARLY NICOLE CUEVAS, Hartnell College — The essential purpose of this research project was to construct and develop a method to quantify nanoparticle concentration using a very sensitive apparatus known as the Quartz Crystal Microbalance (QCM). An airtight glove box was constructed to facilitate sensitive measurements with the QCM. A temperature probe and a inspection camera were added to monitor the environment and the evaporation process of the nanoparticle droplets. The QCM works by a shift in its resonance frequency when small mass of nanoparticles are introduced to it. When the solvent liquid evaporates, the QCM measures the nanoparticle concentration by evaluating the remaining solute residue that is left on the quartz surface. We did extensive measurements using typical alcohol such as methanol and ethanol to determine the sensitivity of the QCM. In this conference we would like to present the data using the QCM with different concentrations of nanoparticles, specifically we would like to present results of titanium dioxide suspensions.

G70.00035: Fabrication and characterization of multicoil neural probes  AMELIA CULP (Presenter), LUKE D'IMPERIO, MICHAEL J NAUGHTON, ANDREW MCCROSSAN, Boston College — There is virtue in long-term neural stimulation for the treatment of symptoms associated with neurological disorders. To date, implanted electrical probes have had great success in mitigating seizures and symptoms of e.g. Parkinson's disease and other pathologies. However, chronic stimulation has proven challenging as electrode performance degrades over time. Alternatively, new technologies are exploring electrical stimulation via changing magnetic fields, harnessing the physical properties set out by Maxwell's equations. Most magnetic neural probes use a single coil design on silicon substrates; multiple coils using substrate materials with increased pliability may improve these technologies. Here, we discuss the modeling, making, and measuring of multicoil magnetic probes microfabricated on flexible polymer substrates for potential long-term neural stimulation. This novel device design is characterized toward the goal of recording of device-driven action potentials in spatially removed neurons.

G70.00036: Phase Transitions in Polymeric Gels Induced by Crosslinking Entropy  JACOB ADAMCZYK (Presenter), MIRON KAUFMAN, KIRIL STRELETZKY, Physics, Cleveland State University — Microgels are polymer-based particles which can change size and shape during volume phase transitions in response to external stimuli. We have specifically investigated microgels which respond to changes in temperature. Hydrodynamic radii were obtained from light scattering data on Hydroxypropylcellulose (HPC) microgels and then modelled with the standard Flory-Huggins theory. We present a numerical study of a thermodynamic theory (M. Kaufman, Entropy, 20(7), 501, 2018) which includes the entropy associated with crosslinking between polyfunctionals and monomers at the ends of linear polymers. This theory predicts a strong first-order transition due to the saturation of possible crosslinks when the number of polyfunctionals is of the same order of magnitude as the number of polymers. We will present numerical results based on this thermodynamic model.

G70.00037: Modeling transport in paper microfluidics  RAYLEIGH PARKER (Presenter), TIM ATHERTON, CHARLES MACE, Tufts University — Paper based microfluidic devices are extremely promising as an inexpensive and highly customizable platform for assays. Flow and particle transport in these highly porous and disordered materials are not well characterized, however, presenting a challenge for the construction of reliable devices that may require well-timed transport of cells and media such as blood. In this work, we identify design and material parameters crucial to transport, and experimentally characterize their influence through a sequence of test devices, where the fluid flow is tracked using our new open-source software package developed for this purpose. Measurements are compared with theoretical modeling to identify the physical processes and relevant timescales involved. Prospects for control and design of future devices will also be discussed.

G70.00038: Development of Cosmic Ray Shower Array and Measurement of the Speed of the Muon  ARAM NINO CANIZAL (Presenter), CHRISTIAN HERNANDEZ, ANDREW REYES, Hartnell College — Supernovae across the universe eject cosmic rays that impact atomic nuclei in Earth's atmosphere to create secondary particles like muons. The muon is an unstable particle that decays quickly and it can penetrate deep into matter. To measure the cosmic rays, we used light sensitive Photomultiplier detectors connected to scintillator sheets by optical fibers enclosed in a light tight box. We assembled multiple detector boxes to measure the high speed muon particles and using 3 different detector boxes we formed an array. In addition, we collected data with a water Cherenkov detector to determine the speed of the muon by varying the distance of separate detectors. By running a program in the Linux OS the speed of the muon was determined and analyzed. In this conference, we present data from our detector array together with our result of the speed of the muon determined to be 99% of the speed of light using the Cherenkov detector.

G70.00039: The Yarkovsky Effect on Near-Earth Asteroid (101955) Bennu, Target of the OSIRIS-Rex Mission: A review of the literature, by Robert Melikyan  ROBERT MELIKYAN (Presenter), Ithaca College — The Yarkovsky effect is a nongravitational phenomenon resulting from anisotropic thermal emissions of rotating asteroids. It took more than 100 years between theory and detection (first seen in asteroid 2489 Golevka in 2003). Now, the near-earth asteroid 101955 Bennu has shown a mean semi-major axis drift da/dt = 284 ± 1.5 m/year due to the Yarkovsky effect. Non-gravitational drift can greatly affect the probability of asteroid impact with earth making accurate modeling of the Yarkovsky effect a high priority for NASA. The OSIRIS-REx mission is currently delivering a satellite into orbit around Bennu. Amongst the mission objectives is the measurement of the asteroid's thermophysical properties that contribute to the Yarkovsky effect, such as the thermal conductivity of the surface. This is important because the observations necessary to measure thermophysical properties from Earth are much more difficult than from a spacecraft platform. Another difficulty is that the highly elliptical orbits of most near-earth asteroids can greatly increase error. Bennu, with the “eyes” of the OSIRIS-REx mission, acts as the perfect aid for observing and understanding the characteristics of this important nongravitational effect that makes asteroid orbits so hard to predict into the future.

G70.00040: Optical Properties of MBE-grown (Bi 1-x Sb x ) 2 Te 3 Thin Films*  PHOEBE KILLEA (Presenter), FRANK C PEIRIS, Kenyon College, ANTHONY R. RICHARDELLA, TIMOTHY PILLSBURY, NITIN SAMARTH, Materials Research Institute, Pennsylvania State University — Spectroscopic ellipsometry was used to determine the dielectric functions of a series of (Bi1-xSbx)2Te3 thin films. The films were grown using molecular beam epitaxy and were deposited on InP substrates. X-ray diffraction, XPS and AFM experiments indicated that the films were of high-quality. Ellipsometry measurements were obtained in the spectral range between 0.05 eV and 6 eV. A standard inversion technique was used to model the ellipsometry spectra, which produced the dielectric functions of each of (Bi1-xSbx)2Te3 thin films. By representing the dielectric function with Kramers-Kronig-consistent oscillators, the fundamental band gap and the higher order transitions of these films were obtained. A Drude oscillator, which represents the absorption of free carriers, was needed to model some films.

* The work at Kenyon is funded by DMR-1609245 and the work at Penn State is funded by DMR-1539916
G70.00041: Developing an Interactive Demonstration for the Science of Smell  
CARISSA GIULIANO, MATTHEW WRIGHT (Presenter), Adelphi University — We present our work towards developing an interactive demonstration for middle school and high school students on the science behind how we smell. We will discuss the results of our literature search which shows there are three models for how we smell: the Lock and Key model, the Vibration Theory model, and the most widely accepted model that combines the two. We will discuss how we plan to demonstrate these three concepts to young science students and how we plan to use it as a tool to generate interest in science.

G70.00042: Progress toward Coherent Control of Ultracold Collisions with Frequency-Chirped Laser Light*  
OLIVIA CHIERCHIO, ZAFIR MOMIN, MICHAEL ROBBINS, AREEBA KHALID, MATTHEW WRIGHT (Presenter), Adelphi University — Frequency-chirped laser light as recently been shown to coherently control collisions and photoassociation. We are planning to use short (~ 3 ns), intense (> 100 mW/cm²), frequency-chirped (~1 GHz in 6ns) laser light to control excited-state collisions between Rb atoms in a MOT. We will discuss our progress towards this aim, including stabilization of our MOT and our computer control system.

*National Science Foundation Award Number: 1803837

G70.00043: ABSTRACT WITHDRAWN

G70.00044: The Effects of Ionized Impurities on the Nanoscale Spatial Distribution of the Schottky Barrier  
STEVEN GASSNER (Presenter), JACK ROGERS, HYEONSEON CHOI, WESTLY NOLTING, VINCENT LABELLA, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Albany, NY — The influence of ionized impurities in the semiconductor upon the local Schottky barrier height of a metal-semiconductor interface is important for contacts in nanoscale devices. A computational model simulates spatially-resolved measurements of the electrostatic potential of various metal-semiconductor interfaces acquired using ballistic electron emission microscopy (BEEM), an STM-based technique. The model assumes a uniform charge density with a set of point charges close to the interface, and generates simulated datasets in the form of Schottky barrier height maps and histograms. The introduction of localized charges causes skewing of the distributions, which are compared to BEEM measurements of Au/Si and Cu/Si Schottky barrier height maps.

G70.00045: A High Power Set-up to Test Optical Coatings  
ANDREW POVERMAN, BRUNO BECHER (Presenter), LOGAN KAEUBLING, ISOBEL CURTIN, RITI BAHL, ANTONIOS KONTOS, Bard College — To detect gravitational waves, the LIGO detectors need to limit the noise from multiple sources. Noise related to the quality and characteristics of the coating that is used on the test masses is one of the most important and most difficult to mitigate. Significant effort is invested in finding new types of coatings that satisfy the many stringent requirements of LIGO, which include low thermal noise, low scattering and low absorption. In addition, these coatings need to withstand high CW power without exhibiting any significant deterioration. It is therefore crucial to develop optical set-ups that will measure all the relevant coating properties, and under conditions similar to LIGO. Here we describe one such set-up at Bard College. The main characteristics of our set-up include a high finesse cavity inside an ultra-high vacuum chamber, in which mirror samples will be tested for scattering and aging over long periods of time.

G70.00046: Directed Self-Assembly of Nanoparticles under Electric Fields  
MATTHEW WITHERS (Presenter), MITCHELL ROBERTS, DAN MAZILU, IRINA MAZILU, Department of Physics and Engineering, Washington and Lee University — We develop an experimental and theoretical approach to study the effect of electric bias on particle-coverage densities produced during nanoparticle self-assembly. Experimentally, we utilize a parallel plate capacitor to allow for the application of a uniform external electric field during the self-assembly of SiO₂ nanoparticles on glass slides. We refer to this procedure as directed self-assembly of monolayers (DSAM). To determine particle-coverage densities, we use scanning electron microscopy. In our theoretical analysis, we modify existing cooperative sequential adsorption models to account for diffusion under an applied electric field. We then apply the mean field approximation to these modified models to obtain master equations, which we solve for particle-coverage densities. To ascertain the validity of these models, we compare computer simulations produced using our theoretical approach to our experimental data.
G70.00047: Modeling Senate Voting Behavior using Mathematical Modeling.  
ANTHONY LORSON (Presenter), SHO GIBBS, JUSTIN PUSZTAY, Washington and Lee University, WILL HANSTEDT, Rockbridge County High School, IRINA MAZILU, Washington and Lee University — Using purely quantitative methods to analyze and explain Congress’ actions is rare, yet has the potential to be extremely valuable. We aim to model the voting patterns of the Senate by adapting the Ising model and incorporating economic game theory, with each individual senator being a node with a voting-state and a partisanship value. Our assumptions include symmetry between voting yes and no before the introduction of partisanship and a lack of an external field. The coupling constants of the Ising model reflect the nature of the issue at hand and are individualized for each senator, reflecting their own partisanship as well as the positions of senators who interact with them. The stochastic model was run using Monte Carlo simulations in Python, with several different graph types allowing for multiple ways for senators to be connected to one another. By looking at the properties of the graph such as magnetization and correlations between nodes, we hope to gain insight into how the Senate operates.

*Washington and Lee Summer Research Scholars and the Washington and Lee 2-Year Fellows Program.

G70.00048: Using an Arduino in a Coupled Logistic Map Circuit to Explore Basins of Attraction for Symmetry-broken States  
MOYI TIAN (Presenter), HOUSSEMEDDINE MHIRI, LARS Q ENGLISH, Dickinson College — L’Her et al. [1] recently constructed a circuit designed to implement the logistic map electronically, and thus generated bifurcation diagrams in growth rate, \( r \), as well as in coupling parameter, \( \varepsilon \), for two coupled maps. We show that in the coupled logistic-map system, the dynamics is not only determined by \( r \) and \( \varepsilon \), but also by the initial conditions, due to the multi-stability of different solutions. By experimentally adding control over initial conditions and incorporating an Arduino Uno Microcontroller, we explore basins of attraction associated with symmetric states, symmetry-broken states and phase-shifted states.


G70.00049: Implementation of a Causal Spectral Decomposition Representation for the Neutron Star Equation of State for Gravitational Wave Parameter Estimation*  
DEVON NOTHARD (Presenter), LESLIE WADE, Kenyon College — On August 17, 2017 LIGO observed a binary neutron star merger 130 million lightyears away by detecting ripples in the fabric of spacetime called gravitational waves. Information about the neutron star equation of state (EOS), an equation relating the state variables of a system, is encoded in these waves. Currently the neutron star EOS is highly unconstrained. However, constraining this equation through gravitational wave measurements may provide us unprecedented knowledge about a naturally occurring source of nuclear matter at densities unachievable in a laboratory. Theoretical physicists use knowledge of microscopic and thermodynamic properties of nuclear matter in order to invent potential candidate EOSs that are consistent with current neutron star observations. Prior to LIGO’s monumental discovery, NS observations and EOS constraints came exclusively via optical telescopes. However, we can extract NS EOS information from gravitational waves as well. In this project, I incorporated an EOS model with physical conditions such as causality and thermodynamic stability built in. I have developed software that will be incorporated into LIGO’s parameter estimation algorithms to measure the neutron star EOS from future gravitational wave observations using this model.

*Kenyon College

G70.00050: 3-Color Two-Beam Broadband Nonlinear Frequency Mixing: From Physics to Applications for Spectroscopy*  
BENNY SCHUNDELMIER (Presenter), LASZLO JANOS UJJ, University of West Florida — We report the theoretical summary of 3-color two-beam broadband nonlinear frequency mixing by using the double-sided Feynman diagrams and the phenomenological picture of the light matter interactions. We measured the intensity dependence of the signal beam via excitation beams and recorded the scattering spectra that originated from molecular solutions and crystals. Pure vibrational spectra were extracted from the measured spectra with model independent phase retrieval methods. We have used our spectroscopy system published recently [1] to characterize the method. We showed that the method is extremely useful to measure molecular vibrational and vibronic spectra in the low frequency, terahertz range.


*The authors acknowledge the financial support from the Department of Physics and the UWF Office of Undergraduate Research.
G70.00051: HIV-1 Gag Protein Nanoparticle Systems: Assembly and Viral Inhibition Strategies*  JAIME GARCIA (Presenter), Physics, St. Mary's University, Texas, DANITZA VASQUEZ, DELVIN CARABALLO, Chemistry, University of Puerto Rico- Rio Pierdas, DELANEY ALEJANDRO, Esc Brígida Alvarez High School, DANIEL RAMOS-PEREZ, MARVIN BAYRO, Chemistry, University of Puerto Rico- Rio Pierdas — Current drug therapies available to individuals infected with the HIV-1 virus work to target reverse transcriptase and the viral protease via a drug cocktail. However, during the process of maturation in HIV-1, viral protease cleaves Gag and initiates conformational changes in CA proteins which foster its assembly into the capsid, a fullerene shaped shell composed of ~1500 copies of CA. This capsid houses the viral genetic information and poses as a viable target for treatment to combat the virus. Current knowledge of the mechanisms and processes of this conformational shift is very limited. To enhance our understanding of the process of maturation we studied the effects of protein crowding by constructing Gag virus-like particles (VLPs) alone (control), in the presence of C-terminal capsid, cytochrome-c, lipids, and ribonucleic acid so we can study the effects the presence may have on Gag's ability to self-assemble. Our results indicate that Gag retains its ability to self-assemble into VLPs despite protein crowding effects and competitive inhibition of its dimerization interface.

*Supported by the NSF Grant 1757365 to University of Puerto Rico- Rio Pierdas.

G70.00052: Molecular Dynamics Simulations of Patterned Complex Coacervates  NATALIA MARKIEWICZ (Presenter), Chemical Engineering, University of Illinois at Urbana-Champaign, TYLER LYTLE, Chemistry, University of Illinois at Urbana-Champaign, CHARLES E. SING, Chemical Engineering, University of Illinois at Urbana-Champaign — Complex coacervation is the liquid-liquid phase separation of polyelectrolytes in aqueous salt solution into a polymer-dense phase (coacervate), and a polymer-dilute phase (supernatant). These materials are simplified analogues of membraneless compartments in cells, where the sequence of charge has been altered to alter resistance to the presence of salt. Previous work using Monte Carlo simulations demonstrated that changing the sequence of charged and neutral monomers while keeping the charge fraction constant alters the phase separation. We have run molecular dynamics simulations to elucidate the interplay between charge fraction and charge sequence, showing comparisons to existing Monte Carlo simulations and experimental data demonstrating that charge blockiness enhances phase separation. This model is then used to demonstrate the structural effects of varying the charge fraction, in particular showing the emergence of microphase separation at low salt concentrations for blocky polyelectrolytes.

G70.00053: Analysis and Comparison of Light Intensity Spectra Using Wavelet and Fourier Analysis.  BRIENA FELTNER (Presenter), JOSEPH TROUT, Richard Stockton College of New Jersey — This is a continuation of research on the analysis of light intensity spectra of stars that began in the Fall 2017. Using Fourier Analysis and Wavelet analysis, both are typically used for analyzing stellar light curves, a comparison of the recorded light spectra can be made between a space telescope and a ground telescope. Long term, continuous time series of light intensities are needed for the analysis of astronomical phenomena such as the orbit of previously unseen planets. Since the space telescope time series records are sometimes missing data, it has been suggested that land based telescopes can be used to fill in the missing data. This poster presents the comparison of data collected and analyzed with Fourier Analysis and Wavelet analysis.

G70.00054: Morlet wavelet analysis of planetary atmospheres.  VATSALA ADILE (Presenter), ESPEN FREDRICK, DARSA DONELAN, Gustavus Adolphus College — This study investigated the use of Morlet wavelet analysis in the detection of gravity wave structure in the atmosphere of terrestrial bodies, primarily Mars, Venus, and Titan. Atmospheric profiles from data collected by planetary probes and satellites were processed to generate 2D images of wave structure in each analyzed atmosphere. The analysis shows a correlation between vertical wave structure at altitudes and wavelengths to those previously found using other methods such as comparing temperature gradient profiles to the dry adiabatic lapse rate. This suggests the use of Morlet wavelet analysis as a viable alternative to previously used methods for detection of small-scale variability.

G70.00055: The Coefficient of restitution by Microcontrollers*  THY DOAN MAI LE (Presenter), DAN A. BRIOTTA, Physics & Astronomy, Ithaca College — The project began with the traditional setup for a coefficiency of restitution experiment that is failing and has been abandoned by students of Advanced Lab, which was a call for a major upgrade. After the project is complete, the experimental set-up now has a completely new circuitry with calibrated frequency responses, the ability to handle a wider range of inputs, a digitizer circuit, an Arduino and an accompanying program for data acquisition and a Python GUI that takes in data via serial connection from the Arduino, plots the live data and analyzes it to find the coefficient of restitution. The goal of the project was to reignite students' interest in the classical experiment, expose students to microcontrollers and give students an opportunity to learn how to program parts of a system to work together, all at a very small cost compared to previous setups using NI devices and Matlab interfaces.

*This project was supported by Ithaca College's Department of Physics & Astronomy, the School of Humanities & Sciences' Summer Scholars Program and the Dana Internship program of Ithaca College.
G70.00056: Effects of structural order on magnetic properties of $S = 1\ \left[\text{Ni(HF}_2\text{)(pyz)}_2\right]\text{PF}_6\ (\text{pyz = pyrazine})^*$

ASHLEY GLOVER (Presenter), JAMIE MANSON, Chemistry, Eastern Washington University, SAM CURLEY, ROBERT WILLIAMS, PAUL GODDARD, Physics, University of Warwick, JOHN SINGLETON, NHMFL, Los Alamos National Laboratory, SAUL H. LAPI DUS, Advanced Photon Source, Argonne National Laboratory, ROGER JOHN SON, PASCAL MANUEL, ISIS Pulsed Neutron Source, Rutherford Appleton Laboratory, WEI ZHOU, National Institute of Standards and Technology, NIST Center for Neutron Research, JESPER BENDIX, University of Copenhagen, Chemistry — We have discovered a third polymorph in the $\left[\text{Ni(HF}_2\text{)(pyz)}_2\right]\text{PF}_6$ family of coordination polymers. As compared to the previously published structures that possess structurally ordered frameworks $^1$, a new example features a disordered, monoclinic unit cell. This new variant allows us to examine the effects of structural order and disorder on superexchange pathways, specifically along the Ni-FHF-Ni and Ni-pyz-Ni directions. We consider the local distortions to the Ni(II) coordination sphere and the geometries afforded by the ligands. This presentation will address the possible discrepancies in magnetic properties for these polymorphs as gleaned by examination of their structures.


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G70.00057: Applying Machine Learning to Ultrasound Computational Simulations to Determine Scattering Location

NAOMI BRANDT (Presenter), NGUYEN NGUYEN, MARIA TERESA HERD, Mount Holyoke College — In the field of ultrasound imaging, it has been theorized that imaging noise, known as speckle, may be the product of unresolvable scatterers. This would result in certain speckling patterns revealing themselves over large datasets, which could be utilized to predict the early formation of tumors. Such a dataset would be difficult to analyze by hand, but machine learning algorithms can be used to recognize these patterns in an effective manner. As of now, few attempts have been made apply machine learning to predict scatterer placement from ultrasound scans.

We have constructed a computational simulation which consistently and accurately reproduces experimental data, and can be used to train a machine learning algorithm. Using Field II, a Matlab-based program for ultrasound modelling, simulations were created to replicate data produced from experimental phantoms composed of glass beads and agarose gel. Simulations were designed to account for bead placement and size, as well as experimental conditions. Comparisons between simulated and experimental data using statistical analysis show that computational methods can accurately predict ultrasound images. This verification allows us to begin training a machine learning algorithm using both simulated and experimental data.

G70.00058: Field Electron Emission of Hafnium Carbide*$^*$

MORGAN CHAMBERLAIN (Presenter), Linfield College, WILLIAM MACKIE, JOSH LOVELL, Applied Physics Technologies — Hafnium carbide, or HfC, is a robust material whose high melting point makes it an advantageous electron source for a variety of uses, including imaging. This research focused on the effects of an applied field at high temperature on HfC crystals, which induces a faceting effect over time. The cause of this faceting was studied to determine whether it could be correlated to evaporation or self-diffusion during use. The method for electrochemically etching hafnium carbide cathodes was also optimized, and the crystallographic geometry of the tip surfaces was studied using field emission microscopy.

$^*$M.J. Murdock Charitable Trust (through the Lynwood W. Swanson Scientific Research Grant)

Applied Physics Technologies

G70.00059: Comparison of Capacitance-Voltage, Current-Voltage, and BEEM Measurements of Metal-Graphene-Semiconductor Schottky Barrier Heights

HYEONSEON CHOI (Presenter), JACK ROGERS, STEVEN GASSNER, WESTLY NOLTING, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, VINCENT LABELLA, Nanoscience, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute — Capacitance-voltage, current-voltage, and ballistic electron emission microscopy (BEEM) measurements were performed to determine the Schottky Barrier Heights of Au/Si and Au/graphene/Si samples. In addition, measurements were performed on a commercial diode for reference. Data were acquired as a function of temperature, which indicate that the graphene had little effect upon the barrier heights that were measured.
G70.00060: Self-Assembly of Spheres on a Cone Surface  
TALHA REHMAN (Presenter), Berea College, NABILA TANJEEM, VINOTHAN N MANOHARAN, Harvard University — Self-assembly in confined space can lead to formation of unique 3-D structures. We study self-assembly of submicron-sized colloidal spheres on the surface of a micron-sized cone. Fabrication of micron-sized cones is challenging using conventional photolithography. We explored alternative techniques for fabrication of cones. By using a 3-D laser lithography tool called Nanoscribe, we successfully manufactured cones of various cone angles and diameters. By using a micropipette puller, we pulled glass capillary tubes into cones with very smooth surfaces. We performed experiments to self-assemble colloidal spheres on both types of conical surfaces. To assemble spheres, we use depletion interaction. It results in a short-ranged attraction between the spheres, and between the spheres and the conical surface. We observed crystal growth on the cones that were fabricated from glass capillary tubes. This result suggests that a smoother cone surface is preferred to study self-assembly on a cone using depletion interaction.

G70.00061: Measurement of the Tissue Properties of Three Cell Lines using Quantitative Ultrasound*  
PENELOPE TAYLOR (Presenter), AMY LONGSTRETH, MARIA TERESA HERD, Mount Holyoke College — We are measuring the ultrasonic characteristics of cells to find the fundamental differences between cancerous and non-cancerous cells by calculating and comparing the attenuation and speed of sound. We are comparing both the attenuation and the speed of sound because these properties are dependent on the medium being used, and thus should have differences in their ultrasonic characteristics. In this experiment, the three cell lines being used are prostate cells, cancerous colon cells, and cancerous prostate cells. To test for these differences, we are using unfocused transducers of 5, 10, and 15 MHz to find the data for the cumulative range of 2 to 18 MHz. These transducers are placed in water and aligned for optimal wave amplitude travelling between them. The results of the comparisons of cell lines shows a noticeable difference between colon cancer and the other two cell lines, prostate and prostate cancer. The difference between prostate cells and prostate cancer cells is much less significant. This research may lead to the ability to better detect whether lesions are cancerous or non-cancerous using the non-invasive method of quantitative ultrasound.

*Mount Holyoke Lynk UAF

G70.00062: Systematic Removal of Self Assembled Monolayers from Au(111) surfaces, investigated via Atomic Force Microscopy and Contact Angle Measurements*  
INDRAJITH SENEVIRATHNE (Presenter), KELLY M GERRITY, Lock Haven University of Pennsylvania — Self-Assembled Monolayers (SAMs) of thiols on Au(111) surface on mica substrates are used in many instances to study various proof of concept devices such as Nanosensors and Nanoelectronics. However, once used, the Au on mica substrate, upon which the SAM layer sits on, is discarded as surface integrity could deteriorate in the cleaning steps. We have used combinations of organic solvents to critically clean and gently remove the SAM surfaces from the Au(111) substrates. Subsequent surfaces were investigated using Atomic Force Microscopy (AFM) and the Contact Angle measurements. Results were compared with Au(111) surface before SAM deposition and after SAM removal. We have used 1-Dodecanethiol as our SAMs on Au(111) surface. AFM was used in intermittent contact mode to image the investigated surfaces. Discussion of the results obtained compared with the existing literature will follow.

*Lock Haven University Nanotechnology Program and Lock Haven University Nano Club.

G70.00063: Optical Tweezer Measurements in Chlamydomonas*  
MAURICIO GOMEZ (Presenter), CORBYN JONES, WYLIE AHMED, California State University, Fullerton — Optical tweezers have been used to study force fluctuations in microscopic systems and to determine the physical properties of complex materials. We implement two calibration methods, the photon-momentum method and the active-passive method, to measure displacements and forces at the nanometer and piconewton scales. Here, we study the force fluctuations of chlamydomonas microswimmers by applying the photon-momentum method. We calculated the stochastic force spectrum (P_{total}) by estimating the power spectral density of the fluctuating force signal. We apply a theoretical framework to extract the non-equilibrium microswimmer forces from the total force spectrum. We then apply a spectrogram analysis to understand the frequency-time dynamics of the chlamydomonas microswimmer. We hope to extract the force kinetics of the agella and molecular motors.

*CSUF Dan Black Family Fellowship
G70.00064: Conductivity vs. Temperature Measurement for PEDOT:PSS
JOSE PERALTA (Presenter), MADISON GUERRERO, PATRICK MILAN, LAYLA LOGLETREE, PROF WEINING WANG, Seton Hall University — Conducting polymers can be applied to a broad range of specialties, such as solar cells, light-diodes, sensors and other optoelectronics. In particular, poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), a conducting polymer, is the most popular due to its high conductivity and stability. It has been used widely as contact material in solar cells, which may operate at different temperatures other than room temperature. Because of this, it is important to examine how the polymer, and its characteristics, are affected at different temperatures, which ultimately affect the performance of the polymer and its application in solar cells.

In this study, we show the temperature dependence of conductivity measurement of the PEDOT:PSS. The PEDOT:PSS samples with different conductivities were studied under different temperatures, using a temperature-varying device. It was found that the PEDOT:PSS samples exhibit an Arrhenius behavior as a function of temperature ($\sigma = \sigma_0 \exp(-E_a/kT)$).

From the results that we collected we were able to obtain the activation energy of the samples.

* Cottrell College Science Award

G70.00065: Development of Apparatus for Simultaneous Measurement of Photocurrent and SHG
AUSTIN KACZMAREK (Presenter), LIUYAN ZHAO, University of Michigan — Many studies have been done investigating the second order nonlinear response of noncentrosymmetric materials to gain insight to the electronic structures of these materials. Photocurrent and optical second harmonic generation (SHG) are two second order nonlinear phenomena that share the same form of the second order nonlinear susceptibility tensor but are sensitive to distinct energy regimes of the electronic structure of the material under investigation. We present the development of an experimental apparatus for the simultaneous measurement of these two nonlinear phenomena using an ultrafast laser-based scanning approach. We show that the laser scanning provides a spatial resolution of these two nonlinear responses down to the optical diffraction limit, and the confocal imaging scheme adopted in our design assures a constant incident electric field over a wide scanning area. We also discuss our effort in enhancing these nonlinear responses, by compressing the laser pulse to its transform limit. Finally, we will discuss future opportunities brought by this apparatus, such as developing time resolved scanning nonlinear optical techniques.

G70.00066: Looking for Variability in Cygnus X1
BAILEY CONRAD (Presenter), ALEX STORRS, Towson University — We present observations of HDE 226868, the companion to Cygnus X-1. Low resolution (R=4.3 Å per pixel) spectra of the visible region, 6500 Å to 3000 Å, made with Maryland Space Grant Consortium’s 0.5-meter telescope at John Hopkins University over the summer. This region includes emissions from hydrogen and helium which are shown to be time variable by Gies et al. (2003). We examined these spectra for variability.

References:

G70.00067: Understanding the determination factors of the formation of large flocks of swimming sperm in viscoelastic fluid
JELANI LYLES (Presenter), North Carolina Agricultural and Technical State University, DANIEL SUSSMAN, Syracuse University, SOON HON CHEONG, SUSAN S SUAREZ, Cornell University, M. LISA MANNING, Syracuse University, CHIH-KUAN TUNG, North Carolina Agricultural and Technical State University —

When bovine sperm swim in viscoelastic fluid, they form dynamic clusters that coexist with individually swimming sperm in a steady state. By tuning the viscoelasticity of the fluid, we are able to generate clusters in the size of ~20 cells. By using a pulse of flow to align them upstream momentarily, we were able to generate large flocks, from a range of 60-200 cells. This large flock formation is also known as mass motility in a clinical setting, which is used for semen motility evaluation from bulls and other ruminants in the field for veterinarians, where environmental control is not available, and sperm die quickly on an optical system. We employ a numerical self-propelled particle (SPP) model to identify the factors that lead to bigger flock formation, or better mass motility. Our model includes nearby sperm orientation alignment and attraction, volume exclusion, and heterogeneity among cells. We will compare the data from the numerical model with the experiments.

*NSF-HRD-1665004, APS Bridge Program MSI Travel Award.
G70.00068: Synthesis and Characterization of Cobalt Ferrite (CoFe$_2$O$_4$) Magnetic Nanoparticles by Ball-Milling and Sol-Gel Techniques

THOMAS LONGO (Presenter), Physics Department, Villanova University, BRYAN EIGENBRODT, Chemistry Department, Villanova University, JEREMY CARLO, ARTHUR VIECAS, GEORGIA C PAPAEFTHYMIOU, Physics Department, Villanova University — Magnetic nanostructures play an important role in nanotechnology allowing for technological advances in electronic devices, photocatalysis, sustainable energy, biotechnology and medicine. In particular, cobalt ferrite (CoFe$_2$O$_4$) magnetic nanoparticles (MNP) have strong uniaxial magnetic moments, which allow for applications in hyperthermia and targeted drug delivery. Therefore, these particles were synthesized using two different techniques: mechanochemical ball-milling and sol-gel. Using Mössbauer Spectroscopy, X-Ray diffraction, Transmission Electron Microscopy, SQUID magnetometry, and Specific Absorption Rate (SAR) measurements, their magnetic, structural, and thermal transfer characteristics were analyzed and compared to maghemite (gamma-Fe$_2$O$_3$) and magnetite (Fe$_3$O$_4$) MNPs. In addition, for cobalt ferrite nanoparticles to be used within the body they must be rendered bio-compatible through surface ligand exchange processes in order to avoid being targeted by the body's auto-defense system. Therefore, different ligands were experimented with to determine an optimal coating for usage in the body.

G70.00069: Establishing Monomer vs. Aggregate Composition of Squaraine-Based Organic Photovoltaics Using Atomic Force Microscopy

ADRIANA CRUZ (Presenter), CATHERINE RYCZEK, Physics, Hamilton College, ZHILA HOOSHANGI, SOUMYA GUPTA, CHRISTOPHER COLLISON, Chemistry, Rochester Institute of Technology, KRISTEN BURSON, Physics, Hamilton College — Organic photovoltaics (OPV) offer exciting possibilities for energy production and in optimizing OPV devices, a greater understanding of the organic solar cells' morphology is needed. Structural order is thought to improve charge mobility and energy transfer. Here we present a method for determining the monomer vs. aggregate composition for squaraine-based thin films using measurements of each film's absorptivity, thickness, and area. Population can be measured through absorption measurement, provided that the extinction coefficient of the species in question (aggregate or monomer) and the path length for the light through the sample are known. Therefore the ability to measure populations depends on an accurate values for the film thickness, typically 50-150 nm. We employ atomic force microscopy (AFM) to measure film thickness and assess two techniques for removing thin-film material to establish accurate heights. Both techniques yield consistent height data and we discuss their merits. AFM measurements yield average thickness measurements for each type of film with an uncertainty under 17% and area measurements with an uncertainty under 3%. These low uncertainties are crucial as they allow for the monomer to aggregate population to be measured with a high level of precision.

G70.00070: Development and Characterization of a Prototype Cosmic Microwave Background Calibration Target

DAVID STILWELL (Presenter), DAVID B GREENE, DAVID CHUSS, MARTIN DEGEORGE, Villanova University, KARWAN ROSTEM, EDWARD J WOLLACK, NASA Goddard Space Flight Center — The capability to construct devices that have low reflectance (and high absorptivity) of electromagnetic radiation at long wavelengths has many potential applications ranging from radar evasion to EMI control to calibration of sensitive detectors for cosmology. In cosmology, characterization of the spectrum and polarization of the cosmic microwave background, the afterglow of the Big Bang, requires measurements that are accurate to one part in 10$^7$. We describe the fabrication of a prototype cosmic microwave background calibration target that consists of an array of 169 cones, each constructed of loaded epoxy that is molded around an aluminum core for mechanical attachment and thermal stability. By testing the target over a range of frequencies, we achieved a reflectance of -50 dB. These processes were developed as a key technology to support a future NASA space mission to measure the spectrum and polarization of the cosmic microwave background to probe the physics of the early universe.

G70.00071: Schottky diode based on large area CVD-grown WSe$_2$

AHMAD MATAR ABED (Presenter), ANAMARIS MELENDEZ, NICHOLAS PINTO, IDALIA RAMOS, Physics and Electronics, University of Puerto Rico at Humacao — Two-dimensional transition metal dichalcogenides have attracted great attention due to their unique optoelectronic applications. Of these, tungsten diselenide (WSe$_2$) is a semiconductor with a trigonal structure, and a small bandgap ~1.6eV. Here we report electronic transport measurements of CVD-grown WSe$_2$ configured as a Schottky diode. To prepare the device, the WSe$_2$ film was transferred onto an n-doped Si/SiO$_2$ wafer with pre-patterned gold electrodes over the oxide surface. The diode parameters were analyzed using the standard thermionic emission model of a Schottky junction. Results obtained at room temperature include a forward turn-on voltage of ~0.46 V, ON to OFF current ratio at ± 1 V of ~1100, barrier height of 0.41 eV and an ideality parameter of n~1.3. The device was tested as a half-wave rectifier showing a rectification ratio of 1150 with an output/input voltage ratio of 46.3%. Efforts to investigate the temperature-dependent transport mechanisms of the device will also be presented.

*The WSe$_2$ films were provided by the PSU 2DCC-MIP, which is supported by NSF cooperative agreement DMR-1539916. Research at UPRH was supported by NSF under grant NSF-DMR-1523463 (PENN-UPRH Partnership for Research and Education in Materials).
G70.00072: In-vitro effects of low intensity ultrasound exposure on prostate cancer cells* BARBARA MARQUEZ (Presenter), MARIA TERESA HERD, Mount Holyoke College — Ultrasound has been utilized in diagnostic and treatment of cancerous lesions. Most research focuses on high intensity focused ultrasound (HIFU) as a viable treatment option; however, there have been studies showing cell apoptosis due to low intensity ultrasound exposure. We have thus studied the effect of low energy ultrasound on cancerous prostate cells compared to healthy prostate cells in vitro. We report on the intensity of ultrasound reaching the cells and attenuation through cell culture flasks. Our study compares cell counts before and after ultrasound exposure with accurate energy measurements as a function of frequency.

*Mount Holyoke College

G70.00073: A Novel Application of Focused Ultrasound for the Treatment of Port Wine Stain Birthmarks KRISTEN DOUCETTE (Presenter), Department of Chemistry and Physics, Simmons University, JOHN O’MALLEY, Department of Dermatology, Brigham & Women’s Hospital, PHILLIP JASON WHITE, Department of Radiology, Brigham & Women’s Hospital — Annually, 0.3-0.5 % of the population is born with a Port Wine Stain (PWS) birthmark. A PWS is a capillary malformation that results in a visible, localized vascular lesion. This lesion is characterized by an increased number of dilated capillaries that give the PWS its red discoloration. The gold standard of PWS treatment is photothermolysis with Pulsed Dye Laser (PDL) emitting at a wavelength of 595 nm. The PDL selectively damages the PWS by using the wavelength at which hemoglobin absorbs light to thermally destroy capillaries. Due to limitations of PDL penetration depth, the deepest capillaries are often left untreated. This can form seed locations where new capillaries can develop, causing the PWS to darken in color over time.

Focused ultrasound therapies are non-invasive alternatives to treating tissue at depth. We investigated a novel application of therapeutic ultrasound to treat PWS. We used a transducer operating at 1.47 and 4.42 MHz and FDA-approved microbubbles to induce cavitation as a non-thermal mechanism of damage to the PWS. An ultrasound phantom was created to mimic the vasculature of the PWS for determining the functional ultrasound parameters. We report on the ability of these parameters to selectively damage vasculature in phantoms and ex vivo animal tissues.

G70.00074: Optimization of nanopillar dimensions for maximum light absorption EVANGELINE BEECHING (Presenter), Slippery Rock University of Pennsylvania — Conductive organic polymers such as Poly(3-hexylthiophene-2,5-diy) P3HT, and Poly(2,2′-[(2,5-bis(2-hexyldecyl)-3,6-dioxo-2,3,5,6- tetrahydropyrrolo[3,4-c]pyrrole-1,4-diy]dithiophene)- 5,5′-diyl-alt-thiophen-2,5-diy) PDPP3T are being studied for use in solar cells due to their flexibility, cost effectiveness, and low environmental impact when compared to traditional inorganic thin films. However, these organic polymers do not yet have the same efficiency as their inorganic counterparts and are not being largely produced. It is established that replacing thin films with nanopillars enhances the light absorption when the diameter of the nanopillar is less than that of the wavelength of light. We fabricate P3HT nanopillars with approximate diameters of 76 nm using a porous alumina template. We will be optimizing the dimensions (diameter, height and interval) of the nanopillars for maximum light absorption of wavelengths between 400-700 nm. The dimensions of the pores can be controlled by varying the timing of the pore widening process which in turn changes the dimensions of the nanopillars. We aim to fabricate nanopillars of various polymers and compare the intensity of absorption of their thin films with the nanopillars using UV-Vis spectroscopy.

G70.00075: Exploring two-dimensional devices† WILLIAM SHANNON (Presenter), BYRON GREENLEE, JOEL TOLEDOUNERA, JOSEPH MURPHY, JENNIFER T. HEATH, Linfield College — Two-dimensional materials and devices are opening up a wide range of possibilities for both fundamental and applied research, yet are accessible to the undergraduate lab. We have built a system to layer two-dimensional exfoliated materials into stacks, opening up the possibility of creating a wide range of device structures. This system has been tested by creating twisted bilayer graphene structures, which are known to exhibit Moiré patterns and have electrical properties that vary with twist angle. These bilayers and other simple field effect devices are being studied further with Atomic Force Microscopy, Kelvin Probe Force Microscopy, and bulk electrical measurements to understand electric field screening and potential barriers. Two-dimensional devices have big potential for the future of electronics, and understanding their behavior is an important first step.

†Work funded by the M. J. Murdock Charitable Trust
G70.00076: Treatment of Pancreatic Cancer Cells with SWCNT-Polymer Nanocomplexes as Drug Carriers

CRISTINA ROSAS (Presenter), JUAN MONTEMAYOR, PAUL A WITHEY, University of Houston, Clear Lake — Recent studies show an alternative treatment for cancer that uses single-walled carbon nanotubes (SWCNTs) as drug delivery agents because of their ability to cross cell membranes easily. SWCNTs were dispersed with polyvinyl alcohol (PVA) and Pluronic biocompatible polymers before introducing anti-cancer drugs in the CNTs. Camptothecin (CPT) and Doxorubicin, the anti-cancer drugs used, formed non-covalent CNT-polymer-drug conjugates in aqueous solution when attached to CNTs with a biocompatible polymer. Near-infrared (NIR) fluorescence emission peaks of (7,5) and (7,6) CNTs verified the polymeric dispersion of SWCNTs by both polymers. Pancreatic cancer cells that came from PaCa-2, a pancreatic cell line, were exposed to various concentrations of PVA and CPT with varying SWCNTs to examine the effectiveness of these complexes. The number of viable cells were observed to also determine how effective the treatment was. Preliminary results demonstrate SWCNTs serve as good drug delivery agents and can help increase the effectiveness of anti-cancer drug on the cancer cells.

G70.00077: Modeling Ultracold Atomic Clouds Confined by Atom-chip Magnetic Traps*

XIAOLE JIANG (Presenter), NATHAN LUNDBLAD, Physics and Astronomy, Bates College — NASA’s Cold Atom Laboratory (CAL) conducts experiments on ultracold atoms in orbital microgravity using microfabricated electromagnets (atom chips). We report on the creation of a generalized model, applicable to CAL experiments, for calculating the properties of magnetic traps associated with Bose-Einstein condensates (BECs). While atom-chip BEC machines offer relative simplicity and compactness, such modeling tools are necessary to elucidate certain features (such as the aspect ratio of the trapped ultracold cloud) which might not be intuitive to typical users of the CAL facility. The model (written in Mathematica) is designed such that its interface and setting is generalized, so that users with different priorities or experimental goals, or who are unfamiliar with the code, could use it. We plan to use this model to inform the creation of radiofrequency-dressed magnetic traps and bubble-geometry BECs aboard CAL.

*NASA Fundamental Physics / JPL RSA No. 1597429

G70.00078: Barrier Height Measurement of Cadmium Telluride (CdTe) Solar Cells*

PATRICK MILAN (Presenter), JOSE PERALTA, MADISON GUERRERO, PROF WEINING WANG, Physics, Seton Hall University — Among the thin film generation, the Cadmium Telluride (CdTe) solar cell is favored for research because it has a low cost and a relatively high efficiency (22.1% in 2016). However, its efficiency is still lower than the theoretical limit. One major problem is at the back-contact junction. Since CdTe solar cells have a high electron affinity (about 4.5 eV), typical back contacts such as metals fail to create good ohmic contacts and as a result a Schottky barrier is formed at the back-contact junction. The Schottky barrier affects charge carrier collections and lowers the efficiency of the cell.

In this work, we show our studies on the effect of the barrier height on the performance of CdTe solar cells. We tested CdTe cells with different back contacts and found they had different characteristics and efficiencies. Using the turning point technique, we were able to obtain the barrier heights at the back-contact junction using the current-voltage characteristics of the solar cells at various temperatures. Our results showed that there is a correlation between the barrier height and cell performance: the lower the barrier height, the better the cell performed. These results yielded parameters that will aid us in choosing a superior back contact material for CdTe solar cells.

*NJSGC-NASA

G70.00079: The Effect of Contact Material on Perovskite Solar Cell Efficiency*

MADISON GUERRERO (Presenter), PATRICK MILAN, JOSE PERALTA, Physics Department, Seton Hall University, HONGKUN CAI, Department of Electrical Science and Engineering, Nankai University, Tianjin, China, WEINING WANG, Physics Department, Seton Hall University — Perovskite solar cells have made tremendous improvements since it was first reported on 2009. Its efficiency has increased from 3% to an outstanding 22.1% in less than eight years. Due to its rapid increase in efficiencies and low cost fabrication process, the perovskite solar cell technology was named as one of the biggest scientific breakthroughs in the year of 2013 by Science. In the Perovskite solar cell structure, poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) is usually used on top of ITO as the conducting electrode.

In this work, we show our study on how the efficiency of the Perovskite solar cells depend on the conductivity and work function of PEDOT:PSS. A series of PEDOT:PSS solutions with different conductivity and work function were used to make the Perovskite solar cells. The Kelvin Probe technique was used to measure the work function of the polymer film and the Keithley sourcemeter was used to measure current-voltage characteristics of the solar cells were. Our results help us gain a better understanding of Perovskite solar cells and give us insight on how to improve the efficiency of those solar cells.

*Clare Booth Luce Program
G70.00080: Image analysis of microgravity Bose-Einstein condensation

MAXWELL GOLD (Presenter), NATHAN LUNDBLAD, Physics and Astronomy, Bates College — With the recent production of Bose-Einstein condensates aboard the International Space Station using NASA's Cold Atom Laboratory (CAL), research is underway focusing on new condensate geometries made available by a microgravity environment. We report fitting analysis and trap frequency characterization of imaging data from condensates in both conventional and rf-dressed magnetic potentials. This information will be used for calibration and design of future experiments with CAL examining ellipsoidal shell condensate geometries.

*We would like to thank NASA Fundamental Physics / JPL RSA Grant No. 1597429.

G70.00081: Modular Smart Home: A proof of concept, by Wyatt Vigilante

WYATT VIGILANTE (Presenter), Ithaca College — Current smart home systems can cost upwards of 15,000. This project seeks to create a similar system for 500 or less. A modular smart home contains a network of smart devices that work together to perform homely functions such as turning on lights or adjusting temperature in a room if movement is detected. To bring costs down an Arduino Mega 2560 microcontroller will be connected to the sensors and output the incoming data to the Raspberry PI which will act as an interface for the user. This system also avoids the use of an internet connection to make it more difficult for potential hacking of the system. To validate the effectiveness of the modular smart home system, devices such as RFID card access, light switches, temperature sensors, fans, sonar sensors, RGB lighting, and motion sensors will be implemented into a 1/32 scale model of a 2-bedroom house. Once the system has been implemented into the scale house, estimates of cost efficiency in the modular smart home will be taken to compare against the $15,000 standard smart home to prove the effectiveness of the system.

G70.00082: Exploring the Structural Transformation of Zirconia Films

MARK LEWIS (Presenter), FRANK C PEIRIS, Physics, Kenyon College, SANTOSH SHAW, LUDOVICO CADEMARTIRI, Materials Science and Engineering, Iowa State — Using a combination of experimental techniques, including Raman spectroscopy, Fourier Transform IR spectroscopy (FTIR), X-ray diffraction, atomic force microscopy (AFM) and ellipsometry, the structural transformation of a series of zirconia films were investigated. The zirconia nanoparticles (diameter of around ~4 nm) were first treated with ligands (either oleic acid or trioctylphosphine oxide), and then were spin-coated onto Si substrates. The as-grown samples were then exposed to an oxygen-plasma, and were subsequently calcined at various temperatures (300° C - 900° C). Raman, FTIR and X-ray diffraction show that the zirconia films transform from amorphous to tetragonal and monoclinic phases as a function of the calcined temperature. Using an effective medium approximation to model the ellipsometry spectra, the porosities of the zirconia films were recovered. While the porosity values decrease for both types of samples, the porosity seems to decrease faster for the samples that were capped with oleic acid. The RMS values determined from AFM measurements optimized the ellipsometry models, which included a surface-roughness layer to fit the experimental spectra.

*The work at Kenyon was supported through funding from American Chemical Society (Petroleum Research Fund Grant).

G70.00083: Single Photons for a Modular Ion Trap Quantum Network

SOPHIA SCARANO (Presenter), MARTIN LICHTMAN, CLAYTON CROCKER, KSENIA SOSNOVA, ALLISON CARTER, CHRISTOPHER ROY MONROE, Physics, Joint Quantum Institute at the University of Maryland — Trapped atomic ions of different species are an ideal candidate for a modular quantum computing network partially due to low crosstalk between memory and communication qubits. A dual species Yb+/Ba+ ion trap is used to create entanglement between memory spin qubits and photonic qubits. The flying qubits are emitted via the 6S_{1/2} ↔ 6P_{1/2} transition in 138Ba+. It is advantageous to excite the atom on the 5D_{3/2} ↔ 6P_{1/2} transition at 650 nm, while still collecting 493 nm photons. This removes the excitation light as a source of noise and reduces double excitation errors. Most significantly, the D ↔ P transition allows us to use a slower excitation, such that instead of requiring a picosecond pulsed laser, we can gate a CW laser using AO modulators. We demonstrate a single photon source for quantum networking based on a trapped barium ion subject to pulsed excitation with a second-order coherence of g^{(2)}(0) ≈ (8.1 ± 2.3) × 10^{-5} without background subtraction, a state-of-the-art result for replicable single photon sources.

*This work is supported by the ARO with funding from the IARPA LogiQ program, the AFOSR, the ARO MURI on Modular Quantum Circuits, the AFOSR MURI on Quantum Transduction, and the ARL Center for Distributed Quantum Information.
G70.00084: Modeling of Cytoskeletal Filaments in C17.2 Cells using ImageJ  JULIA HUTSKO (Presenter), JAY MAGERS, Physics, Susquehanna University, SABRINA JEDLICKA, SWETHA CHANDRASEKAR, Material Science, Lehigh University, SLAVA V. ROTKIN, Material Research Institute, Penn State, LISA SCHNEIDER, Math and Computer Science, Salisbury University, MASSOOMA PIRBHAI, Physics, Susquehanna University — Cytoskeletal filaments, such as actin, and nestin assist in sustaining many cellular function, including: differentiation, motility, cell shape, force generation, etc. Studies on how actin reorganizes can give us insights into how external stimuli affect cellular processes. The external stimuli chosen for this research was carbon nanotubes, which are single atom carbon sheets rolled into cylinders. For this study, neural stem cells, specifically C17.2 cells, were the focus. The goal is to observe how the distribution of actin is altered in the presence of carbon nanotubes. Over the last semester, I collected a catalog of data on the volume of actin in both treated and untreated C17.2 cells. Images of actin were captured using confocal microscopy. ImageJ then characterized the volume of the filaments at each level in the neural stem cells and quantified the actin distribution using thresholding techniques. The results, I obtained from comparing my data, showed how carbon nanotubes impact the distribution of actin throughout the cell.

G70.00085: Application of a Retired Burst Gravitational Wave Data Analysis Method to Investigate the Origin of the Blip Glitch  SARAH CHOATE (Presenter), AMBER L STUVER, Villanova University — The Laser Interferometer Gravitational-Wave Observatory (LIGO) is a collaboration with the goal to observe and study events that create gravitational waves detectable on Earth. During the process of data acquisition, glitches in the data can occur as a result of the observation of transient noise. One class of these glitches that occurs in burst data analysis is the blip glitch, which results in an almost identical signal to that of a gravitational wave detection and has an unknown origin. SLOPE is a data analysis method originally used for gravitational wave detection. This research has redeveloped SLOPE for the purpose of investigating glitches and has readied the algorithm to be applied to auxiliary channels to search for glitches. Results presented includes operating parameters for which SLOPE can be effectively run.

G70.00086: Properties of PVDF Films Blended with Zwitterionic Copolymers*  MIRIAM SALCEDO (Presenter), NELAKA DILSHAN GOVINNA, Physics and Astronomy, Tufts University, SAMUEL LOUNDER, AYSE ASATEKIN, Chemical and Biological Eng., Tufts University, PEGGY CEBE, Physics and Astronomy, Tufts University — Poly(vinylidene fluoride), PVDF, is a semicrystalline polymer used as a membrane for filtration and separation applications. Its properties can be enhanced by blending together with zwitterionic co-polymers which alter the hydrophobicity. In this work, we study the structure and electrical properties of PVDF blended with the random copolymer poly(methylmethacrylate-r-sulfobetaine-2-vinylpyridine). Solutions in dimethylacetamide/ acetone are prepared by varying the concentration of the blend components. Doctor-blading is used to make films of uniform thickness for further investigation by wide angle X-ray scattering, calorimetry, scanning electron microscopy, and dielectric relaxation spectroscopy. The crystalline and glassy structure of these films is determined by the manner in which the solvent is removed from the film, either by slow and continuous evaporation of the solvent, or rapid solvent removal by water immersion. These casting methods create different pore size and distribution which affect the structure and dielectric properties of the films.
*NSF-DMR 1608125; Universidad Autónoma de Madrid; Tufts-Skidmore Spain Program

G70.00087: Microtubule Patterns Through Growth and Crosslinking  AUSTIN MORRISSEY (Presenter), Biochemistry and Molecular Biology, UMass Amherst, LENITA HERBST, Microbiology, UMass Amherst, BIANCA EDOZIE, Biochemistry and Molecular Biology, UMass Amherst, JENNIFER ROSS, Physics, UMass Amherst — Life is never static, and its propagation is possible due to the dynamic dance of continuous cellular motion. Microtubules are a fundamental and dynamic cellular component of eukaryotes. These microfilaments make up essential structures, such as the neuronal axon, and the mitotic spindle. In this study, we explore the self-organized polymerization patterns of microtubules using both macromolecular crowding agents and crosslinking microtubule-associated proteins. Previously, we have found that the phases and patterns depend very sensitively on the filament length and the percentage of MAP65 crosslinkers present. Specifically, there is a range of concentrations that result in spindle-like “tactoids” which could act as model mitotic spindles. Here, we investigate whether similar microtubule organizations are observed when changing the identity of and respective concentration of crowding agents used alongside MAP65. This work will allow further elucidation on self-organization of the mitotic spindle, using a systematically controlled in vitro reconstitution system.
G70.00088: Super-Resolution Patterns in Quantum Dots* HAMID JALILI (Presenter), THOMAS DANZA, RICHARD MOURADIAN, SEAN JAMES BENTLEY, Adelphi University — In this research, quantum dots and other materials were measured for their ability to absorb nonlinearly. Using the second harmonic of a nanosecond Nd: YAG laser an interference pattern was etched onto a quantum nanoparticle thin-film sample and a reference sample which were then compared against linear and nonlinear absorption. After one pattern was formed, a second pattern was interlaced with the first by introducing a phase shift into one arm of the interferometer. Due to the nonlinear nature of the absorption, this allows the formation of a pattern with twice the resolution possible with linear techniques. While the visibility of the combined pattern is reduced as compared to simple interference, it is still sufficiently high for many applications.

*We would also like to thank Adelphi University and the Horace McDonell Summer Fellowship for funding.

G70.00089: Observations of Dislocation Etch Pits in SmB6 SHRIYA SINHA (Presenter), ALEXA RAKOSKI, CAGLIYAN KURDAK, University of Michigan, PRISCILA ROSA, Los Alamos National Laboratory, MONICA CIOMAGA HATNEAN, GEETHA BALAKRISHNAN, University of Warwick, BOYOU N KANG, MYUNG-SUK SONG, BEONGKI CHO, Gwangju Institute of Science and Technology — Samarium hexaboride (SmB6) is a strongly correlated topological insulator, showing insulating behavior from 4-40 K and a conduction plateau below 4 K due to the topological state. Recent transport results on the bulk have demonstrated that SmB6 is not sensitive to point defects but extended defects such as one-dimensional dislocations may still be present. Such dislocations may provide an additional current path beside the topologically protected surface state. The one-dimensional dislocations must terminate on the surface and can be identified by the use of proper chemical etching. In order to characterize the bulk defects in SmB6, we developed an etching technique using equal parts sulfuric acid and nitric acid. Using this etchant we found etch pits in the shape of inverted pyramids aligned with the crystalline axis, which are expected to indicate dislocations. In aluminum flux grown samples, dislocation etch pit densities range from 2x10⁶ to 9x10⁶ cm⁻². A comparison of flux grown samples and floating zone grown samples will be presented.

G70.00090: A demonstration of quantum key distribution with single photons for the undergraduate laboratory* BAIBHAV SHARMA (Presenter), ENRIQUE JOSE GALVEZ, AAYAM BISTA, Physics and Astronomy, Colgate University — The goal of this work was to create a laboratory experiment feasible in an undergraduate setting that demonstrates quantum key distribution and security attacks on quantum key distribution using single photons. The basic principle behind this experiment is that when a measurement is made on a quantum state, it modifies the information it conveys. This principle has been extended to quantum secure communications and is a teaching moment for physicists, computer scientists and engineers alike. We mimicked Eve or the eavesdropper by using an intercept and resend method, which include using an interferometer and a quartz plate. We used polarization entangled photons produced by parametric down-conversion.

*This work was funded by NSF grant PHY-1506321.

G70.00091: ABSTRACT WITHDRAWN —

G70.00092: Lithography-Free Confinement of 2-D Materials Using Precision Laser Ablation* ETHAN RICHMAN, YANPEI DENG, CAMERON MILLER, ZACH WIENER, LI-HENG CHANG, VISHRUT TIWARI, CHRISTOPHER LAFRATTA, PAUL CADDEN-ZIMANSKY (Presenter), Bard College — The ever-expanding array of two-dimensional materials and heterostructures susceptible to alteration in oxygen environments motivates the search for lateral confinement techniques outside conventional lithographic and etching methods. Laser ablation of such materials using a femtosecond pulsed Ti:Sapphire laser and programmable x-y stage is a single-step process that can in principle be used as a flexible tool for device processing. However, scanning probe analysis of sub-micron graphene ribbons fabricated with this technique reveals considerable defect accumulation under ambient condition. We show that such defects are largely alleviated by the simple change in the ablation environment from air to water.

*We thank the Sherman Fairchild foundation and Bard Summer Research Institute for support of this research.
G70.00093: Scanning Electron Microscopy – New Approaches in Imaging Biological Specimens*  INDRAJITH SENEVIRATHNE (Presenter), SYLVIANA HANNA, Lock Haven University of Pennsylvania — Scanning Electron Microscopy (SEM) of biological systems has a long and illustrious history. However due to the inherent complexities of biological hard and soft matter interaction with electrons and with the imaging system, one must overcome certain hurdles. We have attempted to optimize typical biological SEM sample preparation such as critical point drying, fixing of microbes via Osmium Tetroxide and other techniques in this investigation. In the study, we have also focused on the effect of the conductive coating (magnetron sputter deposited) on the specimen. The study concluded with stereoscopic 3D imaging of the specimen acquired by the SEM Secondary Electron and Backscattered Electron Detectors. We will discuss the results and compare them with the current literature.

*Lock Haven University Nanotechnology Program and the Nano Club.

G70.00094: Modulating the Magnetism of LaCoO₃ Thin Films Via Strain Engineering*  RONALDO RODRIGUEZ (Presenter), TOYANATH JOSHI, DAVID LEDERMAN, University of California, Santa Cruz — LaCoO₃ thin films grown on SrTiO₃ (100) single crystals exhibit an anomalous ferromagnetic transition at T_c= 87 K. This material is normally not ferromagnetic and the mechanism of the transition is not well understood, although the O-Co-O bond angle is believed to play a crucial role. It is shown that the compound is not ferromagnetic when grown on LaAlO₃. Further strain, which presumably alters the bonding angle, can be achieved by growing LaCoO₃ on large angle miscut SrTiO₃ substrates in a layer-by-layer growth mode with the angle of miscut being α ~10°. Films are grown using pulsed laser deposition employing a a 248nm KrF excimer laser to ablate a stoichiometric LaCoO₃ target. The growth is studied via in-situ reflection high energy electron diffraction (RHEED), which can detect layer-by-layer growth when the RHEED intensity oscillates as a function of growth time. Crystallinity and topography are measured using X-ray diffraction and atomic force microscopy, respectively, and magnetometry as a function of temperature and magnetic field is measured using a superconducting quantum interference device (SQUID) magnetometer.

*This work was partially funded by the National Science Foundation REU program, grant #1659744.

G70.00095: PHYSICS EDUCATION —

G70.00096: An advanced laboratory course based on the construction and modeling of a magneto-optic atom trap  LEE E HARRELL (Presenter), MARY CLARE CASSIDY, KIRK A INGOLD, DAVID O KASHINSKI, COREY S GERVING, United States Military Academy — Undergraduate physics labs often entail the collection of data using an apparatus that is set up and sometimes even fully adjusted before the students arrive. Various physical phenomena and data analysis techniques can be explored with this approach; however, students are unlikely to develop the experimental design and construction skills that are necessary for conducting original research. We present a magneto-optical atom trap designed and constructed for use in an undergraduate lab class that is organized to address the shortcomings of the more traditional approach. While the basic design and necessary equipment are made available, the students are required to build a working atom trap starting from an empty optics table. Additionally, students must model and simulate the operation of the trap to determine the necessary operating parameters and their tolerances. The results of these simulations provide a basis for interpretation of data collected from the operating trap.
The employment of a glowing LED to determine Planck's constant accurately.  

CHETAN KOTABAGE (Presenter), Department of Physics, KLS Gogte Institute of Technology — Planck’s constant is a fundamental constant in Physical sciences and Millikan was awarded Noble prize for its experimental determination. With the advent of solid state electronic devices, experiments were designed to determine the Planck’s constant utilizing LED [1], [2]. Herrmann, Schätzle [3] and Morehouse [4] have discussed the validity of this experiment. In this article, the validity of this experiment is re-examined. The measurements of the longest wavelength light emitted by LED and precise determination of band gap energy of LED are essential for accurate determination of Planck's constant by utilizing LED [5].


[5] Can a glowing LED light a road to accurate determination of Plank's constant?, Chetan Kotabage, Accepted for Resonance - Journal of Science Education

Physics Education Research on Inexpensive Active-Learning Lab Modules  

ZOE MUTTON, CORINNE RYWALT (Presenter), Physics, Worcester Polytechnic Institute, MEGAN VARNEY, Mathematical Sciences, Worcester Polytechnic Institute, NANCY BURNHAM, Physics, Worcester Polytechnic Institute — Active learning strategies, including hands on activities and lab work, have proved to be beneficial to student comprehension and success in physics classrooms. Despite this, many high school physics classrooms lack lab equipment necessary to supplement learning, mostly due to budget limitations and the high cost of traditional mechanics lab equipment. This project aims to design three modular, inexpensive, and demonstrative labs to enhance student knowledge in friction, conservation of energy, and torque. These labs, including a worksheet for students to complete, are designed to be easily implementable, take 20-30 minutes to complete, and be cost effective. These labs were tested with high school teachers and students to show that they are easy for teachers to implement in their classrooms and that they are easy to understand and effectively demonstrate their respective learning objectives to students. The implementation of these modular labs in high school classrooms will aid learning by kinesthetically illustrating the topics taught in lectures, leading to better student comprehension and higher success rates in introductory mechanics. Furthermore, high schools that cannot afford traditional lab equipment now have the opportunity to provide mechanics lab work to students.

Engaging and Sustainable High School Physics Lab Curriculum Using Smartphones*  

SAVANNAH GRUNHARD, ZAINIL CHARANIA (Presenter), SHENG-CHIANG LEE, Mercer University — The purpose of our research was to develop an engaging and low-cost, hence sustainable physics lab curriculum for implementation in Bibb County, GA, public high schools. Each public high school in Bibb County receives $1000 per year for the whole science curriculum. This is barely enough to restock consumable items in chemistry and biology and leaves nothing for physics. The lack of sufficient funding for proper lab equipment and qualified teachers disadvantages students. We believe that this contributes to the low rate of Bibb County high school students taking at least one physics course before graduating (only half of the national average).

The curriculum is developed to make adoption easy for teachers. It includes student activities (with instructor manuals) and instructions for both class demonstrations and construction of DIY apparatuses. The pedagogical approach of our curriculum is student-centered and inquiry-based. These activities utilize smartphone sensors in place of typical laboratory sensors. The use of existing smartphones in an educational setting serves to engage students and encourages them to explore physics in their everyday lives without adding any financial burden to school budget.

*This work is funded by the Mercer University Research That Reaches Out Office.
Children's interest in science. The results of the surveys show some promising data for this first attempt.

The objective of each survey is to see if the children would retain scientific information after the summer camp, particularly, their science vocabulary, and to see if they can recognize science phenomenon in their everyday lives. This poster will discuss the findings and lessons learned for this past summer camp in an attempt to help us improve the children's interest in science. The results of the surveys show some promising data for this first attempt.

*St. Mary's University

G70.00101: Designing Introductory Physics Experiments for the Visually Impaired  
MORGANNE KENDYLL BENNETT (Presenter), PAUL QUINN, Kutztown University of Pennsylvania — "The only thing worse than being blind is having sight but no vision," is a famous quote from Helen Keller. Teachers of students with visual impairments, must constantly look at the world from a different perspective, one without sight. For these educators, it becomes necessary to adapt the learning environment, making it more accessible to visually impaired students. This becomes more difficult in the STEM fields, particularly physics. This project redevelops some common introductory physics labs in a more tactile fashion, so that the same conclusions can be drawn without visual tools. This involved the design of various pieces of equipment such as a tactile graph board, making it possible for visually impaired students to experience the relationship between variables in the physical world. In this project, we were able to take topics, such as current and resistance, and make them more accessible to the visually impaired population. We discuss the various techniques and pieces of equipment designed to accomplish this goal. Also, the results of these experiments are discussed, after using the more tactile process in collecting and analyzing the physical data.

G70.00102: Learning physics by experiment: IV. Kinematics  
SAAMI SHAIBANI (Presenter), Instruction Methods, Academics & Advanced Scholarship — The trajectory of a ball in sports settings provides extensive opportunities for students to see how principles from physics can be applied to a familiar activity. Advanced equations[1] in mechanics are employed in this research to design an investigation of the relationship between launch speed and launch angle under a variety of circumstances, such as launch height and distance from target. Students are not given access to these theoretical results because they are unduly cumbersome; instead, students identify launch outcomes solely on an empirical basis. Data from such laboratory experiments are high in quality even in the absence of any numerical context, and students report that they are not concerned about the latter because they enjoy the freedom of exploring without constraint. Other educational benefits include a relaxed learning environment and enthusiastic communication between students. Such advantages are further validation of the pedagogy that has been applied to multiple topics[2-7] with considerable success.


G70.00103: Learning physics by experiment: V. Ambulation  
SAAMI SHAIBANI (Presenter), Instruction Methods, Academics & Advanced Scholarship — A multitude of devices associated with developing and maintaining fitness have been introduced in the past decade or so; examples include activity trackers and other wearable instruments, which have the capability of wireless communication for sharing data that they capture. Although the use of such equipment is becoming more widespread, favorable health outcomes (such as weight loss and improved cardiovascular function) have either been too low to be noticeable or have only a small impact[1,2]. The purpose of this study is to compare these devices with those based on much simpler technology (that typically costs an order of magnitude less) to determine to what extent, if any, the considerably greater expense of the former provides commensurately greater benefits than the latter. Experimental procedure is limited to be appropriate for students at the introductory level. Parameters of interest include design, temporal, geometrical, physiological, environmental and human factors. The research conducted here not only expands the number of projects having a similar educational value[3], but also extends the variety.

SAAMI SHAIBANI (Presenter), Instruction Methods, Academics & Advanced Scholarship — A critical piece of medical equipment for use in trauma environments has an inherent, and yet necessary, mechanical instability in its design. This instability can pose danger to operators of the equipment if certain safety measures are not observed; however, it is not always possible to implement every precaution in the high-risk settings usually associated with life-threatening emergencies. The author has direct experience of how the subject equipment is employed during pre-hospital care by first responders, including being present when the equipment caused injury even before it was needed. Application of fundamental principles in this research enables the dynamic properties of the equipment to be calculated with basic calculus and algebra, with the latter being particularly extensive. The behavior of the equipment under recommended procedures is then analyzed to produce a baseline performance, against which the response of the equipment in adverse circumstances is compared. As with other studies conducted throughout this innovative series[1], powerful techniques for superior student understanding are developed from the real world in a manner that transcends the most creative examples in standard textbooks.


JOSEPH TROUT (Presenter), Physics, Stockton University — At Stockton University an interdisciplinary course was developed by a physicist, chemist, and food scientist, which studies the science of ice cream. Ice Cream can be an excellent vehicle for teaching concepts in physics and chemistry. For example the process of the phase change from a liquid to a solid of water in the ice cream mix is an interesting comparison to the process which occurs in pure water. The course is composed of a lecture portion and a lab portion. Topics covered include Newtonian dynamics, fluid mechanics, and thermodynamics. This presentation briefly describes the course and provides a preliminary assessment of the course.

DIEGO VALENTE (Presenter), NIRAJ GHIMIRE, JASON HANCOCK, University of Connecticut — The University of Connecticut is currently in the initial stages of an extensive reform to several of its introductory physics courses seeking to shift away from the traditional framework of isolated lectures and laboratory sessions in favor of a studio-based instructional model blending lectures, problem-solving tutorial sessions and hands-on experimental activities. When completed, we expect this large-scale pedagogical reform spanning a total of 3 introductory sequences and 6 courses to impact approximately 2,000 students each year. In this work we discuss details of our current pilot program preparing us to make the transition to studio-based instruction in our larger introductory courses, as well as some of the challenges we face. We also present preliminary data on student learning comparing normalized gains on concept inventory assessments administered in our pilot courses to similar data collected in previous implementations of these courses taught in a traditional format.

BRIANNA BILLINGSLEY (Presenter), CORY CHRISTENSON, Washington & Jefferson College — If you look through any physics textbook you will encounter canonical names such as Newton and Galileo. While their contributions are indeed significant, presenting the history of physics solely in terms of these western scholars hides a much deeper and complex history that is not often taught. Here we will discuss how to incorporate contributions from Chinese and Arab civilizations. These concepts can be introduced to students through labs, homeworks, and discussion questions. A broader and more culturally diverse scientific history can engage student interest, teach them about how science actually happens, help them to appreciate the value of diversity.

The authors acknowledge the support the Washington & Jefferson College Ken Mason Faculty Development grant.

MATT PREZIOSO (Presenter), CORY CHRISTENSON, Washington & Jefferson College — This poster will explain how computer operated robotic cars can be implemented in college physics lab classes to introduce students to programming while also teaching them about kinematics. Arduino-based toy cars were built that can respond to light and distance stimuli, simulating the effect of traffic lights. The students are provided a basic code and asked to modify it to control the car's motion, and compare the observed motion to the theoretical kinematics equations. This combines the core physics concepts with real-world examples and useful programming skills. These cars can also be used to study traffic flow and energy use in transportation grids.

The authors acknowledge the support of the Washington & Jefferson College Center for Energy Policy and Management (CEPM).
**G70.00109: A Short-Term Physics Study Abroad Experience for General Education Student**  
DAVON W FERRARA  
(Presenter), Chemistry and Physics, Belmont University — Students looking for general education science courses often try to avoid those in physics. However, there are many concepts in physics that students ultimately enjoy learning about once in the course. One way to motivate students to take a conceptual physics course is to teach it while traveling through Italy on a short-term study abroad program. The conceptual laboratory science course described here has been taught four times since 2014 during “Maymester”, a three-week term between spring and summer semesters. The course uses the Galilean scientific revolutions during the Italian Renaissance as a starting point to understanding some of the major developments from classical mechanics to modern physics and the interactions between science and culture, including with respect to religion. Although this short-term study abroad course is in continual development, with changes to the itinerary and pedagogy each year, this presentation will give an overview of the trip, examples of laboratory experiments done while abroad, and a discussion of ways to keep non-science majors engaged in learning physics throughout the trip.

**G70.00110: Common Student Misconceptions in Physics Classes: Mechanics**  
KYLE BAUTISTA (Presenter), CAROLINA C. ILIE, SUNY Oswego — Physics is an important and amazing field of study. However, Physics can be a complicated subject for some students. There are several different topics and areas of physics where students seem to develop or have previously acquired misconceptions. It is possible for these common misconceptions to be found by taking a closer look at what a students’ rational is when they are answering a question. To do this, a Physics survey was created based on several topics in the introductory mechanics unit covered in a college-level physics course. Participants were asked to answer ten questions covering a range of topics including graphs of motion, force, and mechanical energy. Answers to the survey were multiple choice along with a brief explanation with each answer to better identify the cognitive process of participants and diminish guessing. The surveys were collected and all responses were analyzed for any common errors. Using the data collected, we identified the physics misconceptions. We created and implemented new pedagogical strategies aimed to clarify the physics concepts. Some say Physics can be a challenging subject to learn, but with the appropriate student-centered classroom techniques, it is possible for anyone to not only succeed, but find a greater passion for the field.

**G70.00111: A Useful End-of-Semester Physics Course Assessment Survey**  
NORMA CHASE (Presenter), School of Arts and Sciences, MCPHS University - Boston — This scantron-based survey examines the teacher-learner collaboration. It includes questions which probe student preparedness, behaviors, attitudes, and expectations – as well as questions addressing key measures of excellence in teaching and course structure. We find that the most valuable information is revealed when survey responses are displayed at the level of individual students - for it is there that we find data which we can use to improve our guidance of student learning and cognitive development. Bar graphs are used to look for any interdependence between responses to pairs of survey questions. By thus examining the data in its entirety, we obtain insights which might inform future students, as well as faculty and administrators.

**G70.00112: A training course design for developing a student into an academic researcher**  
BING SHEN (Presenter), School of Physics, Sun Yat-Sen University, China — For the undergraduate student who want to enter the academic in the future, the basic scientific training is important and necessary. However, this kind of training is not like the regular course which need design in a different way. In this talk, we study the students from the condensed matter physics. By interviewing the students, teachers and researchers, we found the experiment technique and strategy changing are important to the developing a student into an academic researcher.

**G70.00113: Characterizing Hand-Made Planar Inductor Components in the Series RLC Circuit**  
DANIEL CANSECO-CHAVEZ (Presenter), STEPHEN A TSUI, Physics, California State University San Marcos — In the introductory physics curriculum, students are taught induction and inductance by examining the behavior of the current-carrying coil. As electronic devices approach the nanoscale, one might ask a student how would it be possible to fit an inductor onto an electronic chip. A commercial microelectronics solution is the planar spiral inductor, which are conductive thin film patterns deposited on substrates especially used for high frequency applications. Although synthesizing a thin film is beyond the reach of most classrooms, the principles and advantages of a thin film inductor can be taught using very affordable copper tape. An instructional laboratory activity based on this design introduces students to inductors using a geometry not covered in the introductory text and also offers them insight into the solutions necessary to build devices at the micro- and nanoscale, which would especially be useful to careers in engineering and applied physics. In this work, we demonstrate the construction of macroscale planar spiral inductors using commercially available copper tape and compare their behavior to an off-the-shelf inductor.

*Support provided by the TRIO McNair Scholars Program at California State University San Marcos.

**G70.00114: PHYSICS OUTREACH AND ENGAGING THE PUBLIC** —
G70.00115: Paper-based controllable illumination for multi-mode microscopy  SIMREN KAUR (Presenter), RYAN J. MCGORTY, University of San Diego — A paper-based microscope makes for a rugged and versatile solution to bringing science and science education to a variety of settings including those that are resource-scarce. This has been well demonstrated by the Foldscope project. Here, we describe an extension to that idea. We designed a paper-based method to control the sample illumination in a portable microscope. Controlling the illumination of the sample allows us to employ a variety of microscope imaging modalities including bright-field, dark-field and phase contrast. With this instrument, students can explore those different techniques. Additionally, it can be used to perform advanced imaging, including quantitative phase imaging, in the field, away from advanced and costly instrumentation.

G70.00116: AI framework to solve sustainability issue based on social and political dynamics  DEEDER AURONGZEB (Presenter), University of Maryland, College Park — Sustainable product development requires long term model building that may require social dynamics input. Scaling up temporal causality analysis to very large scale state spaces and extending the framework to handle large relational data is a critical undertaking to create a large scale dynamic model. We extend cross-sectpral model by C Granger, J. of Econometric Soc, V37,N3,424, in light of modern casual models and provide a AI framework on how AI can provide sustainability models in various aspect of social and political conditions using temporal logic.

G70.00117: HISTORY OF PHYSICS  —

G70.00118: Bibliographic Visualizations of Early Work in Neutron Diffraction  MATTHEW MARSTELLER (Presenter), Carnegie Mellon University — The literature of neutron diffraction was explored using Web of Science data and VOSviewer for data visualization. The timespan covered was from the advent of the topic through 1955 when Clifford Shull left Oak Ridge. The search query in Web of Science allowed for either "neutron diffraction" or "neutron scattering" to appear in the resulting records. Visualizations will include networks of co-authors with numbers of documents produced. Co-author groups readily appear in the visualization and allow for identification of important research teams. Shull and Ernest Wollan appear in one cluster. George Bacon of AERE, D.G Hurst and D.G Henshaw of Chalk River are easily visible as well. Other visualizations include citation networks of documents, authors or sources.

G70.00119: EARLY CAREER SCIENTISTS  —

G70.00120: Density Functional Theory Calculations of Stability and Absorption Spectra of Au8- Conjugated Complexes with Met and Trp Amino Acids and Trp-Met Dipeptide  MARWA ABDALMONEAM (Presenter), Physics, Michigan Technological University — Interactions of Au8 (D4h) gold cluster with the functional groups of the amino acids; L-Methionine (Met) and L-Tryptophan (Trp), and the dipeptide L-Tryptophyl-L-Methionine (Trp-Met), in their zwitterionic forms and in presence of solvent have been investigated using the density functional theory (DFT). Specifically, the binding energies and Ultraviolet-Visible (UV-Vis) absorption spectra of the bioconjugated complexes of Au8-Met, Au8- Trp, and Au8- Trp-Met have been analyzed. Our calculations show that; the pristine Au8 (D4h) cluster has strong absorption spectrum in the near-ultraviolet range, in agreement with the literature. The optical activity of the pristine cluster is the major influencing factor on the absorption spectra of the studied bioconjugated complexes, but the spectra of the complexes carry sufficient remarks that allow them to be distinguished from that of the pristine cluster. The interactions of Au8 with each specific functional group (either indole or thiol ether) led to very similar absorption spectra whether this group existed in a mono or in a dipeptide amino acid.

G70.00121: PUBLIC POLICY  —

G70.00122: Research Integrity, the Responsible Conduct of Research, and Plagiarism Analysis  AARON MANKA (Presenter), National Science Foundation — Among its duties, the National Science Foundation (NSF) Office of Inspector General (OIG) is responsible for helping ensure the integrity of research programs at NSF. We investigate allegations of research misconduct (plagiarism, falsification, and fabrication) in NSF proposals and awards. We also handle allegations of conflict of interests and violations of the confidentiality of NSF’s merit review to ensure the integrity of that process. We completed a review of how grantees implemented NSF’s requirement to provide responsible conduct of research training to undergraduate students, graduate students, and postdoctoral researchers. We are currently reviewing our plagiarism cases of the past decade to accumulate data and potentially identify institutional and NSF strategies for preventing and reducing plagiarism. I will briefly discuss these topics and present our results.
Determining the Asymptotic Expansion of Prolate Spin-Weighted Spheroidal Eigenvalues

DANIEL VICKERS (Presenter), GREGORY B COOK, Physics, Wake Forest University — Spin-Weighted Spheroidal Harmonics (SWSHs) are a complete orthonormal basis of tensors on the surface of spheroids. While SWSHs are used in many fields of physics for modeling, this research is focused on their application to describing the normal modes of transmission on the surface of black holes in the Kerr Geometry. Much is known for the oblate case of SWSHs; however, the asymptotic behavior of the prolate case has yet to be well described. In this work, the prolate SWSHs problem was numerically solved, which was used to create a power series approximation for their eigenvalues.

WITHDRAWN ABSTRACT

GRADUATE STUDENT AFFAIRS

Deific Naturalism: A Paradigm Shift from Matter to Consciousness as the Basis of Reality Consistent with all the Scientific Evidence

AMY LANG (Presenter), University of Alabama — “Science has to have a metaphysical framework to operate with confidence.”(Beyond Matter, Trigg) The prevailing scientific philosophy of naturalism assumes only physical causes, excluding any spiritual cause (God) to explain the inherent order of the universe evidenced by the laws of physics. This philosophy conflicts with surveys that show 51% of scientists believe in God or a higher power, with younger scientists at 66%. A paradigm shift to a metaphysical basis would explain this order. Physicists such as Planck have argued that quantum physics infers an observer-dependent reality based in consciousness, not matter. Deific naturalism, as defined by Mary Baker Eddy with her discovery of Christian Science in 1866, defines God as the universal Principle of good which orders the material universe and to which all consciousness, since matter is a mental construct, is steadily yielding. Deific naturalism is also consistent with the growing body of documented evidence anomalous to naturalism and is verified by over 83,000 archived Christian Science healings (many medically documented) where the metaphysical method of prayer applies a spiritual cause to universally and repeatedly restore health and order, and explains Biblical miracles as divinely natural scientific demonstrations.

Selective-Jet Electrochemical Processing for Low-Cost Additive Manufacturing of Metallic Components at Room-Temperature.

WAEL OTHMAN (Presenter), OMAR ALMELHI, LÜTFİYE Y. OZER, Materials Science and Engineering, Khalifa University, MARCO STEFANCICH, Dubai Electricity and Water Authority (DEWA), MATTEO CHIESA, Materials Science and Engineering, Khalifa University — Selective-Jet Electrochemical (SJE) processing has emerged as a novel approach for manufacturing metallic components with a lower cost in comparison with other conventional techniques. In addition, this technique allows metal processing at room temperature, which is considered a benefit as it reduces the need for expensive vacuums and temperature-regulating setups. Basically, SJE performs reduction of metal ions from one electrode and gives it back at the other electrode which is oppositely charged. One of the key characteristics is the capability of adding or subtracting material simply by reversing the polarity applied during the process, which helps in optimizing the AM process. One of the remaining drawbacks of this technique is the slow deposition rate that needs to be enhanced to achieve fully the promises of SJE. In this work, both deposition and etching of copper were monitored by using various polymer-printed nozzles diameters, along with varying current densities and process time. More specifically, relations of the dimensions, density and electrical conductivity of the deposited/etched materials to the mentioned parameters are reported that provide the critical parameter space to be optimized in order to achieve a speedy deposition and obtain the desired density.

Characterizing Uncertainty in Carbon Sources/Sinks using Top-Down Modeling

SIONA PRASAD (Presenter), Thomas Jefferson High School — Carbon dioxide (CO2) emissions, especially from large cities have resulted in the build-up of greenhouse gas concentrations responsible for climate change. Existing sensor technology is too expensive for large-scale use in urban areas, and cannot distinguish between anthropogenic and biogenic emissions. In this paper, we develop a low-cost in-situ sensor for direct CO2 measurements and a spectral imaging system to remotely monitor vegetation phenology. The sensor and camera were installed on a low-powered drone to serve as a mobile platform for accurate measurements and Bayesian models used this data to estimate emission inventories and model uncertainty. The predicted CO2 emission inventory for Washington DC showed a large contribution from the transportation sector. In summary, we demonstrate a methodology to measure and monitor city-wide CO2 emissions by combining low-cost in-situ measurements, multispectral imaging, small drone technology and puff modeling, and taking the first step to targeting specific greenhouse gas sources and reducing overall emissions.

MAGNETISM
G70.00131: FeCo-based Ferrofluid for ELF Transmitter Applications
BRYAN AUGSTEIN (Presenter), WILLIAM ZIMMERMAN, NAVEEN REDDY KADASALA, STEPHEN BLAMA, MARY SAJINI DEVADAS, VERA SMOLYANINOVA, Towson University — Developing compact and efficient extremely low frequency (ELF) transmitter antennas remains a challenge. A rotating magnetic dipole can be used for this application. In our approach we employ magnetic fluid, where suspended single domain nanoparticles act as rotating magnetic moments. The role of particle size and composition needed for optimal performance will be discussed. The FeCo nanoparticles were fabricated by wet chemical synthesis. Static magnetization and AC performance were measured. The role of nanoparticle concentration, type of superparamagnetic behavior, and AC permeability of FeCo magnetic fluid will be discussed.

*This work is supported by DARPA MTO AMEBA grant.

G70.00132: A preliminary investigation of large shift in transition temperature (Tc) in Gd5Si3 nanoparticles
SHIVAKUMAR HUNAGUND (Presenter), SHANE M HARSTAD, Virginia Commonwealth University, SHALABH GUPTA, Ames Laboratory, US Dept. of Energy, Iowa State University, Ames, IA 50011, VITALIJ K PECHE Hur, Dept. of Material Science and Engineering, Ames Laboratory, Iowa State University, Ames, IA 50011, MAGUNDAPPA HADIMANI, Virginia Commonwealth University — Magnetic ordering temperatures in nanostructures depend on size. Curie temperature (Tc) of a bulk material where exchange interactions are comparable to thermal fluctuations tends to decrease in particles. The decrease of ordering temperature with size is described by the scaling theory of Fisher & Barber. However, a large increase in Tc in Gd5Si3 NPs have been observed in the ball-milled gadolinium silicide. SEM images shows particle sizes ranging from 50 nm to >2 μm. XRD analysis on pre-separated sample show that ferromagnetic Gd5Si4 is the major phase while paramagnetic Gd5Si3 is the minor phase. Magnetic properties measured in VSM reveal that the Tc decreases for Gd5Si4 phase from 332K for bulk to 315K for ball-milled sample. Another Tc observed at 80K is attributed to Gd5Si3 phase undergoes large shift in its transition temperature at 110K and remains constant irrespective of particle sizes. Plausible reasons for the increase in Tc for Gd5Si3 NPs could be due to the effect of high energy mechanical ball-milling process that could induce structural changes, lattice strains, exchange interaction between phases in a particle, or formation of new phase.

*Work at the Ames Lab was supported by DOE (contract No. DE-AC02-07CH11358). Work at VCU was funded by NSF, Award No.: 1610967.

G70.00133: Ferrimagnetism of Ti-Adsorbed Graphene
ZHENZHEN QIN (Presenter), Zhengzhou University, MIN FENG, XU ZUO, Nankai University — Using the first-principles calculations, we investigate the magnetism of isolated Ti-adsorbed graphene and the magnetic ground state of Ti adatoms at various concentrations. For isolated Ti adatom on graphene, we analyze the localization of magnetic impurity states and moment formation that can be understood in terms of hybridization between C-pz and Ti 4s-3d orbitals. To examine the magnetic ground state of Ti adatoms, we construct graphene cells with Ti adatom at various concentrations and set up the magnetic configurations for a triangle lattice. It is found that a ferrimagnetic (FI) phase is the most stable in a wide range of Ti concentration by comparing the total energies of different magnetic states. In addition, the exchange integrals between the nearest neighbor and next-nearest-neighbor Ti adatoms are calculated by applying a classical Heisenberg model. The prediction of a graphene-based FI metal monolayer will open the door to applications of spintronics, given that Ti obeys a 2-D growth mechanism on graphene.

G70.00134: Perpendicular magnetic anisotropy in one-dimensional Rashba system under external electric fields: First-principles study
ZHENZHEN QIN (Presenter), Zhengzhou University, GUANGZHAO QIN, University of South Carolina, BIN SHAO, Massachusetts Institute of Technology, XU ZUO, Nankai University — External electric field (EEF) control of magnetization attracts much attention for potential applications in spintronics and is also a key challenge for designing quantum magnetic properties. Noticed, the role of EEF on magnetic properties of one-dimensional (1D) Rashba system has not been explored, even lacking in theoretical. In this work, we comprehensively studied the effect of EEF (parallel or vertical) on the magnetic properties of our previous predicted 1D Rashba system—Gd adsorbed zigzag graphene nanoribbons (Gd-ZGNRs) from first-principles study. Our calculations show that a moderate negative (positive) electric field stabilizes out-of-plane magnetization, where Gd-ZGNR performs perpendicular magnetic anisotropy (PMA) whether the direction of the electric field is vertical or parallel, and intrinsic Rashba effect always exist. It is confirmed that the Rashba spin splitting and PMA are interrelated in 1D Gd-ZGNR, in consistent with previous theoretical models. Furthermore, the (non)-perturbed band structures under EEFs are analyzed to explore the underlying physics of MAE based on our proposed methods combined with traditional second-order theory. Our results would provide a new insight into the mechanism of the magnetoelectric coupling at low-dimensional Rashba system.
STENNING (Presenter), ALEXANDER VANSTONE, JACK C GARTSIDE, LESLEY COHEN, WILL BRANFORD, Physics, Imperial College London reveals that the large spin-orbit coupling of Bi (from non-magnetic elements is an interesting issue recently. Using first-principles calculations based on DFT, we study of $M_z/M_{x,y} \approx 3)$. Our studies provide a potential candidate system for achieving an intrinsic quantum anomalous Hall effect where the in-plane ferromagnetism, giving rise to an exceptionally large magnetic anisotropy energy up to 6.5 meV (with significant ferromagnetic phase transition. Moreover, the relatively large and anisotropic Rashba splitting at the interface shifts towards the higher temperature region and the hysteresis width becomes wider. These size dependencies reproduce that reported experimentally.

**G70.00136: Ice Sculpting: Neuromorphic Training of Geometrically-Frustrated Magnetic Metamaterials**

KILIAN D STENNING (Presenter), ALEXANDER VANSTONE, JACK C GARTSIDE, LESLEY COHEN, WILL BRANFORD, Physics, Imperial College London — Artificial spin ice (ASI) consists of ferromagnetic arrays populated by Ising-like nanopatterned macrospins. The array 'microstate' describes the magnetic orientations of all macrospins, with the ASI microstate manifold notable for its vast range of energetically-degenerate states arising from geometric frustration. ASI has displayed capacity to 'memorise' specific microstates, returning to them with perfect fidelity even under strong magnetic perturbations. This property, termed return point memory (RPM), is a signature of systems which may be trained to act as artificial neural networks.

Today's software-based neural networks are powerful but crucially limited by their non-neuromorphic host hardware. Designing novel computational hardware which is fundamentally neuromorphic in design and operation may greatly enhance the scope and utility of artificial neural networks.

Combining recent development of a nanomagnetic writing technique allowing for access to the entire ASI microstate space and computer-vision microstate recognition with the inherent RPM properties of ASI, we explore the viability of ASI as a hardware platform for directly implementing neural net functionality with no software layer.

*The work was funded by the Leverhulme Trust RPG-2017-257 and an EPSRC DTP award to KS.*

**G70.00137: Magnetic anisotropy driven by enhanced spin-orbital coupling of sp metal Bi on Au /Si(111) root3 surface**

CHONG LI (Presenter), School of physics and engineering, Zhengzhou University, HAN WANG, Renssela Polytechnic Institute, CHUNYAO NIU, FEI WANG, YU JIA, School of physics and engineering, Zhengzhou University, ZHENYU ZHANG, University of Science and Technology of China, SHENGBAI ZHANG, Renssela Polytechnic Institute — Realization of magnetic properties from non-magnetic elements is an interesting issue recently. Using first-principles calculations based on DFT, we study of 1/3 monolayer Bi-covered Au/Si(111) surface and find that such system can be magnetic remarkably. Our further analysis reveals that the large spin-orbit coupling of Bi ($p_x, p_y$) multi-orbitals at the Fermi level leads to an occupancy disparity between spin channels. And this occupancy disparity will break Kramers degeneracy, resulting in a non-magnetic to significant ferromagnetic phase transition. Moreover, the relatively large and anisotropic Rashba splitting at the interface damps the in-plane ferromagnetism, giving rise to an exceptionally large magnetic anisotropy energy up to 6.5 meV (with $M_z/M_{x,y} \approx 3$). Our studies provide a potential candidate system for achieving an intrinsic quantum anomalous Hall effect with temperature up to 70 K.

*NSF of China (grant nos. 11304288, 11774078)*

**G70.00138: Electronic properties of chemically functionalized armchair GaN nanoribbons: A computational study**

NARESH ALAAL (Presenter), IMAN ROQAN, Physical Science and Engineering Division, King Abdullah University of Science and Technology — Graphene synthesis has spurred immense progress in the study of low-dimensional materials, as they offer distinct properties when compared with their three-dimensional bulk counterparts. Nanoribbons (NRs) are quasi-one-dimensional materials that exhibit interesting electronic properties based on their width and edge configurations. Edge functionalization is one of the techniques by which the electronic structure of NRs can be tuned. In this work, we employ first-principles spin-polarized calculations to study electronic and magnetic properties of oxygen- and sulfur-passivated armchair GaN nanoribbons (AGaNNRs). Unlike bare AGaNNR, which is a nonmagnetic semiconductor, oxygen-passivated AGaNNR (O-AGaNNR) displays magnetic behavior with a magnetic moment of 1 $\mu$B, as its band structure splits into spin-up and spin-down channels. Such behavior is caused by additional states that arise from the non-bonding electrons of the edge oxygen atoms. On the other hand, the sulfur-passivated AGaNNR (S-AGaNNR) exhibits semiconducting properties and has a reduced band gap relative to its bare counterpart. Thus, we will discuss the physical mechanism that leads O- and S-AGaNNRs to be good candidates for optoelectronic and spintronic device applications.
**G70.00139: Longitudinal Resonance for Thin Film Ferromagnets with Random Anisotropy**

WAYNE M SASLOW (Presenter), Department of Physics, Texas A&M University, CHEN SUN, Department of Physics, Brown University — At the microscopic level, individual spins in ferromagnets with random anisotropy tip transversely with distinct local angles relative to the magnetization M. When driven by an rf field along the equilibrium M₀, which changes dM = M₀ · dM, the transverse tipplings rotate about M₀, corresponding to a new macroscopic collective angle Ø about M₀. The coupling of dM and Ø leads to a new longitudinal mode, which in bulk has a frequency that is largely independent of field H. A longitudinal mode has been observed in thin films of ferromagnets with random anisotropy, but its frequency is H-dependent; for H at angle θ to the film normal and fixed resonator frequency f₀, H cos θ was constant to angles of 80°, with H saturating for larger angles. When the demagnetization field is included the theory yields such as H vs θ for θ <80°, thus providing evidence for the predicted angle θ. However, lower frequency resonators are needed to manifest the predicted macroscopic anisotropy energy.

**G70.00140: Spin reorientation, magnetocaloric effect and metamagnetic transitions in 50% Mn substituted RFeO₃ (R = Eu, Ho and Er)**

KARTHIKA CHANDRAN (Presenter), SANTHOSH P N, Physics, Indian Institute of Technology Madras — The magnetic and magnetocaloric properties of rare earth orthoferrites are studied with 50% Mn substitution in the Fe site. Polycrystalline samples of RFe₀.₅Mn₀.₅O₃(R=Eu, Ho, Er) were synthesized and the crystal structure was resolved by Rietveld refinement of X-ray diffraction patterns. All samples exhibit a PM to AFM transition near room temperature as follows: Tₙ₁(EuFe₀.₅Mn₀.₅O₃)~280K, Tₙ₁(HoFe₀.₅Mn₀.₅O₃)~290K, Tₙ₁(ErFe₀.₅Mn₀.₅O₃)~245K. As temperature decreases, all samples except HoFe₀.₅Mn₀.₅O₃ show a sudden drop in the magnetization which is similar to the spin reorientation (SR) observed in RFeO₃. As temperature further reduces below SR, ErFe₀.₅Mn₀.₅O₃ shows magnetization reversal for FCW curves taken in fields less than 50 Oe. Both Er and Ho based samples show high isothermal magnetic entropy change values of ∆Sₘₗ= 13.4 J/Kg.K (ErFe₀.₅Mn₀.₅O₃, at ~9.5 K, ΔH = 7 T) and ∆Sₘₗ=11.9 J/Kg.K (HoFe₀.₅Mn₀.₅O₃, at ~9.5 K, ΔH = 7 T). EuFe₀.₅Mn₀.₅O₃ shows a metamagnetic transition at low temperatures. Our studies confirm that, by substituting 50% Mn in Fe site, Tₙ reduces and Tₛᵣ increases. High isothermal magnetic entropy change, room temperature Tₙ and Tₛᵣ make these interesting multifunctional materials.

*PNS thanks DST, India (Project: EMR/2014/000592) for financial support.

**G70.00141: Phase Diagram of Magnetic System Ca₃Co₂-xMnxO₆**

BENJAMIN WHITE (Presenter), JAN JESENOVEC, ALEX MANTILLA, Central Washington University — The crystal structure of Ca₃Co₂O₆ is constructed from relatively isolated chains of Co ions oriented along the c direction. Strong intrachain magnetic exchange interactions and weak interchain coupling lead to a quasi-one-dimensional ferromagnetic ground state. Chemical substitution studies show that Co and Mn ions alternate along the chains in the system Ca₃Co₂-xMnxO₆ and that the magnetic structure is tuned from ferromagnetic to antiferromagnetic. Symmetry breaking through exchange striction also leads to multiferroic states in the vicinity of x = 1. Such a highly complex environment is expected to produce a rich temperature vs. manganese concentration phase diagram. In this study, polycrystalline samples in the system Ca₃Co₂-xMnxO₆ were synthesized via a solid state reaction in the range 0 ≤ x ≤ 1; these samples were studied with measurements of magnetic susceptibility and heat capacity. Using these results, we constructed a temperature-Mn concentration phase diagram.

*Research was supported by the Central Washington University (CWU) Science Phase II Project and CWU Office of Undergraduate Research. Travel support was from CWU COTS and Provost Faculty Development Funds, and a CWU Graduate Studies Faculty Travel Award.

**G70.00142: Room-temperature ferromagnetism induced by boundary defects in graphene oxide nanoplatelets**

JOHN PRIAS (Presenter), HERNANDO ARIZA, Universidad del Quindío, KATHERINE GROSS, PEDRO PRIETO, Universidad del Valle — Graphene oxide nanoplatelets from bamboo pyroligneous acid (GO-BPA) show room-temperature ferromagnetism, by using the double thermal decomposition (DTD) method at different carbonization temperatures from 673 to 973 K. The GO-BPA samples were characterized by using Raman, FTIR, XRD, XPS, HR-TEM, I-V curves, MFM and VSM techniques. Magnetic measurenets suggest that increased carbonization temperature increases graphite conversion, boundary defects, desorption of some organic compounds, phonon response and magnetization saturation, respectively. Room-temperature ferromagnetic behavior was correlated with the variation of the boundary defect density.

*We would like to thank the Interdisciplinary Institute of Sciences and EITP, Universidad del Quindío and the Center of Excellence for Novel Materials at Universidad del Valle, Cali for the financial support.
G70.00143: Many electron, spin-orbit and resonant polaron effects in the THz cyclotron resonance of modulation-doped CdMnTe/CdMgTe Quantum Wells. IMTIAZ TANVEER (Presenter), BRUCE MCCOMBE, University at Buffalo, The State University of New York, ADAMUS ZBYSZEK, MACIEJ WIATER, GRZEGORZ KARCZEWSKI, TOMASZ WOJTOWICZ, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland, XIAOGUANG WU, Chinese Academy of Science, Beijing, China, FRANCOIS M PEETERS, Department of Physics, University of Antwerp, Antwerp, Belgium — We present low temperature THz cyclotron resonance studies of modulation-doped CdMnTe/CdMgTe quantum wells with Mn compositions $x = 1$-3.6% in magnetic fields up to 17T. Electron densities $n_e$ are $(1 - 4) \times 10^{11}$ cm$^{-2}$. We focus on B-regions where the giant Zeeman splitting of Landau levels (LLs) leads to the 1$\parallel$ level crossing 0$\perp$ at a field $B_C$. LLs are resonantly coupled and split by the spin-orbit interaction, and a gap due to many-electron exchange can also occur (Quantum Hall Ferromagnetism) when $B_C$ is close to the field for filling-factor (FF) 2 at low enough temperatures. For $x=2.85\%$ $B_C$ lies at 8.65T, and CR is below our Ge:Ga detector onset. With exchange corrected LLs $B_C$ should occur at ~10T, but no splitting is observed. Between 9 and 15T, FF<1.67 so only spin-orbit coupling is important. Two samples do show a clear splitting of CR into two lines near 15T; strong TO phonon absorption blocks CR transmission at higher B. The origin of this splitting is not understood. For low $x$ samples $B_C$ lies between 3 and 4.5 T, depending upon temperature and sp-d exchange. No LL splittings are observed at 4.2 K, but at 1.5K there is a small splitting near 4.5T. A strong resonant magnetopolaron effect is also observed in all high B in all samples. Effect of e-e exchange will be presented.

G70.00144: The H field dependence of magnon diffusion length basing on Boltzmann transport methods* WEI WANG (Presenter), TAO LIU, YUHENG LI, JIANWEI ZHANG, School of Physics, Tongji University — The urgent demand for high-capacity and high-speed logical storage device gives rise to the further study on spin and magnon. In this abstract, we construct a new magnon Boltzmann equation from full quantum magnon Hamiltonian in magnetic insulator system, which contains the factors related to boundary injection, temperature gradient and magnetic field gradient. In our methods, we first calculate the change of magnon accumulation and magnon current with thickness of magnetic oxide film, under interaction of interface with spin-magnon, which implies that there are two parts in the process of magnon transport: magnon diffusion and magnon relaxation. Second, we calculate the change of magnon current with distance, which explains the dependence of magnon diffusion length on magnetic field theoretically. We find that the magnon diffusion length is inversely proportional to H field which was first observed by experiment [1]. Last but not least, we predict the rate of change of magnon current corresponding to the anisotropy energy change in magnetic insulator with strong anisotropic exchange energy and anisotropy energy.


*This work was supported by NSFC under grant No. 51471119 & 51331004, and by MNSRP under grant No. 2015CB921501.

G70.00145: Interplay between oxygen vacancies, strain, and magnetism in SrMnO$_3$: a self-consistent site-dependent DFT+U study CHIARA RICCA (Presenter), University of Bern, IURII TIMROV, NICOLA MARZARI, Ecole polytechnique federale de Lausanne, ULRICH ASCHAUER, University of Bern, MATTEO COCOCCIONI, Ecole polytechnique federale de Lausanne — Motivated by indications that strain and defects can stabilize a ferromagnetic ground state in normally antiferromagnetic SrMnO$_3$ thin films, we use self-consistent site-dependent (SCSD) DFT+U calculations to investigate the interplay between oxygen vacancies, strain, and magnetism in this material. Already for the stoichiometric material, using a self-consistent U increases the accuracy of lattice parameter predictions, which is crucial to study strain-induced changes in properties and results in critical strain values for the magnetic phase transition in better agreement with experiment compared to previous theoretical studies. Defect formation leads to changes in geometry and occupation on transition metal sites surrounding the defect. We find that taking into account the site-dependence of U around a defect has a strong impact on the computed formation energies and consequently on all related properties. As such $U_{\text{SCSD}}$ prevents overestimating the stability of the ferromagnetic order thanks to a proper description of excess charge localization upon defect formation and helps in rationalizing different ordering of oxygen vacancies depending on the magnetic order in the epitaxial thin film.
G70.00146: Perpendicular magnetic anisotropy and spin mixing conductance in polycrystalline europium iron garnet thin films

JACKSON BAUER (Presenter), ETHAN RAPHAEL ROSENBERG, CAROLINE ANNE ROSS, Materials Science and Engineering, Massachusetts Institute of Technology — Rare earth iron garnets (REIG) are a diverse class of magnetic insulators in which properties such as the anisotropy and magnetostriction can be tuned by choice of rare earth ion. Garnet films with perpendicular magnetic anisotropy (PMA) are attractive for studies of spin orbit torque and chiral spin textures. PMA has been achieved in epitaxial REIG on garnet substrates due to magnetoelastic anisotropy from epitaxial lattice mismatch strain, but for making devices on non-garnet substrates, PMA without epitaxy is essential. Here we report the growth and properties of polycrystalline europium iron garnet (EuIG) with PMA. Films were grown by pulsed laser deposition followed by a rapid thermal anneal. Films on quartz (0001) substrates demonstrated PMA attributed to the in-plane compressive thermal mismatch strain, whereas films on (11-20) quartz, Si, and fused SiO2 exhibited an in-plane easy axis due to tensile strain, consistent with the positive magnetostriction of EuIG. Spin transport measurements on Pt/EuIG/quartz heterostructures gave an anomalous Hall effect-like spin Hall magnetoresistance and spin mixing conductance similar to single crystal epitaxial EuIG. These results show that polycrystalline garnet can be grown with PMA, making it useful for applications in spintronics.

G70.00147: The structural and magnetic properties of the SrTiO3/SrRuO3/SrTiO3(100) Heterostructure

UDDIPTA KAR (Presenter), AKHILESH SINGH, TSUNG-CHI WU, BIPUL DAS, MING-CHIN CHEN, WEI-LI LEE, Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan — The itinerant ferromagnetism in the ultrathin SrRuO3 films, grown by pulsed laser deposition, above a critical thickness of 3-4 unit cell (uc) has been reported previously by few groups[1-3]. On the other hand, in SrTiO3/SrRuO3/SrTiO3(100) heterostructure and (SrRuO3)1–(SrTiO3)5 superlattices grown by oxide molecular beam epitaxy (MBE) technique, the ferromagnetism was found to persist even with a 1-uc of SrRuO3[4]. It was suggested that the RuO6 octahedral tilting angle may be affected by the SrTiO3 capping layer, which in turn influences the ferromagnetism of the underlying SrRuO3[4]. Detailed investigations on the SrTiO3 capped and uncapped SrRuO3 films are required to fully understand the intrinsic mechanism involved for the magnetic properties of ultra-thin SrRuO3 films. In this work, Systematic studies of the structural and magnetic properties of the SrTiO3(x-uc)/SrRuO3(y-uc)/SrTiO3(100) heterostructure with various thicknesses of x-uc and y-uc will be presented and discussed[3, 5].

References
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G70.00148: Current-induced spin polarization and anomalous Hall and Nernst effects in heterostructures with k-cubed Rashba spin-orbit coupling

ANNA DYRDAL (Presenter), Institut fur Physik, Martin-Luther Universitat Halle-Wittenberg, D-06099 Halle, Germany, ANNA KRZYZEWSKA, Faculty of Physics, Adam Mickiewicz University in Poznan, ul. Umultowska 85, 61-614 Poznan, Poland, LUKASZ KARWACKI, Institute of Molecular Physics, Polish Academy of Sciences, ul. M. Smoluchowskiego 17, 60-179 Poznan, Poland, JAMAL BERAKDAR, Institut fur Physik, Martin-Luther Universitat Halle-Wittenberg, D-06099 Halle, Germany, JOZEF BARNAS, Faculty of Physics, Adam Mickiewicz University in Poznan, ul. Umultowska 85, 61-614 Poznan, Poland — We will discuss our recent results on current induced nonequilibrium spin polarization and the anomalous Hall and Nernst effects within the effective models describing 2DEG in semiconductor heterostructures and perovskite oxide interfaces [L. Karwacki et al., Phys. Rev. B 97, 235302 (2018), A. Krzyzewska et al., pss RRL (2018), doi:10.1002/pssr.201800232]. We will focus on the role of k-cubic Rashba spin-orbit interaction which seems to play an important role in these materials. We will present the temperature dependence of the nonequilibrium spin polarization in nonmagnetic and magnetic cases, and indicate the role of the Berry phase on this effect when the system is magnetic. Moreover, we will show that there is a substantial intrinsic contribution to both anomalous Hall and Nernst effects, that are robust against impurity scattering processes. Additionally, the sign of the anomalous Nernst conductivity can be changed by tuning the temperature. This sign change appears below the critical temperature of the magnetic phase transition.

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G70.00149: Effects of second order surface anisotropy in YIG sputtered onto GGG (100) oriented substrate

ROBERTO RODRIGUEZ (Presenter), Physics, Pontificia Universidad Catolica de Chile/Physics, ALEXANDRE OLIVEIRA, CARLOS CHERMAN, RICARDO BORGES DA COSTA, U. C SILVA, NEYMAR DA COSTA, Fisica, Universidade Federal do Rio Grande do Norte, B.G SILVA, R. L SOMMER, Fisica, Centro Brasileiro de Pesquisas, FELIPE BOHN, MARCIO CORREA, Fisica, Universidade Federal do Rio Grande do Norte — In this work, we produced Y$_3$Fe$_5$O$_{12}$ textured films, with thicknesses between 50 nm and 500 nm, onto (100) GdGaO$_3$ by magnetron sputtering and post annealing, and investigated the first and second order surface and cubic anisotropy constants using the ferromagnetic resonance technique. The surface anisotropy constants exhibited different behaviors with film thickness, with the first order presenting the usual inverse of ferromagnetic layer thickness. Besides this inverse of thickness behavior, the second order also came up with a constant value. In the frame of spin reorientation transition phenomenon, we evaluated volume and surface contribution to the surface anisotropy. Although the second order cubic anisotropy constant is one order of magnitude stronger than the first order, they did not show any explicit thickness dependence. As an important finding of this work, in order to correctly characterize the magnetic properties of the YIG films, it is essential to measure both, the out-of-plane and in-plane angular dependence of the FMR resonance field.

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G70.00150: Effect of electron transport on demagnetization on the shortest time scale

GUOPING ZHANG (Presenter), YIHUA BAI, TYLER JENKINS, Indiana State University, THOMAS F GEORGE, University of Missouri-St. Louis — It is generally believed that there are at least two ways to use an ultrafast laser pulse to demagnetize a magnetic sample [1]. One is to directly photo-demagnetize the system through spin-orbit coupling (SOC), and the other is to utilize ultrafast hot electron transport without SOC. The challenge is that these two processes are entangled on the same time scale. However, we do not even know how fast electrons move under laser excitation, nor far they move [2]. Here we carry out a first-principles time-dependent calculation to investigate how fast electrons actually move under laser excitation, and how large the electron transport affects demagnetization on the shortest time scale. To take into account the transport effect, we implement the intraband transition in our theory. For bulk fcc Ni, we find the effect of spin transport on demagnetization to be extremely small, no more than 1% [3].


*Supported by the U.S. Department of Energy under Contract No. DE-FG02-06ER46304.

G70.00151: The magnetic order of antiferromagnetic Mn3NiN thin films under biaxial strain

DAVID BOLDRIN, FREYA JOHNSON (Presenter), Blackett Laboratory, Imperial College London, ANDREI MIHAI, BIN JOU, Department of Materials, Imperial College London, JAN ZEMEN, Faculty of Electrical Engineering, Czech Technical University in Prague, WILL BRANFORD, Blackett Laboratory, Imperial College London, JOERG WUNDERLICH, Hitachi Laboratory, University of Cambridge, LESLEY COHEN, Blackett Laboratory, Imperial College London — We explore the magnetic phase diagram of piezomagnetic antiperovskite Mn$_3$NiN thin films grown on different substrates as a function of the induced biaxial strain using magnetotransport and neutron scattering. We find that the anomalous Hall effect is an effective probe of the out-of-plane magnetisation in our films. Under compressive in-plane biaxial strain, the films support a canted antiferromagnetic (AFM) state with large coercivity at low temperature that transformed at a well-defined Neel transition temperature into a soft ferrimagnetic-like (FIM) state at high temperatures. In stark contrast, under tensile strain the magnetisation value decreases rapidly above the Neel transition. The resulting magnetic phase diagram shares many characteristics with that predicted for thin films of the closely related antiperovskite Mn$_3$GaN.

*UK EPSRC
Long-range, dynamic noncollinear textures \cite{1} can be sustained in ferromagnetic nanowires by the non-local compensation of damping \cite{2}. In contrast to current-driven magnons, noncollinear textures exhibit (1) frequencies under ferromagnetic resonance that are inversely proportional to damping; (2) an excitation threshold that is proportional to the in-plane anisotropy; and (3) coherence over the length of the nanowire. We analytically demonstrate that nonlinearities are fundamental to describe these characteristics. Two generic solutions when the nanowire is subject to spin injection at one edge are found, exhibiting opposite frequency tunabilities. This is in stark contrast to the linear frequency tunability predicted for spin superfluids. By micromagnetic simulations, we show that these predictions hold in the presence of in-plane anisotropy and non-local dipole fields.

References
\cite{1} Iacocca et al., Phys. Rev. Lett. 118, 017203 (2017)
\cite{2} Iacocca et al., Phys. Rev. B 96, 134434 (2017)


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Spin Hall effect is a phenomenon of spin current generation from an applied charge current, arising from the two distinct regimes: intrinsic and extrinsic mechanism. The intrinsic contribution derives from the Berry curvature associated with band structure of the material while extrinsic one originates from spin dependent scattering on structural defects or impurities. In previous reports, SHE has been tuned by alloying, changing the combination of the host and impurity metals or changing the concentration of the impurities in many alloy systems. Nevertheless, the mechanism of SHE is governed by either effect, the crossover between extrinsic and intrinsic regime induced by alloying has remain elusive.

In this study, we focus on AuCu as a material for observation of extrinsic-intrinsic crossover of the SHE. We demonstrate spin Hall angle (SHA) of Au$_{100-x}$Cu$_x$ alloys by changing Cu concentration $x$. The SHA changes the sign only in a limited range of the Cu concentration due to the extrinsic skew scattering, while the intrinsic contribution becomes dominant with increasing the Cu concentration. These results provide an evidence of crossover from extrinsic regime to intrinsic regime in the metallic alloy system.

Electronic vs magnonic contributions to unidirectional magnetoresistance

The effect of spin current on magnetoresistance is of central importance to modern spintronics. We have investigated unidirectional magnetoresistance (UMR) in Permalloy (Py)/Pt bilayers, a magnetoelectronic effect whose origin is currently debated. Two different mechanisms are believed to contribute to UMR. The first mechanism is due to magnon generation/suppression in Py by pure spin current produced by the spin Hall effect in Pt. The second one is due to spin dependent electronic scattering near the Py/Pt interface, where spin accumulation is modulated due to the spin current generated in Pt. By engineering the geometric and material properties of our samples, we enhanced magnon relaxation, thus suppressing the spin current-induced changes of magnon population. We observed a significantly reduced UMR, suggesting that this effect in the studied structures is dominated by the magnon contribution. We also discuss how the dependence of UMR on field temperature provides information about the spectral characteristics of the generated magnons, and their generation mechanisms. Our results suggest the UMR can be utilized as an efficient technique for the characterization of spin current-driven dynamical magnetization states.

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Observation of the evolution of magnetic domain structures related to magnetic polaron cluster formation in a single crystal of EuB$_6$

DIBYA SIVANANDA (Presenter), ANKIT KUMAR, ARIF ALI, Indian Institute of Technology Kanpur, PINTU DAS, Physics, Indian Institute of Technology Delhi, JENS MULLER, Physics, Goethe University, SATYAJIT BANERJEE, Indian Institute of Technology Kanpur — EuB$_6$ is a ferromagnetic semi-metal which shows colossal magnetoresistance at a temperature of $T_c1\approx15.5K$ and also exhibits nanoscale phase separation between conducting ferromagnetic and insulating paramagnetic domains. Here, we have performed high sensitivity magneto-optical imaging of EuB$_6$ which images the local magnetic field distribution on the surface of a sample. From our measurements, we identify three characteristic boundaries, $T^*(H)$, $T_{c1}(H)$ and $T_{c2}(H)$, in a field - temperature magnetic phase diagram and identify their behavior with field. Using scaling and modified Arrott's plot analysis of isothermal bulk magnetization data, we identify critical transition into a ferromagnetic state below $T_{c2} = 12 \pm 0.2K$. High-resolution imaging of magnetic domains reveals large magnetized domains below $T_{c2}$. With increasing $T$ ($>T_{c2}$) the magnetic domains disintegrate into finger-like patterns before fragmenting into disjoint magnetized puddles at $T_{c1}$ and ultimately disappearing at $T^*$. At $T^*_{c1}$ we observe a significant increase in the spatial inhomogeneity of the local magnetic field distribution associated with the magnetic domains disintegrating into smaller magnetized structures. We explain our results via the formation and the subsequent coalescing of magnetic polaronic clusters.

Towards sub-wavelength spin and charge control of nitrogen vacancy centers using super-resolution microscopy

HARISHANKAR JAYAKUMAR (Presenter), SIDDHARTH DHOMKAR, JACOB HENSHAW, CARLOS MERILES, City College of New York — Super resolution microscopy has enabled addressing single nitrogen vacancy centers with a spatial resolution that is an order of magnitude higher than the diffraction limit. Here, we present the latest experimental results towards the utilization of stimulated emission depletion based super resolution techniques to manipulate the charge and spin degrees of freedom of a diamond nitrogen vacancy (NV) center. This technique is applicable to various NV center sensing modalities and data storage applications that demand high spatial resolution with minimal perturbation of the NV environment.

Thermally induced spin polarization in 2D systems with Rashba spin-orbit interaction

ANNA DYRDAL (Presenter), Institut für Physik, Martin-Luther Universität Halle-Wittenberg, D-06099 Halle, Germany, Jozef Barnas, Faculty of Physics, Adam Mickiewicz University in Poznan, ul. Umultowska 85, 61-614 Poznan, Poland, Vitalii Dugaev, Department of Physics and Medical Engineering, Rzeszow University of Technology, Al. Powstancow Warszawy 6, 35-959 Rzeszow, Poland, Jamal Berakdar, Institut für Physik, Martin-Luther Universität Halle-Wittenberg, D-06099 Halle, Germany. — We present the theory of spin polarization induced by a temperature gradient (heat current) in a magnetized two-dimensional electron gas (2DEG) with a Rashba spin-orbit interaction. Within the Matsubara Green's function formalism, we calculated the temperature dependence of the spin polarization not only in non-magnetic case but also in the presence of a nonzero exchange field oriented arbitrarily in the space. For the magnetic system, among others, we identified a term in the spin polarization that stems from the Berry curvature of the corresponding electronic bands. Moreover, we show that the electrically induced and the thermally induced spin polarizations obey the Mott relation in a nonmagnetic 2DEG as well as in the magnetic system but in the latter case only for the spin polarization normal to the electric field and to the thermal gradient. The components along the driving forces in a magnetic system do not obey this relation. This is mainly due to the fact that these components are determined by the Berry curvature of the electronic bands in the presence of both spin-orbit and exchange interactions.

* A. Dyrdal and J. Berakdar acknowledge the support of German Research Foundation (DFG) through SFB 726 and SFB TRR 227
G70.00158: Frustrated bilayer spin one XY model on the honeycomb lattice*  ANTONIO PIRES (Presenter), Universidade Federal de Minas Gerais — The study of quantum magnetism on geometrically frustrated lattices has been an active field of interest due to the possibility of finding new states of matter such as spin liquids and nematic phases. In this context, honeycomb lattices have attracted a lot of attention due to their interesting and poorly understood magnetic properties. The honeycomb lattice has the lowest value $z = 3$ of the coordination number, leading to a strong effect of quantum fluctuations. In contrast to the spin 1/2 model, not so much theoretical attention has been dedicated to the $S = 1$ model in spite of its relevance to several materials with spin one. Here I study the spin one bilayer XY antiferromagnet on the honeycomb lattice at zero temperature, with nearest-neighbor $J_1$ and next-nearest neighbor $J_2$ exchange interactions and single-ion easy plane anisotropy, using the SU(3) Schwinger boson formalism. The ratio between the interlayer to the intralayer nearest neighbor exchange interactions exhibits a quantum phase transition at a critical ratio 13.8 that separates the Neel phase from a quantum disordered paramagnetic phase. The effect of next nearest neighbor interactions is discussed and the phase diagram is presented.

*This work was partially supported by Conselho Nacional de Pesquisa (CNPQ)

G70.00159: Cooperative Two-Sublattice Model for Frustrated Pyrochlore Gd$_2$FeSbO$_7$  SAIKAT NANDI (Presenter), Department of Physics, University of Kalyani — DC and AC magnetization and heat capacity data of frustrated pyrochlore Gd$_2$FeSbO$_7$ are studied within the framework of cooperative two-sublattice model [1] in presence of easy-plane single-ion anisotropy at Gd-site. There are three types of interactions: intra-sublattice Gd-Gd antiferromagnetic interaction, intra-sublattice Fe-Fe ferromagnetic interaction, and inter-sublattice Gd-Fe antiferromagnetic interaction. The interaction between Fe$^{3+}$ $3d$ moments, which is stronger than 4f$^7$ interaction, generates a molecular field at Gd-site through a weaker cooperative Gd-Fe ramification. Fe$^{3+}$ sublattice orders at $T_C \sim 5$ K possibly in ‘two-in, two-out’ spin-configuration due to FM exchange interaction. Gd moments are fixed perpendicular to local <111> axes of tetrahedron due to crystal-field anisotropy and antiferromagnetic Gd-Gd exchange interactions. Such magnetic structure for Gd tetrahedra may resemble the Palmer-Chalker ground state, which is subdued due to stronger B-site Fe-Fe interactions. Saturation magnetization of 13.04μB is expressed as the vector coupling of directional magnetic moments of Gd and Fe. Finally magnetocaloric properties of Gd$_2$FeSbO$_7$ are estimated from magnetization and heat capacity results.


G70.00160: Density functional study of the electronic structure of the non-collinear helical magnet Ba$_3$NbFe$_5$Si$_2$O$_{14}$ (Langasite): Magnetic exchange and Dzyaloshinskii-Moriya interactions*  CHURNA BHANDARI (Presenter), SASHI SEKHAR SATPATHY, University of Missouri — Ba$_3$NbFe$_5$Si$_2$O$_{14}$ is an iron based compound, which consists of a Fe trimer in the ab-plane with a large spin moment $\approx 5$ μB/Fe. The spins of Fe trimer form a 120° non-collinear antiferromagnetic structure in the ab-plane followed by a helical structure with a propagation vector $q = (0,0,1/7)$. We study the electronic band structure using density functional theory (DFT), which shows an insulating gap due to the exchange splitting of the 3d bands. The features of the computed optical spectra are discussed in terms of the band structure. In addition, we study the magnetic exchange parameters by mapping the density functional total energy to exchange models. The absence of inversion symmetry in conjunction with the spin-orbit interaction leads to the Dzyaloshinskii-Moriya interaction (DMI) of the type $D S_1 \times S_2$, which is necessary to explain the observed spin-wave energies. We study the DMI from a model extracted from the DFT in order to gain insight into the magnetic interactions in the system.

*This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Grant No. DE-FG02-00ER45818.
**G70.00161: 'Local-Ising' type magnetism and metamagnetism in the rare-earth pyrogermanates**  KEITH TADDEI (Presenter), LIURUKARA SANJEEWA, Oak Ridge National Laboratory, JOSEPH KOLIS, Chemistry, Clemson University, ATHENA S. SEFAT, CLARINA DELA CRUZ, DANIEL PAJEROWSKI, Oak Ridge National Laboratory — The rare-earth pyrochlores have long been the system of choice for the study of frustrated magnetism due to the inherent geometric frustration of the rare-earth sublattice which can beget 'local-Ising' behavior. The combination of a large local-anisotropy and geometric frustration lead to the famous 'spin-ice' rules and consequently to exotic physics such as magnetic monopoles. The rare-earth pyrogermanate family of materials has seen significantly less study yet has similar potential due to a spiraling triangular rare-earth sublattice. We report the results of neutron scattering experiments on rare-earth pyrogermanate Er$_2$Ge$_2$O$_7$ which reveal a 3D spiral magnetic structure below 1.2 K. Under applied field we find a metamagnetic transition of spin-flip type indicating a large local anisotropy of the rare-earth site. This transition selectively inverts magnetic moments anti-parallel to the applied field yet leaves to moments along their locally determined easy-axis. This describes a local-Ising type behavior as seen in the spin-ice pyrochlores and encourages further study of these materials.

**G70.00162: Observation of magnetoelastic effects in a quasi-one-dimensional spiral magnet**  CHONG WANG, DAIWEI YU, XIAOQIANG LIU (Presenter), RONGYAN CHEN, XINYU DU, BIAOYAN HU, LICHEN WANG, International Center for Quantum Materials, Peking University, KAZUKI IIDA, KAZUYA KAMAZAWA, Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, SHUICHI WAKIMOTO, Materials Sciences Research Center, Japan Atomic Energy Agency, JI FENG, NAN LIN WANG, YUAN LI, International Center for Quantum Materials, Peking University — We present a systematic study of spin and lattice dynamics in the quasi-one-dimensional spiral magnet CuBr$_2$, using Raman scattering in conjunction with infrared and neutron spectroscopy. Along with the development of spin correlations upon cooling, we observe a rich set of broad Raman bands at energies that correspond to phonon-dispersion energies near the one-dimensional magnetic wave vector. The low-energy bands further exhibit a distinct intensity maximum at the spiral magnetic ordering temperature. We attribute these unusual observations to two possible underlying mechanisms: (1) formation of hybrid spin-lattice excitations and/or (2) "quadrumerization" of the lattice caused by spin-singlet entanglement in competition with the spiral magnetism.

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**G70.00163: Effects of boundary on a kagome Ising model with magnetic-charge interaction**  TOMONARI MIZOGUCHI (Presenter), YASUHIRO HATSUGAI, Department of Physics, University of Tsukuba — In frustrated Ising models on kagome and pyrochlore lattices, the system is described by conserved charge degrees of freedom [1]. Conserved charges serve as a "fractionalized" elementary excitation, which characterizes the topological nature of spin liquid state. The conserved charge description is useful to seek novel states induced by perturbations against the conventional nearest-neighbor model. For instance, it has been found that father-neighbor exchange interactions induce an interaction between the charges, which becomes a source of novel spin liquid state [2].

In this presentation, we elucidate the effect of boundary on this novel spin liquid state. The conserved nature of the charges naturally connects the bulk and boundary quantities through "Gauss' law", thus the interplay between interactions of charges and boundary effects is expected to induce a novel physics. By using Monte Carlo simulations, we demonstrate that the spin state at the edges induce a finite bulk charge, which can be regarded as "bulk-boundary correspondence" in an Ising spin system [3].

Spin-flip and magnetoelectric coupling in acentric and non-polar Pb$_2$MnO$_4$*  

HUNG-DUEN YANG  

(Presenter), Physics, National Sun Yat-Sen University, Taiwan, D CHANDRASEKHAR KAKARLA, Center of Crystal Research, National Sun Yat-sen University, Kaohsiung, 804 Taiwan, HUNG-CHENG WU, Texas Center for Superconductivity, University of Houston, Texas 77204, USA, DONG-JIE HSIEH, PO-JUNG SUN, Physics, National Sun Yat-Sen University, Taiwan, JIUNN-YUAN LIN, Institute of Physics, National Chiao Tung University, JIMLONG HER, Division of Natural Science, Chang Gung University, Tao-Yuan 333, Taiwan, YASUHIRO H. MATSUDA, Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan, LIANGZI DENG, GOOCH MELISSA, PAUL C. W. CHU, Texas Center for Superconductivity, University of Houston, Texas 77204, USA — Acentric and non-polar Pb$_2$MnO$_4$ was predicted to exhibit unique multipiezo induced magnetoelectric (ME) phenomena [1]. Here, we present the results of measurements from magnetization as well as the dielectric, as a function of temperature (T), magnetic field (H), pressure (P), and electric field (E) primarily to address the ME coupling and identify the underlying mechanism behind this phenomenon. Magnetization measurements reveal the antiferromagnetic (AFM) ordering of Mn$_4^+$ spins at $T_N = 17$ K. For $T_N = 17$ K, a robustly multiple partial spin-flip transitions were also observed. The existence of ME coupling is supported by the observed dielectric anomaly near $T_N$. The lattice dielectric response is strongly influenced by spin-flip transitions that trigger the pronounced ME coupling below the $T_N$. The magnetic-field-induced ME phenomenon in Pb$_2$MnO$_4$ has been ascribed to the strong coupling of lattice polarization with the magnetic interactions and thereby offers a route to attain novel ME materials.


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G70.00165: Probing variable range hopping lengths by magneto conductance in carbonized polymer nanofibers*  

YUNG PARK (Presenter), Physics and Astronomy, Seoul National University & University of Pennsylvania, KYUNG HO KIM, SAMUEL LARA-AVILA, HANS HE, Microtechnology and Nanoscience, Chalmers University of Technology, HOJIN KANG, Physics and Astronomy, Seoul National University, SERGEY KUBATKIN, Microtechnology and Nanoscience, Chalmers University of Technology — Using magneto transport, we report hopping length scales in the variable range hopping conduction of carbonized polyacetylene and polyaniline nanoribers. In contrast to pristine polyacetylene nanofibers that show zero magneto conductance at large electric fields (it clarifies the charge and spin states of 1-D topological insulator, namely the solitons in polyacetylene nanofibers.), carbonized polymer nanofibers display a negative magneto conductance that decreases in magnitude but remains finite with respect to the electric field. We show that this behavior of magneto conductance is an indicator of the electric field and temperature dependence of hopping length in the gradual transition from the thermally activated to the activation-less electric field driven variable range hopping transport. This reveals magneto transport as a useful tool to probe hopping lengths in the non-linear hopping regime.

Reference: Kyung Ho Kim et. al., Scientific Reports 8, 4948 (2018)

*This work was jointly supported by the Swedish-Korean Basic Research Cooperative Program of the NRF-2017R1A2A1A18070721, Korea and the SSF No. IS14-0053, Sweden.

G70.00166: Single Crystal Synthesis of Frustrated Magnet Y$_{0.5}$Ca$_{0.5}$BaCo$_4$O$_7$  

YUKI TATSUMI (Presenter), LINDA YE, TAKEHITO SUZUKI, JOSEPH CHECKELSKY, Massachusetts Institute of Technology — Neutron scattering experiments on Y$_{0.5}$Ca$_{0.5}$BaCo$_4$O$_7$ powders have reported suppression of magnetic order and flat magnonic bands down to low temperatures [1]. In order to study the physical properties of these materials in greater detail, we have synthesized bulk single crystals of this compound by the optical floating zone method. We present the details of the material preparation and characterization, including the dependence of magnetic properties on the growth conditions as well as plans for probing the unique magnetic dispersion of this system.

Role of anti-site disordering in magnetic properties of Sm2NiMnO6 double perovskite

SUPRIYO MAJUMDER (Presenter), MALVIKA TRIPATHI, R.J. CHOUDHARY, D. M. PHASE, Thin film magnetism group, UGC-DAE Consortium for Scientific Research — We have investigated the structural, magnetic and electronic properties of B-site disordered Sm2NiMnO6 DP oxide. XPS measurements indicate mixed valency of both Ni2+/3+ and Mn4+/3+ species. RE2NiMnO6 ordered DP is commonly believed to show two magnetic phase transitions viz, PM-FM transition at TC due to Ni2+/3+-O-Mn4+/3+ super exchange interaction and at Tf due to coupling of RE spins with Ni-Mn network [1, 2]. In our present study, we have observe that the presence of intrinsic B-site disorder results in an additional AFM coupling [3], mediated by Ni2+/3+-O-Ni2+/3+ and Mn4+/3+-O-Mn4+/3+ pairs. In M(T) measurements we have observed an inverted cusp like trend and thermal irreversibility in FCC and FCW cycles in Tf<T<TC both of which vanishes on application of higher magnetic fields. The observed thermal hysteresis indicates towards the possibility of either coexisting FM-AFM phases or magnetic frustration originating from different exchange interaction paths between mixed valence ions. MH isotherms in Tf<T<TC exhibit two step reversibility loop behavior, which further confirms the presence of competing FM-AFM phases.


Specific heat measurements of Ce2Zr2O7 in magnetic field

ROMAN MOVSHOVICH (Presenter), Los Alamos National Laboratory, ANDREA BIANCHI, JÉRÉMIE DUDEMAIN, Département de physique, Université de Montréal, Montréal, QC, H3T 3J7, Canada, MICHAEL NICKLAS, Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40 D-01187 Dresden, Germany, EVAN SMITH, BRUCE GAULIN, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1, JONATHAN GAUDET, Johns Hopkins University, Baltimore, MD 21218, Institute for Quantum Matter and Department of Physics and Astronomy — We measured specific heat of the pyrochlore Ce2Zr2O7 in magnetic field up to 14 T and temperatures down to 60 mK. In zero field we observe a monotonic rise of the specific heat, with the values of C/T reaching 30 J/mol-K at 100 mK, and without saturation, at least in some compounds. The field was applied in either [100] or [110] directions. Even small magnetic field on the order of a kilogauss pushes the entropy up in temperature, developing a broad maximum in C(T), which moves up in temperature with increasing magnetic field. The calculated entropy is consistent with a doublet ground state. Extreme sensitivity to small magnetic field is consistent with a disordered zero-field ground state, with entropy piling up towards T=0, indicating a possible spin-liquid.

*We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC). Measurements at LANL were supported by the US DOE, Division of Materials Sciences and Engineering.

Monte Carlo Simulations of Classical Spin Liquids

HANNAH PRICE (Presenter), XIAOJIAN BAI, MARTIN MOURIGAL, Georgia Institute of Technology — Using Monte Carlo, we simulate the ground state spin configurations of spin liquids at low temperatures. The program requires only basic unit cell and coupling energy information to be run. Thus, most materials can be easily simulated. We have modeled the frustrated diamond lattice for a range of J2/J1 energies. As well as the frustrated pyrochlore lattice. In particular, we compare the modeled critical temperature and structure factor, with that from previous models and experiments.

Impact of interlayer coupling on magnetic skyrmion size

CANER DEGER (Presenter), ILHAN YAVUZ, Physics Department, Marmara University, FIKRET YILDIZ, Physics Department, Gebze Technical University — We study the magnetic skyrmion formation in thin-film stacks, consist of two magnetic layers separated by a non-magnetic spacer. The Landau-Lifshitz-Gilbert equation, comprising the spin precession term and the damping term with all relevant contributions, is numerically solved within the micromagnetic framework. Through extensive systematic calculations, we find that skyrmion size can be controlled by the interlayer exchange coupling, as well as the external magnetic field. z-component of the magnetization of the layers, which can be tailored by the coupling, strongly affects the skyrmion diameter. The skyrmion phase coexists with the helical phase for both types of coupling, being antiferromagnetic or ferromagnetic, in the absence of the magnetic field. The size of the skyrmions at zero field can also be controlled by the interaction. We anticipate that our predictions not only expand our fundamental understanding of the physical mechanisms responsible for skyrmion formation but also provide rational basis for the next-generation logic/memory device applications.

*This work is supported by Marmara University within the Scientific Research Commission, Turkey, through the Research Projects under Grant FEN-C-DRP-150218-0065 and FEN-A-100616-0275.
G70.00171: Current-driven coherent magnetic skyrmion generation* CANER DEGER (Presenter), ILHAN YAVUZ, Physics Department, Marmara University, FIKRET YILDIZ, Physics Department, Gebze Technical University — The next-generation logic and memory devices which use magnetic skyrmions as the information carrier are frequently studied due to its remarkable magnetic stability, extremely compact size and very-low-cost driving force within the nanostructure. To realize skyrmion-based spintronic devices, it is essential to understand the dynamics of skyrmion generation. In this study, we have carried out a systematic theoretical study on coherent magnetic skyrmion generation by an anti-notch in a channel of finite width. We found that, the coherent skyrmion generation is crucially effected by both damping ($\alpha$) and nonadiabaticity ($\beta$) parameters, as well as the geometry of the anti-notch. The periodicity of the generation is also investigated for certain current densities and $\alpha/\beta$ ratios. We anticipate that our predictions provide rational basis for skyrmion-based devices in which skyrmions are used as information carriers.

*This work is supported by Marmara University within the Scientific Research Commission, Turkey, through the Research Projects under Grant FEN-C-DRP-150218-0065. C. D. is partially supported by the Turkish Funding Agency TUBITAK through the 2211 Graduate Bursary Program.

G70.00172: Topological Hall effect in diffusive ferromagnetic thin films with spin-flip scattering* SHULEI ZHANG (Presenter), OLLE HEINONEN, Materials Science Division, Argonne National Laboratory, Lemont, Illinois, USA — So far, most electrical measurements of magnetic skyrmions have been based on the interpretation that the topological Hall (TH) resistivity is proportional to the number of skyrmions multiplied by the magnetic flux quantum, which only applies to bulk systems in the strong exchange-coupling and nondiffusive regimes. In this work, we theoretically studied the TH effect in diffusive ferromagnetic metal thin films by solving a Boltzmann transport equation in the presence of spin-flip scattering. We found that, even in the strong exchange limit, the TH effect itself is not topologically protected in the presence of spin diffusion, owing to the spin accumulation built up in the vicinity of the skyrmions. A more general formula for the TH resistivity was derived, which establishes the relation between the TH resistivity and the ratio of the spin diffusion length to the skyrmion radius and would be increasingly important for extracting information about skyrmion density from experimental data when the size of room temperature skyrmions is further reduced to tens of nanometers, close to the spin diffusion lengths of most transition metal ferromagnetic thin films.

*This work was supported by the Dept. of Energy, Office of Science, BES, Materials Sciences and Engineering Division.

G70.00173: Robust Hund rule without Coulomb repulsion and exclusion principle in quantum antiferromagnetic chains of composite half spins* SOLOMON DUKI (Presenter), YIKUO YU, National Institutes of Health — Quantum spin chains with composite spins have been used to approximate conventional chains with higher spins. For instance, a spin 1 (or 3/2) chain was sometimes approximated by a chain with two (or three) spin 1/2’s per site. However, little examination has been given as to whether this approximation, effectively assuming the first Hund rule per site, is valid and why. In this work, the validity of this approximation is investigated numerically. We diagonalize the Hamiltonians of spin chains with a spin 1 and 3/2 per site and with two and three spin 1/2’s per site. The low energy excitation spectrum for the composite chain is found to coincide with that of the conventional chain. We find that as the system size increases, an increasingly larger block of consecutive lowest energy states with maximal spin per site is observed, robustly supporting the first Hund rule even though the exclusion principle does not apply and the Coulomb repulsion is absent. We show that this effective Hund rule emerges as a plausible consequence of the Lieb–Mattis theorem, which is originally for the ground state of ferrimagnetic and antiferromagnetic spin systems.

*This research was supported by the Intramural Research Program of the National Institutes of Health, National Library of Medicine.

G70.00174: Quantum phase interference in nanomagnetic particles coupled to the Josephson $\phi_0$ junction GWANG-HEE KIM (Presenter), Department of Physics and Astronomy, Sejong University, Seoul 05006, Republic of Korea, HAN-YONG CHOI, Department of Physics and Institute for Basic Science Research, Sungkyunkwan University, Suwon 16419, Korea/ Asia Pacific Center for Theoretical Physics, Pohang 37673, Korea — We study suppression of magnetization tunneling in nanomagnetic systems coupled to the Josephson $\phi_0$ junction. Employing spin coherent state path integral method, we find that the tunnel splitting is topologically quenched by the bias current applied to the junction as well as an external magnetic field along the hard axis. Considering tunnel splitting as a function of the current, we show that the quenching period is controlled by the external magnetic field and the number of frozen points decreases with increasing the magnetic field. The condition for switching from oscillations to the monotonic growth of the tunnel splitting is presented.
G70.00175: Giant superconducting proximity effect on spintronic anisotropy* KRZYSZTOF WOJCIK, Institute of Molecular Physics Polish Academy of Sciences, Poznan, Poland, MACIEJ MISIORYN, Chalmers University of Technology, Goteborg, Sweden, IRENEUSZ WEYMANN (Presenter), Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — We investigate theoretically the interplay of proximity effects due to the presence of a superconductor and normal ferromagnetic leads on the formation of the spintronic quadrupolar exchange field in a large-spin magnetic molecule. We show that the spintronic anisotropy can be enhanced by a few orders of magnitude, and tuned by changing the strength of coupling to the superconductor. Especially large anisotropy is generated in the vicinity of the charge parity changing transition of the molecule. We also provide predictions of measurable spectral properties being the hallmarks of these phenomena. The calculations are performed with the aid of the numerical renormalization group method.


G70.00176: Phase transitions in the one-dimensional transverse Ising model in a longitudinal magnetic field OSIEL BONFIM (Presenter), Physics, University of Portland, B. BOECHAR, J. FLORENCIO, Physics, Universidade Federal Fluminense — The phase transitions in the one-dimensional transverse Ising model in the presence of a longitudinal magnetic field were studied by the quantum fidelity method. We used exact diagonalization to obtain the ground-state energies and corresponding eigenvectors for lattice sizes up to 24 spins. The maximum of the fidelity susceptibility is used to locate the various phase boundaries present in the system. The type of dominant spin ordering for each phase was identified by examining the corresponding ground-state eigenvector. For a given antiferromagnetic nearest-neighbor interaction ($J_z$), we calculated the fidelity susceptibility as a function of the transverse field ($B_x$) and the strength of the longitudinal field ($B_z$). The phase diagram in the ($B_x$, $B_z$)-plane shows three phases. These findings are in contrast with the published literature that claims the system has only two phases. For $B_z < 1$, we observed an antiferromagnetic phase for small values of $B_x$ and a paramagnetic phase for large values of $B_z$. For $B_x > 1$ and low $B_z$, we found a disordered phase that undergoes a phase transition to a paramagnetic phase for large values of $B_z$.

G70.00177: Spin wave excitation and propagation in ultra-thin nm-thick yttrium iron garnet films* HANCHEN WANG (Presenter), Fert Beijing Institute, BDBC, School of Electronic and Information Engineering, Beihang University, Xueyuan Road 37, Beijing 100191, China, TAO LIU, Department of Physics, Colorado State University, Fort Collins, Colorado 80523, USA, CHUANPU LIU, JILEI CHEN, YOUGUANG ZHANG, WEISHENG ZHAO, Fert Beijing Institute, BDBC, School of Electronic and Information Engineering, Beihang University, Xueyuan Road 37, Beijing 100191, China, MINGZHONG WU, Department of Physics, Colorado State University, Fort Collins, Colorado 80523, USA, HAIMING YU, Fert Beijing Institute, BDBC, School of Electronic and Information Engineering, Beihang University, Xueyuan Road 37, Beijing 100191, China — Magnonics has received increasing attention over the past decades, and it is widely considered to open up new opportunities to transport information by using spin waves (SWs) without charge currents. In our paper, we investigate experimentally the excitation and propagation of SW in 7-nm thick yttrium iron garnet (YIG) thin films with an ultra-low damping constant. On the top of YIG, conventional coplanar waveguides are integrated to excite a large series of short-wavelength spin waves (SWs). The scattering parameters are measured by using a vector network analyzer, which give access to observe the transmission of SW in the films. Consequently, by utilizing the experimental results, we calculate and extract the group velocity as well as the dispersion relation of SWs. Our work may be useful for providing the basis for SW logic devices at GHz rates with low power consumption.

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G70.00178: Local short-scale correlations and the origin of negative magnetization*  
MALVIKA TRIPATHI (Presenter), Thin film magnetization, UGC DAE Consortium for Scientific research, T. CHATTERJI, Institut Laue-Langevin, S. MAJUMDER, R. M. CHAUDHARY, D. M. PHASE, Thin film magnetization, UGC DAE Consortium for Scientific research — Negative Magnetization (NM) defined as the opposite alignment of net magnetization with respect to applied magnetic field in magnetically ordered systems has been associated with a number of unsettled debates regarding the origin and reliability of this phenomena. The presence of two highly neutron absorbing isotopes of natural Gd has prevented to understand the microscopic magnetic structure and consequently the microscopic outlook of NM in GdCrO₃ so far. We have utilized λ = 0.499Å hot neutrons, a value much higher than the resonance energy, to record the thermal evolution of neutron diffraction patterns. Using magnetic pair distribution function analysis, significant local short range Gd³⁺ correlations in disordered state are observed ranging up to ~9 Å. Calculations suggest the frustrated S= 3 ground state of locally ordered Gd ions with competing FM- AFM exchange interactions and states corresponding to NM are comparatively more stabilized. The externally small excitation gap between energy levels is argued to be responsible for the different spin state populations characterized by distinct kinetic rates corresponding to cooling and warming cycles, which explains the observed path dependency of NM in GCO.

*Funding will be received by Department of Science and Technology, India.

G70.00179: Anomalous Nernst effect in a microfabricated Weyl magnet Mn₃Sn  
HIDEKI NARITA (Presenter), TOMOYA HIGO, IKHLAS MUHAMMAD, SATORU NAKATSUJI, YOSHICHIKA OTANI, University of Tokyo — Weyl magnets have attracted much attention in condensed matter physics due to both the fundamental interest and the potential application of a new thermoelectric power generation and heat current sensor. An anomalous Nernst effect is a thermoelectric phenomenon typically observed in ferromagnets under the application of a temperature gradient. The anomalous Nernst effect provides a simple and powerful tool to track the position and motion of a domain wall propagating. Recent theoretical and experimental studies have shown that magnetic domains exist in noncollinear antiferromagnetic Weyl magnets. In this study, we have investigated the anomalous Nernst effect in a microfabricated antiferromagnetic Weyl magnet Mn₃Sn to detect magnetic domains and observed step structures in hysteresis of the anomalous Nernst effect. We discuss the origin of the step structures in the hysteresis and compare the anomalous Nernst effect in the device to that in a bulk single crystal.

G70.00180: Domain wall motion influenced by a standing spin wave in antiferromagnetic systems  
INHYEOK CHOI (Presenter), HYOSEOK KIM, JONGSEOK LEE, Gwangju Institute of Science and Technology — In antiferromagnetic systems, spin dynamics are described by coupled Landau-Lifshitz-Gilbert equation for two order parameters of staggered and magnetic moments. It is also known that the time-varying magnetic field drives a collective motion of domain wall (DW). By using a micromagnetic simulation, we investigate a coupling effect between the spin wave and the DW motion which can be simultaneously driven by the oscillating magnetic field. In an antiferromagnetic nano-rod, a standing spin wave can be formed when its length is multiples of the wavelength of the excited spin wave. Depending on a phase relationship between the DW position oscillation and the standing spin wave, we find that the DW position oscillation is significantly influenced; its oscillation amplitude becomes negligible in the out-of-phase condition, and is enhanced by about twice in the in-phase condition.

G70.00181: Structure and Magnetic Properties of Gd₂₋ₓSrₓNiO₄, a Ruddlesden-Popper type solid solution*  
RENATA MIRANDA (Presenter), RAUL ZÜÑIGA MEDINA, Facultad de Química, Universidad Nacional Autonoma de Mexico, PABLO DE LA MORA, Facultad de Ciencias, National Autonomous University of Mexico, JORGE BARRETO, Instituto de Física, Universidad National Autonoma de Mexico, GUSTAVO TAVIZÓN, Facultad de Química, Universidad Nacional Autonoma de Mexico — Gd₂₋ₓSrₓNiO₄ complex oxide of the Ruddlesden-Popper series, was first prepared by James, M. et al.[1] Several compositions of the Gd₂₋ₓSrₓNiO₄ system were prepared by the complex polymeric route (Pechini). In this work we report the Sr composition stability range for this solid solution. Crystal structure of samples in the 0.75≤x≤1.25 range, were studied by Rietveld structure refinements. Magnetic measurements of samples (2-300 K) show a Curie-Weiss paramagnetic behavior for all x compositions, with a weak antiferromagnetic coupling. Electrical properties were measured in the 20-300 K range and we found that this system displays a metal-insulator transition for x≥1.0. Spectroscopic data (UV-Vis-NIR) at room temperature and magnetic moment measurements of this system reveal the nature of Ni oxidation states of this system.

[1] M. James, J.P. Attfield, Synthesis, crystal structure and magnetic properties of Ln₂₋ₓSrₓNiO₄±δ solid solutions (Ln = La, Nd, Sm and Gd; 1.0≤x≤1.67), J. Mater. Chem. 6 (1996) 57-62.

*Authors of this work acknowledge support from PAPIIT-IN115618 (UNAM).
G70.00182: Structure, Electrical and Magnetic properties of Sm$_{1-x}$Ca$_x$CrO$_3$, orthochromites*  
ALEJANDRO DURAN HERNANDEZ (Presenter), Centro de Nanociencias y Nanotecnología, Universidad Nacional Autonoma de Mexico, JORGE BARRETO, JESÚS ÁNGEL ARENAS, Instituto de Física, Universidad Nacional Autonoma de Mexico, PABLO DE LA MORA, Facultad de Ciencias, National Autonomous University of Mexico, GUSTAVO TAVIZÓN, Facultad de Química, Universidad Nacional Autonoma de Mexico — We have synthesized Sm$_{1-x}$Ca$_x$CrO$_3$ chromite and investigated the influence of calcium (Ca) doping at Sm-sites on the crystal structure, magnetic and electrical properties in a series of compounds in the 0≤x≤2.0 range. No structural transition was observed in this composition range and the doped compound crystallized into distorted orthorhombic structure with Pnma space group, which was confirmed by Rietveld refinement using Mo-Kα X-ray radiation. Samples of the Sm$_{1-x}$Ca$_x$CrO$_3$ series (x=0.0, 0.02, 0.04, 0.10 and 0.20) were prepared by Pechini polymeric precursor method and the polycrystalline samples were characterized by X-ray photoelectron spectroscopy (XPS), Magnetization vs. Temperature measurements, UV-Vis spectroscopy and electrical measurements (10-300 K). The effect of Sm substitution by Ca has important effect on the cell volume; the antiferromagnetic transition decreases from TN= 193K (x=0) to 150K (x=0.20) and the magnetization reversal also decreases from 35K (x=0) to 9K (x=0.20). These changes in magnetic behavior of Sm$_{1-x}$Ca$_x$CrO$_3$ can be associated with the Cr(VI) content in samples.

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G70.00183: A possible Hund's metal and unusual second-order metal insulator transition in perovskite La$_{1-x}$Pr$_x$RuO$_3$*  
ZONGYAO LI (Presenter), University of Texas at Austin, JOSÉ ANTONIO ALONSO, Instituto de Ciencia de Materiales de Madrid, JIANSHI ZHOU, University of Texas at Austin — 4d perovskite LaRuO$_3$ is a paramagnetic metal whereas PrRuO$_3$ is a paramagnetic insulator. Although Ru$^{4+}$ ruthenates have shown very rich physics due to the subtle interplay of Coulomb repulsive potential $U$, Hund's rule coupling $J$, the crystal-field splitting $\Delta$, and the spin-orbit coupling (SOC), limited information of Ru$^{3+}$ perovskite RRuO$_3$ (R=rare earth metals) family has been obtained since these perovskites have to be synthesized under high pressure. We report a successful synthesis of perovskite La$_{1-x}$Pr$_x$RuO$_3$ compounds by spark plasma sintering. A thorough characterization on La$_{1-x}$Pr$_x$RuO$_3$ system has been made by measurements of magnetic and transport properties and specific heat. The samples La$_{1-x}$Pr$_x$RuO$_3$ (0.2 < x < 0.8) exhibit a second-order metal-insulator transition as temperature decreases without any sign of magnetic order in the insulator phase. Due to the reduction of Ru-O-Ru bond angle, substituting La$^{3+}$ ions with smaller Pr$^{3+}$ ions reduces the bandwidth so as to lead to an insulator phase at low temperatures. The strong SOC and Hund's coupling on low spin 4$d^5$ Ru$^{3+}$ are responsible for the anomalous metallic phase found in LaRuO$_3$ and the absence of magnetic ordering in the insulator phase in La$_{1-x}$Pr$_x$RuO$_3$.

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G70.00184: Evidence of Martensitic Phase Transitions in Boron Substituted Ni-Mn-In Thin Films*  
SUDIP PANDEY (Presenter), Department of Physics, Southern Illinois University Carbondale, IL 62901 USA, ALPHA N’DIAYE, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 USA, IGOR DUBENKO, ANIL ARYAL, DIPANJAN MAZUMDAR, Department of Physics, Southern Illinois University Carbondale, IL 62901 USA, SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 USA, SHANE STADLER, Department of Physics & Astronomy, Louisiana State University, LA 70803 USA, NAUSHAD ALI, Department of Physics, Southern Illinois University Carbondale, IL 62901 USA — Ni-Mn-In-B thin films were synthesized on Si substrates using ultra-high vacuum magnetron sputtering. Metamagnetic transitions with thermal hysteresis have been observed on 30 nm thin films using the magnetization measurements. The temperature dependences of the magnetization curves were found to be similar to those of the bulk counterpart. Electronic and magnetic properties of Ni-Mn-In-B thin films were studied using X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD). From the XAS and XMCD spectra, we have observed that Ni plays a dominant role in the overall magnetism. Element-specific XMCD hysteresis loops of Ni in the NiMnInB films were measured as a function of temperature and observed minimum magnetic hysteresis at martensitic transformation. Possible mechanisms responsible for the changes in electronic and magnetic properties of thin films through the effect of redistribution of d electrons are discussed.

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**G70.00185: Beyond spin wave theory on a 5d transition-metal oxide**

JINKWANG KIM (Presenter), Pohang University of Science and Technology, JUNGHO KIM, Advanced Photon Source, Argonne National Laboratory, BUMJOON KIM, Pohang University of Science and Technology — 5d transition metal oxides (TMOs) offer a new playground for quantum magnetism with some unique features. For instance, a Heisenberg antiferromagnet in square lattice iridate Sr2IrO4 reveals similar low-energy effective physics with high-Tc superconductor parent antiferromagnet, La2CuO4, with its spin-orbit coupling driven isospins. However, there are some different features in detailed physics between them, one of which is small deviation of low-energy magnetic dispersion from what spin wave theory gives. In this regard, we used resonant inelastic x-ray scattering to show that the spin wave theory cannot perfectly explain the low-energy magnetic behavior of a 5d transition-metal oxide, Sr2IrO4. The high momentum-resolution low-energy dispersion and its temperature dependent behaviors cannot be fully understood only by spin wave theory, but higher-order exchange order terms should be included to describe these behaviors.

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**G70.00186: Flux-driven and geometry-controlled spin filtering for arbitrary spins in aperiodic quantum networks**

AMRITA MUKHERJEE (Presenter), ARUNAVA CHAKRABARTI, DEPARTMENT OF PHYSICS, UNIVERSITY OF KALYANI, KALYANI, WEST BENGAL-741235, INDIA, RUDOLF ROEMER, DEPARTMENT OF PHYSICS AND CENTRE FOR SCIENTIFIC COMPUTING, UNIVERSITY OF WARWICK, COVENTRY CV4 7AL, U.K. — We demonstrate that an aperiodic array of certain quantum networks comprising magnetic and nonmagnetic atoms can act as perfect spin filters for particles with arbitrary spin state. This can be achieved by introducing minimal quasi-one dimensionality in the basic structural units building up the array, along with an appropriate tuning of the potential of the non-magnetic atoms; the tunnel hopping integral between the non-magnetic atoms and the backbone, and, in some cases, by tuning an external magnetic field. The proposed networks have close resemblance with a family of recently developed photonic lattices, and the scheme for spin filtering can thus be linked, in principle, to a possibility of suppressing any one of the two states of polarization of a single photon, almost at will. We use transfer matrices and a real space renormalization group scheme to unravel the conditions under which any aperiodic arrangement of such topologically different structures will filter out any given spin projection following an energy-independent commutation of the transfer matrices. Our results are analytically exact, and corroborated by extensive numerical calculations of the spin polarized transmission and the density of states of such systems.

*DST-INSPIRE,UGC,India,British Council.University of Warwick

**G70.00187: Spin Hall Torque Mediated by Metallic Antiferromagnet**

YAN WEN (Presenter), FENGJUN ZHUO, AURELIEN MANCHON, XIXIANG ZHANG, King Abdullah University of Science and Technology — We report an enhancement of spin current in //Ta/IrMn/Cu/NiFe multilayer heterostructure. A thin metallic IrMn can enhance the spin current from Ta to NiFe. The spin current enhancement with a pronounced maximum value around the Neel temperature of the thin antiferromagnetic (AFM) layer was found. Through varying the measurement temperature and the thickness of the AFM layer, both electronic and magnonic spin current was observed. At low temperatures, where the convertance is weak, a comparable small spin conductivity is observed. The spin conductivity increases when the temperature rises until Neel temperature due to a more convertance process from electronic spin current to magnonic spin current. The spin conductivity decreases when further rising temperature, in which the AFM order is well-established and magnonic spin current starts to vanish.

*The work reported was funded by King Abdullah University of Science and Technology (KAUST).

**G70.00188: Spin-orbit torque generated by Pd oxides**

SATOSHI HAKU (Presenter), HONGYU AN, AKIRA MUSHA, KAZUYA ANDO, Keio University — Current-induced spin-orbit torques enable the manipulation of magnetization in ultrathin ferromagnetic metals. Recent studies have revealed that the spin-orbit torques can be generated by spin-orbit coupling at ferromagnetic-metal/heavy-metal-oxide interfaces. Here, we report the generation of spin-orbit torques using Pd oxides, PdOx. Pd is known as a heavy metal with high conversion efficiency between charge and spin currents because of the strong spin-orbit coupling. In this work, we quantified the spin-orbit torques generated by PdOx using spin-torque ferromagnetic resonance for NiFe/PdOx bilayers with various oxidation levels. The oxidation level of the PdOx layer was manipulated by varying the oxygen gas flow during the reactive sputtering. By increasing the oxidation level of the PdOx layer, we found that the damping-like torque efficiency is significantly suppressed, showing vanishingly small interface spin-orbit torques in the NiFe/PdOx bilayers. This is in stark contrast to the spin-torque generation in NiFe/PtOx bilayers, where the damping-like torque efficiency is not sensitive to the oxidation level of PtOx. Our results therefore will be essential for fundamental understanding of the spin-orbit torques generated by metal oxides.
First-principles study of the carrier doping effect on all-Heusler GMR junctions

FUMIAKI KURODA
(Presenter), MaDis-CMI2, National Institute for Materials Research, Japan, TETSUYA FUKUSHIMA, Institute of Scientific and Industrial Research, Osaka University, Japan, TAMIO OGUCHI, MaDis-CMI2, National Institute for Materials Research, Japan — In this work, we investigate interfacial magnetic couplings and spin-dependent transport property in all-Heusler based CPP-GMR junctions with a semimetallic \( \text{Fe}_2\text{VAl} \) spacer on the basis of first-principles calculations. A half-metallic ferrimagnet \( \text{Mn}_2\text{VAl} \) is used to investigate interfacial magnetic couplings and spin-dependent transport property in all-Heusler based CPP-GMR junctions. When carriers are introduced in the spacer by a gate voltage, magnetoresistance might be changed significantly. Moreover, from comparison with a spin injector with another half-metallic Heusler alloy \( \text{Co}_2\text{MnSi} \), the chemical trend in this type of CPP-GMR junctions is discussed.

*This work was supported in part by Materials research by Information Integration Initiative (MI²I) project.

Investigation of h-BN/Graphene Spin Valve

TINGYU QU (Presenter), JUNYE HUANG, DEYI FU, JIAWEI LIU, BARBAROS OZYILMAZ, Center for Advanced 2D Materials, National University of Singapore — Spintronics via two-dimensional materials offer promising applications in spin communications. Due to the extraordinary mobility and long diffusion length, graphene is still the subject of intense interest in spin transport. This study focuses on the investigation of the spin lifetime and diffusion length in graphene spin valve, including the extrapolation of the exponential decay of the spin signal with channel length and Hanle precession model. The graphene spin valve exhibits large non-local spin signal up to 40 Ω, with small switching field less than 200 Gauss. The extracted spin lifetime was between 100 and 200 ps, and the diffusion length was more than 4 μm. The spin-injection efficiency in graphene spin valve is further improved by controlling direct current as an injection source and using h-BN as a tunneling barrier.

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Spin transport properties in ultra-thin black phosphorus

JIAWEI LIU (Presenter), Department of Physics, National University of Singapore, DEYI FU, BARBAROS OZYILMAZ, Centre for Advanced 2D Materials, National University of Singapore — The discovery of graphene and two-dimensional materials provided new platforms to study electronic spin transport and to be used for novel spintronics applications. Graphene has been shown to exhibit desirable spin transport properties such as long spin life time\(^1\), long spin relaxation length\(^2\) and up to 100% spin injection efficiency\(^3\), even at room temperature. Beyond graphene, in our previous work, we demonstrated all electric spin injection, transport and detection in ultra-thin black phosphorus. In the non-local spin valve geometry, the measured spin relaxation time is as high as 4ns with spin relaxation lengths exceeding 6 μm\(^4\). In this work, we measured the spin signal and lifetime at different doping level in the black phosphorus. We also studied the relation between the spin and momentum relaxation time as a function of temperature.


The role of the spin-orbit coupling in the Transition metal dichalcogenides vertical spin valves

XINHE WANG (Presenter), XIAOYANG LIN, YUAN CAO, WEISHENG ZHAO, Beihang University — As a family of two-dimensional (2D) layered materials, Transition metal dichalcogenides (TMDCs) MX\(_2\) (M=Mo,W; X=S,Se) have been demonstrated to have potential for applications in the field of spintronics because of their strong spin-orbit coupling, spin-splitting with broken inversion symmetry and spin-valley degrees of freedom. In our work, the 2D MX\(_2\) were grown using chemical vapor deposition, and vertical spin valves with cross-strip geometry were constructed. The spin valve effects are measured, with layer and stacking variations. Which show the signature of the spin-valley coupling and spin-orbit torques. they pave the way for magnetic and electric control of spin and valley-polarized transport in magnetic tunneling junctions. Then, metallic behavior of the junction barrier is discussed; the temperature (50K-300K) dependence of the magnetoresistance ratio is reported; the role of the anisotropic magnetoresistance in the typical cross-strip geometry and the annealing effect on the device is discussed. Finally, the feature of the vertical spin valves based on the different TMDCs are listed and compared.
G70.00193: Edge magnetic properties and transport of spin current in an SU(2)-symmetric Kitaev spin liquid

VANUILDO DE CARVALHO (Presenter), School of Physics and Astronomy, University of Minnesota, HERMANN FREIRE, Institute of Physics, Federal University of Goias, EDUARDO MIRANDA, IFGW, University of Campinas, RODRIGO G PEREIRA, International Institute of Physics, Federal University of Rio Grande do Norte — We investigate the edge magnetism and the spin transport properties of an SU(2)-symmetric Kitaev spin liquid (KSL) model put forward by Yao and Lee [Phys. Rev. Lett. 107, 087205 (2011)] on the honeycomb lattice. In this model, the spin degrees of freedom fractionalize into a $\mathbb{Z}_2$ static gauge field and three species of either gapless (Dirac) or gapped (chiral) Majorana fermionic excitations. We find that, when a magnetic field is applied to a zigzag edge, the Dirac KSL exhibits a nonlocal magnetization associated with the existence of zero-energy edge modes. The application of a spin bias $V = \mu^+ - \mu^-$ at the interface of the spin system with a normal metal produces a spin current into the KSL, which depends, in the zero-temperature limit, as a power-law on $V$ for both Dirac and chiral KSLs, but with different exponents. Lastly, we study the longitudinal spin Seebeck effect, in which a spin current is driven by the combined action of a magnetic field perpendicular to the plane of the honeycomb lattice and a thermal gradient at the interface of the KSL with a metal. Our results suggest that edge magnetization and spin transport can be used to probe the existence of charge-neutral edge states in quantum spin liquids.

G70.00194: Magnetic impurity bands in Ga$_{x-1}$Mn$_x$S: Towards understanding the anomalous spin-glass transition

THOMAS PEKAREK (Presenter), M.C. MASSEY, I. MANUEL, PAUL S. EDWARDS, D. PARKER, JASON HARALDSEN, University of North Florida — We report on magnetic and electronic properties of a quasi-2D single-crystalline Ga$_{0.91}$Mn$_{0.09}$S diluted magnetic semiconductor (DMS) that shows an anomalously high spin-glass $T_c$ at 11.2 K. Using density functional theory (DFT), we characterize the properties contributing to the spin-glass transition through an examination of electronic and magnetic properties for Ga$_{1-x}$Mn$_x$S ($0 < x < 0.18$). The Mn produces impurity bands in the electronic structure, where an analysis of the density of states shows an increase in magnetic impurity bands at the Fermi level that lowers the semiconducting gap consistent with DMS. This is similar to other DMS, where the primary mechanism is likely through magnetic exchange. The increased electron density with Mn doping could explain the anomalously higher $T_c$ in Ga$_{0.91}$Mn$_{0.09}$S. In comparison with the substantially lower transition temperatures in related II-VI based systems (e.g., Zn$_{1-x}$Mn$_x$Te), the high $T_c$ is associated with more metallic spin-glass systems that interact through RKKY exchange, which leads to the conclusion that there may be a combination of interactions occurring in these systems.

*Institute for Materials Science at Los Alamos National Lab, UNF Terry Presidential Prof., FL Space Grant Consortium, & NSF DMR-16-26332 and DMR-14-29428.

G70.00195: Spin pumping driven by magnon-phonon coupled mode

HIROKI HAYASHI (Presenter), KAZUYA ANDO, Applied Physics and Physico-Informatics, Keio University — The properties of magnons and phonons, quasiparticles of spin waves and acoustic waves, have been investigated independently for more than half a century. However, the interaction between magnons and phonons can arise from spin-orbit, dipole-dipole, and exchange interactions in magnetic crystals. The coupling strength is most enhanced in the proximity of the intersection of the uncoupled magnon and phonon dispersions. In the coupling region, the quasiparticle with admixtures of both magnetic and elastic properties, magnon-polarons, is formed.

We report the observation of a resonant enhancement of spin pumping induced by the magnon-phonon coupled mode at room temperature. In this experiment, we measured the spin pumping and inverse spin Hall effect in a Pt/Y$_3$Fe$_5$O$_{12}$ (YIG) bilayer under microwave parametric pumping. We found that spin currents pumped from the YIG layer show an anomaly when the microwave excites dipole-exchange magnons in the proximity of the intersection of the uncoupled magnon and phonon dispersions. Our result shows that the spin pumping driven by the magnon-phonon coupled mode is enhanced compared with the purely magnonic value, consistent with previous works on the spin Seebeck effect.

G70.00196: Computing dynamic spin structure factor using matrix product state method and the time dependent variational principle

LING WANG (Presenter), Beijing Computational Science Research Center — We demonstrate that matrix product state combined with the time dependent variational principle can accurately reproduce a real time evolution of a disturbed ground state. From real time correlation of spin operators respect to the ground state, we compute the dynamic spin structure factor. We will show benchmark results for 1d Heisenberg chain, as well as extensive calculations on 2d square lattice Heisenberg model.

*L.W. is supported by National Natural Science Fundation of China (Grant No. NSFC-11874080).
Critical behavior of the layered ferromagnet $\text{Fe}_{1/4}\text{TaS}_2$*  

CHENHUI ZHANG (Presenter), YE YUAN, YAN WEN, XIXIANG ZHANG, King Abdullah University of Science and Technology — The critical behavior of single-crystalline layered ferromagnet $\text{Fe}_{1/4}\text{TaS}_2$ were studied by bulk dc magnetization around the paramagnetic to ferromagnetic phase transition. Critical exponents $\beta = 0.459(6)$ and $\gamma = 1.205(11)$ are extracted from the Kouvel-Fisher plot, whereas $\delta = 3.69(1)$ is obtained by the critical isotherm analysis at $T_c = 100.7$ K. These critical exponents obey the Widom scaling relation $\delta = 1 + \gamma / \beta$. Moreover, the self-consistency and reliability of the results are further verified by scaling equations. The determined exponents match well with those calculated from the results of renormalization group approach, and our analysis suggests that $\text{Fe}_{1/4}\text{TaS}_2$ possesses three-dimensional long-range magnetic interactions with the exchange distance decaying as $J(r) \approx r^{-4.8}$.

*This research was supported by King Abdullah University of Science and Technology (KAUST)

All-optical Control of the Magnetization in EuS, a Versatile Magnetic Insulator*  

ANDRE HENRIQUES, XAVIER GRATENS, PAVEL USACHEV (Presenter), VALMIR CHITTA, Departamento de Física dos Materiais, Universidade de São Paulo, YUNBO OU, Plasma Science and Fusion Center and Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, JAGADEESH MOODERA, Department of Physics, Massachusetts Institute of Technology — Finding new mechanisms of all-optical control of the magnetic state of matter is highly sought for the development of new devices and for optoelectronic quantum computing. Recently we demonstrated that a single incident photon can generate several thousand spin coherent electrons in antiferromagnetic EuSe, by forming a supergiant spin polaron [1]. Because of the gigantic magnetic moment of the spin polaron, a tiny magnetic field can induce coherence in the spin polaron ensemble. We extend this mechanism of magnetization control with few photons into other materials. Experimentally we show that in the Heisenberg ferromagnetic semiconductor EuS, near the Curie temperature, light induces spin polarons that are even larger than those observed in EuSe. Our Monte Carlo simulation offer a description of the magnetization process. The characteristic times of the spin polaron formation and extinction were measured using time-resolved pump-probe Faraday rotation. We shall present and discuss these results.


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Hybrid quantum-classical method for simulating spin-spin relaxation in solid-state NMR.*  

GRIGORY STARKOV, BORIS FINE (Presenter), Skolkovo Institute of Science and Technology — We propose a new hybrid quantum-classical method for first-principles calculations of NMR free induction decay (FID) in solids where spin-1/2 nuclei form periodic lattices. The method is based on the simulations of a finite cluster of spins 1/2 coupled to an environment of interacting classical spins via a correlation-preserving scheme. Such simulations are shown to lead to accurate FID predictions for one-, two- and three-dimensional lattices with a broad variety of interactions. The accuracy of these predictions can be efficiently estimated by varying the size of quantum clusters used in the simulations.

Reference:

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**G70.00200: Prediction of intrinsic properties of Fe-doped CeCo$_5$**

DURGA PAUDYAL (Presenter), RENU CHAUDHARY, Ames Laboratory — Due to high uniaxial anisotropy and abundant nature of Ce, CeCo$_5$ has become a subject of intense research for getting an excellent permanent magnet with low cost. CeCo$_5$ comes under the materials having a crystal structure of CaCu$_5$-type with space group P6/mmm. The changes in the valence state of the Ce atom from +4 to +3 due to the presence of Cu in CeCo$_5$ can enhance the coercivity of CeCo$_{5-x}$Cu$_x$. The replacement of Co-atom by another transition metal can manipulate the magnetization. The first principles calculations were performed to study the effect of Fe-doping on the magnetic properties of CeCo$_{4.5-x}$Fe$_x$Cu$_{0.5}$ to increase the magnetic moment with sufficient anisotropy. Fe doping increases the total moment. The anisotropy is highly dependent on the sites occupied by Fe and Cu. 20% Fe gives high uniaxial anisotropy in CeCo$_{4.5-x}$Fe$_x$Cu$_{0.5}$ for Cu at the 3g site, whereas 10% Fe in CeCo$_{4.5-x}$Fe$_x$Cu$_{0.5}$ gives high uniaxial anisotropy for Cu at the 2c site. Site preference of Fe is also checked for the compounds separately with Cu at 2c and 3g sites. Depending upon the concentration, Fe prefers both 3g and 2c sites in a CeCo$_{4.5-x}$Fe$_x$Cu$_{0.5}$ indicating the importance of the structural geometry.

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**G70.00201: New roots for synthesis of Cobalt carbide nanoparticles for rare earth free permanent magnets**

EDUARDO MARTÍNEZ-TERÁN (Presenter), AHMED EL-GENDY, University of Texas, El Paso — Magnets have made a great impact in our daily lives, since they are present in all kind of modern devices. However, one of the problems we may encounter in near future is that the supply of materials from which the magnets are made, rare earths, may not be able to supply their demand. In addition, the usual production of magnets involves many steps in between, the melting of raw materials, mold casting, cooling, crushing and then pressing them into the desired shape. For those reasons, we propose the creation of permanent magnets from abundant materials, Cobalt and Carbon. Therefore, we propose synthesis of Co$_x$C nanoparticles using super critical conditions (pressure and temperature). The materials precursors are mixed with solvent and heated up to its supercritical conditions where it decomposes to nanoscaled particles in powder shape, ready for being pressed. The morphology and phase structure were characterized using SEM and XRD to reveal cylindrical like shape and Co$_x$C orthorhombic phase structure respectively. The magnetic properties have been measured to yeild coercivity (Hc) of 760 Oe with saturation magnetization (Ms) of 37.41 emu/g, with an energy product of 2.84 MGOe. This method is still under optimization to reach the single phase of Co3C with higher Hc and Ms.

**G70.00202: Enhanced magnetic anisotropy in Sm–Co magnets due to tensile strain**

SO-YOUNG JEKAL, JÖRG F. LÖFFLER, Department of Materials, ETH Zurich, MICHALIS CHARILAOU (Presenter), Department of Physics, University of Louisiana at Lafayette — The SmCo$_5$ system exhibits one of the strongest magnetocrystalline anisotropy energies (MAE) among the rare-earth based magnets, essentially setting the limit of anisotropy strength in such materials. Based on Density-Functional-Theory calculations, we propose that tensile strain in this compound can in fact increase the MAE [1]. We have found that a tensile strain of 1% is enough to enhance the magnetocrystalline anisotropy by as much as 30%, whereas 5% tensile strain results in a 80% increase of MAE. Further, we predict that such a strain in the structure can be introduced by partial substitution. Specifically, we found that 25% substitution of Sm by Ce, a much lighter element that induces local tensile strain, enhances the magnetocrystalline anisotropy energy by 28%. Preliminary experiments with melt-spun ribbons confirm these predictions and Monte Carlo simulations predict a strong high-temperature performance of magnets based on this material. These findings suggest that it is possible to develop magnets that are substantially more anisotropic by fine-tuning the local atomic arrangements.

corresponding first principles techniques, but with very similar accuracy. The agreement between them is excellent. Thus this realistic tight-binding method provides an effective approach to describe MAE into intra-sublattice and inter-sublattice contributions using both perturbation and scaling procedures, and as FePt and FeNi. This method can accurately calculate the MAE over the whole band filling range. The smaller basis set allows us to efficiently resolve MAE with a very high resolution in reciprocal space. The $k$-resolved MAE using the force theorem and perturbation theory agree well with each other, both reflecting the aspects of the Fermi surface. We resolve MAE into intra-sublattice and inter-sublattice contributions using both perturbation and scaling procedures, and agreement between them is excellent. Thus this realistic tight-binding method provides an effective approach to describe and analyze MAE. Once the real-space Hamiltonian is constructed, this approach is orders of magnitude faster than the corresponding first principles techniques, but with very similar accuracy.

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In conventional spin crossover systems, the vibrational degrees of freedom enhances the entropic effect in excited high-spin terms resulting from the softening of vibrations [1]. Here, we show an opposite effect of vibration on the spin-crossover taking $C_60^{3-}$ as an example [2]. $C_60^{3-}$ anion takes either high ($S = 1/2$) or low ($S = 1/2$) spin state, and in the latter the dynamical Jahn-Teller effect arises. It is found that the large dynamical Jahn-Teller stabilization energy lowers the low-spin levels, resulting in the violation of Hund’s rule. The Jahn-Teller dynamics influences the thermodynamic properties via strong variation of the density of vibronic states with energy. Thus, the vibronic entropy in the low-spin states enhances the effective spin gap of $C_60^{3-}$ quenching the spin crossover. This finding is used for the rationalization of the experimental data on the spin gaps in various fullerenes. The vibronic mechanism is not limited to fullerene: It can play a crucial role when Hund and Jahn-Teller couplings are comparable to each other.


Perpendicular MAE and unconventional MAE contributions in $k$-space are found in the self-assembled Gd-ZGNR system, which presents a remarkable Rashba effect (the estimated strength is 1.89 eV Å) due to the strong SOC and the asymmetric adsorption sites at the nanoribbon edge. Moreover, first-order MAE is connected to the intrinsic Rashba effect beyond the traditional second-order MAE. The dependence on the ribbon width of the first-order MAE and the Rashba effect are also examined. This work not only opens a new gate for designing the 1D Rashba system but also provides insight into the unconventional MAE due to the intrinsic Rashba effect.
In this work, we chemically deintercalated layered ionic compound to an air-stable van-der-Waals material which can be mechanically exfoliated down to thin layers while preserving its magnetic properties. In addition, unlike the materials mentioned above, the material reported here exhibits signs of frustrated magnetism.

Reference:
image spin waves, electric field induced changes in antiferromagnets as well as spin accumulation in non-magnets. magnetization dynamics with a time resolution of the order of 10 ps. We will show results that demonstrate the ability to detect very small changes in the magnetization induced by external stimuli like currents or fields. It also allows to follow becoming a tool available at every synchrotron. The particular capabilities of the instrument discussed here is the ability to polarized X-rays. In this contribution we will present the capabilities of synchrotron based X-ray microscopy, which is needed that provides element-specific information about not only ferromagnetic but antiferromagnetic materials as well.

**References:**
1. K.R. Kumar et al., IEEE Trans. on Magnetics 45, 10 (2009)

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**G70.00210:** Structural and magnetic properties of Co$_{2-x}$Ti$_x$FeGe ($0 \leq x \leq 1$) alloy series with plausible half-metallic behavior

SHAMBUH KC (Presenter), Physics and Astronomy, The University of Alabama — We report the synthesis and characterization of a Co$_{2-x}$Ti$_x$FeGe ($0 \leq x \leq 1$) alloy series by substituting Co with Ti atoms in a stoichiometric Co$_2$FeGe alloy. Based on prior microscopic and structural characterization, Co$_2$FeGe is reported not to be phase pure$^1$. By Ti substitution, however, we investigated and found single-phase behavior for $0.375 \leq x \leq 0.875$, while the other composition studied showed multi-phase behavior, supporting previous work. XRD analysis reveals cubic crystal structure for all single-phase samples with the lattice parameter increasing almost linearly with increasing Ti substitution. The extracted magnetic moments at 5 K show strong agreement with the Slater-Pauling moments. Further, the spin-resolved DOS calculated predicts a gap in the minority channel. Moreover, with the addition of Ti, it is seen that the Fermi level shifts from the right edge of the band gap to the left and it falls exactly in the gap for $x = 0.5$. Our experimental and theoretical studies of different single-phase sample compositions suggest that Co$_{1.5}$Ti$_{0.5}$FeGe is a plausible half metal.

**G70.00211:** Low-damping magnetic materials in FM-NM-FM structures on flexible substrates for RF/microwave applications

XINJUN WANG (Presenter), IVAN LISENKO, NIAN-XIANG SUN, Northeastern University, KATIE HAUCK, KEVIN WALKER, NAVAIR — New magnetic materials can open a way for energy-efficient and flexible antenna and RF microwave devices. Low damping magnetic materials have been attributed to single-crystal magnetic insulators. High-quality with low damping magnetic materials, are deposited on flexible substrates, are needed to enhance the performance of flexible devices. Here, we demonstrated low magnetic damping in a ferromagnetic (FM)/non-magnetic(NM)/ferromagnetic(FM) structure fabricated on a flexible Mica substrate, which comparable with the one found in solid structures. With different Ru thickness, the two FM layers shows parallel(P) and antiparallel(AP) interaction, which is called the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction. For an AP coupling, the linewidth demonstrates a different behavior. For low external fields (and low frequencies in the range 4GHz – 6GHz) the linewidth is practically independent with the frequency, which shows great potential applications for RF/microwave devices and antenna.

**G70.00212:** Tuning structural and magnetic properties by vanadium substitution in Fe$_3$Ge

RABIN MAHAT (Presenter), University of Alabama — The structural and magnetic properties of Fe$_{3-x}$V$_x$Ge intermetallic alloy series (0<x≤1) have been investigated. The samples were prepared by arc-melting under argon atmosphere. After annealing, alloys with 0.375≤x≤0.625 are found to crystallize in the cubic Heusler structure, while alloys with 0<x≤0.25 crystallize in the hexagonal DO$_{19}$, which is the high temperature phase of parent Fe$_3$Ge. Optical microscopy, EDX, and XRD reveal uniform granular microstructures for x≤0.75. The calculated lattice parameter increases linearly with increasing x, while the magnetic moment at 5K decreases linearly for cubic alloys, deviating only about 7% from the Slater-Pauling values, which indicates possible half-metallic behavior. The hexagonal samples have markedly higher moments. The saturation magnetizing field is found to decrease with the increase of x making the system softer at higher V concentrations. The martensitic phase transformation in all stable cubic phases is confirmed by DSC which is being reported for the first time for this system. Vanadium is found to play a crucial role in stabilizing the cubic structure and shifting the martensitic transformation temperature to higher values from that of parent Fe$_3$Ge.

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**G70.00213:** The SSRL BL13 Scanning Transmission X-ray Microscopy for the Study of Magnetic Materials

HENDRIK OHLDAEG (Presenter), Lawrence Berkeley National Laboratory — Today's magnetic device technology is based on complex magnetic alloys or multilayers that are patterned at the nanoscale and operate at gigahertz frequencies. To better understand the behavior of such devices one needs an experimental approach that is capable of detecting magnetization with nanometer and picosecond sensitivity. In addition, since devices contain different magnetic elements, a technique is needed that provides element-specific information about not only ferromagnetic but antiferromagnetic materials as well. Synchrotron based X-ray microscopy provides exactly these capabilities because a synchrotron produces tunable and fully polarized X-rays. In this contribution we will present the capabilities of synchrotron based X-ray microscopy, which is becoming a tool available at every synchrotron. The particular capabilities of the instrument discussed here is the ability to detect very small changes in the magnetization induced by external stimuli like currents or fields. It also allows to follow magnetization dynamics with a time resolution of the order of 10 ps. We will show results that demonstrate the ability to image spin waves, electric field induced changes in antiferromagnets as well as spin accumulation in non-magnets.
G70.00214: Magneto-Raman Spectroscopy on Vanadium-derived Lacunar Spinel GaV$_4$S$_8^*$

CALVERT BARCLAY (Presenter), D. OLOGUNAGUBA, Physics, Florida A&M University, ZHENGUANG LU, Condensed Matter Science, National High Magnetic Field Laboratory, GANESH POKHAREL, HASITHA SURIYA ARACHCHIGE, Materials Science and Engineering, University of Tennessee, ANDREW D CHRISTIANSON, Neutron Scattering Division, Oak Ridge National Laboratory, DAVID MANDRUS, Materials Science and Engineering, University of Tennessee, DMITRY SMIRNOV, Condensed Matter Science, National High Magnetic Field Laboratory, KOMALAVALLI THIRUNAVUKKARASU, Physics, Florida A&M University — Chalcogenides with the GaM$_4$S$_8$ structure are hetero- cubane like [M$_4$X$_4$]$^{n^+}$ cubes (M = Mo, Re,V, Nb, Ta; X = S, Se, Te) and [AX$_4$]$^{n^-}$ tetrahedra (A= Ga, Ge), these adopt the NaCl structure [1,2]. GaV$_4$S$_8$ is a known Mott insulator because of the long inter-cluster distances approximately 4 Å apart [1]. GaV$_4$S$_8$ (GaVS) is a magnetic semiconductor with a Neel-type skyrmion phase displaying multiferroic properties [3]. Magnetic susceptibility measurements showed structural transition at T$_{JT}$ of 42 K followed by a ferromagnetic order at 12 K [4] and 12.7 K [5]. Temperature-dependent infrared and Raman measurements identified phonon modes and Jahn-Teller distortions [6]. For detailed information on the various exchange interactions in GaV$_4$S$_8$, we performed magneto-Raman measurements at magnetic fields up to 20 T and temperatures down to 5 K.

References:

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G70.00215: Characterization of microstructure and residual stresses using Barkhausen noise measurements

NEELAM PRABHU GAUNKAR, Iowa State University, GAJANANA PRABHU GAUNKAR, Mechanical Sciences, Indian Institute of Technology, Goa, DAVID C JILES (Presenter), Iowa State University — Micromagnetic measurement methods based on Barkhausen Noise (BN) measurements are increasingly being used as a versatile and cost effective tool for in-situ examination and evaluation of microstructural changes. They are also used for measurement of surface residual stresses. Interpretation of the observations and measurements, however, require validation with the help of appropriate calibration procedures.

In the present paper, we examine the characterization of a broad spectrum of microstructures such as produced in steels and also lattice strains which sometimes accompany the microstructural changes. Such changes also affect the BN response. Characteristic residual lattice strains or residual stress patterns also get generated around stress raisers including flaws such as surface cracks which need to be detected and evaluated for their consequences during continued service exposure of the material. We will present observations of the mapping of surface residual stress pattern in the vicinity of a part through surface crack produced by controlled fatigue loading of a 15 mm thick martensitic stainless steel plate showing residual stress variations around a dormant crack.

G70.00216: ATOMIC, MOLECULAR, AND OPTICAL (AMO) PHYSICS —

G70.00217: Dynamics of a 2D disordered dipolar interacting spin ensemble on the surface of diamond

KRISTINE REZAI (Presenter), Harvard University, PHILLIP E WEINBERG, Physics, Boston University, SOONWON CHOI, Physics, University of California, Berkeley, MIKHAIL LUKIN, Harvard University, ALEXANDER SUSHKOV, Physics, Boston University — Statistical mechanics has long been the framework which connects the microscopic world to macroscopic observables. However, its fundamental assumption has been shown to break down in a class of strongly disordered systems, resulting in a slowdown or absence of thermalization. In this work, we use a shallow nitrogen-vacancy center to probe the dynamics of disordered dipolar interacting electronic spin-1/2 defects on the diamond surface. Using magnetic resonance techniques, we characterize and control the strength of disorder and dipolar interactions among the electronic spins. We measure the autocorrelation of individual spin projection, which exhibits a decay on a time scale much slower than the inverse interaction strength, indicating a substantial slowdown of thermalization.
Exploring quantum correlations in a many-body localized system

Julian Leonard (Presenter), Matthew Rispoli, Alexander Lukin, Robert Schittko, Sooshin Kim, Joyce Kwan, Markus Greiner, Harvard University — An interacting quantum system that is subject to disorder may cease to thermalize due to localization of its constituents, thereby marking the breakdown of thermodynamics. We realize such a many-body-localized system in a disordered Bose-Hubbard chain and characterize its entanglement properties through particle fluctuations and correlations.

We observe that the particles become localized, suppressing transport and preventing the thermalization of subsystems. Notably, we measure the development of non-local correlations, whose evolution is consistent with a logarithmic growth of entanglement entropy - the hallmark of many-body localization. These results experimentally establish many-body localization as a qualitatively distinct phenomenon from localization in non-interacting, disordered systems.

Furthermore, we study the critical properties of the many-body localization transition. We identify a spatially separated, sparse-resonant structure of the system, which emerges at intermediate disorder strength and drives sub-diffusive particle motion. This structure persists into non-factorizable higher-order correlation functions. Our work identifies the many-body nature of the critical regime and lays a foundation for characterizing dynamic phases via high-order correlation.

Optical black-hole analog in inhomogeneous photonic lattice

Meng Kang (Presenter), Wuhan University, Huaqing Huang, University of Utah, Hongxing Xu, Wuhan University, Feng Liu, University of Utah — Hawking radiation, a key to quantum gravity, has stimulated extensive theoretical and experimental studies of various black-hole analogs. Here we theoretically develop a new laboratory analog of black hole in an inhomogeneous two-dimensional graphyne-like topological photonic lattice. A predesigned lattice transition from type-II to type-I Dirac cone creates an analogous curved space time crossing the event horizon (type-III Dirac cone). Photons tunneling through the horizon emit a spectrum of Hawking radiation with a Hawking temperature of 14 μK. Our approach provides a universal design for the optical black-hole analogs in topological photonic crystals and metamaterials.

Coherent coupling of fluctuations in mesoscopic systems in optomechanics

Devender Garg, Asoka Biswas (Presenter), Indian Institute of Technology Ropar — Interaction between a quantum and a mesoscopic system has always been intriguing in understanding the quantum-classical interface. In this context, we show how the energy fluctuations can be adiabatically exchanged, by using laser pulses, between two mirrors or between the motional degree of freedom of an ion trapped inside the cavity and that of one of the cavity mirrors. In the former case, two membranes are suspended inside a cavity. The zero-eigenvalue eigenstate of the matrix governing their fluctuation dynamics indicates that a suitable sequence of pulses to drive the cavity modes can lead to a deterministic adiabatic transfer of energy fluctuations from one membrane to the other, in a way akin to stimulated Raman adiabatic passage. Similar results can also be obtained in the later setup, in which a single ion is trapped inside an optical cavity, with one of the mirrors oscillating. Our results show that it is possible to coherently couple the fluctuations of two mesoscopic systems. Interestingly, this also indicates that the motion of a trapped ion (a quantum system) can lead to motional fluctuation in a mesoscopic mirror. This opens up possibilities for an ion-controlled long-distance transfer of fluctuations among mirrors, using more cavities.

Emergent Floquet prethermalization signatures in out-of-time ordered correlations

Pai Peng (Presenter), Department of Electrical Engineering and Computer Science, MIT, Xuan Wei, Oles Shtanko, Department of Physics, MIT, Iman Marvian, Departments of Physics & Electrical and Computer Engineering, Duke University, Chandrasekhar Ramanathan, Department of Physics and Astronomy, Dartmouth College, Seth Lloyd, Department of Mechanical Engineering, MIT, Paola Capellaro, Department of Nuclear Science and Engineering, MIT — How a many-body quantum system thermalizes -- or fails to do so -- under its own interaction is a fundamental yet elusive concept. Here we demonstrate nuclear magnetic resonance observation of the emergence of prethermalization by measuring out-of-time ordered correlations. We exploit Hamiltonian engineering techniques to tune the strength of spin-spin interactions and of a transverse magnetic field in a spin chain system, as well as to invert the Hamiltonian sign to reveal out-of-time ordered correlations. At large fields, we observe an emergent conserved quantity due to prethermalization, which can be revealed by an early saturation of correlations. Our experiment not only demonstrates a new protocol to measure out-of-time ordered correlations, but also provides new insights in the study of quantum thermal dynamics.
G70.00224: Rebuilding of destroyed spin squeezing in noisy environments
PENG XU (Presenter), Wuhan University — We investigate the process of spin squeezing in a ferromagnetic dipolar spin-1 Bose-Einstein condensate under the driven one-axis twisting scheme, with emphasis on the detrimental effect of noisy environments (stray magnetic fields) which completely destroy the spin squeezing. By applying concatenated dynamical decoupling pulse sequences with a moderate bias magnetic field to suppress the effect of the noisy environments, we faithfully reconstruct the spin squeezing process under realistic experimental conditions. Our noise-resistant method is ready to be employed to generate the spin squeezed state in a dipolar spin-1 Bose-Einstein condensate and paves a feasible way to the Heisenberg-limit quantum metrology.

G70.00225: On Local Simulations of Local Fluxes in Molecular Junctions*
GABRIEL CABRA (Presenter), University of California, San Diego, ANDERS WESTERGAARD JENSEN, University of Copenhagen, MICHAEL GALPERIN, MASSIMILIANO DI VENTRA, University of California, San Diego — We present a pedagogical review of the current density simulation in molecular junction models indicating its advantages and deficiencies in the analysis of local junction transport characteristics. In particular, we argue that current density is a universal tool which provides more information than traditionally simulated bond currents, especially when discussing inelastic processes. On the other hand, current density simulations are sensitive to the basis set and the electronic structure method utilized. We note that while discussing the local current conservation in junctions, one has to account for the source term caused by the open character of the system and intra-molecular interactions. Our considerations are illustrated with numerical simulations of a benzenedithiol molecular junction.

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G70.00226: Solution of the independent boson model with quadratic coupling
AURELIA CHENU (Presenter), Los Alamos National Laboratory, SHIU-E-YUAN SHIAU, Academia Sinica, MONIQUE COMBESCOT, Sorbonne Universite — We revisit the model of a two-level system coupled to phonons, and provide analytical solutions including a quadratic coupling, which was until now unsolved. Indeed, current techniques to analytically solve this important problem, like the polaron transformation which eliminates what is commonly called system-phonon couplings, hide the fundamental physics. These couplings can be eliminated using a diagonal basis, in which phonons depend on the electronic level. Doing so, we obtain analytical results through a simple algebra, by switching back and forth from ground-phonons to excited-phonons. We easily recover standard results for linear coupling, like state dynamics and correlation functions for absorption/emission lineshapes, in a way far simpler than previous procedures. More importantly, we find solution for the Hamiltonian including quadratic coupling, for which no analytical results have been reported yet. This approach opens a conceptually new route to more complicated matter-boson systems.

G70.00227: A Quantum Mechanical Study of Francium and Radium Clusters*
DAVID NUNN (Presenter), AJIT HIRA, JOSE PACHECO, JARETH BACA, Math and Physics, Northern New Mexico College — This report presents our research on the small atomic clusters of francium (Fr\textsubscript{n}), and radium Ra\textsubscript{n} (n = 1-9), and their hybrids Fr\textsubscript{n}Ra\textsubscript{n} clusters. Francium is a heavy, unstable, radioactive metal with a maximum half-life of only 22 minutes. Radium is the heaviest and most reactive element of the alkaline earth metals family. Hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) were used to derive optimal geometries for the clusters of interest. We compare calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for these clusters. The theoretical study of Fr\textsubscript{n} clusters, such as ours, is particularly important because very little experimental data is available on its physical properties. It is interesting to check the stability of francium in cluster form. The interactions of Fr\textsubscript{n} clusters with O atoms, O\textsubscript{2} molecules, H\textsubscript{2}O molecules, and with some C\textsubscript{n} clusters will be compared to similar interactions for Ra\textsubscript{n} clusters. The possible implications of our computational results for the roles of Radium and Francium as cancer-causing materials will be examined.

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Developments in quantum dynamics of full-dimensional diatom-diatom collisions at pre-exascale*
BENHUI YANG (Presenter), YIER WAN, PHILLIP STANCIL, University of Georgia, BALAKRISHNAN NADUVALATH, University of Nevada Las Vegas, ROBERT C FORREY, Penn State Berks Campus — Accurate rate coefficients for molecular rovibrational transitions due to collisions with H$_2$ are critical for interpreting IR astronomical observations. Theoretical results are the primary source of such rate coefficients. The most accurate theoretical approach is the quantum close-coupling method. Recently we extended full-dimensional quantum dynamics calculations of rovibrationally inelastic scattering large systems including CO-H$_2$, CN-H$_2$, SiO-H$_2$, and CS-H$_2$. The rovibrational cross sections have been computed using various implementations of the TwoBC code based on 6D potential energy surfaces. To date, full-D scattering calculations are mainly focused on the target molecule in its ground and first excited vibrational states with H$_2$ treated as a rigid rotor. To perform scattering computations with larger vibrational excitation of both diatoms further increases the computational demands. This relies on the availability of leadership-class computational resources. We present preliminary results for rovibrational scattering computations on Titan, SummitDev, and Summit with a progression of optimization efforts with MPI, OpenMP, OpenACC, and Magma.

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Multidimensional Bin-Width Optimization for Histogram and Its Application to Four-Dimensional Neutron Inelastic Scattering Data
KENSUKE MUTO (Presenter), HIROTAKA SAKAMOTO, KEISUKE MATSUURA, TAKA-HISA ARIMA, MASATO OKADA, Graduate School of Frontier Sciences, The University of Tokyo — We propose a method for optimizing bin widths for multidimensional histograms. In recent years, a large amount of four-dimensional event data has been obtainable in neutron inelastic scattering experiments conducted by chopper spectrometers[1]. As preprocessing, researchers make histograms from obtained event data. At present, the researchers only empirically select bin widths and slice conditions to get a two-dimensional histogram, while checking the histogram in a visual approach[2]. We propose a method which can automatically make a multi-dimensional histogram from event data. Our method was derived from the one-dimensional bin width optimization method[3]. In this paper, we use artificial data to investigate the behavior of our method. We applied the proposed method to both sliced two-dimensional event data and the whole four-dimensional event data. Comparing their results, we have found that the optimized bin-width strongly depends on the dimensionality of the data. Moreover, the optimum bin widths are affected by the number of events and the magnitude of the white background noise.

[2]Y. Inamura et al., 2013

Diffusion of carbon adatoms on gold ion trap electrode surfaces
HOSSEIN JOOYA (Presenter), ITAMP, Harvard-Smithsonian Center for Astrophysics, KYLE S. MCKAY, NIST, Boulder, Colorado, EUNJA KIM, Department of Physics and Astronomy, University of Nevada, Las Vegas, PHIL WECK, Sandia National Laboratories, DAVID PAPPAS, DUSTIN A HITE, NIST, Boulder, Colorado, HOSSEIN SADEGHPOUR, ITAMP, Harvard-Smithsonian Center for Astrophysics — In ion traps, the electric field noise emanating from the trap electrodes remains as a major obstacle to the realization of ion-trap based scalable quantum computing architectures. The source of this anomalous noise has been identified as the fluctuating surface adatom dipoles (mostly carbon-bearing). The original microscopic theory of fluctuating surface dipoles is static. In order to provide a more realistic picture of the surface dynamics, the mobility of these dipoles whose magnitude change with motion on the electrode surface should also be considered. One of the unknown parameters in the electric field noise spectral power is the diffusion constant of such adsorbates. In this study, classical molecular dynamics (MD) simulations are used to calculate long-time diffusion constant and transition rates of carbon adatoms on various gold surface orientations. The resultant fluctuation in the induced dipole moment is then obtained by computing the work function of the surface, using the density-functional theory method. Such time domain calculations also provide us with a clear picture of carbon structure and cluster formation on various gold surfaces.
According to the mean-field theory, an atomic Bose-Einstein condensate (BEC) will collapse when the interaction between atoms is attractive. However, the mixture of two miscible or phase separated condensates, collapsing, and the droplet of the double BEC of Rb and Na atoms. With the help of an interspecies Feshbach resonance, we have created format of self-bound quantum droplets. In this talk, I will present our progress in studying the heteronuclear quantum BECs with attractive interspecies interaction can be stabilized by the beyond mean-field Lee-Huang-Yang correction in the Einstein condensate (BEC) will collapse when the interaction between atoms is attractive. However, the mixture of two BECs with attractive interspecies interaction can be stabilized by the mean-field Lee-Huang-Yang correction in the format of self-bound quantum droplets. In this talk, I will present our progress in studying the heteronuclear quantum droplet with the double BEC of Rb and Na atoms. With the help of an interspecies Feshbach resonance, we have created double BECs with nearly arbitrary interaction strengths and signs. This should allow us to cover the full phase diagram from two miscible or phase separated condensates, collapsing, and the droplet.

*Wataru Kohno is a JSPS Research Fellow, and this work was supported in part by JSPS KAKENHI Grant Number 18J13241.

Recently, one of the authors has been constructed a variational wave function, which describes weakly interacting Bose–Einstein condensates (BECs) with dynamical 3/2-body correlations, where one of the two colliding non-condensates drops into the condensate and vice versa. In this presentation, we apply the variational method to (1) M-component BEC and (2) BEC trapped by a general trap to investigate the properties of 3/2-body correlations in BECs more qualitatively. From our numerical results in both cases, the 3/2-body correlations lower the ground-state energy in an amount comparable to the mean-field contribution.

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G70.00234: Ground State Properties for a Bose Gas Within a Periodic, Multi-Rods Structure* OMAR ABEL RODRÍGUEZ-LÓPEZ (Presenter), MIGUEL SOLIS, Theoretical Physics, Institute of Physics, Universidad Nacional Autónoma de México — We calculate the ground state (gs) energy and the static structure factor at zero temperature of an interacting Bose gas confined by a one-dimensional, periodic, multi-rod structure created by an external Kronig-Penney potential. We employ the Diffusion Monte Carlo (DMC) method to solve the Schrödinger equation exactly up to a statistical error. The gs energy is compared with the results previously obtained using the Variational Monte Carlo method (VMC), as well with the results obtained using the Mean-Field theory approximation by solving analytically the Gross-Pitaevskii equation. In the limit of zero external potential, we recover the results for the well-known Lieb-Liniger model [1]. For nonzero external potential, we find a phase transition from the superfluid state to a Mott insulator state as the lattice height increases. [1] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).

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G70.00236: Magnetic model for supersolidity* JOSÉ MARTÍNEZ-HERRERA (Presenter), MIGUEL SOLIS, Sociedad Mexicana de Fisica — The well known correspondence between the lattice liquid (or solid) model and a magnetic model like the Ising model, is used to obtain the thermodynamic properties of an one-dimensional quantum crystal whose lattice is divided in two different interpenetrating sublattices α and β. Among others, we introduce a Bose-Einstein condensation and an order-disorder parameters to solve the equilibrium state. Then, we calculate the Helmholtz free energy in a mean field theory approximation and, applying the standard minimization method respect to the condensate and order-disorder parameters, we find a critical temperature different from zero at which the system presents a phase transition like the Bose-Einstein condensation which we connect with the possibility of a supersolid transition.

*We acknowledge partial support from grants PAPIIT IN107616, IN110319 and CONACyT 221030.

G70.00237: Chiral Majorana edge states in the vortex core of a $p + ip$ Fermi superfluid* JING BO WANG (Presenter), University of Science and Technology of China — We study Majorana modes in the vortex core of a two-dimensional $p + ip$ Fermi superfluid interacting with a Bose-Einstein condensate. Under a repulsive $s$-wave contact interaction between fermions and bosons, fermions are depleted from the vortex core when the bosonic density becomes sufficiently large. This gives rise to a dynamically-driven local interface emerges between fermions and bosons, along which chiral Majorana edge states should appear. We examine in detail the variation of vortex-core structures as well as the formation of chiral Majorana edge states with increasing bosonic density, where the circulation of the vortex plays an important role. Whereas both the Majorana modes and vortex-core structures can be controlled and manipulated by tuning the bosonic density and the Bose-Fermi interaction strength, our study presents an illuminating example on how topological defects can be dynamically controlled in the context of cold atomic gases.

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G70.00238: Ultra-cold dysprosium for quantum simulation PIERRE BARRAL (Presenter), MICHAEL A CANTARA, LI DU, WILLIAN LUNDEN, ALAN JAMISON, WOLFGANG KETTERLE, MIT — Dysprosium is in many respects an atom of interest for quantum simulation. Its large angular momentum (J=8) in the ground state gives rise to one of the highest magnetic moments (10 Bohr magneton) in the periodic table, and one can therefore simulate an extended version of the Hubbard model with dipole-dipole interactions. This large angular momentum combined with narrow transitions also allows one to implement strong atom-light coupling with reduced heating. It opens the way to create gauge fields, e.g., spin-orbit coupling. We will report the most recent progress in our dysprosium apparatus.

G70.00239: One-dimensional Bose polarons beyond the Fröhlich paradigm: localized impurities HONG LING (Presenter), Department of Physics and Astronomy, Rowan University, Glassboro, New Jersey 08028, BEN KAIN, Department of Physics, College of the Holy Cross, Worcester, Massachusetts 01610 — Grusdt et al. [New J. Phys. 19, 103035 (2017)] recently made a renormalization group study of a one-dimensional (1D) Bose polaron in cold atoms that goes beyond the usual Fröhlich description. We study the same model in the localized impurity limit where the ground state is described by a multimode squeezed state instead of the multimode coherent state in the static Fröhlich model. We solve the system exactly by applying the generalized Bogoliubov transformation, an approach that can be straightforwardly adapted to higher dimensions. Using our exact solution, we obtain a polaron energy free of infrared divergences and construct analytically the polaron phase diagram. We find the repulsive polaron is stable on the positive side of the impurity-boson interaction but is always thermodynamically unstable on the negative side of the impurity-boson interaction, featuring a bound state, whose binding energy we obtain analytically. We find the attractive polaron is always dynamically unstable, featuring a pair of imaginary energies which we obtain analytically.

G70.00240: ABSTRACT WITHDRAWN —

G70.00241: Quantum Simulation of the Fermi-Hubbard Model GEOFFREY JI (Presenter), CHRISTIE S CHIU, Harvard University, ANNABELLE BOHRDT, Harvard University and Technical University of Munich, MIUQING XU, Harvard University, JUSTUS BRÜGGENJÜRGEN, Harvard University and University of Hamburg, MICHAEL KNAP, Technical University of Munich, EUGENE DEMLER, FABIAN GRUSDT, MARKUS GREINER, DANIEL GREIF, Harvard University — Developments in quantum gas microscopy have enabled detailed studies of the repulsive Fermi-Hubbard model. Using fermionic Lithium-6 in a square lattice, we observe the transition into an antiferromagnet at temperatures below the superexchange energy. We use a novel pattern-finding algorithm to characterize the system’s behavior upon hole-doping. This new observable provides evidence that holes may be hiding the antiferromagnetic order rather than destroying it. We then investigate the deterministic injection of a single mobile dopant into an antiferromagnet and observe how it propagates. Finally, we discuss our progress towards an optical lattice with dynamically tunable interference contrast, which enables several low-entropy state preparation schemes and spin-resolved readout.
**G70.00242: $^6$Li in optical ring lattices**  DANIEL ALLMAN, YANPING CAI (Presenter), KEVIN WRIGHT, PARTH SABHARWAL, Dartmouth College — Optical ring lattices provide a convenient setting for studying, i.e., many-body correlations and emergent topological phenomena in low-entropy, low-temperature Fermi ensembles. Due in part to technical challenges involved in creating and maintaining stable optical ring lattices, there has been no detailed experimental study of the behavior of fermions in periodic lattice geometries. We report on progress toward loading and trapping $^6$Li atoms in optical ring lattices of $\leq 100$ sites. By preparing low-entropy quantum states within the lattice, along with the ability to tune interactions with $^6$Li’s broad Feshbach resonance, we hope to observe a fermionic metal-to-Mott insulating transition in a strictly periodic geometry. We will also have the ability to investigate more exotic lattice structures, potential arenas for realizing several paradigmatic topological lattice models, such as the Su-Schrieffer-Heeger model.

**G70.00243: Boosting the BEC critical temperature of an ideal Bose gas within a crystal with vacancies**  JUAN GARCIA (Presenter), MIGUEL SOLIS, JOSÉ MARTÍNEZ-HERRERA, National Autonomous University of Mexico — We show that an ideal Bose gas in one or two-dimensional imperfect crystal presents Bose-Einstein condensation at a finite critical temperature, which does not happen when the crystal is perfect. For the three-dimensional imperfect crystal case, the BEC critical temperature is higher than that of the gas in the perfect crystal. We have obtained the energy spectrum of the particles using the transfer and dispersion matrix methods as well as the use of the Green function, transfer matrix and dispersion, which we use to calculate, in addition to the critical temperature, the specific heat for the Bose gas within imperfect two-dimensional structures such as multilines or grids, and for three-dimensional cases such as multiplanes, multitubes and multicubes.

*We thank the partial support from grants CONACyT 221030 y DGAPA-PAPIIT IN107616.

**G70.00244: Ultracold YbF molecules for measuring the electron’s electric dipole moment**  MICHAEL TRIGATZIS (Presenter), Centre for Cold Matter, Blackett Laboratory, Imperial College London — Theories that extend the Standard Model (SM) generally contain additional sources of CP-violation and predict the electron to have an electric dipole moment (eEDM) large enough to be measured by today's experiments. The eEDM may be measured by observing spin precession in YbF molecules in an electric field [1]. Recent results [1-4] already strongly constrain beyond-SM theories.

Laser cooling of molecules was first demonstrated in 2010 [5]. An ultracold beam of YbF could increase the eEDM measurement sensitivity by two orders of magnitude [6]. We have demonstrated 1D sub-Doppler transverse cooling of our YbF beam to below 100 $\mu$K [6] and recently extended the technique to 2D.


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**G70.00245: Progress towards quantifying the impacts of state mixing on the Rydberg excitation blockade**  ANDREW LESAK (Presenter), AARON WHTYE REINHARD, Kenyon College — Rydberg atoms are ideal for studying quantum phenomenon due to their exaggerated properties relative to ground-state atoms. During excitation, the highly polarizable atoms interact and the resonant frequencies of the atoms are shifted, leading to a suppression of excitation known as the “Rydberg excitation blockade.” In an ideal blockade, many atoms share one excitation and a more complete blockade is achieved when neighboring atoms interact more strongly. However, near a Forster resonance, stronger interactions can lead to the excitation of unwanted states, breaking the blockade. In order to implement scalable quantum computers, the Rydberg excitation blockade must be used in large samples and therefore state-mixing properties must be rigorously studied in order to minimize their negative impacts. We laser cool rubidium atoms to microkelvin temperatures and use state-selective field ionization spectroscopy to determine the distribution of atoms in each Rydberg state. We present preliminary results in which we seek to quantify exactly how much state-mixing reduces blockade efficiency and to determine the number of interacting bodies that lead to large amounts of state-mixing.

*This work was supported by NSF Grant No. PHY-1553179.
G70.00246: Two-dimensional Condensation of Polar Molecules with Field-induced Dipoles  I-KANG LIU, Department of Physics, National Changhua University of Education, Changhua, Taiwan, DAW-WEI WANG, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, SHIH-CHUAN GOU (Presenter), Department of Physics, National Changhua University of Education, Changhua, Taiwan — We theoretically investigate the ground-state structures of a two-dimensional condensation composed of ultracold polar molecules, in which the condensed particles are subjected to an effective vector potential induced by the Raman coupling between two rotational levels of the molecule. With all dipoles aligned by a DC field in the axial direction and the two counter-propagating Raman beams in the radial direction, the effective dipole moment induced by the light-matter coupling, which is much larger than the intrinsic dipole moment of the molecule, predominates the interaction between molecules. Based on the previous studies, the effective interaction features not only the standard long-range dipolar form but also a spatial dependence on the relative phase between two coupled rotational states. In the mean-field approximation, the ground state is found to possess four phases: plane-wave phase, zero-momentum phase and two of Stoner-type phase. The first two phases appear when the system is in the coupling-dominant regime, while the last two are in the interaction-dominant regime. Numerical results obtained by solving the Gross-Pitaevskii equation agree with the variational analysis. Dynamical stability of the Stoner-type phases is examined via calculating the Bogoliubov spectrum.

G70.00247: Conclusive Precision Bounds for SU(1,1) Interferometers*  CHENGLONG YOU (Presenter), SUSHOVIT ADHIKARI, Louisiana State University, XIAOPING MA, Department of Physics, Ocean University of China, MASAHIDE SASAKI, MASAHIRO TAKEOKA, National Institute of Information and Communications Technology, JONATHAN P DOWLING, Louisiana State University — We revisit the quantum Fisher information (QFI) calculation in SU(1,1) interferometer considering different phase configurations. Firstly, when one of the input modes is a vacuum state, we show by using phase averaging, different phase configurations give same QFI. In this case, the QFI is linearly proportional to the average photon number of the second input state, and quadratically proportional to the average photon number generated by the OPA. This suggests that when fixing the squeezing strength of the OPA, to achieve higher sensitivity, one simply needs to inject a state with higher average photon number. Secondly, we compared the results of the phase-averaging method and the quantum Fisher information matrix method, and then we argued that for a SU(1,1) interferometer, phase averaging or quantum Fisher information matrix method is generally required, and they are essentially equivalent. Finally, we used the quantum Fisher information matrix method to calculate the precision limit for other common input states, such as two coherent state inputs or coherent state with squeezed vacuum inputs.

*CY, SA and JPD would like to acknowledge support from Army Research Office and National Science Foundation.

G70.00248: Phase estimation in an SU(1,1) interferometer with displaced squeezed states*  SUSOHOVIT ADHIKARI (Presenter), NARAYAN BHUSAL, CHENGLONG YOU, HWANG LEE, JONATHAN P DOWLING, Louisiana State University — We study the phase sensitivity of an SU(1,1) interferometer with coherent and displaced-squeezed-vacuum (DSV) states as inputs, and parity and on-off as detection strategies. Our scheme with parity is sub-shotnoise limited and approaches the Heisenberg limit with increasing squeezing strength of the optical parametric amplifier (OPA). Also, for the on-off detection scheme, we show that sub-shotnoise sensitivity is possible by increasing the squeezing strength of the OPA.

*Air Force Office of Scientific Research, Army Research Office

G70.00249: Three-photon molecule generation through coherent scattering process off single dipole emitter in quantum nanophotonics  ZIHAO CHEN (Presenter), YAO ZHOU, JUNG-TSUNG SHEN, Electrical and System Engineering, Washington University in St. Louis — Bound state refers to the quantum state wherein wave function of constituent particles is localized, which typically require interactions between individual particles, e.g., two hydrogen atoms form bound state of a hydrogen molecule due to Coulomb interactions. Thus, photons do not form bound states (also called photonic molecules) easily due to its electric neutrality. Recently, it has been reported that, when three photons interact with a single emitter, photon-photon entanglement mediated by the emitter may induce the formation of 3-photon molecules. However, the underlying generation mechanism is not yet clear.

Here we present a computational study to confirm that, through coherent scattering process for three uncorrelated photons off a single dipole emitter, 3-photon molecule is generated. In particular, three prominent signatures: (1) exponentially decaying wave function as photon distance increases; (2) anti-correlation signature; and (3) pi-phase shift, are unveiled by examining correlation functions and wave functions of scattered photons. Moreover, we show that our results account for recent experiment in ultra-cold atomic gas well. Such a 3-photon molecule has potential applications in designing photonic quantum logic gate and three-photon fluorescence microscopy.
Towards Using Trapped Ions as Memory Nodes in a Photon-mediated Quantum Network

JAMESON O’REILLY (Presenter), Northeastern University, Boston, MA 02115, USA, JACKSON BELL, DANIELA BOGORIN, Air Force Research Laboratory, Rome, NY 13441, USA, BENJAMIN BONENFANT, Northeastern University, Boston, MA 02115, USA, PAUL COOK, Air Force Research Laboratory, Rome, NY 13441, USA, SAVANNAH DECKER, Boston University, Boston, MA 02215, USA, LESTER DISNEY, TYLER DOLEZAL, Air Force Research Laboratory, Rome, NY 13441, USA, BENJAMIN DRIESEN, Northeastern University, Boston, MA 02115, USA, PAIGE HAAS, Air Force Research Laboratory, Rome, NY 13441, USA, NICHOLAS HOUGLAND, Carnegie Mellon University, Pittsburgh, PA 15213, USA, DAVID HUCUL, Air Force Research Laboratory, Rome, NY 13441, USA, BRAD LIU, SPAWAR, San Diego, CA 92110, USA, SAMUEL MARTHAGE, Syracuse University, Syracuse, NY 13244, USA, BRENNAL NELSON, JUSTIN PHILLIPS, Northeastern University, Boston, MA 02115, USA, KAITLIN POOLE, Air Force Research Laboratory, Rome, NY 13441, USA, BRANDON ROBINSON, Northeastern University, Boston, MA 02115, USA, HARRIS RUTBECK-GOLDMAN, LAURA WESSING, KATHY-ANNE SODERBERG, Air Force Research Laboratory, Rome, NY 13441, USA — Quantum networking exploits features of quantum mechanics to provide ultrasecure networks that are both tamper-proof and tamper-evident. Such networks can be implemented as distant memory nodes connected via photon-based interfaces. Trapped ions are nearly ideal quantum network nodes due to the precise control possible over both their internal and external degrees of freedom as well as for their superior performance as long-term quantum memories. Photon-based qubits are the natural choice to transfer information within the network due to their ability to transmit quantum information over long distances and the capability to process information "on-the-fly" between the memory nodes. We present the quantum research being done at the Air Force Research Laboratory (AFRL) with a focus on trapped ion qubits, the short- and long-term goals of the lab, and some of the unique resources we have access to at AFRL. Approved for Public Release [Case # 88ABW-2018-2102] Distribution Unlimited.

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G70.00251: MEST-Spacetime Center, Gluon, and New String Theory

DAYONG CAO (Presenter), Avoid Earth Extinction Association — MEST is a balance systemic model of mass, energy, space, and time.

There is a balance MEST system between gluons and quarks. The gluon is “spacetime”.

According to Einstein field equation and negative Einstein equation, there are massenergy center with massenergy structure and spacetime center with spacetime structure which has gravity of the spacetime (as negative gravity).

The spacetime center structure can explain of dark matter and dark energy.

A balance structure between massenergy and spacetime can explain of the homogeneous, isotropic, and flat structure of the universe. It can suppose a balance system between the sun and a dark sun (as a spacetime center of Oort cloud).

And the quantum spacetime of the wave, new atomic model, and dark atomic model of the dark matter-dark energy had brought forward.

A advanced string theory can explain of the gravitons of the spacetime center, a gravity of the spacetime of the glunos (as one kind of strong force), the gluon field between a quark and an anti-quark, and Regge Trajectories. It also can study the spacetime structure (wave structure) of the quark-gluon plasma.

That can help us to look for big bang of the spacetime and big bang of the massenergy.

http://meetings.aps.org/Meeting/APR16/Session/M13.8
DAYONG CAO (Presenter), AEEA — The thought waves remotely (wireless) simultaneously radiate to increase background photo-voltages of the four solar cells at the same changed rates by cold photoelectric effect.

Because the luminous sensitivities of the solar cells are different and the photo-voltages are nonlinear functions, there are different “changed rates” in general experiments by light.

Brain is made up of balance between stellar matter and dark matter which has spacetime center structure, such as a balance between gluons (spacetime structure) and quarks (massenergy structure), a balance between nucleus structure and electron cloud, and a balance between the basis (massenergy structure of the crystal) and the crystal lattice (spacetime structure of the crystal), and has cold dark radiations.

The cold photoelectric effect of cold dark radiations of brain wave is a probability effect of the spacetime structure (of Confined Structural non-Newtonian Fluids) between brain wave and a balance structure between Electron Clouds and electron holes of P-N Junction.

The relationship between brain wave and consciousness effect will be considered.

As the decade of the brain research and the “BRAIN” Initiative, a “decade of the consciousness research” need be taken.

http://meetings.aps.org/Meeting/APR16/Session/M13.8

WONWOOK LEE (Presenter), SUNGYONG SHIM, CHA-HWAN OH, Physics, Hanyang University — Stark broadening is widely used to determine the electron density of the astrophysical plasmas and the atmospheric pressure plasmas. In low temperature plasmas Doppler broadening is larger than Stark broadening and the Stark broadening can be measured after removing Doppler broadening. In this research, the model for Stark broadening to determine the electron density was discussed in low temperature plasmas when Doppler broadening of plasma radiation was removed. The spectral line broadenings of van der Waals broadening, resonance broadening, natural broadening, and Stark broadening were calculated and compared with each other in low temperature He plasmas. As well the helicon plasma source of which electron density was higher than \(10^{11}\) cm\(^{-3}\) was constructed to investigate the helium Stark broadening. Stark broadening for \(2^1S-4^1P\) was measured using the saturation absorption spectroscopy and the electron density could be determined by analyzing the Stark broadening.

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YONGQIANG LI (Presenter), JIAYU DAI, XIAOWEI WANG, ZENGGXIU ZHAO, JIANMIN YUAN, Department of Physics, National University of Defense Technology — Both coherent pumping and energy relaxation play important roles in understanding physical processes of ultra-intense coherent light-matter interactions. Here, using a large-scale quantum master equation approach [1], we describe dynamical processes of practical open quantum systems driven by both coherent and stochastic interactions. As examples, we investigate coherent dynamics of inner-shell electrons of a neon gas irradiated by a high intensity X-ray laser along with vast number of decaying channels. In these single-photon dominated processes, we find that, due to coherence-induced Rabi oscillations and power broadening effects, the photon absorptions of a neon gas can be suppressed resulting in differences in ionization processes and final ion-stage distributions. Second, we demonstrate a new scheme for the investigation of hole dynamics of complex atoms based on two-color ultrashort X-ray pulses.

REFERENCES


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KUAN-HSUN CHIANG (Presenter), National Central University, IO-CHUN HOI, National Tsing Hua University, YUNG-FU CHEN, National Central University — We study the level structure of a tunable coupling qubit (TCQ) [Ref. 1, 2] by microwave spectroscopy in superconducting circuit architecture. Based on the two independently tunable SQUID loops, the multi-level structure of a TCQ can be tuned in-situ. We demonstrated that a TCQ is a charge qubit while providing tunable selection rule. Accompanied with the mode-tunability in coplanar waveguide design, V-type, lambda-type and many other structures can be achieved in a TCQ-based architecture. TCQs have potential for the application of microwave quantum optics.


*Y.-F. Chen acknowledges the support from Ministry of Science and Technology in Taiwan under Grants No.MOST-107-2112-M-008-003

CHONG YE (Presenter), QUANSHENG ZHANG, YONG LI, Beijing Computational Science Research Center — In the mean-field theory, the stabilization of chiral molecules is understood as a quantum phase transition where the mean-field ground state of molecules changes from the achiral eigenstate of the molecular Hamiltonian to one of the degenerated chiral states due to the increase of the intermolecular interaction. However, the existing mean-field models are either unavailable to chiral molecules whose electric dipoles do not change in sign for |L⟩ and |R⟩ or with free parameters. In this work, starting from the Many-body Hamiltonian with electric dipole-dipole interaction, we give the static Gross-Pitaevskii equations in the vibrational dimension. Our model can be applied to all chiral molecules and has no free parameters.

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SUNGYONG SHIM (Presenter), WONWOOK LEE, CHA-HWAN OH, Department of physics, Hanyang university — Helium 23S metastable atoms play key roles in discharge plasmas because of the long lifetime and large excitation energy. In this research, 23S state helium density in an inductively coupled plasma (ICP) was measured by laser absorption spectroscopy. He plasma was operated at the He pressure of 20~50 mTorr and by a RF power supply with the maximum power of 1.5 kW. Electron temperature and electron density of plasma were 2~3 eV and ~1012 cm⁻³, respectively. Absorption spectra for the 23S₁->23Pᵢ (ᵢ=0, 1, 2) transitions were measured by an external cavity laser diode (ECLD) at 1083 nm. The 23S state helium density was analysed and discussed with the RF power and the radial position in the plasma chamber.

JAMES BOYLE (Presenter), Boyle, PLLC — The bispinor solution to the Dirac equation is used to construct a conserved current. The possibility that the conserved current can take on marginal negative values is addressed as a condition that can be set and altered with constraints. Specifically, a Dirac bispinor solution is constructed and subject to constraints such that the marginal negative probability value in the corresponding conserved current is cancelled completely. Unexpectedly, and for a superposition of positive- and negative-energy states using these bispinor solutions, the conserved current derived here is shown to be completely absent of all Zitterbewegung terms. Various uses of the conserved current and the bispinor solutions derived here are also illustrated in conventional contexts, such as in computing scattering amplitudes across barrier potentials.
We report progress on an ongoing experiment to measure the electron EDM using YbF molecules [1].

We have increased the initial population of YbF molecules in the ground state by a factor of six through a combination of repump lasers, microwaves and rf fields. We have also improved our detection efficiency by a factor of 40. This is due to better collection optics, and a better detection scheme which can scatter many more photons per molecule. The new detection scheme also allows us to measure both quadratures of the interferometer.

Spurious magnetic fields are a major source of random and systematic error in our experiment, and therefore we have improved our control and measurement of magnetic fields. This was done by re-designing the electric field plates for lower magnetic Johnson noise, and by installing several low-noise magnetometers inside the machine.

Together, we will be able to measure the electron EDM at the $10^{-29}$ e cm level, which is competitive with the current limit of $1.1 \times 10^{-29}$ e cm set by the ACME collaboration [2].


*I acknowledge funding from the Controlled Quantum Dynamics Centre for Doctoral Training at Imperial College London.

A broad range of chemical reactions are triggered by the absorption of light. Examples include photosynthesis and charge transfer in semiconductors and molecules. Electronic dynamics which evolve on the few femtosecond to attosecond timescale are expected to play an important role in these processes. We aim to investigate these dynamics with transient X-ray absorption near edge structure (XANES) spectroscopy. XANES spectroscopy uses resonant excitation of particular atoms in a molecule to provide a highly localised probe of electronic structure. By employing attosecond soft x-ray pulses generated via high harmonic generation for XANES spectroscopy this atomic scale spatial resolution can in principle be combined with the attosecond temporal resolution required for tracking electronic dynamics. I shall present development of a beamline for transient XANES spectroscopy and progress towards visible pump, soft x-ray probe experiments in the organic polymer poly(hexylthiophene).

*This research is supported by the EPSRC grants EP/N018680/1 and EP/1032517/1 and the Controlled Quantum Dynamics Centre for Doctoral Training

Electron spin resonance (ESR) lock-in sensing protocols with nitrogen vacancy (NV) centers in diamond allow for wide-field, real time imaging of magnetic fields for biological applications ranging from bio-current imaging to wide-field tracking of magnetic nano-particles. ESR lock-in NV measurements have previously been utilized for the optical detection of firing action potentials in giant axons [1]. By modulating the applied microwave driving field and imaging the NV fluorescence with a specialized lock-in camera, we are able to create real time videos of local magnetic fields with high spatial (~1 μm) and temporal (~1 ms) resolution over a large field of view (~1 mm). Here we show demonstrate a volume-normalized sensitivity of ~100 nT*μm^3/2*Hz^-1/2 and compatibility with living biological systems. This work paves the way for the development of broadband quantum diamond microscopes for imaging bio-magnetic fields from neuronal activity.

References:
VIRGINIA O LORENZ, Physics, University of Illinois at Urbana-Champaign — Deterministic production of high purity photon

SCHLOSS, Massachusetts Institute of Technology, DIANA PRADO LOPES AUDE CRAIK, Physics, Harvard University, RONALD L

WALSWORTH, Harvard-Smithsonian CFA — Magnetic field sensors and imagers employing nitrogen vacancy (NV) centers in
diamond require strong, uniform microwave (MW) fields near 3 GHz. We present a new design for a planar waveguide
structure fabricated on silicon carbide (SiC), which combines homogeneous microwave delivery with the heat-spreading
benefits of SiC. We perform finite element simulations in COMSOL, we fabricate and test MW structures, and we compare
experimental performance with simulation results. We demonstrate optimized MW power delivery and improved MW field
uniformity. We implement these MW delivery structures in quantum diamond microscopes (QDMs) to improve magnetic
imaging performance in fields ranging from Earth and planetary sciences to biology.

KAI SHINBROUGH, BIN FANG, Physics, University of Illinois at Urbana-Champaign, YANTING TENG (Presenter), Physics, Harvard University, YUJIE ZHANG, OFFIR COHEN, VIRGINIA O LORENZ, Physics, University of Illinois at Urbana-Champaign — Deterministic production of high purity photon states is essential for robust quantum communication and information applications. One way to implement the deterministic single photon production is the Duan-Lukin-Cirac-Zoller (DLCZ) protocol via phonon-mediated Raman processes. Although Raman processes have been well demonstrated, the purity of photons has remained largely unexplored. We investigate the effects experimental parameters have on the purity of single photons by using a phenomenological hamiltonian. We show how single photon purity depends on the length of the crystal and the bandwidth of the pump used to generate the photons. We compare our numerical simulations against experimental data showing qualitative agreement.

LIN XIN (Presenter), MICHAEL S CHAPMAN, Georgia Institute of Technology — Squeezing, which redistributes the quantum fluctuations between two noncommuting observables while preserving the minimum uncertainty product, has been extensively studied in boson systems. In addition, research in squeezed spin states (SSSs) is a topical area due to its significant applications in high-precision measurement and in quantum information science. The building block of spin squeezing is One-axis twisting (OAT). A two-axis counter-twisting mechanisms (TAT) is introduced as a natural extension of OAT and is shown to further reduce the quantum noise. So far, there are plenty of experiments that realized OAT while TAT haven't been achieved due to the experimental complexity. In this talk, I will present a way to produce TAT in spin-nematic squeezed system by Floquet driving. Periodically microwave and radio frequency pulse sequence can adjust the direction of spin squeezing and thus generates an effective TAT Hamiltonian. By adapting this method, there is no need to change the setup of the apparatus, but instead, changes only the time sequence, improving the current experimental limit of spin squeezing.

YOUSEF SALAMIN (Presenter), Physics Department, American University of Sharjah — Bessel beams carry orbital angular momentum (OAM). Opening up of the Hilbert space of OAM to information coding makes Bessel beams potential candidates for utility in data transfer and optical communications. The ultra-short and tightly-focused analogue of a non-diffracting and non-dispersing laser Bessel beam is often referred to as a laser bullet. Electromagnetic fields of a laser Bessel-Bessel bullet are presented, following from solution to the wave equations of the scalar and vector potentials in the presence of an under-dense plasma. Intensity distributions based on the derived fields are shown to propagate over many centimeters, without significant diffraction or distortion. The reported fields are derived, to lowest order, from a vector potential containing an ordinary Bessel function of arbitrary order and a zero-order spherical Bessel function, hence the designation Bessel-Bessel bullet.
G70.00268: Supercontinuum generation with octave-spanning bandwidth in the high order mode based Ta2O5 waveguide*  
FU-YAN YAN (Presenter), CHUNG-LUN WU, RARAN FAN, PIN-SHUO HWANG, CHAO-WEI LIU, CHIN-YU LIU,  
Department of Photonics, National Sun Yat-sen University, Taiwan, MIN-HSIUNG SHIH, Research Center for Applied Sciences, Academia Sinica, Taiwan, YI-JEN CHIU, ANN-KUO CHU, CHAO-KUEI LEE, Department of Photonics, National Sun Yat-sen University, Taiwan — Super-continuum generation (SCG) has been attracting plenty of attention due to its wide application, such as OCT and communication. In this work, anomalous dispersion Ta2O5 based waveguide was designed and fabricated for the super-continuum generation (SCG) due to its nature of two-photon absorption free and high optical nonlinearity. The 5mm length air cladding Ta2O5 waveguide with a dimension of 800nm x 700nm was designed and fabricated for fulfilling anomalous dispersion requirement which is crucial for SCG. For excitation laser wavelength of 1056nm, with excitation peak power of around 400W, the 1.5 octave-spanning was demonstrated. Compared to a SiN-based nonlinear waveguide, the resulting exhibit Ta2O5 based waveguide a promising material for SCG.

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G70.00269: GENERAL THEORY AND COMPUTATIONAL PHYSICS  —

G70.00270: Theoretical Prediction of Sulfides Under Pressure  
NISHA GENG (Presenter), Chemistry, SUNY at Buffalo — Inspired by the discovery of high temperature superconductivity in the hydrogen/sulfur system, the XtalOpt evolutionary algorithm has been used to predict the structures of binary and ternary sulfides under pressure. A number of stable and metastable phases with novel stoichiometries are found at pressures attainable in diamond anvil cells. The electronic structure and superconducting properties of these phases are analyzed.

G70.00271: First-principles calculation of third-order elastic constants via numerical differentiation of the second Piola-Kirchhoff stress tensor  
DAVID CUFFARI (Presenter), ANGELO BONGIORNO, College of Staten Island — Third-order elastic constants (TOECs) of materials are difficult to measure experimentally and produce large errors. Computational methods are needed for overcoming these difficulties. Previous methods to calculate TOECs are based on fitting energy-strain and/or stress-strain curves calculated from density functional theory (DFT). These methods rely on symmetry relationships, and for this reason, so far they have been applied mainly to cubic and hexagonal crystals. In this paper, we present a novel method to calculate TOECs that is applicable to any system, regardless of its symmetry and dimensionality. This method relies on second-order numerical differentiation of the second Piola-Kirchhoff stress tensor. In this work, we combine this method to a plane-wave DFT approach to calculate the TOECs of aluminum, diamond, silicon, magnesium, graphene, and graphane. A comparison to experimental results shows that our new method is valid and accurate.

G70.00272: Development of Multiphase EOS Table for Gallium*  
CARRIE PRISBREY (Presenter), CHRISTINE J WU, Lawrence Livermore Natl Lab — We present a multiphase equation of state (EOS) table created at Lawrence Livermore National Laboratory for Gallium (Ga). Gallium is an interesting material as it has a low melting temperature of only a few degrees above room temperature, and the Ga-I solid, found at room temperature and pressure, exhibits the properties of both covalent and metallic bonding. Gallium is unusual in that its liquid phase is more dense than the Ga-I solid, leading to a melt line of negative slope. Our EOS captures the anomalous behavior of the liquid phase as well as the three commonly known solid phases, Ga-I, Ga-II, and Ga-III. The table is constrained by published experimental data such as DAC, isobars, and Hugoniot measurements. In addition, we plan to test our EOS against the newest dynamic measurements taken at the Z facility at Sandia National Laboratory.

*This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344
**Mechanisms of optically initiated decomposition of MgO-PETN and MgO-TNT composites**

ROMAN TSYSHESVSKIY (Presenter), University of Maryland College Park, ANTON S. ZVEREV, ANATOLY Y. MITROFANOV, Kemerovo State University, MAIJA M KUKLA, University of Maryland College Park — Optical initiation to detonation of energetic materials (EMs) opens up new ways for safe handling, storage, and use of high explosives. EM-oxide interfaces have distinct optical and electronic properties because of the alignment of the filled and vacant electronic states of oxides and EMs. These changes are key factor for achieving tunable sensitivity through controllable initiation of decomposition reactions. We report here results of experimental and theoretical study on photoinitiation of PETN-MgO and TNT-MgO composites. We discuss electronic and optical properties of these materials and reveal mechanisms of photoinitiation reactions involving charge transfer from metal oxide to explosive compound. We also show how chemical stability of ionized explosive compounds can be critical for design composite materials with controllable optical sensitivity.

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**Orientation dependence of plasticity and transformation kinetics in Zirconium at higher shock pressure**

HONGXIANG ZONG, University of Edinburgh, TURAB LOOKMAN, Los Alamos National Laboratory, ANDREAS HERMANN (Presenter), GRAEME ACKLAND, University of Edinburgh — We simulated the high pressure phase transformation in zirconium using molecular dynamics with a new EAM potential fitted using force matching. Under quasistatic ("Hugoniostat") conditions the transformation from α-ω follows the phase diagram, as expected. However under directly simulated shock conditions the structure transforms from α-β (hcp-bcc) rather than the expected ω phase. Assuming sudden, isotropic pressurization we trace this to a different phase transformation mechanism (so-called TAO1) in which bcc appears as an intermediate state, and under pressure the barrier hcp-bcc is lower than bcc-ω. The assumption of isotropic loading requires significant plasticity, which we also simulated and found to be of marginal validity. Plasticity depends on the crystal orientation and in the absence of ideal plasticity, so does the transformation path and, indeed, the observed high pressure phase. We have determined the orientational dependence of the transformation kinetics between hcp-ω-bcc and hcp-bcc at higher shock pressure.

*Research funding through the ERC grant HECATE is gratefully acknowledged.

**Electron-Phonon Coupling in Ag-Au Alloys**

SURENDER SINGH (Presenter), DASARI PRASAD, Department of Chemistry, Indian Institute of Technology Kanpur — Superconductivity at ambient temperature and pressure has been recently inferred from the data of electrical resistance and magnetic susceptibility measurements on Ag-Au alloy nanostructures [1]. In view of this, electron-phonon interactions have been calculated by means of density functional perturbation theory to search for the signatures of superconductivity in stable and metastable Ag-Au bulk and nanostructured alloys within the BCS-like pairing mechanism. The electronic structure and phonons of the alloys are found to be similar to that of the constituent elements in their ground states. And, therefore, the estimated superconducting transition temperatures resulted in less than a mK. Our computational results corroborate with the findings of absence of superconductivity in Ag/Au modulated nanostructures grown by pulsed laser deposition [2]. The results will be discussed in detail in two parts: alloy structure solutions and electron-phonon – superconductivity.


*We acknowledge the CC, RNJJ & CHM HPC facilities at IIT Kanpur. S.S. thanks the CSIR-India for a SRF fellowship. D.L.V.K.P. acknowledges Initiation-Grant:IITK/CHM/20130116.
G70.00276: Thermal transport theory of organic semiconductors
NIANDUAN LU, JIAWEI WANG (Presenter), LING LI, MING LIU, institute of microelectronics, chinese academy of sciences — Organic semiconductors (OCSs) have very recently received much attentions as potential thermoelectric materials, originating from the fact that they are both semiconducting and that they exhibit relatively low thermal conductivity than that of inorganic materials. The low thermal conductivity of OCSs can remarkably increase the energy conversion efficiency. Generally, thermal transport in OCSs fundamentally differs from that in inorganic materials and is determined by the charge carriers and phonons in localized states. Understanding thermal transport performance of OCSs is important for a fundamental description of energy flow and then a better design of organic thermoelectric devices. We present a unified theoretical model to describe the thermal transport performance of the OCSs based on hopping transport theory. The proposed model predicts that the contribution from phonon to the thermal conductivity is larger than that from charge carrier in the OCSs. Moreover, the proposed model can well interpret the thermal transport feature of the OCSs by combining the disorder, temperature, and carrier concentration. Simulation results imply that thermal conductivity in the OCSs could be strongly affected under large electric field, high carrier and dopant concentration.

G70.00277: Dimensionality-induced phonon softening: effect on electron-phonon coupling and transport
SUSHANT KUMAR (Presenter), RAVISHANKAR SUNDARARAMAN, Rensselaer Polytechnic Institute — Classical elasticity theory predicts that finite-thickness unstrained materials should exhibit a quadratic flexural phonon mode. However, state-of-the-art computational methods have been largely inconsistent in yielding such a behavior for the phonon dispersion curves of two-dimensional (2D) materials and their heterostructures. Given the enormous attention 2D materials have received in recent decades, it is imperative to understand the impact of this phonon softening on \textit{ab initio} predicted electron-phonon coupling strength and resultant transport properties. Recently, a new formulation of phonon calculations based on internal rather than Cartesian coordinates has observed that capturing rotational invariance in addition to translation invariance captures the quadratic mode correctly. Here, we investigate the role of rotational invariance on predicted phonon dispersion curves rigorously, and systematically quantify its impact on electron-phonon scattering rates. We show that the cross-over from a linear to quadratic dispersion of the transverse acoustic branch strongly affects transport properties such as electrical and thermal conductivity when we move from bulk to few- and single-layer materials.

G70.00278: Laplace transform approach for the dynamics of \( N \) qubits coupled to a resonator
MIRKO AMICO (Presenter), OLEG BERMAN, ROMAN KEZERASHVILI, CUNY Graduate Center — An approach to use the method of Laplace transform for the perturbative solution of the Schrodinger equation at any order of the perturbation for a system of \( N \) qubits coupled to a cavity with \( n \) photons is suggested. We investigate the dynamics of a system of \( N \) superconducting qubits coupled to a common resonator with time-dependent coupling. To account for the contribution of the dynamical Lamb effect to the probability of excitation of the qubit, we consider counter-rotating terms in the qubit-photon interaction Hamiltonian. As an example, we illustrate the method for the case of two qubits coupled to a common cavity. The perturbative solutions for the probability of excitation of the qubit show excellent agreement with the numerical calculations.

G70.00279: Size-Controlled Carrier Multiplication in Graphene Nanoribbons*
JUNHYEOK BANG (Presenter), Korea Basic Science Institute — Carrier multiplication (CM) is a fundamental dynamic process of an excited carrier generating multi-electron-hole pairs from single-photon absorption. As such, CM can improve the efficiency of optoelectronic devices. However, CM is rarely witnessed in conventional semiconductors, calling for the need to discover unconventional materials. Here, using real-time time-dependent density functional theory, we show that CM occurs in armchair graphene nanoribbons (AGNRs). The subband structure of AGNRs plays a key role, as it releases the constraints of energy and momentum conservation in the CM process. The subband structure varies depending on nanoribbon width, and thus it provides the way to control the carrier dynamics and carrier multiplication in AGNRs.

*This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) (NRF- 2018R1D1A1B07044564) and KBSI grant D38614.
However, the adsorption of O2 molecule on monolayer Ti-doped MoS2 shows relatively higher affinity. The results showed perturbative regime.

Ground and excited state energies, our results will give accurate descriptions of light-emission phenomena in the non-perturbative regime.

Beyond accurate calculation of emitter levels and many photon modes that go beyond solvable model systems in quantum optics. One important result is that we arrive at the first theory of Lamb shifts and Casimir-Polder forces in the ultrastrong coupling regime, which reveals new saturation effects that strongly suppress energy shifts as light-matter coupling grows. Beyond accurate calculation of ground and excited state energies, our results will give accurate descriptions of light-emission phenomena in the non-perturbative regime.

*Work funded by the German Research Foundation within the CRC 951

G70.00281: First-principles ultrafast charge carrier dynamics at the hybrid F4TCNQ:H-Si(111) interface

To do so, we adopt the formalism of real-time time-dependent density-functional theory as implemented in the octopus code [2]. Our results offer insights into the earliest-stage formation of the optical excitations in hybrid interfaces.


G70.00280: First-principles photoelectron spectroscopy in molecular solids from multiscale GW-BSE/MM embedding

Here, we present a multiscale study of the photoemission spectra of MADN thin films using a first principle scheme consisting of Metropolis Monte Carlo-based simulated annealing, Many Body Green's Function Theory within the GW approximation, a QM/MM embedding procedure, and explicit treatment of electron-vibrational coupling. We discuss effects of disorder, quasiparticle corrections, and electrostatic embedding on spatially resolved HOMO levels. Predicted UPS signals are in excellent agreement with experiment.

[1] GIANLUCA TIRIMBO (Presenter), XANDER DE VRIES, PETER BOBBERT, REINDER COEHOORN, BJÖRN BAUMEIER, Humboldt Universität zu Berlin — Hybrid inorganic-organic materials are typically characterized by charge-transfer excitations across their interface that make them appealing candidates for opto-electronic applications [1]. However, the fundamental processes leading to the formation and the evolution of these states are still under debate. To address this question, we investigate from first principles the hybrid interface formed by the strong acceptor F4TCNQ adsorbed on the Si(111) surface, which is p-doped in the ground state. Its linear-absorption spectrum exhibits two maxima in the visible region corresponding to transitions between the electronic states across the inorganic and components. We investigate the dynamics of these excitations triggered by resonant ultrafast laser pulses, following the evolution of the charge-carrier population. To do so, we adopt the formalism of real-time time-dependent density-functional theory as implemented in the octopus code [2]. Our results offer insights into the earliest-stage formation of the optical excitations in hybrid interfaces.

G70.00282: Adsorption of molecular oxygen on Ti-doped monolayer MoS2 and effect of applied electric field: A DFT study

XIANGXUAN DENG (Presenter), Department of materials science and engineering, City University of Hong Kong — It is proposed that by tuning the O2 adsorption on Ti-doped MoS2, the resulting materials system can be used as nanocatalyst. To this end, density functional theory calculations was first performed to study the adsorption of molecular oxygen on pristine MoS2 and Ti-doped MoS2. It was found that O2 molecule adsorption energy on pristine MoS2 was very weak. However, the adsorption of O2 molecule on monolayer Ti-doped MoS2 shows relatively higher affinity. The results showed that the Ti-bridge-O2 configuration is most stable. The analysis of molecular projected density of state and charge transfer indicates that the interaction between the O2 molecule and the Ti dopant is chemisorption via two Ti-O bonds, which affects the magnetic, electronic, and atomic properties of Ti-doped MoS2. Furthermore, the adsorption energy and O-O distance of Ti-doped MoS2 under electric field have been studied. It is hoped that together with electric field, the tuned O2 adsorption on Ti-doped MoS2 could become a nanocatalyst.

G70.00283: First principles theory of ground and excited states of correlated light-matter systems in the non-perturbative regime

NICHOLAS RIVERA (Presenter), JOHANNES FLICK, PRINEHA NARANG, Applied Physics, Harvard University — Ultra-strong coupling between light and matter promises to bring about new means to control material properties, concepts for manipulating light at the atomic scale, and insights into quantum electrodynamics (QED). Thus, there is need to develop quantitative theories of QED phenomena in complex electronic and photonic systems. Here, we develop a new variational paradigm to analyze ultra-strongly coupled light-matter systems which gives ground and excited state information as well as real-space information about electromagnetic fields as they are modified by strong light-matter coupling. Our method gives highly accurate energies for both ground and excited states for systems with many emitter levels and many photon modes that go beyond solvable model systems in quantum optics. One important result is that we arrive at the first theory of Lamb shifts and Casimir-Polder forces in the ultrastrong coupling regime, which reveals new saturation effects that strongly suppress energy shifts as light-matter coupling grows. Beyond accurate calculation of ground and excited state energies, our results will give accurate descriptions of light-emission phenomena in the non-perturbative regime.

*N.R. is supported by the DOE Computational Science Graduate Fellowship.
systems. This study, in future, can be applied in the development of the efficient photovoltaic cell. The calculation indicates that there is a linear correlation between electrostatic polarization energy and dipole moments of Sc3NC80 and Sc3NC80_ZnPc with the dielectric permittivity of the solvents. However, the trend for Sc3NC80_Pc is deviated slightly, which is scrutinized in DFT level by considering cationic and anionic clusters to study solvent effect. A comparison of results is made with earlier studies of Sc3NC80 systems using DFT in a gas phase, which established small charge transfer from the external complex to the fullerene, takes place even more rigorously in solvent perturbed Sc3NC80 systems. This study, in future, can be applied in the development of the efficient photovoltaic cell.

*The University of Texas at El Paso.

**G70.00285: Exciton Characteristics in Carbon Nitride and Graphene Quantum Dots**  
NAEEM ULLAH, SHUNWEI CHEN, RUIQIN ZHANG (Presenter), City University of Hong Kong — Graphene quantum dots (GQDs) and Carbon nitride quantum dots (CNQDs), the latest addition to the carbon material family, promise numerous novel applications in optical sensing, photocatalysis, bio-sensing, and photovoltaics. However, understanding the photocatalytic capability of CNQDs compared to the graphene quantum dots (GQDs) have not been investigated thoroughly. Time-dependent density functional tight binding (TD-DFTB) calculations in this work revealed that CNQDs have superior carrier charge separation, sensitive to the size of the QD. Strong localization of the frontier molecular orbitals (FMOs and excited state charge separation was observed in the first excited state due to the relaxation of the structure. The exciton structure reveals spatial confinement to the stretched C-N bonds independent of the size of the QDs while there is no such exciton structure found for GQDs. The optical absorption and emission of CNQDs is sensitive to size, with no dependence on the shape of the QD.

*The work described in this paper was supported by a grant from the Research Grants Council of the Hong Kong SAR [Project No. CityU 11334716].

**G70.00286: Electrical Contacts in Monolayer Blue Phosphorene Devices**  
JINGZHEN LI (Presenter), School of Engineering, Applied Science, Harvard University — Semiconducting monolayer (ML) blue phosphorene (BlueP) shares similar stability with ML black phosphorene (BP) and has recently been grown on the Au surface. Potential ML BlueP devices often need a direct contact with metal to inject carrier. Using *ab initio* electronic structure calculations and quantum transport simulations, we perform a systematic study of the interfacial properties of ML BlueP in contact with metals spanning a wide work function range in a field effect transistor (FET) configuration for the first time. There is a strong Fermi level pinning (FLP) in the ML BlueP FETs due to the metal induced gap states (MIGS). The MIGS are eliminated by inserting graphene between ML BlueP and the metal electrode accompanied by a transition from a strong FLP to a weak FLP. Our study not only provides an insight into the ML BlueP-metal interfaces but also helps to design the ML BlueP device.

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**G70.00287: Deep Bandgap and Band Structure Engineering by Machine Learning**  
ZHE SHI (Presenter), Materials Science and Engineering, Massachusetts Institute of Technology, EVGENII TSYMBALOV, Skolkovo Institute of Science and Technology, MING DAO, Materials Science and Engineering, Massachusetts Institute of Technology, SUBRA SURESH, Nanyang Technological University, ALEXANDER SHAPEEV, Skolkovo Institute of Science and Technology, Ju LI, Materials Science and Engineering, Massachusetts Institute of Technology — The ability to deform and keep silicon at large strains harbingers a new age of deep elastic strain engineering (ESE) of electronic materials. Current strained-Si technology thus represents only "tip of the iceberg" of what silicon can do as the most versatile and processable electronic material. Deep ESE explores the full six-dimensional space of admissible elastic strain and its effect on physical properties, beyond linear elasticity and perturbation theory. Here we present a general method that combines machine learning and *ab initio* calculations to guide rational ESE whereby unprecedented material properties and performance could be designed. This method invokes recent advances in artificial intelligence by utilizing a limited amount of *ab initio* data for the training of a surrogate model. In particular, an artificial neural network predicts the electronic bandstructure within the accuracy of 19 meV. Our model is utilized to discover the indirect-to-direct bandgap transition and semiconductor-to-metal transition in the entire strain space. By finding out the most energy efficient deformation manner to achieve a desirable bandgap, we demonstrate for the first time how to identify novel pathways to tailor any material figure of merit, which is of central importance for ESE.
Machine learning predictions of nuclear stability*  ROBERTO PÉREZ (Presenter), ALEXANDER BALATSKY, Nordic Institute for Theoretical Physics — Machine learning (ML) methods have become a useful tool in many areas of physics, including Nuclear Physics. ML methods’ ability to take in aggregate information about the behaviour of the system and predict trends is able to make relevant and verifiable predictions. The existence of super heavy stable nuclei in currently experimentally inaccessible regions has been predicted by the nuclear shell effect, however, its location and extension are still in dispute by different models (e.g. Z=120 N=172 from relativistic models) [1]. We aim to apply ML tools to develop accurate statistical models to predict isotopic lifetimes in regions of heavy nuclei, such as the fabled stability island. We explore various ML methods, and study the predictive power of different nuclear representations. We use ML models both with and without theoretical bias from nuclear models, such as isotopic magic numbers, over different radioactive decay channels to possibly offer a glimpse of the next stability region.


*Work supported by KAW 2013.0096 and Villum Center for Dirac Materials.

Low-energy physics of the bilinear-biquadratic spin-1 chain  MORITZ BINDER (Presenter), THOMAS BARTHEL, Duke University — The bilinear-biquadratic spin-1 chain features various interesting quantum phases, including the Haldane phase, a dimerized phase, and an extended critical phase. Here, we apply an efficient density matrix renormalization group (DMRG) algorithm utilizing infinite boundary conditions to compute precise dynamic spin structure factors for a comprehensive set of points in the phase diagram. Analyzing both dynamic spin and quadrupolar correlations, we gain detailed insights into the nature of low-lying excitations of the model. We compare our results to Bethe ansatz solutions at the SU(3)-symmetric ULS point and the TB point as well as at the pure biquadratic point, which can be mapped to an anisotropic spin-1/2 XXZ chain in the gapped Néel phase. In the Haldane phase, we relate our results to the approximate description in terms of the non-linear sigma model.

Spin-charge co-operation in even-parity three dimensional nodal superconductivity in strained Sr₂RuO₄*  SWAGATA ACHARYA, CEDRIC WEBER, MARK SCHILFGAARDE (Presenter), King’s College London — We develop a three-tier \textit{ab initio} technique to study the origin and nature of the pairing in Sr₂RuO₄. The technique starts with the quasi-particle self consistent GW (QSGW) approximation to build a reference hamiltonian, augment it with dynamical mean field theory (DMFT) to add spin fluctuations left out of QSGW, and also generate the vertices entering into spin, charge, and pairing susceptibilities. Finally we solve multi-orbital Bethe-Salpeter equations to calculate these properties in both strained and unstrained single crystals. We identify what leads to the recently observed dependence of Tc on strain and also gain insights into what limits it. We find a one-to-one correspondence between Tc and the coherence and intensity of the spin susceptibility under application of strain. Finally, we establish connections between spin fluctuations and superconducting pairing symmetries in Sr₂RuO₄, and dimensionality of the fluctuations associated with these degrees of freedom.

*This work was supported by the Simons Many-Electron collaboration

Optimized higher-order Lie-Trotter-Suzuki decompositions for two and more terms  YIKANG ZHANG (Presenter), THOMAS BARTHEL, Duke University — Lie-Trotter-Suzuki decompositions of operator exponentials have a lot of applications in physics. For example, they are employed to sample equilibrium states in quantum Monte Carlo and to simulate the dynamics of quantum systems on quantum computers or on classical computers using tensor network state techniques. They also provide symplectic integrators for classical physics. Good higher-order decompositions for exponentials of n=2 non-commuting operators are well-known. These cover one-dimensional quantum systems with nearest-neighbor interactions. We present some optimized decompositions for n=2 and new higher-order decompositions for n=3,4 which are needed for one-dimensional systems with longer-ranged interactions or quantum systems in higher dimensions. The ordering of operators in the decompositions turns out to have substantial influence on the attainable approximation order and magnitudes of the leading error terms.
ParaMonte: A user-friendly parallel Monte Carlo optimization, sampling, and integration library for scientific inference

AMIR SHAHMORADI (Presenter), University of Texas at Arlington — At the foundation of predictive science lies the scientific methodology, which involves multiple steps of observational data collection, developing testable hypotheses, and making predictions. Once a scientific theory is developed, it can be cast into a mathematical model whose parameters have to be fit via observational data. This leads to the formulation of a mathematical objective function for the problem at hand, which has to be then optimized to find the best-fit parameters of the model, or sampled to quantify the uncertainties associated with the parameters, or integrated to assess the performance of the model. Toward this goal, a highly customizable, user-friendly high-performance parallel Monte Carlo optimizer, sampler, and integrator library is presented here, which can be used on a variety of platforms with single to many-core processors, with interfaces to popular programming languages including Python, R, MATLAB, Fortran, C/C++. The algorithms implemented in the library include variants of Markov Chain Monte Carlo that utilize Machine Learning techniques to improve the algorithm's performance, as well as Parallel Tempering, and Nested Sampling.

G70.00293: Numeric Analytic Continuation via Rational Function Regression (Padé Regression)

JIAN WANG (Presenter), SUDIP CHAKRAVARTY, physics and astronomy, UCLA — We have developed a simple and natural method to perform numeric analytic continuation of quantum Monte Carlo data. It is based on the Padé approximation, and uses linear regression and bootstrapping statistics to get rid of extreme unstable results, and estimate the error. Unlike maximum entropy method, no prior information is needed here. Test cases have shown that various spectrum is recovered for relative error as large as 0.1%. Physical reasonings are also explained for its success.

Beam Size Prediction and Control using Neural Network

SHUAI LIU (Presenter), University of California, Berkeley, CHARLES MELTON, HIROSHI NISHIMURA, ALEXANDER HEXEMER, SIMON C LEEMANN, Lawrence Berkeley National Lab — Experimental results from beam lines are sensitive to the size of the beam itself. However, predicting and controlling the beam size still prove to be a challenge. Even with the feed-forward strategy using recorded control data (aka look-up tables), the beam size variance on vertical direction is still ~2 μm. Herein, we provide a machine learning based approach to predict the beam size using neural network. We perform a systematic study to optimize the prediction result using different neural network architectures and regularizers. Based on the model, we propose a neural network based beam size stabilization strategy by tuning a certain experimental parameter (dispersion wave parameter). The variance of beam size on vertical direction is reduced to ~0.3 μm in the online test.

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Conservation law presumption from the manifold structure captured by Deep Neural Networks

YOHICHI MOTOTAKE (Presenter), fronteer science, The university of Tokyo — It is suggested that Deep Neural Networks (DNN), which continues to develop in recent years, has a function to extract information of data sets necessary to achieve a given task by modeling the distribution as a manifold. In addition to confirming the usefulness of DNN technology, numerous researchers and engineers are developing various DNN algorithms and tuning parameters. This situation means that enormous knowledge on the manifold structure for various data sets is being accumulated. The purpose of this research is to propose a method to extract manifold structure with complex shape extracted in an interpretable form. Specifically, we propose a method to extract the symmetry of manifold for coordinate transformation. Applying the proposed method to the time series data of the moving object according to the central force potential, it was confirmed that symmetry according to the conservation law of angular momentum could be extracted.
G70.00296: Effect of Different Types of Sulfur Precursors on Chemical Vapor Deposition Synthesis of MoS2 layers: A Reactive Molecular Dynamics Study*  
SUNGWOOK HONG (Presenter), RURU MA, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Layered transition metal dichalcogenides (TMDCs) like MoS2 layers are promising materials for next-generation electronic applications. Large-area monolayer MoS2 samples for these applications are typically synthesized by chemical vapor deposition (CVD) using MoO3 reactants and sulfur precursors. Recent experimental and computational studies have greatly improved our understanding of reaction pathways in CVD synthesis. However, effect of different types of sulfur precursor on CVD synthesis of MoS2 layer has yet to be fully investigated. In this work, we present quantum-mechanically informed and validated reactive molecular dynamics (RMD) simulations to investigate CVD synthesis of MoS2 layer using S2 and H2S molecules. Our goal is to clarify the different sulfidation and reduction rates of MoO3 surface by S2 and H2S precursors. Our RMD results provide an atomic scale understanding of the CVD reactions for higher-quality MoS2 and other TMDCs.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607.

G70.00297: Fracture in α-Quartz under weak shock condition  
SUBODH TIWARI (Presenter), University of Southern California, MASAAKI MISAWA, KYUSHU SANGYO UNIVERSITY, TOMOKO SATO, Hiroshima University, FUYUKI SHIMOJO, Kumamoto University, AIICHIRO NAKANO, University of Southern California, TOSHIMORI SEKINE, Osaka University, PAULO S BRANICIO, PRIYA VASHISHTA, University of Southern California — Shock response of α-Quartz has been extensively studied using both experiment and theory. Here we present a large scale molecular dynamics simulations to study the atomistic mechanism underlying the weak shock response of α-Quartz. First, classical potential (BKS) employed is verified against Density functional theory (DFT). We computed the shock hugoniot curve using BKS potential which show a quantitatively agreement with DFT. Further, we perform non adiabatic molecular dynamics for plane shock loading in [210] direction. Shock simulation reveals the formation of 5 coordinated Si atom in the banded region. 5 coordinated Si relax to form an banded amorphous region in the system. System between these banded amorphous region shows an elastic compression. Further, The generation of shock-induced plastic deformation is characterized using machine learning methods.

G70.00298: Multi-objective forcefield parameterization for thermal transport in 2D materials*  
NICHOLAS GRABAR (Presenter), ANKIT MISHRA, ARAVIND KRISHNAMOORTHY, AIICHIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, University of Southern California — Forcefields for the calculation of thermal properties of nanomaterials must be parameterized to match empirical material properties. Here, the third generation of the Non-Dominated Sorting Genetic Algorithm (NSGA-III) is used to construct forcefields to model 2D semiconducting materials by optimizing structure parameters (lattice constants), mechanical properties (elastic modulus) and vibrational behavior (phonon dispersion curve) from ab initio simulations. The algorithm is a parallelized, cross-platform workflow, written in C, that uses GULP as the engine for validating constructed forcefields. NSGA-III is a reference-point-based many-objective algorithm emphasizing population members that are non-dominated, yet close to a set of supplied reference points. It can handle up to fifteen variables and reference point tuning allows for user tuned diversity in the end product. This will allow for future expansion into forcefields finely-tuned over additional variables.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607. The simulations were performed at the Center for High Performance Computing of the University of Southern California.
G70.00299: Learning Structure-Thermal Property Relationships in 2D Materials* NITISH BARADWAJ (Presenter), ARAVIND KRISHNAMOORTHY, AIICHIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, University of Southern California — Two dimensional monolayer semiconductors, alloys and patterned lateral heterostructures are extremely promising candidates for the next generation of nanoelectronic devices. Quantification of thermal transport of such two dimensional materials and heterostructures is necessary for the design of such nanoelectronic and thermoelectric devices. However, direct experimental measurements of intrinsic thermal conductivity is challenging at these length scales and, therefore, the role of material stoichiometry and phase distribution on thermal transport properties of these materials remains unknown.

Here, we use fully atomistic non-equilibrium molecular dynamics simulations to compare the calculated intrinsic thermal conductivity of a Mo$_{1-x}$W$_x$Se$_2$ monolayer alloy with that of a self-similar fractal MoSe$_2$/WSe$_2$ heterostructure. Machine learning applied to the compositional phase space of these materials is used to predict heterostructures with desired thermal transport properties.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC00014607

G70.00300: Global warming impact on low frequency acoustic propagation in Pacific Ocean equatorial surface ducts: a potential paradox. DAVID BROWNING (Presenter), Browning Biotech — A typical Pacific Ocean pH profile has a value of 8.1 at the surface decreasing to 7.7 at the axis of the SOFAR channel (400m). Absorption in seawater of low frequency sound is pH dependent, so that the low frequencies that are contained in a surface duct will be absorbed at twice the rate of those in the SOFAR channel. Global warming is producing ocean acidification which is reducing the pH, hence the low frequency sound absorption, and this will first impact the surface duct. But global warming is also predicted to increase the rainfall and as these equatorial surface ducts are produced from monsoon conditions, the surface duct would be deepened and thus expand the low frequencies contained in it, which would now be absorbed at a higher rate than in the SOFAR channel. This is just a first look into one aspect of what may prove to be a multifaceted and complex interaction of global warming on acoustic propagation conditions in the ocean.

G70.00301: Aimsbg: An algorithm and open-source python library to generate periodic grain boundary structures* KESONG YANG (Presenter), JIANLI CHENG, University of California, San Diego — An algorithm implemented in an open-source python library was developed for building periodic grain boundary models in a universal fashion. The software framework, aimsbg, aims to generate tilt and twist grain boundaries from an input cubic or non-cubic crystal structure for ab-initio and classical atomistic simulation. It can output a coincidence site lattice (CSL) grain boundary for a cubic input structure and a non-CSL grain boundary for a non-cubic input structure. This framework has two useful features: (i) it can calculate all the CSL matrices for generating CSL from a given Sigma (Σ) value and rotation axis, allowing the users to build the specific CSL and grain boundary models; (ii) it provides a convenient command line tool to enable high-throughput generation of tilt and twist grain boundaries by assigning an input crystal structure, Σ value, rotation axis, and grain boundary plane. The developed algorithm in the open-source python library is expected to facilitate studies of grain boundary in materials science. The software framework is available on the website: aimsbg.org.

*The author acknowledges support by National Science Foundation under award number ACI-1550404.

G70.00302: Electrochemical Stability Window of Polymeric Electrolytes LIHUA CHEN (Presenter), SHRUTI VENKATRAM, CHIHO KIM, ANAND CHANDRASEKARAN, RAMAMURTHY RAMPRAKASH, Georgia Institute of Technology — The electrochemical stability window (ESW) is a fundamental consideration while choosing polymers for electrolytes in lithium-ion batteries. In this work, we propose two computational procedures, viz. first-principles density functional theory (DFT) computations coupled with classical molecular dynamics (MD) simulations and machine learning (ML) methods to efficiently and accurately estimate ESW of polymers electrolytes. Six model polymers were investigated, namely, polyethylene (PE), polyethylene oxide (PEO), polyvinyl alcohol (PVA), poly(methyl methacrylate) (PMMA), polycaprolactone (PCL) and polyvinyl chloride (PVC). The role of polymer chemistry and the morphological complexity in determining ESW of these polymers have been elucidated. Comparison with established experimental values revealed that the ESW can be accurately predicted using DFT calculations coupled with MD simulations. However, this method is still time-consuming and the relevant force fields are limited, therefore ML methods are proposed to predict the ESW of single chain models with a first-order accuracy instantaneously. Overall, these two computational procedures proposed in this work can assist the rational design of novel solid polymer electrolytes with desired ESW values.
Co-evolutionary search for Cu-Pd-Ag nanoparticle ground states accelerated with neural network potentials

AIDEN CULLO (Presenter), SAMAD HAJINAZAR, ERNESTO D. SANDOVAL, ALEKSEY KOLMOGOROV, Physics, Applied Physics and Astronomy, Binghamton University — Unconstrained optimization of nanoparticles requires advanced search methods capable of locating global minima in large configuration spaces. In this study, we demonstrate that algorithm efficiency can be improved substantially if ground state searches are performed across a range of nanoparticle sizes simultaneously. In this symbiotic co-evolutionary approach implemented in our MAISE package [1], stable motifs are periodically exchanged among tribes with neighboring nanoparticle sizes. The algorithm was extensively tested on elemental Cu, Pd, and Ag nanoparticles up to 80 atoms using both traditional classical potentials and our neural network models. Examination of the lowest-energy configurations revealed that the neural network set was consistently more stable at the density functional theory level. Lastly, we used our Cu-Pd-Ag neural network model to identify stability regions in binary and ternary systems.

[1]: https://github.com/maise-guide/maise

Are Small Polarons Always Detrimental to Transparent Conducting Oxides?

GUILLAUME BRUNIN (Presenter), GIAN-MARCO RIGNANESE, GEOFFROY HAUTIER, Universite catholique de Louvain — Transparent conducting oxides (TCOs) are critical components in many devices like solar cells or touchscreens. The search and development of new TCOs combining high conductivity and transparency is a major endeavor of modern Materials Science. Novel p-type TCOs are especially greatly sought for as they lie much behind their n-type counterpart and the discovery of a high performance p-type TCO would enable important technological breakthroughs. There are two types of carrier transport mechanism in materials: band transport involves delocalized carriers while small-polaron transport involves carriers trapped in the crystalline lattice. Materials exhibiting transport through small polarons have been traditionally disregarded for TCO applications as they offer small mobilities. In this work, we use well-established physical models to compare the performances of TCOs based on band- and small-polaron transports. Surprisingly, we demonstrate that small-polaron TCOs can outperform band TCOs in terms of transparency and conductivity, especially p-type. Using our analysis, we outline the materials properties necessary for high performance small-polaron TCOs, leading to a series of design principles for the search of new efficient small-polaron p-type TCOs.

Point charged defects in 2D and 3D h-BN: A density functional theory study

PRADIP NIRAULA (Presenter), ANGELO BONGIORNO, College of Staten Island — In this work, we first calibrated a density functional theory (DFT) approach, and then I carried out DFT calculations to study the properties of charged point defects in monolayer, bilayer, and bulk h-BN. In particular, we considered a DFT approach using a semiempirical scheme to account for Van der Waals forces, and we optimized the dispersive coefficient of B to obtain a description of the structural and mechanical properties of bulk h-BN in agreement with the experiments. The resulting optimized DFT scheme was used to calculate formation energies and electronic properties of neutral and charged B and N vacancies, as well as C substitutional defects for both N and B sites. To correct the formation energies of charged defects, we used a novel polarizable force field. Our calculations show that, due to electrostatic polarization, the formation energy of charged defects in bilayer h-BN is about 0.5 eV lower than in monolayer h-BN. Furthermore, we found that assuming that the aforementioned four types of point defects are present with a finite concentration in mono- and bi-layer h-BN, there is always a class of defects that is likely to be charged, regardless of the position of the Fermi level.

Is Defect Segregation Facile in the Grain Boundary of Methylammonium Lead Iodide?

XIN HE (Presenter), Jilin University, WISSAM SAIDI, University of Pittsburgh, LJUN ZHANG, Jilin University — Methylammonium Lead Iodide (MAPbI3) is emerging as one of the most promising materials for solar cells. Grain boundaries (GBs) and native point defects are ubiquitous in MAPbI3 given that solution-based methods generate polycrystalline materials. Our previous study has shown that there is a strong thermodynamic preference of iodine point defects to exist in the GB region rather than in the interior of the MAPbI3 grain [Shan and Saidi, J. phys. Chem Lett. 8, 5935 (2017)]. This would generate defect segregation to the GB, provided that defect diffusion is not hindered at room temperature. In this talk, we examine the energy barriers and possible kinetic limitations of the diffusion of iodine interstitials and vacancies in Σ5 (210) MAPbI3 GB, and contrast the results with their diffusion in crystalline system.

*Work at Jilin University is supported by National Natural Science Foundation of China under Grant Nos. 61722403 and 11674121.
G70.00307: Lone-pair electrons induced anomalous enhancement of thermal transport in strained planar two-dimensional materials GUANGZHAO QIN (Presenter), MING HU, University of South Carolina — Manipulating heat conduction is an appealing thermophysical problem with enormous practical implications, which requires insight into the lattice dynamics. Strain engineering is one of the most promising and effective routes towards continuously tuning the thermal transport properties due to the flexibility and robustness. However, previous studies mainly focused on quantifying how the thermal conductivity is affected by strain, while the fundamental understanding on the electronic origin has yet to be explored. In this talk, I would like to show that the thermal conductivity (κ) of planar monolayer group III-nitrides is unexpectedly enlarged by one order of magnitude with bilateral tensile strain applied, which is in sharp contrast to the strain induced κ reduction in graphene despite their similar planar honeycomb structure. The anomalous positive response of κ to tensile strain is attributed to the attenuated interaction between the lone-pair s electrons around N atoms and the bonding electrons of neighboring (B/Al/Ga) atoms, which reduces phonon anharmonicity. The microscopic picture for the lone-pair electrons driving phonon anharmonicity would have great impact on future research in materials design with targeted thermal transport properties.

G70.00308: Surface plasmon polariton excitation in exfoliated MoS2 flakes on Au nanogratings SOYEONG KWON (Presenter), MIN HEE KWON, JUNG EUN SONG, BO RA KIM, EUNAHAH KIM, SANG WOOK LEE, DONG WOOK KIM, Physics, Ewha Womans University — We prepared MoS2 flakes on Au nanogratings to investigate how the surface plasmon polariton (SPP) excitation can affect physical properties of MoS2. SPP – the propagating electromagnetic and charge wave at metal/dielectric interface – can be excited using grating structures by overcoming the momentum mismatch between the impinging photons and the SPPs. The MoS2 flakes were exfoliated from its bulk and transferred on the Au nanogratings (period: 500 nm) fabricated by electron beam lithography. The number of MoS2 layers was identified using micro-Raman and atomic force microscopy measurements. Finite-difference time-domain simulations showed clear signature of the SPP excitation in the electric field intensity distributions and optical reflection spectra of the Au nanogratings. The work function of the MoS2 flakes was measured using Kelvin probe force microscopy, and its variation in dark and light was studied to understand the interaction between the SPPs at the MoS2/Au interface and charge carriers in the MoS2 flakes. This study can help us to develop new kinds of 2D transition metal dichalcogenide semiconductor-based plasmonic devices.

G70.00309: Giant effect of spin-lattice coupling on the thermal transport in two-dimensional ferromagnetic CrI3 GUANGZHAO QIN, MING HU (Presenter), Department of Mechanical Engineering, University of South Carolina — Recently, two-dimensional monolayer chromium triiodide (CrI3) with intrinsic magnetism was experimentally discovered, which shows promising applications in many technologies ranging from sensing to data storage where thermal transport plays a critical role. However, so far, the effect of spin-lattice coupling on the thermal transport properties has not been explored yet. In this talk, I will present the giant effect of spin-lattice coupling on the lattice thermal conductivity (κL) of monolayer CrI3. The lattice thermal conductivity is more than two orders of magnitude enhanced by considering the spin-lattice coupling. The effect is found to be especially stronger for the acoustic phonon modes, which dominates thermal transport with spin-lattice coupling. The mechanism lies in the weakened phonon anharmonicity by spin-lattice coupling. The bond angle and atomic position are changed due to the spin-lattice coupling, making the structure much stiffer and more symmetric, which lead to the weaker phonon anharmonicity, and thus the enhanced thermal conductivity. This study uncovers the effect of spin-lattice coupling on the thermal transport, which would deepen our understanding on thermal transport and shed light on future research of thermal transport in magnetic materials.

G70.00310: Size and Substrate effect on excitation dynamics of 2D materials* SUBODH TIWARI (Presenter), University of Southern California, HIROYUKI KUMAZOE, SHOGO FUKUSHIMA, Kumamoto University, ARAVIND KRISHNAMOORTHY, University of Southern California, FUUYUKI SHIMOJO, Kumamoto University, RAJIV KALIA, AILICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Excitation dynamics of 2D materials has been extensively studied by different theoretical and experimental methods. However, effect of substrate and size effect on the excitation dynamics of 2D materials has not been well delineated due to large number of atoms. We perform quantum molecular dynamics simulations at high electron temperatures within the density functional theory framework to understand the effect of substrate and size. We computed the intralayer mean square displacement and Debye-waller factor of top and bottom layer of WSe2. The simulation results show that interaction between substrate and transition metal dichalcogenide layers create distinct anisotropy in electronic excitation-induced lattice dynamics that may be experimentally observable.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, and Basic Energy Sciences, under Award Number DE-SC0014607. The simulations were performed at the Argonne Leadership Computing Facility under the DOE INCITE program and at the Center for High Performance Computing of the University of Southern California.
G70.00311: Ab-initio Study of Electronic Properties of Ti-doped VO₂ Nanowire* PRABAL BHUYAN (Presenter), Department of Physics, Gujarat University, Ahmedabad, India, SANJEEV K. GUPTA, Department of Physics, St Xavier’s College, Ahmedabad, India, YOGESH SONVANE, Department of Applied Physics, SV National Institute of Technology, Surat, India, P. N. GAJJAR, Department of Physics, Gujarat University, Ahmedabad, India — Vanadium oxide (VO₂) nanowire undergoes a phase transition at 341K and shows metal-insulator transition (MIT). We have considered high-temperature VO₂-NW structure, which is stable in rutile form. The state of art density functional calculation has shown metallic in VO₂ (R) rutile structure nature. Further, we have investigated the doping effect of Ti substitution for V in VO₂-NW. A transition of metallic to semiconducting behaviour is observed by the presence of Ti-3d orbital and it is also confirmed by the partial density of states (PDOS) that contribution of Ti-3d orbital near the Fermi level at conduction band. We have observed band gap of 1.83eV, however band gap decreases with the increase in Ti concentration. Furthermore, Ti-doped VO₂-NW shows adsorption energy at visible region, which attributes to its potential application in nano-optoelectronic devices.

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G70.00312: Lithium adsorption and diffusion on Janus Mo/WXY (X,Y = S, Se, Te) GRACIE CHANEY (Presenter), FATIH ERSAN, CAN ATACA, University of Maryland, Baltimore County — One of the most important factors in improving the efficiency of anode materials for Li-ion batteries is the mobility of Lithium atoms in these materials. On the basis of first-principles plane-wave calculations, we examined the adsorption and diffusion of lithium atoms on the hexagonal Janus Mo/WXY (X,Y=S, Se and Te) monolayers. We found the lowest energy adsorption positions of the Li adatom to be on the top site of the transition metal atom, on both sides of all considered Janus monolayers. Due to electronegativity differences of the chalcogenides in the Janus structures and induced dipole moment, both the Li adatom adsorption and the diffusion barrier energies on the surfaces of Janus structures differ from the bare Mo/WX₂ monolayers. For instance, Li diffusion barrier energy for the Tellurium sides of the Mo-Janus structures are about 0.09-0.12 eV lower than that of MoTe₂ monolayers which is 0.23 eV. Also, Li diffusion barrier energy on the Sulfur sides of the Mo-Janus monolayer is about 0.04-0.08 eV larger than its MoS₂ energy value. All considered structures turn to metal after Li atom absorption. Our electronic transport calculations concluded inn an increase in conductivity. This makes them superb candidate materials for the electrodes of Li-ion batteries.

G70.00313: WITHDRAWN ABSTRACT —

G70.00314: Electronic structure and optoelectronic properties of 4',5'-dibromo-2',7'-dinitro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3',6'-dialate JEAN BAPTISTE FANKAM FANKAM (Presenter), Physics, University of Yaounde I — The molecular structure, electric parameters and optoelectronic properties of 4',5'-dibromo-2',7'-dinitro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3',6'-dialate have been theoretically studied. We used the RHF and DFT (PBE1PBE, MPW1PW91, B3PW91 and B3LYP) approach to calculate the optimized parameters, molecular structure, electric parameters and optoelectronic properties of the tilted compound with cc-pVDZ basis set. The larger the HOMO-LUMO energy gap, the harder and more stable (less reactive) the compounds. The lowest value (3.78eV) is shown in B3LYP is most stable and the highest value (8.81eV) in RHF is least stable. The effect of correlation decreased the value of HOMO-LUMO energy. Our results suggest that this molecule have potential applications as linear and nonlinear optical materials. Due to the large hyperpolarizability of this molecule, we think that these molecules have potential applications in thoptoelectronic and can be a promising material for optical limiting applications.
G70.00315: High-accuracy large-scale DFT calculations using localized orbitals in complex electronic systems: The case of graphene-metal interfaces*  CARLOS ROMERO-MUÑIZ (Presenter), Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, AYAKO NAKATA, National Institute for Material Science (NIMS), PABLO POU, Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, DAVID R BOWLER, Physics & Astronomy, University College London, TSUYOSHI MIYAZAKI, National Institute for Material Science (NIMS), RUBEN PEREZ, Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid — Over many years, computational simulations based on Density Functional Theory (DFT) have been used extensively to study many different materials at the atomic scale. However, its application is restricted by system size, leaving a number of interesting systems without a high-accuracy quantum description. In this work, we calculate the electronic and structural properties of a graphene-metal system significantly larger than in previous plane-wave calculations with the same accuracy. For this task we use a localized basis set with the Conquest code, both in their primitive, pseudo-atomic orbital form, and using a recent multi-site approach [1]. This multi-site scheme allows us to maintain accuracy while saving computational time and memory requirements, even in our exemplar complex system of graphene grown on Rh(111) with and without intercalated atomic oxygen. This system offers a rich scenario that will serve as a benchmark, demonstrating that highly accurate simulations in cells with over 3000 atoms are feasible with modest computational resources.


G70.00316: GTPack: A Mathematica group theory package for application in solid-state physics and photonics*  RICHARD GEILHUFE, Nordic Institute for Theoretical Physics, KTH Royal Institute of Technology, Stockholm University, WOLFRAM HERGERT (Presenter), Martin-Luther University Halle-Wittenberg — We present the Mathematica group theory package GTPack providing about 200 additional modules to the standard Mathematica language. The content ranges from basic group theory and representation theory to more applied methods like crystal field theory, tight-binding and plane-wave approaches capable for symmetry based studies in the fields of solid-state physics and photonics. GTPack is freely available via http://gtpack.org. The package is designed to be easily accessible by providing a complete Mathematica-style documentation, an optional input validation and an error strategy. We illustrate the basic framework of the package and show basic examples to present the functionality.


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G70.00317: Band structure theory of twisted bilayer graphene  XING-JU ZHAO (Presenter), DONG-BO ZHANG, Simulation of Physical Systems Division, Beijing Computational Science Research Center — Twisted bilayer graphene show various interlayer interaction under different rotation angles, which make the system presents nontrivial physical properties, such as unconventional quantum hall effect and berry's phase, correlated insulator behaviour and unconventional superconductivity in magic angle graphene superlattice, et al. However, when the rotation angle is small, the electronic structure, such as band, can’t be simulated by the first-principles method. In this project, combine tight-binding method and first-principles simulation, we construct interlayer Hamiltonian matrix element and improve the effective continuum model in band structure theory. Based on this, we construct the wavefunction of each layer in superlattice and then build the Hamiltonian matrix, which further simplify the band structure theory model. Finally, we extend this model to other 2D bilayer systems. The success implementation of this project will construct a simple, cheap and general method for band structure simulation of twisted bilayer graphene, and provide a useful tool for the relative physical effects study of 2D bilayer materials.
G70.00318: Is self-interaction corrected density functional theory straying from the path toward the exact functional? SEBASTIAN SCHWALBE, TORSTEN HAHN, JENS KORTUS, Theoretical Physics, TU Bergakademie Freiberg, KAI TREPTÉ (Presenter), KOBLAR ALAN JACKSON, Physics, Central Michigan University — As recently pointed out [1] higher rung functionals (e.g. MGGA or hybrids) may deliver a better description of the total energy but not necessarily a better description of the density for the calculated systems. We present an additional perspective to this discussion and present the performance of self-interaction corrected densities for LDA, GGA and MGGA rungs of density functionals for an extended benchmark set considering atoms, molecules and stretched bond situations.


G70.00319: Strong correlation effect on the Seebeck coefficient from Density Functional Theory* ROBERTO D’AGOSTA (Presenter), University of the Basque Country, KAIKE YANG, Chinese Academy of Science, ENRICO PERFETTO, GIANLUCA STEFANUCCI, University of Rome “Tor Vergata”, STEFAN KURTH, University of the Basque Country — Density Functional Theory (DFT) has become the standard for transport calculations due to its simplicity and widespread implementations. It has been shown that the theory fails, especially when dealing with strongly correlated systems. The standard approximations associated with the theory are the culprit for most of these failures, but we should also realize that static DFT should not deal with transport problems. In this talk, we will discuss how to build a DFT theory that is able to describe strongly correlated effects [1]. In particular, we will discuss the correction for the Seebeck coefficient in the Coulomb blockade regime in a quantum dot in linear response [2]. We will show how the theory can compare with experiments and outline future research lines to extend the methods beyond linear response.


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G70.00320: ABSTRACT WITHDRAWN —

G70.00321: Self-Interaction Error Free Magnetic Exchange Couplings: LSDA vs PBE vs SCAN.* RAJENDRA JOSHI (Presenter), KOBLAR ALAN JACKSON, JUAN ERNESTO PERALTA, Department of Physics and Science of Advanced Materials, Central Michigan University, Mt. Pleasant, MI, 48858 — We analyze the effect of self-interaction error removal from density functional theory on magnetic exchange couplings using Fermi-Lowdin orbital self-interaction correction (FLOSIC) methodology. We compare self-interaction corrected LSDA, PBE, and SCAN exchange couplings to the respective uncorrected ones and to more accurate quantum chemistry calculations and experiments. In addition, we discuss the effect of spin projection on magnetic exchange couplings.

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G70.00322: Crossover Behavior of Entanglement Entropy for Energy Eigenstates of 1d and 2d Fermionic Systems QIANG MIAO (Presenter), THOMAS BARTHEL, Department of Physics, Duke University — The entanglement entropy in ground states of typical condensed matter systems obeys the area law or a log-area law for critical systems. Subsystem entropies in random and thermal states obey a volume law. Here, we discuss the distribution of entanglement entropy in energy eigenstates of quasi-free fermionic systems as a function of energy and subsystem size. Numerical results are obtained with a Monte Carlo approach. We characterize the crossover behavior from the area or log-area law in the vicinity of the ground state and for small subsystem size to the volume law at higher energy and larger subsystem size. The coefficients of the volume law scaling can be matched to entropy densities in equilibrium thermal ensembles. For critical 1d systems at low energies, the universal crossover function matches the prediction from 1+1d conformal field theory for systems at nonzero temperatures. For 2d systems, we find a similar crossover behavior.
**G70.00323: Large N Tensor and SYK Models**  
JAEWON KIM (Presenter), University of California, Berkeley, IGOR R KLEBANOV, Physics, Princeton University — The SYK model consists of Majorana fermions that interact randomly four at a time. A holographic dual may exist for this model, which makes it interesting in the study of quantum gravity. It has been found that the SYK model is similar to large N tensor models: in both models, only the melonic diagrams survive in the large N limit. In this paper, we explore the large N tensor model with O(N)^3 symmetry containing two flavours of Majorana fermions in the fundamental representation, the quartic Hamiltonian of which depends on a real parameter. We derive the kernels of the four point functions. With these, we calculate the scaling dimensions of several types of conformal primaries. We also find a duality relation between two Hamiltonians of different real parameters. This is not a perfect duality, because the normalization of energy scales with the transformation. Nevertheless, the ratios of the energies are the same, and the operator dimensions are preserved. Last, for real parameters > 1 or < 0 the scaling dimensions of one of the conformal primaries become complex, rendering the model unstable.

**G70.00324: Molecular dynamics simulation for collective phenomena in collisionless plasmas**  
RYUSUKE NUMATA (Presenter), YUTARO IKEHATA, University of Hyogo — Plasmas are constituted of many charged particles interacting via the long range Coulomb force, and exhibit various collective phenomena. To describe plasma dynamics, we usually utilize some theoretical models, such as fluid models, or kinetic models, depending on the scale we are focusing on. Those theories are developed by employing some coarse-graining assumptions. However, essentially, plasma dynamics can be understood by individual particle dynamics. Particle based simulations for macroscopic plasma dynamics are still computationally demanding, yet they become feasible (eg. [1]) thanks to the rapid growth of computation technology and simulation techniques.

In this work, we develop a molecular dynamics simulation code for collisionless plasmas using FDPS [2] (a framework for developing parralel particle simulation codes). The aim of this study is to demonstrate collective phenomena in plasmas, such as Debye shielding, waves, and Landau damping, from the first principle. This code will provide a useful tool to study multiscale nature of plasmas.


**G70.00325: The von Neumann and Double Slit Paradoxes Lead to a New Schrödinger Wave Mathematics**  
JEFFREY BOYD (Presenter), Retired — John von Neumann states a paradox. Why does measuring something disrupt the smooth Schrödinger wave, causing it to collapse for no mathematical reason? This paradox is embedded in the double slit experiment. When a dot appears on the target screen, how does that cause the Schrödinger wave to collapse everywhere else, faster than the speed of light? Von Neumann didn't follow his mathematics to its logical conclusion. If wave function collapse irreversibly changes reality, then the math is telling us that the timing and location of that event cannot be at the target screen. An event fitting that description happens only once: at the gun. A gunshot CAN change history. We propose a new mathematics of Schrödinger waves. Zero energy waves from the target screen pass backwards through the double slits and impinge on the gun prior to the gun firing. A particle randomly chooses one to follow backwards. The particle's choice of wave is proportional to the amplitude squared of that wave at the gun, determined by the superposition of the two waves moving backwards through the two slits. Why follow a wave of zero energy? Because Schrödinger waves convey amplitudes determining the probability density of that path.

*None*

**G70.00326: Effect of Electron-electron Scattering on Linear Conductivity for Graphene-like Band Structure**  
FERESHTEH MEMARIAN (Presenter), University of California, Merced, BEN YU-KUANG HU, Physics, University of Akron — We study theoretically the effect of electron-electron scattering on the electrical conductivity of two-dimensional materials with linear bands such as graphene, both with and without a perpendicular magnetic field. The Boltzmann transport equation was utilized, where phonon and impurity scattering are modeled using the relaxation-time approximation. In graphene-like materials with linear bands, for a constant relaxation time, the conductivity decreases as the temperature increases from absolute zero. Furthermore, in linear band materials, the electron-electron scattering also decreases the conductivity. This is in contrast to parabolic band materials, where the conductivity for a constant relaxation time does not depend on temperature or the electron-electron scattering rate. We also investigate the magneto-conductance for linear band materials in the absence and presence of electron-electron scattering.
G70.00327: Efficient Calculation of Lattice Thermal Conductivity by Molecular Dynamics Simulation: Role of Isobaric-Isothermal Relaxation and Potential Cutoff Distance

SANGWOO KWON (Presenter), WON BO LEE, Seoul National University — This work studied the Green-Kubo approach of calculating thermal conductivity with molecular dynamics (MD) simulation. In MD lattice thermal conductivity calculation, zero-pressure volume relaxation in the isobaric-isothermal (NPT) ensemble which determines lattice parameters, is often not included in standard procedure. Several MD simulations of fcc-based structures with different lattice parameters were performed to calculate lattice thermal conductivity and phonon density of states. The results were compared to experimental references and ab initio datas to suggest that NPT relaxation is crucial for accurate thermal conductivity calculation. Moreover, dependency between potential cutoff and lattice thermal conductivity in MD simulation was also studied. The results suggested that lattice thermal conductivity is not strictly dependent on potential cutoff distance, but exactly function of lattice parameters given by NPT relaxation. We concluded that properly reducing the cutoff distance can greatly improve computation cost of thermal conductivity calculation without sacrificing the accuracy.

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G70.00328: Electronic Band Structure of ZnO, CdO, MgO and related alloys

NICK BOECKER (Presenter), MACK ADRIAN DELA CRUZ, GARY PENNINGTON, Physics, Towson University — The electronic band structure of rocksalt CdO, ZnO, MgO and their ternary alloys are investigated using the empirical pseudopotential method and the virtual crystal approximation. This method is computationally efficient and highly advantageous when the band structure is needed on a very fine k-space mesh. A nonlocal pseudopotential correction with l = 2 symmetry is included for CdO and ZnO to account for the interaction between d and p electrons known in these materials. Additionally, an alloy compositional disorder potential term is included. Results are shown to agree well with known experimental band gap and band spacing energies. The cross over between direct and indirect minimum band gaps along with the conduction and valence band effective masses is studied for CdO, ZnO, MgO and their ternary alloys. Results have potential applications in optoelectronic devices.

*We acknowledge support from NSF grant DMR 1709781 and the Fisher General Endowment grant from the Jess and Mildred Fisher College of Science and Mathematics at Towson University.

G70.00329: Nonequilibrium Electric Current-induced Phonon Distribution in Microscale Metallic Structures

GUANXIONG CHEN (Presenter), SERGEI URAZHDIN, Emory University — The downscaling of modern electronic circuits places an increasing demand on the efficiency of heat dissipation. Electric current-induced heating is generally described in terms of Joule heating – an increase of phonon temperature due to the scattering of electrons on impurities and phonons. We experimentally demonstrate that this interpretation is not universally applicable to microscopic metallic structures. We study the current-dependent resistance R(I) in Pt nanowires. For a 7 μm-long nanowire, we observe a parabolic dependence R(I) at all temperatures T=5 K – 295 K, consistent with the Joule heating. A 1 μm-long nanowire exhibits a similar dependence at T=295 K. In contrast, we observe a singular piecewise-linear dependence at 5 K. As consequence, current-induced resistance increase is much larger than expected from Joule heating at small I, but smaller at large I. The linear dependence persists at modestly increased temperatures, but the singularity becomes broadened, reminiscent of common spectroscopic effects. Our observations are consistent with the non-thermal phonon distribution produced by electron scattering on impurities. The demonstrated effects provide an approach to characterizing and controlling thermal energy dissipation mechanisms.

*DOE grant DE-SC2218976
G70.00330: Ionization energies and excited state lifetime of charged defects in Two-dimensional Materials*  
YUAN PING (Presenter), TYLER SMART, Department of Chemistry and Biochemistry, University of California Santa Cruz, MARCO GOVONI, Institute for Molecular Engineering and Materials Science Division, Argonne National Laboratory, FENG WU, Department of Chemistry and Biochemistry, University of California Santa Cruz — Defects in 2D materials such as ultrathin h-BN have been found to be promising candidates for single-photon emitters and quantum bits. However, first-principles prediction of accurate defect properties in 2D materials remains challenging, mainly because of the highly anisotropic dielectric screening and strong many body interactions in 2D materials. In our previous work[1], we solved the numerical convergence issues for defect charge transition levels in 2D materials at both DFT and many body perturbation theory (MBPT) levels; in this talk we will compare different levels of theory and propose the fundamental principles to obtain reliable ionization energies of charged defects in 2D materials. Next, we will show preliminary results of radiative exciton recombination lifetime based on MBPT and phonon-assisted non-radiative recombination lifetime of defects in 2D materials. We compared different recombination processes between defect-defect and defect-band edge states for complex defects in monolayer BN. With our methods, we will design promising quantum defects that have deep defect levels, weak electron-phonon coupling and long excited state lifetime. [1] F. Wu et al, Phys. Rev. Mater. 1, 071001(R), (2017)

*National Science Foundation under grant No. DMR-1760260 and DMR-1747426

G70.00333: Ab-initio study of new, correlated color pigments*  
ANNA GALLER (Presenter), SILKE BIERMANN, Centre de Physique Théorique, Ecole Polytechnique — Conventional color pigments used in plastics, ceramics, paint or coatings often contain toxic heavy metals. Recently, the search for non-toxic and environmentally-benign alternatives has led to the experimental discovery of several new pigments, among them blue Y11-xMnxO3 and several rare-earth fluorosulfides. Here, we present first results of a theoretical study of these compounds by means of combined density functional and dynamical mean-field theory.

*FWF - Fonds zur Förderung der wissenschaftlichen Forschung (Austria)
G70.00334: Structural, vibrational, electrical and optical properties on Cr-doped LaAlO$_3$* ROMUALDO SANTOS SILVA JUNIOR, RAFAEL SILVA GONÇALVES, PETRUCIO BARROZO DA SILVA (Presenter), Physics Department, Federal University of Sergipe — The oxides with perovskite-type structure have been largely studied in last decades. This classes of materials show a large variety of properties such as ferroelectricity, superconductor, multiferroic, transparent conductor oxides among other properties. The perovskite compound LaAlO$_3$ has been used as a substrate in many applications. The high dielectric constant observed in this compound is ideal to reduce the loss of energy in devices working at high frequency. In this work, we will report the structural, vibrational, electric and optical of Cr-doped LaAlO$_3$ ceramics produced by combustion method. We observe a structural phase transition from rhombohedral to an orthorhombic structure with the increase of the Cr amount. It was possible to observe a reduction of the optical bandgap as well as a reduction of the resistivity of the compound. The Raman spectrum as a function of temperature reveals the nature of the structural transition in this compound. The change of the Cr amount can be used to produce new color pigments range from orange/yellow to green/blue.

*Thanks to Brazilian fund agencies CNPq and CAPES

G70.00335: Molecular influence on dynamic stiffening of synthetic polyurethanes through laser-induced supersonic microscale impact tests* YUCHEN SUN (Presenter), Chemistry, MIT, DAVID VEYSSET, Institute for Soldier Nanotechnologies, MIT, YOU-CHI MASON WU, Chemistry, MIT, ALEX J HSIEH, US Army Research Laboratory, RDRL-WMM-G, STEVEN E KOOI, Institute for Soldier Nanotechnologies, MIT, A A MAZNEV, Chemistry, MIT, JAN W ANDZELM, US Army Research Laboratory, RDRL-WMM-G, TIMOTHY M SWAGER, KEITH ADAM NELSON, Chemistry, MIT — High-strain-rate response is an important characteristic of protective elastomers. To discern the molecular influences on dynamic stiffening in polyurethane (PU), we synthesized two-component PUs from poly(tetramethylene oxide) (PTMO) and either hexamethylenediisocyanate (HDI) or 4,4'-methylenediphenyldiisocyanate (MDI). From dynamic mechanical analysis, HDI-PU displays semicrystallinity while MDI-PU appears amorphous. We also synthesized three-component PUs with the chain extender butanediol (BD) to introduce segmented hard domains. We performed supersonic microscale impacts with a laser-induced particle impact test in which a silica microsphere is accelerated up to ~1000 m/s. The impact is recorded with micron spatial resolution and nanosecond temporal resolution on an ultra-high-speed camera. In a velocity range of 50 to 1000 m/s, we show that MDI-PU exhibits greater dynamic stiffening than HDI-PU. We hypothesize that greater intermolecular hydrogen bonding in MDI-PU plays an important role. Finally, we discuss the role of segmented hard domains in dynamic stiffening of polyurethanes.

*This material is based upon work supported in part by the U. S. Army Research Office through the Institute for Soldier Nanotechnologies, under Cooperative Agreement Number W911NF-18-2-0048.

G70.00336: Anomal behavior of tellurium under pressure JAIME OLIVEIRA, Centro Brasileiro de Pesquisa Física, Rio de Janeiro, Brasil, MARCUS MOUTINHO, CARSTEN ENDERLEIN, Campus de Duque de Caxias, UFRJ, Rio de Janeiro, Brasil, ELISA BAGGIO-SAITOVOITCH (Presenter), Centro Brasileiro de Pesquisa Física, Rio de Janeiro, Brasil — Elemental tellurium is a small bad-gap semiconductor with a unique chiral crystal structure and a spin texture of the valence bands, which allows in-parallel current-induced magnetization of p-doped samples. Under pressure the band gap narrows and the structure of the valence band changes from a narrow camel-back close to the H-point to a single maximum with radial spin texture. Here, we present a theoretical and experimental study of the low-temperature behavior of the chemically extremely pure, but doped by vacancies, tellurium under pressure. We identify an anomaly at low temperatures, which is related to the orbital structure of the vacancy states and the respective spin texture. The pressure induced change of the valence band leads to the emergence of a change of the orbital structure of the vacancies, effectively leading to an exotic quantum critical point. At one side of the transition strong weak antilocalization is observed, which is consistent with our DFT-calculations, which show a change in spin texture.
G70.00337: Structural and dynamic properties of Fe\((1-x)S_x\) melts at core conditions* ALDEMAR DE MOYA CAMACHO (Presenter), Ciencias Naturales y Exactas, Universidad de la Costa, GUILLAUME MORARD, Institut de Minérologie, de physique de Matériaux, et de Cosmochimie, Sorbonne Université, CARLOS PINILLA, Universidad del Norte, Colombia — Earth’s core is subjected to conditions of 320-350 GPa and 5000-6500 K. The core is lighter than the density of pure iron by around 5% to 10%. In addition, the density jump between inner and outer core is 4.5%, being too large to be explained by simple solid-liquid phase transitions. Because of this, it has been suggested that the outer and inner core contain a percentage of light elements (5-10wt% and 2-3wt% respectively). These light elements affect processes from core’s dynamics to recrystallization of the inner core. One of the candidates to be part of the core is Sulphur. In this work, we used \(ab-initio\) Molecular Dynamic methods to study structural and dynamical properties of liquid Fe\((1-x)S_x\) alloys with S concentrations from 5.8 to 16wt%. We looked at the behavior of structural properties as a function of \(x\), \(P\) and \(T\) as well as to provide information on diffusion and viscosity coefficients. A P-V-T equation of state for melts whose S concentration falls within 5-10wt% is reported. We find density values in agreement with other theoretical and experimental results and show that concentrations between 10-12wt% of S agree with the densities expected for the outer core.

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G70.00338: Anisotropy in shock compression of different polymorphs of SiC* NILANJAN MITRA (Presenter), DIPAK PRASAD, Indian Institute of Technology Kharagpur — High hardness and melting point makes SiC an important ceramic material having wide application in defense industry. Typically, SiC utilized for armor and or other applications in defense is a polycrystal having different polymorphs and with numerous defects and thereby the properties of these materials have significant scatter. It can be quite anticipated that the response of the polymorphs of SiC exhibit significant differences in response. In this study anisotropy in shock Hugoniot response of SiC is shown not only amongst the different polymorphs but also between different orientations of the same polymorph. It is expected that this molecular dynamic study will lay the fundamental grounds explaining the scatter is experimental observations of SiC under different loading conditions. However, it should be noted that the study is only limited to considering pristine single crystal materials with no defects.

*None

G70.00339: Kinetic Monte Carlo Simulation of Oxygen Diffusion in Yttrium Monosilicate BRIAN GOOD (Presenter), NASA Glenn Research Center — Ceramic Matrix Composite (CMC) materials are of interest for use in next-generation turbine engines, offering a number of significant advantages, including reduced weight and high operating temperatures. However, in the hot environment in which such components operate, the presence of water vapor can lead to corrosion and recession, limiting the useful life of the components. Such degradation can be reduced through the use of Environmental Barrier Coatings (EBCs) that limit the amount of oxygen and water vapor reaching the component. Candidate EBC materials include Y and Yb mono- and disilicates. In order to better understand the diffusion of oxygen in such coatings, kinetic Monte Carlo computer simulations are performed for vacancy mechanism oxygen diffusion in Y monosilicate. Oxygen vacancy formation energies and migration barrier energies are computed using density functional theory, showing that all reasonably short migration paths involve relatively large barrier energies. In addition, the vacancy formation energies are relatively large as well, indicating that intrinsic vacancy concentrations will be small, leading to the conclusion that oxygen permeation associated with vacancy-mechanism oxygen diffusion will be small in this material.

G70.00340: An Atomistic Study of the Incorporation and Diffusion of Noble Gases in Silicate Minerals* CARLOS PINILLA (Presenter), ALFREDO LORA, Physics and Geosciences, Universidad del Norte, NEIL ALLAN, Chemistry Department, University of Bristol — Trace elements are widely used to unravel magmatic processes and constrain the chemical differentiation of the Earth. Central to this enterprise is understanding the controls on trace element fractionation between solid and liquid phases and thus the energetics of incorporating trace elements into crystals. In this contribution we focus on the incorporation of noble gases into crystals. We use \(ab-initio\) simulations to study the uptake of noble gases (He, Ne, Ar) into solid silicates. We calculate defect energies of incorporation both at vacancies and at interstitial positions in the solid and use these energies to estimate the total uptake of the noble gases into the crystal as a function of temperature. Such concentrations are found to be very low \((10^{-3} \text{ and } 10^{-10} \ \text{ppm})\) for He up to Ar respectively with the noble gases incorporated predicted to be more favorable at intrinsic vacancies or interstitials sites. We also look at the diffusion of these elements within the lattice and estimate activation energies for such processes. Our results support the hypothesis that noble gases have very low solubilities in bulk solid minerals.

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Complicated diffusions of dense hydrogen in accurately predicted liquid-liquid phase transition

JIAYU DAI (Presenter), ZENGXIU ZHAO, National University of Defense Technology, Department of Physics — We present results of extensive calculations of the liquid-liquid phase transition (LLPT) in dense liquid hydrogen by path-integral molecular dynamics simulations. The satisfactory nonlocal density functional rVV10 and the hybrid functional PBE0 are used to improve the description of electronic structure of hydrogen. Within density functional theory calculations, we report the best consistent results to the quantum Monte Carlo and coupled electron-ion Monte Carlo results so far of the LLPT in dense liquid hydrogen. The critical point at temperature between 1500 K and 2000 K is estimated according to the equation of state. Interestingly, we find that the self-diffusion coefficients of dense liquid hydrogen exhibit complicated behaviors in the vicinity of the transition point, which can be used as a criterion to diagnose the phase transition, and the first-order LLPT and metallization of dense hydrogen do not occur simultaneously.

WITHDRAWN ABSTRACT

A Stochastic approach to thermal DFT

YAEL CYTTER (Presenter), Chemistry, Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Israel, DANIEL NEUHAUSER, Department of Chemistry and Biochemistry, University of California Los Angeles, USA, ERAN RABANI, Chemistry, University of California and Lawrence Berkeley National Laboratory, USA, ROI BAER, Chemistry, Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Israel — Despite progress in observational astronomy, some elements such as the internal composition of planets are still not well-understood. A root cause is our limited understanding of matter under extreme conditions (MEC) - pressures in the GPa-TPa range and temperatures (T) up to $10^5$ K. Due to the difficulty in preparing MECs, the experimental input is limited, and ab initio calculations are sometimes the only source of information. The Kohn-Sham density functional theory (KS-DFT) seems as a reliable and useful tool for obtaining information on MEC. Calculations in finite temperatures, however, are expensive due to the large number of fractionally occupied KS orbitals involved. A stochastic method developed recently\cite{1},\cite{2}, appears to be a fitting approach to this problem. By performing a stochastic trace, the KS Hamiltonian is directly obtained from the density, resulting in a scaling of $T^{-1}$.

I will introduce the convergence and errors involved in calculations of the canonical free energy. In addition, a stochastic approach to calculate the Kubo-Greenwood conductivity will be presented.


External Electric Field Driving the Ultra-low Thermal Conductivity of Silicene

GUANGZHAO QIN (Presenter), MING HU, University of South Carolina — Manipulation of thermal transport (pursuing ultra-high or ultra-low thermal conductivity) is on emerging demands, since heat transfer plays a critical role in enormous practical implications, such as efficient heat dissipation in nano-electronics and heat conduction hindering in solid-state thermoelectrics. It is well established that the thermal transport in semiconductors and insulators (phonons) can be effectively modulated by structure engineering or materials processing. However, almost all the existing approaches involve altering the original atomic structure, which would be frustrated due to either irreversible structure change or limited tunability of thermal conductivity. Motivated by the inherent relationship between phonon behavior and interatomic electrostatic interaction, we comprehensively investigate the effect of external electric field, a widely used gating technique in modern electronics, on the lattice thermal conductivity ($k$). Taking two-dimensional silicon (silicene) as a model system, we demonstrate that, by applying electric field ($E_z = 0.5 \, \text{V/Å}$) the thermal conductivity of silicene can be reduced to a record low value of $\sim 0.091$ W/mK. Our study paves the way for robustly tuning phonon transport in materials without altering the atomic structure.

QUANTUM INFORMATION, CONCEPTS, AND COMPUTATION
**G70.00346: Yield Analysis of Superconducting Qubit Fabrication in KRISS**

GWANYEOL PARK (Presenter), Korea University Sejong Campus & KRISS, JIMAN CHOI, University of Science and Technology (UST) & KRISS, GAHYUN CHOI, Ulsan National Institute of Science and Technology (UNIST), SOON-GUL LEE, Korea University Sejong Campus, KIBOG PARK, Ulsan National Institute of Science and Technology (UNIST), WOON SONG, Korea Research Institute of Standards and Science (KRISS), YONUK CHONG, Korea Research Institute of Standards and Science (KRISS) & UST — In order to achieve scalable quantum circuits, large-scale qubit fabrication capability is essential. We have been working on superconducting transmon qubits, and in this study we will present our process' yield analysis on our wafer-scale qubit fabrication. Our qubit fabrication uses 3 inch wafers, either sapphire or silicon, and tunnel junctions are made by two-angle evaporation using the Dolan bridge. We checked the tunnel resistances on the wafer at room temperature and we typically get 5 to 6% standard deviation across the wafer. For targeting, we usually get resistance within 10% of the target value. We also have a couple of outliers on the wafer, typically less than 5 out of ~100 junctions, in which we need improvements. There are many control parameters to improve the yield and spread, so in the end we will discuss the substrate cleaning, e-beam patterning, deposition and oxidation conditions, which are to be controlled tightly in order to get a robust large scale fabrication process of the Josephson junctions.

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**G70.00347: Superconducting qubit-qutrit circuit: A toolbox for efficient quantum gates**

THOMAS BÆKKEGAARD (Presenter), LASSE BJØRN KRISTENSEN, NIELS JAKOB LOFT, Department of Physics and Astronomy, Aarhus University, CHRISTIAN KRAGLUND ANDERSEN, Department of Physics, ETH Zurich, DAVID PETROSYAN, Institute of Electronic Structure and Laser, FORTH, NIKOLAJ T ZINNER, Department of Physics and Astronomy, Aarhus University — We propose a superconducting circuit which implements an effective tunable spin chain consisting of a qutrit (three-level system) coupled to two qubits (spin-1/2). In our paper [1] we show the derivation leading to an effective spin-model system which has highly tunable qutrit energy levels and Heisenberg XXZ-like interactions between the three effective degrees of freedom.

Our system can very efficiently accomplish various quantum information tasks, including entanglement of the two qubits and conditional three-qubit quantum gates such as the Toffoli and Fredkin gates. Furthermore, our system realizes a double-conditional non-adiabatic holonomic quantum gate.

The efficiency, robustness, and universality of our circuit makes it a promising candidate to serve as a building block for larger spin networks capable of performing involved quantum computational tasks.

We are currently working on a system implementing two qutrits, realizing an effective AKLT spin model.


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**G70.00348: Enhancement in the cross-resonant gate performance**

XUEXIN XU (Presenter), MOHAMMAD H. ANSARI, Peter Grünberg Institute, Forschungszentrum Julich — In this poster we describe how the performance of two qubit gates in a superconducting circuits made of capacitive shunted flux qubits and transmons sharing interaction with a bus resonator, can get boosted up as the direct result of capacitive direct coupling between the qubits. For this aim we consider circuit parameters that allow small capacitive coupling between qubits and after quantizing the circuit Hamiltonian within the dispersive regime we make comparison the gate performance with a typical all transmon circuit.
G70.00349: Hole spins in Ge/Si nanowires  FLORIAN NM FRONING, MIRKO REHMANN, Physics, University of Basel, J RIDDERBOS, Physics, University of Twente, MATTHIAS BRAUNS, Physics, Institute of Science and Technology, FLORIS ZWANENBURG, Physics, University of Twente, ANG LI, Physics, Beijing University of Technology, ERIK P. A. M. BAKKERS, Physics, TU Eindhoven, DOMINIK ZUMBUHL, FLORIS BRAAKMAN (Presenter), Physics, University of Basel — Single hole spins confined in quantum dots (QDs) in Ge/Si core/shell nanowires (NWs) combine several properties which make them potentially very unique qubits. The natural abundance of non-zero nuclear spins in both Si and Ge is small and can be further reduced to a negligible amount by isotopic purification. Furthermore, hole spins have no contact hyperfine interaction due to their p-type wavefunction. These properties make hole spin qubits in Si and Ge resilient against dephasing via interaction with nuclear spins.

A particularly promising feature of hole spins in Ge/Si core/shell NWs is the nature of spin-orbit interaction (SOI) in this system. Confinement to one dimension gives rise to an SOI in the valence band, which is predicted to be both strong and electrically tunable. This promises electrical gating of the SOI, allowing to switch to a large SOI for high interaction strengths and fast quantum operations, or to turn off SOI for increased qubit coherence.

We demonstrate and characterize single, double and triple QD arrays in Ge/Si NWs, all with low hole occupation numbers. In the double QD configuration, we observe Pauli spin blockade and see indications of a sizeable SOI causing spin flips. Finally, we report progress towards electrically tuning the SOI.

G70.00350: Emission of entangled photons via the biexciton formation and decay in core/shell nanoplatelets  MATTHEW OTTEN, XUEDAN MA, CNM, Argonne National Lab, PATRICK SERAFIN, GERMAN KOLMAKOV (Presenter), Physics, New York City College of Technology, STEPHEN K GRAY, CNM, Argonne National Lab — Quasi-two-dimensional nanoplatelets (NPLs) possess fundamentally different excitonic properties from zero-dimensional quantum dots including exceptionally narrow spectral features and large lateral carrier mobility. We numerically study carrier dynamics of individual CdSe/CdS NPLs in an optical microcavity and find the emitted photon statistics using the density matrix formalism. We find that, due to formation of biexcitons in an NPL and their subsequent decay, the emitted pairs of cavity photons are entangled at temperatures below 20 K. Under favorable conditions the photon pair can be nearly maximally entangled with the relative photon pair population ~0.5. We also show that second-order photon correlation (g(2)) can be used as a measure of the photon pair entanglement. At temperatures higher than 20 K, the photon entanglement is suppressed due to dephasing caused by thermal fluctuations. Finally, we discuss possible experiments, in which the NPL generated photon pair entanglement can be observed, as well as potential applications in integrated quantum photonics.

G70.00351: State Recognition of qubits in Two-Dimensional Quantum Dots Arrays with Machine learning  ALI RAD (Presenter), Physics, University of Maryland, College Park — Application of quantum dot is not limited to a one-dimensional array. For the purpose of quantum computation, we need to deal with a two-dimensional array of quantum dots. The technical difficulty of large-scale and higher dimensional arrays of quantum dots lies a the grow of parameter space substantially with the number of qubits. fortunately, we are able to use machine learning techniques to recognize the pattern of dots and find the tune parameters more efficiently.

G70.00352: Measurement and advances in hybrid quantum system with P1 centers and superconducting qubits  ZHILING WANG (Presenter), TIANQI CAI, XIYUE HAN, IIS, Tsinghua University, MAODONG GAO, Department of Physics, Tsinghua University, HONGYI ZHANG, YIPU SONG, LUMING DUAN, IIS, Tsinghua University — A hybrid quantum system which contains spin ensembles, superconducting resonators and superconducting qubits, has been proposed as a way to realize quantum computer. In the first part of this poster, we coupled substitutional nitrogen centers (P1 centers) in diamond to a superconducting resonator with Zeeman effect. We observed a fast relaxation of spin population on the millisecond scale, which is much faster than the intrinsic spin longitudinal relaxation of P1 centers. By pump-probe experiments we attributed this process to a cross relaxation among different hyperfine splitted spin subensembles. In the second part, we demonstrate iSWAP gate and CR gate by using a 5-qubit quantum processor. The qubit anharmonicity is enhanced by using a parallel capacitor, meanwhile the qubit is still operated in transmon regime. Furthermore, we have proposed a new architecture of scalable superconducting qubits based on ring network structures. This design can efficiently avoid breakpoints of superconducting patterns and significantly improve the robustness of intra-connections of qubits. We will demonstrate a quantum processor based on this architecture, to implement a fault-tolerant operating scheme with fourteen transmon qubits, which support reliable logical qubits and universal gates.
G70.00353: Heralded Bell State of Dissipative Qubits Using Classical Light  XIN ZHANG (Presenter), HAROLD U BARANGER, Duke University — Maximally entangled two-qubit states (Bell states) are one of the most exotic states in the quantum world and have important applications from testing quantum foundations to quantum information processing. Here we show that a Bell state can be generated using classical light by coupling two qubits to a one-dimensional (1d) waveguide. Even though the steady state of the qubits is a trivial product state with no coherence or entanglement, continuous monitoring unravels the steady state nontrivially such that a Bell state is generated in its trajectories and heralded by a reflected photon. This provides a particularly sharp illustration that information gained by measuring an open quantum system can affect its physical state and lead to surprising and useful results. Further, the specific role of information in our system is explored by including imperfect photon detection as a source of information loss.

G70.00354: Floquet-engineered quantum state preparation in a noisy qubit  ERIC BOYERS (Presenter), MOHIT PANDEY, DAVID K CAMPBELL, ANATOLI S POLKOVNIKOV, Department of Physics, Boston University, DRIES SELS, Department of Physics, Harvard University, ALEXANDER SUSHKOV, Department of Physics, Boston University — The ability to manipulate quantum states is important to many areas of quantum science including quantum simulation and computation. Adiabatic evolution is a common strategy for preparing quantum states, but it is slow and susceptible to decoherence. Existing methods for speeding up adiabatic evolution require complex multi-qubit gates or are difficult to construct for many-qubit systems. Our approach for constructing approximate fast-forward (FF) protocols uses the tools of Floquet engineering utilizing only the interactions in the original Hamiltonian. We apply this approach to a two level system and demonstrate it experimentally using the electronic spin of a Nitrogen-vacancy center in diamond. We show that our Floquet-engineered FF protocol performs comparably to the conventional FF protocol, achieving target state preparation with an upper bound on infidelity (1-F) of 0.01 at the 1σ level. We study the performance of our protocol when external noise acts on the qubit and find that it is significantly more robust than the conventional FF protocol.

G70.00355: Quantum interpolation for digital quantum simulation  JORDAN HINES (Presenter), Physics, Massachusetts Institute of Technology, YI-XIANG LIU, Nuclear Science and Engineering, Massachusetts Institute of Technology, ASHOK AJOY, University of California Berkeley, PAOLA CAPPELLARO, Nuclear Science and Engineering, Massachusetts Institute of Technology — Quantum simulation enables understanding complex dynamics with experimentally implementable dynamics. Digital quantum simulation enabled by Trotter expansion finds many applications due to its flexibility and universality. However, Trotter expansion higher than second order requires complicated coefficients that are hard to implement in experiment. Here we present Quantum Interpolation, a new exponential product second order approximation of exponential operators, motivated by realistic experimental limitations. We show that Quantum Interpolation has higher fidelity than the most commonly used second order Trotter expansion without any complicated coefficients. We also present the application of Quantum Interpolation in nano nuclear magnetic resonance imaging.

G70.00356: Spooky Action at a Distance is Not Spooky—It Is Knowledge: Combining Entanglement And Negative Observation To Show How The Einstein-Podolsky-Rosen Experiment Works, Not Just How It Doesn't Work  DOUGLAS SNYDER (Presenter), independent research — EPR considered positive measurement (where there is a physical interaction between the measuring device and the particle measured). EPR did not consider that knowledge is responsible for the effect of one of the entangled particles on the other entangled particle. If they had considered negative measurement (where there is no physical interaction between a measuring device and the particle measured), they would have deduced that knowledge is responsible for the effect of a negative measurement on one particle on the other particle. They would have seen that knowledge is also responsible in the case of positive measurements, that the essence of a positive measurement is that it supplies information just as negative measurements do. A sample experiment has been presented to show how the above points work in practice. Implications for the relationship between knowledge and reality are presented. The term “reality” is substituted for “physical reality” since physical reality is not independent of knowledge.
G70.00357: Does Unitarity Necessitate That an Entanglement Cannot be Destroyed Until a Measurement of 1 of the Entangled Particles is Made? The Answer Is No.  DOUGLAS SNYDER (Presenter), none, independent — The generally held view is that an entanglement of two particles cannot be broken until a measurement is made on one of the entangled particles. One reason given for the above thesis is unitarity. Great empirical evidence does indicate the importance of unitarity in the evolution of the wave function itself and also for the mathematical processes for making a measurement prediction. Both unitarity in wave function evolution before measurement and also the mathematical processes for making measurement predictions are supported by great empirical evidence. The view of entanglement that it cannot be broken until a measurement is made on one of the entangled particles is an extension of the view that a wave function is not destroyed until a measurement associated with the wave function is made. It is proposed that one lose or destroy an entangled particle and any which-way information the particle holds (and that the particle supplies to the other entangled particle before any measurements are made) through the use of a large system interacting with the particle to be destroyed. Whether or not the entangled particles is destroyed in the manner noted is correlated to different distributions of the other entangled particle.

G70.00358: A single-world consistent interpretation of quantum mechanics from fundamental time and length uncertainties  LUIS PEDRO GARCIA-PINTOS (Presenter), University of Massachusetts Boston, RODOLFO GAMBINI, Instituto de Fisica, Universidad de la Republica, JORGE PULLIN, Louisiana State University - Baton Rouge — Within unitary quantum mechanics there exist global protocols that allow to verify that no definite event ---an outcome to which a probability can be associated--- occurs. Instead, states that start in a coherent superposition over possible outcomes always remain as a superposition. We show that, when taking into account fundamental errors in measuring length and time intervals, that have been put forward as a consequence of a conjunction of quantum mechanical and general relativity arguments, there are instances in which such global protocols no longer allow to distinguish whether the state is in a superposition or not. All predictions become identical as if one of the outcomes occurs, with probability determined by the state. We use this as a criteria to define events, as put forward in the Montevideo Interpretation of Quantum Mechanics, analizing in detail the occurrence of events in the case of a particle in a superposition of two different locations. We argue that our approach provides a consistent (C) single-world (S) picture of the universe, thus allowing an economical way out of the limitations imposed by a recent theorem by Frauchiger and Renner showing that having a self-consistent single-world description of the universe is incompatible with quantum theory.

G70.00359: Review Article on Quantum Entanglement & Growing Quantum Information  ADITYA CHINCHOLE (Presenter), ELECTRONICS AND TELECOMMUNICATION, YESHWANTRAO CHAVAN COLLEGE OF ENGINEERING,NAGPUR,INDIA, SHUBHAM REDDY, Computer Science and Engineering, Ramdeobaba College of Engineering & Management, Nagpur, India — This paper presents the study on quantum entanglement till date, its applications and the research going on in the quantum communication field. It highlights the work on quantum Satellite "Micius" and the future scope of quantum communication. Quantum Information science is also discussed broadly. EPR paradox and Bell inequalities, quantum measurement theory and conceptual work in quantum interpretations mainly many worlds interpretation and Niels Bohr’s copenhagen interpretation are also covered. Future applications of the quantum entanglement including the quantum computers is displayed in this paper.

G70.00360: Universe’s Order Based on the Quantum Disorder  HASSAN GHOLIBEIGIAN (Presenter), AmirKabir University of Technology — One of the central challenge in physics is to understand how the ordered systems in macro scales in the universe can arise and how these systems can be characterized from disordered quantum systems in depth of the matter. In other words, how the quantum confuse systems are transformed to the macro scale ordered systems which we see in our daily life in the universe.

If the universe is a symphony of fundamental particles (vibrating strings), how is led this symphony orchestra?

On the other hand, the life need to the ordered systems for its evolution. In this way, it seems that, transformation of disordered quantum systems to the large scale ordered systems should be led by communication of information process. Because, fundamental particles need to know their next quantum states. In this process, fundamental particles get packages of information by sub-particles (quantum soft particles) from dimension of information for analysis and drawing the road map of the quarks.

It seems these are four sub-particles of mater, plant, animal and human in substructure of each quark as the origins of the life and cause of differences between spins of those elementary particles.[Gholibeigian, 2015 APS. APR. L1027G].

G70.00361: Counterfactual Assessment of The Quantum Zeno Effect  ONOFRIO RUSSO (Presenter), OKTAY H GOKCE, New Jersey Institute of Technology — We consider counterfactual measurements of the decay process for an unstable quantum mechanical system. In particular, there is a region during the decay process for which frequent observations or measurements of the initial decay states result in a delay in the decay time. The phenomenon is referred to as the quantum Zeno effect. We contend that this can be achieved counterfactually.
Subsequently, we use a generalized Wilson-loop order-parameter, namely, the equal-time Fredenhagen-Marcu order parameter, to distinguish between the different phases. Furthermore, we calculate perturbatively the energy gap of the toric code in the presence of Cooper-pair tunneling. Our results are relevant for the current efforts to experimentally realize the Majorana toric code.

* A.R. acknowledges the support of the Alexander von Humboldt foundation.

In this mapping, a successful decoding of the error syndrome of the TQC corresponds to a certain phase of the corresponding SPM. The error-correction performance of several TQC-s have been analyzed using Monte Carlo (MC) simulations.

We, on the other hand, use high-temperature series expansion to analyze the decoding performance of the toric code. In contrast to zero temperature simulations, which estimate the threshold of the minimum-weight perfect-matching decoder, our method naturally provides an estimate of that of the maximum-likelihood decoder. First, we analyze the phase diagram of the 2D random-bond Ising model to a higher order than previously performed. Our results provide an estimate of the decoding threshold of the toric code in absence of measurement imperfections. We compare our result to those obtained by MC simulations and network model analysis. Then, we perform the analysis of the free-energy and the Wilson loop order parameter in the 3D Ising gauge theory in the presence of quenched disorder. The latter model describes the decoding of the toric code subject to measurement errors.

*AR is funded by the Huboldt Foundation. NPB is a UCLQ Fellow at UCL.

We developed the mathematical framework for extending Harlow’s results to the more physical case where a Von Neumann algebra on the bulk, but assumes a simple tensor product structure on the boundary Hilbert space. In this work, we developed the mathematical framework for extending Harlow’s results to the more physical case where a Von Neumann algebra is also given on the boundary CFT. We showed that the resulting code more accurately captures the properties of AdS/CFT.

G70.00365: Quantum machine learning for electronic structure calculations* RONGXIN XIA (Presenter), Department of Physics and Astronomy, Purdue University, SABRE KAIS, Department of Chemistry, Department of Physics and Astronomy and Birck Nanotechnology Center, Purdue University — Considering recent advancements and successes in the development of efficient quantum algorithms for electronic structure calculations—alongside impressive results using machine learning techniques for computation—hybridizing quantum computing with machine learning for the intent of performing electronic structure calculations is a natural progression. Here we report a hybrid quantum algorithm employing a restricted Boltzmann machine to obtain accurate molecular potential energy surfaces. By exploiting a quantum algorithm to help optimize the underlying objective function, we obtained an efficient procedure for the calculation of the electronic ground state energy for a small molecule system. Our approach achieves high accuracy for the ground state energy for H2, LiH, H2O at a specific location on its potential energy surface with a finite basis set. With the future availability of larger-scale quantum computers, quantum machine learning techniques are set to become powerful tools to obtain accurate values for electronic structures.

*Sabre Kais and Rongxin Xia are grateful for the support from Integrated Data Science Initiative Grants, Purdue University.
G70.00366: Quantum Linear Regression With Regularization  XIAOKAI HOU (Presenter), XI HE, CHUFAN LV, DINGDING WEN, XIAOTING WANG, University of Electronic Science and Technology of China — The problem we are trying to solve in this article is how to execute linear regression algorithm with regularization based on quantum mechanics system. In the field of machine learning, linear regression is a powerful tool modeling input and output variables using the least squares function of linear equations. And regularization is a technical method to solve the overfitting phenomenon which can be caused when the training data is lack or not universal. The approach we mainly adopt to transform classical linear regression to quantum version is to construct Hamiltonian containing the training data information. And via HHL algorithm and swap test, we can accomplish the training process and also make a prediction with input variable state. Compared with classical analogue, the quantum linear regression algorithm demonstrates quadratic speed up.

G70.00367: Decomposable Coherence and Quantum Fluctuation Theorems*  ERICK HINDS MINGO (Presenter), Imperial College London, DAVID JENNINGS, Physics, University of Leeds — How can one define work on a quantum system without requiring the existence of a classical agent manipulating macroscopic equipment? To answer this question, we formulate the problem as can be done in Newtonian mechanics - by introducing a `weight system' with strict global energy conservation. By allowing a system in an arbitrary pure quantum state to interact with a weight system prepared in a well defined state, we are able to study the structure of `coherent energy transfers'. We then define a coherent work process and show that this is related to the notion of decomposability of a classical random variable. Maintaining the nomenclature, we introduce the notion of decomposable coherence. Furthermore, we show that coherent work processes can only map coherent states to coherent states, and they become classical work processes in a conservative potential as h goes to 0.

We then relate this framework to recent work in the study of quantum fluctuation theorems [1,2]. We find an induced definition of coherent work consistent with the previous framework. Furthermore, we show that entanglement generation is exponentially more probable than de-correlating dynamics.


*EPSRC - Centre for doctoral training.

G70.00368: An iterative variational algorithm for optimization on near-term quantum devices  OMID KHOSRAVANI (Presenter), Georgia Institute of Technology — Hybrid quantum-classical optimization algorithms have recently attracted interest for applications in the noisy intermediate-scale quantum devices (NISQ) era of quantum computing. However, as it has been recently shown by Jarrod McClean et. al. (arXiv:1803.11173v1), many such algorithms could suffer from the issue of Barren Plateaus even at shallow depth circuits, which corresponds to the phenomenon of vanishing of gradients in training classical deep neural networks. Here we introduce a variational method which restricts the entropy of the batch Hamiltonian per circuit complexity and propose an algorithm that attempts to avoid this issue by iteratively recombining the solutions while approaching an optimal solution. Finally we compare the performance of our algorithm with existing variational and quantum approximate optimization algorithms.

G70.00369: Separating Quantum and Classical Entropies: A unified treatment of quantum and classical information  AMRO DODIN (Presenter), ADAM P. WILLARD, Massachusetts Institute of Technology — Information in open quantum systems can be influenced by the presence of classical and quantum sources of uncertainty, complicating the quantification of the information encoded in such systems. By considering classical distributions on quantum state space, quantum and classical uncertainty can be separated, allowing for the simultaneous treatment of quantum (von Neumann) and classical (Shannon) entropies. In this presentation, a method for simultaneously quantifying quantum and classical entropies of quantum ensembles will be presented and the manner in which quantum operations (e.g. measurements and dynamical channels) transform one form of entropy into another will be discussed.
Superadiabatic quantum friction suppression in finite-time thermodynamics

SHUJIN DENG, East China Normal University, AURELIA CHENU, Los Alamos National Laboratory, PENG PENG DIAO, FANG LI, SHI YU, East China Normal University, IVAN COULAMY, Universidade Federal Fluminense, ADOLFO DEL CAMPO (Presenter), University of Massachusetts Boston, HAIBIN WU, East China Normal University — Optimal performance of thermal machines is reached by suppressing friction. Friction in quantum thermodynamics results from fast driving schemes that generate nonadiabatic excitations. The far-from-equilibrium dynamics of quantum devices can be tailored by shortcuts to adiabaticity to suppress quantum friction. We experimentally demonstrate friction-free superadiabatic strokes with a trapped unitary Fermi gas as a working substance and establish the equivalence between the superadiabatic mean work and its adiabatic value.


Optimal Quantum Approximate Optimization Algorithm: Success Probability and Runtime Dependence on Circuit Depth

MURPHY YUEZHEN NIU (Presenter), Physics, Massachusetts Institute of Technology, SIRUI LU, Physics, Tsinghua University, ISAAC CHUANG, Physics, Massachusetts Institute of Technology — Due to its simplicity, universality and optimality, quantum approximate optimization algorithm (QAOA) has been considered a useful near-term algorithm for conducting classical optimization and quantum simulation. We answer an open question of how the success probability and runtime of QAOA depend on the quantum circuit depth by focusing on a specific problem: state transfer in one-dimensional spin chain. We provide an analytic proof on the success probability scaling by leveraging the spectral property of the XY Hamiltonian. We show both analytically and numerically a Grover like quadratic dependence on the circuit depth in the short circuit depth limit and an exponential scaling in the large circuit depth limit. We prove the perfect state transfer needs $O(N)$ time using Lieb-Robinson bound for a spin chain of length $N$ and confirm this numerically.

Locally accurate matrix product state approximations with constant bond dimension for ground states of gapped 1D models

ALEXANDER DALZELL (Presenter), FERNANDO BRANDAO, Caltech — The numerical success of the DMRG method has been explained by the observation that it can be recast as a variational algorithm over the set of matrix product states (MPSs) with a specified bond dimension. The bond dimension need only increase like a polynomial in the number of sites on the 1D chain to guarantee that some element of the MPS manifold represents a good approximation to the ground state of a given gapped local Hamiltonian. But DMRG is often successful even for very small values of the bond dimension. We provide a partial justification for this success by showing that the MPS bond dimension may be kept constant as the number of sites increases if one desires an approximation that is good only in a local sense, that is, the reduced density matrix of the true ground state is close to that of the approximating MPS when all but a constant segment of the chain is traced out. While a similar result was known for matrix product operator (MPO) approximations, MPSs are superior to MPOs as an ansatz for variational algorithms since verifying that a certain MPO is positive (and thus represents a valid quantum state) is difficult, whereas MPSs do not have this issue.

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G70.00373: Quantum enhanced metrology with noise assistance and error correction  
YU CHEN (Presenter), HAI-DONG YUAN, Mechanical and Automation Engineering, The Chinese University of Hong Kong — Quantum metrology has seen various important applications in science and engineering, ranging from atomic frequency estimation to gravitational wave detection. It has been shown that quantum resources can outperform their classical counterparts as regard to improving the precision of parameter estimation. However, there is inevitable difficulty in manipulating a quantum system because the system keeps leaking out information to the environment that it is coupled to, making superiority brought by the "quantumness" disappear beyond decoherence time. Therefore, it is critical to protect the system from noise, which can be achieved by means of adding control signals.

Most of the previous work has a focus on time-invariant parameter-independent Hamiltonian and noise. By contrast, in this paper we provide a sufficient and necessary condition under which one can employ control to recover the Heisenberg precision limit for systems with time-invariant parameter-dependent Hamiltonian and noise. We further consider the case where both Hamiltonian and noise are time-varying and parameter-dependent. We show a detailed technique via quantum error correction to harvest, or even beat the optimal quantum Fisher information in the noiseless case.

G70.00374: Dark matter search with the Cosmic Axion Spin Precession Experiment (CASPeR)  
DENIZ AYBAS (Presenter), Department of Physics, Boston University — The nature of dark matter is an open question in fundamental physics. The Cosmic Axion Spin Precession Experiment (CASPeR) is a laboratory scale search for the axion as a dark matter candidate [D. Budker, et al., Phys. Rev. X 4, 021030]. The range of axion-like dark matter masses to which CASPeR is sensitive extends from feV to μeV with sensitivity beyond current astrophysical limits. CASPeR uses Nuclear Magnetic Resonance (NMR) techniques and precision magnetic sensors, such as Superconducting Quantum Interference Devices (SQUIDs). The current status and preliminary results of CASPeR will be presented.

G70.00375: Josephson Metamaterial with a Tunable Kerr Constant*  
MATTHEW BELL (Presenter), WEN TING HSIEH, University of Massachusetts Boston — Superconducting circuits rely heavily on the non-linearity inherent in Josephson Junctions. The magnitude of this nonlinearity can be set either at fabrication or tuned with a superconducting quantum interference device (SQUID). Generally, the sign of the Kerr coefficient in the cosine energy phase relation for Josephson junctions cannot be tuned. Here we will present a unit cell design of a metamaterial which allows the Kerr coefficient to be tuned over a wide range in magnitude and can even change sign from positive to negative. Experimental results will be presented showing agreement with theory for the Josephson chain. We will also demonstrate how this metamaterial can be applied to recent efforts in realizing large superinductors and efficient traveling-wave parametric amplifiers (TWPA), two applications which have heavily relied on series arrays of Josephson junctions.

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G70.00376: Practical algorithm for determining Hamiltonian identifiability*  
XIAOYANG HUANG (Presenter), Physics, Massachusetts Institute of Technology, ROBERTO GAUNA, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, AKIRA SONE, PAOLA CAPPELLARO, Nuclear Science and Engineering, Massachusetts Institute of Technology — We demonstrate a practical algorithm for determining the identifiability of Hamiltonian parameters with local accessibility. We consider the problem of estimating the parameters of the Hamiltonian of one-dimensional spin chain systems with nearest-neighbor interaction and assume that we only have access to a single quantum probe coupled to the target system. We demonstrate a practical implementation of Hamiltonian identifiability by the eigensystem realization algorithm and Gröbner basis. Furthermore, we also provide a practical code to estimate the Hamiltonian parameters from the experimental results. XH and RG equally contributed to this work.

*This work was supported in part by the U.S. Army Research Office through Grants No. W911NF-11-1-0400 and W911NF-15-1-0548 and by the NSF PHY0551153. AS acknowledges Thomas G. Stockham Jr. Fellowship.
G70.00377: Room-Temperature Quantum Non-Demolition Measurement Enhanced by Machine Learning  
MO CHEN (Presenter), YI-XIANG LIU, PAOLA CAPPELLARO, Massachusetts Institute of Technology — Projective measurements of qubits are a key resource for quantum computation. For qubits based on Nitrogen-Vacancy centers in diamond at room-temperature, projective measurement has been achieved using quantum non-demolition measurement schemes enabled by an ancillary qubit. In this scheme, the nuclear spin (qubit) state is repetitively read out by a mapping to the NV electronic spin (ancillae) until the photon number distribution from one qubit state is distinguishable from the other in a single shot. High readout fidelity requires a few to tens of thousands of repetitive readouts. This, unfortunately, imposes a heavy time overhead to any quantum algorithms. The readout time is on the same order of the decoherence time of the best physical qubit in the system, preventing feed forward protocols. In this work, we describe a method to improve the single shot readout fidelity using machine learning with information already recorded, but traditionally discarded in the experiment. Hence, our method does not impose an additional experimental time penalty. Combined with photonic structures that enhance photon collection efficiency, we expect this technique will enable room-temperature feed forward quantum information processing.

G70.00378: Integrated Fibre Detection Architectures for Distributed Quantum Magnetometry*  
CHRISTOPHER FOY (Presenter), SHAI MAAYANI, DIRK R. ENGLUND, YOEL FINK, Massachusetts Institute of Technology — Distributed magnetic sensing over large distances is of interest for a diverse range of applications including remote detection of ferrous metals, geophysics, and biosensing. Unfortunately, the capability to measure magnetic fields over large distance is unrealized. Here, we address this problem by introducing a diamond spin magnetometer directly embedded into an optical fibre alongside high-performance optoelectronic devices. Our magnetometer relies on the translation of an ensemble of nitrogen vacancy (NV) centers in micro-diamonds within a microfluidic channel. The NV's spin-dependent fluorescence is detected by embedded Si photodiodes. This device allows for distributed magnetic field measurements along a 300 meter-long fibre with a DC sensitivity of 81 nT Hz-1/2. We will discuss next steps and the deployment of this technology. 

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G70.00379: Single-photon switching inside a polarizatcavityion-selective*  
JEREMY FLANNERY (Presenter), MICHAL BAJCSY, University of Waterloo — We propose a scheme for single-photon switching that employs the phenomenon of vacuum induced transparency (VIT) and an ensemble of a three-level atoms in a polarization-selective cavity. In this system, light of one polarization (H) couples to one of the atomic transitions with high single-atom cooperativity, while the orthogonal polarization (V) couples to the other atomic transition. When both a weak probe and the cavity mode are resonant with their respective transitions, the otherwise opaque system becomes transparent to the probe through VIT. By setting the cavity mode and probe field far detuned, the regime of a Raman two-photon absorption (TPA) is reached, however because we use a vacuum cavity mode, this may be referred to as a vacuum induced Raman absorption (VIRA). The benefit of this regime is that the resonance condition for the VIT, allowing for full transmission, and the VIRA, resulting in a large absorption, can be very close in frequency. We exploit this by setting the probe photon on the VIRA resonance. The optical switch can then be opened by injecting a single photon into the cavity mode, shifting the VIRA resonance such that the probe field is instead at the VIT resonance, allowing for large transmission. 

*Industry Canada, NSERC's Discovery grant., OGS.

G70.00380: Time-resolved probing of many-body states in circuit-QED systems  
KIRILL SHULGA (Presenter), RIKEN Center for Emergent Matter Science, IHOR VAKULCHYK, MIKHAIL FISTUL, Center for Theoretical Physics of Complex Systems, Institute for Basic Science (IBS), YASUNOBU NAKAMURA, RIKEN Center for Emergent Matter Science — Circuit-QED quantum simulators based on superconducting circuits provide a tool to study many-body phenomena in strongly interacting qubit systems. In this work, we perform experimental studies of time-resolved dynamics of superconducting qubit arrays embedded in a superconducting resonator. We demonstrate an occurrence of many-body Rabi oscillations and complex dynamics in the dispersive and the resonant regimes. At variance with single qubit Rabi oscillations, the many-body Rabi oscillations emerge as the amplitude of applied microwave pulse exceeds the critical value. The magnetic field tunable crossover between many-body and single particle Rabi oscillations is obtained. We also experimentally explore a possibility to realize a time crystalline order in an array of superconducting qubits by applying periodic sequence of pulses with excitation of nonequilibrium states in the system.
G70.00381: Fast dispersive, Purcell-filtered measurement and reset using smooth and simple analytic pulse shapes
LUKAS F BUCHMANN, FELIX MOTZOI (Presenter), Aarhus University, CHRISTIAN DICKEL, TU Delft — We present a dispersive, measurement pulse shaping technique that allows for arbitrarily fast quantum non-demolition, single-quadrature measurements of non-linear systems and unconditionally leaves the measurement resonator empty. Leftover cavity population from short measurements with square or composite digital pulses can be suppressed using instead simple smooth pulse shapes from an analogous family of DRAG shapes; here, it can be derived exactly for arbitrarily many measured modes. The results are easily generalizable, including single-shot, single-quadrature, measurements of multi-qubit and multi-state (leakage) systems. One can also straightforwardly incorporate Purcell filter cavities, which can be depopulated simultaneously via the same technique. Finally, we show how to apply the technique to cascaded cavity networks, e.g. for fast remote entanglement generation, or in non-dispersive single-photon networks, and discuss applicability to single flux quantum (SFQ) readout.

G70.00382: Deep Learning-Based Prediction and Optimal Sequential Measurement of a Quantum Dot*
DOMINIC LENNON (Presenter), HYUNGIL MOON, Materials, University of Oxford, MICHAEL OSBORNE, Department of Engineering, University of Oxford, LEON CAMENZIND, LIUQI YU, DOMINIK ZUMBUHL, Department of Physics, University of Basel, GEORGE ANDREW DAVIDSON BRIGGS, Materials, University of Oxford, EDWARD LAIRD, Department of Physics, Lancaster University — Spin qubits defined in quantum dots are promising for creating a scalable quantum computer. However, they are time-consuming to characterise, and as the size of these systems increases, this task will become intractable without the aid of automation. We present a machine learning algorithm that decides where to measure next and demonstrate it operating on a real quantum dot device in real-time. The algorithm utilises a probabilistic deep-generative model to make reconstructions of a full current map given partial measurement and information theory to select the most informative measurements to perform next. We demonstrate, for two different measurement configurations, that the algorithm outperforms standard grid scan techniques, reducing the number of measurements required by up to 4 times and the measurement time by 3.7 times.

*We acknowledge J. Zimmerman and A. C. Gossard for the growth of the AlGaAs/GaAs heterostructure.

G70.00383: Tunneling-noise-induced spin dephasing of two electrons in an arbitrarily detuned double quantum dot
PEIHAO HUANG (Presenter), Shenzhen Institute for Quantum Science and Engineering, and Department of Physics, Southern University of Science and Technology — Recent progress enables operations of a two-qubit gate for two electron spin qubits in a double quantum dot (DQD), which is an important step towards scalable semiconducting quantum computing. In an asymmetric DQD, it has been shown that 1/f charge-noise-induced tunneling noise can dominate spin decoherence under condition relevant in a two-qubit experiment. Here, we study spin decoherence due to 1/f charge noise for two electrons in a DQD with arbitrary detuning. We show that, in a symmetric DQD, charge-noise-induced tunneling noise can have a profound contribution compared to detuning noise, where the contribution of detuning noise is vanished due to the destructive interference while the contribution of tunneling noise remains finite. We study the spin decoherence for various detuning and tunneling and discuss its consequence on the figure of merit of a two-qubit gate.

G70.00384: 12-photon entanglement and scalable scattershot boson sampling with optimal entangled photon pairs from parametric down-conversion
HAN-SEN ZHONG (Presenter), YUAN LI, WEI LI, LI-CHAO PENG, ZU-EN SU, YI HU, YU-MING HE, XING DING, Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, WEIJUN ZHANG, HAO LI, LU ZHANG, ZHEN WANG, LIXING YOU, State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Micro system and Information Technology (SIMIT), Chinese Academy of Sciences, JUN ZHANG, XI-LIN WANG, LI LI, YU-AO CHEN, NAI-LE LIU, CHAO-YANG LU, JIAN-WEI PAN, Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China — Spontaneous parametric down-conversion (SPDC), one of the most popular entanglement source, enable thousands of quantum optics experiment during the past few decades. We have been devoted on optimizing the property of SPDC. One of the major task is to design a near perfect SPDC entanglement source with high indistinguishability and high efficiency simultaneously. Recently, an SPDC entangled photon pair source of which the heralding efficiency is 97% and the indistinguishability is 96% has been developed.

To prove the powerful of this SPDC source, we produced the first 12-photon entangled GHZ state and implement 3-, 4-, and 5-photon scattershot boson sampling experiment. In 12-photon entanglement experiment, we extend the previous scheme directly. We measured the population and coherence of the GHZ state, and then calculated the fidelity of 0.576(24), which exceed the threshold 0.5 more than 3 times of standard deviation. In scattershot boson sampling experiment, 12 SPDC photon pair sources are employed. The count rate of 3-, 4-, and 5-photon coincidence is 3.9 kHz, 44 Hz and 0.3 Hz, respectively. We validate the sampling result with a modified likelihood ratio test. All of them show a continual deviation from distinguishable particle.
G70.00385: Investigating the Effectiveness of Measurement-Device-Independent Quantum Key Distribution with Weak Coherent Pulses

ANNIKA DUGAD (Presenter), JOSEPH CHAPMAN, ANDREW CONRAD, PAUL G KWIAT, University of Illinois at Urbana-Champaign, DANIEL J GAUTHIER, Dept. of Physics, OSU — Quantum key distribution (QKD) is a quantum cryptographic task that allows a random secret key to be generated and communicated between two parties in the presence of an eavesdropper. Although QKD systems are theoretically foolproof and completely secure according to the laws of quantum mechanics, many security loopholes have been found in practice. Measurement-device-independent quantum key distribution (MDI-QKD) improves upon previous QKD systems by removing all detector side-channels, therefore rendering many of the loopholes obsolete. However, in order to successfully implement MDI-QKD, the sources (representing the two communicating parties) must be indistinguishable. We will be implementing MDI-QKD with two independent sources of light coming from attenuated laser pulses, or resonant cavity LEDs; as a result, the sources will be rigorously tested and characterized to determine how indistinguishable they truly are.

*This work is supported by the ONR MURI program on Wavelength-Agile Quantum Key Distribution in a Marine Environment, Grant #N00014-13-1-0627.

G70.00386: Why We Should Be Skeptical of Quantum Computing

ALAN M. KADIN (Presenter), Consultant, Princeton Junction, NJ 08550 — It is widely believed that quantum computing is on the threshold of practicality, with performance that will soon surpass that of classical computing. On the contrary, it is argued that both the present and the future of quantum computing may be highly uncertain, for the following reasons:

1) The promised performance depends on entanglement-based scaling to massive parallelism, which has not been verified, and may be tested [1].
2) Even if the theory were correct, exponential sensitivity to noise for highly entangled states could make the technology impractical [2].
3) Evidence for entanglement in superconducting qubits can be explained using the nonlinear properties of classical Josephson junctions [3].
4) Evidence for entanglement in arrays of coupled qubits can be explained using conventional energy-band theory with delocalized states.


G70.00387: Single-channel Hadamard gate through single-photon Raman Scattering in Chiral Quantum Nanophotonics

ZHIAO CHEN (Presenter), YAO ZOU, JUNG-TSUNG SHEN, Washington University in St. Louis — Hadamard gate (H-gate) is indispensable to constitute complete sets of logic gates for universal quantum computing. Practical implementations can be classified into atom- and photon-based. While atom-based techniques are rather mature by employing consecutive electromagnetic pulses to drive qubit rotations on Bloch sphere, it is of limited coherent time, and may not be compatible with photon-based quantum communication protocol in scalable quantum internet blueprint. Henceforth, photon-based implementations may play significant roles, which are typically realized by using linear optical elements. However, such schemes require different photonic channels to accommodate binary qubits, thus resulting in limited spatial utility.

To enhance spatial utility, we propose a novel single-channel H-gate scheme by chirally coupling Lambda-type atoms to 1D waveguide, and exploiting photon frequency degree of freedom as qubit. The underlying physics of gate operations here, is frequency conversion through single-photon Raman scattering. The single-channel feature enhances the spatial utility to be highly scalable. Such a scheme is readily feasible due to the advent of chiral coupling technique using photon spin-momentum locking and polarized dipole moment in quantum nanophotonics.
G70.00388: Quantum computing methods for electronic states of the water molecule*  TENG BIAN (Presenter), Physics, Purdue University, DANIEL MURPHY, Physics, Georgia Institute of Technology, RONGXIN XIA, Physics, Purdue University, AMMAR DASKIN, Computer Engineering, Istanbul Medeniyet University, SABRE KAIS, Chemistry, Purdue University — We compare recently proposed methods to compute the electronic state energies of the water molecule on a quantum computer. The methods include the phase estimation algorithm based on Trotter decomposition, the phase estimation algorithm based on the direct implementation of the Hamiltonian, direct measurement based on the implementation of the Hamiltonian and a specific variational quantum eigensolver, Pairwise VQE. We explain how each method works and compare the simulation results in terms of gate complexity and the number of measurements. In conclusion, among methods based on the phase estimation algorithm, the second order direct method provides the most efficient circuit implementations in terms of the gate complexity. With large scale quantum computation, the second order direct method seems to be better for large molecule systems. Moreover, Pairwise VQE serves the most practical method for near-term applications on the current available quantum computers. Finally, the possibility of extending the calculation to excited states and resonances is discussed. This work is posted on arXiv: Quantum computing methods for electronic states of the water molecule.

*Sabre Kais and Teng Bian are grateful for the support from Integrated Data Science Initiative Grants, Purdue University.

G70.00389: Quantum Bernoulli Factories in a Classical Setting*  THOMAS HEBDIGE (Presenter), Controlled Quantum Dynamics Theory Group, Imperial College London, DAVID JENNINGS, School of Physics and Astronomy, University of Leeds — Recently a novel quantum advantage over classical information processing has been developed in the context of randomness processing, under the title of “Bernoulli factories”. Bernoulli Factories find modern application in classical Bayesian statistics, such as in genetics when one encounters intractable likelihood functions. However, since quantum Bernoulli factories are more powerful than their classical counterparts, an open question is if this advantage can be exploited within the classical setting. Here we present work towards an implementation of a quantum Bernoulli factory on near-term quantum devices, and contrast this formalism with the quantum resampling protocol of Webb & Kitaev.

*TH is funded by the EPSRC Centre for Doctoral Training in Controlled Quantum Dynamics. DJ is supported by the Royal Society.

G70.00390: Scaling Hypothesis of Spatial Search on Fractal Lattice Using Quantum Walk  SHOHEI WATABE (Presenter), SHU TAMEGAI, REI SATO, TETSURO NIKUNI, Tokyo University of Science — We investigate a quantum spatial search problem on a fractal lattice. A recent study for the Sierpinski gasket and tetrahedron made a conjecture that the dynamics of the search on a fractal lattice is determined by spectral dimension for the optimal oracle calls, and not by the fractal dimension [A. Patel and K. S. Raghunathan, Phys. Rev. A 86, 012332 (2012)]. We tackle this problem for the Sierpinski carpet, and we find that our simulation result may support the conjecture. We also propose a scaling hypothesis of oracle calls for the quantum amplitude amplification in a fractal lattice, which is given by the Euclidean dimension, fractal dimension, spectral dimension, and the scale factor of a fractal lattice. We have confirmed that our scaling hypothesis holds in the Sierpinski carpet, gasket, and tetrahedron.

G70.00391: Quantum Theory of Entanglement and Brain Physics  SHANTILAL GORADIA (Presenter), Gravity Research Institute, Inc. — Despite decades of hard work by Penrose-Hameroff Hypothesis (ORCH OR) about consciousness, the hypothesis is not universally accepted. We formulate our hypothesis dubbed as “orchestrated subjective experience (ORCH SE)” based on our theory of quantum gravity (explaining the abundance of dark matter) to address the subject disconnect in our recent article, “Quantum Theory of Entanglement and Brain Physics,” in an open minded, OPEN ACCESS Journal of Clinical Reviews and Case Reports 2018, Volume 3, Issue 7. Since dark matter exists in the universe, there is no reason why it would not be present in the brain, to some extent.

G70.00392: FLUID DYNAMICS  —
G70.00393: Pulsatile Flow Through Multi-Coupled Idealized Renal Tubules: Fluid-Structure Interaction and Dynamics Pathologies

NIKSA PRALJAK (Presenter), Department of Physics, Cleveland State University, ANDREW H RESNICK, Department of Physics, Center for Gene Regulation in Health and Disease, Cleveland State University — Kidney tubules are known to have flow-sensing structures, yet information about the flow itself is very fragmentary. Our aim is to generate a biomechanical model for analyzing fluid flow within an elastic kidney tubule when the driving pressure is pulsatile. We created finite-element numerical models of coupled kidney tubules and determined the flow dynamics and wall stresses over a range of driving frequencies and wall compliances. The results form a basis for including elasto-hydrodynamic coupling by neighboring tubules via the interstitium. As well, the results analyze how elastic tubes interact with different frequency phases that alter the hydrodynamics of the fluid in the interior and exterior. Overall, we are interested in exploring the idea of ‘dynamics pathology’ to better understand the progression of certain kidney diseases, for example, Polycystic Kidney Disease.

*This work was supported by the National Science Foundation Research Experience for Undergraduates grant number 1659641.

G70.00394: Particle Collisions During Multiphase Flow

SURESH AHUJA (Presenter), XEROX CORPORATION — Applications of granular materials range from food grains, ores, and coal to pharmaceutical powders and digital printing. High definition digital imaging is enabled in printers by using small micron and nano toner particles. Use of small particles in a housing presents challenges in particle flow as large particles break and small particles tend to aggregate, clog and impact either on the wall of the housing or on other surfaces. Solids are known to undergo brittle – ductile transition depending on the size of a particle, elastic plastic behavior and strain rates under which they are deformed.

Particulate flow can some cases result in jamming and has been analyzed using Lattice- Boltzmann (LB) or DEM (Discrete Element Methods) involving deformation from collisions resulting from hydrodynamic forces. Consequence of particle impaction on surfaces is a reduction in particle charge with wider distribution causing shortfalls in electro-photographic development and image quality. An elasto-plastic model is developed for particle impaction for a particulate flow that depends on particle radius, incident particle speed and yield stress of the material. The model predictions are compared with experimental data on particle impaction.

G70.00395: Foam films and liquid bridges formed by aqueous sodium naphthenate solutions

CHRYSTIAN OCHOA (Presenter), ELIZABETH JOHN, JELENA DINIC, VIVEK SHARMA, Chemical Engineering, University of Illinois at Chicago — Sodium Naphthenates found in crude oils can act as surfactants and self-assemble in aqueous solutions to form micelles and liquid crystals. Understanding and controlling the drainage kinetics of thin films is an important problem that underlies the stability, lifetime and rheology of petroleum foams and emulsions. Here, we show that foam films formed by aqueous solutions of sodium naphthenates exhibit step-wise thinning or stratification. We utilize Interferometry, Digital, Imaging, Optical Microscopy protocols, previously developed by our group, to investigate the drainage and stratification in micellar foam films (< 100 nm) with high spatial (thickness < 10 nm) and temporal resolution (< 1 ms). We determine how the concentration of added sodium naphthenates influences the nanoscopic topography, stratification kinetics and step size of foam films. Finally, we show that visualization and analysis of capillary-driven thinning and pinch-off dynamics of the columnar neck in an asymmetric liquid bridge created by dripping-onto-substrate (DoS) of sodium naphthenate solutions can be used for characterizing the change in shear viscosity, extensional viscosity and microstructure in such surfactant solutions.

G70.00396: Holographic Rheology of Viscoelastic Fluids in Microfluidic Geometries

SIDDHARTHA GUPTA (Presenter), SIVA A VANAPALLI, Texas Tech University — To explore the kinematics and rheology of viscoelastic flows it is critical to map three-dimensional (3D) velocity fields. The 3D flow information can be used for understanding phenomena such as elasticity-driven instabilities, slip and shear-banding. Digital holography microscopy (DHM) with particle tracking velocimetry (PTV) is an interferometry technique which can provide real-time 3D flow information by recording holograms of the flow. We demonstrate the robustness of holography in characterizing the kinematics of polymeric and Newtonian fluids in rectilinear channels, contraction-expansion and curved microchannels, which provide for shear, extensional and curvilinear flow behavior respectively. Using DHM-PTV, we recover the full 3D velocity field which is in good agreement with analytical results and flow simulations. Additionally, we demonstrate a digital holography driven rheology (DHR) approach for quantifying shear viscosity curves of complex fluids in thin-slit geometries. The DHR approach does not make a-priori assumptions about material properties and is thus independent of slip which has been found to affect narrow gap rheology. In sum, we conclude that digital holography microscopy has powerful applications for investigation of complex fluids in complex geometries.
**G70.00397: Effects of nanoparticles on the stability of polymer fibers**

TAEJIN KWON (Presenter), BONG JUNE SUNG, Sogang University — Soft matters in confinement may deform easily upon small perturbation. Especially, polymer fibers are unstable due to a large surface area. Recent studies showed that the addition of nanoparticles (NPs) could control the stability of polymer fibers. It remains elusive how NPs would affect the disruption of polymer fibers. In this work, we perform molecular dynamics simulations for polymer fibers with NPs of different interaction types. We prepare unstable polymer fibers that disrupt into globules. We find that upon the addition of NPs, the disruption of fibers is hindered and the breakup time ($t_b$) of polymer fibers increases. We find that polymer fibers with NPs are more likely to retain their morphology. The free energy barrier between the fiber and the globule would increase due to NPs. The mechanism for the stability differs for the different interaction types of NPs. When the interaction between polymers and NPs is attractive (non-attractive), $t_b$ increases (decreases) with a decrease in temperature. We show that different spatial arrangement of NPs leads to the different temperature dependence of $t_b$.

*This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2018R1A6A1A03024940).*

**G70.00398: Experimental Investigation of Droplets Impacting on Inclined Heated Surfaces with Varying Wettability**

QIANG MA (Presenter), XIAOMIN WU, Department of Energy and Power Engineering, Tsinghua University — Droplets impacting on heated surfaces is a common phenomenon in spray cooling, which can remove very high heat flux. Since the surface wettability has a significant effect on the heat transfer performance by directly changing the droplet spreading, rebounding and boiling behaviors, it has drawn much attention. However, the surface roughness changes simultaneously when changing the surface wettability in most researches. Thus, the influence factors of wettability and roughness are coupled. In this work, the test surfaces were fabricated by spray-coating a thin film on the aluminum substrates and the roughness of each surface is small enough. Therefore, the influence of wettability on droplets impacting on inclined heated surfaces have been experimentally studied. The experiments were carried out with different inclination of 0°, 30° and 60°, with different surface temperature from 100°C to 400°C and with different surface contact angle of 10°, 78°, 95° and 122°. The droplet spreading, rebounding and boiling behaviors have been observed by a high speed camera. The droplet spreading factors, advancing and receding contact angles have been measured and the droplet boiling regimes have been identified.

*National Natural Science Foundations of China (No.51476084).*

**G70.00399: Simulation of Droplet Impact on a Spherical Surface**

XIN LIU (Presenter), XUAN ZHANG, JINGCHUN MIN, Tsinghua University — Droplet impact phenomenon is widely found in nature, production and life. Due to the complexity of the actual surface structures, the droplet may impact not only on a flat surface but also on surfaces of various shapes and the one typical example is a sphere. In this study, the droplet impact process on a spherical surface is simulated using the VOF multiphase model coupled the dynamic contact angle model, which is compared with our experimental data to verify the model. Based on this model, the impact processes of droplets with different We numbers on spherical surfaces with different diameters and contact angles are simulated. The results indicate that the maximum spreading factor increases significantly with the increase of We and the decrease of contact angle while it is little influenced by the sphere diameter. The droplet may break up at the spreading or receding stage during the whole impact process. Compared with impacting on the flat surface, the droplet is more likely to break up when impacting on a sphere due to the gravity and the critical We number for breaking up is smaller. The droplet breaking-up diagram is obtained, which provides reference for the droplet impact study.

*This work is funded by the National Key Basic Research Program of China (No. 2015CB755800).*
G70.00400: Coalescence Dynamics of Near-Critical Sulfur Hexafluoride in Microgravity*  
CHRISTIAN HAWKINS (Presenter), ANA OPRISAN, College of Charleston, DANIEL A BEYSENS, Université Pierre et Marie Curie, YVES GARRABOS, CAROLE LECOUTRE, Institut de Chimie de la Matière Condensée de Bordeaux — Critical fluids have a variety of applications from manufacturing high-tech materials to industrial lubrication and extracting oils from foods. Phase separation of critical fluids cannot be studied on earth due to the increase in compressibility near the critical point and stratification of fluids by density in gravity. We used direct imaging to record snapshots of phase separation that takes place in sulfur hexafluoride (SF6) in weightlessness conditions on the International Space Station (ISS). The system was at liquid-vapor equilibrium slightly below the critical temperature and further cooled down by a 0.2-mK quench that produced a new phase separation. Both full view and microscopic views of the direct observation cell were analyzed to determine the evolution of the radii distributions. In addition, in microscopic view, we measured the diameter of droplets and bubbles in the system throughout multiple coalescence events leading to further support of the coalescence-induced-coalescence model.

*We would like to thank the College of Charleston School of Science and Mathematics for the Dean's Funding grant which funded this research. Furthermore, Y.G., C.L., and D.B. acknowledge a research grant from CNES, and wish to thank the CNES and NASA teams involved in the DECLIC project.

G70.00401: Strategies for Microparticle Manipulation by Rectified Inertial Forces  
SIDDHANSH AGARWAL, University of Illinois at Urbana-Champaign, BHARGAV RALLABANDI, Mechanical Engineering, University of California, Riverside, SASCHA HILGENFELDT (Presenter), University of Illinois at Urbana-Champaign — Oscillating interfaces in a liquid give rise to inertial effects that manifest as multiple physical phenomena on slower (steady) time scales, including streaming flow and force actuation on immersed particles. While these effects have traditionally been treated separately, we develop a timescale separation formalism that puts streaming motion of fluid elements and rectified motion of particles on the same footing. Using ultrasound-driven microbubble oscillations in microfluidic devices allows for flexible and specific manipulation of particles: depending on parameters, microparticle reaction is selective by size or by density, results in attraction to or repulsion from the bubble, and can be focused on particle trapping or deflection. Thus, a device can be tailored to desired applications by changing easily controlled parameters like flow speed and driving frequency.

G70.00402: Throughput enhancement of parallel step emulsifier devices by shear-free and efficient nozzle clearance  
ELAD STOLOVICKI (Presenter), ROY ZIBLAT, DAVID A WEITZ, Harvard University — Step emulsification is an attractive method for production of monodisperse drops. Its main advantage is the ability to parallelize many step emulsifier nozzles to achieve high production rates. However, step emulsification is sensitive to any obstructions at the nozzle exit. At high production rates, drops can accumulate at nozzle exits, disturb the formation of subsequent drops and impair monodispersity. As a result, parallelized step emulsifier devices typically do not work at maximum productivity. Here a design is introduced that parallelizes hundreds of step emulsifier nozzles, and effectively removes drops from the nozzle exits. The drop clearance is achieved by an open collecting channel, and is aided by buoyancy and does not apply shear on forming drops. The clearance method avoids the use of a continuous phase flow for drop clearance. The method works well for a wide range of drops, sizing from 30 to 1000 µm at production rates of 0.03 and 10 L per hour and achieved by 400 and 120 parallelized nozzles respectively.

G70.00403: WITHDRAWN ABSTRACT

G70.00404: Experimental investigation into a nanoparticle based direct absorption solar oscillating heat pipe  
HAIE YANG (Presenter), HAICHUAN JIN, GUIPING LIN, DONGSHENG WEN, Beihang University — Nanoparticle-based volumetric solar absorption has been shown to be an effective technique to realize efficient solar harvesting. However, most of such systems under study are stationary and cannot realize solar energy transport, which limits their potential applications to a large extent. A novel idea of using directive absorptive nanofluids in oscillating heat pipes (OHP) is investigated in this work, which would achieve efficient solar energy capture and transportation simultaneously without the use of any additional pumping power. The influence of a variety of parameters such as nanoparticle type, nanoparticle concentration, nanofluids filling ratio and solar radiation intensity on the performance of OHPs are investigated. Very high effective thermal conductivity is observed. It is found that strong absorption of solar energy, efficient vapor generation inside the OHP and proper configuration of the OHP should be responsible for the efficient operation of this system.
G70.00405: Fluidic wrench: Precise control over the position and orientation of anisotropic colloids using fluid flow*  
DINESH KUMAR (Presenter), ANISH SHENOY, SONGSONG LI, CHARLES SCHROEDER, University of Illinois at Urbana-Champaign — A grand challenge in the field of directed assembly is to precisely assemble chemically and structurally distinct anisotropic particles into functional hierarchical structures. Such complex assembly schemes will require precise control over both the position and orientation of individual rods. In this work, we demonstrate simultaneous control over the 2D center-of-mass position and orientation of anisotropic colloidal particles using only fluid flow. We use a 4-channel microfluidic device with a model-predictive control scheme to generate a flow pattern that translates and rotates rod-like particles from their initial state to a final desired position and orientation. Unlike alternative techniques that exploit intrinsic material properties of particles (e.g. index of refraction, magnetic properties, surface charge) to control position and orientation, our method imposes no restrictions on the physical or chemical properties of the particles, and hence, can be used for rods of any material and size, assuming they can be imaged. Moving forward, this approach could be further engineered to achieve fluidic-directed assembly of asymmetric objects on a meso- to micro-scale level.

*NSF CBET PMP #1704668 for funding.

G70.00406: Microporosity Evolution and Powder-Powder Interaction in Selective Laser Melting Process  
JIQIN LI (Presenter), LU LI, TAI-HSI FAN, Mechanical Engineering, Univ of Connecticut, Storrs, CT — Additive manufacturing in aerospace and biomedical applications is challenging due to the need of superior quality and liability of end products. A critical concern about the process is the formation of surface defects due to incomplete melting of powders and gas trapping between powders, which significantly weakens the mechanical performance of the raw products. Better understanding of the process dynamics can help to mitigate the defects and determine process control parameters. We present phase-field modeling of the powder-powder interaction and the formation of micropores during selective laser melting of pure titanium powders. The solid-liquid phase transition is coupled with thermal transport, capillary flow, and liquid-gas interfacial deformation. The change of morphology and the evolution of pores highly depend on the interplay of the fusion dynamics, configuration of powders, and laser control parameters.

G70.00407: Gravity and Flow Effects on Coarsening Dynamics in Crystal-Liquid Mixtures  
TAI-HSI FAN (Presenter), JIQIN LI, ELIZABETH SOHA, Mechanical Engineering, Univ of Connecticut, Storrs, CT — Coarsening of crystals can be driven by cooling, Ostwald ripening, or interfacial kinetics in crystal-liquid mixtures. The relevant phenomena appear in many manufacturing processes involving metals and alloys, or nonmetallic materials. The degree of coarsening determines the size of crystals and microstructural pattern, and thus understanding coarsening dynamics is important in controlling the uniformity of microstructure and properties of the end products. We present a phase-field theoretical framework to investigate coarsening dynamics in symmetric and asymmetric binary systems. The phase transition and microstructure evolution are coupled with fluid flow, trajectory motion of the crystals, thermophysical properties of the materials, interfacial energy, and the relevant heat and mass transport phenomena. Specifically, we focus on crystal morphology and the fluid flow induced by density variation and gravity acceleration. The flow and collective motion of crystals also influence the heat and mass transfer around the interstitial space between crystals and should be resolved simultaneously. The theoretical analysis and 2d computational results based on spectral method will be presented.

G70.00408: Geometry and Topology of Collective 2D Vortex Dynamics*  
ALEXANDER BOGATSKII (Presenter), PAVEL WIEGMANN, University of Chicago — We consider the coarse-grained dynamics of many quantized chiral vortices on a 2D surface.

There are two groups of emergent phenomena. First, coupling the incompressible Euler equation to a metric in the presence of point vortices involves important ambiguities reminiscent of spin in quantum 2D systems. We obtain the coarse-grained flow of the vortex fluid, observe the effective negative temperature envisioned by Onsager in 1952, and discuss the curvature effects.

Secondly, vortices can form bounded drops of nonzero vortex density. The quantization of vortices leads to the presence of an "overshoot" in the vortex density at the boundary of the drop, also observed in Quantum Hall droplets. The Euler dynamics generates a remarkable edge wave in the overshoot density that obeys the integrable Benjamin-Ono equation. The mass of the soliton in this equation is quantized in units of one vorticity quantum, representing the topological nature of vortices.

Based on work with prof. Paul Wiegmann.

*A.B. has been supported by The University Of Chicago.
G70.00409: Ellipsometric Characterization of Monolayer MoSe$_2$ from 31 to 300K

HOANG TUNG NGUYEN, HAN GYEOL PARK, TAE JUNG KIM, VAN LONG LE, Kyung Hee University, FARMAN ULLAH, YONG SOO KIM, University of Ulsan, MAENG-JE SEONG, Chung Ang University, YOUNG-DONG KIM (Presenter), Kyung Hee University — The layered transition metal dichalcogenides (TMDCs) has recently gained significant interest due to their distinctive physical properties. Molybdenum diselenide (MoSe$_2$) is well known as one of transition metal dichalcogenides, which suggests promise as a potential substitute for silicon in state-of-the-art transistors, sensors, and photodetectors. A systematic study on temperature dependence of the dielectric function and critical point energies of MoSe$_2$ is therefore strongly needed.

In this work, we investigate the dielectric function of 2D MoSe$_2$ in 0.74 to 6.42 eV energy range at temperatures from 31 to 300 K by spectroscopic ellipsometry. The CP transitions are observed and their energies are obtained by fitting standard analytic expressions to second energy derivatives of the data. We found six new CPs at low temperature beside another six CPs realized at room temperature. Blue shift and enhancement of most CP energies at low temperatures were observed and understood by the reduced lattice constant and electron-phonon interaction. The temperature dependences of these CPs were determined by fitting the data to the coefficients in a phenomenological expression that contains the Bose-Einstein statistical factor.

G70.00410: Anisotropic Phononic Bandgap Formation of Nano-Dicolloid Crystals

HOJIN KIM (Presenter), ERIC M FURST, Department of Chemical and Biomolecular Engineering, University of Delaware, GEORGE FYTAS, Max Planck Institute for Polymer Research — Self-assembly of colloidal nanoparticles form periodic building blocks and the fabricated crystalline structures exhibit useful photonic and phononic properties because of the periodicity of their structure. Such phononic properties are broadly applicable in technologies such as hypersonic and thermal cloaking materials, heat management systems, and metamaterials. To guide the propagation of acoustic waves to targeted direction, we investigate the potential of self-assembled anisotropic colloidal particles. Colloidal crystals consisted of nano-dicolloids are fabricated using directed self-assembly technique under electric field and their hypersonic phonon spectra are measured by Brillouin light scattering (BLS). The anisotropy of dicolloidal particle shape enables crystals to have different periodicity depending on the direction of phonon propagation. We show that the fabricated crystals have anisotropic phononic bandgaps due to both hybridization and Bragg scattering.

G70.00411: Examining the Feasibility of Room-Temperature Exciton-Polariton Lasers Based on III-V Microcavities

ANIRUDDHA BHATTACHARYA (Presenter), Department of Electrical Engineering and Computer Science, The University of Michigan at Ann Arbor, ALEXEY KAVOKIN, Institute of Natural Sciences, Westlake University, No.18, Shilongshan Road, Cloud Town, Xihu District, Hangzhou, China — Exciton-polaritons are light-matter dressed bosonic quasiparticles. Electrically energized room-temperature GaN-based polariton lasers have been recently demonstrated. Nevertheless, further improvements in the laser characteristics can be brought about by implementing them on state-of-the-art GaAs-based microcavities. In particular, GaAs-based microcavities have vanishingly small values of dislocation densities and extremely high values of intra-cavity photon lifetimes. Demonstration of strong coupling and polariton lasing effects in GaAs-based devices at room temperature is limited mainly by the rather small values of the free excitonic Rydberg energies. To that end, we would give an overview of several strategies for enhancing the binding energy of the excitonic component of the lower-polaritons and comment on their respective merits and demerits. Among others, methodologies for squeezing the spatial extent of the excitonic wavefunctions, such as by application of out-of-plane magnetic fields and in-plane lateral confinement of 2D excitons in quantum wells, respectively, and the stabilization effect of the strong exciton-photon coupling on the excitonic binding shall be discussed. We believe that the latter is, probably, the most promising for future device applications.

Tuesday, March 5, 2019 2:30 PM - 5:18 PM

Session H01 DCMP: Fermi Surface and Excitations of Weyl Systems

BCEC 106 - Ryo Okugawa, Tohoku University - Tag(s): Focus

2:30PM H01.00001: Semi-Quantized Pumping and Spin-Orbit Torque in Topological Dirac Semimetals

TAKAHIRO MISAWA (Presenter), Institute for Solis State Physics, University of Tokyo, KENTARO NOMURA, Institute for Materials Research, Tohoku University — We study the spin/charge transport phenomena and magnetization switching in a topological Dirac semimetal attached to a ferromagnetic insulator. Topological Dirac semimetals manifest a large inverse spin Hall effect when a spin current is pumped from the attached ferromagnetic insulator with a precessing magnetization, compared to conventional normal metals. We show that the induced charge current is semi-quantized because it originates to topological nature. We also show that an applied electric field in the topological Dirac semimetal generates the spin-orbit torque which reverses the magnetization in the ferromagnet.
2:42PM H01.00002: Disordered fermionic quantum critical points  
HENNADII YERZHAKOV (Presenter), JOSEPH MACIEJKO, University of Alberta — We study the effect of short-range quenched disorder on the semimetal-superconductor quantum phase transition in a model of two-dimensional Dirac semimetal with N flavors of two-component Dirac fermions, using perturbative renormalization group methods at one-loop order in 4-ε spatial and ετ time dimensions. Depending on the value of N, the model is applicable to topological insulators (odd N), graphene (N=4), and possibly other systems and type of transitions. For N≥2 we find that the Harris-stable clean critical behavior gives way, past a certain critical disorder strength, to a finite-disorder critical point characterized by non-Gaussian critical exponents, a noninteger dynamic critical exponent, and a finite Yukawa coupling between Dirac fermions and bosonic order parameter fluctuations. For sufficiently large N the disordered quantum critical point is described by a renormalization group fixed point of stable-focus type and exhibits oscillatory corrections to scaling.

2:54PM H01.00003: Chirality Josephson current in inversion-asymmetric Weyl semimetals  
SONGBO ZHANG (Presenter), JOHANNA ERDMENGER, BJ"ORN TRAUZETTEL, Institute for Theoretical Physics and Astrophysics, University of Würzburg — In this report, I will talk about Josephson junctions based on inversion-asymmetric but time-reversal symmetric Weyl semimetals under the influence of Zeeman fields. Due to distinct spin textures, the Weyl nodes of opposite chirality respond differently to an external magnetic field. Remarkably, a Zeeman field perpendicular to the junction direction results in a phase shift of opposite sign in the current-phase relations of opposite chirality. This leads to a finite chirality Josephson current even in the absence of a phase difference across the junction. In the long junction and zero temperature limit, the chirality Josephson current embodies a novel quantum anomaly at π phase difference which is associated with a Z2 symmetry at low energies. It can be detected experimentally via an anomalous Fraunhofer pattern.

3:06PM H01.00004: Generalized Triple-Component Fermions: Lattice Model, Fermi arcs and Anomalous Transport  
SNEHASISH NANDY (Presenter), Department of Physics, Indian Institute of Technology Kharagpur, SOURAV MANNA, Max Planck Institute for the Physics of Complex System, DUMITRU CALUGARU, Cavendish Laboratory, University of Cambridge, BITAN ROY, Max Planck Institute for the Physics of Complex System — A generalization of time-reversal symmetry-breaking triple-component semimetals, transforming under the pseudo-spin-1 representation, to arbitrary (anti-)monopole charge , with n = 1, 2, 3 in the crystalline environment will be presented. The quasiparticle spectra of such systems are composed of two dispersing bands with pseudo-spin projections and one completely flat band at zero energy with . In this talk we will show simple tight-binding models for such spin-1 excitations in a cubic lattice and address the symmetry protection of the generalized triple-component nodes. In accordance to the bulk-boundary correspondence, triple-component semimetals support branches of topologically protected Fermi arc surface states and accommodate a large anomalous Hall conductivity (in the xy plane), given by . Furthermore, we compute the longitudinal magneto-, planar Hall and magneto thermal-conductivities in this system, which increase as (due to the non-trivial Berry curvature in the medium) with the external magnetic field (B), when it is sufficiently weak. A generalization of our construction to arbitrary integer spin system is also highlighted.

3:18PM H01.00005: Magnetic field induced valley polarization in a Weyl semimetal with tilted cones.*  
SIMON BERTRAND (Presenter), RENE COTE, ION GARATE, Universite de Sherbrooke — We present a theory of the optical conductivity in time-reversal symmetric Weyl semimetals with tilted cones placed under strong magnetic fields. Our theory incorporates long range Coulomb interactions treated within the generalized random phase approximation. Under irradiation by circularly polarized light, we predict a 100% valley polarization for significant intervals of the incident photon frequency. This polarization, which occurs between nodes related by time-reversal, originates from interband transitions involving the chiral Landau level. We propose observable signatures of this polarization in the optical conductivity and comment on its manifestation in TaAs and related materials.

*We acknowledge financial support from Québec’s Réseau Québécois des Matériaux de Pointe and Canada’s National Science and Engineering Research Council.
Thermoelectric transport in torsional strained Weyl semimetals* ENRIQUE MUNOZ (Presenter), Pontifical Catholic University of Chile, RODRIGO SOTO GARRIDO, Universidad San Sebastian — We recently1 studied the electronic transport properties in Weyl semimetals submitted to the combined effects of torsional mechanical strain and magnetic field, showing that this configuration induces a node-polarization effect on the current that can be used to measure the torsion angle from transmission experiments. In this talk, we extend our previous work to study thermoelectric transport in Weyl semimetals2 (WSM) under torsional strain and an external magnetic field. We provide exact analytical expressions for the transmitted heat current, in order to calculate the thermal conductance and the Seebeck coefficient under this configuration. Our results suggest that thermoelectric transport coefficients in these materials can be engineered by appropriately tuning the magnitude of the magnetic field, torsional strain and the applied bias or thermal gradient, leading to a potentially very high figure of merit.

References

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First-Principles Studies of Topological Semimetal Features in the Nonpolar Phase of Ferromagnetic Hexagonal Manganites YXO₃ (X=V-Co) SOPHIE WEBER (Presenter), University of California, Berkeley,CA, SINEAD MAGELLA GRIFFIN, JEFFREY B NEATON, Lawrence Berkeley National Lab, Berkeley, CA — Hexagonal Manganites have garnered much attention in the condensed matter community due to their multiferroic properties. Here, we use first principles calculations to examine the topological properties of their band structures. While the noncollinear antiferromagnetism common in this compound class generally yields insulating states, we find that energetically-nearby ferromagnetic ordering can cause metallic band structures with topological nodal features in the nonpolar P6₃/mmc phase. Starting with YMnO₃ we substitute different 3d transition metals for Mn and examine the resultant trends in band structure as a function of B site cation. In particular we find that YVO₃ and YCrO₃ have nodal lines near the Fermi level due a band inversion which can be tuned via biaxial strain. Based on our findings, stabilizing YXO₃ compounds in the hexagonal ferromagnetic phase, for example via epitaxial growth, can offer a promising platform for studying the interplay of topology and multiferroicity.

Topological nodal phases in non-Hermitian systems with parity-time and parity-particle-hole symmetries RYO OKUGAWA (Presenter), WPI-AIMR, Tohoku university, TAKEHITO YOKOYAMA, Department of Physics, Tokyo Institute of Technology — Exceptional points emerge from band touching in non-Hermitian systems. We study band degeneracy in non-Hermitian systems with parity-time and parity-particle-hole symmetries. When parity-time or parity-particle-hole symmetry is present, it is shown that exceptional lines and surfaces can appear in two-dimensional and three-dimensional non-Hermitian systems, respectively. We also investigate topological properties of the nodal band structures. We demonstrate the non-Hermitian topological nodal phases by using lattice models of a topological semimetal and a superconductor.

Berry curvature and Hall viscosities in an anisotropic Dirac semi-metal FRANCISCO PENA-BENITEZ, KUSH SAHA, PIOTR SUROWKA (Presenter), Max Planck Institute for the Physics of Complex Systems — We investigate parity-odd non-dissipative transport in an anisotropic Dirac semi-metal in two spatial dimensions. The analysis is relevant for interacting electronic systems with merging Dirac points at charge neutrality. For such systems the dispersion relation is relativistic in one direction and non-relativistic in the other. We give a proposal how to calculate the Berry curvature for this system and use it to derive more than one odd viscosities, in contrast to rotationally invariant systems. We observe that in such a model the odd part of stress tensor is parameterised by two independent transport coefficients and one that is identically zero.
the external magnetic field \( B \) and increases as \( B^2 \), at least when it is sufficiently weak (the semi-classical regime). In the longitudinal magnetoconductivity (LMC), bearing the signature of the chiral anomaly, is insensitive to the direction of the magnetic field even though the distribution of the underlying Berry curvature is anisotropic, the corresponding intrinsic component of arbitrary integer charge \( n \), with \( n=1, 2 \) and \( 3 \) in a crystalline environment, will be presented. We will show that for any \( n > 1 \), the anomalous contribution, arising from the chiral anomaly.

4:42PM H01.00010: Magnetotransport in multi-Weyl semimetals: A kinetic theory approach

RENAITO DANTAS (Presenter), FRANCISCO PENABENITEZ, PIOTR SUROWKA, BITAN ROY, Max Planck Institute for the Physics of Complex System — Longitudinal magnetotransport in three-dimensional multi-Weyl semimetals, constituted by a pair of (anti)-monopole of arbitrary integer charge \( n \), with \( n=1, 2 \) and \( 3 \) in a crystalline environment, will be presented. We will show that for any \( n > 1 \), even though the distribution of the underlying Berry curvature is anisotropic, the corresponding intrinsic component of the longitudinal magnetoconductivity (LMC), bearing the signature of the chiral anomaly, is insensitive to the direction of the external magnetic field \( B \) and increases as \( B^2 \), at least when it is sufficiently weak (the semi-classical regime). In addition, the LMC scales as \( B^2 \) with the monopole charge. We demonstrate these outcomes for two distinct scenarios, namely when inter-particle collisions in the Weyl medium are effectively described by (a) a single and (b) two (corresponding to inter-valley and intra-valley) scattering times. While in the former situation the contribution to LMC from chiral anomaly is inseparable from the non-anomalous ones, these two contributions are characterized by different time scales in the later construction. Specifically for sufficiently large inter-valley scattering time the LMC is dominated by the anomalous contribution, arising from the chiral anomaly.

4:44PM H01.00011: Geometric signatures of topological origin in the particle-hole continuum of Weyl semimetals

ANIRUDH CHANDRASEKARAN (Presenter), STEFANOS KOURTIS, Boston University — We present a full geometric description of the particle-hole continuum in Weyl semimetals, emphasizing distinctive features in the joint density of states for particle-hole excitations across nodal points. These are shown to arise as a geometric consequence of the linear effective Hamiltonian around nodal points, and are thus characteristic of Weyl semimetals. We discuss how such geometric characteristics of the particle-hole continuum of Weyl semimetals can be present in resonant inelastic X-ray scattering (RIXS) spectra. Our work provides signatures of the presence of Weyl nodes in bulk band structures, and indicates that RIXS is a promising tool that can potentially be used to identify and characterize nodal points in materials, especially in settings that are difficult to access with other spectroscopies. The calculation presented here also serves as a first checkpoint for comparison with ongoing RIXS experiments.

4:54PM H01.00013: Non-abelian braiding of Weyl points

ADRIEN BOUHON (Presenter), Nordita, ROBERT-JAN SLAGER, Max Planck Institute for the Physics of Complex Systems, TOMAS BDUSEK, Physics Department, Stanford University — We discuss the realization of non-abelian braiding of Weyl points in a two-dimensional crystal. This proposal is based on a refined homotopy characterization of band structures that goes beyond the current classification of crystalline topological phases of matter.

*Nordita, Stockholm.

5:06PM H01.00014: The disordered single Weyl cone

JED PIXLEY (Presenter), JUSTIN WILSON, Rutgers University, New Brunswick, DAVID HUSE, Physics, Princeton University, SANKAR DAS SARMA, Physics, University of Maryland — We numerically study a single Weyl cone in the presence of short-range disorder. By representing the Hamiltonian in a \`mixed\’ way between real and momentum space we are able to invoke fast Fourier transforms to take advantage of efficient numerical routines (such as Lanczos and the kernel polynomial method) that rely on sparse matrix-vector multiplications. As a result, we reach sufficiently large system sizes that are comparable to lattice model simulations. We study the distinctions that arise between lattice models that contain band curvature and multiple Weyl nodes that have internode scattering with the case of a single Weyl node with a perfectly linear dispersion. We will report results on the nature of rare regions and the density of states as a function of the strength of disorder as well as compare and contrast single node and multinode situations.
Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H02 DMP: Topological Metamaterials and Functional Nanostructures BCEC 107A -
Yongmin Liu, Northeastern University - Tag(s): Focus

2:30PM H02.00001: Topological Metamaterials [Invited] ANDREA ALU (Presenter), Photonics Initiative, Advanced Science Research Center at CUNY GC — In this talk, I discuss our recent research activity in electromagnetics, nano-optics, acoustics and mechanics, showing how suitably tailored meta-atoms and arrangements of them open exciting venues to induce topological order for light, radio-waves and sound, mimicking the response of electronic topological insulators. Our approaches are based on using suitably tailored mechanical motion, spatio-temporal modulation, large nonlinearities in coupled resonator systems, and bianisotropy in order to induce the required symmetry breaking in periodic systems that yields topologically nontrivial wave propagation. In the talk, I will also discuss the impact of these concepts from basic science to practical technology.

3:06PM H02.00002: Two-dimensional mechanical metamaterials with unusual Poisson ratio behavior* DAVID TOMANEK (Presenter), DAN LIU, ZHIBIN GAO, Michigan State University — We design two-dimensional mechanical metamaterials that may be deformed substantially at little or no energy cost. Examples of such deformable structures are assemblies of rigid isosceles triangles hinged in their corners on the macro-scale, or polymerized phenanthrene molecules forming porous graphene on the nano-scale. In these and in a large class of related structures, the Poisson ratio ν diverges for particular strain values. ν also changes its magnitude and sign, and displays a shape memory effect.

*NSF/AFOSR EFRI 2-DARE grant number EFMA-1433459 and China Scholarship Council grant number 201706260027

3:18PM H02.00003: A programmable modular metamaterial with alterable Poisson's ratio and multi-stability* XIAOYI JIANG, JIAYAO MA, YAN CHEN (Presenter), Mechanical Engineering, Tianjin University — Modular metamaterials are artificially designed materials constructed by linked modules, often with properties surpassing these constituent modules. To achieve certain required deformation modes and mechanical properties, the modules are usually linked to form a mobile mechanism or a deformable structure. Here we present a novel 3D modular metamaterial constructed of hinged blocks, which utilizes both to realize alterable Poisson's ratio and multi-stability. We demonstrate through theoretical analysis and experiments that upon axial compression, a single unit of the new metamaterial has two distinct mechanism motion stages with positive and negative Poisson's ratio, respectively. And in between there exist a structure deformation stage, thereby forming a mechanism-structure-mechanism transition with bi-stability. Both the magnitude of Poisson's ratio and the energy needed to bypass the structure deformation stage is programmable through two design parameters. In addition, the single unit can be stacked axially to form a tubular metamaterial with progressive folding deformation mode and multi-stability.

*The authors acknowledge the financial support from the Natural Science Foundation of China (Projects No. 51721003, 51575377).

3:30PM H02.00004: Seeded glancing-angle deposition of nanoparticle-nanowire hybrid structures* KAI TREPKA (Presenter), YE TAO, Harvard University — The controllable handling of an arbitrary single particle of matter < 50 nm is an essential but unsolved technological challenge. Applications are wide, ranging from fabrication of functionalized scanning probe tips and samples to the sorting of biological particles such as enzymes and viruses for research and drug development [1-4]. Here, we demonstrate a method to handle single copies of nanoparticles (NP) with diameters from 10-100 nm. The procedure is based on the production of nanoparticle-nanowire hybrid structures using glancing-angle deposition (GLAD), with arbitrary NP seeds. The result is a nanoparticle tip attached to a silicon oxide nanowire handle for facile manipulation. To showcase the generality and versatility of the process, we demonstrate its applicability to a range of NP sizes and compositions (FeO, Au, and Fe@C NP). Such tip-handle growth using arbitrary NPs enables manipulation and heterostructure creation at nanoscale, with wide-ranging applications.

[1] 10.1038/s41565-018-0150-y
[4] 10.1038/nnano.2014.140

3:42PM H02.00005: Passive Radiative Thermostat Enabled by Phase-Change Photonic Nanostructures*  WILTON DE MELO KORT-KAMP (Presenter), SHOBHITA KRAMADHATI, ABUL K AZAD, MATTHEW T REITEN, DIEGO A R DALVIT, Los Alamos National Laboratory — A thermostat senses the temperature of a physical system and switches heating or cooling devices on or off, regulating the flow of heat to maintain the system’s temperature near a desired set point. Taking advantage of recent advances in radiative heat transfer technologies, here we propose a passive radiative thermostat based on phase-change photonic nanostructures for thermal regulation at room temperature. By self-adjusting their visible to mid-IR absorptivity and emissivity responses depending on the ambient temperature, the proposed devices use the sky to passively cool or heat during day-time using the phase-change transition temperature as the set point, while at night-time temperature is maintained at or below ambient. We simulate the performance of a passive nanophotonic thermostat design based on vanadium dioxide thin films, showing daytime passive cooling (heating) with respect to ambient in hot (cold) days, maintaining an equilibrium temperature approximately locked within the phase transition region. Passive radiative thermostats can potentially enable novel thermal management technologies, for example, to moderate diurnal temperature in regions with extreme annual thermal swings.

*The authors thank LANL LDRD program and the Center for Nonlinear Studies for support.

3:54PM H02.00006: Quantum electrodynamics of photonic Weyl points  IÑAKI GARCIA-ELCANO, Condensed Matter Theory Department, Universidad Autonoma de Madrid, ALEJANDRO GONZALEZ-TUDELA, Instituto de Fisica Fundamental IFF-CSIC, JORGE BRAVO-ABAD (Presenter), Condensed Matter Theory Department, Universidad Autonoma de Madrid — The recent realization of photonic Weyl points in three-dimensional photonic crystals [1,2] has drawn significant interest due to their potential as highly controllable platforms to explore topological phenomena [3]. In this talk, we present a systematic study of the decay dynamics of quantum emitters embedded in Weyl-point photonic materials. By combining both analytical and numerical approaches [4], we show how the unique dispersion of photonic Weyl points enables the emergence of a novel light-matter bound state, which cannot be described by conventional perturbative treatments. Potential applications of these findings in emerging quantum technologies are also discussed.


4:06PM H02.00007: Control of radiative processes using periodic arrays of plasmonic nanostructures*  YUWARAJ ADHIKARI, Department of Physics and Materials Science, University of Memphis, YING LI, CHRISTOS ARGYROPoulos, Department of Electrical and Computer Engineering, University of Nebraska-Lincoln, THANG HOANG (Presenter), Department of Physics and Materials Science, University of Memphis — The radiative processes of a quantum emitter can be profoundly altered by its surrounding photonic environment. In this report we explore fundamentals of the light-matter interactions between quantum emitters (such as semiconductor quantum dots or organic molecules) and periodic lattices of plasmonic nanostructures. A lattice of metallic nanostructures provide high photonic density of states via local and lattice plasmon resonances. Via computational and experimental studies, we demonstrate the emission rate enhancement of quantum emitters by integrating them with arrays of plasmonic nanostructures. A set of parameters including size, shape, and lattice constant will be discussed. In particular, an array of plasmonic nanostructures operating near their cut-off frequency can exhibit effective epsilon-near-zero which is expected to trigger both enhanced spontaneous emission and superradiance.[1] Control of radiative processes using local and lattice plasmon resonances also benefits from possibilities of leveraging multiple energy bands.


*This work is supported by the National Science Foundation (NSF) (Grant No. DMR-1709612)
4:18PM H02.00008: Topological Phononic Logic* JENNIFER WANG (Presenter), Physics, Wellesley College, HARRIS PIRIE, SHUVOM SADHUKA, JENNIFER HOFFMAN, Physics, Harvard University — Topological metamaterials have protected dissipationless boundary modes engineered from their macroscopic arrangement, rather than their microscopic constituency. They can be designed by breaking either symmetry-enforced or accidental degeneracy in Dirac metamaterials. The latter case provides greater flexibility because a large number of tuning parameters can break the degeneracy to induce a topological phase. However, the design of a topological logic element, a switch that can be controlled by the output of a separate switch, remains elusive. Here we numerically demonstrate a topological phononic logic gate by exploiting the large phase space of accidental degeneracies in a honeycomb lattice. We find that a degeneracy can be broken by six physical parameters, and we tune these parameters to create a topological phononic switch that can be triggered by ultrasonic heating. Our design scheme is directly applicable to photonic crystals and may guide future designs of electronic topological transistors [1].


*This work was supported by the Center for Integrated Quantum materials under NSF grant DMR-1231319 and by the Gordon and Betty Moore foundation under grant GBMF4546.

4:30PM H02.00009: Photonic implementation of algebraic number theory SEAN GORSKY (Presenter), FABRIZIO SGRIGNUOLI, LUCA DAL NEGRO, Boston University — We study the unique spectral and optical features of a new class of aperiodic arrays generated from the distribution of prime numbers in complex quadratic fields as well as quaternion primes. By using a multiple scattering spectral method, we have discovered several unique spectral properties, such as light localization, critical level statistics, and the existence of critical modes, i.e. extended fractal modes with long lifetime that cannot be supported in traditional systems. A systematic analysis based on LDOS calculations unveil the new functionalities of these complex aperiodic platforms for lasing applications. Our results unveil the importance of aperiodic structures characterized by a coexistence of singular and continuous spectral components for the engineering of new photonic architectures based on algebraic number theory.

4:42PM H02.00010: “Fractional Photonics”: designing light transport in complex aperiodic media LUCA DAL NEGRO (Presenter), Boston University — Space-time fractional transport equations are integro-differential equations with power-law kernels that naturally account for the non-local and memory effects that become important in strongly non-homogeneous environments. In this talk I will discuss the applications of fractional calculus methods to photonics, with emphasis on the physics of multiple light scattering in structurally-complex, aperiodic optical structures and metamaterials. I will focus on our recent results on tunable, sub-diffusive photon transport of ultra-short pulses a across deterministic aperiodic media with multifractal energy spectra and critical mode localization. I will discuss fractional photon diffusion in the presence of optically amplifying media, thus generalizing Letokhov’s treatment of non-resonant uniform random structures to disordered media with arbitrary correlations. The concept of a “fractional random laser” will be introduced along with detailed predictions on its laser threshold and dynamical behavior. The combination of fractional calculus with photonic devices represents a novel and effective approach for the engineering of complex optical structures with anomalous photon transport and amplification properties leading to enhanced light-matter interaction across multiple spectral bands.

4:54PM H02.00011: Topological Photonics* [Invited] CHE-TING CHAN (Presenter), Hong Kong University of Science and Technology — We will begin with 1D photonic crystals, in which the Zak phase of the bulk bands can be used to predict the existence of boundary modes. For 2D systems, we show that meticulously designed photonic crystals can achieve the duality condition, enabling the realization of photonic topological insulators which can be regarded as classical wave counterparts of electronic topological insulator. We will also see that symmetry-protected pseudospin states that are guided in air ican be realized simply by imposing certain special electromagnetic boundary conditions. Such systems are unique to EM wave and do not have electronic counterparts. We then discuss the realization of Weyl points in 3D photonic crystals carrying chiral structures. One-way edge modes are found on the boundary of these systems as a result of the synthetic gauge flux emerging from the Weyl nodes. These structures possess single Weyl points, including “type-II” nodes, and Weyl points with topological charges higher then one. Weyl points can also be found in some woodpile photonic crystals. The sign of topological charge will change when the constituent materials change, leading to a topological phase transition and the bands change from topologically trivial to nontrivial. We will see that Weyl-like nodal points can be found in the parameter space of a 1D photonic crystals with complex unit cells. The reflection at the surface of these photonic crystals exhibits phase vortexes, which guarantees the existence of interface states between photonic crystals and any reflecting substrates. In addition, we will see that helical structures that be used to realize three-dimension photonic Dirac points, with four-fold symmetry stabilized by electromagnetic duality symmetry. These systems carry spin-polarized surface arcs that can be realized experimentally.

*Work supported by the Hong Kong Research Grants Council (AoE/P-02/12).
2:30PM H03.00001: Surfaces of axion insulators* NICODEMOS VARNAVA (Presenter), DAVID VANDERBILT, Rutgers University, New Brunswick — Axion insulators (AXIs) are magnetic topological insulators in which the non-trivial \(Z_2\) index is protected by inversion instead of time-reversal (TR) symmetry. The naturally gapped surfaces of AXIs give rise to a half-quantized surface anomalous Hall conductivity (SAHC), but its sign cannot be determined from topological arguments. To be explicit, we construct a minimal tight-binding model on the pyrochlore lattice and investigate the all-in-all-out and ferromagnetic spin configurations. We show that the Wilson loop eigenvalues are not required to wind for an AXI in contrast with their TR-invariant cousin. We also implement a method that lets us calculate the SAHC directly, which allows us to explore how the interplay between surface termination and magnetic ordering determines the sign of the half-quantized SAHC. We find that it is possible to construct a topological state with no protected metallic states on boundaries of any dimension, although chiral hinge modes do occur for many surface configurations. Finally, we find that rotation of the magnetization by an external field offers promising means of control of chiral hinge modes, which can also appear on surface steps or where bulk domain walls emerge at the surface.

*This work was supported by grant NSF DMR-1408838.

2:42PM H03.00002: Failure of Nielsen-Ninomiya theorem and fragile topology in two-dimensional systems with space-time inversion symmetry: application to twisted bilayer graphene at magic angle* JUNYEONG AHN, SUNGJOON PARK (Presenter), BOHM-JUNG YANG, Seoul National University — We examine the band topology of two dimensional real fermions in systems with space-time inversion (STI) symmetry. We show that a two-band system with a nonzero Euler class cannot have STI symmetric Wannier representation. Moreover, a two-band system with the Euler class \(e_2\) has band crossing points whose total winding number is equal to \(2e_2\). Thus the conventional Nielsen-Ninomiya theorem fails in systems with a nonzero Euler class. We propose that the topological phase transition between insulators carrying different Euler classes can be described by pair creation and annihilation of vortices across Dirac strings.

For a multiband system, the \(Z_2\) invariant called the second Stiefel-Whitney class \((w_2)\) can be defined, which is equal to \(e_2 \mod 2\) for a 2-band system. Although \(w_2\) remains robust against adding trivial bands, it does not impose Wannier obstruction when the total number of bands is greater than two. However, when the resulting multi-band system with the nontrivial second Stiefel-Whitney class is supplemented by additional mirror and chiral symmetries, a nontrivial second order topology and the associated corner charges are guaranteed. We discuss the implications to the nearly flat bands of twisted bilayer graphene at magic angle.

*S.P. was supported by IBS- R009-D1

2:54PM H03.00003: Topological phase transitions induced by tunable magnetization direction in Chern insulators RUI-AN CHANG (Presenter), CHING-RAY CHANG, National Taiwan University — Quantum anomalous Hall effect (QAHE), the quantum Hall effect without Landau levels, has been widely studied in 2D electron systems for its nontrivial topology and promising applications in future technology. Magnetic topological insulators are very typical systems exhibiting QAHE phase [1].

With recent intense study of spintronics such as spin-orbit torque (SOT) or spin-transfer torque (STT), SOT or STT is anticipated as a proper way to manipulate the magnetization direction and trigger the topological phase transitions [2]. Following the preceding idea, we present a 2D QAHE system, possibly realizable in semiconductor heterostructure, with inversion symmetry breaking and Dresselhaus spin-orbit coupling (SOC). Topological phase diagrams are obtained by the calculation of Chern number in a totally analytical way. We find that this system is topologically trivial with in-plane magnetization and undergoes a topological phase transition that makes this system transform into a topologically nontrivial phase when the magnetization is deviated from the in-plane direction. Therefore, the control of the topological phases and corresponding chiral edge states can be achieved by tuning the magnetization degrees of freedom.

[1] Science 329 (5987), 61-64.
3:06PM H03.00004: Topological Superconductivity and Density Waves on the surface of Topological Kondo Insulator
YI LUO (Presenter), Physics and Astronomy, Johns Hopkins University, PREDRAG NIKOLIC, Physics & Astronomy, George Mason University — We study the weak-coupling instabilities in the particle-particle and particle-hole channels on the surface of a prototype Kondo topological insulator. We draw inspiration from samarium hexaboride (SmB6), and the possible observation of its correlation physics through magnetoresistance hysteresis[1]. We work on the 100-surface, which has square C4v symmetry and contains three Dirac cones (electron or hole pockets) at Γ and two X points in momentum space. For superconducting order, we find phases supporting non-zero magnetization and spin current in the ground state, with certain symmetries broken by the condensates of inter-pocket order parameters. The intra-pocket pairings in general lead to a non-zero Chern number in Bogoliubov band, hinting topological superconductivity and the presence of Majorana zero modes bounded to defects. For exciton pairings, similar symmetry breaking phases are discovered.


3:18PM H03.00005: Higher-Order Topology of Three-Dimensional Strong Stiefel-Whitney Insulators*
JUNYEONG AHN (Presenter), BOHM-JUNG YANG, Seoul National University — The Stiefel-Whitney insulator (SWI) is a two-dimensional topological phase protected by the symmetry under the combination of time reversal and a two-fold rotation C2. This phase has got attention because it shows new aspects of topological crystalline insulators such as fragile topology and higher-order topology. In this talk, we study the three-dimensional generalization of the Stiefel-Whitney insulator. We show that a C2T-symmetric insulator in 3D can have a stable topological invariant, contrary to its two-dimensional counterpart having fragile band topology. To characterize the bulk band topology further, we develop a new method based on the homotopy class of the symmetry representation for C2T in a smooth gauge, instead of examining the obstruction to constructing smooth wavefunctions compatible with the reality condition. By using the new method, we show that the 3D topological insulator, dubbed 3D strong SWI, is characterized by the quantized magnetoelectric polarizability, which induces anomalous chiral hinge states along the edges parallel to the C2 rotation axis and massless Dirac fermions on the surfaces normal to the C2 axis. This establishes that a 3D strong SWI is a second-order topological insulator.

*J.A. was supported by IBS-R009-D1.

3:30PM H03.00006: Revisiting topological property of a \((t_{2g})^5\) system with a honeycomb lattice
BEOM HYUN KIM (Presenter), School of Computational Sciences, Korea Institute for Advanced Study, KAZUHIRO SEKI, TOMONORI SHRAKAWA, International School for Advanced Studies, SEIJI YUNOKI, Computational Condensed Matter Physics Laboratory, RIKEN Cluster for Pioneering Research — Na2IrO3 is the transition-metal system with a honeycomb lattice in which five electrons per site are occupied in Ir \(t_{2g}\) bands. It was firstly proposed as a candidate to show the quantum spin Hall (QSH) phase because spin-orbital entangled \(J_{\text{eff}} = 1/2\) bands across the Fermi level can be map into the Kane-Mele model. However, its topological phase has not been reported yet. Contrarily, Na2IrO3 and its isostructural systems have turned out to be Mott insulator with antiferromagnetic order. Nevertheless, the possibility of the QSH phase in these systems is still an interesting subject. State-of-the-art structural controlling with high pressure, chemical substitution, or substrate engineering can potentially manipulate their electronic kinetics and correlation effect.

In the study, we revisit the topological property of a \((t_{2g})^5\) system with a honeycomb lattice. We explore the topological phase transition with respect to a relative strength of two types of nearest neighboring hopping channels: the hopping mediated by edge-shared ligands with pdp bonding and the direct hopping between \(t_{2g}\) orbitals with ddσ bonding. Moreover, we investigate topological properties in the presence of Coulomb repulsion with help of variational cluster perturbation theory.
prototypical TI Bi\textsubscript{2}Te\textsubscript{3} films, we find from our angle-resolved photoemission spectroscopy (ARPES) measurements of thickness (3 – 10 quintuple layers) on top of bulk Nb film. Moreover, by carefully controlling the growth conditions of the DU, DOUGLAS NATELSON, Rice University — We report preliminary shot noise measurements in InAs/GaInSb quantum well and for clarifying the pairing in these heterostructures for applications in topological quantum computing.

states in these doped TI/SC thin-film heterostructures. Our study underlines methods for realizing superconductivity in TIs ARPES and STM measurements would clarify the mechanism of coupling between the SC and the topological surface dimensions. We investigate the universal behaviour of a density-driven Chern and Z\textsubscript{2} glass transitions by carrying topological matter. In this work we introduce a scaling theory of amorphous topological phase transitions in two dimensional systems. We investigate the universal behaviour of a density-driven Chern and Z\textsubscript{2} glass transitions by carrying out a finite-size scaling analysis of topological invariants averaged over random geometries. We find that the universal properties of continuum problems can be captured by studying random geometries generated by percolation lattices. Strikingly, our results show that even for short-range hopping the topological phase may persists down to the classical site percolation threshold. Furthermore, our theory suggests that the value of the critical exponent describing the diverging localization length near the critical density is close to that of the exponent of the correlation length of the critical percolation cluster. Our theory supports the conclusion that density-driven amorphous topological transitions have their unique properties not shared by disordered systems and occupy separate universality classes.

3:54PM H03.00008: Current Noise in InAs/GaInSb Corbino structures  LOAH STEVENS (Presenter), TINGXIN LI, RUI-RUI DU, DOUGLAS NATELSON, Rice University — We report preliminary shot noise measurements in InAs/GaInSb quantum well interfaces. The band structure of these composite quantum wells is inverted, and electron and hole densities are equal at the cross point of the valence and conduction bands. The holes in the strained GaInSb layer couple strongly to the electrons in the InAs layer, opening a gap in the spectrum of the 2d bulk. At low temperatures or when gated into the appropriate regime, bulk transport is greatly suppressed as the hybridized gap is opened. Corbino disk devices consist of concentric rings, meaning no edge conduction is present. Therefore, in these structures, noise measurements examine transport through the bulk and the role played by contacting electrodes. We will compare current noise measurements of samples in the nominal Quantum Spin Hall Insulator state and in the lower-resistance, bulk transport state.

4:06PM H03.00009: Superconducting proximity effects and pairing in (Bi\textsubscript{1-x}Sb\textsubscript{x})\textsubscript{2}Te\textsubscript{3} films on niobium  JOSEPH HLEVYACK (Presenter), YANG BAI, MENG-KAI LIN, PENG CHEN, DAVID FLÖTOTTO, RO-YA LIU, Department of Physics, University of Illinois-Urbana-Champaign, AYKHIRO TSUZUKI, KOZO OKAZAKI, SHIK SHIN, Institute for Solid State Physics, The University of Tokyo, JAMES N ECKSTEIN, TAI-CHANG CHIANG, Department of Physics, University of Illinois-Urbana-Champaign — Interfacing a topological insulator (TI) with an s-wave superconductor (SC) can favor the formation of helical-Cooper pairing in the topological surface states. However, realizing this system is often challenging, due to the impracticality of growing TIs on most SCs and possibly defects and Fermi surface/lattice mismatch at the TI/SC interface. By developing a novel cleavage-based “flip chip” approach, we have successfully fabricated single-crystalline (Bi\textsubscript{1-x}Sb\textsubscript{x})\textsubscript{2}Te\textsubscript{3} thin films of a predetermined thickness (3 – 10 quintuple layers) on top of bulk Nb film. Moreover, by carefully controlling the growth conditions of the prototypical TI Bi\textsubscript{2}Te\textsubscript{3} films, we find from our angle-resolved photoemission spectroscopy (ARPES) measurements of Bi\textsubscript{2}Te\textsubscript{3}/Nb that the Fermi level can lie in the band gap, giving rise to a lightly n-doped TI on a SC substrate. Ongoing laser ARPES and STM measurements would clarify the mechanism of coupling between the SC and the topological surface states in these doped TI/SC thin-film heterostructures. Our study underlines methods for realizing superconductivity in TIs and for clarifying the pairing in these heterostructures for applications in topological quantum computing.

4:18PM H03.00010: Theory of topological glass transitions in amorphous topological matter  ISAC SAHLBERG, Department of Physics, Tampere University, ALEX WESTSTRÖM, KIM PÖYHÖNEN, Aalto University, TEEMU OJANEN (Presenter), Department of Physics, Tampere University — Amorphous systems have recently been identified as promising platforms for topological matter. In this work we introduce a scaling theory of amorphous topological phase transitions in two dimensional systems. We investigate the universal behaviour of a density-driven Chern and Z\textsubscript{2} glass transitions by carrying out a finite-size scaling analysis of topological invariants averaged over random geometries. We find that the universal properties of continuum problems can be captured by studying random geometries generated by percolation lattices. Strikingly, our results show that even for short-range hopping the topological phase may persists down to the classical site percolation threshold. Furthermore, our theory suggests that the value of the critical exponent describing the diverging localization length near the critical density is close to that of the exponent of the correlation length of the critical percolation cluster. Our theory supports the conclusion that density-driven amorphous topological transitions have their unique properties not shared by disordered systems and occupy separate universality classes.
4:30PM H03.00011: Anomalous scaling law in the quantum Hall plateau-plateau transitions of topological insulator Sn-Bi$_1$.1Sb$_{0.9}$Te$_2$S devices  
FAJI XIE (Presenter), SHUAI ZHANG, FENGQI SONG, Nanjing University — The surfaces of three dimensional topological insulators are two dimensional electron gases of Dirac fermions without electron-phonon scattering contamination. In the quantum Hall states of the surface states system, the mechanism of transport dispassion change from thermal activation to the variable range hopping at a critical temperature 20K. The quantum Hall plateau-to-plateau transition behavior in the temperature regime below 20K gives with a universal exponent $k=0.20$. It indicates that only electron-electron interaction dominates the inelastic scattering mechanism in the two dimensional topological electron system.

4:42PM H03.00012: Mirror Chern number in the hybrid Wannier representation  
TOMÁŠ RAUCH, University of Jena, Germany, THOMAS OLSSEN, Technical University of Denmark, DAVID VANDERBILT, Rutgers University, USA, IVO SOUZA (Presenter), University of the Basque Country, Spain — We formulate the mirror Chern number (MCN) of a two-dimensional insulator with reflection symmetry $M_z$ in terms of hybrid Wannier functions (the eigenfunctions of $P_zP$, the position operator projected onto the valence bands). Because $P_zP$ and $M_z$ anticommute, the spectrum of "Wannier bands" is symmetric about the mirror plane, and an excess of one mirror eigenvalue over the other in the occupied manifold leads to the appearance of flat bands on the mirror plane. (This structure is reminiscent of the energy bands of a bipartite lattice, where the Hamiltonian anticommutes with the sublattice symmetry operator.) In the absence of flat bands, pairs of dispersive bands may touch at isolated points on the mirror plane. These Dirac cones are protected by symmetry, and the MCN is given by the sum of their winding numbers. When flat bands are present the Dirac cones are no longer protected, and the MCN is related instead to the Chern number of the flat bands. In three dimensions, the present formalism reveals a simple relation between the MCNs and the quantized axion angle $\theta$, whose expression in the hybrid Wannier representation was previously obtained.

4:54PM H03.00013: Strongly enhanced Berry-dipole at topological phase transitions in BiTeI*  
JORGE FACIO (Presenter), DMITRI EFERMOV, KLAUS KOEPERNIK, JHIH-SHIH YOU, IFW - Dresden, INTI SODEMANN, Max Planck Institute for the Physics of Complex Systems, Dresden, JEROEN VAN DEN BRINK, IFW - Dresden — Transitions between topologically distinct electronic states have been predicted in different classes of materials and observed in some. A major goal is the identification of measurable properties that directly expose the topological nature of such transitions. Here we focus on the giant-Rashba material bismuth tellurium iodine (BiTeI) which exhibits a pressure-driven phase transition between topological and trivial insulators in three-dimensions. We demonstrate that this transition, which proceeds through an intermediate Weyl semi-metallic state, is accompanied by a giant enhancement of the Berry curvature dipole which can be probed in transport and optoelectronic experiments. From first-principles calculations, we show that the Berry-dipole --a vector along the polar axis of this material-- has opposite orientations in the trivial and topological insulating phases and peaks at the insulator-to-Weyl critical points, at which the nonlinear Hall conductivity can increase by over two orders of magnitude (arXiv:1805.02680).

*J.v.d.B. acknowledges support from the German Research Foundation (DFG) via SFB 1143.

5:06PM H03.00014: Contrasting the Surface Phonon Dispersion of the Topological Crystalline Insulator Pb$_{0.7}$Sn$_{0.3}$Se in its Topologically Trivial and Nontrivial Phases*  
SAMUEL KALISH (Presenter), Physics, Boston University, LUIZ SANTOS, Physics, Emory University, RAMAN SANKAR, FANGCHENG CHOU, Center of Condensed Matter Sciences, National Taiwan University, CLAUDIO CHAMON, MAGED MANSOUR EL-BATANOUNY, Physics, Boston University — We report inelastic He atom surface-scattering measurements of the (001) surface phonons dispersion of the topological crystalline insulator Pb$_{0.7}$Sn$_{0.3}$Se. Because this material exhibits a temperature-dependent topological transition, we measure the surface dispersion curves in both the trivial and topological phases. Peculiarly, most surface phonon modes appear as resonances, rather than pure surface states. We find that a vertical shear surface resonance branch around 1.9 THz dramatically changes on going from the trivial to the topological phase. We associate this remarkable change with a strong interaction of the emergent surface Dirac fermions with the modes of this branch. We use the measured dispersion of this resonance branch to determine the corresponding mode-dependent electron-phonon coupling $\lambda_m$.$(q)$.

*C.C. was supported by the U.S. Department of Energy under Grant No. DE-FG02-06ER46316. L.H.S. is supported by a fellowship from the Gordon and Betty Moore Foundations EPiQS Initiative through Grant No. GBMF4305 at the University of Illinois and by a faculty startup at Emory University.
Localization-Driven Correlated States of Two Isolated Interacting Helical Edges

YANG-ZHI CHOU

Presenter, University of Colorado, Boulder — We study the localization-driven correlated states among two isolated dirty interacting helical edges as realized at the boundaries of two-dimensional $\mathbb{Z}_2$ topological insulators. We show that an interplay of time-reversal symmetric disorder and strong inter-edge interactions generically drives the entire system to a gapless localized state, preempting all other intra-edge instabilities. For weaker interactions, an anti-symmetric interlocked fluid, causing a negative perfect drag, can emerge from dirty edges with different densities. We also study the stability of the inter-edge correlated states against finite size and/or finite temperature corrections. The corresponding experimental signatures are discussed.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H04 DMP: Dirac/Weyl Semimetals -- Type-II Topological Semimetals

Polar domains and domain walls in MoTe$_2$ with Weyl semimetallic and trivial semimetallic phases

Fei-Ting Huang (Presenter), Seong Joon Lim, Sobhit Singh, Jinwoong Kim, Department of Physics and Astronomy, Rutgers University, New Jersey, Lunyong Zhang, Laboratory for Pohang Emergent Materials and Max Planck POSTECH Center for Complex Phase Materials, Pohang University of Science and Technology, JAE-Wook Kim, David Vanderbilt, Sang-Wook Cheong, Department of Physics and Astronomy, Rutgers University, New Jersey — Quantum materials with non-trivial electronic topologies are one of the most active fields of current condensed matter research. Among them, Weyl semimetal (WSM) behavior can be realized quite generally in a semimetallic crystal with large spin-orbit coupling by breaking either time-reversal or space inversion symmetry. Interestingly, those known WSMs through the space inversion breaking mechanism often crystallize in polar structures, and thus they are polar WSMs. The question that naturally arises is the possible existence of polar domains and domain walls (DWs), which is particularly important because the Weyl points and the surface Fermi-arcs can depend on the domain reorientation and accompany with intriguing properties. Here, we focus on the type-II WSM MoTe$_2$, which has recently drawn an immense attention due to its phase tunability and unique physical properties. Utilizing in-situ cryogenic transmission electron microscopy, we unveil intriguing polar domain structures in MoTe$_2$. We also discover unexpected domain kinetics under electron beams. Using spatially resolved tunneling spectroscopy, we observe distinct electronic responses of those domains and DWs. These findings are a key step toward engineering the Weyl-node-pair-related physical properties in such polar WSMs.

Novel structure in the Mo$_{1-x}$W$_x$Te$_2$ family

Yu Tao (Presenter), John Schneeloch, Chunruo Duan, University of Virginia, Masaaki Matsuda, Sachith Dissanayake, Oak Ridge National Lab, Despina Louca, University of Virginia — Mo$_{1-x}$W$_x$Te$_2$ belongs to the family of 2-dimensional transition metal dichalcogenides that are of wide interest because of their fascinating topological properties. Mo$_{1-x}$W$_x$Te$_2$ undergoes a structural phase transition from the monoclinic 1T' phase at high temperatures, to the orthorhombic T$_d$ phase at low temperatures through a first-order structural phase transition. Both phases consist of nearly-identical layers which differ primarily by the layers' in-plane positioning. With elastic neutron scattering, we study the transition between these two structures on single crystals of MoTe$_2$ with and without W-doping. Structural changes including changes in interlayer disorder were observed from the elastic scattering along (2, 0, L) on cooling and warming through the hysteresis. We observed a thus far unreported unit cell doubling phase, T$_d$*, that emerges without disorder on warming from T$_d$ and deduced its layer stacking pattern as 'AABB' rather than the 'ABAB' and 'AAAA' orders for the 1T' and T$_d$ phases. We describe the transition in terms of a 1-dimensional Ising model whose interaction coefficients change with temperature. These results clarify in microscopic detail the nature of these phase transitions.

*This work is supported by the Department of Energy, Grant number DE-FG02-01ER45927.
Doping dependence of the sliding-layer phase transitions in (Mo,W)Te₂

JOHN SCHNEELOCH (Presenter), YU TAO, DESPINA LOUCA, CHUNRUO DUAN, University of Virginia — The electronic properties of materials composed of weakly-bound layers can change substantially depending on how the layers are stacked. For example, the monoclinic 1T' phase of MoTe₂ is reported to become a Weyl semimetal when cooled below 250 K into its orthorhombic T₉ phase, which differs from 1T' mainly by in-plane displacements of the layers. Substituting Mo for W raises the transition temperature. In this talk, we will focus on the effect of W-doping on Mo₁₋ₓWₓTe₂ crystals up to x=0.5, using neutron scattering to investigate structural changes. The transition temperature continues to increase to at least ~460 K, approximately linearly, as a function of W-doping (as estimated from the c-axis lattice constant). The monoclinic beta angle steadily decreases with doping, from 93.9 to 93.2 degrees. The T₉* phase (a thus far unreported phase which will be discussed in Yu Tao's talk) was present on warming up to x~0.3, but was not seen above this point. Some MoTe₂ crystals had broad transitions, likely due to Te vacancies; the existence of a T₉* phase in these crystals could not be determined. We discuss these tendencies and their implications for finding new phases in materials with weakly-bound layers.

*We acknowledge funding from the U.S. Department of Energy.

Fermi Surfaces and Topological Character of Dirac and Weyl Type-II Semimetals as Revealed by the de Haas-van Alphen Effect

LUIS BALICAS (Presenter), National High Magnetic Field Laboratory — The texture of the Berry phase curvature has led to the observation of novel, but controversial, electrical transport properties in the so-called topological semimetals. Examples include the so-called Weyl orbits that explore the Fermi arcs on the surfaces of Weyl semimetals, the observation a planar Hall-effect in non-magnetic compounds, or the observation of a negative magnetoresistivity ascribed to the axial current between Weyl points resulting from the suppression of their chiral symmetry. We have studied the transport properties of some of these compounds as well as their Fermi surfaces through quantum oscillatory phenomena, finding both marked disagreements with calculations and photoemission (e.g. MoTe₂), as well as good agreements (e.g. PdTe₂). Here, we will focus on the semimetals MAl₃ (where, M = V, Nb and Ta) which were predicted to be candidates for a Dirac type-II state. We find that the angular-dependence of their Fermi surface (FS) crosssectional areas reveals a remarkably good agreement with first-principle calculations. Therefore, dHvA supports the existence of tilted Dirac cones with Dirac type-II nodes located at 100, 230 and 250 meV above the Fermi level for VAl₃, NbAl₃ and TaAl₃ respectively. However, for all three compounds the cyclotron orbits on their FSs, including an orbit nearly enclosing the Dirac type-II node, yield trivial Berry phases. We explain this via an analysis of the Berry phase where the position of this orbit, relative to the Dirac node, is adjusted within the error (of ~10 meV) implied by the small disagreement between our calculations and the experiments.

*This work was supported by DOE-BES through award DE-SC0002613. A portion of this work related to two-dimensional materials was supported by US Army Research Office MURI Grant W911NF-11-1-0362 and is currently supported by NSF-DMR 1807969.

Chemical Bonding Induced Topological Lifshitz Transition in Type-II Dirac Semimetal VAl₃

YI-YUAN LIU, YU-FEI LIU, Physics, Peking University, GUI XIN, Chemistry, Louisiana State University, CHENG XIANG, HUIBING ZHOU, Physics, Peking University, WEIWEI XIE, Chemistry, Louisiana State University, CHUANG-HAN HSU, Physics, National University of Singapore, HSIN LIN, Institute of Physics, Academia Sinica, TAY-RONG CHANG, Physics, National Tsing Hua University, SHUANG JIA (Presenter), Physics, Peking University — We report a chemical bonding induced Lifshitz transition of Ti₁₋ₓVₓAl₃ in which the compounds evolve from p-type trivial metal to n-type robust Dirac semimetal. This topological transition is concomitant with an anomalous structural distortion which stems from the interplanar V-Al bond formation. The V-Al bonds in Ti₁₋ₓVₓAl₃ are built up as long as the bonding orbitals of V atoms are fully populated by the electrons. In other words, the type-II Dirac semimetal state of VAl₃ is protected by the V-Al bonds whose molecular orbitals are the “gravity center” of the topological electron and hole bands.

*This work was supported by the National Natural Science Foundation of China No.11774007 and No. U1832214, the National Key R&D Program of China (2018YFA0305601) and the Strategic Priority Research Program of Chinese Academy of Sciences, Grant No. XDB28000000. T.-R.C. were supported by the Ministry of Science and Technology under MOST Young Scholar Fellowship: the MOST Grant for the Columbus Program NO. 107-2636-M-006-004-, National Cheng Kung University, Taiwan, and National Center for Theoretical Sciences (NCTS), Taiwan.
3:54PM H04.00006: Fermiology and evidence of conventional superconductivity in the type-II Dirac semimetal PdTe₂ AMIT VASHIST (Presenter), RADHA KRISHNA GOPAL, YOGESH SINGH, Department of Physical Sciences, Indian Institute of Science Education and Research, Mohali — We use electrical transport and heat capacity measurements on high-quality single crystals of the recently discovered superconducting type-II Dirac semimetal PdTe₂, to probe the nature of its superconducting phase. The magnitude of the electronic heat-capacity anomaly at Tc, the low temperature exponential T dependence of the heat capacity, the linear H dependence of the T = 0 electronic Somerfield coefficient, and a conventional H − T phase diagram establish that the superconductivity in PdTe₂ is conventional in nature despite the presence of a topologically nontrivial Fermi surface band, which contributes to the electrical conduction. The Fermi surface of PdTe₂ is investigated by the dHvA oscillations.

4:06PM H04.00007: Topological Nontrivial Surface Plasmon on a Type-II Weyl Semimetal XUN JIA (Presenter), XUETAO ZHU, JIANDONG GUO, Institute of Physics, Chinese Academy of Sciences — Type-II Weyl semimetals (WSMs), with the Lorentz invariance broken and hosting tilted Weyl cones giving rise to non-point-like Fermi surfaces (FSs), have attracted plentiful attention recently. The orthorhombic phase of (W, Mo)Te₂ is predicted to be a prototypical system of Type-II WSM. However, the topological signatures are not clear enough from the single-electron measurements due to its complicated band structure. Meanwhile, measurements of electronic collective excitations (i.e. plasmons) in topological bands may provide more evidence of the topological nature, since they possess some exotic properties distinct from those in standard electron gases. Here, using momentum resolved inelastic electron scattering, we report an observation of a topological nontrivial surface plasmon mode originated from the topological bands of MoTe₂, which displays unique super-linear temperature-dependence matching the predictions for that in a WSM. Moreover, the damping of this nontrivial mode matches well with the boundary of electron-hole particle continuum from Weyl band. These findings provide consolidated evidences of the existence of topological nontrivial bands in MoTe₂.

4:18PM H04.00008: Inversion Symmetry Breaking in the Monoclinic Phase of MoTe₂* CHUNRUO DUAN (Presenter), JOHN SCHNEELOCH, YU TAO, University of Virginia, JUNJIE YANG, Central Michigan Univ, XIAOPING WANG, FENG YE, Oak Ridge National Laboratory, DESPINA LOUCA, University of Virginia — Among the layered material transition metal dichalcogenides, MoTe₂ shows a complex phase diagram and many interesting properties such as magnetoresistance, superconductivity, and potentially Weyl semimetal property. If synthesized by furnace cooling, MoTe₂ is stabilized in a hexagonal phase (2H). Quenching from above 1000 °C results in a metastable monoclinic phase (1T'), which becomes orthorhombic (Td) in a first order phase transition when cooled below room temperature. The phase transition is accomplished through layer shifting along the monoclinic tilting direction, and the structure within each layer is not changed. The reported crystal structures indicate that the layer shifting from 1T' (P2₁/m) to Td (Pnm2₁) breaks the inversion symmetry and allows the Weyl physics to emerge. Single crystal neutron diffraction performed at SNS, ORNL provided evidence on a lower symmetry (P2₁) in the 1T' phase which is non-centrosymmetric. Ab initio calculations and molecular dynamics simulations based on the refined structure will be discussed.

*This work has been supported by the Department of Energy, Grant number DE-FG02-01ER45927.

4:30PM H04.00009: Pressure evolution of the low temperature crystal structure of superconducting Weyl semimetal candidate MoTe₂ COLIN HEIKES (Presenter), National Institute of Standards and Technology, I-LIN LIU, Center for Nanoscale and Advanced Materials, University of Maryland, TANER YILDIRIM, NICHOLAS BUTCH, WILLIAM RATCLIFF, National Institute of Standards and Technology — Orthorhombic MoTe₂ has been proposed to be a type II Weyl semimetal. This classification is supported by the observation of rare topological phenomena such as Fermi arcs and Weyl nodes through ARPES measurements. Superconductivity is also observed in this material, with a drastic pressure enhancement of the superconducting transition temperature often associated with a first-order structural transition from the non-centrosymmetric orthorhombic phase to a centrosymmetric monoclinic phase with uncertain band topology. I will discuss the temperature-pressure structural phase diagram of this system as determined by neutron scattering at conditions relevant for superconductivity. I will also comment on possible implications of the structural evolution on the ground state electronic structure.
4:42PM H04.00010: Anomalous Transport Properties in Dirac/Weyl Semimetals [Invited]  TIAN LIANG (Presenter), RIKEN — Topological semimetals, notably Dirac/Weyl semimetals have become one of the central fields in modern physics. In this talk, I will talk about two examples of Dirac/Weyl semimetals, ZrTe5 [1] and PbSnTe under pressure [2]. In ZrTe5, in-situ double-axis rotator was employed to detect the full 4π solid angular dependence of the anomalous Hall signals, or effectively the strength of the Berry curvature. Interestingly, the system shows large in-plane anomalous Hall signals, the direct evidence of the Berry curvature coming from the Weyl nodes. In order to further investigate and manipulate the Weyl nodes in the momentum space, pressure measurements of Pb1−xSnxTe were performed. Using pressure to tune the gap, we have tracked the nucleation of a Fermi surface droplet that rapidly grows in volume with P. In the metallic state, we observe a large Berry curvature, which dominates the Hall effect. The results confirm the existence of a topological metallic phase protected by the Weyl nodes over a finite pressure interval. [1] T. Liang et al., Nat. Phys. 14, 451 (2018) [2] T. Liang et al., Sci. Adv. 3, e1602510 (2017)

5:18PM H04.00011: Electronic structure of the candidate Weyl phase in MoTe2  I-LIN LIU (Presenter), University of Maryland, College Park, COLIN HEIKES, NIST, CHRIS ECKBERG, University of Maryland, College Park, NICHOLAS BUTCH, WILLIAM RATCLIFF, NIST, JOHNPIERRE PAGLIONE, University of Maryland, College Park — Orthorhombic MoTe2 has been proposed to be a type II Weyl semimetal. This classification is supported by the observation of rare topological phenomena such as Fermi arcs and Weyl nodes through ARPES measurements. A first-order structural transition from the centrosymmetric monoclinic phase at room temperature to the orthorhombic phase, without inversion symmetry, was found through both magnetoresistance and neutron scattering measurements. I will discuss quantum oscillations measurements and their ramifications for the electronic band structure, and how this relates to the topological state and corresponding novel quantum phenomena

Tuesday, March 5, 2019 2:30 PM - 5:18 PM

Session H05 DMP: Topological Superconductivity: 2D, Junctions BCEC 108 - Adrian Feiguin, Northeastern University - Tag(s): Focus

2:30PM H05.00001: Emergent two-dimensional superconductivity in few-layer stanene [Invited]  DING ZHANG (Presenter), State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University — The two-dimensional crystalline superconductors possess a variety of exotic properties such as the Griffiths singularity, the quantum metal phase as well as the strongly enhanced in-plane critical field [1]. Here we report the discovery of superconductivity in few layer stanene—ultrathin gray tin (111)—and the complete phase diagram in the magnetic field and temperature plane. The emergence of superconductivity in stanene is unexpected. Bulk gray tin is non-superconductive [1] and stanene attracts attention mostly because of its topological properties. Instead, we found superconductivity by growing few-layer stanene on PbTe/Bi2Te3/Si(111) substrate via molecular beam epitaxy [2][3]. The superconducting properties can be further modulated by varying the substrate thickness. Our experimental studies are further supported by first-principles calculations, which suggest that superconductivity occurs in a doped quantum spin Hall insulator.

References

3:06PM H05.00002: Growth and low temperature STM study of Stanene  JINFENG JIA (Presenter), Shanghai jiao Tong University — Stanene and its derivatives can be 2D topological insulators (TI) with a very large band gap as proposed by first-principles calculations, or can support enhanced thermoelectric performance, topological superconductivity and the near-room-temperature quantum anomalous Hall (QAH) effect. Here, we report a successful fabrication of 2D stanene by MBE. The atomic and electronic structures determined by STM and ARPES agree well with the predictions by first-principles calculations. Bulk band gap and edge states are also observed. On stanene thicker than 2 layers, superconductivity is also observed, which suggests stanene is a good candidate for topological superconductor.
3:18PM H05.00003: Tracking the motion of Josephson vortices and the Majorana fermion states bound to them in S-TI-S junctions networks designed for braiding*  
GILBERT ARIAS (Presenter), ERIK HUEMILLER, CHAD GERMANY, GUANG YUE, JESSICA H MONTONE, DALE J VAN HARLINGEN, Physics, University of Illinois Urbana Champaign — Networks of S-TI-S (Superconductor-Topological Insulator-Superconductor) lateral Josephson junctions provide a potential platform for nucleating, manipulating, and braiding Majorana fermion states (MFs) for quantum information processing. In this system, the MFs are bound to the cores of Josephson vortices where the phase difference across the junction is an odd multiple of \( \pi \) and can be manipulated by moving the vortices. To assist in the design of braiding circuits, we are exploring ways to monitor the position of Josephson vortices in junction networks. A direct approach is to image the location of the vortices via Scanning SQUID Microscopy (SSM), for which we are developing an ultralow temperature SSM with sub-micron resolution based on a pickup coil fabricated by electron-beam lithography and focused ion-beam etching and an optical interferometer approach mechanism. We can also indirectly determine the vortices configuration by measuring the modulation of the supercurrent vs. magnetic field modulation patterns. We report on progress toward implementing these techniques.

*NSF DMR 17-45304, DOE DE-SC0017888

3:30PM H05.00004: Electron waiting times in hybrid junctions with topological superconductors*  
SHUO MI (Presenter), INAC/PHELIQS/GT, Grenoble Alpes University, PABLO BURSET, CHRISTIAN FLINDT, Department of Applied Physics, Aalto University — We investigate the waiting time distributions (WTDs) of superconducting hybrid junctions, considering both conventional and topologically nontrivial superconductors hosting Majorana bound states at their edges. To this end, we employ a scattering matrix formalism that allows us to evaluate the waiting times between the transmissions and reflections of electrons or holes. Specifically, we analyze normal-metal--superconductor (NIS) junctions and NISIN junctions, where Cooper pairs are spatially split into different leads. The distribution of waiting times is sensitive to the simultaneous reflection of electrons and holes, which is enhanced by the zero-energy state in topological superconductors. For the NISIN junctions, the WTDs of trivial superconductors feature a sharp dependence on the applied voltage, while for topological ones they are mostly independent of it. This particular voltage dependence is again connected to the presence of topological edge states, showing that WTDs are a promising tool for identifying topological superconductivity.

*European Union's Horizon 2020 research and innovation program under Marie-Curie Grants No. 753906 and No. 743884, Academy of Finland (Research Council for Natural Sciences and Engineering) No. 312299

3:42PM H05.00005: Study of Josephson trijunction constructed on Bi\(_2\)Te\(_3\) surface  
GUANG YANG (Presenter), ZHAOZHENG LYU, JUNJUA WANG, JIANGHUA YING, XIANG ZHANG, GUANGTONG LIU, JIE FAN, ZHONGQING JI, XIUNIAN JING, FANMING QU, LI LU, Institute of Physics, Chinese Academy of Sciences — In 2008, Fu and Kane proposed that Josephson trijunctions constructed on the surface of topological insulators could host Majorana zero modes [1]. Such trijunctions could potentially serve as the basic components in a two-dimensional platform for realizing universal topological quantum computing [2]. In this talk, we will present the results of experimental investigations on trijunctions constructed on the surface of Bi\(_2\)Te\(_3\). And we will compare the experimental results with Fu and Kane's theory as well as with the results of numerical simulations based on a lattice model.


3:54PM H05.00006: Observation of perfect Andreev reflection due to Klein paradox in a topological superconducting state in SmB\(_6\)/YB\(_6\) heterostructures*  
SEUNGHUN LEE (Presenter), VALENTIN STANEV, XIAOHANG ZHANG, JOSHUA S HIGGINS, VICTOR M YAKOVENKO, JOHNPIERRE PAGLIONE, RICHARD L. GREENE, VICTOR GALITSKI, ICHIRO TAKEUCHI, University of Maryland, College Park — Topological insulator, whose boundary states are described by the massless Dirac equation, is of great interest to realize unusual states of quantum matter. We report the observation of perfect Andreev reflection as a manifestation of Klein tunneling (perfect transmission of massless Dirac particles through any potential barrier) at the interface between a normal metal and a SmB\(_6\)/YB\(_6\) heterostructure. We have previously demonstrated proximity-induced superconductivity in the surface state of SmB\(_6\). Conductance spectra of point contact junctions between a Ptn tip and the surface of the superconducting SmB\(_6\) show perfect conductance doubling within the induced superconducting gap (\( \Delta \)). The absence of electron reflection under such finite Z is attributed to the interplay of the Dirac material in Andreev reflection process i.e., Klein tunneling. The observation can be described by a modified BTK theory with Dirac Hamiltonian, Dirac-BTK theory.

*This work was funded by ONR N00014-13-1-0635, ONR N00014-15-1-2222, AFOSR No. FA9550-14-10332, and C-SPIN.
4:06PM H05.00007: Meissner screening of Proximity coupled Topological Insulator/Superconductor Heterostructures* SEOKJIN BAE (Presenter), SEUNGHUN LEE, ICHIRO TAKEUCHI, STEVEN ANLAGE, University of Maryland, College Park — Meissner screening of proximity coupled SmB$_6$/YB$_6$ topological insulator-superconductor (TI/SC) thin-film bilayers is studied through the temperature dependence of the effective penetration depth. A microwave resonator technique is used in which the bilayers are exposed to the rf magnetic field. The study is conducted by systematically varying the thickness of the SmB$_6$ layer on top of the YB$_6$ layer. Unconventional thickness dependence of the temperature profile of the effective magnetic penetration depth of the TI/SC bilayer is observed, which is distinctly different from that of the conventional metal/superconductor bilayers. This provides evidence for Meissner screening in the presence of bulk insulating states in the SmB$_6$. Through an electromagnetic screening model, key parameters such as normal screening length, normal coherence length, thickness of the surface states, and Fermi velocity of SmB$_6$ are extracted and found to be in reasonable agreement with previous studies.

*This work is supported by NSF Grant DMR-1410712, DOE Grants DE-SC 0012036T, DE-SC 0018788

4:18PM H05.00008: Experimental evidence of proximity induced odd-frequency superconductivity in a topological insulator* JONAS KRIEGER, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, SEAN GIBLIN, School of Physics and Astronomy, Cardiff University, THOMAS PROKSCHA, ANDREAS SUTER, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, THORSTEN HESJEDAL, Department of Physics, University of Oxford, ZAHER SALMAN (Presenter), Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute — At an interface between a topological insulator (TI) and a conventional superconductor, the topological surface states have been predicted to rearrange in an interesting fashion. The induced superconductivity between an s-wave superconductor and a TI surface state is expected to develop a complex p-wave order parameter which may allow to create a Majorana Fermions inside the core of a vortex. These collective excitations are their own antiparticles and are the basic element in a proposal for fault-tolerant quantum computing. Here we present experimental evidence for proximity induced superconductivity in a thin layer of the TI Bi$_2$Se$_3$ grown on top of Nb. From depth-resolved measurements in the Meissner state, we observe a local enhancement of the magnetic field in Bi$_2$Se$_3$ that exceeds the externally applied field, thus supporting the existence of an intrinsic paramagnetic Meissner effect arising from an odd-frequency superconducting state.

*This work is supported by the Swiss National Science Foundation (SNF-Grant No. 200021_165910).

4:30PM H05.00009: How to systematically map out a Majorana island* JIE SHEN (Presenter), FRANCESCO BORSOI, SEBASTIAN HEEDT, Delft University of Technology, BERNARD VAN HECK, Station Q, Microsoft Research, SASA GAZIBEGOVIC, ROY L. M. OP HET VELD, Eindhoven University of Technology, JOHN A LOGAN, MIHIR PENDHARKAR, University of California, Santa Barbara, MARINA QUINTERO PEREZ, Station Q, Microsoft Research, NICK VAN LOO, Delft University of Technology, ALEXANDRA FURSINA, KEVIN VAN HOOGDALEM, Station Q, Microsoft Research, CHRIS PALMSTROM, University of California, Santa Barbara, ERIK P. A. M. BAKKERS, Eindhoven University of Technology, LEO KOUWENHOVEN, Station Q, Microsoft Research — As a high-quality hybrid system, InSb nanowires with epitaxial-grown Al shells reveal ballistic superconductivity and quantized zero-bias conductance peak. This holds great promise for the realization of Majorana-based topological quantum computing. Building block for a topological qubit is a superconductor-semiconductor island hosting a pair of Majorana zero modes (called Majorana island). The state of the topological qubit is the combination of the even/odd parity of such Majorana islands. Therefore, to understand the status of the topological qubit, systematic studies of a Majorana island are crucial. First, by performing tunnelling spectroscopy measurements, we use the ballistic superconductivity and quantized zero-bias peak to support the high-quality and potential ‘Majorana’ properties of the island. Secondly, the even-odd ground state phase diagram as a function of chemical potential is mapped out and provides a guideline for the topological qubit. Thirdly, how the superconducting gap and effective g-factor influence the phase diagram is also studied. Such a systematic mapping of the Majorana island is also suitable for double islands, leading towards topological qubits based on multiple islands.

*Dutch Organization for Scientific Research and Microsoft Corp. Station Q.
4:42PM H05.00010: Realization of Majorana Zero Modes within a Topological Hinge State* BERTHOLD JAECK (Presenter), YONGLONG XIE, Princeton University, JIAN LI, Westlake Institute for Advanced Study, SANGJUN JEON, ANDREI B BERNEVIG, ALI YAZDANI, Princeton University — Higher order topological insulators (HOTI) host helical edge modes along its hinges that are protected by crystal and time-reversal symmetry. Proximity induced superconductivity on these hinge states is predicted to be topological in nature and provides a platform for the realization of Majorana zero modes (MZM). Theoretical modeling shows the emergence of MZMs in the hinge states at an interface where they are influenced by superconductivity and magnetism. Recently, bismuth was identified as a HOTI where scanning tunneling microscopy (STM) studies revealed the existence of hinge states on its surface (1). To realize this MZM platform, we grow bismuth thin films and iron clusters on a niobium surface. Using high-resolution spectroscopic mapping and spin-polarized STM, we characterize the influence of superconductivity and magnetism on the hinge states. Our measurements show the presence of localized zero energy states at the interface between superconducting hinge states and the iron clusters. Comparing various measurements with theoretical models, we will discuss how our observations are consistent with the presence of MZM.


*This work is supported by the ONR, the Moore foundation, NSF-DMR, NSF-MRSEC & the Humboldt foundation

4:54PM H05.00011: Radio frequency methods for Majorana based quantum computing: fast charge sensing and phase diagram mapping* DAVYDAS RAZMADZE (Presenter), DEIVIDAS SABONIS, FILIP MALINOWSKI, GERBOLD MENARD, Center for Quantum Devices, Niels Bohr Institute, SEBASTIAN PAУKA, ARC Centre of Excellence for Engineered Quantum Systems, The University of Sydney, HUNG NGUYEN, DAVID VAN ZANTEN, Eoin C O'FARREL, Judith Tabea Suter, Peter Kroegstrup, Ferdinand Kuemmeth, Charles M Marcus, Center for Quantum Devices, Niels Bohr Institute — We employ radio frequency techniques to demonstrate two measurements: first, by embedding an InAs/Al nanowire directly into a resonant circuit, it is possible to map key features of the conductance vs. gate-voltage phase diagram approximately 40 times faster than conventional lock-in methods; second, by capacitively coupling the same nanowire to a radio-frequency single electron transistor, fabricated from another nanowire, we demonstrate detection of single electron inter-island transitions, with signal-to-noise ratios exceeding 5 for an integration time below 1 μs at axial (parallel to nanowire) magnetic fields of 0.6T. Latter results will be the requirements for implementing Majorana based quantum computation in hybrid superconductor-semiconductor nanowire devices, and demonstrates the full compatibility of the high-bandwidth sensing techniques. Presented device geometries are similar to that have previously shown signatures of Majorana-like bound states.

*Research is supported by Microsoft Project Q, the Danish National Research Foundation and by the Australian Research Council Centre of Excellence for Engineered Quantum Systems (project ID CE170100009). CMM acknowledges support from the Villum Foundation.

5:06PM H05.00012: Advanced hybrid InSb/Al nanowires devices for topological parity readout (Part 1)* FRANCESCO BORSOI (Presenter), SEBASTIAN HEEDT, JIE SHEN, SENJA RAMAKERS, KUN ZUO, Delft University of Technology, QuTech, KEVIN VAN HOOGDALEM, MARINA QUINTERO PEREZ, Microsoft Station Q Delft, SASA GAZIBEGOVIC, ROY L. M. OP HET VELD, Eindhoven University of Technology, Department of Applied Physics, JOHN A LOGAN, MIHIR PENDHARKAR, University of California Santa Barbara, Materials Engineering, BERNARD VAN HECK, Microsoft Station Q Santa Barbara, CHRIS PALMSTROM, University of California Santa Barbara, Materials Engineering, ERIK P. A. M. BAKKERS, Eindhoven University of Technology, Department of Applied Physics, LEO P KOUWENHOVEN, Microsoft Station Q Delft — Majorana bound states (MBS) in hybrid semi-superconducting systems have been proposed to be the building blocks of the next quantum computers. Quantum information can be stored in the fermionic parity degree of freedom, shared in two well-separated MBS. A promising method to readout such parity is to measure the conductance through an Aharonov-Bohm (AB) interferometer, hosting a pair of MBS in one of the interfering arms. Here, we report our progress in the realization of such device based on InSb/Al islands. We first investigate the electron-phase evolution in a normal quantum dot embedded in an InSb nanowire network by mapping the phase of AB oscillations. Phase lapse and winding are extracted from the shift of these oscillations and from the associated Fano effect. Secondly, we study the energy spectrum of proximitized InSb nanowires in Coulomb blockade revealing gate-dependent ground state parity transitions as a function of magnetic field. Based on these results and on the development of a new nanofabrication technique, interferometric readout can be performed in both nano-networks and single-nanowire architectures.

*European Research Council, Dutch Organization for Scientific Research, Office of Naval Research, Laboratory for Physical Sciences, Microsoft Corp. Station Q.
2:30PM H06.00001: Intermediate gapless phase and topological phase transition of the Kitaev model in a uniform magnetic field* SHUANG LIANG (Presenter), MING-HONG JIANG, WEI CHEN, JIAN-XIN LI, QIANG-HUA WANG, Physics, Nanjing University and National Laboratory of Solid State Microstructures — We study the Kitaev model in a [001] magnetic field employing the mean-field theory(MFT) in the Majorana fermion representation. We discover a robust gapless regime in the intermediate magnetic field for both gapless and gapped antiferromagnetic(AFM) Kitaev models with \( J_x = J_y \) before the system is polarized in a high magnetic field. A topological phase transition connecting two gapless phases with a nodal line phase takes place at a critical magnetic field \( h_{c1} \) in this regime. While the nodal line phase at \( h_{c1} \) disappears when the mirror symmetry \( J_x = J_y \) is broken, the nodal point gapless phase can exist at intermediate fields even without the mirror symmetry. We reveal that the phase evolution of the system in the magnetic field is driven by the competition between the magnetic field and the particle-hole asymmetry of the normal state of the BdG Hamiltonian. For the ferromagnetic case, there is no intermediate phase transition before polarization. The above phase diagrams are confirmed by dynamical MFT results.

*NSF of China under Grants No. 11504195 (W.C.), No.11774152 (J.X.L.), and No. 11574134 (Q.H.W.); The National Key Projects for Research and Development of China under Grants No. 2016YFA0300401 (J.X.L. and Q.H.W.); A grant from Jiangsu Province Educational Department (W.C.).

2:42PM H06.00002: Majorana representations of spin and an alternative solution of the Kitaev honeycomb model* JIANLONG FU (Presenter), School of Physics and Astronomy, University of Minnesota, JOHANNES KNOLLE, Blackett Laboratory, Imperial College London, NATALIA PERKINS, School of Physics and Astronomy, University of Minnesota — Based on the Dirac spinor representation of the SO(4) group, we discuss the relationship between three types of representation of spin in terms of Majorana fermions, namely the Kitaev representation, the SO(3) representation, and the SO(4) chiral representation. Comparing the three types, we show that the Hilbert space of the SO(3) representation is different from the other two by requiring a pairing of sites, but it has the advantage over the other two in that no unphysical states are involved. As an example of its application, we present an alternative solution of the Kitaev honeycomb model. Our solution involves no unphysical states which enables a systematic calculation of physical observables. Finally, we discuss an extension of the model to a more general exactly soluble \( \mathbb{Z}_2 \) gauge theory interacting with complex fermions.

*We acknowledge the support from NSF DMR-1511768 Grant

2:54PM H06.00003: Algebraic Quantum Spin Liquid from an Exactly Solvable Spin-1/2 Kitaev Model JIAN-JIAN MIAO (Presenter), Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, HUI-KE JIN, Zhejiang University, FU-CHUN ZHANG, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, YI ZHOU, Zhejiang University — We propose an exactly solvable quantum spin-1/2 model with time reversal invariance on a two dimensional brick-wall lattice, where each unit cell consists of three sites. We find that the ground states are algebraic quantum spin liquid states. The spinon excitations are gapless and the energy dispersion is linear around two Dirac points. The ground states are of three-fold topological degeneracy on a torus. Breaking the time reversal symmetry opens a bulk energy gap and the \( \mathbb{Z}_2 \) vortices obey non-Abelian statistics.
3:06PM H06.00004: Topological superconductivity in the Kondo-Kitaev model*  WONJUNE CHOI (Presenter), Physics, University of Toronto, PHILIPP WILHELM KLEIN, ACHIM ROSCH, Physics, University of Cologne, YONG-BAEK KIM, Physics, University of Toronto — We investigate possible topological superconductivity in the Kondo-Kitaev model on the honeycomb lattice, where the Kitaev spin liquid is coupled to conduction electrons via the Kondo coupling. The self-consistent mean-field theory gives three distinct quantum phases as the Kondo coupling is increased: the fractionized Fermi liquid, where the Kitaev spin liquid and conduction electrons remain decoupled, the ferromagnetic topological superconductor with a single chiral Majorana edge mode, and the paramagnetic topological superconductor with a single pair of helical Majorana edge modes. In this talk, we discuss the connection between topological nature of the Kitaev spin liquid and two emergent topological superconductors obtained in this model. These findings offer a novel route to topological superconductivity in the Kondo lattice system.

*This work was supported by the NSERC of Canada and Center for Quantum Materials at the University of Toronto (W.C. and Y.B.K.), and DFG Project C02 of CRC1238 (P.W.K. and A.R.). P.W.K. acknowledges support from the German Academic Scholarship Foundation and the Bonn-Cologne Graduate School of Physics and Astronomy (BCGS).

3:18PM H06.00005: Emergent interacting two-fluids in a disordered Hubbard model*  KYUNGMIN LEE (Presenter), Ohio State University, AAVISHKAR PATEL, Harvard University, NANDINI TRIVEDI, Ohio State University, SUBIR SACHDEV, Harvard University — Recently a number of theoretical studies of models containing lattices of Sachdev-Ye-Kitaev (SYK) islands have brought in a fresh perspective on the problem of non-Fermi liquids. Motivated especially by a two-fluid model, with localized SYK islands and itinerant fermions, that captures the physics of the ‘‘strange’’ metal state of high temperature superconductors, here we discuss the possibility of such a separation of fermionic degrees of freedom starting from a disordered Hubbard model. Our numerical studies indicate that a disordered Hubbard model can lead to the emergence of localized SYK-like islands that interact with itinerant fermions. We also discuss the implications of disorder of the temperature-dependent transport properties.

*K. L. and N. T. have been supported by the National Science Foundation Grant No. DMR-1629382. A.A. P. and S. S. have been supported by the Department of Energy Grant No. DE-SC0019030.

3:30PM H06.00006: Many-body localization in a modified SYK model  HANTENG WANG (Presenter), ALEX KAMENEV, University of Minnesota — We investigate the many-body spectrum and eigenfunctions of Sachdev-Ye-Kitaev model with additional random hopping terms. To preserve the symmetry class of the original model, the additional term we add is the square of standard two Majorana hopping which is integrable on its own. We examine the level statistics of the many-body energy spectrum of this model numerically and find the crossover from Poisson statistics to Wigner-Dyson statistics when tuning the total energy of the system with finite number of Majorana. We study relations of the transition in level statistical transition to Anderson localization in the Fock space by examining the inverse partition ratios (IPR) and information entropy of the eigenstates with different total energy. Fitting IPR and information entropy with a scaling ansatz, one can access degree of the Fock space localization of the many-body eigenstates. We found that there exist three different regimes: ergodic delocalized, non-ergodic delocalized and localized, which closely resembles findings for the Anderson model on Bethe lattice and random regular graphs.

3:42PM H06.00007: Strong impact of all-in all-out magnetic order on magnetic and lattice dynamics in pyrochlore iridates studied by Raman spectroscopy*  KENTARO UEDA (Presenter), RYOMA KANEKO, University of Tokyo, ALASKA SUBEDI, Universite Paris-Saclay, MATTEO MINOLA, Max-Planck-Institut, BUMJOON KIM, Pohang University, JUN FUJIOKA, University of Tsukuba, YOSHINORI TOKURA, University of Tokyo, BERNHARD KEIMER, Max-Planck-Institut — We perform Raman spectroscopy on pyrochlore Eu2Ir2O7 which undergoes a paramagnetic-to-antiferromagnetic transition, as well as paramagnetic counterpart Pr2Ir2O7. The first polarization analysis combined with density functional theory allows us to assign all observed peaks to six optical phonons without any ambiguity. An additional peak clearly shows up below the transition temperature TN at 210 cm-1 which is reasonably close to the single-magnon excitation energy estimated from the resonant inelastic x-ray scattering. Simultaneously, the Eg phonon, involving Ir-O-Ir bond bending motion, exhibits a remarkable softening by 35 cm-1 that is by one order of magnitude larger than those in 3d magnets. These findings imply that the magnon-phonon coupling is unconventionally strong in this system, and intriguingly, the combination of the antiferromagnetic super-exchange and Dzyaloshinskii-Moriya interaction can play a vital role in the all-in all-out magnetic order, providing an important insight into the exotic phase transition in 5d transition metal oxides.

*This work is supported by JSPS Grant-in-Aid for Scientific Research (No. 26103006, No. 24224009, 18H04214, and 16H00981) and by PRESTO (No. JPMJR15RS) and CREST (No. JPMJCR16F1 and JPMJCR1874) in Japan.
3:54PM H06.00008: Linear magnetoresistance in the all-in-all-out antiferromagnet Cd$_2$Os$_2$O$_7$  
YISHU WANG (Presenter), The Johns Hopkins University, YEJUN FENG, Okinawa Institute of Science and Technology Graduate University, FELIPE GOMEZ, DANIEL SILEVITCH, California Institute of Technology, JIAQIANG YAN, Oak Ridge National Lab, DAVID GEORGE MANDRUS, University of Tennessee, Knoxville, PATRICK LEE, Massachusetts Institute of Technology, THOMAS F ROSENBAUM, California Institute of Technology — The pyrochlore Cd$_2$Os$_2$O$_7$ undergoes a metal-insulator transition at 227 K, concomitant with a formation of all-in-all-out magnetic ordering. Here, we explore the magnetoresistance associated with this magnetic order, which manifests an odd-parity linear functional form. This form, recently reported in the related compounds Eu$_2$Ir$_2$O$_7$, is allowed by the Onsager relationship for antiferromagnetic materials; however the microscopic origin is still unclear. By systematically studying a range of galvanomagnetic measurement configurations, we are able offer potential mechanisms for understanding this linear magnetoresistance involving transport both in the bulk and along the magnetic domain walls.

4:06PM H06.00009: Visualizing Kondo lattice behavior in the frustrated pyrochlore iridate Pr$_2$Ir$_2$O$_7$ using scanning tunneling spectroscopy and machine learning*  
MARIAM KAVAI (Presenter), KYLE G SHERMAN, JUSTIN LESHEN, JOEL FRIEDMAN, IOANNIS GIANNAKIS, Binghamton University, SATORU NAKATSUJI, Advanced Materials Science, The University of Tokyo, MICHAEL J LAWLER, PEGOR AYNAJIAN, Binghamton University — Pyrochlore iridates have attracted great interest due to their geometrically frustrated lattice with potential for realizing metallic spin liquid behavior. Pr$_2$Ir$_2$O$_7$ is uniquely located near the quantum critical point of antiferromagnetic metal to insulator transition. We carried out STM experiments on the [111] Kagome surface of the pyrochlore iridate Pr$_2$Ir$_2$O$_7$. STM topographs show the six-fold atomic structure expected from the [111] surface demonstrating atomic resolution STM images on a pyrochlore iridate. At low temperature, the tunneling density of states reveal Kondo behavior with Fano lineshape near the Fermi energy that exhibit strong electronic inhomogeneity. The large quantity of generated data and the intrinsic electronic inhomogeneity in this system introduce enough complexity to render conventional data analysis inadequate. Using machine learning of large data, we discover these rather seemingly random spectra to form nanoscale patterns, which may be related to electronic entanglement.

*We acknowledge support from the U.S. National Science Foundation (NSF) CAREER under award No. DMR-1654482

4:18PM H06.00010: Using quantum typicality to compute the thermodynamics of the frustrated spin compound SrCu$_2$(BO$_3$)$_2$  
ALEXANDER WIETEK (Presenter), Flatiron Institute, Simons Foundation, ANDREAS HONECKER, Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, PHILIPPE CORBOZ, Institute for Theoretical Physics and Delta Institute for Theoretical Physics, Universiteit van Amsterdam, STEFAN WESSEL, Institut für Theoretische Festkörperphysik, RWTH Aachen University, FREDERIC MILA, Institute of Physics, École Polytechnique Fédérale de Lausanne, BRUCE NORMAND, Neutrons and Muons Research Division, Paul Scherrer Institute — The concept of quantum typicality presents a novel route to computing finite temperature properties of quantum many-body systems. We demonstrate, how to use the Lanczos method in conjunction with quantum typicality to extract thermodynamic quantities at arbitrary temperatures without a full diagonalization of the Hamiltonian. This technique is applied to compute the thermodynamics of the frustrated spin compound SrCu$_2$(BO$_3$)$_2$, where recently a pressure-induced quantum phase transition has been observed. Our results are compared to Quantum Monte Carlo and iPEPS simulations.
4:30PM H06.00011: Partial order in the extended Hubbard model on a triangular lattice  MATTHEW ENJALRAN  
(Presenter), Physics, Southern Connecticut State University — The list of new materials which possess charge, spin, and orbital degrees of freedom all competing within a geometrically frustrated environment continues to grow. Such systems are intriguing because they are apt to exhibit new collective phases of matter. Theoretical work in this area has increased too, but theoretical and numerical studies of frustrated models of interacting fermions are difficult for a host of reasons. The application of mean-field theory is typically a good starting point for the study of the phase diagram of a strongly correlated many-body model. Hence, focusing on charge and magnetic degrees of freedom of fermions, we present results from Hartree-Fock calculations of the extended Hubbard model on the triangular lattice. We emphasize the case of $1/3$ filling where a finite temperature metal-insulator transition can be induced for select values of the on-site ($U$) and nearest-neighbor ($V$) Coulomb repulsions, including a phase with partial order confined to the honeycomb substructure of the parent triangular lattice.

4:42PM H06.00012: Supersymmetry in an interacting Majorana model on the kagome lattice*  CHENGSHU LI  
(Presenter), ÉTIENNE LANTAGNE-HURTUBISE, MARCEL FRANZ, University of British Columbia — We construct a supersymmetric model of interacting Majorana modes on the kagome lattice. The supersymmetry is manifest in the infinite-coupling limit, which exhibits an exponential ground state manifold separated in two parity "supersectors". An exact solution for thin torus geometries allows us to analytically construct the entire ground state manifold. Upon inclusion of weak two-fermion terms, the supersymmetry is broken for finite systems but recovered in the thermodynamic limit. We also briefly discuss the non-interacting limit of the model, which exhibits a zero-energy flat band and Majorana Chern bands.

*The work described in this article was supported by NSERC and CifAR. C. L. and É. L.-H. were also supported by the QuEst scholarship at the University of British Columbia.

4:54PM H06.00013: Majorana-Hubbard model on the triangular lattice  TARUN TUMMURU (Presenter), ALBERTO NOCERA, IAN AFFLECK, University of British Columbia — Majorana fermions are known to arise as emergent particles in certain condensed matter systems. One such realization involves inducing superconductivity on the surface of a 3-dimensional topological insulator, in the presence of a magnetic field. The resulting Abrikosov lattice has a Majorana zero mode (MZM) localized at the core of each vortex. It has been shown that the interaction between MZMs falls off exponentially with the superconducting coherence length. This enables one to write a tight-binding model to describe the system and some of these models have rich phase diagrams that exhibit emergent supersymmetry. Given that in experiments the vortex lattice usually has a triangular geometry, we construct a model for interacting MZMs in this setup. With the interaction strength as a tunable parameter, we study the phase diagram numerically using the density-matrix renormalization group.

5:06PM H06.00014: Possible gapless spin liquid in a rare-earth kagome lattice magnets Tm$_3$Sb$_3$Zn$_2$O$_{14}$*  ZHAOFENG DING  
(Presenter), YANXING YANG, JIAN ZHANG, CHENG TAN, ZIHAO ZHU, GANG CHEN, LEI SHU, Fudan University — We report the thermodynamic and muon spin relaxation ($\mu$SR) evidences for a possible gapless spin liquid in Tm$_3$Sb$_3$Zn$_2$O$_{14}$, with the rare-earth ions Tm$^{3+}$ forming a two-dimensional kagome lattice. We extract the magnetic specific heat of Tm$_3$Sb$_3$Zn$_2$O$_{14}$ by subtracting the phonon contribution of the non-magnetic isostructural material La$_3$Sb$_3$Zn$_2$O$_{14}$ and obtain a clear linear-T temperature dependence of magnetic specific heat at low temperatures. The absence of magnetic order is confirmed by specific heat, A.C. susceptibility and $\mu$SR measurements down to 20 mK. We find that the spin-lattice relaxation time remains constant down to the lowest temperature. The possibility of disorder induced effect could not be excluded due to the possible Tm/Zn site-mixing disorder in Tm$_3$Sb$_3$Zn$_2$O$_{14}$.

*The National Key Research and Development Program of China Nos.2016YFA0300503 and 2016YFA0301001, the start-up fund and the first-class university construction fund of Fudan University, the thousand-youth-talent program of China, the National Natural Science Foundation of China: No.11474060 and No.11774061.

Tuesday, March 5, 2019 2:30 PM - 5:18 PM
**Session H07 DCMP: Ruthenates and Nickelates** BCEC 109B - David Parker, Oak Ridge National Laboratory

**2:30PM H07.00001: Current-controlled switching of diamagnetism in Ca$_3$(Ru$_{1-x}$Ti$_x$)$_2$O$_7$**

*YOSHITERU MAENO (Presenter), CHANCHAL SOW, RYO NUMASAKI, GIORDANO MATTONI, SHINGO YONEZAWA, Department of Physics, Kyoto University, Kyoto 606-8502, Japan, NAOKI KIKUGAWA, SHINYA UJI, Quantum Transport Properties Group, National Institute for Materials Science (NIMS), Tsukuba 305-0003, Japan — It was recently shown that a strong Landau diamagnetism may emerge in strongly correlated electron systems (SCES) under nonequilibrium steady state (NESS) conditions. However, due to high resistivity of the insulating state, in situ sign-switching of magnetism was not possible in the previous study. Here, we demonstrate that DC current can trigger in situ switching between the impurity-induced Mott insulating state and diamagnetic semimetallic state of the bilayered ruthenate Ca$_3$Ru$_2$O$_7$. By performing simultaneous magnetic and resistive measurements, we map out the temperature vs current-density phase diagram in the NESS of this material. The present results open up the possibility of creating novel electronic states in a variety of SCES by NESS conditions under DC current.*

*This work was supported by JSPS Grant-in-Aids KAKENHI Nos. 26247060, 15H05852 and 17H06136.

**2:42PM H07.00002: How does optical response of SrRuO$_3$ and CaRuO$_3$ thin films deviate from Fermi liquid predictions?**

YOUCHENG WANG (Presenter), GRACE BOSSÉ, Department of Physics, Institute for Quantum Matter, Johns Hopkins University, HARI NAIR, Department of Materials Science and Engineering, Kavli Institute at Cornell for Nanoscale Science, Cornell University, JACOB P RUF, Department of Physics, Laboratory of Atomic and Solid State Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University, BING CHENG, Department of Physics, Institute for Quantum Matter, Johns Hopkins University, DARRELL G. SCHLOM, Department of Materials Science and Engineering, Kavli Institute at Cornell for Nanoscale Science, Cornell University, KYLE M SHEN, Department of Physics, Laboratory of Atomic and Solid State Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University, NORMAN ARMITAGE, Department of Physics, Institute for Quantum Matter, Johns Hopkins University — Orthorhombic perovskites SrRuO$_3$ and CaRuO$_3$ are strongly correlated metals with unusual transport properties. Previous optics studies in the infrared and terahertz range shows non-Drude dynamics and fractional scattering rates at low temperatures which seems to contradict a Fermi-liquid picture with long-lived quasiparticles. Here we present time domain THz measurements of clean thin films of SrRuO$_3$ and CaRuO$_3$. Our results demonstrate for both materials the low temperature conductivity shows a narrow Drude-like peak and can be fitted with two Drude terms. The conductivity crosses over to become less coherent at higher temperatures. Comparison with Fermi liquid scaling theories shows that CaRuO$_3$ is more anomalous than SrRuO$_3$ probably owing to spin fluctuations in the paramagnetic phase.

**2:54PM H07.00003: $^{17}$O NMR Studies Applied to the Uniaxial Stress-Tuned Fermi-Liquid Crossover in Sr$_2$RuO$_4$**

AARON CHRONISTER (Presenter), ANDREJ PUSTOGOW, YONGKANG LUO, University of California, Los Angeles, NAOKI KIKUGAWA, National Institute for Materials Science, DMITRY SOKOLOV, FABIAN JERZEMBECK, ANDREW MACKENZIE, CLIFFORD HICKS, Max Planck Institute for Chemical Physics of Solids, ERIC BAUER, Los Alamos National Laboratory, STUART E BROWN, University of California, Los Angeles — Application of in-plane uniaxial stress to the quasi two-dimensional strongly correlated system Sr$_2$RuO$_4$ results in substantial changes of the physical properties, including a more than doubled superconducting transition temperature as well as normal state transport properties deviating from conventional Fermi-liquid behavior. Both observations are attributed to a nearby Lifshitz transition, associated with moving the Fermi energy through a van Hove singularity (vHs). $^{17}$O NMR measurements reveal that the Lifshitz point is accompanied by strong field and temperature dependence of the spin susceptibility, persisting to temperatures less than 100 mK. Our NMR measurements indicate that the non-Fermi-liquid behavior is strongly influenced by the proximity of the Lifshitz transition and a large Stoner enhancement, in a system where three energy scales are nearly balanced: width of vHs, as well as Zeeman and thermal energies.

*This work was supported by the National Science Foundation (DMR-1709304) and Los Alamos Laboratory Directed Research and Development (LDRD) program.
3:06PM H07.00004: Collective modes in Sr$_2$RuO$_4$ measured with momentum-resolved EELS (M-EELS)* ALI HUSAIN
(Presenter), MATTEO MITRANO, MELINDA RAK, SAMANTHA RUBECK, Department of Physics and Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, FUMIHIKO NAKAMURA, Department of Education and Creation Engineering, Kurume Institute of Technology, CHANCHAL SOW, YOSHITERU MAENO, Department of Physics, Graduate School of Science, Kyoto University, PETER ABBAMONTE, Department of Physics and Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign — Measurements of the charge susceptibility $\chi(q,\omega)$ of the high-$T_c$ cuprate Bi-2212 using Momentum-resolved inelastic electron scattering (M-EELS) have shown that bad-metallic behavior can be characterized by a continuum of non-propagating density fluctuations, in stark contrast to the plasmons of simple metals [1]. Here, we report on M-EELS measurements of Sr$_2$RuO$_4$, a bad metal which crosses over to a Fermi Liquid at $T=40$K. Like Bi-2212, we find that the bad metal phase of Sr$_2$RuO$_4$ exhibits a continuum of density fluctuations. However, below 40K, spectral weight is redistributed to form a plasmon-like excitation around 1.4 eV. Surprisingly, we also discover a coherent low-energy (sub-80meV) 2D acoustic plasmon in the bad metal phase, whose velocity is strongly renormalized from 0.7 to 0.4eV Å below the Fermi liquid crossover, indicating a coupled 2D Fermi Liquid and 3D bad metal in a single solid. We will contrast this coupled system to a closely related ruthenate, the Mott-insulator Ca$_2$RuO$_4$.


*This work was supported by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF-4542. An early prototype of the M-EELS instrument was supported by the DOE CES under award DE-AC02-98CH10886.

3:18PM H07.00005: Magnetisation density and electronic structure of Sr$_3$Ru$_2$O$_7$.* JONATHAN DUFFY (Presenter), University of Warwick, STEPHEN DUGDALE, University of Bristol, SEAN GIBLIN, University of Cardiff, JONATHAN TAYLOR, European Spallation Source, ROBIN S. PERRY, UCL, YOSHITERU MAENO, Kyoto University, MATTHEW BUTCHERS, University of Bristol, TED FORGAN, University of Birmingham — Sr$_3$Ru$_2$O$_7$ is itinerant metamagnet, exhibiting a sharp increase in magnetisation in a field of 5.5 – 7.7 T (depending on the applied field direction) at temperatures around 1 K. This metamagnetic transition is thought to be related to the behaviour of the density of states near the Fermi level. We have performed a study of the magnetisation density in the metamagnetic state combining a magnetic Compton scattering experiment with electronic structure calculations. Our initial density functional calculations were fixed to reproduce the value of the experimentally determined spin moment, but do not agree well with the experimentally measured spin density. In the talk, we will show how it is possible to gain a good agreement with the experimental spin densities from the calculations and the consequences of this in relation to the electronic structure and underlying physics.

*We are very grateful to the Japan Synchrotron Radiation Institute (JASRI) for providing beamtime at SPring-8 via projects 2012B00045 and 2016A0131.

3:30PM H07.00006: DMFT+NRG study of orbital differentiation in three-orbital Hubbard models FABIAN B. KUGLER (Presenter), SEUNG-SUP B. LEE, Ludwig-Maximilians-Universität München, Munich, Germany, MANUEL ZINGL, ANTOINE GEORGES, Flatiron Institute - Simons Foundation, New York, USA, GABRIEL KOTLIAR, Rutgers University, New Jersey, USA, JAN VON DELFT, Ludwig-Maximilians-Universität München, Munich, Germany, ANDREAS WEICHSELBAUM, Brookhaven National Laboratory, New York, USA — The orbital-selective Mott phase (OSMP) in multi-orbital Hubbard models has been of high interest for a long time. While it has early been understood [1] that different bandwidths of the orbitals can lead to different critical interaction energies, the OSMP solely driven by crystal-field splitting (CFS) is more intricate. Here, we present a real-frequency dynamical mean-field theory and numerical renormalization group (DMFT+NRG) analysis of the OSMP driven by CFS in a three-orbital model and illustrate the singular Fermi-liquid properties of this phase [2]. On the example of Sr$_2$RuO$_4$, we show how our method can be used to study low-energy physics in a real-materials framework.

Multi-Wavelength Near-Field Imaging of the Temperature & Current Induced Metal to Insulator Transitions in Ca$_2$RuO$_4$

ROCCO VITALONE (Presenter), BENJAMIN AARON FOUTTY, ALEXANDER SWINTON MCLEOD, JEDRZEJ WIETESKA, Department of Physics, Columbia University, CHANCAL SOW, Department of Physics, Kyoto University, FUMIHIKO NAKAMURA, Department of Education and Creation Engineering, Kurume Institute of Technology, YOSHITERU MAENO, Department of Physics, Kyoto University, ABHAY PASUPATHY, DIMITRI BASOV, Department of Physics, Columbia University — Ca$_2$RuO$_4$, a strongly correlated metal oxide and Mott Insulator, exhibits an insulator to metal transition and a large structural distortion along the c-axis concurrently at 365K with a hysteresis of about 30K. In this study, we examine the temperature driven insulator-metal transition (IMT) in single crystals of Ca$_2$RuO$_4$ at the nanoscale with wavelengths ranging from 10 µm to 16 µm, where a strong phonon resonance characterizes the insulating phase. Through this study, we clearly resolve the phonon mode at 16 µm among insulating domains coexisting with the metallic phase, in accord with the far-field optical response of this material. We also resolve a novel pattern of striped phase coexistence emerging on the sub-micron scale that we attribute to the large strain induced by the structural difference between the metallic and insulating phases. We discuss how the development of this stripe pattern spontaneously minimizes strain energy within the crystal. Our interrogation of the metallic and phonon responses of these coexisting phases provides nano-imaging evidence that the temperature and current driven IMTs proceed through fundamentally different microscopic mechanisms.

Effect of uniaxial strain on the metal-insulator transition in Ti-substituted Ca$_3$Ru$_2$O$_7$

JEDRZEJ WIETESKA (Presenter), ALEXANDER SWINTON MCLEOD, BEN FOUTTY, ROCCO VITALONE, Columbia University, JIN PENG, Physics, Tulane University, YU WANG, ZHIQIANG MAO, Physics, Pennsylvania State University, DIMITRI BASOV, ABHAY P NARAYAN, Columbia University — We present results of electrical transport studies on the metal-insulator transition (MIT) in 10% Ti-substituted Ca$_3$Ru$_2$O$_7$ under uniaxial strain. We observe a large (~10K) modulation of the Mott transition temperature under application of high (<1%) ab-plane uniaxial strain. For low strains we find an anomaly across $T_{MIT}$ in the linear response elastoresistive susceptibility. Complementary scanning near-field optical microscopy measurements have been performed on the same samples.

Novel uniaxial strain device for transport and scanning probe experiments

BEN FOUTTY (Presenter), JEDRZEJ WIETESKA, DREW A EDELBERG, ALEXANDER SWINTON MCLEOD, ROCCO VITALONE, SIMON TURKEL, ABHAY P NARAYAN, DIMITRI BASOV, Physics, Columbia University — In recent years uniaxial strain has emerged as an important probe of condensed matter systems, coupling to phenomena such as nematicity [1], superconductivity [2], magnetism [3], and metal insulator transitions [4]. Existing methods for in-situ application of high strains generally have been based off of extension piezoelectric actuators [5]. We present a method of strain application that relies on stacks of shear piezoelectric actuators to apply up to 1% uniaxial extension and compression at cryogenic temperatures homogeneously to up to 100 um square regions of materials ranging from transition metal dichalcogenides to ruthenates. Our method has been successfully applied to electrical transport, scanning tunneling microscopy, and scanning near-field optical microscopy measurements. Some early results using this device include measurement of a large strain effect on superconductivity in 2H-NbSe$_2$, the formation of solitons in 2H-MoSe$_2$, and the insulator-metal transition in 10% Ti-doped Ca$_3$Ru$_2$O$_7$.

4:18PM H07.00010: Nano-resolved strain control and polar modulation of the Mott transition in a bilayer ruthenate  
ALEXANDER SWINTON MCLEOD (Presenter), RAN JING, JEDRZEJ WIETESKA, BENJAMIN AARON FOUTTY, Physics, Columbia University, SHIMING LEI, RUI ZU, LEIXIN MIAO, KLEYSER E AGUEDA LOPEZ, JIN PENG, ZHIQIANG MAO, Physcis, Pennsylvania State University, DANIO PUGGIONI, JAMES M RONDINELLI, Materials Science and Engineering, Northwestern University, NASIM ALEM, VENKATRAMAN GOPALAN, Physics, Pennsylvania State University, DIMITRI BASOV, Physics, Columbia University — The 4d transition metal oxides of the Ca_{n+1}Ru_{n}O_{3n+1} perovskite family have recently garnered interest for their correlated electron physics and strong sensitivity to external stimuli like strain, temperature, and even electric current. These place the n=1,2 members in a rich phase diagram of competing and tunable metallic, magnetic, and insulating phases. The bilayer ruthenate Ca_{2}Ru_{2}O_{7} exhibits a structural distortion producing a polar metal and, under Ti substitution for Ru, a polar Mott insulator. We report cryogenic (T<100K) infrared nano-imaging (nano-IR) of 5% and 10% Ti-doped crystals revealing spontaneous patterns of striped phase coexistence through the thermal first-order Mott transition, and demonstrate nucleation and manipulation of metallic stripes through in situ uniaxial strain. Energy-resolved nano-IR imaging combined with surface work function mapping reveal suppression or enhancement of the Mott insulating state at polar domain boundaries in the crystal. Verified by second-harmonic polarimetry and transmission electron microscopy, we find the polar orientation and state of charge at these polar domain walls can selectively modulate the Mott transition, thus opening new routes towards manipulation of this canonical insulator-metal transition at sub-micron scales.

4:30PM H07.00011: Ionic gating of correlated perovskite nickelates  
YIFEI SUN (Presenter), ZHEN ZHANG, Purdue University - USA, HUA ZHOU, Argonne National Lab, SHIRIYAM RANAMATHAN, Purdue University - USA — In this work, we demonstrate that an ionic liquid gate can drive the fast motion of Li+ into and out of correlated perovskite nickelates such as SmNiO_{3} and NdNiO_{3}. This modulation effect can successfully engineer the phase of the material and tune the effective gap by nearly 3 eV. X-ray absorption spectra characterization showed that the Ni-site orbital occupancy control upon the gate modulation is the primary reason for the phase transition. Electrical transport measurements illustrated that such liithiation behavior induced the drastic change in electronic transport by several orders of magnitude and is independent of temperature. The lattice dilatation can be monitored as a function of Li+ doping concentration via synchrotron spectroscopy and provides structural insights during the phase transition. We will discuss hydrogen versus lithium doping of the nickelates and discuss the strain-orbital filling relationships.

ABRAHAM LEVITAN (Presenter), JARUI LI, Massachusetts Institute of Technology, KEVIN MERTES, Los Alamos National Laboratory, MARC ALLAIN, Institut Fresnel, ASH TRIPATHI, Los Alamos National Laboratory, WEN HU, Brookhaven National Laboratory, RICHARD L SANDBERG, Los Alamos National Laboratory, CLAUDIO MAZZOLI, Brookhaven National Laboratory, RICCARDO COMIN, Massachusetts Institute of Technology — Cubic perovskite nickelates with a rare earth ion (ANiO_{3}) exhibit both a metal to insulator transition and a transition to antiferromagnetic order, which coincide in the case of NdNiO_{3}. The many-body nature of these oxides and the interplay between antiferromagnetic order and charge disproportionation leads to a complex landscape involving significant inhomogeneity at the nanoscale. This is exhibited in the form of phase segregation near both the antiferromagnetic and metal to insulator transitions [1]. We report on a first step towards fully characterizing that nanoscale texture using resonant soft x-ray coherent Bragg ptychography at the CSX beamline of NSLS-II. In addition, our work demonstrates for the first time the feasibility of Bragg ptychography in the soft x-ray regime using the weak resonant scattering signals associated with electronic ordering wavevectors.

4:54PM H07.00013: Similarities and Differences Between the Nickelate LaNiO_{2} and Isoelectronic Cuprate Superconductors*  
MATTHIAS HEPTING (Presenter), DANFENG LI, HAIYU LU, CHUNJING JIA, XIAO FENG, YASUYUKI HIKITA, BRIAN MORITZ, SIMES, SLAC National Accelerator Lab, EUGENIO PARIS, YI TSENG, Paul Scherrer Institut, ZAHID HUSSAIN, YI-DE CHUANG, Advanced Light Source, Lawrence Berkeley National Laboratory, ZHIXUN SHEN, SIMES, SLAC National Accelerator Lab, SCHMITT THORSTEN, Paul Scherrer Institut, THOMAS DEVEREAUX, HAROLD HWANG, WEI-SHENG LEE, SIMES, SLAC National Accelerator Lab — It is an open question whether layered nickelate compounds and derived heterostructures could mimic a set of distinct properties which are suspected to invoke high-temperature superconductivity in cuprates, that is, a 2D layered crystal structure, spin 1/2 and strong antiferromagnetic correlations in the parent compound, absence of orbital degeneracy, and hybridization with oxygen ligands. To address this issue, we have investigated LaNiO_{2} and isostructural SrCuO_{2} thin films by x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS) at the O K -and Ni L-edges. Despite several formal similarities between the nickelate and the cuprate, our study unveils severe differences in orbital configuration, antiferromagnetic order, and ligand-hybridization.

*This work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under contract DE-AC02-76SF00515
5:06PM H07.00014: On the mysterious magnetic susceptibility of LaNiO$_3$  
OLEKSANDR FOYEVTSOV (Presenter), Physics, 
University of British Columbia, JOHN MITCHELL, Argonne National Lab, GEORGE ALBERT SAWATZKY, Physics, University of British Columbia — Ever since Mott's time, understanding of the enhanced Pauli susceptibility observed in many metallic compounds has remained a great challenge[1]. This, in particular, holds in regard to the temperature dependence of the magnetic susceptibility of LaNiO$_3$, which, up until recently, was thought to be greatly enhanced yet almost temperature independent. However, recent advances in growth of highly stoichiometric LaNiO$_3$ single crystals have revealed that the magnetic susceptibility of LaNiO$_3$ has in fact a much more complex temperature dependence[2,3], which has invoked a renewed theoretical interest in the basic electronic structure of this material. In this talk, we propose an explanation of the recent data assuming temperature dependent disproportionation of localized magnetic moments.


Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H08 DCMP: Superconductivity: Copper Oxide - Stripes, CDW and local probes BCEC

2:30PM H08.00001: Doping-dependent precursor charge density wave correlations in La$_{2-x}$Ba$_x$CuO$_4$*  
HU MIAO (Presenter), Brookhaven National Laboratory, GIACOMO GHiringHELLI, Dipartimento di Fisica, Politecnico di Milano, MARK DEAN, Brookhaven National Laboratory — Recently using resonant inelastic x-ray scattering (RIXS), we discovered, in La$_{2-x}$Ba$_x$CuO$_4$ x=0.125, precursor charge density wave (CDW) correlations that exist above the CDW transition temperature and observed that its wavevector varies with temperature and becomes unlocked from the spin wavevector [1]. This observation may help to reconcile the distinct doping-dependence of CDW wavevector in different cuprates families [1,2]. Here we show our new RIXS study that reveals the doping-dependent evolution of precursor CDW in La$_{2-x}$Ba$_x$CuO$_4$.


*This material is based upon work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Early Career Award Program under Award No. 1047478. Work at Brookhaven National Laboratory was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-SC0012704.

2:42PM H08.00002: Temperature Dependence of CDW phenomena in optimally-doped Bi2212 via RIXS*  
WEI-SHENG LEE (Presenter), MATTHIAS HEPTING, SLAC National Accelerator Laboratory, JIEMIN LI, ABHISHEK NAG, ANDREW WALTERS, MIRIAN GARCIA-FERNANDEZ, Diamond Light Source, MAKOTO HASHIMOTO, SLAC National Accelerator Laboratory, YOSHIYUKI YOSHIDA, HIROSHI EISAKI, AIST, BRIAN MORITZ, SLAC National Accelerator Laboratory, EDWIN HUANG, Stanford University, ZHIHUN SHEN, SLAC National Accelerator Laboratory, KEJIN ZHOU, Diamond Light Source, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory — Charge density wave (CDW) in double-layered Bi-2212 copper oxide superconductor has long been studied by STM; yet the questions of how the CDW's origin and how it interacts with other degrees of freedom as a function of temperature still remain largely unexplored. Here we utilize high-resolution resonant inelastic x-ray scattering (RIXS) at the Cu L-edge to investigate the CDW in optimally-doped Bi2212. A CDW scattering in the quasi-elastic region can be clearly observed, unambiguously demonstrating that CDW is a bulk property and exist in the optimally-doped Bi2212. Its temperature dependence and interaction with the phonon degrees of freedom will also be discussed.

*This work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under contract DE-AC02-76SF00515

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Orbital symmetries of charge density wave order in \( \text{YBa}_2\text{Cu}_3\text{O}_{6+x} \)

2:54PM H08.00003: CHRISTOPHER M. MCMAHON, ANDREW ACHKAR, Physics and Astronomy, University of Waterloo; EDUARDO H. DA SILVA NETO, Stuart Blussom Quantum Matter Institute, University of British Columbia; ISAIAH DJIANTO, YLER MENARD, Physics and Astronomy, University of Waterloo; FEIZHOU HE, RONNY SUTARTO, Canadian Light Source; RICCARDO COMIN, RUIXING LIANG, DOUGLAS ANDREW BONN, WALTER N HARDY, ANDREA DAMASCELLI, Stuart Blussom Quantum Matter Institute, University of British Columbia; DAVID G. HAWTHORN (Presenter), Physics and Astronomy, University of Waterloo — Charge density wave (CDW) order has been shown to compete and co-exist with superconductivity in underdoped cuprate superconductors. Moreover, the CDW order has been proposed to exhibit a novel \( d \)-symmetry form factor—a quadrupolar modulation of the charge on oxygen sites surrounding each Cu site — evidence for which has emerged from STM measurements in BSCCO, NCCOC and from resonant x-ray scattering measurements of \( \text{YBa}_2\text{Cu}_3\text{O}_{6+x} \) (YBCO). Here, we revisit resonant x-ray scattering measurements at the Cu \( L \) edge of the CDW form factor in YBCO, utilizing a variation in the measurement geometry to provide enhanced sensitivity to the CDW orbital symmetry. Contrary to previous reports, the (0 0.31 \( L \)) peak measured at the Cu \( L \) edge is dominated by a simple \( s \) form factor, revealing no evidence for a dominant \( d \) form factor CDW. However, by measuring the CDW orbital symmetry at both the (0.31 0 \( L \)) and (0 0.31 \( L \)) peaks, we identify a pronounced difference in the orbital symmetry of the CDW order propagating along the \( a \) and \( b \) axes, with the CDW propagating along the \( a \)-axis exhibiting some form of orbital order in addition to charge order. Model calculations indicate that a candidate for the unusual orbital symmetry of the \( a \)-axis CDW to break \( ac \) and \( ab \) plane mirror symmetries.

Ground states of striped cuprates at high magnetic fields (\( H \))*

3:06PM H08.00004: PAUL G. BAITY (Presenter), ZHENZHONG SHI, DRAGANA POPOVIC, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ.; TAKAO SASAGAWA, Tokyo Inst. of Tech. — The interplay of superconductivity and charge orders found in all hole-doped cuprates remains an open question in the limit of high \( H \). To address this issue, we have investigated the \( H \)-tuned superconducting-normal phase transitions in ultra-high-quality single crystals of \( \text{La}_{1.7}\text{Eu}_{0.2}\text{Sr}_{0.1}\text{CuO}_4 \) and \( \text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4 \), which have a striped charge order, under extreme conditions (temperatures \( T \) down to 0.016 K and \( H \) up to 45 T). A variety of linear and non-linear transport measurements have been performed, and the results reveal a full sequence of states in the \( T=0 \) limit as a function of \( H \): a superconductor, a wide regime of 2D superconducting phase fluctuations, and a high-\( H \) normal state. Within the phase-fluctuations regime, an unanticipated insulatinglike region emerges that is consistent with a novel type of ordering of localized Cooper pairs within the charge stripes in \( \text{CuO}_2 \) planes. This regime appears to compete with the \( H=0 \) superconductivity. We will present our results and discuss the role of disorder, as well as the similarities to other 2D systems and materials with competing orders that undergo superconducting phase transitions.


Stripes and superconductivity in the two-dimensional Hubbard model

3:18PM H08.00005: CHIA-MIN CHUNG (Presenter), Department of Physics, Ludwig-Maximilians-Universität München (LMU); MINGPU QIN, Department of Physics, College of William and Mary; HAO SHI, Center for Computational Quantum Physics, Flatiron Institute; ETTORE VITALI, Department of Physics, College of William and Mary, CLAUDIUS HUBIG, Max-Planck-Institut für Quantenoptik, ULRICH JOSEPH SCHOLLWOECK, Department of Physics, Ludwig-Maximilians-Universität München (LMU), STEVEN ROBERT WHITE, University of California, Irvine; SHIWEI ZHANG, Department of Physics, College of William and Mary — The stripes have been shown the ground state in the doped two-dimensional Hubbard model for a particular interaction. In this work we discuss the superconductivity in the stripes. We employ two of the most powerful methods, density matrix renormalization group and constrained-path auxiliary-field Monte Carlo to study the superconductivity in the stripes on finite-size cylinders and in the thermodynamic limit. By studying the pair-pair correlation and the local pairing order, we show that no long-range superconductivity exists in the ground-state stripes. In addition we discuss the mixture of stripes with different stripe fillings, and the effect on the superconductivity.
3:30PM H08.00006: Temperature and field dependence of the intrinsic tunneling structure in overdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$

TIMOTHY BENSEMAN (Presenter), Physics, CUNY Queens College, JOHN ROBERT COOPER, Cavendish Laboratory, University of Cambridge, GEETHA BALAKRISHNAN, Physics, University of Warwick — Tunneling in stacked ‘intrinsic’ junctions in the high-$T_c$ superconductor doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ is a bulk probe of the quasiparticle density of states, which can be used to complement surface spectroscopic techniques such as ARPES and scanning tunneling microscopy. However, in order for this technique to give useful data above the superconducting sum-gap voltage, stacks with area of less than 1 $\mu$m$^2$ and containing approximately 10 or fewer intrinsic junctions must be used in order to ensure negligible self-heating.

Here we present intrinsic tunneling data for mesa structures fabricated on three over- and optimally-doped Bi$_{2+\delta}$Sr$_{1+\delta}$CaCu$_2$O$_{6+\delta}$ crystals, with 0.16–0.19 holes per CuO$_2$ unit, for a wide range of temperature ($T$) and applied magnetic field ($H$). The differential conductance above the gap edge shows a clear dip structure which is highly suggestive of strong coupling to a narrow boson mode. Data below the gap edge gives clear evidence for strong $T$-dependent pair breaking. These findings could help theorists make a detailed Eliashberg analysis and thereby contribute towards understanding the pairing mechanism.

*The work at the University of Warwick is supported by EPSRC, UK, Grant No. EP/M028771/1, while that at Cambridge was supported by EPSRC, UK, Grant No. EP/C511778/1.

3:42PM H08.00007: Bosonic Mode in the Tunneling Spectra of Fe-based and Cuprate Superconductors

JOHN ZASADZINSKI (Presenter), NOAH SAMUELSON, Physics, Illinois Institute of Technology, BEVERLY LOWELL, Physics, Northwestern University, MARIA IAVARONE, Physics, Temple University — The above-gap, SIN tunneling spectral dip feature in the bilayer cuprate Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) is highly reproducible and unambiguously linked to the resonance spin excitation. The search for similar bosonic mode features in the tunneling spectra of Fe-based and other cuprate superconductors is presented. The single-layer cuprate Hg1201Tc (94K) exhibit sharp spectra and a well resolved bosonic mode feature similar to Bi2212. STS data on FeSe (Tc = 8.9K) reveal a bosonic mode feature quite similar to Bi2212, also linked to the neutron resonance mode. It is demonstrated that SIS break junctions or intrinsic c-axis junctions reveal a strongly enhanced dip feature allowing the observation of a bosonic mode in strongly disordered Bi2201 with Tc values ≤ 5K. Over a wide range of Tc values the mode energy $\Omega$ remains inside the superconducting gap $2\Delta$ as found in high Tc cuprates. The conclusion is that irrespective of Tc, composition and degree of disorder, the bosonic mode $\Omega$ retains its character as a spin exciton and appears to be a universal signature of unconventional superconductivity.

3:54PM H08.00008: Can Short-Range CDW Order Cause the Fermi Surface Reconstruction in the Cuprates?*

YUVAL GANNOT (Presenter), STEVEN KIVELSON, Stanford University — In the cuprates, short-range charge density wave (CDW) order is generally thought to account for the reconstructed Fermi surface apparent in quantum oscillation (QO) experiments. However, since the measured CDW correlation length may sometimes be shorter than the cyclotron radius, it is unclear whether sharp QOs reflecting the reconstructed Fermi surface are theoretically expected. In this work, we derive a simple quantization rule appropriate for disordered CDWs and show that it involves a random Berry phase. We demonstrate that under most circumstances, the predicted QO amplitude is not easily reconciled with observations in the cuprates.

*This work supported by NSF award number DMR-1608055.

4:06PM H08.00009: Visualizing the electronic structure of infinite-layer cuprate by scanning tunnelling spectroscopy*

YONG ZHONG (Presenter), RUIFENG WANG, ZIYUAN DOU, CANLI SONG, XUCUN MA, QIKUN XUE, State Key Laboratory of Low-dimensional Quantum Physics, Department of Physics, Tsinghua University — Infinite layer Sr$_{1-x}$La$_x$CuO$_{2+\delta}$ is a prototype to study the high-$T_c$ superconductivity in cuprates. Using oxide-MBE technique, we fabricate Sr$_{1-x}$La$_x$CuO$_{2+\delta}$ films with different doping levels. Mottness has been observed in lightly electron-doped Sr$_{1-x}$La$_x$CuO$_2$ by in-situ STM. We also find a phase transition to hole-doped Sr$_{1-x}$La$_x$CuO$_{2+\delta}$ when $x$ exceeds 0.1. Apical oxygens are responsible for this electron- to hole-cuprate transition, which is supported by transmission electron microscope measurements. By comparing the electronic structures in electron- and hole-doped Sr$_{1-x}$La$_x$CuO$_{2+\delta}$, we give some clues to understand the e-h asymmetry in cuprates.

*This work is financially supported by the Ministry of Science and Technology of China (Grants No. 2017YFA0304600, 2015CB921001, 2016YFA0301004), the National Natural Science Foundation of China (Grants No. 11427903, 11504196, 11634007, 11774192), and in part by the Beijing Advanced Innovation Center for Future Chip (ICFC).
4:18PM H08.00010: Real-Space Characterization of Charge Ordering in Epitaxial La_{2-x}Sr_xCuO_4 films  YANG WANG (Presenter), YONG ZHONG, ZHILING LUO, MENGHAN LIAO, RUIFENG WANG, ZIYUAN DOU, DING ZHANG, CANLI SONG, XUCUN MA, QIKUN XUE, Tsinghua University — Injection of charge carriers into the parent Mott insulator gives rise to a plethora of electronic orders in cuprates. Investigation of the behaving and relationship of these exotic orders with high-T_c is of pivotal importance in solving the cuprate conundrum. For this, we present a detailed study of the doping dependent charge orderings in the canonical La_{2-x}Sr_xCuO_4 cuprate thin films. By in-situ STM, we unveil a 4a_0-modulated stripe phase in the vicinity of 0.125 doping, whose commensurability is lost with decreasing Sr concentration. When heavier doped, a grid phase appears whose size is averaged to 4 nm. In the lightly doped regime, on the other hand, a Wigner crystal phase with a distorted-hexagonal patterned electronic structure is captured. Our results contribute to the construction of electronic landscape in the cuprate doping phase diagram, and is of help in illuminating its interplay with superconductivity.

4:30PM H08.00011: Charge trapping and super-Poissonian noise centers in a cuprate superconductor  KOEN BASTIAANS (Presenter), DOOHEE CHO, TJERK BENSCHOP, IRENE BATTISTI, DAMIANOS CHATZOPoulos, Leiden University, YINGKAI HUANG, MARK GOLDEN, University of Amsterdam, QUAN DONG, YONG JIN, C2N, University Paris-Saclay, JAN ZAANEN, MILAN P ALLAN, Leiden University — We present new insight into the mystery of highly anisotropic transport in the cuprates and how they can trap additional charges. Above the superconducting transition these materials are perfectly metallic along the crystal planes (ab-plane), but are insulating in the c-axis, with ratios between in-plane and perpendicular resistance exceeding 10^4. This anisotropy has been identified as one of the key mysteries in the cuprates and has been connected to the mechanism of high-temperature superconductivity. Here, we employ our newly developed scanning noise spectroscopy technique, for which we combined a scanning tunneling microscope (STM) with a novel MHz frequency amplifier to bring noise-spectroscopy measurements to the atomic scale [1]. We discover surprising deviations from the expected Poissonian noise of uncorrelated electrons. A behavior that can only happen in highly polarizable insulators and represents strong evidence for trapping of charge in the charge reservoir layers of the cuprates. We will show how these new observations connect to the mystery of anisotropic transport in high-temperature superconductors and shed new light onto this issue [2].


4:42PM H08.00012: Towards the development of YBa_2Cu_3O_7-based S-I-S tunneling Josephson junction device  HOM KANDEL (Presenter), Physics, University of Wisconsin-Parkside, ZHONGRUI LI, University of Michigan, Ann-Arbor, TARPIN CHEN, University of Arkansas — Josephson junctions are used to fabricate superconductor quantum interference devices (SQUIDs), qubits, and terahertz frequency devices. YBa_2Cu_3O_7 (YBCO)-based S-I-S tunneling Josephson junctions offer many advantages over the conventional low temperature superconductor-based Josephson junctions including low cost, cryogenic system simplicity, and high J_cR_n product value (with J_c being the junction critical current and R_n the normal resistance). However, the development of a well-controlled and reproducible YBCO based S-I-S tunneling Josephson junction is very challenging since the thickness of the electrical insulation layer (I) on the junction has to be only about a nanometer and it must provide a very high potential barrier in the junction.

Here, we present our work towards the development of the YBCO based S-I-S tunneling Josephson junction device by discussing growth, structure, and electrical transport properties of (110)-YBCO, various metals (M) doped PrBa_2(Cu_0.8M_0.2)O_7 (PBCMO), and heterostructures of YBCO and PBCMO. In particular, we discuss thin film deposition of (110)-oriented YBCO, PBCMO, and heterostructures of YBCO and PBCMO and their electrical transport properties including the electrical resistivity, conduction mechanism, and proximity effects.

4:54PM H08.00013: Quantum Sensing of Layered Superconductor at the Nanoscale  CHUNHUI DU (Presenter), RUOLAN XUE, MARK KU, FRANK ZHAO, NICOLA POCCIA, Harvard University, RUIDAN ZHONG, Brookhaven National Laboratory, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, GENDA GU, Brookhaven National Laboratory, PHILIP KIM, RONALD L WALSWORTH, AMIR YACOBY, Harvard University — We introduce single spin magnetometry based on nitrogen-vacancy (NV) centers in diamond as a new platform to probe the microwave response of a two-dimensional layered high Tc superconductor Bi_2Sr_2CaCu_2O_{8+x} (BSCCO) flake at the nanoscale. We observed a temperature-dependent spatial profile of the microwave field around the BSCCO flake, which can be attributed to the variation of the conductivity in BSCCO. Our technique provides a novel method to characterize the superconducting phase transitions without making electrical contacts and opens up new possibilities for nanoscale imaging of the charge dynamics in layered materials.
5:06PM H08.00014: High temperature superconducting oxychlorides: a light element model for cuprates  BLAIR LEBERT (Presenter), University of Toronto, MATTEO D’ASTUTO, Institut Néel — The copper oxychloride cuprate Ca$_2$CuO$_2$Cl$_2$ (CCOC) system, with vacancy or Na doping on the Ca site, is unique among the high temperature superconducting cuprates (HTSCs) since it: lacks high Z atoms; has a simple I4/mmm 1-layer structure at all doping and temperatures; and has a strong 2D character due to its apical chlorine. Due to the reduced number of electrons, advanced calculations that incorporate correlation effects, such as quantum Monte Carlo [1], are now feasible which makes CCOC a model system to gain insight into the 30-year-old mystery of HTSCs. But relatively little is known about CCOC so we are now filling this gap by a comprehensive experimental study covering the whole phase diagram, in particular the (para)magnon dispersion using RIXS [2] and the phonon dispersion using IXS [3]. We are also investigating the electron-phonon coupling using RIXS and searching for a bulk signature of the charge modulation (stripes) from x-ray resonant scattering close to the 1/8 doping.


5:18PM H08.00015: Emergent superconductivity upon disordering a charge density wave ground state  ANURAG BANERJEE (Presenter), Indian Institute of Science Education and Research, Kolkata, ARTI GARG, Theoretical Condensed Matter Physics Division, Saha Institute of Nuclear Physics, Kolkata, AMIT GHOSAL, Indian Institute of Science Education and Research, Kolkata — We explore the interplay of a charge density wave (CDW) order and s-wave superconductivity in a disordered system. Recent experiments on 1T-TiSe$_2$, where the pristine sample has a commensurate CDW order and the superconductivity appears upon copper intercalation, motivates our study. Starting with an extended Hubbard model, with parameters which yield a CDW ground state within Hartree-Fock-Bogoliubov formalism in pure systems, we show that the addition of disorder quickly wipes out the global charge order by disrupting periodic modulation of density at some (low) strength of disorder. Along with this, the subdominant superconducting order emerges in regions that spatially anticorrelate with islands of strong local CDW order. The short-range density modulations, however, continue to persist and show discernible effects up to a larger disorder strength. The local CDW puddles reduce in size with increasing disorder and they finally lose their relevance in effecting the properties of the system. Implication of our model calculations on the experimental findings of transition-metal-dichalcogenides will also be discussed.

Tuesday, March 5, 2019 2:30 PM - 5:18 PM

Session H09 DCOMP: Superconductivity: Sr$_2$RuO$_4$ and other Triplet Candidates  Liuyan Zhao, University of Michigan

2:30PM H09.00001: Investigating the Pairing Symmetry in Uniaxially Strained Sr$_2$RuO$_4$ by $^{17}$O NMR Shifts* ANDREJ PUSTOGOW (Presenter), YONGKANG LUO, AARON CHRONISTER, YUE-SHUN SU, University of California, Los Angeles, NAOKI KIKUGAWA, National Institute for Materials Science, Tsukuba, DMITRY SOKOLOV, FABIAN JERZEMBECK, ANDREW MACKENZIE, CLIFFORD HICKS, Max Planck Institute for Chemical Physics of Solids, ERIC BAUER, Los Alamos National Laboratory, STUART E BROWN, University of California, Los Angeles — The unconventional superconductor and Fermi liquid Sr$_2$RuO$_4$ exhibits clear effects of electronic correlations associated with Hund’s Rule coupling. In the superconducting (SC) state, several experiments produced evidence for time reversal symmetry breaking, and nuclear magnetic resonance (NMR) Knight shift measurements were consistent with an equal-spin pairing triplet state. To that end, Sr$_2$RuO$_4$ is widely considered as a potential candidate for a chiral $p$-wave pairing with an order parameter of $p_x \pm ip_y$ symmetry - a solid state analog to $^3$He-$^3$He. Motivated by the recent observation of a strong peak in $T_c$ across a strain-induced Lifshitz transition associated with a van Hove singularity, we studied the $^{17}$O NMR shifts in the SC state of Sr$_2$RuO$_4$. Our low-temperature experiments at high strain reveal a drop of spin susceptibility below $T_c$ evidenced by unambiguous reduction of Knight shifts for the in-plane O sites. Most pronounced at the Lifshitz point, the loss of spin susceptibility on entering the SC state is reduced on lowering the strain, while no evidence for a phase transition between distinct SC states is observed.

*This work was supported by the National Science Foundation (DMR-1709304) and Los Alamos Laboratory Directed Research and Development (LDRD) program.
2:42PM H09.00002: Microscopic model of the Knight shift in an anisotropic type-II superconductor  RICHARD KLEMM (Presenter), AIYING ZHAO, physics, University of Central Florida, JINGCHUAN ZHANG, QIANG GU, physics, University of Science and Technology Beijing, Beijing, PR China — We have simplified our model of the Knight shift in an anisotropic metal and superconductor by forcing the Hamiltonian for an electron in the Landau orbits for an ellipsoidal anisotropic single electron Hamiltonian and the Zeeman interaction to be relativistically consistent. The resulting Hamiltonian with three effective masses in the three directions of an orthorhombic crystal is invariant under the most general proper Lorentz transformation involving general rotations about all three crystal axes and general boosts in all three directions. The non-relativistic limit then has the following general properties: there is no Zeeman interaction for a one-dimensional metal, and for a two-dimensional metal, the Zeeman interaction is only present for the magnetic field applied perpendicular to the conducting plane. These exact results show that for the field parallel to the layers of a highly layered superconductor or for any field direction in a quasi-one-dimensional superconductor, the temperature dependence of the Knight shift in the superconducting state should either vanish or be very weak. Hence, many Knight shift measurements on such superconducting materials, while correct, have been misinterpreted in the literature.

2:54PM H09.00003: Possible three-dimensional nematic odd-parity pairing in Sr$_2$RuO$_4$ evidenced by uniaxial strain measurements  WEN HUANG (Presenter), Institute for Advanced Study, Tsinghua University, YI ZHOU, Department of Physics, Zhejiang University, HONG YAO, Institute for Advanced Study, Tsinghua University — In the presence of a nontrivial three-dimensional (3D) spin-orbital entanglement, the superconducting pairing in Sr$_2$RuO$_4$ is inherently 3D, consisting both in-plane and out-of-plane channels: $(k_x, k_y)\hat{z}$ and $(k_x, k_y)\hat{z}$. When the latter dominates, the system may develop a time-reversal invariant nematic pairing. We show that, as the out-of-plane pairing lacks a linear-order coupling to certain symmetry-lowering perturbations such as in-plane uniaxial strains, the nematic state may observe a superconducting $T_c$ enhancement indistinguishable from a quadratic function of the strain. Further, in contrast with the chiral pairing, the nematic pairing shall exhibit only a single phase transition or a comparatively less robust secondary transition under the stated perturbations. In combine these may be consistent with several recent experiments on uniaxially-strained samples of Sr$_2$RuO$_4$, thereby providing stronger support for the 3D nematic $p$-wave pairing in this material.


3:06PM H09.00004: Upper critical field of Sr$_2$RuO$_4$ under uniaxial stress  FABIAN JEREMBECK (Presenter), ALEXANDER STEPPKE, YOU-SHENG LI, DMITRY SOKOLOV, Max-Planck-Institut for Chemical Physics of Solids, NAOKI KIKUGAWA, National Institute for Material Science, Tsukuba, Ibaraki, ANDREW MACKENZIE, CLIFFORD HICKS, Max-Planck-Institut for Chemical Physics of Solids — Through application of in-plane uniaxial stress, the unconventional superconductor Sr$_2$RuO$_4$ can be driven through a Lifshitz transition and associated Van Hove singularity (VHS) in the density of states. At this point, its $T_c$ is enhanced by a factor of about 2.5, and $H_{c2}$ by about twenty. Here, we present data on $H_{c2}$ at intermediate strains, and observe that the peak in $H_{c2}$ is much sharper than that in $T_c$. The ratio $H_{c2}/T_c^2$ increases in the close vicinity to the VHS, providing information on the evolution of the superconducting gap as the VHS is approached.


3:18PM H09.00005: Superconducting penetration depth measurement and zero field muon spin relaxation experiments on Sr$_2$RuO$_4$ under uniaxial strain*  SHREENANDA GHOSH (Presenter), VADIM GRINENKO, RAJIB SARKAR, FELIX BRÜCKNER, Institut für Festkörper- und Materialphysik, Technische Universität Dresden, JEAN-CHRISTOPHE ORAIN, HUBERTUS LUETKENS, NIKITIN ARTEM, MATTHIAS ELENDER, Paul Scherrer Institute, Villigen, Switzerland, JOONBUM PARK, MARK E BARBER, NAOKI KIKUGAWA, DMITRY SOKOLOV, ANDREW MACKENZIE, CLIFFORD HICKS, Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany, YOSHITERU MAENO, Department of Physics, Graduate School of Science, Kyoto University, Kyoto, Japan, HANS-HENNING KLAUSS, Institut für Festkörper- und Materialphysik, Technische Universität Dresden — To probe its superconducting order parameter, we have performed muon spin relaxation (muSR) measurements on samples of Sr$_2$RuO$_4$ placed under uniaxial stress. Previous studies on unstressed Sr$_2$RuO$_4$ have revealed enhanced relaxation in the superconducting state, which is interpreted as evidence for a chiral $px \pmipy$ order parameter. With this order parameter, uniaxial stress is expected to induce a splitting between $T_c$ and the onset of chirality. muSR requires large samples, so to perform these measurements, we have developed piezoelectric-based apparatus capable of applying forces of up to ~ 500 N.

*We are grateful to the Deutsche Forschungsgemeinschaft through grants GRK 1621 and SFB 1143, GR 4667 and to the Max Planck Society.
Electronic correlations and enhanced spin-orbit coupling in Sr$_2$RuO$_4$ determined from high-resolution laser-based ARPES.  

**ANNA TAMAI (Presenter), Department of Quantum Matter Physics, University of Geneva, MANUEL ZINGL, Center for Computational Quantum Physics, Flatiron Institute, MINJAE KIM, College de France, ANTOINE GEORGES, Center for Computational Quantum Physics, Flatiron Institute, FELIX BAUMBERGER, Department of Quantum Matter Physics, University of Geneva —** We combine laser-based angle-resolved photoemission and dynamical mean-field theory calculations to study the interplay of electron-electron correlations and spin-orbit coupling (SOC) in the model Fermi liquid Sr$_2$RuO$_4$. Analyzing the experimental Fermi surface, we show that correlations enhance SOC by a factor of $\sim 2$ over the bare value. We further reveal that the real part of the self-energy of the $\beta$ and $\gamma$ sheet is momentum dependent and strongly non-linear down to low energies, in contrast to widely held believes about the phenomenology of Fermi liquids. Introducing a new method to determine orbital self-energies from quasiparticle states with multi-orbital composition, we demonstrate that the anisotropy of the self-energy does not imply momentum dependent many-body interactions. The non-linearity of the self-energy is reproduced by single-site dynamical mean field theory, which provides strong evidence for a dominantly electronic origin of ‘kinks’ in the quasiparticle dispersion of Sr$_2$RuO$_4$.

Sr$_2$RuO$_4$ Josephson junctions built in epitaxial films  

**MASAKI UCHIDA (Presenter), IKKEI SAKURABA, University of Tokyo, MINORU KAWAMURA, RIKEN CEMS, MOTOHARU IDE, University of Tokyo, KEI TAKAHASHI, YOSHINORI TOKURA, RIKEN CEMS, MASASHI KAWASAKI, University of Tokyo —** A layered-perovskite superconductor Sr$_2$RuO$_4$ has attracted continuing interest as a leading candidate with chiral $p$-wave symmetry, which is one of topological superconductors potentially hosting Majorana fermions. For further investigation and possible applications of the unique state, the use of Sr$_2$RuO$_4$ thin films for junctions has been increasingly demanded. While growth of the superconducting Sr$_2$RuO$_4$ films had been extremely difficult over the past decades [1,2], the reproducible and controllable growth has been recently achieved by refining molecular beam epitaxy techniques [3]. In this talk, we report fundamental superconducting properties of Sr$_2$RuO$_4$ thin films and also Josephson junctions as revealed by systematic ultralow-temperature transport measurement. The Sr$_2$RuO$_4$-Sr$_2$RuO$_4$ Josephson junctions built in the epitaxial films have some advantages in investigating the possible multicomponent order parameter. The observed $I_cR_n$ product is as high as 2 $\mu$eV and its temperature dependence shows clear deviations from the conventional Ambegaokar-Baratov model.


**[3] M. Uchida et al., APL Mater. 5, 106108 (2017).**

Spontaneous emergence of Josephson junctions in homogeneous rings of single-crystal Sr$_2$RuO$_4$  

**YUUKI YASUI, Dept. of Physics, Kyoto University, KAVEH LAHABI, Huygens-Kamerlingh Onnes Laboratory, Leiden University, VICTOR FERNANDEZ BECERRA, Dept. of Physics, University of Antwerp, MUHAMMED SHAHBAZ ANWAR, Dept. of Materials Science and Metallurgy, University of Cambridge, SHINGO YONEZAWA, TAKAHITO TERASHIMA, Dept. of Physics, Kyoto University, MILORAD MILOSEVIC, Dept. of Physics, University of Antwerp, YOSHITERU MAENO, Dept. of Physics, Kyoto University, JAN AARTS (Presenter), Huygens-Kamerlingh Onnes Laboratory, Leiden University —** Sr$_2$RuO$_4$ is expected to be a spin-triplet chiral $p$-wave superconductor, where the chirality means that the ground state is two-fold degenerate, with two different directions of the Cooper-pair orbital angular momentum. We fabricated Sr$_2$RuO$_4$ microrings and performed resistance ($R$) and critical-current ($I_c$) measurements in an axial magnetic field. In some such rings, Little-Parks magnetoresistance oscillations are observed close to the transition temperature $T_c$ as recently reported [1]. In other rings, however, we find that $I_c$ oscillates with a period corresponding to the fluxoid quantization down to temperatures far below $T_c$. This behavior resembles that of a superconducting quantum interference device (SQUID) and suggests that a pair of weak links of an intrinsic origin is spontaneously formed in the arms of the ring. Such weak links are most naturally attributable to domain walls separating domains with different chirality, which is also the outcome of order parameter calculations. We believe this to be strong new evidence for the chiral superconducting state in Sr$_2$RuO$_4$.

4:06PM H09.00009: Signature of Unconventional Superconductivity in a Metal-Organic Framework with a Perfect Kagome Structure  
TAKAAKI TAKENAKA (Presenter), KOTA ISHIHARA, YIJIE MIAO, Department of Advanced Material Science, University of Tokyo, XING HUANG, WEI XU, DAOBEN ZHU, Institute of Chemistry, Chinese Academy of Sciences, NA SU, JINGUANG CHENG, Institute of Physics, Chinese Academy of Sciences, TAKASADA SHIBAUCHI, Department of Advanced Material Science, University of Tokyo — Recently, the superconductivity in a Metal-organic framework (MOF) has been discovered for the first time in copper(II) benzenehexathiolate ([Cu₃(C₆S₆)]ₙ, Cu-BHT). A theoretical study predicts that the electron-phonon coupling constant of 0.51 for bulk Cu-BHT can lead to superconductivity at $T_c \sim 1.58$ K, thus conventional s-wave superconducting state has been proposed as a candidate of the pairing state. Meanwhile, recent measurements revealed strong quantum spin fluctuation possibly related to the 2D Kagome lattice of Cu atoms with $S = 1/2$ spin. Quantum spin fluctuations can promote unconventional superconducting pairing states, and it is therefore important to experimentally determine whether the superconductivity in Cu-BHT has conventional or unconventional nature. Here we present measurements of in-plane magnetic penetration depth $\lambda$ in Cu-BHT films down to 40 mK. The temperature dependence of $\lambda$ shows a non-exponential, quasi-linear behavior at low temperatures. Our finding suggests that not only unconventional superconductivity with low-energy quasiparticle excitations is realized in this system but also MOFs can provide a flexible platform to investigate the superconducting pairing mechanisms in the presence of spin frustration and strong quantum fluctuations.

4:18PM H09.00010: Spin Polarized Triplet Supercurrent in Ferromagnetic-Superconducting Josephson Junctions*  
MADISON SUTULA (Presenter), Physics, Materials Science and Engineering, Massachusetts Institute of Technology, MIRKO ROCCI, Francis Bitter Magnet Laboratory, Plasma Science and Fusion Center, Massachusetts Institute of Technology, NILADRI BANERJEE, Physics, Loughborough University, CUI-ZU CHANG, Physics, Penn State University, F. SEBASTIAN BERGERET, Centro de Fisica de Materiales CFM, Centro Mixto CSIC-UPV/EHU, JAGADEESH MOODERA, Physics, Francis Bitter Magnet Laboratory, Plasma Science and Fusion Center, Massachusetts Institute of Technology — Proximity coupling across superconductor-ferromagnet bilayers can give rise to the triplet component of the superconducting condensate [1]. Superconductivity and ferromagnetism have been reported to coexist in a Ni/Bi bilayer system [2]. We investigated Josephson and quasiparticle tunneling across such ferromagnetic-superconducting layers in Bi/Ni/Insulator/Ni/Bi junctions. The superconductivity in the Ni/Bi bilayer is expected to be topological [3]. Moreover, the observed Josephson current could be spin polarized, as superconducting quasiparticles originating from Ni in the Ni/Bi bilayer have been shown to also exhibit spin polarization [2]. The occurrence of conductance at zero bias in these junctions points to odd-frequency symmetry in the superconducting condensate, supporting the presence of a non-zero component associated with a triplet pair superconductivity insensitive to disorder.  
*We acknowledge funding from NSF (DMR-1700137) and ONR (N00014-16-1-2657) as well as MIT UROP funding.

4:30PM H09.00011: Unconventional superconductivity near frustrated orders in quasi-one-dimensional CrAs based systems  
KEITH TADDEI (Presenter), Oak Ridge National Laboratory, GUANGZONG XING, JIFENG SUN, YUHAO FU, YUWEI LI, Physics, University of Missouri, QIANG ZHENG, ATHENA S. SEFAT, Oak Ridge National Laboratory, DAVID SINGH, Physics, University of Missouri, CLARINA DELA CRUZ, Oak Ridge National Laboratory — Even in the absence of a microscopic theory, a generalized recipe has emerged for unconventional superconductivity. In the common scenario, some ordered phase in a strongly-ish correlated material is suppressed giving rise to quantum fluctuations which can act as a possible pairing mechanism. The nature of these fluctuations – whether they are of the ordered phase, resultant of a quantum critical point or some more exotic pair density wave – is still hotly debated. Therefore, it is useful to find new unconventional superconductors which can provide further insight into the most relevant components of this recipe. The recently discovered family of $A_xTM_3As_3$ ($A = \text{Alkali, } x = 1,2 \text{ and } TM = \text{Cr, Mo}$) superconductors provides such an opportunity in a system with a novel quasi-one-dimensional structure. In this presentation the latest results of joint $\text{ab initio}$ and neutron scattering studies will be discussed which reveal a frustrated structural instability in $K_2\text{Cr}_3\text{As}_3$. Together with our previous reports of spin-fluctuations, this observation indicates a rich phase diagram for this system analogous to the traditional unconventional superconductors.
4:42PM H09.00012: Spontaneous magnetisation in the superconducting state of LaNiGa2*  
GABOR CSIRE, Physics, University of Bristol, SUDEEP GHOSH, PHILIP WHITTLESEA, JORGE QUINTANILLA, Physics, University of Kent, BALAZS UJFALUSSY, Wigner Research Center for Physics, KAZUMASA MIYAKE, Ctr Adv High Maget Field Sci, Osaka University, JAMES ANNETT (Presenter), Physics, University of Bristol — Muon spin relaxation shows spontaneous magnetism in the superconducting state of LaNiGa2. Symmetry analyses imply nonunitary triplet pairing with line nodes and predict a sub-dominant magnetisation consistent with SQUID measurements. In contrast, there is evidence from penetration depth and specific heat for two-gap, nodeless superconductivity. It was proposed to reconcile this by assuming equal-spin inter-orbital pairing. Here we show within a mean-field framework, that this gives rise to a nodeless, two-gap spectrum. We probe the state's stability in the presence of finite inter-orbital energy splitting and derive an analytical expression for the resulting spontaneous magnetisation. Furthermore, we present a detailed calculation combining a realistic first-principles band structure with a phenomenological pairing interaction. We find that equal-spin pairing between certain Nickel d-orbitals can describe the specific heat quantitatively. We predict the two-gap structure in differential tunnelling conductance and the size of the spontaneous magnetic moment.

*We acknowledge support from EPSRC (EP/P007392/1, EP/P00749X/1) and the Hungarian National Research, Development and Innovation Office (contract K115632).

4:54PM H09.00013: Nodeless bulk superconductivity in the time-reversal symmetry breaking Bi/Ni bilayer system*  
PRASHANT CHAUHAN (Presenter), FAHAD MAHMOOD, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD, United States, DI YUE, PENGCHAO XU, XIAOFENG JIN, Department of Physics, Fudan University, Shanghai, China, PETER ARMITAGE, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD, United States — Epitaxial bilayer films of Bi(110) and Ni host a time-reversal symmetry (TRS) breaking superconducting order with an unexpectedly high transition temperature Tc = 4.1K. Using time-domain THz spectroscopy, we measure the low energy electrodynamic response of a Bi/Ni bilayer thin film from 0.2THz to 2THz as a function of temperature and magnetic field. We analyze the data in the context of a BCS-like superconductor with a finite normal-state scattering rate. In zero magnetic field, all states in the film become fully gapped, providing important constraints into possible pairing symmetries. Our data appears to rule out the odd-frequency pairing that is natural for many ferromagnetic-superconductor interfaces. By analyzing the magnetic field-dependent response in terms of a pair-breaking parameter, we determine that superconductivity develops over the entire bilayer sample which may point to the p-wave like nature of unconventional superconductivity.

*Experiments at JHU were supported by the Army Research Office Grant W911NF-15-1-0560. Film growth at Fudan was supported by the National Basic Research Program of China (Grants No. 2015CB921402 and No.2011CB921802), and the National Science Foundation of China (Grants No. 11374057, No. 11434003, and No.11421404)

5:06PM H09.00014: Nontrivial effects of point-like disorder on critical fields and pinning in s± superconductors*  
RUSLAN PROZOROV (Presenter), Ames Laboratory, MARCIN KONCZYKOWSKI, Ecole Polytechnique, VLADIMIR G. KOGAN, MAKARIY TANATAR, Ames Laboratory — In most superconductors non-magnetic point-like defects enhance pinning and upper critical field. However, in s± superconductors, for example iron-based compounds, point-like disorder influences not only intra-band potential scattering, but also inter-band pair-breaking scattering rates. The latter leads to suppression of Tc, Hc2 and the condensation energy. The balance between these opposite effects leads to an increase of (dHc2/dT)T=Tc slope with the decrease of Tc, opposite to what is observed as a function of doping. Even more unusual, it may also lead to a suppression of strong pinning believed to be responsible for a sharp peak in magnetization near H=0. In our experiments controlled disorder was induced by 2.5 MeV electron irradiation.

*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract #DE-AC02-07CH11358.

Tuesday, March 5, 2019 2:30 PM - 5:06 PM

Session H10 DMP: Fe-based Superconductors IV
2:30PM H10.00001: Pairing mechanisms in iron-based superconductors: variations on the s+- theme*  [Invited]  PETER HIRSCHFELD (Presenter), University of Florida — I will review some of the recent developments in the theory of superconductivity of iron-based systems that go beyond the s+- paradigm established in the early days of the field. These include: a) prediction of and evidence for T-breaking mixed symmetry pair states; b) influence of orbital selective correlations on pairing; c) competition and cooperation of nematic order and superconductivity; and d) new pair states possibly stabilized by spin-orbit coupling. A main focus will be a critical look at the of whether Fe-pnictide based materials are fundamentally different from Fe-chalcogenides.

*Research supported by the Department of Energy under Grant No. DE-FG02-05ER46236.

3:06PM H10.00002: Fermi surface pockets in iron pnictides revised by screened exchange dynamical mean-field theory*  STEFFEN BACKES (Presenter), Ecole Polytechnique, AMBROISE VAN ROEKEGHEM, LITEN, CEA, SILKE BIERMANN, Ecole Polytechnique — Until today our understanding of iron based superconductors is hampered by a persistent systematic discrepancy between theory and experiment: the size of the Fermi surface pockets consistently turn out too large in theoretical calculations[1]. Here we show that this puzzle can be solved when taking into account the effect of nonlocal exchange beyond the Density Functional Theory plus dynamical mean-field theory(DFT+DMFT) approach. As it turns out, the nonlocal exchange properties in DFT+DMFT are rather poorly described, leading to an overestimation of the size of Fermi surface pockets. We show that an approximative treatment within screened exchange dynamical mean-field theory gives rise to momentum dependent Fermi surface modifications leading to a significant improvement with experiment. Additionally, we observe a Fermi surface modification in paramagnetic BaFe2As2, where the Fe 3d_{xy} hole pocket in the Brillouin zone center vanishes completely. Reinterpreting existing angle-resolved photoemission (ARPES) experiments, we propose that indeed the Fe 3d_{xy} states are located below the Fermi level, in contrast to previous belief[2].


*ERC 617196, CORRELMAT

3:18PM H10.00003: Doping dependence of the electronic structure and superconductivity of FeSe thin films by Cobalt dopant  SHIYONG TAN (Presenter), XINGYU JI, XINCHUN LAI, China Academy of Engineering Physics — Both superconductivity and structural transition/orbital order are found to be suppressed by Co doping in FeSe single crystal. We have grown FeSe thin films on STO substrates using MBE, and studied the doping dependence of the electronic structure and superconductivity of FeSe thin films by Cobalt dopant. For single layer FeSe, the electron pockets at M point are enlarged when doped with cobalt, and the Tc is slightly increased. When the 2.5 UC, 3.25 UC and 4 UC FeSe sample are electron doped by cobalt, the nematic order is suppressed and superconductivity can be detected. For the multi-layer FeSe thin films, the electronic structure turns out to be alike of single layer FeSe when they are effectively Co doped. But it is not superconducting at the largest doping level, which indicates that the interface effect plays an important role for the high Tc in 1UC FeSe/STO system.

*ERC 617196, CORRELMAT
3:30PM H10.00004: Phase diagram of compressed RbEuFe₄As₄ and CsEuFe₄As₄: Coexistence of superconductivity and magnetism∗

DANIEL JACKSON (Presenter), Pulsed Field Facility, National High Magnetic Field Laboratory, Los Alamos National Lab, DERRICK VANGENNEP, Department of Physics, University of Florida, WENLI BI, Advanced Photon Source, Argonne National Laboratory, DONGZHOU ZHANG, Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, PHILIPP MATERNE, Advanced Photon Source, Argonne National Laboratory, YI LIU, GUANG-HAN CAO, Department of Physics, Zhejiang University, SAMUEL T WEIR, Physics Division, Lawrence Livermore National Laboratory, YOGESH KUMAR VOHRA, Department of Physics, University of Alabama at Birmingham, JAMES HAMLIN, Department of Physics, University of Florida — RbEuFe₄As₄ and CsEuFe₄As₄ are members of the recently discovered 1144 superconducting family, they exhibit the unusual combination of superconductivity (Tc ~ 35 K) and ferromagnetism (Tm ~ 15 K). We performed a series of measurements under compression including x-ray diffraction, magnetic susceptibility, and electrical resistivity. Compression monotonically suppresses Tc and enhances Tm. Near 7 GPa, Tc onset and Tm become comparable, at higher compression evidence of bulk superconductivity gradually disappears. Room-temperature x-ray diffraction measurements provide evidence of a transition from tetragonal to a half-collapse-tetragonal structure near 10 GPa for RbEuFe₄As₄ and near 12 GPa for CsEuFe₄As₄. The cross-over from ferromagnetic superconductor (Tc > Tm), to superconducting ferromagnet (Tm > Tc) occurs before the structural transition, suggesting that RbEuFe₄As₄ and CsEuFe₄As₄ are an ideal system for studying the interplay between superconductivity and magnetism.

∗Equipment development partially supported by the NHMFL User Collaboration Grants Program, NSF Cooperative Agreement DMR-1157490 and the State of Florida, as well as DOE-NNSA DE-NA0002928. Measurements supported by NSF DMR-1453752, NSF EAR-1606856, and DFG MA 7362/1-1. DEJ acknowledges support from LDRD XWR500.

3:42PM H10.00005: Specific heat under pressure on selected iron-pnictide superconductors∗

ELENA GATI (Presenter), GIL DRACHUK, LI XIANG, ANNA BOEHMER, SERGEY BUDKO, PAUL CANFIELD, Ames Laboratory/Iowa State University — The phase diagrams of iron-pnictide superconductors manifest a complex interplay of superconductivity, magnetism and structure which can typically be tuned by external tuning parameters, such as pressure. In this contribution, we report a study of the specific heat under pressure on selected iron-pnictide superconductors, such as FeSe, as well as pure and Co-doped BaFe₂As₂. We will compare pressure-dependent phase diagrams, as well as provide further characterization of the superconducting properties. The latter will, in particular, include a discussion of the evolution of the specific heat jump sizes at the superconducting transition with pressure.

∗This work was carried out at Iowa State University and supported by Ames Laboratory, US DOE, under Contract No. DE-AC02-07CH11358. L. X. was supported, in part, by the W. M. Keck Foundation.

3:54PM H10.00006: Specific heat evidence for rotational symmetry breaking in RbFe₂As₂

OHEI TANAKA (Presenter), YUTA MIZUKAMI, KOUSUKE ISHIDA, MASAYA TSUJII, Department of Advanced Materials Science, University of Tokyo, SHIGEYUKI ISHIDA, AKIRA IYO, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, THOMAS WOLF, KAI GRUBE, HILBERT LOEHNEYSEN, Karlsruhe Institute of Technology, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, University of Tokyo — RbFe₂As₂ has the 3d⁵.₅ electronic configuration, which corresponds to the most heavily hole-doped system among 122-type iron-based superconductors. In this system, a large mass enhancement has been observed, and the importance of the vicinity to the Mott insulator phase at 3d⁵ configuration has been suggested [1]. Recently, we have observed nematic fluctuations along the Fe-As direction, 45° tilted from the nematic direction usually found in other iron-based superconductors. Although the two-fold symmetry along the Fe-As direction has also been suggested from STM measurements [2], the bulk evidence for nematic ordering has not been reported. Here, we perform field-angle-resolved specific heat measurements in RbFe₂As₂ single crystals by using a high-resolution long-relaxation calorimeter. We choose tiny crystals of about 10 μg to avoid cancellation effect of multiple nematic domains. We find clear two-fold oscillations as a function of in-plane field angle near the superconducting transition. This provides bulk evidence for long-range nematic ordering along the Fe-As direction in RbFe₂As₂.

4:06PM H10.00007: Specific heat in strongly hole-doped Iron-based superconductors  DMITRY CHICHINADZE (Presenter), ANDREY CHUBUKOV, University of Minnesota — In our work we compute the specific heat $C(T)$ in an Fe-based superconductor with only hole pockets. We use a three orbital/three pocket model with two smaller hole pockets made out of $d_{xz}$ and $d_{yz}$ orbitals and a larger pocket made out of $d_{xy}$ orbital. We use the experimental fact that the mass of $d_{xy}$ fermion is much heavier than that of $d_{xz}/d_{yz}$ fermions as an input. We argue that the heavy $d_{xy}$ band contributes most to the specific heat in the normal state, but the superconducting gap on the $d_{xy}$ pocket is parametrically smaller than that on $d_{xz}/d_{yz}$ pockets. We also argue that in this situation the jump of $C(T)$ at $T_c$ is determined by $d_{xz}/d_{yz}$ fermions, and the ratio $(C_s - C_n)/C_n$ is a fraction of that in a one-band BCS theory. Below $T_c$, $C(T)$ remains relatively flat down to some $T^*$, below which $C(T)$ rapidly drops. This behavior is consistent with the data for KFe$_2$As$_2$ and related materials. We claim that the data on $C(T)$ can be reproduced without assuming that the quasiparticle residue $Z$ on $d_{xy}$ band is small. We further argue that the very existence of a finite $T^* < T_c$ favors $s^+$ gap structure over $d$-wave, because in the latter case $T^*$ would vanish.

4:18PM H10.00008: Coexistence of superconductivity and magnetism in CaK(Fe$_{1-x}$Ni$_x$)$_4$As$_4$ as probed by $^{57}$Fe Mössbauer spectroscopy* SERGEY BUDKO (Presenter), VLADIMIR G. KOGAN, RUSLAN PROZOROV, WILLIAM MEIER, MINGYU XU, PAUL CANFIELD, Ames Laboratory, Iowa State University — Temperature dependent $^{57}$Fe Mössbauer spectroscopy and specific heat measurements for CaK(Fe$_{1-x}$Ni$_x$)$_4$As$_4$ with $x = 0$, 0.017, 0.049 are presented. No magnetic hyperfine field (i.e. no static magnetic order) was detected down to 5.5 K for $x = 0$ and 0.017 in agreement with the absence of any additional feature below superconducting transition temperature, $T_c$, in the specific heat data. The evolution of magnetic hyperfine field with temperature was studied for $x = 0.033$ and 0.049. The long-range magnetic order in these two compounds coexists with superconductivity. The magnetic hyperfine field, $B_{hf}$, ordered magnetic moment) below $T_c$ in CaK(Fe$_{0.967}$Ni$_{0.033}$)$_4$As$_4$ is continuously suppressed with the developing superconducting order parameter. The $B_{hf}(T)$ data for CaK(Fe$_{0.967}$Ni$_{0.033}$)$_4$As$_4$, and CaK(Fe$_{0.951}$Ni$_{0.049}$)$_4$As$_4$ can be described by Machida’s model for coexistence of itinerant spin density wave magnetism and superconductivity [K. Machida, J. Phys. Soc. Jpn. 50, 2195 (1981)].

*This work was supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Contract No. DE-AC02-07CH11358. W. R. M. was supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant No. GBMF4411

4:30PM H10.00009: Nuclear magnetic resonance techniques for in-situ strain measurements using surface coils CHARLES SNIDER (Presenter), ERICK GARCIA, Brown University, JOHANNA PALMSTROM, IAN R FISHER, Stanford University, VESNA F MITROVIC, Brown University — Widespread efforts have been made to study the role of nematic order in the high temperature superconductivity of iron-based pnictides. This includes the increasing use of strain to explore the anisotropies in electronic states and the nematic susceptibility. Nuclear magnetic resonance (NMR) is the ideal probe to explore such properties because it is sensitive to spin and charge degrees of freedom while allowing the measurement of nematic properties in the superconducting state. It has been shown that strain can be fully transmitted to samples up to approximately 100 μm thick using piezoelectric stacks [J.H. Chu et al. Science 2012], but there are practical limitations in the application of such techniques in NMR. The nontrivial issue of probing such small samples can be overcome by the novel use of surface coils that enhance the signal to noise ratio [W. Liu et al. Rev. Sci. Instrum. 2017] and allow for in-situ sample rotations and controllable application of strain. In this talk, we demonstrate how to simultaneously implement such techniques in NMR experiments.

4:42PM H10.00010: Switching effect in metal-superconductor-metal Fe(0.7Se0.3) nanojunction* YUN LING (Presenter), Suzhou University of Science and Technology, ANDREW STEELEY, ABIN JOSHY, Tulane University, ZHIQIANG MAO, Pennsylvania State University, JIANG WEI, Tulane University — We report our transport study on the metal-superconductor-metal (MSM) device based on Fe(0.7Se0.3) nanoflakes. An unusual switching behavior in I-V characteristics for flakes with a thickness below 10nm has been observed. Furthermore, we discovered that such switching behavior could be controlled by an external magnetic field and bias voltage. Given the traditional understanding that superconductivity in Fe(0.7Se0.3) manifests as the collective effect from clusters of nanoscale superconducting domains, we proposed a self-heating model to explain such switching behavior. Our work demonstrates that nanoscale junction between superconducting and normal metal naturally exists in thin Fe(0.7Se0.3) nanoflakes, which provides an opportunity to study transport behavior MSM junction in nanoscale.

*This work was supported by the DOE under grant DESC0014208 and by the Board of Regents Support Fund (BoRSF) under grant LEQSF(2015-18)-RD-A-23.
4:54PM H10.00011: Nodeless superconductivity with broken time reversal symmetry*  HUIQIU YUAN (Presenter),
Center for Correlated Matter/ Department of Physics, Zhejiang University — In unconventional superconductors, additional
symmetries, e.g., rotational symmetry and time reversal symmetry (TRS), may be broken below the superconducting
transition temperature. In the past, evidence for TRS breaking was observed in a few nodal superconductors with a
possible triplet pairing state. Recently, there are a growing number of compounds which behave like a simple s-wave BCS
superconductor, but break TRS below $T_c$. How to reconcile these seemingly contradictory feature is currently an
interesting problem. In this presentation, we will present our recent results on a few Re- and La-based nodeless
superconductors with broken TRS at $T_c$, including a few new examples. We will try to summarize their common features
and discuss the possible pairing states and origin of the TRS breaking.

This work is in collaboration with M. Smidman, A, Wang, P. R. Zhang, Z. Y. Nie, W. Xie, G. M. Pang (Zhejiang University), T.

*This work was supported by the National Key R&D Program of China, the National Natural Science Foundation of China
and the Science Challenge Project of China.

Tuesday, March 5, 2019 2:30 PM - 4:54 PM

Session H11 DMP DCOMP FIAP: Defects in Semiconductors -- Quantum Materials BCEC 152 -

Cyrus Dreyer, Stony Brook University - Tag(s): Focus

2:30PM H11.00001: Scaling Study of Disordered Antiferromagnetic Systems of Acceptors in p-Type Semiconductors
ADAM DURST (Presenter), ALI HYDER, Hofstra University — We consider the low temperature magnetic properties of a system
of randomly-distributed interacting acceptor atoms in a p-type semiconductor. For the equivalent n-type system, where
donor interactions are well described by a spin-1/2 Heisenberg model with a single antiferromagnetic exchange coupling
that varies exponentially with donor separation, the classic work of Bhatt and Lee [Phys. Rev. Lett. 48, 344 (1982)] provides
an iterative numerical procedure for discarding irrelevant high energy excitations of strongly interacting donor pairs while
renormalizing the remaining donor couplings. Due to valence band degeneracy and spin-orbit coupling, acceptor
interactions are known to be more complex. Recent computations thereof suggest a six-level energy spectrum
characterized by five distinct coupling parameters and a nontrivial degeneracy structure. By employing an interaction
model that respects this degeneracy structure, we extend the Bhatt-Lee renormalization procedure to the acceptor case,
studying the evolution of the distribution of exchange couplings, and calculating magnetic susceptibility, as a function of
decreasing temperature. Results are compared with that of spin-1/2 and spin-3/2 Heisenberg models.

2:42PM H11.00002: Theory of Hyperfine Interactions and Electrically Detected Magnetic Resonance (EDMR) for
Phosphorus-Doped Silicon*  NICHOLAS HARMON (Presenter), MICHAEL FLATTÉ, Physics and Astronomy, University of Iowa —
EDMR is a useful tool to sensitively study a spin pair's local environment as well as spin-dependent recombination.
Theoretical treatments have focused on resonances originating from differences between g-factors of two recombining
spins [1]. Recently hyperfine interactions were included but in a classical manner [2]. We present a theory of EDMR where
transitions take place via differences in g-factor or hyperfine interactions. The stochastic Liouville formalism is suited to
account for hyperfine interactions involving multiple nuclei where each nuclear spin is a quantum spin. For a single spin-
1/2 nucleus, expressions for resonances at any field are determined and agree with most measured resonances in
phosphorus-doped silicon [3]. Comparisons between the model and observations lead to new understandings of the
defect-induced recombination pathways.


*The project or effort depicted was or is sponsored by the Department of the Defense, Defense Threat Reduction Agency.
The content of the information does not necessarily reflect the position or the policy of the federal government, and no
official endorsement should be inferred.
2:54PM H11.00003: The Interplay among Localization Spin-Orbit Coupling and Ferromagnetism in the Diluted Magnetic Semiconductor (Ga,Mn)As* YI ZHANG (Presenter), Louisiana State University, UNJONG YU, Department of Physics and Photon Science, GIST, HANNA TERLETSKA, Middle Tennessee State Univ, KA-MING TAM, MARK JARRELL, Louisiana State University — We combine the typical medium analysis and dynamical mean field approximation to study the electronic and magnetic properties of the diluted magnetic semiconductor Ga$_{1-x}$Mn$_x$As. We use the $k$-$p$ model to describe the electronic structure of GaAs with spin-orbit coupling. By using the typical medium analysis, localization due to disorder induced by the Mn doping is appropriately captured, which allows us to study the interplay among the localization, spin-orbit coupling and ferromagnetism. This study can serve as a guidance to the more realistic first-principles calculation of Ga$_{1-x}$Mn$_x$As.

*This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0017861.

3:06PM H11.00004: Spontaneous defect formation on the polar surface of giant Rashba semiconductors BiTeX*

[Invited] WEIDA WU (Presenter), WENHAN ZHANG, Physics and Astronomy, Rutgers University, New Brunswick, DAMIEN WEST, Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, CHEN CHEN, JINWOONG KIM, SANG-WOOK CHEONG, DAVID VANDERBILT, Physics and Astronomy, Rutgers University, New Brunswick, SHENGBAI ZHANG, Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute — Defects in semiconductors are crucial for the performance of modern electronics. Although there are tremendous progress on theoretical understanding of defect formation and kinetics in functional materials, visualizing the kinetics of the defect formation remains a great challenge. Herein, we report an exciting discovery of spontaneous formation of point defects below room temperature on the surface of polar semiconductors BiTeX (X=Cl, Br and I), where giant Rashba splitting of bulk bands was reported. The defect density increases over three order of magnitudes when the surface temperature increases from ~10 K to room temperature. Our scanning tunneling microscopy studies reveal formation of Frenkel pairs of Bi vacancies and interstitial Bi atoms, followed by the formation of BiTe antisites. Combined with first principle calculations, our results reveal a significant reduction of formation energy of Frenkel pairs due to surface band bending of polar surface. Our results demonstrate a dramatic modulation of defect formation via surface bending of polar surface, which is crucial for the potential technological application of giant Rashba systems.

*The STM works at Rutgers were supported by NSF Grant No. DMR-1506618. S.B.Z. was supported by the Department of Energy under Grant No. DE-SC0002623. D.W. was supported by NSF under Grant No. EFMA-1542789. The supercomputer time was provided by the CCNI at RPI and NERSC under DOE Contract No. DE-AC02-05CH11231. The single crystal synthesis works were supported by NSF under Grant No. DMR-1629059.

3:42PM H11.00005: 3D imaging and manipulation of subsurface selenium vacancies in PdSe$_2$* GIANG NGUYEN, LIANGBO LIANG, QIANG ZOU, MINGMING FU, AKINOLA OYEDELE, BOBBY G SUMPTER, Oak Ridge National Laboratory, ZHENG LIU, Nanyang Technological University, ZHENG GAI, KAI XIAO, AN-PING LI (Presenter), Oak Ridge National Laboratory — We report 3D imaging and manipulation of individual Se vacancies in PdSe$_2$ using a STM. By imaging the characteristic charge rings of defects arising from a tip-induced band bending effect, we first determine the lateral and depth location of V$_{Se}$ precisely in the 3D lattice. We then use a STM tip as a movable electrostatic gate to manipulate V$_{Se}$ by reversibly switching the charge states of defects between neutral and negative states. We find a slightly higher bias voltage (~2.0 V) can trigger vacancy migrations, which allows us to demonstrate both direct "writing" and "erasing" of atomic defects from a particular lattice site in PdSe$_2$. The results are corroborated by first-principles calculations that unveil the formation energy and diffusion barriers of Se vacancies in PdSe$_2$. This work opens an opportunity for defect engineering at the atomic level to achieve controlled phase transformations, or on-demand switchable states for such as neuromorphic computing and quantum bits.

*This research was performed at the Center for Nanophase Materials Sciences which is a DOE Office of Science User Facility.
**3:54PM H11.00006: Colossal thermopower from defect-induced in-gap states in FeSb$_2$**  
QIANHENG DU (Presenter), Department of Materials Science and Chemical Engineering, Stony Brook University, CEDOMIR PETROVIC, Brookhaven National Laboratory — The thermoelectric properties of FeSb$_2$ are attracting attention due to its colossal thermopower and record-high thermoelectric power factor. Although this colossal thermopower was attributed to phonon-drag effect, the factors that affect the phonon-drag effect remains unclear and further. By changing the amount of defects in different FeSb$_2$ crystals we show that thermopower maxima around 10 K change between relatively small 14 μV/K and colossal values of about 20 mV/K. The effect of crystallographic defects and impurities on the colossal thermopower coefficient is studied in single crystals of FeSb$_2$. From the Hall effect, all the crystals show clear two-bands behavior. Defect-induced vacancy band with low Hall mobility dominates the thermal transport. Defects influence considerably phonon mean free path and low mobility band carrier concentration, revealing the source of the in-gap states that govern thermopower size. Our results explain the strong sample dependence of Seebeck coefficient in FeSb$_2$ crystals and give a possible way to furtherly improve the thermal performance of this correlated semiconductor.

**4:06PM H11.00007: Anisotropic defects and assisted scattering in InAs/GaSb superlattices**  
FRANCESCA CAROSELLA (Presenter), Ecole Normale Superieure, HERMANN DETZ, CEITEC, Brno University of Technology, GÉRALD BASTARD, ROBSON FERREIRA, Ecole Normale Superieure — Heterostructures containing antimonide-based compounds received in the last decade much attention because of their potential for designing new devices. Moreover, some InAs/GaSb heterostructures are also topological insulators thus attracting interest for fundamental research. We performed a thorough multi-scale study of the structure and electronic states of InAs/GaSb superlattices (SL). We have implemented the envelope function formalism for the calculation of the electronic states in these SL, taking into account the strong coupling between conduction and valence states. To improve the description of interface roughness, we performed atomistic simulations (using empirical interaction potentials as well as a Monte Carlo based algorithm) of the growth of InAs/GaSb short-period SL. In particular, we found that the simulated growth of InAs on GaSb along the usual [0,0,1] axis leads to the formation of elongated islands, one ML height, one ML thick, but with a much bigger average length along the direction [1,1,0]. Finally, we tackled the effect of the interface disorder on the electronic properties of these heterostructures. To this end, we present a model to perturbatively evaluating scattering rates by an inhomogeneous ensemble of defects with such a particular aspect ratio.

**4:18PM H11.00008: Scanning Tunneling Microscopy Studies of Er Adatoms on GaAs (110)***  
REBEKAH SMITH (Presenter), ANNE BENJAMIN, KEVIN WERNER, ENAM CHOWDHURY, JAY A GUPTA, Ohio State University — Rare earth dopants in III-V semiconductors are of interest as high quality optical sources due to the preservation of sharp intra-$f$-shell transitions. Here we investigate Er interactions with host GaAs (110) surface with atomic resolution using STM. Er atoms were deposited via electron beam evaporation onto the GaAs surface at 5 K. We find three different Er$_{\text{ad}}$ configurations with varying abundance upon deposition, each with a different surface site location. All three configurations exhibit long-range depressions in STM topographic images, attributed to band bending associated with a positive adatom charge state. Individual Er adatoms can be switched between these states by applying a positive voltage pulse with the STM tip. Tunneling spectroscopy on Er adsorbed at the interstitial sites reveals prominent states within the GaAs bandgap, but no evidence of sharp $f$-shell transitions inferred from bulk optical studies. We also form substitutional Er$_{\text{Ga}}$ by applying a larger positive voltage pulse. Substitutional Er appears neutral, which we attribute to it being isoelectronic with Ga. We will also present preliminary studies with concurrent optical excitation. Shifts in Er defect states are interpreted as a surface photovoltage effect.

*We acknowledge funding from DOE-DE-SC0016379.
We propose a self-consistent site-dependent (SCSD) DFT+U approach for calculations of defects in transition-metal oxides. Defect formation in these materials induces local perturbations in the chemical environment of Hubbard sites around the defect that may not be properly described by applying a global U value on all sites as done in conventional DFT+U. Here, U is treated as an intrinsic response property of the material and computed from first principles using density-functional perturbation theory. SCSD U values are obtained starting from a DFT ground state by an iteration of perturbing all inequivalent Hubbard sites followed by geometry relaxation with the determined U values until convergence of the geometry and U. Changes in U due to excess charge localization and lattice relaxation in defective structures are hence properly accounted for.

After discussing the approach, we highlight some results, showing that U values depend on the distance of the Hubbard site from the defect, its coordination number, its oxidation state, and on the magnetic properties of the material. This site-dependence is particularly important in the case of semiconductors, where filled localized defect states may form in the band gap, and strongly influences all properties related to defect energetics.

**Novel II-VI compound based organic-inorganic hybrid semiconductors: intrinsic properties, defects, and long-term stability**

TANG YE (Presenter), MARGARET KOCHERGA, ANDREI NESMELOV, THOMAS A. SCHMEDAKE, YONG ZHANG, University of North Carolina at Charlotte — The hybrid structures in this study are a family of sub-nanoscale II-VI layers or chains interconnected or coordinated with smaller organic linkers.[1] They were shown to exhibit a very high degree of structural ordering (e.g., the most perfect man-made semiconductor superlattices), and a number of extraordinary properties such as much-greater-than-kT exciton binding energy, exceedingly strong excitonic absorption, and zero thermal expansion.[2,3] Comparison between Raman, PL and XPS spectra of freshly made and approximately 15-year old samples of a prototype hybrid structure β-ZnTe(en)0.5 have revealed defect related spectroscopy signatures that appear in both newly made defective samples and aged samples. Although the old samples typically show varying degree of degradation, some are found to be as pristine as high-quality freshly made samples. The study suggests that the initial state of the defect level is pertinent to the material's long-term stability. This is a rare example of hybrid materials exhibiting recorded long-term stability. This study has a broad impact on the long-term stability of a wide range of hybrid materials, including perovskites.


*Funding Acknowledgement: ARO Materials Science

**Tuesday, March 5, 2019 2:30 PM - 5:30 PM**

**Session H12 DMP: Devices from 2D Materials -- Theory**

BCEC 153A - Yang Gao, Carnegie Mellon University - Tag(s):

Focus

**2:30PM H12.00001: Theory of 2D Materials: Excitons, Valley-Spin Physics, and Magnetism.** [Invited] TING CAO (Presenter), Physics Department at UC Berkeley and Geballe Laboratory for Advanced Materials at Stanford University — Recent advances in the experimental and theoretical studies of atomically thin two-dimensional (2D) materials have opened up opportunities in exploring new phenomena and properties as well as related applications absent in conventional bulk materials. In the first part of my talk, we will present theoretical studies on the optical responses of monolayer transition metal dichalcogenides. By ab initio GW-BSE calculations, we demonstrate a previously unrecognized valley-spin character of bright excitons, which leads to interesting ultrafast phenomena in monolayer transition metal dichalcogenides [1]. We then discuss the theory of dark excitons and trions, and how they could be brightened by applying an external magnetic field [2] or using other approaches. In the second part of my talk, we will discuss theoretical studies of magnetism in 2D materials. We discuss the physical origins and control of ferromagnetism in materials with different chemical species and structural configurations. We further connect our theoretical discoveries to experimental results and explore their potential applications.


*This work was supported by U. S. Department of Energy and National Science Foundation. I would like to acknowledge collaborations with Louie, Fleming, and Heinz groups, as well as support from a GLAM postdoctoral fellowship at Stanford University.
3:06PM H12.00002: A theoretical proposal of gate-induced quantum anomalous hall effect in 2D ferromagnetic multilayers  
YUAN GAO (Presenter), Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, DI XIAO, Department of Physics, Carnegie Mellon University, WENGUANG ZHU, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China — The quantum anomalous hall effect (QAHE) is the manifestation of topological electronic structure characterized by a finite Chern number and helical edge electron states and may have potential applications in future electronic devices with low energy consumption. However, the QAHE so far can only be achieved at very low temperatures. Thus, the search for new quantum anomalous hall systems with elevated temperature is in demand. Here we propose a new design based on recently discovered 2D ferromagnetic semiconductors. Using first-principles calculations, we demonstrate that by applying a moderate electric field a 2D ferromagnetic multilayer can be converted into the quantum anomalous hall state. The topological nature and band gap as a function as the applied electric field and film thickness are systematically investigated in details.

3:18PM H12.00003: Simulating the nanomechanical response of cyclooctatetraene molecules on a graphene device*  
SEHOON OH (Presenter), MICHAEL F CROMMIE, MARVIN L COHEN, Department of Physics, University of California at Berkeley — We have investigated the atomic and electronic structures of cyclooctatetraene molecules on graphene and analyzed their dependence on external gate voltage using first-principles calculations. The external gate voltage is simulated by adding or removing electrons using density functional theory calculations. This allowed us to investigate how changes in carrier density modify the molecular shape, orientation, adsorption site, diffusion barrier, and diffusion path. The results of the calculation imply that the shape and mobility of the adsorbed molecules can be controlled by externally gating graphene devices.

*This work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under contract no. DE-AC02-05CH11231 within the Nanomachine program, and by the National Science Foundation under Grant No. DMR-1508412.

3:30PM H12.00004: Universal scaling laws of electron emission phenomena in two-dimensional material electrical contacts*  
YEE SIN ANG (Presenter), Science and Math, Singapore University of Technology and Design, HUI YING YANG, SUTD-MIT International Design Center, Singapore University of Technology and Design, LAY KEE ANG, Science and Math, Singapore University of Technology and Design — Electrically contacting two-dimensional (2D) material with another material often leads to the formation of an interfacial Schottky barrier. Charge injection across such barrier is commonly analysed using the classic Richardson-Dushman (thermionic emission) and Fowler-Nordheim (field emission) models despite the fact that the assumptions underlying such models are often inconsistent with the physical properties of most 2D materials. Here we formulate generalized models of electron injection across 2D material interfaces. We show that the thermionic transport across a 2D material Schottky contact is governed by universal scaling laws broadly applicable for large classes of 2D systems. We further uncover a new universal scaling behavior in the vertical electron tunneling across 2D material van der waals heterostructures. Our models signal the breakdown of century-old classic electron emission models in 2D materials, and paves the way towards the better understanding and design of 2D material electronic devices.


*This work is supported by A*STAR IRG (A1783c0011) and AFOSR AOARD (FA2386-17-1-4020).
Design of Atomically Precise GNR-Based Negative Differential Resistance Device

ZHONGCAN XIAO (Presenter), North Carolina State University, CHUANXU MA, JINGSONG HUANG, LIANGBO LIANG, Oak Ridge National Laboratory, WENCHANG LU, North Carolina State University, KUNLUN HONG, BOBBY G SUMPTER, AN-PING LI, Oak Ridge National Laboratory, JERRY BERNHOLC, North Carolina State University — Down-scaling device dimensions to the nanometer range raises significant challenges to traditional device design, due to potential current leakage across nanoscale dimensions and the need to maintain reproducibility while dealing with atomic-scale components. Here we investigate negative differential resistance (NDR) devices based on atomically precise graphene nanoribbons. Our computational evaluation of the traditional double-barrier resonant tunneling diode NDR structure uncovers important issues at the atomic scale, concerning the need to minimize the tunneling current between the leads while achieving high peak current. We propose a new device structure consisting of multiple short segments that enables high current by the alignment of electronic levels across the segments while enlarging the tunneling distance between the leads. The proposed structure can be built with atomic precision using a scanning tunneling microscope (STM) tip during an intermediate stage in the synthesis of an armchair nanoribbon. An experimental evaluation of the band alignment at the interfaces and an STM image of the fabricated active part of the device are also presented. This combined theoretical-experimental approach opens a new avenue for the design of nanoscale devices with atomic precision.

Deep Learning Assisted Optical Identification of Exfoliated Two-Dimensional Crystals

BINGNAN HAN, School of Astronautics, Beihang University, YUXUAN LIN (Presenter), Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, WENYUE LI, School of Astronautics, Beihang University, NANNAN MAO, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, YAFANG YANG, Department of Physics, Massachusetts Institute of Technology, HAOZHE WANG, WEI SUN LEONG, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, PABLO JARILLO-HERRERO, Department of Physics, Massachusetts Institute of Technology, TOMAS PALACIOS, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, JIHAO YIN, School of Astronautics, Beihang University, JING KONG, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology — Up to now, hundreds of two-dimensional materials are being studied in the fields of condensed matter physics, material sciences and electrical engineering. The overwhelming approach to obtain 2D crystals in laboratory is a combination of the mechanical exfoliation and the exhaustive search under an optical microscope by a well-trained researcher. Here we report a generic flake-hunting approach assisted by deep learning that can achieve the automatic, real-time, accurate, and robust optical identification of the type and the thickness of various 2D crystals. A semantic segmentation method using the encoder-decoder convolutional neural networks (SegNet) was developed and trained to identify the type and the thickness of the mechanically exfoliated 2D crystals on a SiO2/Si wafer. Besides the commonly used parameters such as the optical contrasts of the 2D crystals, deep graphical features can also be extracted and harnessed by the SegNet for accurate and robust identification. Our proposed method can be used for a wide range of research topics where initial screening and identification of nanomaterials are necessary.

Ab Initio Study of the Mechanisms of Nitrogen Functionalization of Graphene*

OLIVIER MALENFANT-THUOT (Presenter), MICHEL COTE, Universite de Montreal — Our research aims to better understand the process of nitrogen functionalization of graphene, at the atomic level. We conducted electronic structure calculations, in the Density Functional Theory framework, to study the dynamics of different incorporation mechanisms of nitrogen atoms. We used the Nudged Elastic Band module, available in the BigDFT ab initio code, to calculate reaction pathways and energy barriers for a diverse set of migration and incorporation reactions, with or without the presence of native defects in the graphene sheet. By analyzing these results, we can predict which processes and functionalization configurations are more likely to be obtained in particular conditions.

*This research was enabled in part by support provided by Calcul Québec (www.calculquebec.ca) and Compute Canada (www.computecanada.ca) and has been supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) under grants RGPIN-2016-06666.

Model for the metal-insulator transition in graphene superlattices and beyond

NOAH YUAN (Presenter), LIANG FU, Massachusetts Institute of Technology — We propose a two-orbital Hubbard model on an emergent honeycomb lattice to describe the low-energy physics of twisted bilayer graphene. Our model provides a theoretical basis for studying metal-insulator transition, Landau level degeneracy lifting, and unconventional superconductivity that are recently observed.
may lead to important electronic and spintronic devices. The coupling condition provides important insights in the design and manufacture of two-dimensional heterostructures where no significant p-d coupling exist. This discovery largely widens the scope of periodic structures and the general coupling with substrate and explains why the incommensurate bilayer is even more stable than an AB stacking bilayer, where the top layer to couple and form a gap at the M point of the lower layer. This mechanism also enhances a p-d orbital.

On our first principles calculations, we found that such a coupling mechanism allows a coupling of K and K’ wave vectors of any two vectors of one layer, if their difference equals the difference between the reciprocal vectors of the two layers, for any two vectors of one layer, if their difference equals the difference between the reciprocal vectors of the two layers. Based on our first principles calculations, we found that such a coupling mechanism allows a coupling of K and K’ wave vectors of the top layer to couple and form a gap at the M point of the lower layer. This mechanism also enhances a p-d orbital coupling with substrate and explains why the incommensurate bilayer is even more stable than an AB stacking bilayer, where no significant p-d coupling exist. This discovery largely widens the scope of periodic structures and the general coupling condition provides important insights in the design and manufacture of two-dimensional heterostructures that may lead to important electronic and spintronic devices.

Since the advent of exfoliated graphene on SiO2/Si substrates, the identification process of graphene has relied on the feature extraction algorithm, enabling highly accurate classification of monolayer, bilayer, and trilayer graphene. The analysis can be applied to substrates with differing SiO2 thickness, which demonstrates the generality of the approach.

*This work was supported by the Core Research for Evolutional Science and Technology (JPMJCR15F3), Japan Science and Technology Agency (JST).

4:54PM H12.00011: Theoretical investigation of 30 degree twisted bilayer graphene* KEJIE BAO (Presenter), YIOU ZHANG, JUNYI ZHU, Physics, Chinese University of Hong Kong, SHUYUN ZHOU, Physics, Tsing Hua University — To understand the unique stability and coupling mechanism in the interesting incommensurate bilayer graphene on top of Pt substrate with 30 degree twisting angles, we performed theoretical derivations and discovered a general interlay scattering mechanism: for any two vectors of one layer, if their difference equals the difference between the reciprocal vectors of the two layers, they can be coupled via a scattering of another layer. This scattering condition is general for any bilayer structures. Based on our first principles calculations, we found that such a coupling mechanism allows a coupling of K and K’ wave vectors of the top layer to couple and form a gap at the M point of the lower layer. This mechanism also enhances a p-d orbital coupling with substrate and explains why the incommensurate bilayer is even more stable than an AB stacking bilayer, where no significant p-d coupling exist. This discovery largely widens the scope of periodic structures and the general coupling condition provides important insights in the design and manufacture of two-dimensional heterostructures that may lead to important electronic and spintronic devices.

*start-up HKRGC funding with the Project Code of 1431916.
General Research Fund (Grant 2130490) from Research Grants Council in Hong Kong.

5:06PM H12.00012: Unconventional superconductivity and density waves in twisted bilayer graphene* HIROKI ISOBE (Presenter), NOAH YUAN, LIANG FU, Massachusetts Institute of Technology — We study electronic ordering instabilities of twisted bilayer graphene with n=2 electrons per supercell, where correlated insulator state and superconductivity are recently observed. Motivated by the Fermi surface nesting and the proximity to Van Hove singularity, we introduce a hotspot model to study the effect of various electron interactions systematically. Using the renormalization group method, we find d/p-wave superconductivity and charge/spin density wave emerge as the two types of leading instabilities driven by Coulomb repulsion. The density wave state has a gapped energy spectrum at n=2 and yields a single doubly-degenerate pocket upon doping to n=2. The intertwine of density wave and superconductivity and the quasiparticle spectrum in the density wave state are consistent with experimental observations.

*This work is supported by the DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award de-sc0010526. LF is partly supported by the David and Lucile Packard Foundation.
5:18PM H12.00013: Twisted bilayer graphene as a phononic metamaterial* WILLIAM DORRELL (Presenter), HARRIS PIRIE, BOWEI LIU, YU LIU, NATHAN DRUCKER, ALEX J KRUCHKOV, JENNY HOFFMAN, Harvard University — The twist angle within stacked van der Waals materials represents a novel degree of freedom to tune electronic properties. In bilayer graphene, varying the twist angle hybridizes the Dirac cones from each layer, resulting in flat bands that localize charge and induce unconventional superconductivity. Recently, graphene-like Dirac cones were observed in the phononic band structure of a metamaterial consisting of a honeycomb lattice of steel pillars in air. However, varying the twist angle has not been explored in metamaterials, due to the difficulty in coupling two macroscopic layers. Here we develop a method to couple layered phononic metamaterials using intermediary membranes, and we numerically demonstrate a classical system with flat phononic bands analogous to the electronic structure at magic angle twisted bilayer graphene. Our results provide a more tangible route to comprehending the behavior of quantum materials and may yield applications in super-resolution imaging.

*This work was supported by the Center for Integrated Quantum Materials, NSF grant DMR-1231319. HP was funded by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4536.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H13 DMP: 2D Materials (General) -- Defects BCEC 153B - Victor Brar, Caltech - Tag(s): Focus

2:30PM H13.00001: Combining nitrogen substitutional defects and oxygen intercalation to control corrugation and doping level in graphene on Rh(111) JOSE-MARIA GOMEZ-RODRIGUEZ (Presenter), ANA MARTIN-RECIO, Dept. Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Spain, CARLOS ROMERO-MUÑIZ, PABLO POU, RUBEN PEREZ, Dept. Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, Spain — By means of STM experiments and first-principles calculations, we demonstrate the synergetic effect of combining two different strategies to modify the properties of graphene supported on a strongly interacting substrate. A complete control of the corrugation and doping level is achieved by the introduction of nitrogen defects and oxygen intercalation. First, we use ion bombardment to obtain purely-substitutional N-doped graphene on Rh(111) with tunable dopant concentration. Second, the interaction with the substrate is controlled by the amount of intercalated oxygen atoms. Unlike weakly interacting substrates, the highly corrugated structure of G/Rh(111) leads to remarkable variations of the electronic properties associated with N defects created in the high and low areas of the moire. After oxygen intercalation, the N-doped graphene layer decouples from the substrate preserving the incorporated N atoms, which display a subtle dependence of the STM contrast. First principles calculations confirm the identification of substitutional N defects and the recovery of the Dirac cone with a tunable shift governed by N concentration. Our results support the combination of different modification techniques to tailor structural and electronic properties of graphene and other 2D materials.

2:42PM H13.00002: Observation of superlattice periodicity on the surface of highly-doped MoS2 STEVEN SCHOFIELD (Presenter), MOHAMMED BIN SUBHAN, ASIF SULEMAN, GARETH MOORE, PETER PHU, HIDEKAZU KUREBAYASHI, CHRIS A. HOWARD, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London — We have used low temperature (~5 K) scanning tunnelling microscopy (STM) and spatially-resolved tunnelling spectroscopy (STS/CITS) to investigate the surface of highly-doped molybdenum disulphide (MoS2). In agreement with previous STM investigations of intrinsic MoS2 we find the surface exhibits a large density of charged point defects [e.g., ACS Appl. Mater. Interfaces, 9, 19278 (2017)]. Fourier analysis of our atomic-resolution imaging and spectroscopy data from the doped MoS2 surface reveals two separate superlattice periodicities in addition to the 1x1 sulphur lattice, one of which is enhanced in the vicinity of the charged defects. We present an interpretation of the observed superlattices consistent with prior DFT and ARPES data.
In this work, we employ a combination of theoretical calculations to explore the electronic properties of donor and acceptor states of substitutional impurities in h-BN, a wide-gap 2D insulator. We find that the structure of the impurity levels that appear inside the electronic gap strongly depends on the atom replaced by the impurity. For instance, when an acceptor replaces a N atom, the intervalley interaction induced by the impurity is found to be strong and the resulting level structure consists only of non-degenerate levels with strong valley and spin splittings. On the other hand, when an acceptor replaces a B atom, the intervalley interaction is much weaker and a near-valley-degenerate ground state is found. Donor impurities behave on a similar fashion. We show that the differences between these level structures can be traced to the peculiar sublattice-resolved electronic structure of pristine h-BN. In fact, these exotic impurity levels may also be present in other 2D semiconductors and insulators with similar bandstructures, such as other hexagonal III-V compounds, and their optical properties may be engineered for applications in future optoelectronic devices.

*This research was supported by the Office of Naval Research (ONR N00014-17-1-2993) and the National Science Foundation Materials Research Science and Engineering Center at Northwestern University (NSF DMR-1720139).
3:54PM H13.00006: Point defects in 1T'-MoS2 from first principles  MICHELE PIZZOCHERO (Presenter), OLEG YAZYEV, Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland — Monolayers of group VI Transition Metal Dichalcogenides (TMDs) exist in either the semiconducting 2H phase or semimetallic 1T' phase. While the stable 2H phase has been extensively investigated due to prospective optoelectronic applications, the metastable 1T' phase has appeared in the spotlight only recently, mainly due to its topological properties. In this talk, I will provide an overview on the formation of point defects in 1T'-MoS2 within two experimentally-relevant situations, i.e. under thermodynamic equilibrium and under electron beam irradiation. First, I will address the stability of point defects, exploring several configurations of vacancy, adatom and antisite defects. All considered defects exhibit lower formation energies in the 1T' phase compared to the 2H phase, suggesting that the 1T' polymorph is more susceptible to lattice imperfections. Next, the response of 1T'-MoS2 to the electron irradiation will be examined. The range of electron beam energies needed to carry out imaging without inducing any damages in the sample and some guidelines for the controlled creation of defects in the electron microscope are discussed. Throughout my talk, I will draw comparisons between local disorder in the two phases to portray a complete picture of the role of defects in TMDs.

4:06PM H13.00007: Correlating Microscopic Electronic Features with Macroscopic Transport in Defective Graphene* JAKE RIFFLE (Presenter), CAITLYN MEDITZ, ALANA GUDINAS, SHAWNA HOLLEN, University of New Hampshire — Past studies on graphene show that intervalley and intravalley scattering off atomic defects and impurities change the electronic transport properties and give rise to weak Anderson localization at low temperatures. We will present our studies on the interactions and correlations between electron-hole charge puddles and the weakly localized regions. Using a low temperature scanning tunneling microscope (STM) on graphene field effect transistors, we present experiments which aim to study the effects of point defects and to employ simultaneous STM and electronic transport measurements to directly associate microscopic electronic interactions with macroscopic transport. These experiments will show strides toward mapping out the phase space of defect-populated graphene in our investigation of the prospect of a metal-insulator quantum phase transition.

*This work supported by NSF DMR (1709029)

4:18PM H13.00008: Atomic manipulation of defects in the layered semiconductor 2H-MoTe2* SARA MUELLER (Presenter), Ohio State University, BENJAMIN ST. LAURENT, University of New Hampshire, YAXIAN WANG, WOLFGANG E WINDL, Ohio State University, SHAWNA HOLLEN, University of New Hampshire, JAY A GUPTA, Ohio State University — Here we demonstrate control over the charge state and layer position of individual defects in the layered semiconductor, 2H-MoTe2. Pristine surfaces were revealed at room temperature in ultrahigh vacuum by cleaving the top few layers from the crystal. STM images and spectroscopy were performed with a cut PtIr tip at 9K. Two classes of native defects were observed in large area STM images, appearing in both near-surface and sub surface layers with progressively fainter contrast. One class of defect images as a bright protrusion with a nm-scale fall-off in STM topography, indicative of band bending associated with a charged defect. Spectroscopic imaging reveals a ring-shaped feature associated with these defects, consistent with tip-induced ionization between two defect charge states. Consistent with studies in other semiconductor systems, the rings depend on the STM imaging conditions and tip apex. We find that subsurface defects exhibit discrete increases in apparent height following large positive voltage pulses, suggesting migration between layers near the surface. We compare with DFT calculations to identify these defects and estimate the energy barriers for inter-layer migration.

*Funding by NSF MRSEC DMR-1420451.

4:30PM H13.00009: Defect Characterization and Engineering in Black Phosphorus  BEN ST LAURENT (Presenter), JAKE RIFFLE, CAMERON C FLYNN, Physics, University of New Hampshire, CHARLIE AYOTTE, CHRISTINE CAPUTO, Chemistry, University of New Hampshire, SHAWNA HOLLEN, Physics, University of New Hampshire — A tunable band gap and high carrier mobility make black phosphorus (BP) attractive for device applications. To effectively engineer micron scale BP devices, it is essential to understand defects down to the atomic level. The most prominent defects on the surface of BP exhibit a large electronic signature in scanning tunneling microscopy (STM) images. We previously found that the predominant defects in BP are vacancies and are the source of p-doping in the material. These studies demonstrate the need for vacancy formation control during synthesis. Here, we will describe STM experiments of BP that further characterize the defects and explore defect control and creation through ultra high vacuum annealing.
4:42PM H13.00010: Direct correlation of defects with photoluminescence and electrical conductivity in monolayer transition metal dichalcogenides*  MATTHEW ROSENBERGER (Presenter), HSUN-JEN CHUANG, KATHLEEN MCCREARY, SAUJAN SIVARAM, CONNIE LI, BEREND JONKER, Materials Science and Technology Division, U.S. Naval Research Laboratory — Transition metal dichalcogenides (TMDs) are promising candidates for emerging applications such as transparent and flexible optoelectronics and electronics. Understanding the impact of defects on TMD properties is essential for the advancement of these materials. Here, we demonstrate the ability to observe electronically active defects in monolayer TMDs using conductive atomic force microscopy in ambient conditions, and we correlate defect density with local potential gradients, corresponding to high resistivity. This suggests that the defects responsible for decreased PL intensity are also responsible for decreased electrical conductivity.

*M.R. and S.S. hold NRC fellowships, H.C. holds an ASEE fellowship

4:54PM H13.00011: Spatially Selective Enhancement of Photoluminescence in MoS2 by Photo-mediated Adsorption and Defect Passivation  SAUJAN SIVARAM (Presenter), AUBREY HANBICKI, MATTHEW R. ROSENBERGER, HSUN-JEN CHUANG, KATHLEEN MCCREARY, BEREND T. JONKER, United States Naval Research Laboratory — Monolayers of transition metal dichalcogenides (TMD) are promising components for optoelectronic devices due to their direct band gap and atomically thin nature. Their photoluminescence (PL) is strongly dependent on mid-gap defects which serve as non-radiative recombination sites for excitons. We demonstrate up to a 200x increase in PL intensity by exposing MoS2 synthesized by chemical vapor deposition (CVD) to laser light in ambient. This spatially resolved passivation treatment is air and vacuum stable, which indicates strong bonding of moieties from ambient. A wavelength dependent study confirms that this PL brightening is concomitant with exciton generation in the MoS2; laser light below the optical band gap of MoS2 fails to brighten the TMD. We highlight the photo-sensitive nature of the process by successfully brightening with a broadband white light source (< 10 nW/mm²). We decouple changes in absorption from defect passivation by examining the degree of circularly polarized PL. This measurement, which is independent of exciton generation, confirms that the laser brightening reduces non-radiative recombination sites in the MoS2. We propose that H2O molecules passivate sulfur vacancies in the MoS2 but requires photo-generated excitons to overcome the adsorption barrier.

5:06PM H13.00012: Defect-related photoluminescence from networks of suspended 2D crystal membranes*  ANDREW L YEATS (Presenter), JOSE FONSECA VEGA, JOEL Q GRIM, SAMUEL CARTER, CORY D CRESS, JAMES CLIFFORD CULBERTSON, MAXIM ZALALUTDINOV, JEREMY T ROBINSON, Naval Research Laboratory — Luminescent defects in 2D semiconductors hold promise for applications in photonics and quantum communication. For instance, strain-induced defects in WSe2 have attracted attention as narrow line-width single photon sources. We present a series of low-temperature photoluminescence (PL) microscopy studies on networks of suspended 2D crystal membranes formed by controlled dewetting and recrystallization of an underlying metal film. For monolayer membranes of WSe2 and heterojunctions of WSe2/MoS2 formed on a porous Au film, we find a strong (1000x) enhancement of PL intensity from the suspended regions, as well as the appearance of relatively sharp (< 1 meV) emission lines. The crystallographic texturing of the metal under-layer may also lend itself to low-loss propagation of surface plasmon polaritons (SPP), offering a means for energy transfer between discrete luminescent centers. We use a split excitation/collection imaging approach to characterize nonlocal luminescence in this unique material system, and discuss the outlook for studying networks of interconnected defects in 2D materials.

*JF acknowledges the NRC Research Associateship Program. Work performed at NRL was supported through Base Programs funded by the Office of Naval Research.

5:18PM H13.00013: Nano-imaging of local strain in hexagonal boron nitride  BOSAI LV (Presenter), HONGYUAN LI, Shanghai Jiao Tong University, LILI JIANG, UC Berkeley, WANFEI SHAN, Shanghai Jiao Tong University, HANS BECHTEL, MICHAEL CROCKER MARTIN, Lawrence Berkeley National Laboratory, WEIDONG LUO, Shanghai Jiao Tong University, FENG WANG, UC Berkeley, ZHIWEN SHI, Shanghai Jiao Tong University — Strain plays an important role in condensed matter physics. Strain effect becomes more interesting in two-dimensional materials, both because an unusually large strain can be achieved without breaking the material, and because the strain can lead to novel behavior such as the generation of pseudomagnetic field in graphene. Here, we report an ultra-sensitive nanometer scale mapping and a quantitative analysis of local strain field in atomically thin hexagonal boron nitride.
2:30PM H14.00001: Shape of the zeroth Landau level in graphene with non-diagonal disorder* RAJESH MALLA (Presenter), MIKHAIL RAIKH, University of Utah — Non-diagonal (bond) disorder in graphene broadens Landau levels (LLs) in the same way as random potential. The exception is the zeroth LL, n=0, which is robust to the bond disorder, since it does not mix different n = 0 states within a given valley. The mechanism of broadening of the n = 0 LL is the inter-valley scattering. Several numerical simulations of graphene with bond disorder had established that n = 0 LL is not only anomalously narrow but also that its shape is very peculiar with three maxima, one at zero energy, E = 0, and two others at finite energies ± E. We study theoretically the structure of the states in n = 0 LL in the presence of bond disorder. Adopting the assumption that the bond disorder is strongly anisotropic, namely, that one type of bonds is perturbed much stronger than other two, allowed us to get an analytic expression for the density of states which agrees with numerical simulations remarkably well. On the qualitative level, our key finding is that the delocalization of E = 0 state has a dramatic back effect on the density of states near E = 0. The origin of this unusual behavior is the strong correlation of eigenstates in different valleys.

*Department of Energy, Office of Basic Energy Sciences, Grant No. DE-FG02-06ER46313.

2:42PM H14.00002: Measuring Hall Viscosity of Graphene's Electron Fluid* ALEXEY BERDYUGIN (Presenter), School of Physics & Astronomy, University of Manchester, SHUIGANG XU, National Graphene Institute, University of Manchester, FRANCESCO PELLEGRINO, Dipartimento di Fisica e Astronomia, Università di Catania, ROSHAN KRISHNA-KUMAR, ALESSANDRO PRINCIPI, School of Physics & Astronomy, University of Manchester, IACOPO TORRE, ICFO - Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, MOSHE BEN SHALOM, School of Physics & Astronomy, University of Manchester, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, IRINA GRIGORIEVA, MARCO POLINI, ANDRE GEIM, DENIS BANDURIN, School of Physics & Astronomy, University of Manchester — In this work, we report the violation of the conventional Hall Effect (HE) in a viscous electron fluid. We show that the latter reacts to oppose the HE, producing an opposite electric field, which is proportional to the so-called Hall viscosity, a dissipationless transport coefficient emerging as a result of time-reversal symmetry breaking. By studying the response of a viscous electron fluid in monolayer (MLG) and bilayer (BLG) graphene to a weak (not quantizing) magnetic field in a suitable measurement geometry we were able to identify the anomalous contribution to the measured Hall signal arising from viscous electron flow. We probe this anomaly over a wide range of temperatures and carrier densities and compare it with theoretical calculations based on magnetohydrodynamic equations, which allows us to extract the Hall viscosity from our measurements. Our findings pave the way for investigations of magnetohydrodynamic of viscous electron fluids in two dimensions.

*The authors acknowledge support from the Lloyd’s Register Foundation.

2:54PM H14.00003: The role of edge effects in magnetotransport measurements of graphene hall bars OLIVIA GHOSH (Presenter), YI-HANG ZENG, J.I.A. LI, Department of Physics, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, CORY DEAN, Department of Physics, Columbia University — The development of the Van der Waals (VdW) assembly technique has led to greatly improved bulk quality of graphene devices. However, little is known about the quality of the sample edge. Here we investigate how the nature of the sample edge affects transport measurements, particularly for the case of the quantum Hall effect regime where the chiral edge modes are presumed to be topologically protected and therefore insensitive to details of the edge. We compare in a single device the transport response along electrostatically-defined versus naturally occurring boundaries, and discuss possible implications for the measurement of boundary edge modes more generally.
3:30PM H14.00006: Extraordinary magnetoresistance in encapsulated monolayer graphene  BOWEN ZHOU (Presenter), Washington University, St. Louis, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, Japan, ERIK HENRIKSEN, Washington University, St. Louis — We report a study on the phenomenon of extraordinary magnetoresistance (EMR) in boron nitride encapsulated monolayer graphene devices. Each device is circular, with an internal circular metal shunt made by edge contact to the graphene. Extremely large EMR values—calculated as (R(B) - R(0)) / R(0), can be found in these devices due to the vanishingly small resistance values at zero field. In many devices the zero-field resistance can become negative, likely due to ballistic carrier transport. This enables R(0) to be chosen arbitrarily close to zero depending only on measurement precision, resulting in very large EMR; conversely, small values of R(0) can have large uncertainty in short term measurements, leading to very large error bars on the EMR. We critically discuss the dependence of EMR on measurement precision and device asymmetry. Finally, the gate-voltage-dependent resistance at zero field also shows a strong electron-hole asymmetry, which we trace to the nature of the metal-graphene edge contact: as in the well-studied case of metals deposited on graphene, the graphene at one-terminal contacts also appears to be heavily electron-doped ~100s of nm away from the contact. We also report measurements on the Landau level energy gaps of bilayer graphene adjacent to 1-2 layer WSe₂ through van der Waals stacking. In comparison to pristine samples, a significant enhancement of the orbital splitting between the N=0 and N=1 levels was observed. The coincidence point of the ν=0 gap splits at field as low as 4 T. Meanwhile, the magnitude of the large ν=2 gap was reduced to roughly half of its value in pristine bilayer. Using thermally activated transport and a pair of top and bottom gates, we performed a set of gap measurements at ν=1, 2, 3 as a function of the carrier density and the applied perpendicular electric field D. We analyze the dependences, compare to the results in pristine bilayer and discuss the impact of WSe₂.


*This work was supported by the National Science Foundation (grant DMR-1507788).
3:54PM H14.00008: Observation of Cyclotron Resonance in Dual-Gated Bilayer Graphene* JORDAN RUSSELL (Presenter), JORDAN PACK, YASHIKA KAPOOR, Physics, Washington University, St. Louis, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ERIK HENRIKSEN, Physics, Washington University, St. Louis — We present measurements of the cyclotron resonance in boron nitride encapsulated, dual-gated bilayer graphene by way of infrared transmission magnetospectroscopy. We have observed both intra- and inter-band resonances, and study these as a function of the Landau level filling factor, $\nu - n/B$, for zero electric displacement field, $D$, and constant magnetic field, $B$. The magnetic field dependence and effects of nonzero displacement field on the Landau level resonances will also be discussed.

*Washington University in St. Louis
Institute for Materials Science and Engineering, Washington University in St. Louis

4:06PM H14.00009: Graphene Quantum Point Contact for Quantum Hall Interferometry THOMAS WERKMEISTER (Presenter), Applied Physics, Harvard University, YUVAL RONEN, SI YOUNG LEE, YOUNG JAE SHIN, Physics, Harvard University, DANIAL HAEI NAJAFABADI, University of Massachusetts Lowell, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, PHILIP KIM, Physics and Applied Physics, Harvard University — Anyons are particles which possess exchange properties beyond the typical bosonic and fermionic quantum statistics. Several varieties of anyons are expected to emerge as quasi-particles in the regime of the fractional quantum Hall effect (FQHE) where strong magnetic fields are applied on a 2-dimensional electron gas with strong electron-electron interactions. Traditionally, experiments in GaAs heterostructures have attempted to demonstrate anyonic exchange properties via quantum Hall interferometry, but results remain inconclusive. Recently, graphene based heterostructures have emerged as an alternative platform for studying these exotic anyonic quasi-particles within several robust FQHE phases that show larger gaps, particularly in even-denominator states. Here we present preliminary results utilizing hBN-encapsulated monolayer graphene with top and bottom graphite gates to electrostatically define interferometers in the FQHE regime. We will present a quantum point contact (QPC) that functions in the quantum Hall regime, a necessary ingredient for interferometers, and several devices that we characterize through transport measurements at cryogenic temperatures and strong magnetic field.

4:18PM H14.00010: Aharonov-Bohm Phase and Valley Splitting in Strained Graphene P-N Junction* RABINDRA NEPAL (Presenter), SANJAY PRABHAKAR, University of Nebraska - Lincoln, RODERICK MELNIK, The MS2Discovery Interdisciplinary Research Institute, Wilfrid Laurier University, ALEXEY KOVALEV, University of Nebraska - Lincoln — Veselago lens focusing on a graphene P-N junction is promising for the realizations of electron-optical devices such as electron lenses and electron beam splitters. We study two effects in a strained graphene layer with P-N junction: the Lorentz force due to fictitious magnetic fields and Aharonov-Bohm (AB) phase. In a strained P-N junction graphene layer, the strain induced magnetic field modifies the electron trajectories. Furthermore, the Lorentz force on electrons engenders the valley-splitting of electron beams as well as the shifting of caustics formed by refracted electron waves. We also calculate a non-zero AB phase associated with the electron beams due to a localized in-plane strain produced by a ripple. This non-zero phase is accumulated from the electrons that avoid traversing through the locally strained region and experience a non-vanishing vector potential associated with the fictitious magnetic field induced by the localized strain. We believe that these effects can be realized in a simple ballistic experiment and might be useful for mapping strain profiles by analyzing the interference pattern observed in electron-optical devices.

*NSF MRSEC Grant No. DMR-1420645, DOE DE-SC0014189, Canada Research Chair Program

4:30PM H14.00011: Influence of a Gaussian nanobubble on quantum Hall conductance across a p-n junction in graphene* NOJOON MYOUNG, physics education, chosun university, HEE CHUL PARK (Presenter), Institute for Basic Science — Structural deformations in graphene can emerge during the fabrication processes. Although the nanobubbles in graphene has a capability to be applied in valleytronics and nano electromechanics, they also act as disorders causing inelastic scatterings in Dirac fermion transport. It is important to locate where the nanobubbles are formed in graphene surface not only for exploiting them to applications but also for avoiding them to acheive ballistic transport. Here, we report a theoretical investigation of influence of a Gaussian nanobubble on quantum Hall conductance with a p-n junction in graphene, showing strain-induced conductance oscillations as the position and strain strength of the Gaussian nanobubble vary. We reveal that the reported conductance oscillations stem from the rotation of valley isospin along the p-n junction interface. Due to the pseudo-magnetic field produced by the Gaussian nanobubble, there are localized states for given strain strengths, and Fano resonances can appear in the quantum Hall conductance as a consequence of coupleline between the localized and extended states.

*National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT and MOE) (2017R1C1B5076824, Project IBS-R024-D1,NRF2016-R1D1A1B04-935798) and Chosun University (2017).
4:42PM H14.00012: Splitting of conductance resonance through a magnetic quantum dot in graphene*  NOJOON MYOUNG, Physics education, Chosun University, JUNG-WAN RYU, HEE CHUL PARK, PCS, Institute for Basic Sciences, SEUNG JOO LEE, Dongguk University, SUNGJONG WOO (Presenter), PCS, Institute for Basic Sciences — We report a dual resonance feature in ballistic conductance through a quantum Hall graphene nanoribbon with a magnetic quantum dot. Such a magnetic quantum dot localizes Dirac fermions exhibiting anisotropic eigenenergy spectra with broken time-reversal symmetry. Interplay between the localized states and quantum Hall edge states is found to be two-fold, showing Breit-Wigner and Fano resonances, which is reminiscent of a double quantum dot system. By fitting the numerical results with the Fano-Breit-Wigner lineshape from the double quantum dot model, we demonstrate that the two-fold resonance is due to the valley mixing that comes from the coupling of the magnetic quantum dot with quantum Hall edge channels; an effective double quantum dot system emerges from a single magnetic quantum dot in virtue of the valley degree of freedom. It is further confirmed that the coupling is weaker for the Fano resonance and stronger for the Breit-Wigner resonance.

*This work is supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT and MOE) (2017R1C1B5076824, Project IBS-R024-D1,NRF2016-R1D1A1B04-935798) and Chosun University (2017).

4:54PM H14.00013: Giant pseudo-magnetic fields, valley polarization and topological channels by nanoscale strain engineering of monolayer graphene*  CHEN-CHIH HSU (Presenter), JIAQING WANG, MARCUS TEAGUE, NAI-CHANG YEH, Physics, Caltech — We report the use of nearly strain-free PECVD-grown graphene [1] to induce controllable strain and pseudo-magnetic fields (Bs) by placing graphene on periodic nanostructure arrays [2]. We fabricated these arrays using focused ion beam and electron-beam lithography. These nanostructures were covered by a monolayer h-BN followed by a monolayer graphene, we found that graphene appeared to wrinkle up along the nanostructures. Each wrinkle results in four parallel channels of alternating positive and negative pseudo-magnetic fields, which are natural topological channels for valley-polarized propagation. Properly designed arrays of nanostructures could induce the desirable Bs values and spatial distributions, which can function as a valley splitter to separate valley-unpolarized currents, or a valley propagator to guide valley-polarized currents. To enable valleytronic applications, we pattern strained graphene with these topological channels into Hall bar geometry to study the valley Hall effect.


*This work was supported by the Army Research Office, National Science Foundation and Kavli Foundation.

5:06PM H14.00014: Scaling and quantum phase transitions of disordered graphene in the quantum Hall regime.*  TATIANE DOS SANTOS (Presenter), LEANDRO LIMA, CAIO LEWENKOPF, Instituto de Física, Universidade Federal Fluminense — We investigate the magneto-transport properties of disordered graphene samples in the quantum Hall (QH) regime. Despite the huge attention that the QH effect in graphene has received in the past decade, there are still open questions about the effects of the disorder on the transition states between Hall plateaus, especially regarding scaling properties. Such transition states have been intensively studied in the context of two-dimensional electron gases and found to exhibit universal scaling behavior. The situation is less clear in graphene, which displays an anomalous quantum Hall effect as a consequence of the valley degeneracy. For a sufficiently strong disorder that causes valley mixing, theoretical works have predicted Landau level splittings and even a transition to the conventional quantum Hall regime. The latter behavior has not been experimentally reported. To elucidate this issue, we address the problem by calculating the longitudinal and Hall resistances of graphene systems up to 10^5 atoms in a Hall bar geometry via the Landauer-Büttiker formalism. We consider both scalar and chiral disorder with different disorder correlation lengths. Finally, we discuss how intervalley/intravalley scatterings affect the QH transition states in graphene.

*Funded by CNPq and FAPERJ.
5:18PM H14.00015: Spin-relaxation in superconducting graphene*  DENIS KOCHAN (Presenter), JAROSLAV FABIAN, University of Regensburg — 2D materials in the proximity to a superconductor are expected to host a wide spectrum of different phenomena. In my talk I will focus on spin-relaxation in graphene proximitized by an s-wave superconductor. Adatom impurities can affect spin-relaxation via locally enhanced spin-orbit coupling (SOC) and local magnetic moments. I will discuss their impact on quasiparticle spin-relaxation with an attempt to disentangle contributions from the local SOC and local magnetic moments. Moreover, I will analyze the stability of the induced local magnetic moments and the emergence of Yu-Shiba-Rusinov (YSR) bound states in such proximity induced superconducting systems.

*This research was supported by DFG SFB 1277 and GRK 1570 and by the European Union's Horizon 2020 research and innovation programme under Grant agreement No. 696656.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H15 DMP: 2D Materials (Semiconductors) -- Optical Properties II BCEC 154 - Hiroshi Idzuchi


*This research was supported by NSF under award number DMR-1753054 and Texas A&M High Performance Research Computing.

2:42PM H15.00002: Exciton-dynamics of molybdenum disulfide on gallium nitride  YUBA RAJ POUDEL (Presenter), SEETHARAAN SAIRAMAN, Physics Department, University of North Texas, ZACHARIAH HENNIGHAUSEN, SWASTIK KAR, Physics Department, Northeastern University, FRANCIS D’SOUZA, ARUP NEOGI, Physics Department, University of North Texas — Layered transition metal dichalcogenides (TMD) have generated significant research interest because of interesting optical properties that are strongly dependent on the substrate. The integration of two dimensional (2D) materials with the bulk semiconductors provides an attractive platform to enhance the device functionality. Of all the 2D/3D heterostructures, MoS$_2$/GaN structures are at the top because of strong lattice matching and direct gap structures of both semiconductors. The properties of the heterostructures are governed by the excitons, which are weakly bound in nitrides but are strongly localized in MoS$_2$. Here we present the exciton dynamics of single layer MoS$_2$ on GaN. We studied the non-equilibrium exciton-dynamics with pump-probe spectroscopy using a tunable laser as a pump and a supercontinuum white light probe. The transient absorption spectrum shows different excitonic states. We will discuss the evolution of these states at different delay times starting as early as 200 fs and the corresponding decay kinetics. Our study will be useful to understand the energy transfer as well as the charge transport across the junction in the heterostructure which is crucial to enhance the performance of the device.
2:54PM H15.00003: Influence of the electric field on the optical properties of bilayer graphene nanoribbons*

TRUONG VAN TRAN, SRMP, CEA Saclay, SRMP, CEA Saclay, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France — Increasing attention has been paid to multilayer graphene, especially to bilayer graphene nanoribbons (BLGNRs)[1]. The interlayer interactions in BLGNRs result in a deformation of the electronic band structure with a change in the slope of the subbands. Recent studies show that the bandgap of BLG is widely tunable by external electric fields (EF) [2,3]. Here, the optical properties of BLGNRs under effects of EF are investigated by using a tight-binding model and the gradient approximation. The EF can induce the subband (anti)crossing, change the subband spacing, cause the oscillating bands, and distort the band-edge states as well. Our results demonstrate that the optical absorption spectra exhibit rich prominent peaks that mainly stem from the subbands. In addition, the number, spectral intensity, and energy of the absorption peaks are strongly dependent on the interlayer atomic interactions and the ribbon width. The dependence of the optical excitations on both the magnitude and direction of the EF is studied as well. This study could be validated by optical spectroscopy measurements. These results provide a view of the possibilities for applying future optoelectronic applications base on BLGNRs.

*This research is funded by NAFOSTED under grant No. 103.01-2015.98

3:06PM H15.00004: Excitation Density-Dependent Exciton Transport in a h-BN Encapsulated WSe2 Monolayer*

ZIDONG LI ( Presenter), Department of Electrical and Computer Engineering, University of Michigan, DARWIN FERNANDO CORDOVILLA LEON, Applied Physics Program, University of Michigan, SUNG WOON JANG, PARAG BHASKAR DEOTARE, Department of Electrical and Computer Engineering, University of Michigan — We report an excitation density-dependent visualization of excitonic energy diffusion in a h-BN encapsulated WSe2monolayer. At low excitation densities, we observe a linear evolution of the mean-squared displacement of the exciton density with a diffusivity of 0.5 cm²/s and a mono-exponential decay (300ps) of time-resolved photoluminescence (TRPL). At high excitation densities, however, the TRPL splits into two regimes: an excitation density-dependent, short-lived regime (150ps to 80ps), and an excitation-independent, long-lived regime (300ps). This observation and the fact that the exciton density preserves its initially Gaussian profile suggest that the results are not due to exciton-exciton annihilation but due to the remaining density of unfilled trap states. We also observe an excitation density-dependent increase in exciton diffusivity in the short-lived regime that saturates at 3 cm²/s and eventually transitions into the long-lived regime with a diffusivity of 0.5 cm²/s. At the transition point, the exciton density corresponds to the trap density in the WSe2monolayer which was measured to be 5*10¹¹/cm².

Z.L, D.C-L, S.J contributed equally to this work.

*3:18PM H15.00005: Ultrafast carrier and structural dynamics of supported monolayer MoS2*

XING HE (Presenter), MAZHAR CHEBL, DING-SHYUE YANG, Chemistry, University of Houston — Two-dimensional materials, such as graphene and transition metal dichalcogenides, have been considered promising for novel (opto)electronic and energy applications due to their unique properties at the mono- to few-layer limit. A thorough understanding of their carrier dynamics and energy transport behavior is therefore needed. Here, we present ultrafast carrier and energy-transport dynamics observed in sapphire-supported monolayer MoS2 following photoexcitation, using femtosecond transient reflectivity and ultrafast electron diffraction (UED). In particular, both monolayer MoS2 and the sapphire substrate were probed by reflection UED, which allows direct monitoring of structural motions at the interface. It is determined that dissipation of the photoexcitation energy undergoes a few steps with their characteristic time constants: ultrafast carrier relaxation and recombination as well as carrier-phonon coupling in MoS2, energy transport from the monolayer to the substrate on a 10-ps time scale, and slower thermal diffusion in bulk sapphire. Temperature-dependent observations will also be discussed.

*We acknowledge the support from the R. A. Welch Foundation and Samsung Global Research Outreach Program and the partial support from a National Science Foundation CAREER Award.
3:30PM H15.00006: Optical absorption in 2D MoS2 monolayers conformally grown on 3D Si and SiO2 nanocone arrays
EUNAH KIM (Presenter), Physics, Ewha Womans University, JIN-WOO CHO, Applied Physics, Kyung Hee University, TRI NGUYEN, Physics and Energy Harvest Storage Research Center, University of Ulsan, TRANG THI THU NGUYEN, SEOKHYUN YOON, Physics, Ewha Womans University, SUN-KYUNG KIM, Applied Physics, Kyung Hee University, YONG SOO KIM, Physics and Energy Harvest Storage Research Center, University of Ulsan, DONGWOOK KIM, Physics, Ewha Womans University — We prepared 2D MoS2 monolayers conformally coated on Si and SiO2 nanocone (NC) arrays using metal organic chemical vapor deposition technique, and investigated the influences of the refractive indices of 3D NCs on the optical properties of 2D MoS2 monolayers. The height, bottom diameter, and the period of the hexagonal Si NC array were 460, 250, and 300 nm, respectively. The SiO2 NC array was prepared by thermal oxidation of the Si NC array. The photoluminescence and Raman intensities of the MoS2 monolayer on the SiO2 NC were higher than those on the Si NC, although the Si NC exhibited much lower optical reflectivity in the visible wavelength range compared with the SiO2 NC. Numerical calculations showed that the strongly confined light in the high refractive index Si NC prevented a large electric field formation at the NC surface. In contrast, the weak light confinement in the low refractive index SiO2 NC resulted in a large electric field intensity and enhanced absorption in the MoS2 monolayer on the SiO2 NC. This work demonstrates that the 2D MoS2 and 3D Si hybrid nanostructures can provide a useful means to realize high-performance optoelectronic devices.

3:42PM H15.00007: Photocurrent Measurement of Monolayer Transition Metal Dichalcogenides*
TIANMENG WANG (Presenter), ZHIPENG LI, Rensselaer Polytechnic Institute, ZHENGGUANG LU, National High Magnetic Field Laboratory, YUZE MENG, YANWEN CHEN, Rensselaer Polytechnic Institute, DMITRY SMIRNOV, National High Magnetic Field Laboratory, SUFEI SHI, Rensselaer Polytechnic Institute — Monolayer transition metal dichalcogenides (TMDs) exhibit unique excitonic physics due to the reduced screening and enhanced Coulomb interactions. The strong light matter interaction in monolayer TMDCs gives rise to large response of photocurrent which involves carrier extraction after the excitation of the exciton. Photocurrent measurement thus provides a unique tool to investigate the combined effects of optical absorption and gain mechanism, revealing the spatial electric field distribution and photocurrent generation mechanism. The monolayer TMDs based photodetector exhibits large signal to noise ratio and can be exploited for sensitive photon sensor. The photocurrent measurement can also read out the valley degree of freedom of monolayer TMDs, excited by light of certain helicity.

* We acknowledge support from the AFOSR through Grant FA9550-18-1-0312.

3:54PM H15.00008: Exciton Up-conversion in Transition Metal Dichalcogenide Monolayers
XAVIER MARIE (Presenter), BO HAN, CEDRIC ROBERT, INSA/CNRS, MICKAEL GLAZOV, LEONID GOLUB, Ioffe Institute, MARCO MANCA, SHIVANGI SHREE, EMMANUEL COURTADE, PIERRE RENUCCI, BERNHARD URBASZEK, THIERRY AMAND, INSA/CNRS, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS/Tsukuba — The optical properties of Transition Metal Dichalcogenide (TMD) monolayers are governed by robust excitons. We have systematically investigated the excited exciton states by photoluminescence up-conversion spectroscopy in high quality MoS2, MoSe2, MoTe2 and WSe2 monolayers (MLs) encapsulated in hBN [1]. The excitation laser is tuned into resonance with the A:1s exciton ground state transition, and we observe for all the investigated MLs clear emission of excited exciton states (A:2s, A:3s...) up to 450 meV above the laser energy. The optical transitions are further investigated by reflectivity, photoluminescence excitation, and resonant Raman scattering, confirming their origin as excited excitonic states. We interpret the efficient up-conversion process as the consequence of exciton-exciton interactions where one of the excitons is annihilated while the second exciton acquires large extra energy. This mechanism is expected to be quite weak because it should satisfy both energy and momentum conservation laws. However our model calculations suggest an efficient exciton-exciton (Auger) scattering mechanism specific to TMD monolayers involving an excited conduction band, thus generating high-energy excitons with small wave vectors.

4:06PM H15.00009: Valley Polarized Excitonic Complexes in Monolayer TMD alloy* YUZE MENG (Presenter), Nanjing University, TIANMENG WANG, ZHIPENG LI, Rensselaer Polytechnic Institute, YING QIN, Arizona State University, ZHEN LIAN, YANWEN CHEN, MICHAEL C LUCKING, KORY BEACH, Rensselaer Polytechnic Institute, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, SEFAATTIN TONGAY, Arizona State University, FENGQI SONG, Nanjing University, HUMBERTO TERRONES, SUFEI SHI, Rensselaer Polytechnic Institute — Monolayer transition metal dichalcogenides (TMDs) have superior optical properties. Particularly, Tungsten based TMDs are known for their excellent valley polarization due to the strong spin-orbit coupling. However, the optical bandgap is limited by these two materials, which hinders the valleytronics applications that rely on the resonant excitation. We explore the possibility to overcome this limitation through the monolayer alloy, WS2xSe2(1-x), which promises an atomically thin semiconductor with tunable bandgap. We find that the high-quality BN encapsulated monolayer alloy WS0.6Se1.4 inherits the superior optical properties of tungsten-based TMDs, including a trion splitting of ~ 6 meV and valley polarization as high as ~60%. In particular, we demonstrate the emerging interlayer electron-phonon coupling in the BN/WS0.6Se1.4/BN van der Waals heterostructure. This coupling can be sensitively tuned by electrostatic gating and renders the otherwise optically silent Raman modes visible.

*S.-F. Shi acknowledges support from the AFOSR through Grant FA9550-18-1-0312. HT, MCL and KB acknowledge support from NSF grant EFRI-1433311. Y.M. acknowledges support from China Scholarship Council.

4:18PM H15.00010: Ultrafast charge dynamics and photoluminescence in bilayer MoS2* NASEEM UD DIN (Presenter), VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Physics, University of Central Florida — In a recent experiment it was shown that despite having an indirect band gap, the dominating peak in the emission spectrum of bilayer MoS2 corresponds to direct transitions. [1] To understand this phenomenon, we have applied density-matrix based time-dependent density-functional theory to examine ultrafast charge dynamics and emissive properties of bilayer MoS2. In particular, we demonstrate that despite initial accumulation of excited charge at the valleys between the K and Γ points of the two-dimensional Brillouin zone, photoemission takes place through direct charge recombination at the K and K' points. Analysis of the phonon spectrum suggests that the main reason for the direct emission is phonon-assisted transfer of the excited electrons to the K and K' valleys. We also analyze the role of the spatial structure of the electron and hole excitations in the ultrafast charge dynamics and hence photoemission to find that d(Mo)-p(S) hybridized character of the holes facilitates inter-layer charge transfer. Our results thus reveal the importance of ultrafast charge dynamics in photoemissive properties of a few-layer transition-metal dichalcogenides.

[1] K. Xiao et al., private communication

*Work support in part by DOE grant DE-FG02-07ER46354

4:30PM H15.00011: Polarisation switching and electrical control of interlayer excitons in two-dimensional van der Waals heterostructures ALBERTO CIARROCCHI (Presenter), DMITRII UNUCHEK, AHMET AVSAR, Ecole polytechnique federale de Lausanne, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ANDRAS KIS, Ecole polytechnique federale de Lausanne — Interlayer excitons in van der Waals heterostructures of transition metal dichalcogenides are of great interest due to their fascinating spin-valley and moiré physics. These aspects could be implemented to realize next-generation photonic and valleytronic devices, as well as exploring new physical phenomena. However, the efficient manipulation of the exciton valley-state, a necessary requirement for valley information encoding, is still lacking. In this talk, we will demonstrate electrical control of interlayer excitons in a MoSe2/WSe2 heterostructure. Encapsulation of aligned monolayers with boron nitride allows to resolve two separate interlayer transitions with opposite helicities under circularly polarized excitation, either preserving or reversing the polarization of incoming light. By electrically modulating these resonances, we realize a polarization switch with tuneable emission intensity and wavelength in the near-infrared. By applying magnetic fields, we assign the origin of the effect to the moiré-induced brightening of forbidden optical transitions, as also predicted by recent theoretical works. The ability to control the polarization of interlayer excitons is a step forward towards the practical manipulation of the valley degree-of-freedom in device applications.
4:42PM H15.00012: Intrinsic multi-particle bound-state luminescence emission from high-quality monolayer tungsten diselenide*  JUN YAN (Presenter), SHAO-YU CHEN, THOMAS A GOLDSTEIN, Physics, University of Massachusetts - Amherst, ZHENGGUANG LU, DMITRY SMIRNOV, National High Magnetic Field Lab, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan — Monolayer WSe$_2$ is an interesting semiconductor that hosts versatile light emitting manybody states. While the bright exciton photoluminescence (PL) is ubiquitous, PL at higher energies are challenging to observe due to Kasha's rule, and PL at lower energies are often plagued by extrinsic peaks from trapped excitons. In this talk, I'll show that with our high-quality samples, excited Rydberg exciton PL up to the 4s exciton become visible, and in the lower energy window PL due to four-particle biexcitons and five-particle exciton-trions are resolved. In magnetic fields up to 31 Tesla, the Rydberg exciton energy displays increasing curvature against magnetic field strength from 1s to 4s, reflecting their increasingly larger diameter. The biexciton and the exciton-trion are found to be intervalley complexes composed of a dark exciton in one valley and a bright exciton / trion in the other valley. This spin-valley configuration gives rise to counter-intuitive inverted PL valley polarization as compared to the two-particle bright and dark excitons.


*This work is mainly supported by the University of Massachusetts Amherst and NSF ECCS-1509599.

4:54PM H15.00013: Room-Temperature Valley Coherence in a Polaritonic System*  LIANGYU QIU (Presenter), CHITRALEEMA CHAKRABORTY, SAJAL DHARA, NICK VAMIVAKAS, University of Rochester — In the flourishing field of valleytronics, demand for coherently manipulating valley information at elevated temperature continues to escalate. Monolayer transition metal dichalcogenide, due to its strongly bonded excitons and degenerated valleys, nominates itself as a promising candidate for room temperature operation of valley degree of freedom (DOF). Through the hybridization of valley-resolved exciton and helicity-resolved photon mode, the valley DOF will be inherited by half-light, half-matter polaritons. Here, we demonstrate non-vanishing valley coherence of exciton-polaritons at room temperature in a cavity-embedded monolayer Tungsten Diselenide. The extra decay path through the exciton-cavity coupling, which is free of decoherence, is the key for intervalley phase correlation. These observations pave the way for room temperature valleytronic devices.

*Air Force Office of Scientific Research (AFOSR)
Materials Research Science and Engineering Centers (MRSEC)

5:06PM H15.00014: Exciton behaviors at the metal-semiconductor interface*  JAYDEEP JOSHI (Presenter), George Mason University, SERGIY KRYLYUK, ALBERT DAVYDOV, Functional Nanostructured Materials Group, NIST, PATRICK VORA, George Mason University — The application of transition metal dichalcogenides in optoelectronics technology requires an understanding of how metal-semiconductor contacts impact exciton photophysics. In this study we explore changes in excitons at the interface of monolayer tungsten diselenide (1L-WSe$_2$) and a series of conventional metals. Low-temperature hyperspectral PL measurements reveal intriguing changes in exciton linewidth and energy on approach to the junction that persist over multiple microns. In particular, the neutral exciton experiences a blueshift as the interface between the metal and WSe$_2$ is approached, a phenomenon that persists at higher temperatures. These results are difficult to rectify as a charge doping effect since electrostatic gating of WSe$_2$ leads to insignificant shifts of the exciton. Lattice strain from the contact is also not responsible since a redshift would be expected. The precise mechanisms governing this effect therefore remain an open question but a critical one for the 2D community.


*Funded by : NSF EAGER grant #1748650.
Valley-selective exciton bistability in a suspended monolayer semiconductor

HONGCHAO XIE (Presenter), Penn State & Cornell University, SHENGWEI JIANG, JIE SHAN, KIN FAI MAK, Cornell University — Monolayer transition metal dichalcogenide (TMD) semiconductors such as WSe$_2$, are direct band gap materials, which exhibit over 80% reflectance contrast at the fundamental exciton resonance. This extremely strong light-matter interaction can lead to optical nonlinearity or even bistability at high optical pump intensity. Furthermore, the valley degree of freedom (DOF) carries valley contrasting orbital magnetic moments, which enables K and K' valleys of the Brillouin zone exclusively coupled to the incident light with opposite helicity. Valley-selective exciton bistability can be achieved, in principle, by combining the above two properties of monolayer TMD semiconductors. In this work, we demonstrate robust bistable exciton resonance by continuous-wave (cw) optical excitation in a suspended WSe$_2$ sample. The detailed excitation wavelength and power dependence studies of the sample reflectance, as well as numerical simulation, quantitatively support a photothermal mechanism with internal feedback contributing to the observed excitonic bistability. The presence of external magnetic field further allows control of the sample reflectivity purely by varying the polarization of incident light.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H16 DMP: Computational Materials Design and Discovery -- Structure Prediction and Optimization

BCEC 155 - Ramamurthy Ramprasad, University of Connecticut

Solving Unknown Crystal Structures in a High-Throughput Manner*

SEAN GRIESEM (Presenter), LOGAN WARD, CHRISTOPHER WOLVERTON, Northwestern University — Databases of density functional theory (DFT) calculations, such as the Open Quantum Materials Database (OQMD), have paved the way for accelerated materials discovery. DFT requires a crystal structure as input; however, due to inherent challenges in solving a compound's structure from powder diffraction data alone, there are thousands of known compounds whose structures remain unsolved. Although structure solution methods involving DFT-based algorithmic optimization have been demonstrated, their computational cost limits their applicability. We present a more rapid DFT-based structure solution method in which we search the OQMD for structure types that match the cell geometry and stoichiometry of the compound, and evaluate them as possible solutions using DFT and match to diffraction pattern. As this approach is straightforward and inexpensive, we employed it in a high-throughput manner to solve hundreds of previously-undetermined structures from the Powder Diffraction File, including many new elpasolites, transition metal oxides, and mixed anion structures, as well as wide range of scarcely explored structure types.

*We acknowledge funding by the Center for Hierarchical Materials Design (CHiMaD), which is supported by U.S. Department of Commerce, NIST under Award No. 70NANB14H012.

Determining nanoparticle structures using FANTASTX

ISAAC MALSKY (Presenter), SPENCER T HILLS, FATIH SEN, MICHAEL STERNBERG, GRACE LU, ALPER KINACI, KENDRA LETCHWORTH-WEAVER, MARIA CHAN, Argonne National Laboratory — Determining the atomistic structures of nanoparticles is a fundamental problem. Their structures determine their functionality, and therefore their effectiveness in applications. Although there are both experimental and computational methods to determine these nanoscale structures, they both possess limitations. We develop FANTASTX (Fully Automated Nanoscale To Atomistic Structure from Theory and eXperiment) to overcome the limitations of either by combining both experimental and computational data. We demonstrate the effectiveness of FANTASTX by determining the structures of Au and IrO$_2$ nanoparticles from x-ray pair distribution function (PDF) data and density functional theory (DFT) calculations, using multi-objective optimization and a variety of canonical and grand canonical sampling algorithms.
2:54 PM H16.00003: Evolutionary Niching in the GAtor Genetic Algorithm for Molecular Crystal Structure Prediction
TIM C ROSE (Presenter), FARREN CURTIS, NOA MAROM, Carnegie Mellon University — The goal of molecular crystal structure prediction is to find all plausible polymorphs for a given molecule. This requires performing global optimization over a high dimensional search space. Genetic algorithms (GAs) perform global optimization by mimicking evolution. New structures are generated by breeding the fittest structures in the population. Typically, the fitness function is based on relative lattice energies, such that structures with lower energies have a higher probability of being selected for mating. GAs may be adapted to perform multi-modal optimization by using evolutionary niching methods that support the formation of several stable subpopulations and suppress the over-sampling of densely populated regions. Evolutionary niching is implemented in the GAtor molecular crystal structure prediction code by using machine learning to dynamically cluster the population by structural similarity. A cluster-based fitness function is constructed such that structures in less populated clusters have a higher probability of being selected for breeding. Using evolutionary niching increases the success rate of generating the experimental structure of 1,3-dibromo-2-chloro-5-fluorobenzene and additional low-energy structures with similar packing motifs.

3:06PM H16.00004: First-principles study on electrode – solid electrolyte interfaces in solid-state battery via efficient structure prediction method
BO GAO (Presenter), Center for Materials research by Information Integration (CMI2), Research and Services Division of Materials Data and Integrated System, National Institute for Materials Scie, RANDY JALEM, Center for Green Research on Energy and Environmental Materials & Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute, YANMING MA, State Key Laboratory of Superhard Materials, Jilin University, YOSHITAKA TATEYAMA, Center for Green Research on Energy and Environmental Materials & Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute — Understanding the origin of high interfacial resistances between electrodes and solid-electrolytes is crucial for commercial application of solid-state batteries (SSBs). [Chem. Mater. 26, 4248-4255] [ACS Appl. Mater. Interfaces 9, 286-292]. Here we utilized the CALYPSO structure prediction method [Physical Review B 82, 094116] to investigate the interface structures between LiCoO2 cathode and β-Li3PS4 sulfide electrolyte. About 20000 configurations are sampled to search the stable interface structures. The results show that the interfacial reaction layer is formed accompanied by the cation mixing and anion mixing. It is confirmed that the preferential Li depletion can occur at interface upon charging, even in very distorted region. Furthermore, CALYPSO interface structure prediction method can be applied to the solid-solid interface systems beyond the SSBs.

*This research has been supported by National Institute for Materials Science (NIMS) - “Materials research by Information Integration” Initiative (MI2I).

3:18PM H16.00005: An efficient algorithm for novel two-dimensional crystal structure prediction
KISUNG CHAE (Presenter), YOUNG-WOO SON, Korea Institute for Advanced Study — Two-dimensional (2D) materials are promising for their intriguing standalone properties and a number of combinatorial heterostructures. In this regard, crystal structure prediction (CSP) can enhance both material and property spaces significantly, accelerating innovative materials discovery. However, conventional approaches based on global optimization may be inefficient for 2D CSP due to enormously enhanced search space. Here, we will discuss an efficient algorithm for predicting novel 2D materials based on spatial symmetry of the atomic arrangements. We show the method was used to predict a number of novel 2D silicon crystals [1] and group IV and group VI compounds (namely, TXene) [2]. In addition, we will show that the method is efficient and transferable, and can be further applied to propose novel 2D materials.

3:30PM H16.00006: From Pentagonal Geometries to Two-Dimensional Materials
LEI LIU (Presenter), IMMANUELLA KANKAM, HOULONG ZHUANG, Arizona State University — Most of the most popular two-dimensional (2D) materials, such as semiconducting MoS2 and magnetic CrI3, adopt hexagonal structures. Inspired by the geometries of the existing 15 types of convex pentagons that can tessellate a plane without creating a gap or overlap, we combined these pentagonal geometries and density functional theory (DFT) calculations to predict novel 2D materials. We showed that this combination leads to a new direction in the field of 2D materials. In particular, we discovered a hidden pattern of pentagons called the Cairo tessellation in a group of bulk materials with the pyrite structure. We predicted single-layer PtP2 to exhibit a completely planar, pentagonal structure and a direct band gap. Our work shows that encoding quantum mechanics into pentagonal geometries and with the help of DFT calculations open up a novel route for accelerating discovery of new 2D materials.

*We thank the Fulton Undergraduate Research Initiative (FURI) and the start-up funds from Arizona State University. This research used computational resources of the Texas Advanced Computing Center under Contracts No. TG-DMR170070.
**3:42PM H16.00007: Dominant in-plane cleavage direction of CrPS₄**

MINWOONG JOE (Presenter), JINHWAN LEE, CHANGGU LEE, School of Mechanical Engineering, Sungkyunkwan University — In-plane cleavage directions of two dimensional (2D) crystals are displayed and often well-defined in their flakes exfoliated by the mechanical exfoliation method. Here, we investigate the correlation between dominant in-plane cleavage direction and elastic properties in different directions. CrPS₄ flakes show a preferential in-plane cleavage direction of 67.5°, corresponding to <110> direction. To explain it, we calculated the directional dependence of Young's modulus and fracture energy using first-principles density functional theory calculations. We found that fracture energy is directly relevant to the in-plane cleavage direction of CrPS₄. Our study can provide a facile approach to figure out the direction of 2D crystals without complex characterization process, which is valuable for material processing of 2D materials.

*M. J. acknowledge the National Research Foundation of Korea (NRF-2016R1A6A3A11934734) and the KISTI grant (KSC-2014-C2-041).

**3:54PM H16.00008: Conformations, electronic, and mechanical properties of monolayer diamene**

TENGFEI CAO (Presenter), ANGELO BONGIORNO, chemistry, college of staten island — Experiments show that diamond-like (diamene) films can be obtained from multilayer graphene, either by compression or surface passivation. Based on DFT calculations, we predict that diamene assumes various conformations, requiring either one or both surfaces being passivated. Conformations with surfaces fully passivated exhibit insulating properties, whereas diamene films presenting a clean surface show variable electronic properties, from insulating to semiconducting and metallic. Interestingly, regardless being monolayers or having a clean surface, all conformers of diamene exhibit elastic moduli comparable to those of the corresponding sp³ bulk phase, retaining Young's moduli along their transverse direction that are between 50% and 80% of bulk phases. Moreover we suggest that diamene film can be obtained from multilayer graphene by means of compression and/or wear without the need of chemical passivants, and the energies and pressures involved in the transformation depend critically on the structure and chemistry of the interface with the substrate.

*We acknowledge the support of the NSF grant CMMI-1436375. We also acknowledge support from the CUNY High Performance Computing Center and the Extreme Science and Engineering Discovery Environment (XSEDE).

**4:06PM H16.00009: Inverse Design for Self-assembly of Materials with Targeted Mechanical Properties**

PENGJI ZHOU (Presenter), Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, USA, JAMES C PROCTOR, Department of Materials Science & Engineering, University of Michigan, Ann Arbor, MI, USA, JULIA DSHEMUCHADSE, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, USA, GREG VAN ANDERS, Department of Physics, Engineering Physics, and Astronomy, Queen's University, Kingston, ON, Canada, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, USA — Inverse design is a promising yet challenging approach to develop new materials. To create materials with new properties, several inverse approaches have been proposed to design building blocks for target structures. However, the relationship between a material's structure and its properties is often unknown for novel materials. This calls for the development of inverse approaches that can directly target materials properties without having to target structures as the intermediary. Here, we present an inverse-design approach for particles with interacting potentials to self-assemble crystal structures with targeted mechanical properties. We do so through a novel molecular dynamics implementation of the 'digital alchemy' inverse-design approach. We give examples in which model particles interact via isotropic pair potentials that are designed to yield structures with a desired bulk modulus. Our results demonstrate that we can directly target mechanical properties via inverse materials design, and that our algorithm can be generalized to other properties.
Effect of alloying concentration on the mechanical properties of $B_2Cr_{1-x}Mo_x$* VIVIANA DOVALE-FARELO (Presenter), PEDRAM TAVADZE, ALDO H ROMERO, West Virginia University —

Transition metal borides as $Mo_2FeB_2$, $Mo_2NiB_2$, and $WCoB$ have recently caught attention because they exhibit excellent mechanical properties for wear resistant applications. On the other hand, it is widely known that the addition of Cr and/or Mo as alloying elements improves the mechanical properties and corrosion resistance of some alloys. In this investigation, first principles calculations were performed to study the structural properties of the ternary $B_2Cr_{1-x}Mo_x$ within DFT formalism. The $B_2Cr_{1-x}Mo_x$ compounds were studied for a concentration $x$ of 25%, 50%, and 75%. The Minima Hopping method was used to search over the stable and metastable structures for each concentration. $B_2Cr_{1-x}Mo_x$ structures were optimized to obtain the lattice parameters, total energies and formation enthalpies in each case. The elastic constants were calculated to verify the mechanical stability of the compounds, as well as the bulk modulus, shear modulus, Young's modulus, and Poisson's Ratio. The mechanical strength of the ternary was maximized as a function of the alloying concentration. Free energies were also calculated to study the thermal stability of the found crystal phases.

* Bridges and Stampede XSEDE-NSF supercomputers and the DMREF-NSF 1434897, NSF OAC-1740111 and DOE DE-SC0016176 projects.

Amorphous materials modeling and classification for low mechanical loss mirror coatings using machine learning methods* JUN JIANG (Presenter), MAHER YAZBACK, ALEC MISHKIN, Department of Physics and Quantum Theory Project, University of Florida, KIRAN PRASAI, RICCARDO BASSIRI, MARTIN FEJER, E. L. Ginzton Laboratory, Stanford, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — Instead of the well-defined atomic structures of crystals, amorphous materials are more complicated due to intrinsic randomness. Modeling and predicting the properties of amorphous materials (amorphous $Ta_2O_5$, doped $Ta_2O_5$) are important to understand experimental results and to find lower mechanical loss mirror coatings to reduce thermal noise in the next generation of LIGO laser interferometer gravitational wave detectors. In our work, thousands of atomic models of amorphous materials are generated using reverse Monte Carlo (RMC) and molecular dynamics (MD) simulations based on experimental data. Classifying them into different groups according to their properties and features with the help of machine learning, enables us to understand the differences between these models and use the information from these structures to find the best materials for low mechanical loss mirror coating.

*NSF/PHY 1707870 and NSF/PHY 1404110. Thanks Ximing Wang for the discussion and the help with the machine learning method.

Discovery of Novel Layered Heteroanionic Materials from Pauling's Rules* JAYE HARADA (Presenter), KENNETH POEPPELMIEIER, JAMES M RONDINELLI, Northwestern University — Heteroanionic materials, such as oxyfluorides and oxynitrides, display a myriad of functional properties derived from the presence of two anions of difference size, charge, and electronegativity. To aid synthetic efforts focused on compound discovery, we propose a workflow that can be used to predict new and stable $n = 1$ Ruddlesden-Popper type heteroanionic materials using principles from inorganic chemistry and supported with density functional theory calculations. We show that a simple structural optimization scheme based on Pauling's rules is an effective method to evaluate the stability of novel heteroanionic materials and predict new stable oxyfluorides. Last, we describe some of the properties exhibited by the newly identified compounds.

*This work is supported by the National Science Foundation Grant No. DMR 1454688.
Pressure-induced dimerization of the hyperkagome framework in Na$_3$Ir$_3$O$_8$

ERNESTO SANDOVAL (Presenter), ALEKSEY KOLMOGOROV, Department of Physics, Applied Physics and Astronomy, Binghamton University, FEI SUN, Center for High Pressure Science and Technology Advanced Research (HPSTAR), JOHN MITCHELL, Materials Science Division, Argonne National Laboratory, DANIEL HASKEL, Advanced Photon Source, Argonne National Laboratory — The ambient-pressure cubic Na$_3$Ir$_3$O$_8$ phase has been observed to undergo a symmetry-breaking transformation around 10 GPa [1]. Structure determination proved to be a challenge due to the large system size and the low symmetry of the new ground state. We performed extensive ab initio evolutionary searches [2] without any input from the high-pressure experiment and identified a complex monoclinic phase with 56 atoms per unit cell that agreed well with the collected XRD patterns. According to our ab initio calculations, the monoclinic phase features a dimerized Ir hyperkagome framework and a lower bulk modulus compared to that of the starting cubic phase. Study of the compound's electronic structure revealed significant convergence problems in the DFT+U approach.


Numerical Studies of Thermal Conductivity in Functionalized Carbon Nanotubes

ALEXANDER KERR (Presenter), KIERAN MULLEN, DANIEL T. GLATZHOFER, LIANGLIANG HUANG, University of Oklahoma — Although carbon nanotubes (CNTs) possess a large thermal conductivity, when they are incorporated in a polymer matrix their severe boundary resistance makes them ineffective at improving the thermal conductivity of the resulting composite. This resistance at CNT interfaces can be altered via chemical functionalization using mixed molecular chains to match the thermal impedance between CNTs and their environment. We explore the vast chemical space of possible configurations through meta-heuristics such as genetic algorithms and present candidate structures with optimal thermal conductance. We make comparisons of these CNT systems to certain harmonic lattices and look for important correlations among molecule parameters that contribute to the thermal conductivity, as is done in machine learning. We will summarize these results in general design rules for improving the thermal conductivity across molecular interfaces.

*This work was supported by NSF grant DMR-1310407.

On the Superconductivity in Ag-Au Alloys

DASARI PRASAD (Presenter), SURENDER SINGH, Department of Chemistry, Indian Institute of Technology Kanpur — In light of the recent reports on the evidence [1] and absence [2] of room temperature superconductivity at 1 atm pressure in Ag-Au nanostructured materials synthesized using colloidal and pulsed-laser deposition techniques, respectively, we have extensively investigated and predicted Ag-Au bulk and two-dimensional alloys for superconductivity. The structures are predicted by means of data-mining and evolutionary algorithms. The energies and forces are calculated at DFT-PBE and electron-phonon matrix elements are solved at DFPT. Superconducting transition temperatures are estimated within the BCS-like formalism. In our calculations, it is found that among all the stable and metastable structures resulted, only a few are found to be superconductors with Tc not more than one mK. No significant improvements noted in Tc when electrons and holes are externally injected to the bands near Fermi energy [3].


*D.L.V.K.P. acknowledges financial support through Initiation Grant No. IITK/CHM/20130116. S.S. thanks the CSIR, India for a SRF fellowship. We acknowledge CC/CHM-IITK, and RNJH HPC facilities.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H17 DCOMP: Matter in Extreme Environments: Iron in Planetary Interiors

BCEC 156A

- Xiaoyu Wang - Tag(s): Focus
2:30PM H17.00001: Chemical equilibrium in the Earth’s core* [Invited] DARIO ALFE (Presenter), MONICA POZZO, University College London, CHRIS DAVIES, DAVID GUBBINS, University of Leeds — The core of the Earth is a source of thermal energy for the mantle, helping to drive convection, plate tectonics and volcanism. It is mainly formed by iron, but is also contains light impurities. The exact chemical inventory of the core is unknown, but it is believed that oxygen may be present in relatively large quantities, as it is a major element in the mantle. Freezing of the inner core causes oxygen to be released in the liquid, which is thought to be the main form of energy driving core convection at the present day, responsible for the generation of the magnetic field. One of the fundamental questions is therefore how oxygen entered the core in the first place.

Using first principles calculations of chemical potentials we put contraints on the equilibrium concentrations of oxygen between liquid iron and a liquid silicate mixture, representative of long lived magma ocean (MO) at the base of the mantle. We show that the presence of a large fraction of oxygen in the core can be explained by a relatively large thermodynamic advantage of partitioning from the MO into the liquid core.

We also computed chemical potentials in solid ferropericlase, thought to be one of the main constituents of the Earth’s mantle, and found that the current oxygen concentration in the core is lower than its equilibrium concentration, suggesting that the mantle may be continually pumping oxygen into the core, even at the present day. This has important consequences for our understanding of convection in the core, supporting the idea of the presence of a stratified, oxygen rich, layer at the top of the core, which may have been observed in the seismological record.

*NERC-UK, NE/M000990/1, NE/R000425/1, NE/L011328/1
EPSRC-UK, MMM hub EP/P020194/1
Oak Ridge Leadership Computing Facility, DE-AC05-00OR22725

3:06PM H17.00002: Transport properties of iron under Earth’s core conditions* RONALD COHEN (Presenter), Geophysical Laboratory, Carnegie Institution for Science, RONALD COHEN, Earth and Environmental Sciences, LMU Munich — Transport properties of iron in Earth’s core control the dynamo that generates Earth’s magnetic field. If the thermal conductivity is high, heat transport is through conduction, and if low by convection. Conventional dynamo theory considered thermal convection primarily to drive the dynamo, but it is also possible to sustain a dynamo through chemical segregation, such as growth of Earth’s inner core. We computed the electrical resistivity and thermal conductivity of solid and liquid iron under core conditions, including both electron-ion (electron-phonon) and electron-electron scattering (Xu et al., PRL 121 096601, 2018). We have included saturation effects in different approximations. We find somewhat higher resistivity than recent resistivity measurements and somewhat higher thermal conductivity than recent thermal conductivity measurements. Thermal conductivities are lower than would be obtained using an ideal Wiedemann-Franz Lorenz factor. Electron-electron scattering also decreases the thermal conductivity. Our results are consistent with a convection driven dynamo.

*This work is supported by the ERC Advanced grant ToMCaT, the Carnegie Institution for Science, and the Gauss Centre for Supercomputing.

3:18PM H17.00003: Ab initio study of iron isotope fractionation during Earth’s core-mantle segregation* TIAN QIN (Presenter), Department of Earth Sciences, University of Minnesota, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics, Columbia University, MICHEL MARCONDES, Lamont-Doherty Earth Observatory, Columbia University, GAURAV SHUKLA, Physics, Bennett University — Recent studies have revealed that the iron isotope composition of mid-ocean ridge basalts (MORBs) is +0.1‰ richer in heavy Fe isotope (56Fe) relative to primitive chondritic meteorites, while basalts from Mars and Vesta have similar Fe isotopic composition as these meteorites. Here we investigate the hypothesis that iron isotope fractionation may have occurred during core formation on Earth. In particular, we compute Fe isotope fractionation factors among the lower mantle phases, bridgmanite (Bdg) and ferropericlase (Fp), and the metal phase at relevant pressure-temperature conditions. We pay particular attention to the effect of the spin crossover in Fe in Bdg and Fp on these fractionation factors. In addition, Fe in Bdg can occupy more than one crystalline site and can be in more than one valence state. In the metal phase, we consider variable amounts of Ni, the other metallic element expected to alloy with Fe in the core. Considering all these possible states of Fe in the silicate, oxide, and metallic phase, we show that the spin crossover in Fe, which does not occur in Mars or Vesta, may have played an important role in the Fe isotope fractionation during core-mantle segregation in the Earth.

*NSF grant EAR-1503084
4:18PM H17.00008: Viscosity of the Inner Core*  ANATOLY BELONOSHKO (Presenter), Royal Institute of Technology, Sweden, JIE FU, Department of Physics, Ningbo University, China, TARAS BRYK, Institute of Condensed Matter Physics, Ukraine, SERGUEI I SIMAK, Department of Physics, Linköping University, Sweden, MAURIZIO MATTESINI, Department of Earth’s Physics and Astrophysics, Complutense University of Madrid — The Earth solid inner core (IC), composed mostly by iron, is a highly attenuating medium. This property of the core is at odds with the widely accepted paradigm of the hexagonal close-packed (hcp) phase stability under the inner core conditions, because sound waves propagate through the hcp iron without energy dissipation. We show by first-principles molecular dynamics that the body-centered cubic (bcc) phase of iron, recently demonstrated to be thermodynamically stable under the IC conditions, is considerably less elastic than the hcp phase. Being a crystalline phase, the bcc iron possesses the viscosity close to that of a liquid iron. The attenuation of the inner core is due to the unique diffusion characteristic of the bcc phase. The liquid-like nature of the bcc phase at extreme pressures and temperatures allow to resolve a number of controversies and explain enigmatic features of the Core.

*We thank VR (grants 2013-5767, 2014-4750, and 2017-03744), Scientific Research Foundation of Ningbo University (grant 421708130), Olle Engkvist Byggmästare Foundation, Swedish Government Strategic Research Area in Materials Science at LIU (grant SFO-MatLiU No. 2009 00971), and Spanish Ministry of Economy and Competitiveness (CGL2013-41860-P and CGL2017-86070-R) for financial support.

4:30PM H17.00009: Exploring Thermal Conductivity of h.c.p. Iron (ε-Fe) at the Earth’s Core Conditions from Direct ab initio Molecular Dynamics Simulations  SHENG-YING YUE, Department of Mechanical Engineering, University of California Santa Barbara, MING HU (Presenter), Department of Mechanical Engineering, University of South Carolina — The exact value of electronic thermal conductivity ($\kappa_{\text{el}}$) of ε-Fe under the extreme pressure and temperature conditions still remains poorly known both experimentally and theoretically. Previous experiments reported quite scattered results of $\kappa_{\text{el}}$ of ε-Fe, which could differ by several folders. By utilizing our newly developed methodology based on direct non-equilibrium ab initio molecular dynamics (NEAIMD) simulation coupled with the concept of electrostatic potential oscillation (EPO), we evaluate the electronic thermal conductivity of iron in h.c.p phase without any artificial manipulation of computational parameters. Unlike the previous theoretical studies, our methodology inherently includes all possible interactions and scattering of electrons under extreme conditions. The results of electronic thermal conductivity of iron in the Earth’s core are consistent with some previous theoretical and experimental results. More importantly, our study provides a totally new physical picture of heat transfer process in iron at Earth’s core conditions from the electrostatic potential oscillation point of view. This simulation methodology offers a new approach to study thermal transport property of pure metals in planet’s cores with different temperature and pressures.

4:42PM H17.00010: Electrical conductivity of silicate liquids at extreme conditions and planetary dynamos*  LARS STIXRUDE (Presenter), Earth, Planetary, and Space Sciences, University of California, Los Angeles, ROBERTO SCIPIONI, Earth Sciences, University College London, MICHAEL PAUL DESJARLAIS, Pulsed Power Sciences Center, Sandia National Laboratory, EERO HOLMSTRÖM, Earth Sciences, University College London, A. S. FOSTER, Applied Physics, Aalto University — We find that Earth’s earliest magnetic field may have been produced in a deep magma ocean, and that silicate dynamos may exist in super-Earth exoplanets as well. Our conclusions are based on ab initio molecular dynamics simulations and Kubo-Greenwood computations of the electrical conductivity. These show that silicate liquids are semi-metallic at the extreme pressure and temperature conditions characteristic of planetary interiors with conductivity exceeding 10,000 S/m. In silica, the electrical conductivity shows a remarkable non-monotonic dependence on pressure that reveals connections to the underlying atomic structure, and highlights broken charge ordering as a novel compression mechanism. We compare the behavior of silica liquid with that of (Mg,Fe)O liquid and a multi-component composition (MgO-FeO-CaO-Al2O3-Na2O-SiO2) representative of the bulk silicate Earth.

*Research supported by the European Research Council under Advanced Grant 291432 MoltenEarth (FP7/2007-2013)
Structure Evolutions of Iron Compounds under Pressure Show an Unusual Chemistry in Deep Earth

MAOSHENG MIAO (Presenter), California State University, Northridge, XIAOLI WANG, Institute of Condensed Matter Physics, Linyi University, XIAOLEI FENG, Center for High Pressure Science and Technology Advanced Research (HPSTAR), JIANFU LI, Institute of Condensed Matter Physics, Linyi University, MATTHEW JACKSON, FRANK SPERA, Department of Earth Science, University of California Santa Barbara, SIMON REDFERN, Department of Earth Sciences, University of Cambridge — The terrestrial abundance of many elements, including heavy halogens Cl, Br, and I is approximately one order of magnitude lower than that predicted from their volatilities. One possible explanation is that these heavy elements are sequestered into the Earth’s core. This suggestion is supported by recent computational studies showing that heavy p elements may combine with iron at high pressure. Using first-principles electronic structure calculations and the automatic crystal structure search method based on particle swarm optimization algorithm, we also studied the stability and structures of Fe-halogen compounds under high pressure up to 350 GPa. Our calculations show that the compounds with higher Fe composition become more stable with increasing pressure and the reaction propensity of Fe might become opposite to ambient pressure. Our detailed electronic structure analysis reveals that the charge capture by Fe 3d orbitals and the reduction of the lone pair electrons in halogens are the major factors that govern the structure evolution under increasing pressure. Our results suggest that the distribution of many p-block elements in the Earth core might be much higher than we usually believe.

Thermal equation of state of ε-Fe at exoplanetary interior conditions

JINGYI ZHUANG (Presenter), HONGJIN WANG, QI ZHANG, KANCHAN SARKAR, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics, Columbia University in the City of New York, 500 W. 120th St., Mudd 200, MC 4701 New York, NY 10027, USA — The equation of state (EoS) of hcp-iron (ε-Fe) is essential for investigating physical properties of planetary cores. Despite its importance to geophysics and planetary astronomy, experimental investigations of ε-Fe at relevant conditions are still challenging. Therefore, ab initio calculations can contribute decisively to elucidating the equation of state (EoS) and other properties of this system. In this study, we present ab initio results of the properties of ε-Fe covering a wide range of pressures (0 - 1,400 GPa) and temperatures (300 - 8,000 K). Two new techniques are employed: i) a PAW dataset for iron specially designed for very high-pressure calculations [1], and ii) a free energy calculation approach based on the phonon gas model compatible with temperature dependent phonon frequencies, here produced by thermal electronic excitations. These new features of the calculation produce an isentropic EoS in good agreement with data from recent ramp compression experiments up to 1,400 GPa conducted at the National Ignition Facility (NIF)[2].


Vibrational spectrum throughout the iron spin crossover in ferropericlase (Mg_{1-x}Fe_xO)

MICHEL MARCONDES (Presenter), Department of Earth and Environmental Sciences, Columbia University, FAWEI ZHENG, Institute of Applied Physics and Computational Mathematics, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics, Columbia University — Ferropericlase (Fp), (Mg_{1-x}Fe_x)O, is the second most abundant phase in the Earth’s lower mantle. At relevant pressure-temperature conditions, iron in Fp undergoes a high spin (HS), S=2, to low spin (LS), S=0, state change. The nature of this phenomenon is quite well understood now, but there are still basic questions regarding the structural stability and the existence of soft phonon modes during this iron state change. General theories exist to explain the volume reduction, the large elastic anomalies, and the broad nature of this HS-LS crossover. These theories make extensive use of the quasi-harmonic approximation (QHA), therefore, dynamical and structural stability are essential to the validity of these theories. Here, we investigate the vibrational spectrum of Fp throughout this spin crossover using ab initio DFT+Usc calculations. We address vibrational modes associated with isolated and (2nd) nearest neighbor Fe atoms undergoing the HS-LS state change. As expected, acoustic modes of this solid solution reproduce the well-known elastic anomalies, but optical modes display unusual features. We show that there are no soft phonon modes across this HS-LS crossover and Fp is dynamically stable at all mantle pressures and relevant iron concentrations.

Tuesday, March 5, 2019 2:30 PM - 5:06 PM

Session H18 DCOMP DCMP DAMOP: Machine Learning Quantum States III

BCEC 156B - Juan Carrasquilla, Vector Institute - Tag(s): Focus
2:30PM H18.00001: Hybrid neural network - quantum simulator [Invited ] GIACOMO TORLAI (Presenter), Center for Computational Quantum Physics, Flatiron Institute — The recent advances in qubit manufacturing and coherent control of synthetic quantum matter are leading to a new generation of intermediate-scale quantum hardware, with promising progress towards scalable quantum simulation of strongly-correlated systems. In order to enhance the capabilities of this class of quantum devices, some of the more arduous experimental tasks can be off-loaded to classical algorithms running on conventional computers. In particular, generative neural networks trained on measurement data can be implemented to obtain an approximate reconstruction of the experimental wavefunction, allowing specialized measurements which are either costly or not accessible in the experimental setup. I will present this classical-quantum hybridization for quantum hardware based on trapped ultra-cold atoms and superconducting qubits.

3:06PM H18.00002: Reinforcement Learning Decoders for Fault-Tolerant Quantum Computation* RYAN SWEKE, MARKUS KESSELRING, Dahlem Center for Complex Quantum Systems, Freie Universitaet Berlin, EVERT VAN NIEUWENBURG (Presenter), Caltech, JENS EISERT, Dahlem Center for Complex Quantum Systems, Freie Universitaet Berlin — Topological error correcting codes, and particularly the surface code, provide a promising and feasible roadmap towards large-scale fault-tolerant quantum computation. Obtaining fast and flexible decoding algorithms for these codes, within the experimentally relevant context of faulty syndrome measurements, is therefore an important milestone. The problem of decoding such codes, in the full fault-tolerant setting, can be naturally reformulated as a process of repeated interactions between a decoding agent and a code environment. Reinforcement learning can then be used to obtain such a decoding agent, and can successfully learn to decode in the fault-tolerant setting.

*This research was supported by the Swiss National Science Foundation through grant P2EZP2-172185, the DFG (CRC 183, EI 519/14-1, and EI 519/7-1), the ERC (TAQ), the Templeton Foundation, and the BMBF (Q.com). This work has also received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 817482 (PASQUANS).

3:18PM H18.00003: The recoverable quantum information: A smart reward for reinforcement learning of quantum error correction THOMAS FOESEL (Presenter), PETRU TIGHINEANU, Max Planck Institute for the Science of Light, TALITHA WEISS, IQOQI, University of Innsbruck, FLORIAN MARQUARDT, Max Planck Institute for the Science of Light — Quantum information can be encoded in a complex manner in entangled multi-qubit states. But how well is this information preserved, given the dissipative time evolution of a system? In order to address this question, we have developed a new quantity, which we call the recoverable quantum information.

Beyond the possibility to judge how well existing techniques perform, it is particularly useful for the autonomous discovery of new quantum error correction strategies, by using it as an immediate reward scheme for a reinforcement learning approach as demonstrated in [1]. The recoverable quantum information is applicable generically, i.e. independent of the concrete hardware platform, noise model, etc. In this talk, this quantity will be introduced and motivated, an intuitive interpretation is given, it is shown how it evolves in some exemplary systems, and I will sketch how it can be computed numerically.


3:30PM H18.00004: Quantum error correction for the Toric code using Deep reinforcement learning PHILIP ANDREASSON, SIMON LILJESTRAND, JOEL JOHANSSON, MATS GRANATH (Presenter), University of Gothenburg — We implement a quantum error correction algorithm for the Toric code using Deep reinforcement learning. An action-value Q-function encodes the discounted value of moving a defect to a neighboring site on the square grid (the action) depending on the full set of defects on the torus (the syndrome or state). The Q-function is represented by a deep convolutional neural network. Using the translational invariance on the torus allows for viewing each defect from a central perspective which crucially simplifies the Q-function representation independently of the number of defect pairs.

The training is done using experience replay, where data from the algorithm being played out is stored and used for batch upgrade of the Q-network.

Performance is close to that achieved by the Minimum Weight Perfect Matching algorithm for moderate system sizes and for the uncorrelated noise model.
3:42PM H18.00005: Restricted Boltzmann Machines and Matrix Product States of 1D Translational Invariant Stabilizer Codes*  
YUNQIN ZHENG (Presenter), HUAN HE, Princeton University, NICOLAS REGNAULT, Laboratoire Pierre Aigrain, Ecole normale superieure, ANDREI B BERNEVIG, Princeton University — We discuss the relations between the restricted Boltzmann machine (RBM) states and the matrix product states (MPS) for the ground states of 1D translational invariant stabilizer codes. A generic translational invariant and finitely connected RBM state can be expressed as an MPS, and the matrices of the resulting MPS are of rank 1. We dub such an MPS as an RBM-MPS. This provides a necessary condition for exactly realizing a quantum state as an RBM state, if the quantum state can be written as an MPS. We mostly focus on generic 1D stabilizer codes having a non-degenerate ground state with periodic boundary condition. We obtain an expression for the lower bound of their MPS bond dimension, and also an upper bound for the rank of their MPS matrices. In terms of RBM, we provide an algorithm to derive the RBM for the cocycle Hamiltonians whose MPS matrices are proved to be of rank 1. Moreover, the RBM-MPS produced by our algorithm has the minimal bond dimension. A family of examples is provided to explain the algorithm.

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The National Science Foundation EAGER Grant No. NOA-AWD1004957  
Simons Investigator Grant No. ONR-N00014-14-1-0330, NSF Grant No. NSF-MRSEC DMR-1420541  
The Packard Foundation  
The Schmidt Fund for Innovative Research

3:54PM H18.00006: Neural loop algorithm for square ice model*  
YING-JER KAO (Presenter), KAI-WEN ZHAO, WEN-HAN KAO, National Taiwan University — We discuss how to apply a reinforcement learning framework on the square spin ice model. Spin ice is a frustrated magnetic system with a strong topological constraint on the low-energy configurations called the ice rule. The conventional single spin-flip Monte Carlo update breaks this constraint. We exploit a reinforcement learning method that parameterizes the transition operator with neural networks. By extending the Markov chain to a Markov decision process, the algorithm can adaptively search for a global update policy through its interactions with the physical model. We find that the global loop update emerges without the explicit knowledge of the ice rule. This method might serve a general framework to search for efficient update policies in other constrained systems.

*This work is supported by MOST of Taiwan under Grants No. 105-2112-M-002-023-MY3, and 104-2112-M-002-022-MY3.

4:06PM H18.00007: Variational optimization in the AI era: supervised wave-function optimization and computational graph states.*  
DMITRII KOCHKOV (Presenter), BRYAN CLARK, Physics, University of Illinois at Urbana-Champaign — An important approach to the quantum many-body problem is to write down a compact variational ansatz which represents the target quantum state. The success of a particular model depends on its ability to capture the structure of the state and optimize all variational parameters. We introduce a machine learning inspired computational framework that works with wave-functions represented as differentiable computational graphs and develop a novel optimization algorithm Supervised Wave-function Optimization, that allows for effective optimization of such models. We present results on several architectures showing the efficiency of our approach.

*Blue Waters sustained petascale computing project.

4:18PM H18.00008: Generalized Transfer Matrix States from Artificial Neural Networks  
LORENZO PASTORI (Presenter), Institute of Theoretical Physics, TU Dresden, RAPHAEL KAUBRUEGGER, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, JAN CARL BUDICH, Institute of Theoretical Physics, TU Dresden — We propose and investigate a new family of quantum states, coined generalized transfer matrix states (GTMS), which bridges between tensor network states and states derived from artificial neural networks (ANNs). In particular, we show by means of a constructive embedding that the class of GTMS contains generic matrix product states while at the same time being capable of capturing more long-ranged quantum correlations that go beyond the area-law entanglement properties of tensor networks. While generic deep ANNs are hard to contract, meaning that the corresponding state amplitude can not be exactly evaluated, the GTMS network is shown to be analytically contractible using transfer matrix methods. With numerical simulations, we demonstrate how the GTMS network learns random matrix product states in a supervised learning scheme, and how augmenting the network by long-ranged couplings leads to the onset of volume-law entanglement scaling. We argue that this capability of capturing long-range quantum correlations makes GTMS a promising candidate for the study of critical and dynamical quantum many-body systems.
4:30PM H18.00009: Construction of Hamiltonians by supervised learning of energy spectra* HIROYUKI FUJITA, YUYA NAKAGAWA, Institute for Solid State Physics, University of Tokyo, SHO SUGIURA (Presenter), Physics, Harvard University, MASAKI OSHIKAWA, Institute for Solid State Physics, University of Tokyo — Handling the large number of degrees of freedom with proper approximations, namely the construction of the effective Hamiltonian is at the heart of the (condensed matter) physics. Here we propose a simple scheme of constructing Hamiltonians from a given energy spectrum [1]. The sparse nature of the physical Hamiltonians allows us to formulate this as a solvable supervised learning problem. Taking a simple model of correlated electron systems, we demonstrate the data-driven construction of its low-energy effective model. We present potential applications for the construction of entanglement Hamiltonians and materials discovery through the construction of parent Hamiltonians from effective models of topological matters. [1]H.Fujita et.al., Phys. Rev. B 97, 075114 (2018).

*H. F. and Y. O. N are supported by Advanced Leading Graduate Course for Photon Science (ALPS) of Japan Society for the Promotion of Science (JSPS). The works of H. F., Y. O. N., and S. S are supported by JSPS KAKENHI Grant-in-Aid for JSPS Fellows Grant No. JP16J04752, No. JP16J01135, and No. JP15J11250, respectively. The work of M. O. is supported in part by JSPS KAKENHI Grant No. 16K05469.

4:42PM H18.00010: Backflow Transformations via Neural Networks for Quantum Many-Body Wave-Functions* DI LUO (Presenter), BRYAN CLARK, University of Illinois at Urbana-Champaign — Obtaining an accurate ground state wave function is one of the great challenges in the quantum many-body problem. In this paper, we propose a new class of wave functions, neural network backflow (NNB). The backflow approach, pioneered originally by Feynman, adds correlation to a mean-field ground state by transforming the single-particle orbitals in a configuration-dependent way. NNB uses a feed-forward neural network to learn the optimal transformation via variational Monte Carlo. NNB directly dresses a mean-field state, can be systematically improved and directly alters the sign structure of the wave-function. It generalizes the standard backflow[1] which we show how to explicitly represent as a NNB. We benchmark the NNB on a Hubbard model at intermediate doping finding that it significantly decreases the relative error, restores the symmetry of both observables and single-particle orbitals, and decreases the double-occupancy density.


*The Blue Waters sustained-petascale computing project supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the State of Illinois.

The U.S. Department of Energy, Office of Science under Award Number FG02-12ER46875.

4:54PM H18.00011: Contrasting the Building Blocks of Grain Boundaries using Local vs. Multi-Scale Universal Descriptors* DEREK HENSLEY (Presenter), CONRAD W ROSEN BROCK, ANDREW H NGUYEN, GUS HART, ERIC HOMER, Brigham Young University — The behavior and properties of Grain Boundary (GB) Systems arise from a myriad of atomistic interactions. Is it possible to describe the properties of any GB in the system using knowledge of only a few? If so, which GBs have these essential, atomistic “building blocks” from which all other GB properties can be predicted? Previously, a universal similarity metric for GBs based on the Smooth Overlap of Atomic Positions (SOAP) descriptor was shown to effectively discover the underlying physics of GBs and find these atomistic building blocks. We present another universal GB representation using a multi-scale, scattering transform that also discovers GB building blocks. We contrast the building blocks discovered by SOAP with those of scattering transform to show the merits of local vs. multi-scale universal descriptors in describing the physics of GB.

*Funding from ONR (MURI N00014-13-1-0635)

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H19 DCOMP DCMP: Precision Many Body Physics VI BCEC 156C - Shiwei Zhang - Tag(s): Focus
2:30PM H19.00001: Precision spectral densities in correlated systems* [Invited] KAREN HALLBERG (Presenter), YURIEL NÚÑEZ FERNÁNDEZ, Condensed Matter Theory, Centro Atómico Bariloche and Instituto Balseiro, CNEA, CONICET — We develop an efficient numerical method to calculate spectral densities of complex impurities based on the Density Matrix Renormalization Group (DMRG) and use it as the impurity solver of the Dynamical Mean Field Theory (DMFT). By using a self-consistent bath configuration with very low entanglement, we take full advantage of the DMRG to calculate dynamical response functions paving the way to treat large effective impurities such as those corresponding to multi-orbital interacting models and multi-site or multi-momenta clusters. It also solves for complex impurities using ab-initio input which opens its realm of applications to real materials. This method leads to reliable calculations of non-local self energies on the real frequency axis directly, at zero temperature, arbitrary dopings and interactions and at all energy scales. We will show results for multi-site and multi-orbital models in which interesting features arise such as emergent low-energy bound states.

*We acknowledge support from projects PICT 2012-1069 and PICT 2016-0402 from the Argentine ANPCyT and PIP 2015-2017 11220150100538CO (CONICET). This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562

3:06PM H19.00002: Approximation to an exchange-correlation functional on the basis of renormalization-group theory* [Invited] LUIZ OLIVEIRA (Presenter), KRISZIA ZAWADZKI, Sao Carlos Institute of Physics at the University of Sao Paulo — Approximations to the exchange-correlation functional are central to Density Functional Theory. Generalizations of the Local-Density Approximation typically describe electronic systems very well. Nonetheless, many exceptions are known. The molecular junction offers an outstanding example, one in which nonlocal correlations stem from the Kondo effect. The junction comprises two metallic leads bridged by a molecule. At low temperatures, the molecular-orbital spin and the low-energy conduction-electron spins lock into a singlet, an entangled state that renders local approximations inadequate, so large is its diameter. To take a nonlocal approach, we resort to renormalization-group concepts. As the temperature $T$ is reduced, the junction crosses over from the vicinity of a high-$T$ fixed point, in which the molecular spin and lead electrons are decoupled, to a low-$T$ fixed point, in which they are strongly coupled. The high-$T$ fixed point is devoid of entanglement, hence well described by local approximations. We can therefore set up and solve the Kohn-Sham equations for that fixed point. We then combine the resulting Kohn-Sham eigenstates with the molecular spin to define a single-impurity Anderson Hamiltonian. Numerical renormalization-group diagonalization of the latter depicts the crossover to the low-$T$ fixed point and yields the ground-state and temperature-dependent zero-bias transport properties of the junction. As an illustration, results for an inhomogeneous Hubbard model will be presented and compared with experimental data.

*Financial support by the CNPq (grant 312658/2013-3), and FAPESP (grants 20111/20865-0 and 2012/02702-0) is acknowledged. This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001.

3:42PM H19.00003: Sign-blessed Diagrammatic Monte Carlo Method for Electrons Interacting with the Long-range Coulomb Repulsion KUN CHEN (Presenter), KRISTJAN HAULE, Department of Physics, Rutgers University — We show that combining a variational approach with a new diagrammatic quantum Monte Carlo method results in a powerful and accurate solver to the generic solid state problem, in which a macroscopic number of electrons interact by the long range Coulomb repulsion. We apply the solver to the quintessential problem of solid state, the uniform electron gas (UEG), which is at the heart of the density functional theory (DFT) success in describing real materials, yet it has not been adequately solved for over 90 years. While some wave-function properties, like the ground state energy, have been very accurately calculated by the diffusion Monte Carlo method (DMC), the static and dynamic response functions, which are directly accessed by the experiment, remain poorly understood. Our method allows us to calculate the momentum-frequency resolved spin response functions for the first time, and to improve on the precision of the charge response function. The accuracy of both response functions is sufficiently high, so as to uncover previously missed fine structure in these responses. This method can be straightforwardly applied to a large number of moderately interacting electron systems in the thermodynamic limit, including realistic models of metallic and semiconducting solids.
3:54PM H19.00004: First principles study of correlation effects in solids* SERGEI ISKAKOV (Presenter), ALEXANDER RUSAKOV, EMANUEL C GULL, DOMINIKA ZGID, University of Michigan — Designing reliable, predictive, and computationally affordable methods to address electronic correlations in realistic solids is an ongoing challenge for quantum chemistry, condensed matter physics, and material science. Recent advances have made computations with density functional theory (DFT) routine and Green’s function based approaches such as GW feasible. In this talk we present the finite-temperature statistical mechanics formulation of perturbation theory self-consistently to second order, and obtain a solution for periodic three-dimensional solids in a fully self-consistent conserving approximation.

*This project was supported by the Simons Foundation via the Simons Collaboration on the Many-Electron Problem.

4:06PM H19.00005: Theory of Time-Resolved Raman Scattering in Correlated Systems: Ultrafast Engineering of Spin Dynamics and Detection of Thermalization* CHENG-CHIEN CHEN (Presenter), University of Alabama at Birmingham, YAO WANG, Harvard University, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory — Ultrafast characterization and control of elementary excitations are critical to understanding and manipulating emergent phenomena in correlated systems. In particular, spin interaction plays an important role in unconventional superconductivity, but efficient tools for probing spin dynamics especially out of equilibrium is still lacking. Here we develop the theory of time-resolved Raman scattering, which can be a powerful tool for nonequilibrium studies. We also simulate a pumped single-band Hubbard model using exact diagonalization. Different ultrafast processes are shown to exist in the time-resolved Raman spectra and dominate under different pump conditions. For high-frequency and off-resonance pumps, the Floquet theory is shown to work well in capturing the bimagnon softening. We also show that effective heating dominates at small pump fluences, while many-body effect takes over at larger pump amplitudes and frequencies resonant to the Mott gap. Time-resolved Raman scattering thereby provides the platform to explore ultrafast processes and design material properties out of equilibrium.

*This work was supported by NSF Grant No. OIA-1738698. Y.W. is supported by the Harvard-MPQ Center Postdoctoral Fellowship. T.P.D. acknowledges support from DOE Contract No. DE-AC02-76SF00515.

4:18PM H19.00006: Charge self-consistent DFT + DMFT study on magnetism of transition metals* MANCHEON HAN (Presenter), HYOUNG JOON CHOI, Department of Physics, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University — Density functional theory (DFT) is a static approximation, so it describes system with static magnetic moment quite well. However, if spin fluctuation is much larger than static moment, DFT is not appropriate tool for investigate such material. For example, the high-temperature paramagnetic state of a magnetic material can not be adequately described by DFT alone. Dynamical Mean Field Theory (DMFT), which accounts the local dynamic correlation effects exactly, can be used to account such fluctuation effects. We studied the magnetic properties of period 4 transition metals using our charge self-consistent density function theory + dynamical mean field theory (DFT + DMFT) program. Our calculation shows temperature dependence of magnetism, which is not observed in ordinary DFT calculation. Moreover, paramagnetic phase was investigated by calculating total spin angular momentum and magnetic susceptibility for several temperatures.

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4:30PM H19.00007: Almost exact energies for the G1/G2 set with the semistochastic heat-bath configuration interaction method* YUAN YAO (Presenter), JUNHAO LI, CYRUS JEHANGIR UMRIGAR, Cornell University — The recently developed semistochastic heat-bath configuration interaction (SHCI) method is a systematically improvable selected configuration interaction plus perturbation theory method capable of giving essentially exact energies for larger systems than is possible with other such methods. We compute SHCI atomization energies for the 55 molecules in the G1/G2 set, for which accurate experimental data are available. Basis sets from cc-pVDZ to cc-pV5Z are used, totaling up to 500 orbitals and a Hilbert space of $10^3$ determinants for the largest molecules. To speed up convergence, we first optimize orbitals using 1-body and 2-body reduced density matrices constructed from SHCI wavefunctions with a large convergence threshold. For each of the basis sets, the extrapolated energy is within chemical accuracy (1 kcal/mol) of the exact energy for that basis using only a tiny fraction of the entire Hilbert space. The energies are extrapolated to the basis set limit and compared to the experimental atomization energies. We also use our almost exact energies to benchmark coupled cluster theory (CCSD(T)) energies.

*This work was supported by the AFOSR through grant FA9550-18-1-0095.
4:42PM H19.00008: One-electron spectral properties of self-assembled structures and defects on semiconductors*
JOSE CARMELO (Presenter), Department of Physics, Boston University, TILEN CADEZ, CSRC, Beijing, YOSHIYUKI OHTSUBO, SHIN-ICHI KIMURA, DAVID K CAMPBELL, Department of Physics, Osaka University — Twin grain boundaries in monolayers of transition metal dichalcogenides such as molybdenum diselenide [MoSe(2)] and self-assembled atomic structures on the surface of semiconductors such as a bismuth-induced anisotropic structure on indium antimonide [Bi/InSb(001)] are exceptional candidates for truly one-dimensional metals. The microscopic mechanisms behind their exotic spectral properties involve long-range interactions of electrons confined to one-dimensional channels. We extend the universal theory for the finite-energy spectral properties of a wide class of one-dimensional correlated lattice systems whose microscopic mechanisms involve phase shifts imposed by a mobile quantum impurity to electronic lattice systems with long-range interactions. In contrast to theoretical schemes that do not account for the effects of long-range interactions, our theoretical predictions agree quantitatively with the observed one-electron spectral properties of one-dimensional metallic states in MoSe(2) line defects and in Bi/InSb(001).

* J. M. P. C. would like to thank Boston University's Condensed Matter Theory Visitors Program for support and the Portuguese FCT through the Grants UID/FIS/04650/2013, PTDC/FIS-MAC/29291/2017, and SFRH/BSAB/142925/2018

4:54PM H19.00009: On the limitations of cRPA downfolding CARSTEN HONERKAMP (Presenter), RWTH Aachen University, HIROSHI SHINAOKA, Department of Physics, Saitama University, FAKHER F. ASSAAD, Theoretical Physics, University of Würzburg, PHILIPP WERNER, Department of Physics, University of Fribourg — We check the accuracy of the constrained random phase approximation (cRPA) downfolding scheme by considering one-dimensional two- and three-orbital Hubbard models with a target band at the Fermi level and one or two screening bands away from the Fermi level. Using numerically exact quantum Monte Carlo simulations of the full and downfolded model we demonstrate that depending on filling the effective interaction in the low-energy theory is either barely screened, or antiscreened, in contrast to the cRPA prediction. This observation is explained by a functional renormalization group analysis which shows that the cRPA contribution to the screening is to a large extent cancelled by other diagrams in the direct particle-hole channel. We comment on the implications of this finding for the ab-initio estimation of interaction parameters in low-energy descriptions of solids.

5:06PM H19.00010: Maximum quantum entropy method: the analytic continuation of matrix-valued Green's functions* JAE-HOON SIM (Presenter), MYUNG JOON HAN, Department of Physics, KAIST — Analytic continuation of the quantum Monte Carlo data written in the imaginary-frequency to the real-frequency axis is one of the difficult numeric problems, due to the ill-conditioned nature of the kernel matrix. While the maximum entropy method (MEM) is one of the most suitable choices to gain information from the noisy input data, its applications are limited by the non-negative condition of the output spectral function. Here we have extended the MEM to the matrix-valued function, introducing quantum relative entropy as a regularization function [1]. As a true matrix-valued method, our maximum quantum entropy method (MQEM) is invariant under the arbitrary unitary transformation of the input matrix. Without introducing further ambiguity, Bayesian probabilistic interpretation can be applied to the MQEM. Using our DFT+DMFT package, DMFTpack, the MQEM is applied for real materials, namely Sr₂IrO₄. The application shows that the generalized method provides a reasonable band structure without introducing a material specific base set.


*This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2018R1A2B2005204).

5:18PM H19.00011: Diagrammatic Quantum Monte Carlo for Molecular Systems JIA LI (Presenter), MARKUS WALLERBERGER, EMANUEL C GULL, University of Michigan — Electron correlations in chemical systems give rise to a wide range of interesting physical properties. Although traditional mean-field quantum chemical algorithms can reliably calculate ground state observables, finite temperature and spectral properties are only accessible with explicit inclusion of electron correlations. Diagrammatic Monte Carlo (DiagMC), which expands the physical observable in terms of connected Feynman diagrams and samples the resulting series stochastically, is a powerful technique for studying electron correlations and does not suffer from numerical sign problem which worsens with increasing system size. Recent developments in DiagMC algorithms have greatly improved their numerical efficiency. In this talk, we aim to introduce our DiagMC implementation for multi-orbital systems, and discuss the difficulties and potentials when it is applied to realistic molecular systems.
2:30PM H20.00001: Non-orthogonal configuration interaction for molecular excited states: Valence and core excitations and strong correlations* [Invited] MARTIN HEAD-GORDON (Presenter), University of California, Berkeley — Most electronic structure methods are designed using a single set of orthogonal orbitals. Using multiple sets of orbitals, that are orthogonal within a given configuration, but non-orthogonal from one configuration to another, is an interesting alternative that is the basis of the non-orthogonal configuration interaction (NOCI) approach to electronic structure. NOCI provides great flexibility to compactly incorporate the different physics of different configurations. A very simple example is a molecule in which an ionic configuration (e.g. Li⁺F⁻) competes with a covalent configuration (e.g. LiF). Orbital relaxation is very different in the two configurations, and accounts for a large part of what would conventionally be termed dynamic correlation. Far more complicated examples natural arise in mixed valent systems, and systems with low-lying charge-transfer excited states. Core excitations are another natural class of examples. I shall discuss the NOCI method, ways in which it can be made nearly black-box for interesting classes of valence and core excitations, and how to describe remaining dynamic correlation effects using a generalized second order perturbation theory. A variety of molecular examples will be shown for each of these types of NOCI. I hope to convey the message that the NOCI framework can be very useful for both computing and interpreting electronic structure, with bright prospects for further developments in the future.

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3:06PM H20.00002: Quantum embedding for excited states in molecular and periodic systems XUELAN WEN (Presenter), DHABIH CHULHAI, JASON GOODPASTER, Department of Chemistry, University of Minnesota, Twin Cities — Projection-based quantum embedding methodologies provide a framework for performing DFT-in-DFT and wavefunction-in-density functional theory (WF-in-DFT) calculations. The previous application of using absolute localization on the ground states of molecular systems\(^1\) and periodic systems\(^2\) showed high accuracy and improved computational efficiency.

In this work, we extend the absolute localization method to study localized excited states in molecular and periodic systems. We show the accurate embedding results on small organic molecules and green fluorescent protein (GFP). We are further extending our methods to periodic systems. Ray et al.\(^3\) found that different density functionals have to be used for CsM\(_3\) (M = Ge, Sn, Pb, Mg, Ca, Sr and Ba) to reproduce the experimental band gaps. Not a single exchange-correlation functional can give consistently good results among these inorganic perovskites.\(^3\) We discuss our progress of making periodic WF-in-DFT embedding methods applicable to such systems.

3:18PM H20.00003: Coupled cluster theory for coupled electron-photon systems  ULIANA MORDOVINA (Presenter), HEIKO APPEL, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany, FREDERIK R. MANBY, Centre for Computational Chemistry, School of Chemistry, University of Bristol, Bristol, UK — Recent experiments show that properties of materials and energy landscapes of chemical reactions can change drastically when put inside a high-Q optical cavity. Understanding these phenomena require novel theoretical approaches, where both parts of the problem, light and matter, are treated on an equal quantum mechanical footing. Extension of existing electronic structure methods to include photons provides one route in this direction.

One prominent tool in electronic structure theory is coupled cluster (CC) theory which is often called the gold-standard in quantum chemistry, as it is a robust polynomial-scaling approach for handling weak correlations.

In the present work we develop methodology to extend CC theory to coupled electron-photon systems. We show benchmark results for model molecular hamiltonians coupled to cavity photons. By comparing to full configuration interaction results, we study the accuracy of the proposed method. We show that our method includes effects like multiphoton processes, which ab-initio methods so far fail to describe. Therefore, not only does our method go beyond standard quantum optical approaches, since it includes an accurate treatment of electronic structure, it also goes beyond existing methods such as QEDFT in terms of its description of light.

3:30PM H20.00004: A quantum embedding theory in the screened Coulomb interaction: Combining configuration interaction with GW/BSE†  MARC DVORAK (Presenter), PATRICK RINKE, Aalto University — We present a new quantum embedding theory called dynamical configuration interaction (DCI) that combines wave function and Green’s function theories. DCI captures static correlation in a correlated subspace with configuration interaction and couples to high-energy, dynamic correlation outside the subspace with many-body perturbation theory based on Green’s functions. DCI takes the strengths of both theories to balance static and dynamic correlation in a single, fully ab-initio embedding concept. We show that treating high-energy correlation up to the GW and Bethe-Salpeter equation level is sufficient even for challenging multi-reference problems. Our theory treats ground and excited states on equal footing, and we compute the dissociation curve of N$_2$, vertical excitation energies of N$_2$ and C$_2$, and the ionization spectrum of benzene in excellent agreement with high level quantum chemistry methods and experiment.

*The research is supported by Academy of Finland grant no. 316347.

3:42PM H20.00005: Locality and Computational Reliability of Linear Response Calculations for Molecular Systems  LUIGI GENOVESE (Presenter), INAC, CEA Grenoble, MARCO D’ ALESSANDRO, ISM, CNR — We explore the interplay between locality of the response density operator and numerical convergence of Linear Response quantities. We show that for frequencies below the first ionization potential (IP) of the system, it is possible to express the response density by employing localized states only. Above this threshold energy, such a locality property cannot be achieved. Such considerations may be transposed in terms of the molecule’s excited states. We show that not all the system's excitations can be considered on equal footing. There is a discrete sector of excitations - which may extend above IP - that can be parametrized by observable, localized states, which can be computationally expressed with high precision, provided an adequate level of completeness. The remaining excitation modes belong to a continuum spectrum that, on the contrary, is not directly associated to observable properties and can only be effectively represented in a given computational setup. Such considerations are important not only for reproducibility of the results among different computer codes employing diverse formalisms, but also in view of providing a deeper understanding on the impact of models' approximations on the scientific outcomes of the simulation.
ARKAJIT MANDAL

CS-RPMD also holds a very promising method to apply in non-equilibrium dynamics. With a two-state model system show very good agreement with the exact quantum results. Besides the equilibrium regime, multiple beads for nuclei, CS-RPMD preserves detailed balance and an approximate QBD. Numerical tests of this method sampled distribution with an additional phase factor. In a special limit that there is one bead for mapping variables and oscillations. At the time equivalent to zero, the quantum Boltzmann distribution (QBD) is recovered by reweighting the not contain any inter-bead coupling term in the state-dependent potential and correctly describes electronic Rabi quantum effects. This new approach is derived by using coherent-state mapping representation for the electronic degrees of freedom. Direct simulations of the exact quantum dynamics remains to be computationally challenging. Here we propose to develop an efficient simulating quantum dynamics effects is one of the central challenges in modern theoretical chemistry. Direct approach, a diabatic quantum dynamics method, with Density Functional Tight Binding, an electronic structure approach diabatization or to formulate them back to the adiabatic representation. We combine Partial Linearized Density Matrix interface diabatic quantum dynamics approaches with adiabatic electronic structure calculation. This scheme uses the crude adiabatic basis as a diabatic basis for a short-time nuclear dynamics propagation and updates it in each consecutive nuclear step. This scheme extends the scope and applicability of the diabatic quantum dynamics approaches and allows us to propagate on-the-fly quantum dynamics with them, avoiding any additional non-trivial efforts to perform diabatization or to formulate them back to the adiabatic representation. We combine Partial Linearized Density Matrix approach, a diabatic quantum dynamics method, with Density Functional Tight Binding, an electronic structure approach to demonstrate the applicability of our proposed scheme.

4:06PM H20.00007: Coherent State Mapping Ring Polymer Molecular Dynamics for Nonadiabatic Quantum Propagations SUTIRTHA CHOWDHURY (Presenter), PENGFEI HUO, Chemistry, University of Rochester — Accurately and efficiently simulating quantum dynamics effects is one of the central challenges in modern theoretical chemistry. Direct simulations of the exact quantum dynamics remains to be computationally challenging. Here we propose to develop a classical trajectory based method to accurately describe electronic non-adiabatic dynamics as well as capture nuclear quantum effects. This new approach is derived by using coherent-state mapping representation for the electronic degrees of freedom (DOF) and the ring-polymer path-integral representation for the nuclear DOF. The CS-RPMD Hamiltonian does not contain any inter-bead coupling term in the state-dependent potential and correctly describes electronic Rabi oscillations. At the time equivalent to zero, the quantum Boltzmann distribution (QBD) is recovered by reweighting the sampled distribution with an additional phase factor. In a special limit that there is one bead for mapping variables and multiple beads for nuclei, CS-RPMD preserves detailed balance and an approximate QBD. Numerical tests of this method with a two-state model system show very good agreement with the exact quantum results. Besides the equilibrium regime, CS-RPMD also holds a very promising method to apply in non-equilibrium dynamics.

4:18PM H20.00008: Quasi-Diabatic scheme for on-the-fly quantum dynamics propagation ARKAJIT MANDAL (Presenter), PENGFEI HUO, Chemistry, University of Rochester — We develop a nonadiabatic quantum dynamics scheme to interface diabatic quantum dynamics approaches with adiabatic electronic structure calculation. This scheme uses the crude adiabatic basis as a diabatic basis for a short-time nuclear dynamics propagation and updates it in each consecutive nuclear step. This scheme extends the scope and applicability of the diabatic quantum dynamics approaches and allows us to propagate on-the-fly quantum dynamics with them, avoiding any additional non-trivial efforts to perform diabatization or to formulate them back to the adiabatic representation. We combine Partial Linearized Density Matrix approach, a diabatic quantum dynamics method, with Density Functional Tight Binding, an electronic structure approach to demonstrate the applicability of our proposed scheme.

4:30PM H20.00009: Electronic Non-Adiabatic Dynamics: memory-dependence and electron-nuclear correlation ALI ABEDI KHALEDI (Presenter), Max Planck Institute for Microstructure Physics — Time-Dependent Density Functional Theory (TDDFT) is one of the most promising theoretical tools in describing the electronic dynamics. In spite of its great success calculating spectra in the linear response regime, it performs poorly in the case of the strong-field dynamics of atoms and molecules. Two main obstacles concerning the application of TDDFT to atoms and molecules in ultrashort intense laser pulses are:

i) Lack of memory dependence in the usual exchange-correlation approximations. The exact functional depends on the history of the density that is neglected in almost all of the existing approximations.

i) Lack of a proper description of the electron-ion correlation.

Towards tackling these problems, we have developed a memory-dependent functional for two-site Hubbard model that fulfills the recently proposed exact condition (Fuks et al. PRL 114, 183002 (2015)). Furthermore, by utilising the Exact-Factorization framework, we have studied the exact potential acting on the electron in charge-resonance enhanced ionization in H2+ molecule and showed that there can be significant differences between the exact potential and that used in the traditional quasistatic analyses, arising from non-adiabatic coupling to the nuclear system (Khosravi, Abedi, Maitra, PRL 115, 263002 (2015)).
4:42PM H20.00010: Optical conductivity and charge fluctuation spectroscopy in the time domain*  
ALEXANDER KEMPER (Presenter), ANKIT KUMAR, North Carolina State University — Using ultrashort laser pulses it is possible to study the dynamics of many-body systems in the time domain. The response functions are often two-particle correlation functions, including optical or terahertz transmission spectroscopy (current) and charge fluctuation spectroscopy momentum resolved EELS (charge). We have studied two-particle response functions using functional derivatives within a non-equilibrium Keldysh Green's function method. This has several advantages over common approaches, most notably the natural inclusion of vertex corrections. We present the equilibrium and non-equilibrium response of a few model systems including electrons interacting with each other and with a bath of phonons, and discuss the implications for experiments.

*This work is supported by NSF DMR-1752713.

4:54PM H20.00011: Ab initio study of photo-induced phase transitions*  
CHAO LIAN (Presenter), BRYAN M WONG, University of California, Riverside — Ultrafast real-time lattice dynamics is a powerful tool to study the fundamental properties and behavior of solids. Ultrafast electronic dynamics in solids lies at the core of modern condensed matter and materials physics. To construct a practical ab initio method for studying solids under photoexcitation, we developed a momentum-resolved real-time time-dependent density functional theory algorithm using a numerical atomic basis, together with the implementation of both length and vector gauges of an electromagnetic field. When applied to the simulation of elementary excitations in both bulk and two-dimensional materials, different excitation modes are only distinguishable in momentum space. We also discuss various examples of photoinduced phase transitions such as amorphizations, charge density wave enhancements, and ultrafast solid-solid transitions.

*The authors acknowledge the support of the U.S. Army Research Office under grant number W911NF-17-1-0340.

5:06PM H20.00012: Modeling Excitation Energies of Quantum Dots based on First Principles Data  
EZEKIEL OYENIYI, Dept. of Physics, University of Ibadan, NIGERIA, OMOLOLU AKIN-OJO (Presenter), University of Rwanda, East Africa Institute for Fundamental Research (EAIFR) — Wave function ab initio methods are prohibitively expensive for determination of excited states of large systems such as quantum dots. In this work, we present a method for determination of excitaton energies of large systems having more than 10,000 electrons. The method is based on the use of a semi-empirical hamiltonian appropriately parameterized to reproduce ab initio "EOM-CCSD" excitation energies of small systems. The same set of parameters is then extended to the calculation of excited state properties of large systems. Our results compare well with EOM-CCSD, TDDFT, and CIS(D) results whenever they are available.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H21 DCOMP DCMP GSNP: Advances in Computational Methods for Statistical Physics and Their Applications III  

JONATHAN MACHTA (Presenter), CHRIS AMEY, University of Massachusetts Amherst, NATHAN ROSE, 1QBit — Population annealing is an algorithm that is well-suited for sampling equilibrium distributions for systems such as spin glasses and configurational glasses with rough free energy landscapes. Population annealing is massively parallel and easily implemented either on large clusters or GPUs. In addition to being massively parallel, population annealing has several attractive features: (1) it gives direct access to thermodynamic potentials, (2) multiple independent runs can be combined using weighted averaging to improve both statistical and systematic errors and (3) equilibration can be assessed with an intrinsic measure. In this talk population annealing will be introduced and put in the context of other sequential Monte Carlo and annealing algorithms. Applications to spin glasses, configurational glasses and first order transitions will be discussed.

*This work was supported by the National Science Foundation (Grant No. DMR-1507506).
3:06PM H21.00002: Population annealing: A massively parallel algorithm for simulating systems with rough free energy landscapes*  CHRIS AMEY (Presenter), University of Massachusetts Amherst, NATHAN ROSE, 1QB Information Technologies, JONATHAN MACHTA, University of Massachusetts Amherst, Santa Fe Institute — Population annealing is a massively parallel sequential Monte Carlo algorithm that is designed to sample equilibrium states of systems with rough free energy landscapes. Population annealing is closely related to simulated annealing. In population annealing, the relevant equilibrium ensemble is represented by a large population of replicas of the system. The population is initialized in an easy to equilibrate region of parameter space and is then "annealed" in parameter space to a more difficult, target region. Resampling the population of replicas during each annealing step ensures that the population remains near equilibrium. The entropy and thermodynamic potentials together with intrinsic estimates of systematic errors are readily accessible from the simulations. We will describe both canonical and microcanonical versions of the population annealing algorithm, and discuss applications to spin glasses, binary hard sphere fluids in the glassy regime, and large q Potts models.

*This work was supported by the National Science Foundation (Grant No. DMR-1507506).

3:18PM H21.00003: Quantum Free Energy Differences from Non-Equilibrium Path Integral Methods*  LISANDRO HERNANDEZ DE LA PENA (Presenter), Kettering University, RAMSES VAN ZON, University of Toronto, JEREMY SCHOFIELD, Chemistry, University of Toronto, GILLES PESLHERBE, Chemistry and Biochemistry, Concordia University — In this work, we discuss how the imaginary-time path integral representation of the quantum canonical partition function and non-equilibrium work fluctuation relations can be combined to yield methods for computing free energy differences in quantum systems using non-equilibrium processes. The path integral representation is isomorphic to the configurational partition function of a classical field theory to which a natural Hamiltonian dynamics can be associated. It is then shown that both, Jarzynski nonequilibrium work relation and Crooks fluctuation relation, formally hold for this classical field theory. Since the energy diverges in canonical equilibrium, regularization methods need to be introduced in order to limit the number of degrees of freedom M to be finite. The convergence of the work distribution as M tends to infinity is demonstrated analytically for a system composed of a quantum particle trapped in a harmonic well, and numerically for a quartic double-well potential with varying asymmetry. Finally, the method is used to study the relevance of protonic quantum effects in ionic water clusters.

*Natural Sciences and Engineering Research Council of Canada (NSERC)  National Science Foundation (NSF)  American Chemical Society Petroleum Research Fund (ACS PRF)

3:30PM H21.00004: Stable Recursion Relation for the Canonical Partition Function of Non-Interacting Fermions*  JIANGYONG YU (Presenter), HATEM BARGHATHI, ADRIAN DEL MAESTRO, University of Vermont — While the thermodynamics of a system of non-interacting fermions can be straightforwardly determined in the grand canonical ensemble, results for a specific number of N particles are more difficult to obtain. In this talk we will present a general recursion scheme for the canonical partition function of free fermions with a quadratic energy level spacing as might be present for ultracold fermionic atoms confined inside a box trap. Exact results for the entropy, specific heat and one and two particle occupation probabilities are numerically obtained to arbitrary precision and compared with their corresponding grand canonical values. The numerical stability of the recursion relation allows us to quantify deviations from Wicks theorem in the canonical ensemble for a variety of temperatures and densities.

*This work was supported in part by the NSF through grants No. DMR-1553991 and No. OAC-1827314.

3:42PM H21.00005: New Approaches to Tensor Network Simulation of 2D Quantum Systems  KATHARINE HYATT (Presenter), MILES STOUDENMIRE, Center for Computational Quantum Physics, Flatiron Institute — Accessing generic many-body quantum ground states in two full dimensions remains an outstanding problem in numerical condensed matter physics. Quantum Monte Carlo suffers from the sign problem, exact diagonalization cannot access large systems, DMRG struggles to reach beyond quasi-1D ladders, and many existing 2D tensor network approaches still have much room for improvement in terms of computational costs and numerical stability. We develop a PEPS approach, inspired by successful DMRG methods in one spatial dimension, which has much better performance than DMRG while retaining many of its advantages. We discuss the benefits and some drawbacks of the method, and we present some preliminary successes in fully two dimensional simulations with an eye to working towards simulating models on the frontier of numerical and analytical understanding.
3:54PM H21.00006: Accelerating Monte Carlo Simulations of Two-Dimensional Spin Models using GPUs  
BENJAMIN HIMBERG (Presenter), Physics, University of Vermont, SANGHITA SENGUPTA, Physics, Institut quantique de l'Université de Sherbrooke — Utilizing the vast computational power of Graphics Processing Units, we develop novel algorithms in both OpenCL and CUDA to study the statistical mechanical properties of two-dimensional spin models. Our basic technique is the general Markov chain Monte Carlo method which uses a Metropolis-Hastings step. In contrast to the popular method of checkerboard updates, we have devised an unconventional procedure that traverses rows to generate the spin configurations. This special implementation allows us to simulate large system sizes (~ 10^9 spins) and, when tested on our fastest GPU, produces an average time per spin-flip of 0.005 ns with a speed-up factor of 600 compared to an optimized single-core CPU algorithm. We test the performance characteristics of our techniques for simulating 2D spin models such as the Ising, XY, and Potts on hexagonal and square lattices. Finally, as a theoretical proof of our computational concept we present critical temperatures of the models based on finite-size scaling methods.

4:06PM H21.00007: Accelerated simulation of gelation  
ROMAIN DUPUIS (Presenter), CNRS/MIT/AMU Joint Laboratory MultiScale Materials Science for Energy and Environment, UMI 2, LAURENT BELAND, Department of Mechanical & Materials Engineering, Queens university, ROLAND JM PELLENQ, CNRS/MIT/AMU Joint Laboratory MultiScale Materials Science for Energy and Environment, UMI 2 — The formation of gels is a complex issue that has to be resolved to investigate manifold synthetic materials - among them: porous materials such as cement, high-quality glass fiber and geomaterials for radioactive waste sealing.

Being able to simulate the structural, mechanical and dynamical properties of gels would have far-reaching consequences to improve the synthetization of materials and to lengthen their lifetime. This requires rather demanding computational power, which is worsen by the fact that gels have weak long-distance ordering (which requires large simulation cells) and that the gelation is a slow process due to high energy barrier for bond formation.

In order to reproduce the gelation we coupled GCMC and Parallel tempering methods to enhance the formation of silicate chains and reduce the computational costs. Using such cost-efficient method, we were able to study the formation of alkali-silica gels that is key to understand concrete structures failure.

4:18PM H21.00008: Heuristic optimization and sampling with tensor networks for quasi-2D spin glass problems  
MASOUD MOHSENI (Presenter), Google AI Quantum, MAREK RAMS, Institute of Physics, Jagiellonian University, BARTEK GARDAS, Institute of Physics, University of Silesia — We devise a deterministic classical algorithm to reveal the structure of low energy spectrum for certain spin-glass systems that encode classical optimization problems. We employ tensor networks to represent probability distributions of all possible configurations. We then develop efficient techniques for approximately extract the relevant information from the networks for a class of quasi-two-dimensional Ising Hamiltonians. To this end, we apply a branch and bound approach over marginal probability distributions by approximately evaluating tensor contractions. Our approach identifies configurations with the largest Boltzmann weights corresponding to low energy states. We discover spin-glass droplet structures at finite temperatures, by exploiting local nature of the problems. This droplet finding algorithm naturally encompass sampling from high quality solutions within a given approximation ratio. It is, thus, established that tensor networks techniques can provide profound insight into the structure of large low-dimension spin-glass problems, with ramifications both for machine learning and noisy intermediate-scale quantum devices. Moreover, limitations of our approach highlight alternative directions to establish quantum speed-up and possible quantum supremacy experiments.
4:30PM H21.00009: Studying the finite temperature properties of ferroelectrics*
KRISHNA CHAITANYA PITIKE (Presenter), Materials Science and Technology Division, Oak Ridge National Laboratory, YING WAI LI, National Center for Computational Sciences, Oak Ridge National Laboratory, SIMUCK F YUK, Basic and Applied Molecular Foundations, Pacific Northwest National Laboratory, MARKUS EISENBACh, National Center for Computational Sciences, Oak Ridge National Laboratory, SERGE M NAKHMANSOn, Department of Materials Science and Engineering, University of Connecticut, VALENTINO R. COOPER, Materials Science and Technology Division, Oak Ridge National Laboratory — ABO₃ perovskite ferroelectrics, as well as their solid solutions, exhibit rich transitional behavior patterns that can be exploited, e.g., to obtain large piezoelectric and dielectric responses. Due to the complexity of the phase diagrams of these materials, mesoscale-level parameterizations capable of accurately reproducing their finite temperature properties are difficult to develop. Furthermore, obtaining such parameters from first principles calculations is complicated by the large number of available exchange correlation (XC) functionals. We investigate the influence of XC functionals on the prediction accuracy of ferroelectric phase transitions in PbTiO₃. LDA, PBE, PBEsol and vdW-DF-C09 XC functionals are evaluated utilizing constant-temperature molecular dynamics, in comparison with Wang-Landau (WL) Monte Carlo and Replica Exchange WL simulations. We find that LDA, PBEsol and vdW-C09 provide good estimates of physical properties near the phase transition, as compared with experiments, while PBE significantly overestimates the transition temperature.

* KCP, YWL and VRC acknowledge financial support from the LDRD program at ORNL. SFY and ME were supported by the U.S. DOE, Office of Science, BES, MSED. The authors acknowledge computational resources provided by NERSC and OLCF.

4:42PM H21.00010: Predicting the surface phase diagram of Ag(111) using ab initio grand canonical Monte Carlo*
ROBERT WEXLER (Presenter), TIAN QIU, ANDREW RAPPE, University of Pennsylvania — The structure of a surface can dramatically affect its properties. For example, surface reconstructions can occur that change band alignments and/or catalytic activity. Currently, ab initio thermodynamics is the method of choice for determining the stable surfaces of a material, however, the selection of surfaces to study is done manually, which induces bias that can prevent one from finding global minima in the surface energy. We present an implementation of ab initio grand canonical Monte Carlo (GCMC) that automatically predicts surface phase diagrams and apply it to the Ag(111) system. We obtain an Ag₇O₁₀ overlayer, which is consistent with the most stable reconstruction found experimentally and computationally. We extracted structure-stability trends from our simulation data using machine learning and find that surface coordination and bond angles are important descriptors for stability. We analyzed the stochastic evolution of the surface and discovered a possible mechanism for the formation of the Ag₇O₁₀ overlayer. Ab initio GCMC therefore offers a rich set of possibilities for studying interfacial systems.

* Department of Energy, Division of Basic Energy Sciences, DE-SC0019281
High-Performance Computing Modernization Office
National Energy Research Scientific Computing Center

4:54PM H21.00011: A Lattice Boltzmann Method for Simulating Dry and Dense Active Fluids
DAVID NESBITT (Presenter), Bioengineering, Imperial College London, GUNNAR PRUSSNER, Mathematics, Imperial College London, CHIU FAN LEE, Bioengineering, Imperial College London — Symmetry serves a foundational role in all areas of physics today. In classical many-body problems, by first clarifying the underlying symmetries of a system of interest, one can derive the hydrodynamic equations of motion that govern the dynamics of the system. Analysis of a hydrodynamic theory can elucidate the universal behavior exhibited by all generic systems respecting the prescribed set of symmetries; conversely, any particular many-body system defined by microscopic rules that respect the same set of symmetries can also be used to study the associated universal behavior in the hydrodynamic limit. An example of the latter is the use of lattice gas cellular automata to study the Navier-Stokes equations. Superseding the lattice gas cellular automata is the celebrated lattice Boltzmann method, which led to a drastic improvement in computational efficiency. Surprisingly, the development of a lattice Boltzmann method for dry active fluids is still lacking, which is what we accomplish here. We will demonstrate the usefulness of our approach by clarifying the phase behaviour of polar active fluids and motility-induced phase separation. In particular, we show that there are generically three distinct phases in polar active fluids separated by two discontinuous phase transitions.
Spin-flop transition in the 3D anisotropic Heisenberg antiferromagnet: Finite size scaling for a first order transition where a continuous symmetry is broken

JIAHAO XU (Presenter), SHAN-HO TSAI, DAVID P LANDAU, Center for Simulational Physics, University of Georgia, KURT BINDER, Institut für Physik, Johannes Gutenberg Universität Mainz — We use Monte Carlo simulations to explore the 3D anisotropic Heisenberg antiferromagnet in a field in order to study the finite size behavior of the first order "spin-flop" transition between the Ising-like antiferromagnetic state and the canted, XY-like state[1]. Finite size scaling for a first order phase transition where a continuous symmetry is broken is developed using an approximation of Gaussian probability distributions with a phenomenological "degeneracy" factor, q, included. Our theory yields q = π, and it predicts that for large linear dimension L the field dependence of all moments of the order parameters as well as the fourth-order cumulants exhibit universal intersections. The values of these intersections at the spin-flop transition point can be expressed in terms of the factor q. Our theory and simulation imply a heretofore unknown universality can be invoked for first order phase transitions.


Evaluating the Jones polynomial with tensor networks*

KONSTANTINOS MEICHANETZIDIS (Presenter), School of Physics & Astronomy, University of Leeds, STEFANOS KOURTIS, Physics, Boston University — We introduce tensor network contraction algorithms for the evaluation of the Jones polynomial of arbitrary knots. The value of the Jones polynomial of a knot maps to the partition function of a q-state Potts model defined as a planar graph with weighted edges that corresponds to the knot. For any integer q, we cast this partition function into tensor network form and employ fast tensor network contraction protocols to obtain the exact tensor trace, and thus the value of the Jones polynomial. By sampling random knots via a grid-walk procedure and computing the full tensor trace, we demonstrate numerically that the Jones polynomial can be evaluated in time that scales subexponentially with the number of crossings in the typical case. This allows us to evaluate the Jones polynomial of knots that are too complex to be treated with other available methods. Our results establish tensor network methods as a practical tool for the study of knots.

*EPSRC Doctoral Prize Fellowship 2017-2019
Boston University Center for NonEquilibrium Systems and Computation
An optimal approach to computing phonons and their interactions via finite displacements*
LYUWEN FU (Presenter), MORDECHAI C KORNBLUTH, ZHENGQIAN CHENG, CHRIS MARIANETTI, Columbia University — Phonons and their interactions are critical to predicting a wide range of materials properties. Therefore, efficiently extracting a high resolution Taylor series expansion of the Born-Oppeheimer surface from an arbitrary first-principles approach is of great importance. Here we present an optimal formalism to compute phonons and their interactions at arbitrary order and crystal dimension on a regular grid using finite displacements; yielding a Taylor series purely in terms of group theoretically irreducible derivatives. Building on a key theorem we derive, our approach ensures that a given derivative can always obtained from the smallest possible supercell dictated by the translation group. Our approach maximally exploits any derivatives the first-principles approach can efficiently deliver perturbatively (e.g. Hellman-Feynman forces, etc) to obtain higher order derivatives. We prove that our approach is superior to any single-supercell finite displacement approach. Applications are presented for graphene, computing and tabulating the irreducible derivatives up to 5th order. A number of critical tests are performed to demonstrate the fidelity of our results.

*This work was supported by the grant DE-SC0016507 funded by the U.S. Department of Energy, Office of Science.

New Thermal Transport Regime for Partial-Crystalline Partial-Liquid Materials [Invited]  MING HU (Presenter), Department of Mechanical Engineering, University of South Carolina — Materials in partial-crystalline partial-liquid (PCPL) state are now widely used as thermoelectrics and battery electrodes, due to their low thermal conductivity and high ionic conductivity, respectively. However, the well-developed computational methods for pure crystalline materials such as anharmonic lattice dynamics coupled with Boltzmann transport equation cannot be used to study such systems. By performing first-principles and molecular dynamics simulations, we give a robust explanation of the thermal transport mechanism in PCPL material Li₂S. At the temperature range where the system can be regarded as a solid, the large hopping of Li is found to be responsible for phonon thermal conductivity's deviation from the traditional 1/T relationship. At high temperatures, the contribution of convection and liquid-phonon interaction increase significantly due to the fluidization of Li ions. Furthermore, there is an interplay between the enhanced phonon scattering and the increased force hopping between neighboring atoms as temperature arises, which results in a dip in the evolution of the virial term around 1200K. When the temperature is even higher, the virial term increases with temperature due to the contribution of vibrations with extremely short mean free path (diffusons). This point is validated by the evolution of the accumulative thermal conductivity with mean free path. At 1300 K, more than 46% of the heat carried by the S sublattice is contributed by the carriers with mean free path smaller than a few angstroms, which is the typical hopping distance. Our study [1] provides a clear physical map of the heat transport in PCPL materials and describes the key mechanism to guide the design of future thermoelectric materials and battery electrodes.


Observation of second sound in graphite at temperatures up to 100 K* RYAN DUNCAN (Presenter), SAMUEL HUBERMAN, KE CHEN, BAI SONG, VAZRIK CHILOYAN, ZHIWEI DING, ALEXEI MAZNEV, GANG CHEN, KEITH ADAM NELSON, Massachusetts Institute of Technology — Wavelike thermal transport in solids, referred to as second sound, has until now been an exotic phenomenon limited to a handful of materials at low temperatures. This has restricted interest in its occurrence and in its potential applications. Through time-resolved optical measurements of thermal transport on 5-20 μm length scales in graphite, we have made direct observations of second sound at temperatures above 100 K. The results are in qualitative agreement with ab initio calculations that predict wavelike phonon hydrodynamics on ~ 1-μm length scale up to almost room temperature. The results suggest an important role of second sound in microscale transient heat transport in two-dimensional and layered materials in a wide temperature range.

*S.H., V.C., Z.D., and G.C. acknowledge support from the office of Naval Research (MURI grant N00014-16-1-2436) and from the Solid State Solar-Thermal Energy Conversion Center (S³TEC), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (Award DE-SC0001299). R.A.D., A.A.M., and K.A.N. acknowledge support from the U.S. National Science Foundation (EFRI-2-DARE Award No. 1542864).
3:54PM H22.00006: First-principles study of lattice thermal conductivity in concentrated solid solution alloys*  
SAI MU (Presenter), LUCAS LINDSAY, RAINA OLSEN, BENNETT C LARSON, GEORGE MALCOLM STOCKS, Oak Ridge National Laboratory — Energy dissipation of concentrated solid solution alloys can be controlled by the number and types of alloying elements and has impacts on the defect formation and recombination after radiation. Here we use an ab-initio supercell method combined with a phonon unfolding technique to access the effects of disorder on the lattice-mediated thermal conductivity in a series of 2-4 component equiatomic alloys (e.g. NiFe, NiCo, NiCoCr, NiFeCo, NiFeCoCr) where the mass disorder is small while the force constant disorder is pronounced. We demonstrate that force constant disorder itself can efficiently reduce the thermal conductivity. We further show that the low-conductivity Cr-containing alloys present the largest force constant fluctuations across the studied alloys and that this is electronically driven. The results provide a new tuning parameter, based on the electronic structure, to manipulate the force constant disorder, thereby facilitating the design of materials with desirable thermal transport properties.

*This work was supported as part of the Energy Dissipation to Defect Evolution (EDDE), an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences under contract number DE-AC05-00OR227.

4:06PM H22.00007: The influence of interfacial structure and strain energy on phonon transport*  
RILEY HANUS (Presenter), JEFF SNYDER, Northwestern University — Phonon transport across interfaces is an inherently complex topic of great scientific and technological importance. Several experimental and theoretical results which aim to establish a fundamental understanding of heat transfer across interfaces will be presented. First, I will demonstrate how phonon diffraction and dimensionality crossover effects arise when the nanoscale structure and strain field of interfaces and grain boundaries (GBs) are considered. Next, an experimental study is presented where the thermal boundary resistance is measured on individual Si-Si twist GBs at different twist angles. The thermal boundary resistance at GBs, again, seems to be dominated by the interfacial strain field. Finally, it is shown how the thermal boundary resistance can be controlled by modifying the GB with 2D materials. Several layers of graphene were introduced into the GBs of skutterudite materials which dramatically increases the materials thermal boundary resistance, negligibly effecting electronic transport, resulting in a 24% improvement in measured thermoelectric device efficiency.

*GJS and RH acknowledge EFRC Solid-State Solar-Thermal Energy Conversion Center (S3TEC) Grant DE-SC0001299. RH acknowledges support from the Johannes and Julia Randall Weertman Graduate Fellowship.

4:18PM H22.00008: Thermal properties of magnetic materials from first principles*  
MATTHEW HEINE (Presenter), Physics, Boston College, OLLE HELLMAN, Linkoping University, DAVID A BROIDO, Physics, Boston College — In addition to representing an active area of physics research, magnetic materials are used in finite temperature applications such as computer memory technology. In this study we use the Temperature Dependent Effective Potential (TDEP) approach to calculate finite temperature properties of magnetic materials from first principles. In this approach, thermal disorder of the lattice and magnetic moments are incorporated self consistently to yield temperature-dependent properties. Calculations are performed within the framework of Density Functional Theory (DFT) using constrained, fully noncollinear magnetic moments. The effects of such thermal disorder are demonstrated across a range of temperatures spanning the magnetic transition temperature.

*Dissertation Fellowship Award (Boston College)

4:30PM H22.00009: Nonperturbative modeling of high-frequency Holstein-coupled modes using matrix product states  
BENEDIKT KLOSS (Presenter), DAVID REICHMAN, ROEL TEMPELAAR, Columbia University — Many nonequilibrium phenomena of current interest involve coupling of electronic coordinates to vibrational modes whose frequency and reorganization energy are high or comparable to other relevant energies. A proper theoretical account of such modes needs to be non-perturbative and non-classical. The commonly applied direct diagonalization approach rapidly becomes prohibitively expensive with increasing system sizes. We present an alternative approach based on tensor network states, merging concepts from the condensed matter physics and molecular quantum dynamics communities. Focusing on the one-particle (electronic) sector, relevant for exciton and polaron dynamics, we construct the vibronic wavefunction as a set of matrix product states, representing the vibrational degrees of freedom surrounding the particle. This approach allows for an exact treatment of Holstein-driven processes at an unprecedented scale.
4:42PM H22.00010: Accuracy of Lorenz number estimates based on transport data* ADITYA PUTATUNDA (Presenter), DAVID SINGH, University of Missouri — Determination of the thermal conductivity (κ) and its separation into its major constituent lattice and electronic parts is of importance in certain materials. In this work, we study the Wiedemann-Franz law which is used broadly by experimentalists to estimate these parts to investigate κ. For a group of known thermoelectric materials, we investigated the temperature and doping dependence of the Lorenz number (L). In relation to this, we examined the accuracy of an expression proposed by Kim et al. relevant in the literature which is used frequently to estimate L. Solving the Boltzmann transport equations for first-principles band-structure results, we find that this expression, despite being mathematically simple, captures the observed variations of L with satisfactory accuracy for wide band gap materials. It does not work as well for some other materials e.g. PbTe and MgSb2 which primarily have non-parabolic band structures.

* Work at the University of Missouri is supported by the Department of Energy, Basic Energy Sciences, Award DE-SC0019114

4:54PM H22.00011: Automatic ab initio calculations of electronic transport of semiconductors HENRIQUE MIRANDA (Presenter), GUILLAUME BRUNIN, MATTEO GIANTOMASSI, GIAN-MARCO RIGNANESE, GEOFFROY HAUTIER, Universite catholique de Louvain — We address the problem of calculating electronic transport quantities on semiconductors of technological interest (Si,GaAs,MoS2) with minimal user intervention. An important technical challenge is to accurately obtain quantities that depend on integrations on the band-structure. Several methods have been proposed based on Wannier functions or atomic orbitals with the drawback that they often require time-consuming user intervention. For automatic calculations, we use the Shankland-Koelling-Wood interpolation as implemented in the Boltztrap2[1] code. We will discuss some often seen interpolation artifacts, its limitation in reproducing band-crossings and how those affect the final results. We compare these with calculations done using a newly developed driver to obtain electron velocities within the Abinit[2] code on large k-point meshes integrated using the tetrahedron method. We will then show the importance of the accuracy of these quantities when performing calculations including the electronic lifetimes due to electron-phonon scattering.


5:06PM H22.00012: Evidence for the weak coupling scenario of the Peierls transition in the blue bronze K0.3MoO3* BOGDAN GUSTER, MIGUEL PRUNEDA, PABLO ORDEJON (Presenter), Catalan Institute of Nanoscience and Nanotechnology, ENRIC CANADELL, ICMAB-CSIC, JEAN-PAUL POUGET, Laboratoire de Physique des Solides, Université de Paris-Sud — In this work we confirm the interband nesting mechanism for the Charge Density Wave in the blue bronze K0.3MoO3 by a direct calculation of the Lindhard function using the DFT band structure [1]. Furthermore, our calculation of the thermal dependence of the Lindhard function allows to quantitatively account for the standard weak coupling scenario of the Peierls transition. To the best of our knowledge, this type of validation of the weak coupling scenario based on actual data for a real material has never been reported in the literature [2].


*Work supported by European Union H2020-EINFRA-5-2015 MaX Center of Excellence (Grant No.824143) and Spanish MINECO (Granta No. FIS2015-64886-C5-3-P and FIS2015-64886-C5-4-P). Funding by the Severo Ochoa Centers of Excellence Program under Grants SEV-2013-0295 and SEV-2015-0496, and by Generalitat de Catalunya (Grant 2017SGR1506) is also acknowledged. ICN2 is funded by the CERCA Program/Generalitat de Catalunya.
A model to incorporate electron-phonon coupling into classical molecular dynamics

ARTUR TAMM (Presenter), Quantum Simulations Group, Lawrence Livermore National Laboratory, MAGDALENA CARO, Department of Mechanical Engineering, Virginia Polytechnic Institute, ALFREDO CARO, Virginia Science and Technology Center, George Washington University, ALFREDO A. CORREA, Quantum Simulations Group, Lawrence Livermore National Laboratory — We have developed a new model to incorporate equilibration of ions and electrons at the corresponding timescales into classical molecular dynamics (MD) simulations. The model is based on Langevin dynamics where the stochastic description does not generate any linear momentum nor torque in the system. This is achieved by introducing spatial correlations into friction and random forces which have a range described by atomic electron density.

All the model parameters can be described fully by using results from first principles realtime time-dependent density functional theory calculations. We use this model to study the phonon lifetimes due to electron-phonon coupling in classical MD simulations in large and complex systems. Particularly, our model is able to capture the wavevector and polarization dependence of phonon lifetimes in qualitatively good agreement with more exact methods.

Finally, we apply the model to study the laser heating of a material similar to pump-probe laser experiments. In conclusion, this model should be used to study the dynamics of any metallic system where the electronic and lattice temperatures diverge due to fast phenomena, like, radiation damage, laser-material interaction, and compressions shocks.

Tuesday, March 5, 2019 2:30 PM - 5:06 PM

Session H23 GMED: Physics in Medicine: Imaging, Therapy, and Disruptions on the Horizon

BCEC 158 - Thomas Bortfeld, Harvard Medical School - Tag(s): Focus

Magnetic Resonance Relaxometry and Macromolecular Mapping: An Inverse Problem Framework, with Applications to Alzheimer's Disease and Osteoarthritis

RICHARD G SPENCER (Presenter), Magnetic Resonance Imaging and Spectroscopy Section, National Institute on Aging, National Institutes of Health — Quantification of changes in the macromolecular constituents of tissue is a major theme in biomedical magnetic resonance (MR). In many cases, constituents can only be distinguished through their differing water transverse relaxation times, instead of by frequency differences as is more familiar in MR spectroscopy. However, this requires implementation of multiexponential transverse relaxation analysis (METRA), a special case of the inverse Laplace transform, a notoriously ill-posed and unstable inverse problem. Our work in this area combines basic science studies with methodologies that carry immediate translational potential. We will discuss METRA as a means to quantify the myelin water fraction (MWF) of total brain water as a marker for myelin, a critical element of signal transmission within the central nervous system, in the mathematical setting of a linear inverse problem. In addition, we have stabilized MWF estimates using a rapid steady-state MR pulse sequence through Bayesian analysis of the corresponding non-linear inverse problem. With this, we provide the first report of myelination deficits using direct MWF measurements in subjects with mild cognitive impairment and Alzheimer's disease. We have implemented similar methods to map cartilage proteoglycan, the macromolecule most vulnerable to loss in osteoarthritis, obtaining results indicating the potential for improved detection of this condition. Finally, we describe extensions of METRA to higher dimensional experiments, with two or more independent time variables. We discuss the stability of parameter estimates from these experiments, as well as correlation experiments providing insight into chemical exchange between macromolecular constituents. All of these studies are directed toward the clinical goal of improving the ability of MR to diagnose pathology and monitor disease progression, and to define therapeutic targets for treatment.

*Prepared by LLNL under Contract DE-AC52-07NA27344.

*Intramural Research Program, National Institute on Aging, NIH
3:06PM H23.00002: Fractional Anisotropy by DTI in Patients with Myotonic Distrophy Type I*  
MARGARITA LOPEZ (Presenter), Instituto de Neuroetología, Universidad Veracruzana, ROSALINDA DÍAZ, CARLOS HERNÁNDEZ, Facultad de Medicina, Universidad Nacional Autónoma de México, JONHATAN MAGAÑA, Instituto Nacional de Rehabilitación, JUAN FERNÁNDEZ, Instituto de Neuroetología, Universidad Veracruzana — Myotonic Distrophy Type I (DM1) is a neurodegenerative and hereditary disorder; its more typical symptoms are muscle weakness and hypotonia, which may lead to several complications like respiratory failure and cardiac arrest. The aim of this study is to find biomarkers that help us to characterize the evolution of this disorder related to white matter. In the present work 74 volunteer participants (37 DM1 patients and 37 healthy control subjects) were matched by age, gender and level education, then underwent an MRI session in a 3T Philips Ingenia scanner with 32 channel head sense coil. Diffusion Tensor Images (DTI) were acquired with 33 diffusion direction (64 axial slices with spatial resolution of 3mmx3mmx3mm). The image post-processing analysis was done with specialized software FSL 5.0.8. The DTIs were reoriented to the standard space, then artifact corrected and the Fractional Anisotropy maps was obtained. For the statistical analysis a t-test for unpaired samples was applied.

*We want to thank to CONACYT a JFR N°220871 and DGAPA-PAPIIT IN 214716 a JFR.

3:18PM H23.00003: Stability of Parameter Estimates from Multieponential Decay in MR Relaxometry and Related Experiments in One, Two, and Three Dimensions*  
RICHARD G SPENCER (Presenter), MUSTAPHA M BOUHRARA, National Institute on Aging, National Institutes of Health — Analysis of one-dimensional (1D) multieponential decay has remained a topic of active research for over 200 years. This attests to the ubiquity of such signals as well as the difficulty in deriving parameters of the underlying monoexponential decays. However, we have shown in the context of nuclear magnetic resonance (NMR) relaxometry that parameter estimates derived from two-dimensional (2D) exponential decays, with two distinct time variables, exhibit substantially greater accuracy than those obtained from analysis of 1D data with a single time variable [1]. Here, we present statistical underpinnings of this remarkable fact and indicate applications in 2D NMR relaxometry and related experiments. These may be constructed, for example, as T1-T2 experiments correlating longitudinal (T1) and transverse (T2) relaxation times or as T2-diffusion (T2-D) correlation experiments. These results are readily generalizable to higher dimensions and may provide a means of circumventing conventional limits on multieponential parameter estimation.


*Intramural Research Program, National Institute on Aging, NIH

3:30PM H23.00004: Mote-carlo simulation to reduce sensor dimension of EEG neurofeedback device*  
PRASANTA PAL (Presenter), Radiology, University of Massachusetts Medical School, DANIEL L. THEISEN, MICHAEL DATKO, Center for Mindfulness, University of Massachusetts Medical School, REMKO V LUTTERVELD, ALEXANDRA ROY, JUDSON BREWER, Center for Mindfulness, Brown University — Neuro-feedback (NF) training using EEG device is finding wide acceptance for treatment of ADHD, epilepsy, anxiety, dyslexia, schizophrenia etc. In realistic clinical practice, high quality delivery of NF signal is possible only with high sensor density devices. Unfortunately, these are often cost-prohibitive, time consuming and unmanageable due to large number of sensors. So, reduction of sensor dimension without compromising the quality of the signal is an important clinical problem.

On the contrary, inexpensive low density devices lacks clinical precision. This can be solved by generating reduced dimension sensor configuration by Monte Carlo (MC) sampling of high-quality data. In our experiment, high quality EEG data was collected from NF sessions with 72 subjects. MC sampling of all possible 32 configurations were used to generate a targeted set of montages to produce NF source signal equivalent to those from the original high-density configuration.

We found a large pool of potential montage configurations with only 32 sensors that can reproduce results from high density sensor system with more than 80%. Thus, MC sampling can be utilized to design low cost clinical grade EEG devices without compromising the quality.

*Fetzer trust
LUKE D’IMPERIO (Presenter), JUAN M. MERLO, CHAOBIN YANG, YITZI M CALM, Physics, Boston College, MEGI MACI, Biology, Boston College, MICHAEL J BURNS, Physics, Boston College, TIMOTHY CONNOLLY, THOMAS C CHILES, Biology, Boston College, MICHAEL J NAUGHTON, Physics, Boston College — Diagnostic tools e.g., those used in the biomedical field, have greatly benefited from taking advantage of the properties of plasmonic phenomena in micro- and nano-scale thin films and structures [1]. Here, we discuss the considerations involved in the design and fabrication of a previously reported plasmonic microstructure towards the goal of sensitive detection of disease biomarkers [2]. We show current fabrication results and motivate relevant processes, parameters and materials therein. We describe our measurement setup and provide comparison to a commercially available system, particularly to motivate how our device can extend existing detection tools to point-of-care applications. We introduce preliminary device responses and our approaches to current obstacles of the project.

[3] The authors thank Dr. Fan Ye and Steve Shepard for beneficial communications.

*M. MILANIC (Presenter), JOST STERGAR, LUKA ROGELJ, ROK DOLENEC, MARTIN HORVAT, University of Ljubljana — Hyperspectral imaging (HIS) is an optical technique providing both spectral and spatial information in one measurement. A big challenge in the medical HIS (diagnostics and surgery) is effective processing of a huge amount of data and extraction of relevant parameters.

An analytical solution of the 2D radiative transfer equation (RTE) was derived for a multi layered biological tissue. The solution represents reflectance from the tissue surface. Each tissue layer was specified by a set of optical properties including refractive index. The solution served as an azimuthal single scattering approximate inverse light transport model for analyzing HSI.

Hyperspectral images of a human forearm were recorded in the 400–1000 nm spectral range. A cuff test was performed to simulate hypo-, hyper- and normoxia of the skin. The inverse RTE was used to determine physiological parameters of the skin (e.g., oxygenation, hemoglobin concentration). A good agreement with the parameters reported in the literature was obtained.

The RTE solutions can be effectively used to analyze medical HIS. The RTE is as accurate but significantly less computationally demanding as the alternative Monte Carlo approach.

*ARRS grants P1-0389 and J2-8171.

LJUBICA PETROVIC (Presenter), University of Massachusetts Boston — This study uses a 3D cell culture approach to study the impact of gold nanoparticles (GNP) uptake and localization on radiation dose enhancement, as well as on combined photodynamic (PDT)/photothermal treatment (PTT). The use of 3D cell cultures reveals that GNP resides in the extracellular matrix (ECM) for surprisingly long durations after initial delivery and prior to localization in tumor nodules, an effect which, as it will be shown here, has a big impact on the treatment outcomes for nanoparticle-aided therapy.

Here we show that heavy metal such as gold in a form of gold nanorods (GNRs) influences PDT outcome. GNRs were used to excite surface plasmon resonance (SPR) and consequently, to induce heat via PTT, which combined with PDT raises treatment response. It turned out that presence of GNRs does enhance PDT outcome, not via thermal effect, but rather because of gold photochemistry and the appearance of the heavy atom effect\(^1\), which efficiency depends on the amount of GNRs present in the 3D cancer nodule itself.

In combined x-ray/GNP treatment, GNPs act as a source of short-range secondary radiation effects\(^2\), where disproportionate accumulation of GNP in ECM significantly reduces radiation response in 3D tumor spheroids.

MRI-guided focal proton radiation therapy for locally advanced prostate cancer  MARYAM MOTEABBED (Presenter), Radiation Oncology, Massachusetts General Hospital, MUKEH HARISINGHANI, Radiology, Massachusetts General Hospital, JASON A EFSTATHIOU, HSIAO-MING LU, Radiation Oncology, Massachusetts General Hospital — We investigate the dosimetric efficacy and clinical implications of proton radiation therapy of prostate cancer with dose microboost to the MRI-defined dominant intraprostatic lesions (DIL).

For 6 patients with high-risk prostate cancer, DILs were delineated using multiparametric MRI based on hypointense appearance on T2-weighted and apparent diffusion coefficient maps. After transferring the contours to CT via image registration, conventional and boosted pencil beam scanning proton treatment plans were created. Dose-volume histograms were analyzed. Tumor control probability (TCP) and normal tissue complication probability (NTCP) were compared between the two scenarios.

In all cases the addition of up to 60% (of prescribed dose) boost to the DILs was achievable without violating the organs at risk (OAR) planning constraints. The increase in OAR mean dose was within 1.5 Gy, and all volume indices remained within clinical tolerance for all cases. TCP of DILs increased by at least 59% depending on the boost amount and model parameters. Bladder and rectum NTCP increase remained negligible.

Proton therapy of high-risk prostate cancer with MRI-guided focal boost to highly malignant DILs is feasible and could yield significant improvement in treatment outcome without increasing toxicities.

Radiation cabinet to study the effect of Low-dose radiation on cells  BISHWAMBHAR SENGUPTA (Presenter), DONALD MEDLIN, XIAORAN ZHENG, ENDRE TAKACS, Clemson University — Exposure to ionizing radiation comes from many sources: medical imaging, radiotherapy, nuclear fallout, and natural or background radiation. However, the biological effects of ionizing radiation can be paradoxical. In fact, the current radiation risk assessment model - the Linear No Threshold model - has been challenged by recent research that shows evidence of radiation hormesis at low-doses. To better understand the biological effects of radiation the primary aim of our research group is to study the effects of low-dose, well-characterized radiation on various cell cultures. The biological effects of irradiations vary with radiation type, energy, total dose delivered and dose rate; however, most research in this field is focused only on the total dose, and thus most irradiators used are not well characterized. The goal of this study was to develop a spectrally and dosimetrically well-characterized X-ray irradiation cabinet to explore the relationships of these variables and their biological effects in a systematic manner. Here we report the overall design, hardware used, calibration methods, and the dose calculation methods used for this study.

A new entropic algorithm to measure of the impact of magnetic field on dose distribution: application to MRI-guided radiotherapy*  JEAN-LUC FEUGEAS (Presenter), CELIA, Université de Bordeaux — Purpose - The integration of magnetic resonance imaging, providing an efficient soft-tissue contrast opens real perspective for a better radiotherapy-based treatment. However, the magnetic fields will modify the localization of radiation dose always induced by charged particles. The fast development of these new facilities is one of the recent challenges for the next generation of treatment planning softwares.

Material and methods - Our theoretical physics group proposes a direct resolution of linear Boltzmann transport equation thanks to an angular momentum closure based on the principle of entropy maximization [1,2,3,4]. This algorithm, originally developed for the energetic particle transport in magnetized plasmas, is perfectly suited for modeling dose deposition for MRI-guided radiotherapy [3,4].

Results - We confirm the ability of our entropic closure to take efficiently into account magnetic effects on dose deposition for complex realistic geometries [3,4].

References

*Aquitaine Regional Council and the European Fund for the Regional Development supports.
**4:54PM H23.00011: A Vector-Space Representation of Cytoskeletal Drug Mechanisms for Intracellular Doppler Spectroscopy**  
ZHE LI (Presenter), Department of Physics and Astronomy, Purdue University, JOHN TUREK, Department of Basic Medical Sciences, Purdue University, DAVID NOLTE, Department of Physics and Astronomy, Purdue University — Biodynamic imaging is sensitive to intracellular transport and has been successfully used to profile drug effects in 3-D cell culture. We report the use of biodynamic imaging to provide phenotypic profiles of cytoskeletal drugs that have a wide range of mechanisms of action (MoA). These profiles serve as “fingerprints” of the drug MoA and can be queried by machine learning clustering algorithms. In this study, 7 cytoskeletal drugs are used, including cytochalasins and latrunculin that inhibit the polymerization of actin, jasplakinolide that enhances actin polymerization, colchicine and nocodazole that inhibit microtubule polymerization, and taxanes that stabilize microtubules. In contrast, blebbistatin is a molecular motor inhibitor that inhibits ATPase activity. Biodynamic imaging is sensitive to subtle changes in intracellular motion, and drugs that affect the cytoskeleton are particularly strong inducers of biodynamic fingerprints. Biodynamic imaging uses short-coherence digital holography to profile cytoskeletal drug responses of 3D cultured tumor spheroids. Drug responses and their relations are examined in a high-dimensional space spanned by vectors of biomarkers and related with their mechanism of actions and targeted cytoskeletal components.

**Tuesday, March 5, 2019 2:30 PM - 5:30 PM**

**Session H24 DAMOP DCMP: Non-Equilibrium Physics in AMO Systems II**  
BCEC 159 - Johannes Motruk, Lawrence Berkeley National Laboratory - Tag(s): Focus

**2:30PM H24.00001: Phonon excitations in a one dimensional Bose gas**  
FEDERICA CATALDINI (Presenter), BERNHARD RAUER, THOMAS SCHWEIGLER, SICONG JI, MOHAMMADAMIN TAJIK, JOAO SABINO, JOERG SCHMIEDMAYER, Technical University of Vienna — Cold atomic gases provide a powerful tool to investigate quantum many-body systems [1]. Phonons, which are low-energy collective excitations for one dimensional superfluids, play a major role in the relaxation dynamics of such systems. It has been shown that mechanisms of phonon dephasing and rephasing generate, respectively, losses and recurrences of coherence in a quantum isolated system, and that the long time behavior of the system itself is determined by the spectrum of the phononic modes [2]. In our experiment we are able to excite and detect phonon modes individually and to monitor them over time.

Our system consists in a 1D BEC of $^{87}$Rb atoms confined in a box trap, which provides a dispersion relation where the phonon energies are commensurate. We implement a shaking process that modulates the box walls symmetrically at a fixed frequency. The density profile of the cloud can be obtained via absorption imaging at different times. Doing so, we are able to investigate, within a reasonably broad range of frequencies, the growth of the lower symmetric modes when the system is excited, and their subsequent evolution and damping after the end of the shaking.


*FWF, CoQuS, VCQ*

**2:42PM H24.00002: Exact strong-ETH violating eigenstates and quasiparticle descriptions of many-body scar states in the Rydberg-blockaded atom chain**  
CHENG-JU LIN (Presenter), OLEXEI I MOTRUNICH, Caltech — A recent experiment in the Rydberg atom chain observed unusual oscillatory quench dynamics with a period-2 charge density wave initial state (Z2 state), and theoretical works identified a set of many-body “scar states” in the Hamiltonian as potentially responsible for the atypical dynamics. In the same nonintegrable Hamiltonian, we discover several eigenstates at infinite temperature that can be represented exactly as matrix product states with finite bond dimension, for both periodic boundary conditions (two exact $E = 0$ states) and open boundary conditions (two $E = 0$ states and one each $E = \pm \sqrt{2}$). This discovery explicitly demonstrates violation of strong eigenstate thermalization hypothesis in this model. These states show signatures of translational symmetry breaking with period-2 bond-centered pattern, despite being in 1d at infinite temperature. We show that the whole tower of Z2 many-body scar states can be excellently approximated as single or multiple “quasiparticle excitations” on top of our exact $E = 0$ states, and propose a quasiparticle explanation of the strong oscillations observed in experiments. We also discuss the possibility of similar construction for Z3 many-body scar states relevant for quench with period-3 CDW initial state.
2:54PM H24.00003: Observation of Non-Gaussian Statistics and Levy Flights in Nitrogen Vacancy Centers*  DAVID LEVONIAN (Presenter), Harvard University, MICHAEL L GOLDMAN, Physics, University of Maryland College Park, KRISTIAAN DE GREVE, SUSANNE F YELIN, MIKHAIL LUKIN, Harvard University — A nitrogen-vacancy center can be used as a probe of the interacting 13C nuclear spins in a diamond crystal. Under the right conditions, its behavior can be described as a random walk with step sizes drawn from a distribution without a well-defined mean or standard deviation. Its behavior is then described by Levy statistics, providing an opportunity to study Levy statistics in a well understood system.

*DL acknowledges support by the National Defense Science and Engineering Fellowship

3:06PM H24.00004: Detection of quantum phases via out-of-time-order correlators  CEREN DAG (Presenter), KAI SUN, Physics Department, University of Michigan, LUMING DUAN, Center for Quantum Information, IIIS, Tsinghua University — We elucidate the relation between out-of-time-order correlators (OTOCs) and phase transitions via analytically studying the OTOC dynamics both in non-degenerate and degenerate spectra. Our method indicates that for a wide variety of quantum phase transitions, OTOCs can directly characterize various quantum phases as well as their symmetry breaking patterns. Key ingredients about how to utilize OTOC to detect and characterize a quantum phase transition are presented. We further discuss how our method could be useful to understand the dynamical features of the OTOCs.

3:18PM H24.00005: Beyond Bose Fireworks: Stimulated Emission of Exotic Shaken Condensates  HAN FU (Presenter), JOOHEON YOO, LEI FENG, CHENG CHIN, KATHRYN LEVIN, University of Chicago — Periodic modulation of the two-body interaction in a Bose condensate has led to the interesting observation of “Bose fireworks” [Nature 551, 356–359 (2017)]; these were later shown to be well captured by our time-dependent Gross-Pitaevskii simulations [prXiv:1807.08781]. The promise of these experiments is that this stimulated emission may, through the process of parametric amplification, make it possible to unravel the structure (i.e., wavefunction amplitude and phase) of an unknown condensate. We seek to fulfill this promise by presenting numerical simulations of analogous fireworks patterns in more complex systems. We consider single and multiple imprinted vortices (giving rise to "chiral jets") as well as more exotic states. Using the far-field jets to reveal the character of the initial condensate is reminiscent of established procedures in particle physics and we address how this expertise can be exploited.

3:30PM H24.00006: Dynamical critical behavior of long-range spin models  PARAJ TITUM (Presenter), Joint Quantum Institute/ NIST University of Maryland, College Park, MOHAMMAD MAGHREBI, Michigan State University — Long range interacting spin models exhibit a variety of order-to-disorder phase transitions. We consider prototypical long-range spins models, and investigate dynamical properties of the order parameter as well as entanglement after a sudden quench in the Hamiltonian. The quench dynamics is studied through a combination of exact numerics and analytical calculations. We show that, depending on the nature of quench, different dynamical critical behavior arises. Specifically, we identify regimes when the stationary state at long times exhibits a non-thermal scaling behavior, and describe the signatures in the entanglement. Our results are amenable to realization in experiments with trapped-ion experiments where long-range interactions naturally arise.

3:42PM H24.00007: Floquet resonances from integrability: Spin polarization in a driven central spin model*  PIETER W. CLAEYS (Presenter), Boston University, STIJN DE BAERDEMACKER, Ghent University, JEAN-SEBASTIEN CAUX, University of Amsterdam — Adiabatically varying the driving frequency of a periodically driven many-body quantum system can induce controlled transitions between resonant eigenstates of the time-averaged Hamiltonian, corresponding to adiabatic transitions in the Floquet spectrum and presenting a general tool in quantum many-body control. Using the central spin model as an application, we show how such controlled driving processes can lead to a polarization-based decoupling of the central spin from the decoherence-inducing environment at resonance. While it is generally impossible to obtain the exact Floquet Hamiltonian in driven interacting systems, we exploit the integrability of the central spin model to show how techniques from quantum quenches can be used to explicitly construct the Floquet Hamiltonian in a restricted many-body basis and model Floquet resonances.

*P.W.C. gratefully acknowledges a Francqui Foundation Fellowship from the Belgian American Educational Foundation.
3:54PM H24.00008: Floquet-Induced Superfluidity with Periodically Modulated Interactions of Two-Species Hardcore Bosons in a One-dimensional Optical Lattice* SHIJIE HU (Presenter), Physics Department, Univ. Kaiserslautern, TAO WANG, School of Science, Wuhan Institute of Technology, SEBASTIAN EGGERT, AXEL PELSTER, Physics Department, Univ. Kaiserslautern, XUEFENG ZHANG, Department of Physics, Chongqing University — We consider two species of hard-core bosons in a one-dimensional optical lattice with periodically modulated repulsive interactions. Using Floquet theory the periodic can be mapped to an effective Hamiltonian for high frequencies, which is described by a static interaction and hopping parameters that depend on the local densities. In particular, if the density difference of one species is non-zero on neighboring sites, the effective hopping of the other species is reduced and can even take on negative values. Using a combination of analytic calculations and different numerical simulations we establish the full quantum phase diagram for half-integer filling for this system. The density-dependent reduction of hopping drives a quantum phase transition into a superfluid phase. For negative hopping a previously unknown state is found, where one species induces a gauge phase of the other species, which leads to a new superfluid phase. The corresponding experimental signatures in time-of-flight experiments are calculated and show characteristic signatures of the different phases.

*This research was supported by the Special Foundation from NSFC (No 11647165), by the Nachwuchsring of the TU Kaiserslautern, by the German Research Foundation (DFG) via SFB/TR49 and SFB/TR185 (OSCAR).

4:06PM H24.00009: Analysis of weakly-driven multi-emitter cQED systems* RAHUL TRIVEDI (Presenter), MARINA RADULASKI, KEVIN A FISCHER, JELENA VUCKOVIC, SHANHUI FAN, E. L. Ginzton Laboratory, Stanford University — In this work, we show that a weakly driven multi-emitter cQED system can be analyzed by approximating the driving coherent state with a single- and two-photon Fock state, and using the Scattering matrix formalism to analyze the response of this system to these Fock states. This is a significantly more computationally feasible approach than the master equation formalism, allowing the analysis of multi-emitter systems with ~50 emitters. We use this approach to analyze the transmission and second order correlations induced in the incident coherent state by the multi-emitter system. In particular, we show that for identical emitters, increasing the number of emitters does not improve the polaritonic photon blockade. Moreover, we analyze the impact of inhomogeneous broadening on the second order correlation function of the light emitted by the multi-emitter system with large number of emitters, and analyze the emergence and behaviour of subradiant photon blockade in such multi-emitter systems.

*We gratefully acknowledge financial support from the Air Force Office of Scientific Research (AFOSR) MURI Center for Quantum Metaphotonics and Metamaterials. RT acknowledges support from Kailath Stanford Graduate Fellowship.

4:18PM H24.00010: The Density Matrix Renormalization Group for Periodically Driven Many-Body Systems SHAON SAHOO (Presenter), IMKE SCHNEIDER, SEBASTIAN EGGERT, University of Kaiserslautern — Driving a quantum system periodically in time can profoundly alter its long-time dynamics and trigger exotic quantum states of matter. We propose a new DMRG method which directly deals with the Fourier components of the eigenstates of a periodically driven system using Floquet theory. With this new method we can go beyond effective Hamiltonians and take into account higher Floquet modes. Numerical results are presented for the isotropic Heisenberg antiferromagnetic spin-1/2 chain under both local (edge) and global driving for energies, spin-spin correlation and temporal fluctuations. As the frequency is lowered, the spin system enters into a Floquet regime with a coherent exciations of a large number of Floquet modes, which shows characteristic quantum correlations that cannot be described by any effective static model.

4:30PM H24.00011: Effective Cross Section Enhancement from Embedded Atomic Lattice Impurities* TAYLOR PATTI (Presenter), DOMINIK S WILD, EPHRAIM SHAHMOON, MIKHAIL LUKIN, SUSANNE F YELIN, Physics, Harvard University — Atoms arranged in a two-dimensional lattice strongly interact with light via collective excitations. Such lattices can be supplemented with impurity atoms which couple to the collective array modes and permit the manipulation of emission properties. In particular, the combination of strong array-light coupling and large impurity atom non-linearity enable highly nonlinear responses to collimated, far-field radiation. We explore the effective enhancement of impurity cross section which results from this coupling in a variety of lattice potentials and parameter regimes. Higher-order photon correlations are calculated and pertinent extensions, such as long-lived photon bound states and multi-impurity systems, are discussed.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE1745303.
**4:42PM H24.00012: Scrambling dynamics across a thermalization-localization quantum phase transition**

SUBHAYAN SAHU (Presenter), SHENGLONG XU, Condensed Matter Theory Center and Department of Physics, University of Maryland, College Park, BRIAN SWINGLE, Condensed Matter Theory Center, Maryland Center for Fundamental Physics, Joint Center for Quantum Information and Computer Science, and Department of Physics, University of Maryland — We study quantum information scrambling, specifically the growth of Heisenberg operators, in large disordered spin chains using matrix product operator dynamics to scan across the thermalization-localization quantum phase transition. We observe ballistic operator growth for weak disorder, and a sharp transition to a phase with sub-ballistic operator spreading. The critical disorder strength for the ballistic to sub-ballistic transition is well below the many body localization phase transition, as determined from finite size scaling of energy eigenstate entanglement entropy in small chains. In contrast, at the eigenstate localization transition, the operator dynamics changes from a power-law behaviour to logarithmic, which is hard to detect from our numerics. These data are discussed in the context of a universal form for the growing operator shape and substantiated with a simple phenomenological model of rare regions.

*This material is based on work supported by the Simons Foundation via the It From Qubit Collaboration, by the Air Force Office of Scientific Research (FA9550-17-1-0180), and by the NSF Physics Frontier Center at the Joint Quantum Institute (PHY-1430094).

**4:54PM H24.00013: Quantum Brownian motion in a quasiperiodic potential**

AARON FRIEDMAN (Presenter), Rudolf Peierls Centre for Theoretical Physics, Oxford University, ROMAIN VASSEUR, University of Massachusetts Amherst, AUSTEN LAMACRAFT, TCM Group, Cambridge University, SIDDHARTH A PARAMESWARAN, Rudolf Peierls Centre for Theoretical Physics, Oxford University — We study the behavior of a quantum particle in one dimension subject to Ohmic dissipation, moving in a bichromatic quasiperiodic potential. The bath is described by the Caldeira-Leggett model; absent the potentials, the particle-bath system resolves the Langevin equation in the classical limit. In a single-period potential, the particle undergoes a zero-temperature localization-delocalization transition as dissipation strength is decreased. We show that the delocalized phase is absent in the quasiperiodic case, even when the deviation from periodicity is infinitesimal. Using the renormalization group, we determine how the crossover time to the localized phase depends on the dissipation strength and incommensurability of the two frequencies, and from this, extract a localization length. Finally, we show that a similar problem can be realized as the strong-coupling limit of a mobile impurity moving in a periodic optical lattice and immersed in a one-dimensional Fermi or Bose gas.

**5:06PM H24.00014: Design and characterization of a quantum gas heat pump**

ARKO ROY (Presenter), DANIEL VORBERG, ANDRE ECKARDT, Quantum Chaos and Quantum Dynamics, Max Planck Institute for the Physics of Complex Systems — We propose a novel scheme for quantum heat pumps powered by weak rapid time-periodic driving that enables extraction of heat from fermionic reservoirs at finite temperatures and chemical potentials. We focus our investigation on a system consisting of two coupled driven quantum dots in contact with the reservoirs. Experimentally, such a configuration can be realized in a quantum-gas microscope. To this end, we theoretically characterize the device by describing the coupling to the reservoirs using the Floquet-Born-Markov approximation. For weak driving, we reveal that an optimal temperature and chemical potential difference between the two reservoirs facilitates the working of the heat-pump with minimal particle loss in the reservoirs. Furthermore we show that for strong driving, the device departs away from working as a heat-pump. The genesis lies in the coupling of the higher energy Floquet states with the reservoir energy states. Finally, we discuss the optimal system parameters in which the proposed heat-pump is most useful for refrigeration. That is, one can attain temperature as low as ~0.05 T_F. With the aid of two such pumps combined in series, the minimum temperature that could be achieved is ~0.01 T_F.
5:18PM H24.00015: Memories of Initial States in the Dynamics of Disordered Systems*  
AHANA CHAKRABORTY (Presenter), Department of Theoretical Physics, Tata Institute of Fundamental Research, India, PRANAY GORANTLA, Department of Physics, Princeton University, New Jersey, USA, RAJDEEP SENSARMA, Department of Theoretical Physics, Tata Institute of Fundamental Research, India — We consider the dynamics of a one dimensional closed disordered system of non-interacting bosons/fermions which is initialized to a Fock state with a pattern of 0 and 1 particles on alternating sites. We show that in the long time limit, the imbalance between the densities in the two sublattices reach a finite value in the localized phase given by, $I(\infty) = \tanh \left( \frac{1}{2} \xi \right)$, where $\xi$ is the localization length. For a chain with random potential disorder, the imbalance is finite for any disorder, whereas for the Aubrey Andre model, it shows a localization-delocalization transition. For a modified Aubrey Andre model, the imbalance as a function of the disorder shows a kink when the mobility edge first appears. We find that in this case, $I(\infty) = \sum_i \tanh \left( \frac{1}{2} \xi_i \right)$, where $\xi_i$ is the localization length corresponding to each of the three bands in the model. Our work relates experimentally measurable non-equilibrium quantities in these systems to the localization length and hence shows a new method for extracting the localization length in these systems.

* TIFR Computational Facility

Tuesday, March 5, 2019 2:30 PM - 5:06 PM

Session H25 DAMOP: Trapped Ions and Polaritons

2:30PM H25.00001: Electric-field noise from thermally-activated fluctuators in a surface ion trap*  
MAYA BERLIN-UDI (Presenter), CRYSTAL NOEL, CLEMENS MATTHIESEN, University of California, Berkeley, VINCENZO LORDI, Lawrence Livermore National Laboratory, HARTMUT HAEFFNER, University of California, Berkeley — Electric-field noise originating from surfaces is a major source of motional decoherence in ion trap chips. A better understanding of this noise is important for the fabrication of low-noise quantum devices. We probe electric-field noise near the aluminum-copper surface of an ion trap chip in a previously unexplored high-temperature regime. A saturation of the noise amplitude occurs around 500 K, which, together with a small change in the frequency scaling, points to thermally activated two-state fluctuators as the origin of the noise. We find intriguing similarities in the distribution of activation energies extracted from our data and corresponding data from resistance fluctuation measurements for polycrystalline aluminum films. These similarities suggest atomic motion as a relevant microscopic mechanism, likely taking place at the metal trap surface.

* NSF, Lawrence Livermore National Laboratory, ONR

2:42PM H25.00002: An Ion-trap Collider: Entangling Distant Atomic Ions by Direct Collisions  
LINGZHEN GUO (Presenter), Max Planck Institute for the Science of Light (MPL), PENGFEI LIANG, Department of Physics, Beijing Normal University (BNU) — We propose a novel scheme to entangle two atomic ions in linear Paul traps. The two traps are designed capable of merging into one single trap allowing two ions to be accelerated and collide periodically in the trap, which we call the Ion-trap Collider. We show that the direct collisions of two ions induce an effective spin-spin interaction due to the exchange effect, which decreases with the third power of the two ions’ trapping distance instead of the conventional exponential behaviour of static exchange interaction. The collision-induced spin-spin interaction is about 9 orders of magnitude stronger than the direct spin-spin interaction through the magnetic dipole-dipole coupling. It possible to generate entangled pairs of atomic ions with very large distance for quantum information processing, and realize universal two-qubit square root of SWAP gate for quantum computing.

2:54PM H25.00003: Zero-temperature properties of the long-range transverse-field Ising model on the triangular lattice  
JAMES GARRISON (Presenter), KEVIN WANG, ALEXEY V GORSHKOV, Joint Quantum Institute and Joint Center for Quantum Information and Computer Science, NIST/University of Maryland — We investigate the ground state properties of the transverse-field Ising model with long-range, antiferromagnetic interactions on the triangular lattice. Our study is motivated by experiments on trapped beryllium ions, where the ions form a 2D Wigner crystal with tunable $1/r^\alpha$ Ising interactions in the range $0 \leq \alpha \leq 3$, where $r$ is the distance between two spins. Our results are obtained using a projector variant of the stochastic series expansion (SSE) Monte Carlo method, which allows direct access to ground state properties throughout the phase diagram.
1.3 x 10^5 A m^{-2} sr^{-1} eV^{-1} and a maximum continuous current of 1.16 ± 0.06 nA. These values significantly surpass previous present the design and detailed characterization of 7Li magneto-optical trap ion source (MOTIS) with a peak brightness of.

High-field photoionization of Beryllium using a low-cost solid-state laser*

Portables quantum technologies based on trapped ions. Development of an ultranarrow laser compatible with integrated photonic resonators is a key part of the design of future suppress temperature fluctuation of the central frequency of the fiber resonator to enable precise control of ions. The to achieve lasing at a linewidth comparable to that of a ULE cavity-stabilized laser. Additionally, we apply a novel technique scattering (SBS) nonlinearity in a fiber-based cavity with a quality factor similar to those of integrated photonic resonators quality factors as high as those in ULE cavities. In this work, we demonstrate the application of the stimulated Brillouin scattering (SBS) nonlinearity in a fiber-based cavity with a quality factor similar to those of integrated photonic resonators to achieve lasing at a linewidth comparable to that of a ULE cavity-stabilized laser. Additionally, we apply a novel technique to suppress temperature fluctuation of the central frequency of the fiber resonator to enable precise control of ions. The development of an ultranarrow laser compatible with integrated photonic resonators is a key part of the design of future portable quantum technologies based on trapped ions.

Quantum Control of a Trapped Ion using a Stimulated Brillouin Scattering Laser JULES STUART (Presenter), Massachusetts Institute of Technology, WILLIAM LOH, COLIN BRUZEWICZ, ROBERT MCCONNELL, ROBERT NIFFENEGGER, MIT Lincoln Laboratory, GAVIN WEST, GARRETT SIMON, Massachusetts Institute of Technology, JEREMY SAGE, JOHN CHIAVERINI, MIT Lincoln Laboratory — Trapped ions are natural qubit candidates for quantum information processors and sensors, but high-fidelity quantum operations require high quality laser oscillators. In typical trapped-ion experiments, high finesse, free-space optical cavities made of ultralow expansion (ULE) glass are used to reduce the emission linewidth of commercial lasers to the level of the ion's natural linewidth. Integration of these narrow laser systems into compact or scalable platforms presents a challenge, since it is not currently possible to fabricate integrated photonic resonators with quality factors as high as those in ULE cavities. In this work, we demonstrate the application of the stimulated Brillouin scattering (SBS) nonlinearity in a fiber-based cavity with a quality factor similar to those of integrated photonic resonators to achieve lasing at a linewidth comparable to that of a ULE cavity-stabilized laser. Additionally, we apply a novel technique to suppress temperature fluctuation of the central frequency of the fiber resonator to enable precise control of ions. The development of an ultranarrow laser compatible with integrated photonic resonators is a key part of the design of future portable quantum technologies based on trapped ions.

High-field photoionization of Beryllium using a low-cost solid-state laser* ROBERT WOLF (Presenter), CHRISTIAN MARCINIAK, MICHAEL JORDAN BIERCUK, School of Physics, The University of Sydney — The generation of a pure sample of ions is a prerequisite for a variety of experiments in atomic and molecular physics, in particular using ion traps. Resonant laser photoionization has the advantage of being element and isotope selective, therefore permitting precise control of the composition of the generated ionic species. In this talk we describe experiments employing a novel system for the photoionization of Beryllium at a 2T magnetic field in a Penning trap. Our system is based on injection-locking of a low-cost, high-power multimode diode at 470nm which can then be frequency doubled to the relevant wavelength near 235nm. The optical setup and its application will be presented.

*This research was supported by the Australian Research Council Centre of Excellence for Engineered Quantum Systems (project ID CE170100009).

Characterization of a High-Brightness, Laser-Cooled Li+ Ion Source JAMIE GARDNER (Presenter), WILLIAM McGEHEE, JABEZ J MCCLELLAND, National Institute of Standards and Technology — Ion sources based on laser cooling have recently provided new pathways to high-resolution microscopy, ion milling, and ion implantation. Here, we present the design and detailed characterization of 7Li magneto-optical trap ion source (MOTIS) with a peak brightness of. 1.3 x 10^5 A m^2 sr^{-1} eV^{-1} and a maximum continuous current of 1.16 ± 0.06 nA. These values significantly surpass previous Li MOTIS performance benchmarks. Using simple models, we discuss how the performance of this system relates to fundamental operating limits. This source will support a range of projects using lithium ion beams for surface microscopy and nanostructure characterization, including Li+ implantation for studies of ionic transport in energy storage materials.
4:06PM H25.00009: Mitigation of frequency noise due to mechanical vibration in a cryogenic trapped-ion quantum processor  COLIN BRUZEWICZ (Presenter), JULES STUART, GARRETT SIMON, ROBERT NIFFENEGGER, ROBERT MCCONNELL, JEREMY SAGE, JOHN CHIAVERINI, MIT Lincoln Laboratory — Trapped-ion systems equipped with closed-cycle cryocoolers confer several cost-efficient advantages over traditional room-temperature designs. For example, operation of ion traps at cryogenic temperatures has been shown to lower rates of anomalous motional heating, a limit to multi-qubit logic fidelity, by up to two orders of magnitude. This environment also permits the use of superconducting materials to shield the ion qubits from magnetic field fluctuations. Additionally, cryopumping quickly produces ultrahigh vacuum conditions without the need for extended high-temperature chamber bakeouts, greatly reducing the cycle time of ion trap prototyping. However, mechanical vibrations caused by the cryocooler compressor can degrade quantum gate performance. Specifically, we have identified uncompensated Doppler shifts due to the relative motion of the ion with respect to the laser driving our gates as a leading source of decoherence. Here we describe the recent implementation of an interferometric stabilization scheme that actively modulates the qubit laser frequency to compensate for the motion induced by the cryocooler vibration. We observe a significant increase in the laser-ion coherence time and investigate the effect of this frequency stabilization on two-qubit gate performance.

4:18PM H25.00010: Observation of the Polariton Drag Effect*  BURCU OZDEN (Presenter), DAVID MYERS, JONATHAN BEAUMARIAGE, DAVID SNOKE, Physics, University of Pittsburgh, LOREN PFEIFFER, Physics, Princeton University, KENNETH WEST, Physics, University of Pittsburgh — In this work, we report the observation of polariton drag effect in a semiconductor structure that has been designed to maximize the light-matter coupling, the namely strong coupling of exciton-polaritons in a solid-state microcavity. We show that collisions of polaritons with the free electrons results in a change in the angle of emission of the photons from the cavity structure. The effect is asymmetric, significantly slowing down the polaritons when they move oppositely to the electrons, while the polaritons are only slightly accelerated by electrons moving in the same direction. In conclusion, we have demonstrated proof of principle that a DC current can directly alter the momentum of photons moving in the cavity; this has the direct effect of changing the angle of emission. This polariton drag effect is beam steering using a DC current to tune the angle of a light beam since the experiment is a photon-in, photon-out system.

*The work at Pittsburgh was funded by the Army Research Office (W911NF-15-1-0466). The work of sample fabrication at Princeton was funded by the Gordon and Betty Moore Foundation (GBMF-4420) and by the National Science Foundation MRSEC program through the Princeton Center for Complex Materials (DMR-0819860)

4:30PM H25.00011: Exciton-Polariton Condensate in a Ring Microcavity*  SHOUVIK MUKHERJEE (Presenter), DAVID MYERS, Physics and Astronomy, University of Pittsburgh, ROSARIA LENA, Physics and SUPA, University of Strathclyde, BURCU OZDEN, JONATHAN BEAUMARIAGE, Physics and Astronomy, University of Pittsburgh, MARK STEGER, National Renewable Energy Laboratory, ZHENG SUN, Physics and Astronomy, University of Pittsburgh, LOREN PFEIFFER, KENNETH WEST, Electrical Engineering, Princeton University, ANDREW DALEY, Physics and SUPA, University of Strathclyde, DAVID SNOKE, Physics and Astronomy, University of Pittsburgh — Ring microchannels for exciton-polaritons were created using optical photolithography followed by an inductively coupled plasma etch to pattern the top mirror of the microcavity in a ring shape. Due to the variation in the thickness of the microcavity across the ring, there was a gradient of potential energy across each ring. Polariton condensates were created by non-resonantly pumping the ring at the highest energy region using short laser pulses. A polariton condensate was formed at the location of the pump spot which flowed towards the minimum energy region. We observed natural oscillations of the condensate about this energy minimum by time resolving the photoluminescence using a streak camera. The time period of the oscillations was in good agreement with the numerical simulation of the time evolution of a wave packet in a rigid pendulum potential. A time-reversal -symmetry-broken rotational mode was also observed in the ring. The temporal oscillations in energy and density of the polaritons at a given spatial point provide a direct measurement of the exciton-exciton interaction strength (~ 5 μeV-μm²) in a GaAs quantum well.

*Authors acknowledge funding from ARO (W911NF-15-1-0466), Gordon and Betty Moore Foundation (GBMF-4420) and by the NSF MRSEC program (DMR-0819860).
The development of high-Q microcavity quantum well samples has led to long lifetime polaritons, thus allowing for long distance propagation of polaritons. However, long lifetime polaritons have very narrow line widths, as a result we can no longer resolve the polariton branches in the reflectivity spectrum of these samples. This makes accurately determining the detuning of polariton populations difficult. Accurate detuning information is essential for quantitative work involving absolute density of the polariton population. In this work, we will discuss our modern characterization techniques. We have two methods which we currently use. One method involves fitting large angle dispersion curves of the lower polariton with the theoretical predictions of a two state model. The other method involves measuring accurate dielectric functions for our materials, and then comparing experimental reflectivity data to the predictions of a transfer matrix model to determine the cavity mode. Both of these methods depend on the measurement of the rabbi splitting by photoluminescent emission scans. We found these two methods agree well with each other.

*Supported by the Army Research Office (W911NF-15-1-0466)

4:54PM H25.00013: Long-Range Exciton Transport in Microcavity Exciton-Polariton Systems*  
DAVID MYERS (Presenter), SHOUVIK MUKHERJEE, JONATHAN BEAUMARIAGE, University of Pittsburgh, MARK STEGER, National Renewable Energy Lab, LOREN PFEIFFER, KENNETH WEST, Princeton University, DAVID SNOKE, University of Pittsburgh — It has previously been assumed that the transport distance of excitons in microcavity exciton-polariton systems is limited by the bare exciton diffusion length (≤ 1 μm). In the case of non-resonant excitation, this implies that excitons created by the pump laser would be mostly confined to the pump location. While this is clearly generally true given the close similarities between the spatial pump and lower polariton potential profiles, we show that there is an important minority population of slightly polaritonic excitons that can move distances similar to those of the much more photonic polaritons (~ 30 μm). This population, which resides in the bottleneck region of the lower polariton branch, is often not detected in a typical photoluminescence experiment due to limited numerical aperture. While small in number compared to the total population of excitons, they can substantially outnumber the polaritons below the bottleneck. This has significant implications for creating potential landscapes using a non-resonant pump, and for measurements of the interaction strength between polaritons.

*This work was supported by the Army Research Office Project W911NF-15-1-0466, the Gordon and Betty Moore Foundation (GBMF-4420), and the National Science Foundation MRSEC program (DMR-1420541).

Tuesday, March 5, 2019 2:30 PM - 5:06 PM

Session H26 GIMS: Advances in Scanned Probe Microscopy II: High Frequency, and Optical and Low Temperature Measurements  
BCEC 160B - Tag(s): Focus

2:30PM H26.00001: What limits time resolution in AFM?*  
PETER GRUTTER (Presenter), McGill University — Developing a technique that combines nanometer spatial and sub-femtosecond temporal sensitivity is a crucial step towards exposing the inner mechanisms of chemical reactions, single molecule motion, electron dynamics in solids, and the effects of defects or trap states on electron motion and behavior, amongst many other questions relating to the most fundamental processes in molecular systems.

Our most recent advances in mechanically detecting ultrafast events will be presented. In particular, a non-linear optically induced polarization in a solid will directly lead to a force which can be detected by AFM with its intrinsic nanometer spatial resolution. I will show how one can mechanically measure a change in the sample response as a result of a delay time as short as 25 atto seconds between a pump and probe stimulation pulse on LiNbO3 or monolayers of MoSe2.

The realization of ultrafast AFM opens the door to understanding ultrafast electron dynamics on surfaces. As such, we are able to demonstrate that the lower limit of timing precision in mechanical detection in a pump-probe experiment is determined by the smallest detectable signal, and not, as might be expected, by the mechanical resonance frequency of the oscillator.

Work done in collaboration with Z. Schumacher, R. Rejali, R. Pachlatko, A. Spielhofer, Y. Miyahara, and D. Cooke

*Supported by NSERC, FRQNT and CFI
3:06PM H26.00002: Subsurface Second Harmonic Speckle Defect Microscopy* FARBOD SHAFIEI, The University of Texas at Austin, TOMMASO ORZALI, SEMATECH, ALEXEY VERT, P Y HUNG, SEMATECH/Sunny Polytechnic Institute, GENNADI BERSUKER, The Aerospace Corporation, MICHAEL C DOWNER (Presenter), The University of Texas at Austin — Growing crystals epitaxially over substrates is a critically important process for opto-electronic applications. Due to generally occurred atomic-level mismatches between the crystal and substrate, these semiconductor thin films are vulnerable to varieties of defects (like threading dislocation in GaAs-Si), which act as scattering sites for electrons and photons. Multi-scattering from these defects can result in the localization of the light. We demonstrate that a signature of this localization (in the case of III-V films) can be picked by a fiber scanning probe microscope in nonlinear regime. The size of these light localizations, which optically appear like speckles, have strong correlation to the density of the film dislocations. We introduce this noninvasive optical technique capable of identifying the presence of threading dislocations, their density, as well as orientation and structural arrangements of these defects.

*Welch Foundation

3:18PM H26.00003: Optical evolution of dislocation speckle imaging inside and outside of thin films* FARBOD SHAFIEI, The University of Texas at Austin, TOMMASO ORZALI (Presenter), SEMATECH, ALEXEY VERT, SEMATECH/Sunny Polytechnic Institute, MAN HOI WONG, SEMATECH, GENNADI BERSUKER, The Aerospace Corporation, MICHAEL C DOWNER, The University of Texas at Austin — We have employed a fiber scanning probe microscopy to study light localization due to multi-scattering of light by dislocation defects in III-V films (in particular, GaAs-Si). By sputtering the film down to the semiconductor-substrate interface we observe how the nonlinear optical signature of the dislocation defects changes with the increasing density of a dislocation area. The same probe microscopy approach was used to track the evolution of the propagating optical fields from these dislocation speckles, outside the thin film. Such approach can be used as an extremely high resolution monitoring tool of propagating electromagnetic fields.

*Welch Foundation

3:30PM H26.00004: Vibration measurements of a scanning SQUID microscope in a cryogen-free dilution refrigerator* DAVID LOW (Presenter), GEORGE FERGUSON, ALEXANDER B JARJOUR, RACHEL RESNICK, BRIAN SCHAEFER, ERIC N SMITH, KATJA NOWACK, Cornell University — Scanning probe microscopy is more challenging in cryogen-free systems due to vibrations introduced at the sample by the cryocooler. We built a cryogen-free scanning superconducting quantum interference device (SQUID) magnetic probe microscope operating in a cryogen-free dilution refrigerator with a base temperature of 10 mK. We report characterization of both the vibrations at the mixing chamber plate and of probe-to-sample vibrations. For the latter, we follow Schliessl et al. (Appl. Phys. Lett. 109, 232601 (2016)) and measure noise spectra at multiple locations above a sample where strong magnetic field gradients are present. This allows us to disentangle vibrations in different spatial directions. We find that the most pronounced vibrations are below 10 nm/Hz^{1/2} and occur at low harmonics of the pulse tube cycle. We will also discuss future improvements to our microscope and refrigerator that will further reduce the vibrations in our system.

*Work was supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Award DE-SC0015947 (vibration characterization, mK microscope) and by the Cornell Center of Materials Research with funding from the NSF MRSEC program under Award DMR-1719875 (microscope design).

3:42PM H26.00005: Upgrading a low-temperature scanning tunneling microscope for electron spin resonance experiments* FABIAN NATTERER (Presenter), University of Zurich, FRANÇOIS PATTHEY, TOBIAS BILGERI, PATRICK FORRESTER, NICOLAS WEISS, HARALD BRUNE, Ecole polytechnique federale de Lausanne — We describe the upgrade of a helium-3 STM to an electron spin resonance enabled apparatus [1]. We are able to transmit RF power to the tunnel junction at frequencies of up to 30 GHz. Our apparatus is benchmarked via magnetic field sweep ESR on the model system TiH/MgO/Ag(100) [2] for which we find a magnetic moment of (1.00±0.001) μB. We can chose a DC mode for regular STM operation or an ultra-fast mode for pump-probe spectroscopy or the reading of spin-states. In both modes, simultaneous radiofrequency excitation is possible, which we add via a resistive pick-off tee to the bias voltage path. We discuss our transmission, indicate potential pitfalls in the upgrade and demonstrate how to synchronize the arrival times of RF and DC pulses coming from different paths to the STM junction, a prerequisite for future pulsed ESR experiments.


*Support from the Swiss National Science Foundation under project numbers PZ00P2_167965 and 200020_176932 is appreciated.
3:54PM H26.00006: An Ultra-High Vacuum Cryogen-free Low Temperature Proximal Probe System for the Exploration of Low Dimensional Materials and Nano-devices* ANGELA COE (Presenter), GUOHONG LI, EVA ANDREI, Rutgers University, New Brunswick — We introduce a new design concept that combines into one instrument, several scanning probe microscopy modules, ultra-high vacuum, low temperature, magnetic field, and cryogen free operation. The integration of these capabilities is made possible by the realization of an ultra-compact scanning probe microscopy (SPM) head with a modular design for accommodating interchangeable probes including STM, AFM, and MFM. A novel transfer mechanism makes it possible to transfer the SPM head between various chambers of a compact UHV system for loading probes, tips, and samples. The instrument is equipped with stages for sputtering, e-beam film deposition, and exfoliation for in-situ sample preparation and tip conditioning. Following the UHV room-temperature assembly, the entire SPM with the loaded sample is transferred without breaking vacuum to a variable temperature cryogen-free cryostat and magnet. The integration of all these capabilities into one instrument enables in-situ nano-scale characterization of low dimensional systems and devices in an ultra-clean environment, and under controlled temperature and field conditions.

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

4:06PM H26.00007: Low temperature magnetic force microscope with simple design.* JEFFREY VIT (Presenter), University of Texas at Austin, KWOK-WAI NG, University of Kentucky, ALEJANDRO DE LOZANNE, University of Texas at Austin — We present a new design for a magnetic force microscope that will operate at variable temperatures down to liquid helium in fields up to 8 Tesla. As with our previous designs, the temperature/field design goals are achieved most efficiently by maintaining everything within a one-inch cylinder. [Rev. Sci. Instrum. 78, 053710 (2007)] Unlike other designs, this one has an open architecture that results in simplified machining, assembly, modification/repair, and daily operation. The new microscope has three homemade stick-slip stages that provide several millimeters of relative travel between tip and sample.

*Supported by NSF DMR-1507874

4:18PM H26.00008: Advances in SQUID-detected Magnetic Resonance Force Microscopy MARTIN DE WIT (Presenter), GESA WELKER, FREDERIK HOEKSTRA, TJERK OOSTERKAMP, Leiden University — Magnetic Resonance Force Microscopy (MRFM) is a technique that combines magnetic resonance protocols with an ultrasensitive cantilever to measure the forces exerted by extremely small numbers of spins. The fundamental limit for the sensitivity of MRFM is given by the thermal force noise, so experiments should be performed at the lowest possible temperature. For this reason, we have developed a three stage mechanical low pass filter, which combines good vibration isolation (expected attenuation > 100 dB at 100 Hz) with a high thermal conductance (cooling power 113 μW at 100 mK). The MRFM can be operated at temperatures around 20 mK thanks to a SQUID-based detection scheme and the mechanical generation of the alternating B1 fields required for the magnetic resonance. We use these technical advances to perform MRFM experiments on a thin copper film, where we obtain frequency-shift signals from the Boltzmann polarization of spins in a volume as small as (40 nm)3. We propose an experiment on a sample containing protons where magnetic resonance imaging with a voxel size < (10 nm)3 should be possible.

4:30PM H26.00009: Incommensurate surface superstructure observed on epitaxially grown Al(111) films by scanning tunneling microscopy at mK temperature SUNGMIN KIM (Presenter), JOHANNES SCHWENK, WILLIAM G CULLEN, Physical Measurement Laboratory, National Institute of Standards and Technology, YOUNG KUK, Department of Physics and Astronomy, Seoul National University, JOSEPH A STROSCIO, Physical Measurement Laboratory, National Institute of Standards and Technology — Superconducting aluminum samples are generally used as a standard reference for testing the energy resolution of cryogenic scanning tunneling microscopes operating at ultra-low temperatures by measuring its superconducting tunneling gap spectrum. However, only a few of the atomic structure of the aluminum surface have been reported in those studies because of the difficulties in preparing atomically clean surfaces due to its strong reactivity. In this presentation, we report the observation of an incommensurate superstructure on Al(111) films grown epitaxially on graphene on SiC substrates. The observed superstructure has 3-fold symmetry with a 3.3 periodicity. The superstructure closely resembles a charge density wave structure, for example, similar to that typically observed on NbSe2. We therefore speculate that possibly Al(111) may support a surface CDW at ultra-low temperatures due to same electron-phonon coupling which is responsible its superconductivity. Other possible explanations for a surface or bulk CDW phase include such soft phonons resulting from strain effects [1], which will be discussed.

4:42PM H26.00010: Photonic crystal fiber assisted nano-antenna for tip-enhanced Raman spectroscopy

KHANT MINN, BLAKE BIRMINGHAM, BRYNNA R NEFF, Department of Physics, Baylor University, MARLAN O SCULLY, The Institute for Quantum Science and Engineering, Texas A&M University, HOWARD HO WAI LEE, ZHENRONG ZHANG (Presenter), Department of Physics, Baylor University — Metallic plasmonic nano-probes can efficiently excite and detect the near-field at nanoscale for near-field imaging and sensing applications such as tip-enhanced Raman spectroscopy (TERS). In this paper, we report the design, fabrication and far-field characterization of a photonic-plasmonic probe. In our device, light in a photonic crystal fiber (PCF) couples with the surface plasmons of a nano-antenna. The needle-shaped antenna is grown by electron beam assisted chemical deposition of platinum on the PCF's end facet. Plasmonic resonance conditions can be optimized by controlling the deposition parameters, height, and base diameter of the antenna. Far field emission to the side of the probe, optical spectra and mode profiles transmitted through the probe demonstrate the excitation of surface plasmons on the antennae. The probe can be implemented into TERS setup to obtain spectroscopic information at the nanoscale.

4:54PM H26.00011: Cryogen-free variable temperature scanning SQUID microscope*

LOGAN BISHOP-VAN HORN (Presenter), ZHENG CUI, JOHN KIRTLEY, KATHRYN ANN MOLER, Stanford University — Scanning Superconducting QUantum Interference Device (SQUID) microscopy is a powerful tool for imaging local magnetic properties, but it requires a low-vibration cryogenic environment, traditionally achieved by thermal contact with a bath of liquid helium or the mixing chamber of a "wet" dilution refrigerator. We mount a SQUID microscope on the 3 K plate of a Bluefors pulse tube cryocooler and characterize its vibrational spectrum by measuring SQUID noise in a region of sharp flux gradient. By implementing passive vibration isolation, we reduce relative sensor-sample vibrations to 20 nm in-plane and 15 nm out-of-plane. A variable-temperature sample stage that is thermally isolated from the SQUID sensor enables measurement at sample temperatures from 2.8 K to 110 K. We demonstrate these advances by imaging inhomogeneous susceptibility and vortex pinning in optimally doped YBCO above 90 K. Together with sub-micron spatial resolution and 350×350 μm² scan range, these advances position us for further studies of magnetic and superconducting materials and devices over a temperature range not previously accessible to scanning SQUID microscopy.

*This work was supported by the DOE Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, DE-AC02-76SF00515.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H27 DQI: Quantum Information in Relativistic and Condensed Matter Systems

BCEC 160C - Shenglong Xu, University of Maryland, College Park - Tag(s): Focus

2:30PM H27.00001: Quantum Interferometry Meets General Relativity

IGOR PIKOVSKI (Presenter), Stevens Institute of Technology — The interplay between Einstein's theory of gravity and quantum mechanics remains one of the open questions in physics. Each of the theories has been confirmed individually, but phenomena described by the two usually take place at very different physical regimes. Nevertheless, gravity can affect quantum systems and some aspects of the interplay can be probed in experiments. In this talk, I will discuss a quantum version of the “twin paradox” in which a clock is brought in superposition of being at two different gravitational potentials. The effect leads to new and measurable consequences at the interplay between quantum theory and general relativity and causes decoherence of composite quantum systems. I will also discuss how these effects can be accessed in quantum interference experiments.
2:42PM H27.00002: Gravitational entanglement with Gaussian states*  
SOFIA QVARFORT (Presenter), SOUGATO BOSE, ALESSIO SERAFINI, University College London — Is gravity a quantum force? This question was recently addressed by two proposals (see [1] and [2]) which explored the possibility of detecting entanglement as generated by gravity. Successful detection of entanglement due to a gravitational interaction would imply that gravity is fundamentally a quantum force, since only quantum systems can mediate entanglement.

In my talk, I will show how the experimental scheme in [1] can be modeled for Gaussian states in the continuous variable framework using massive optomechanical spheres for two different settings: trapped systems and freely-falling systems. We evaluate the entanglement generated by the Newtonian potential for both cases and propose the use of two specific continuous variable entanglement witnesses to simplify the detection. The approach also allows us to include other central-potential interactions, such as the attractive Casimir effect.


*SQ acknowledges funding from EPSRC.

2:54PM H27.00003: General relativistic time dilation and spacetime uncertainty in quantum clocks*  
SHISHIR KHANDELWAL (Presenter), Institute for Theoretical Physics, ETH Zürich, MAXIMILIAN P. E. LOCK, Institute for Quantum Optics and Quantum Information (IQOQI), Vienna, Austria, MISCHA WOODS, Institute for Theoretical Physics, ETH Zürich — The general theory of relativity associates a proper time with each object via its spacetime trajectory. In quantum theory on the other hand, such trajectories are forbidden. Here we demonstrate that, in the weak-field and low-velocity limit, all "good" quantum clocks experience the time dilation dictated by general relativity for the most classical states of motion. For nonclassical states of motion, on the other hand, we find that quantum interference effects give rise to a significant discrepancy between the proper time and the time measured by the clock. Moreover, we show how our ignorance of the clock's state of motion leads to a larger uncertainty in time measurements with the clock, a consequence of entanglement between the clock time and its center-of-mass degrees of freedom.

*Swiss National Science Foundation

3:06PM H27.00004: Ontological models for relativistic quantum information*  
[Invited] IAN DURHAM (Presenter), Saint Anselm College — Epistemic models of nature prove to be problematic in many settings, particularly in those for which measurement procedures are ill-defined. By contrast, in ontic models of nature, measurement results are independent of the procedure used to obtain them. If we assume that all measurement results can be expressed in terms of pointer readings, then any useful ontology would need to unambiguously specify the positions of things. We review a number of proposals for such ontologies in the context of relativistic quantum information and quantum many-body theories, and we propose a new ontology based on the Wheeler-DeWitt equation that overcomes some of the problems inherent in existing models. Our model includes a set of deterministic constraints for the geometry, matter field, and action.

*Funding provided by FQXi and the Silicon Valley Community Fund, Grant No. 2016-165593.

3:42PM H27.00005: Relativistic wave equations from quantum walks  
TODD BRUN (Presenter), LEONARD MLODINOW, University of Southern California — Quantum walks are unitary analogues of classical random walks. We examine the quantum walk on the 3D body-centered lattice, and show that a set of natural symmetry assumptions lead, in the long wavelength limit, to its wave functions becoming solutions to the Dirac equation. These assumptions require at least a four-dimensional internal space. Taking this as a model of a particle propagating in discrete spacetime, we show that the discreteness could be detected in non-parallel matter interferometers. We also look at the problem of generalizing to the many-body case, by replacing the quantum walk with a quantum cellular automaton that gives the same evolution as the quantum walk for the single-particle sector. This automaton approaches a quantum field theory in the long-wavelength limit.
4:06PM H27.00007: Locality and digital quantum simulation of power-law interactions  MINH TRAN (Presenter), ANDREW Y GUO, QuICS/JQI, University of Maryland, College Park, YUAN SU, QuICS, University of Maryland, College Park, JAMES GARRISON, ZACHARY ELDREDGE, QuICS/JQI, University of Maryland, College Park, MICHAEL FOSS-FEIG, United States Army Research Laboratory, ANDREW CHILDS, QuICS, University of Maryland, College Park, ALEXEY V GORSHKOV, QuICS/JQI, University of Maryland, College Park — The propagation of information in non-relativistic quantum systems obeys a speed limit known as a Lieb-Robinson bound. We derive a new Lieb-Robinson bound for systems with interactions that decay with distance $r$ as a power law, $1/r^\alpha$. The bound implies an effective light cone tighter than all previous bounds. Our approach is based on a technique for approximating the time evolution of a system, which was first introduced as part of a quantum simulation algorithm by Haah et al. To bound the error of the approximation, we use a known Lieb-Robinson bound that is weaker than the bound we establish. This result brings the analysis full circle, suggesting a deep connection between Lieb-Robinson bounds and digital quantum simulation. In addition to the new Lieb-Robinson bound, our analysis also gives an error bound for the Haah et al. quantum simulation algorithm when used to simulate power-law decaying interactions. In particular, we show that the gate count of the algorithm scales with the system size better than existing algorithms when $\alpha>3D$ (where $D$ is the number of dimensions).

4:18PM H27.00008: Composite quantum systems at the interface with general relativity* [Invited] MAGDALENA ZYCH (Presenter), The School of Mathematics and Physics, The University of Queensland — A major goal of modern physics is to understand and test the regime where quantum mechanics and general relativity both play a role. However, new effects of this regime are usually thought to be relevant only at high energies or in strong gravitational fields, beyond the reach of present-day experiments. I will discuss a novel framework for achieving this goal, focused on low-energy but composite quantum systems and using the tools of quantum information science. Quantum coherence of composite particles can be measurably affected by general relativity even at low-energies and in weak gravitational fields through time dilation. I will explain the resulting new phenomena and how they can be tested. I will discuss broader relevance of the approach for quantum sensing, communication and quantum information processing.

*ARC Discovery Early Career Researcher Award (DECRA) DE180101443

4:54PM H27.00009: Signature of quantum chaos in operator entanglement in 2d conformal field theories+ LAIMEI NIE (Presenter), MASAHIRO NOZAKI, Kadanoff Center for Theoretical Physics, University of Chicago, SHINSEI RYU, Kadanoff Center for Theoretical Physics and James Franck Institute, University of Chicago, MAO TIAN TAN, Kadanoff Center for Theoretical Physics, University of Chicago — We study operator entanglement measures of the unitary evolution operators of $(1+1)$-dimensional conformal field theories (CFT), aiming to uncover their scrambling and chaotic behaviors. In particular, we compute the bi-partite and tri-partite mutual information for various configurations of input and output subsystems, and as a function of time. We contrast three different CFTs: the free fermion, the compactified free boson at various radii, and CFTs with holographic dual. We found that the bi-partite mutual information exhibits distinct behaviors for these CFTs, reflecting the different information scrambling capabilities of these unitary operators; while a quasi-particle picture can describe well the case the free fermion and free boson CFTs, it completely fails for the case of holographic CFTs. Similarly, the tri-partite mutual information also distinguishes the unitary evolution operators of different CFTs. In particular, its late time behaviors, when the output subsystems are semi-infinite, are quite distinct for these theories. We speculate that for holographic theories the late time value of the tri-partite mutual information saturates the lower bound among quantum field theories.

*Simons Foundation; Kadanoff Fellowship from University of Chicago.
5:06PM H27.00010: Exact bosonization in two and three spatial dimensions and new classes of lattice gauge theory
YU-AN CHEN (Presenter), ANTON KAPUSTIN, Caltech, DJORDJE RADICEVIC, Physics, Perimeter Institute — We will describe 2d (3d) analogs of the Jordan-Wigner transformation which maps an arbitrary fermionic system on a 2d (3d) lattice to a lattice gauge theory while preserving the locality of the Hamiltonian. The lattice gauge theory can be understood as a stabilizer code. When the space is simply-connected, this bosonization map is an equivalence. On 2d square lattice, our bosonization mapping is equivalent to Bravyi-Kitaev "Superfast simulation of Fermions" and it has possible applications on quantum simulation of fermions. We also describe Euclidean actions for the corresponding lattice gauge theories and find that the (2+1)D theory contains Chern-Simons-like terms, which can be considered as Z/2Z version of particle-vortex duality.

5:18PM H27.00011: Momentum-space entanglement of disordered non-interacting one-dimensional fermions after a quantum quench
REX LUNDGREN (Presenter), FANGLI LIU, Joint Quantum Institute, NIST/UMD, PONTUS LAURELL, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, GREGORY FIETE, Department of Physics, The University of Texas at Austin — We investigate the momentum-space entanglement entropy and spectrum of several disordered one-dimensional free-fermion systems that circumvent Anderson localization, such as the random-dimer model, after a quantum quench. We numerically observe two different types of momentum-space entanglement entropy dynamics, an interesting slow logarithmic-like growth followed by saturation or rapid saturation. The type of dynamics one observes depends on the Fermi level of the intial state and the scattering matrix element structure in momentum-space. We then discuss when the momentum-space entanglement spectrum reveals the presence of delocalized states after a quench in these systems. We find if there are vanishing momentum-scattering states, the momentum-space entanglement spectrum clearly reveals the presence of delocalized states for long times.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM
Session H28 DQI: Qubit Readout and Open Systems BCEC 161 - Archana Kamal - Tag(s): Focus

2:30PM H28.00001: Nonequilibrium thermodynamics and many-body dynamics in open quantum systems* [Invited]
MASAHITO UEDA (Presenter), University of Tokyo — Quantum gas microscopy has revolutionarized our view on quantum many-body systems where atoms trapped in an optical lattice can be observed in real time at the single-particle level. At such extreme precision, the measurement backaction due to Heisenberg's uncertainty relation can no longer be ignored. One should naturally led to the question of whether or not nonequilibrium thermodynamics and statistical physics should be modified be modified and, if so, in what way and, in particular, how thermalization proceeds under continuous observation. A similar situation has emerged in a system of superconducting qubits under feedback control. I will address these issues and closely related problems of thermalization, heating and many-body localization in isolated and open quantum systems.

*This work was supported by KAKENHI Grant. No. JP18H01145 and a Grant-in-Aid for Scientific Research on Innovative Areas “Topological Materials Science” (KAKENHI Grant No. JP15H05855) from the Japanese Society for the Promotion of Science.

3:06PM H28.00002: Multiplexed Readout of Superconducting Qubits in 3D cQED Architecture Using Impedance Engineered Broadband JPA*
SUMAN KUNDU (Presenter), DCMP&MS, Tata Institute of Fundamental Research, Mumbai, NICOLAS GHEERAERT, Neel institute, CNRS and University Grenoble-Alpes, Grenoble, France, SUMERU HAZRA, DCMP&MS, Tata Institute of Fundamental Research, Mumbai, TANAY ROY, Department of Physics, University of Chicago, USA, KISHOR SALUNKHE, MEGHAN P. PATANKAR, RAJAMANI VIJAYARAGHAVAN, DCMP&MS, Tata Institute of Fundamental Research, Mumbai — We propose and demonstrate a frequency-multiplexed readout scheme in 3D cQED architecture. We use four transmon qubits coupled to individual rectangular cavities which are aperture-coupled to a single rectangular waveguide feedline. A coaxial to waveguide transformer at the other end of the feedline allows to launch and collect the multiplexed signal. The reflected readout signal is amplified by an impedance engineered broadband parametric amplifier with 380 MHz of bandwidth. This provides us high fidelity single-shot readout of multiple qubits using compact microwave circuitry, an efficient way for scaling up to more qubits in 3D cQED. We also discuss possible designs for multiplexing larger number of qubits. Finally, we discuss the saturation properties of our broadband JPA and explore a few approaches to improve them to increase the number of qubits that can be measured simultaneously.

*This work is financially supported by Department of Atomic Energy, Government of India, India.
Increasing qubit readout fidelity and efficiency with two-mode squeezed light

XI CAO (Presenter), GANGQIANG LIU, TZU-CHIAO CHIEN, PINLEI LU, MICHAEL HATRIDGE, Physics and Astronomy, University of Pittsburgh — Implementing quantum information processing on a large scale with flawed components requires highly efficient, quantum non-demolition (QND) qubit readout. In superconducting circuits, qubit readout using coherent light with fidelity above 99% has been achieved by using a quantum-limited parametric amplifier such as the Josephson Parametric Converter (JPC), as the first stage amplifier. However, further improvement of such measurement is fundamentally limited by the vacuum fluctuations on the ports of the JPC. Alternatively, readout with squeezed input can entangle the vacuum fluctuations in different modes, thus allowing for the reduction of the noise by controlling their interference. In this talk, we demonstrate a dispersive qubit readout scheme which exploits the two-mode squeezed light generated by a first JPC and processed by a second JPC to form an amplified interferometer [1]. We have observed a 22% improvement in the voltage Signal-to-Noise Ratio (SNR) of the measurement compared to coherent light. We can also extend this scheme to generate remote entanglement. We will discuss how the role of losses changes in this system for coherent vs two-mode squeezed light.


*Work supported by: ARO, NSF and the Kauffman Foundation.

cross-resonance-based readout scheme of a superconducting flux qubit

FUMIKI YOSHIHARA (Presenter), National Institute of Information and Communications Technology, SAHEL ASHHAB, Qatar Environment and Energy Research Institute, TOMOKO FUSE, KOUICHI SEMBA, National Institute of Information and Communications Technology — We propose a cross-resonance-based readout scheme of a superconducting flux qubit, in which a flux qubit is coupled to a resonator, and a microwave flux pulse tuned to the resonator is applied to the flux qubit. At the optimal flux bias, the persistent current of the flux qubit is an increasing or decreasing function of the flux bias, depending on the state of the qubit. When a microwave flux drive is applied to the qubit, the phase of the induced microwave signal felt by the resonator depends on the state of the qubit, and the difference between the two values is 180 degrees. Since this qubit-state-dependent phase difference is larger than that of dispersive-interaction schemes [1], the proposed cross-resonance-based readout scheme has the potential to be faster. The proposed scheme takes advantage of the large contrast of the flux-bias dependence of the persistent current, and, hence, faster readout is expected compared to the alternative readout schemes [2, 3], which are mainly for transmon qubits.


*This work was supported by Japan Science and Technology Agency Core Research for Evolutionary Science and Technology (Grant No. JPMJCR1775).

Continuous joint measurement of two-qubit fluorescence: quantum dynamics and entanglement

PHILIPPE LEWALLE (Presenter), ANDREW N JORDAN, Physics and Astronomy, University of Rochester — We consider a continuous weak measurement scheme in which two qubit-cavity systems are allowed to fluoresce, and their fluorescence signals are mixed before being routed to a measurement apparatus. We theoretically investigate the stochastic quantum trajectories, qubit state dynamics, and entanglement dynamics between the qubits under such a joint-measurement scheme. Equivalent systems should be experimentally realizable with existing circuit-QED technologies.

*We acknowledge funding from NSF DMR-1809343. PL acknowledges additional partial support as a GAANN fellow (US Dept. of Education GR506598).
Qubit measurements in a computational basis are a necessary component of quantum computation. Examples include measurement at the end of a quantum algorithm and projective measurements during teleported operations. Although qubit readout suffers from errors, they may be repeated if the readout is quantum non-demolition (QND). In this way, individual imperfect readouts can be combined via methods such as majority voting to form a more accurate measurement. The measurement fidelity will be limited, however, by state transitions between qubit basis states. For two-level qubits, a single relaxation event destroys the information in the qubit. An increased distance in the Hilbert space between basis states for qubits encoded in bosonic modes, however, exponentially suppresses this infidelity limit due to transitions. In this talk, we present a measurement scheme in the circuit quantum electrodynamics (cQED) platform that utilizes repeated QND readouts to suppress measurement infidelity due to both individual readout errors and relaxation. [1] We characterize the fidelity of this scheme in terms of experimental parameters for various encodings.

[1] Hann et al, PRA 98 022305

*US ARO grant W911NF-18-1-0212
AFOSR grant FA9550-14-1-0052 & FA9550-15-1-0015
NSF GRFP grant DGE1752134 (C. Hann)
4:30PM H28.00009: Measuring qubit quasi-probability distributions behind out-of-time-ordered correlators*  
RAZIEH MOHSENINIA (Presenter), JOSE RAUL GONZALEZ ALONSO, MORDECAI WAEGELL, Chapman University, NICOLE YUNGER HALPERN, California Institute of Technology, JUSTIN DRESSEL, Chapman University — The non-classicality of the quasi-probability distribution (QPD) behind an out-of-time-ordered correlator (OTOC) is a more nuanced witness for information scrambling than the OTOC itself. We use the method introduced in Phys. Rev. A 98, 012132 (2018) to provide different experimental protocols for obtaining such a QPD in a multi-qubit system. We show that by strategically averaging sequential measurements of any strength, we can reconstruct both OTOCs and QPDs in spite of disturbances caused by intermediate strong measurements.

*Army Research Office (ARO) grant No. W911NF-18-1-0178

4:42PM H28.00010: Time-resolved single-shot single-gate RF spin readout in silicon*  
PRASANNA PAKKIAM (Presenter), ANDREY V. TIMOFEEV, MATTHEW HOUSE, MARK HOGG, TAKASHI KOBAYASHI, MATTHIAS KOCH, SVEN ROGGE, MICHELLE Y SIMMONS, Univ of New South Wales — For solid-state spin qubits, single-gate RF readout can minimise the number of gates required for scale-up since the readout sensor can integrate into the existing gates used to manipulate the qubits [1][2]. However, state of the art topological error correction codes benefit from the ability to resolve the qubit state within single-shot, that is, without repeated measurements [3]. Here we show single-gate, single-shot readout of a singlet-triplet spin state in silicon, with an average readout fidelity of 82.9% at 3.3kHz measurement bandwidth. We use this technique to measure a triplet T to singlet S0 relaxation time of 0.62ms in precision P-donor quantum dots. We also show that the use of RF readout does not impact the spin lifetimes (S0 to T decay remained 2ms at zero detuning). This establishes single-gate sensing as a viable readout method for spin qubits.


*Research supported by ARC CoE for Quantum Computation and Communication Technology (Project No. CE110001027) and U.S. ARO under Contract No. W911NF-17-1-0202. The device is fabricated at the NSW node of ANFF. M.Y.S. acknowledges an ARC Laureate Fellowship.

4:54PM H28.00011: Radio-frequency reflectometry of a quantum dot using an ultra-low-noise SQUID amplifier*  
FELIX SCHUPP (Presenter), NATALIA ARES, AQUILA MAVALANKAR, Oxford University-USE 4643, JONATHAN GRIFFITHS, GEB JONES, Physics, Cambridge University, IAN FARRER, Physics, Sheffield University, DAVID A RITCHIE, CHARLES G SMITH, Physics, Cambridge University, GEORGE ANDREW DAVIDSON BRIGGS, Oxford University-USE 4643, EDWARD LAIRD, Physics, Lancaster University — Fault-tolerant spin-based quantum computers will require fast and accurate qubit readout. This can be achieved using radio-frequency reflectometry given sufficient sensitivity to the change in quantum capacitance associated with the qubit states. Here, we demonstrate a 23-fold improvement in capacitance sensitivity by supplementing a cryogenic semiconductor amplifier with a SQUID preamplifier. The SQUID amplifier operates at a frequency near 200 MHz and achieves a noise temperature below 550 mK when integrated into a reflectometry circuit, which is within a factor 115 of the quantum limit. It enables a record sensitivity to capacitance of 0.07 aFHz^-0.5 and a sensitivity to oscillating charge of 5.9 x 10^{-24}Chz^{-0.5}. We use this circuit to measure the stability diagram of a gate-defined quantum dot, and show that the sensitivity should be sufficient for single-shot readout of a singlet-triplet qubit in GaAs without a charge sensor.

*The work was funded by DSTL (contract 1415Nat-PhD 59), EPSRC (EP/J015067/1, EP/N014995/1), the Royal Academy of Engineering, a Marie Curie Fellowship and Templeton World Charity Foundation.
Advantages of Independent Heat Sinking of a Two-Stage Cryogenic Amplifier for Quantum Dot Readout

JOELLE CORRIGAN (Presenter), TREVOR KNAPP, JOHN DODSON, NATHAN HOLMAN, BRANDUR THORGRIMSSON, THOMAS MCJUNKIN, SAMUEL NEYENS, E. R. MACQUARRIE, RYAN FOOTE, Department of Physics, University of Wisconsin-Madison, LISA EDGE, HRL Laboratories, LLC, SUSAN COPPERSMITH, MARK ALAN ERIKSSON, Department of Physics, University of Wisconsin-Madison — Reduced device electron temperature while using a cryogenic HEMT amplifier is achieved by moving the amplifier to an adjacent PCB electrically connected to the sample PCB. The amplifier PCB is directly heat sunk to the mixing chamber of a dilution refrigerator, and connects to the sample through a short stainless steel coax. Using straightforward measurements of gain and RMS noise, the two stages are tuned separately to minimize the input-referred noise for a given level of power dissipation. A single shot measurement with 650 ns rise time using 10 µW of power results in a 2.3:1 SNR and 150mK electron temperature. An electron temperature of 115 mK is achieved with lower power, and the effect of these various powers on SNR is examined for bandwidths of 540kHz and 170kHz. The large amplifier bandwidth enables high frequency lock-in measurements, resulting in lower noise data than possible without such an amplifier. The ease of use of cryogenic amplification combined with relatively low electron temperature and large bandwidth provides a useful tool for characterization of semiconductor quantum dot qubits.

Fast high fidelity qubit readout of a transmon molecule using longitudinal coupling

VLADIMIR MILCHAKOV (Presenter), REMY DASSONNEVILLE, OLIVIER BUISSON, LUCA PLANAT, SÉBASTIEN LÉGER, JAVIER PUERTAS, KARTHIK SRIKANTH BHARADWAJ, FARSHAD FOROUGHI, CECILE NAUD, WIEBKE HASCH-GUICHARD, NICOLAS ROCH, Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France — The most common technique of qubit readout in cQED relies on the transverse dispersive coupling between a qubit and a microwave cavity. However, despite important progresses, implementing fast high fidelity readout remains a major challenge. Indeed, inferring the qubit state is limited by the trade-off between speed and accuracy due to Purcell effect and unwanted transitions induced by readout photons in the cavity. To overcome this, we introduce a transmon molecule based on two transmons coupled by a large inductance, which is inserted inside a 3D-cavity. The full system presents one transmon –used as qubit– with a large direct cross-Kerr(longitudinal) coupling to a non-linear readout resonator, called polaron mode. This polaron mode results from the hybridization between the microwave cavity and the second mode of the transmon molecule circuit. The direct cross-Kerr coupling is a key point of our readout scheme since it protects the qubit from Purcell effect. We will present qubit readout performance with fidelity as high as 95.7% in 120ns and discuss the quantum non-demolition properties of this novel readout.

* R. Dassonneville thanks CFM recherche foundation. This work is supported by the French Agence Nationale de la Recherche (ANR-CE24-REQUIEM).

Tuesday, March 5, 2019 2:30 PM - 3:30 PM

Session H29 APS: Strategic Plan Town Hall BCEC 162A

2:30PM H29.00001: Strategic Plan Town Hall — APS President David Gross and CEO Kate Kirby will present and answer questions about the new APS strategic plan. The strategic plan will lay out APS’ goals and priorities for the next several years.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H30 GSOFT DPOLY DBIO: Organization and Dynamics of Functional Liquid Crystals, Polymers, and Biological Assemblies I BCEC 162B - Cecilia Leal, University of Illinois at Urbana-Champaign -

Tag(s): Focus
2:30PM H30.00001: Assembling and organizing block copolymer nanostructures with the aid of liquid crystals

CHINEDUM OSUJI (Presenter), Chemical and Biomolecular Engineering, University of Pennsylvania, YOUNGWOO CHOO, MANESH GOPINADHAN, Yale Univ, MASAFUMI FUKUTO, RUIPENG LI, Brookhaven National Lab, DENNIS NDAYA, REUBEN BOSIRE, University of Connecticut, YEKATERINA ROKHLENKO, Yale Univ, KEN KAWAMOTO, JEREMIAH JOHNSON, Massachusetts Institute of Technology, RAJESWARI KASI, University of Connecticut — Attaching mesogens to block copolymer backbones (BCP) can result in a rich interplay of self-assembly on multiple lengthscales, and provides new opportunities to control nanostructure development. We examine the self-assembly and directed-self assembly under magnetic fields of LC BCPs and BCP-analogous macromolecules containing mesogens. We observe a rich phase behavior, including the formation of gyroid morphologies and highly asymmetric phase diagrams, and we encounter systems with structural periodicities as small as ~6 nm. We consider the phase behavior and field alignment of a cylinder-forming system in the presence of labile mesogens that swell the LC block. The system transitions from hexagonal cylinders to FCC spheres beyond a critical mesogen concentration. Despite the isometric nature of the cubic lattice, the system aligns with the [100] axis parallel to the applied magnetic field, resulting in a degenerate, fiber-like texture. We speculate that this response may originate from symmetry breaking due to the action of the field that leads to a 2-step ordering process of the spherical microdomains. Alternatively, the response may indicate the presence of an unexpected magnetic easy axis in this cubic system.

*NSF DMR-1410568

2:42PM H30.00002: Bipolar to Radial Drop Transitions in the Presence of Novel Surfactants

JAKE SHECHTER (Presenter), BENJAMIN STRAIN, LINDA OSTER, University of Massachusetts Amherst, JESSICA SLEATOR, Springfield College, FNU MANISHA, UMA SRIDHAR, University of Massachusetts Amherst, JUAN DE PABLO, University of Chicago, SANKARAN THAYUMANAVAN, JENNIFER ROSS, University of Massachusetts Amherst — Liquid crystals (LCs) are a class of molecules that can form a variety of phases that can be influenced by external interactions. We are interested in controlling the phase of a liquid crystal droplet by controlling the interface between the organic liquid crystal (5CB) and the aqueous surfactant medium. This is an interesting physical system because the molecules at the surface can alter the phase of the LC throughout the interior by balancing the elastic energy of splay, twist, and bend against the interfacial tension. Here, we test the effects of novel amphiphiles, in the presence of SDS, on the phase of the LC droplets. We have synthesized molecules with various triggerable stimuli, such as pH, light, and protein binding. To help us understand the dynamics of the phase changes, we compare our experiments to simulations. We find that the phase transition is triggered by the addition of SDS, but not the novel surfactants. The concentration at which the phase transition occurs does not appear to depend on the droplet size, but does depend on the novel surfactant in the solution. Interestingly, we find a hysteresis in the concentration of the phase transition, from bipolar to radial and back again, that depends on the novel surfactant used.

*DoD ARO MURI 67455-CH-MUR

2:54PM H30.00003: Physical insights on the self-assembly of myelin sheaths: what drives healthy lamellar stacks to disrupted inverted hexagonal phase

ROY BECK (Presenter), RONA SHAHARABANI, Tel Aviv University — Myelin sheath is a multimilayer complex of various lipids and proteins that surrounds axons and acts as an insulating layer for proper nerve conduction. In multiple sclerosis (MS), the myelin structure is disrupted impairing its function. Previous studies showed that MS is correlated with a small lipid composition variation and a reduction in the adhesive myelin basic protein (MBP). We show that such alterations result in structural instabilities and phase transition from a lamellar to inverted hexagonal phase, in accordance with pathological in vivo studies. Moreover, alteration in local environmental conditions, such as elevated salinity and temperature, drive the myelin system further into the inverted hexagonal phase [2]. Finally, we will demonstrate that the self-assembly of such complex system presents ion-specific structural modulation that is physiologically relevant. Since the etiology and recovery pathways of MS are currently unclear, these findings delineate novel functional roles to dominant constituents in cytoplasmic myelin sheaths.


*ISF (571/11 and 550/15)
Mechanics and Ion Transport in Dynamic Polymer Networks based on Metal-Ligand Coordination in Polymeric Ionic Liquids* [Invited] RACHEL SEGALMAN (Presenter), NICOLE MICHENFELDER-SCHAUSER, SEAMUS JONES, RAM SESHADRI, University of California, Santa Barbara — Polymers that contain ionic liquid constituent retain many of the properties of ionic liquids including ionic conductivity. Further, the polymerized cation (such as imidazolium) forms transient ligand bond interactions with dissolved metal ions allowing them to conduct while also forming a dynamic network. Dynamic polymer networks based on metal-ligand coordination are promising materials to accomplish such decoupling due to the transient nature of the coordination interaction. The general system of interest comprises a metal salt mixed in a polymeric medium with ligands located either along the backbone or on pendant side-chains. The molecular design of these materials allows for precise and independent control over the nature and concentration of ligand and metal, the salt dissolution, and the binding energy between the ligand and metal, all of which shown to be critical for controlling bulk ion conduction and polymer mechanics. Salt dissociation is universally governed by coordination number, equilibrium constant, and initial salt and ligand concentrations. Salt dissociation is enhanced by larger equilibrium constants and higher cation valency. The sensitivity of the ionic conductivity on equilibrium constant, coordination number, and the ratio of cation to anion diffusion coefficients is much higher for monovalent salts compared to divalent or trivalent salts. In a model system composed of poly(ethylene oxide) with tethered imidazole moieties that facilitate salt dissociation of both nickel (II) bis(trifluoromethylsulfonyl)imide (NiTFSI) and lithium bis(trifluoromethylsulfonyl)imide (LiTFSI), the nickel-imidazole interactions physically crosslink the polymer, increase the number of elastically active strands, and dramatically enhance the modulus while allowing Li⁺ to conduct quickly through the matrix.

*This work was supported by the MRSEC Program of the National Science Foundation under Award No. DMR 1720256.

Orientation of hard semiconducting nanoparticles by soft lyotropic lipid constructs* DYLAN STEER (Presenter), JOSEPH C FLANAGAN, MARILYN PORRAS GOMEZ, MOONSUB SHIM, CECILIA LEAL, University of Illinois at Urbana-Champaign — Quantum nanorods (QnR) are fluorescent nanoparticles with tunable optoelectronic properties depending on size and shape. These properties make them attractive in many biotechnology applications but due to their hydrophobic nature they are often hybridized by a shell of soft amphiphilic molecules. Anisotropic nanocrystals have orientation dependent properties, however controlling QnR alignment when drying from an organic solvent is difficult. We investigate the ability of amphiphilic molecules that are mostly known as stabilizers of QnRs in water to act as a matrix to guide QnR orientational order. Lipids are amphiphilic molecules that rapidly assemble into hierarchic liquid crystalline structures with various levels of positional and orientational order. These structures rapidly experience phase transitions depending on lipid composition, relative humidity, and temperature. Here we use glancing-incidence small angle X-ray diffraction (GI-SAXS) and fluorescence microscopy to study the co-assembly of lipid – QnR composites in highly concentrated regimes. Conditions are found to promote either the separation into lipid and highly ordered QnR domains, or the mixture of these components into a single phase with distinct structural characteristics.

*Office of Naval Research N000141612886

Elementary smectic ordering of “gapped” DNA duplexes* PRABESH GYAWALI (Presenter), RONY SAHA, Department of Physics, Kent State University, Kent, OH USA, MIREK SALAMONCZYK, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA USA, JAMES GLEESON, Department of Physics, Kent State University, Kent, OH USA, ANTAL ISTVAN JAKLI, Chemical Physics Interdisciplinary Program, Liquid Crystal Institute, Kent State University, Kent, OH USA, HAMZA BALCI, SAMUEL SPRUNT, Department of Physics, Kent State University, Kent, OH USA — We used small angle X-ray scattering and optical microscopy to study the liquid crystalline behavior of “gapped” DNA duplexes in aqueous solution. Our previous work revealed the occurrence of a smectic-A phase for DNA concentrations in the range ~230 to ~300 mg/ml and for a single-strand “gap” between duplexes of 20 thymine bases. Here we describe evidence for two coexisting/competing smectic-A-like layer structures, whose relative population varies with temperature and “gap” length. Smectic layering occurs for gap lengths down to 4 bases but disappears when the gap is reduced to 2 bases. Transitions from smectic to cholesteric/nematic state are observed as a function of temperature.

Reference

*Supported by NSF under grant no. DMR13-07674
4:06PM H30.00007: Lipid-driven Crystallization of Block Copolymers in Lipid-Polymer Alloys*. YOO KYUNG GO
(Presenter), CECILIA LEAL, Department of Materials Science and Engineering, University of Illinois, Urbana Champaign — Tailoring crystallinity of blocks in crystalline-crystalline diblock copolymers (BCPs) is a route to gain control over the material's optical and mechanical properties. One methodology that has successfully tuned BCPs crystallinity is to include additives to the assembly.[1] In this work, we investigate the crystallization behavior of BCPs as tuned by the addition of a biological lipidic component. We adopted 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) as an additive to induce crystallization-driven self-assembly of poly(ε-caprolactone)-b-poly(ethylene oxide) (PCL-b-PEO). Herein, we scrutinize the effects of the lipids on crystallization of each block in PCL-b-PEO at multiple length scales by IR spectroscopy, differential scanning calorimetry, wide-angle X-ray scattering, small-angle X-ray scattering, and polarization optical microscopy. We discovered that DPPC and BCPs assemble in a uniform alloy with a lamellar structure at the mesoscale. Within this structure, the lipid can enhance crystallinity of PCL while suppressing that of PEO. The crystalline domains appear tubular at the nanoscale and the alloy displays large platelet morphologies at the microscale compared to pure neat polymeric systems. [1] ACS Nano 2015, 9, 4, 3627-3640

*National Science Foundation (DMR-1554435)

4:18PM H30.00008: Molecular Dynamics Simulations of Elastic Capsomeres Self Assembling into a Virus Capsid*
LAUREN NILSSON (Presenter), JAYANATH CHAMINDU KADUPITIGE, Intelligent Systems Engineering, Indiana University Bloomington, MARTIN JARROLD, Department of Chemistry, Indiana University Bloomington, VIKRAM JADHAO, Intelligent Systems Engineering, Indiana University Bloomington — Viruses are an important class of soft biological materials that are capable of self-assembling into capsids that are often icosahedral-shaped. However, this self-assembly process is not completely understood in part due to the arduousness and simulation cost of correlated investigations between experiments and rigid-body models of constituent capsomere subunits. Experimentally-informed, hybrid OpenMP/MPI parallelized molecular dynamics simulations of a coarse-grained model composed of elastic capsomeres are used to investigate the assembly pathway of heterogeneous icosahedral viruses, focusing on Hepatitis B virus (HBV) as a first application. Simulation results are correlated to data from charge detection mass spectrometry. Based on the time-dependent mass spectrums and steady-state phase diagrams associated with the self-assembly of HBV at 5-100 micromolar protein and 100-500 millimolar salt concentrations, we propose that the formation of both 90- and 120-capsomere (T3, T4) structures in 100-500 micromolar salt concentrations, we propose that the formation of both 90- and 120-capsomere (T3, T4) structures at the nanoscale and the alloy displays large platelet morphologies at the microscale compared to pure neat polymeric systems. [1] ACS Nano 2015, 9, 4, 3627-3640

*This work is supported by the National Science Foundation through Awards 1720625 and 1753182.

4:30PM H30.00009: Luminescent Liquid Crystals Based on Platinum(II) Complexes* XINGTIAN HAO, HAIYAN PENG (Presenter), XIAOLIN XIE, Huazhong University of Science and Technology — Luminescent liquid crystals, which hold outstanding optical anisotropy, fluidity and intrinsic photoluminescence characteristic, show a great potential to be widely applied in liquid crystal display, organic light-emitting diode, optical information storage, etc. Yet, it still remains a big challenge to enhance and tune the luminescent properties. Herein, we report a highly luminescent liquid crystals based on platinum(II) complexes. These complexes are able to relax from the excited state back to the ground state through spin-forbidden transitions, giving rise to distinct photochemical and photophysical features in comparison with traditional organic fluorophores. Flexible side chains are found to play a significant role in enabling the liquid crystal phase due to the strong intermolecular interaction between the complex's square-planar structure.

*NSFC (51503045, 51433002 and 51773073)

4:42PM H30.00010: Effect of Lipid Headgroup on Polymer-Lipid Bilayer Association WENJIA ZHANG (Presenter), FRANK BATES, TIMOTHY LODGE, University of Minnesota — Cell membrane composition plays an important role in binding to polymers. We have investigated the effect of lipid headgroup on the interaction between model membranes and amphiphilic and biocompatible diblock and triblock polymers composed of ethylene oxide and propylene oxide. Large unilamellar phospholipid vesicles were used as model membranes to mimic the lipid bilayer structure of cell membranes. The composition of the lipid headgroup was manipulated by altering the amount of phosphatidylcholine and phosphatidylglycerol in the lipid bilayers, thereby varying the molar ratio of choline to glycerol headgroups. Polymer binding to lipid bilayers was quantified by pulsed-field-gradient NMR, which differentiated the polymers bound to lipid bilayers from free polymers based on their distinct diffusivities. It was observed that polymer binding significantly increases as the concentration of glycerol in the lipid bilayer increases, which could be due to the hydrogen bonds formed between poly(ethylene oxide) and the glycerol group of phosphatidylglycerol.
Spontaneous and diverse morphological transitions of nematic liquid crystal oligomer micro-droplets

WEI-SHAO WEI (Presenter), Department of Physics and Astronomy & LRSM, University of Pennsylvania, Philadelphia, PA, USA, YU XIA, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA, SOPHIE ETTINGER, Department of Physics and Astronomy & LRSM, University of Pennsylvania, Philadelphia, PA, USA, SHU YANG, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA, A. G. YODH, Department of Physics and Astronomy & LRSM, University of Pennsylvania, Philadelphia, PA, USA — Viruses and pollen grains are known for their diverse morphologies and surface patterns, which play important roles to their functions. It begs the questions how the patterns were originated and then evolved. Here, we report the spontaneous morphological transformations from micro-droplets, consisting of polydisperse nematic liquid crystal oligomers (NLCOs) suspended in water, to a strikingly rich set of nematic structures, including roughened spheres, flowers, and filamentous structures. We investigate the interplay of elasticity and interfacial tension within the drop as a function of temperature, surfactant concentrations, and the LCO chain length distribution. We show that heterogeneity of LCO chain length is a feature leading to segregation of LCOs within the micro-droplet. The transformed morphologies are highly uniform in size and can be locked via UV curing. The study of synthetic systems offers a first attempt to understand the origin of complex morphologies in biological world.

Design Diblock Copolymers for More Efficient Encapsulation

BILIN ZHUANG (Presenter), Materials Science and Engineering, Institute of High Performance Computing, MINH TUAN NGUYEN, National Junior College, Singapore, FREDA C.H. LIM, Materials Science and Engineering, Institute of High Performance Computing — The encapsulation of active molecules is often a crucial step in pharmaceutical and consumer care formulation processes. Diblock copolymers, with the right chemical structures, are potentially effective in encapsulating various hydrophobic active molecules. A model that predicts the encapsulation efficiency of diblock copolymers would therefore be helpful to guide the design of the diblock copolymers so that the encapsulation of specific active molecules can be maximized. Here, by combining group contribution method and self-consistent-field theory, we develop a model for computing the encapsulation free energy of drug molecules by diblock copolymers in a solution, based on the chemical structures of the constituents in the system. We systematically explore how the encapsulation free energy and the resulting morphology of the encapsulates depend on the variation in the chemical structures of the diblock copolymers.

Deciphering and Engineering Reentrant Phase Transition of Intrinsically Disordered Proteins

PRIYA BANERJEE (Presenter), Department of Physics, University at Buffalo, The State University of New York — Formation of intracellular RNA- and protein-rich granules (RNP granules) are primarily driven by liquid phase condensation of Intrinsically Disordered Proteins (IDPs). What are the molecular driving forces that control the material properties and morphology of RNP granules? Using mixtures of multivalent charged IDPs and RNA that display reentrant phase behavior, we show that (a) the condensed phase is predominantly droplet-like under equilibrium conditions, and (b) the material properties are primarily tuned by the charge regulated electrostatic interactions. Unexpectedly, hollow condensates are formed under non-equilibrium conditions by RNA influx into RNP droplets. We propose that this spontaneous morphological transformation of RNP droplets is actuated by RNA-mediated mixing phase transition at the droplet center. By controlling the RNA inflow using simple microfluidic designs, complex patterns of hollow condensates can be generated stochastically. Our results suggest that cellular processes that can drive an active RNA influx into RNP droplets, such as transcription, can spatiotemporally control their material properties and morphology.


College of Arts and Sciences, University at Buffalo
Improving the prediction of magnetic interactions from DFT methods: Non-collinear magnetization and self-interaction

JUAN PERALTA (Presenter), RAJENDRA JOSHI, KAI TREPTE, KOBLAR JACKSON, Department of Physics, Central Michigan University — Electronic structure methods are routinely used to predict magnetic properties of diverse materials, including molecular nanomagnets, clusters, and crystals. Density functional theory (DFT) has been one of the workhorses of modern electronic structure methods, and as such, it has been used extensively for the prediction of magnetic properties. In this talk I will summarize our efforts to improve the prediction of magnetic exchange couplings J from DFT methods in two fronts. First, I will show a proposed method to extract J based on differential rotations of the local atomic magnetization. This method avoids the explicit evaluation of energy differences, which can become impractical for large complexes and clusters. Our approach is based on the evaluation of the transversal magnetic torque between magnetic centers using constraints of the local magnetization direction via Lagrange multipliers and involves non-collinear spin DFT.[1] This, combined with a local partitioning of $\langle S^2 \rangle$, [2] makes possible the evaluation of J couplings entirely from first principles without ad-hoc nominal spin values. Second, I will show how self-interaction error (SIE) impacts the prediction of J couplings using an efficient implementation for SIE removal based on Fermi-Löwdin orbitals (FLOSIC).[3] Using this method, removing SIE from the simple local spin density approximation improves calculated J couplings,[4] in line with previous observations for small model systems.


Efficient Implementation of RT-TDDFT on Siesta 4.0

FERNANDO VILA (Presenter), MARILENA TZAVALA, JOHN REHR, University of Washington — Real-time time-dependent DFT (RT-TDDFT) provides a versatile method for computing electronic response in both linear and non-linear regimes. Here we introduce RT-Siesta4, an efficient implementation of RT-TDDFT which combines the LCAO approach for electronic structure in Siesta 4.0 with an efficient Crank-Nicolson time-evolution operator to propagate Kohn-Sham states in the presence of an external electric field. This development extends our previous implementation with Siesta 2.0. RT-Siesta4 uses a predictor-corrector scheme to ensure time-reversibility, thus enabling long time steps. Its capabilities include full spectrum linear optical response, single frequency NLO response, and response to shaped pulses. Benchmarks for typical systems are presented showing how the faster evaluation of the TD Hamiltonian in Siesta 4.0 improves the performance of our real-time implementation. Finally, we discuss the need to extend scalability into the peta- and exa-scales.


*Supported as part of the Comput. Chem. Sci. Program funded by the U.S. DOE, Office of Science, BES, CSGB Division in the Center for Scalable and Predictive methods for Excitations and Correlated phenomena (SPEC) at PNNL, and with computer support from DOE-NERSC.

Performance of Generalized Gradient Approximations with Nearly Correct Asymptotic Potentials on Molecular and Solid-State Properties

ALBERTO VELA (Presenter), ANGEL ALBAVERA-MATA, Department of Chemistry, Cinvestav, KARLA BOTELLO MANCILLA, Escuela Superior de Ingeniería Química e Industrias Extractivas, IPN, JAVIER CARMONA-ESPÍNDOLA, Department of Chemistry, UAM-Iztapalapa, SAM B TRICKEY, Quantum Theory Project, Department of Physics and Department of Chemistry, University of Florida, JOSE L GAZQUEZ, Department of Chemistry, UAM-Iztapalapa — The recently developed nearly correct asymptotic potential (NCAP) and its predecessor (CAP) are generalized gradient approximations (GGAs) for exchange and correlation designed to capture the asymptotic behavior of the exchange potential [1,2]. Compared to more common GGAs, they improve the description of frequency-dependent response properties in molecules, yet provide good accuracy of thermodynamic and kinetic properties. NCAP incorporates a potential shift accounting for the derivative discontinuity of the potential and has an overall performance, for molecules, competitive with current meta-GGAs. In this work, we present and discuss the performance of these GGAs on extensive tests involving lattice constants, bulk moduli, and cohesive energies for a set of solids and compare that performance with molecular results.


*Conacyt Proyecto Fronteras 867
4:06PM H31.00005: Ionization potentials and static dipole polarizabilities of polyacenes using Fermi-Lowdin self-interaction corrected density functional approximation*  SHARMIN AKTER, YOH YAMAMOTO, LUIS BASURTO, TUNNA BARUAH (Presenter), RAJENDRA ZOPE, University of Texas, El Paso — We study the static electric dipole polarizabilities and the first ionization potentials of polyacenes from benzene to pentacene using the Fermi-Lowdin Orbital based self-interaction corrected (FLOSIC) density functional method. Most common density functional approximations (DFA) that often accurately predict equilibrium properties show deviation from the piecewise exact linear behavior between integer electron numbers. These functionals favor fractional charges and cause excessive electron delocalization resulting in incorrect electron densities. Due to delocalization errors, the ionization potentials obtained using the LDA and PBE functionals rapidly decrease as a function of length. The application of the FLOSIC method shows that it corrects for this many-electron self-interaction error in ionization potentials of polyacenes. Furthermore, it is observed that the FLOSIC corrected electron density when used in simple LDA functionals results in a remarkably accurate prediction of the ionization potentials of polyacenes.

*This work was supported by the Office of Basic Energy Sciences, US Department of Energy, DE-SC0002168, DE-SC0006818 and DE-SC0018331.

4:18PM H31.00006: Enhancing the efficiency of density functionals with a novel iso-orbital indicator*  JAMES FURNESS (Presenter), JIANWEI SUN, Tulane University — The accuracy and efficiency of a density functional depends on the basic ingredients it uses and how the ingredients are built into the functional as a whole. An iso-orbital indicator based on the electron density, its gradients, and the kinetic energy density, has proven an essential dimensionless variable allowing density functionals to recognise various types of chemical bonding, both strong and weak. Density functionals constructed around the iso-orbital indicator usually require dense real-space grids for numerical implementation that deteriorate computational efficiency, compromising the improved accuracy. A novel iso-orbital indicator is proposed based on the same ingredients that retains the capability to identify the same chemical bonds while relieving the requirement of dense grids. The novel iso-orbital indicator improves recognition of electron density tail regions and is constraint-free for the exchange-correlation potential. The novel iso-orbital indicator is therefore expected to be the prime choice for density functional development and we discuss aspects of its use in cutting edge meta-generalised gradient approximations.

*Support from start-up funding from Tulane University and the U.S. DOE, Office of Science, Basic Energy Sciences DE-SC0019350(core research).

4:30PM H31.00007: Density driven error and many-body dispersion in the calculation of protobranching energies in alkanes*  JORGE NOCHEBUENA (Presenter), ALBERTO VELA, Center for Research and Advanced Studies of the National Polytechnic Institute — It is well known that branched alkanes are more stable than their linear isomers. Protobranching energies are energetic footprints of this isomeric preference. They have been estimated accurately (compared to experimental values) through highly correlated wave function methods. In contrast, calculations based on density functional approximation (DFA) errors can be classified as errors due to the density (density-driven error) and errors due to the functional (functional error). Functional errors can be related to the inability of common DFAs to describe long-range electronic correlations (dispersion forces). Such forces can be efficiently included in DFT calculations through the many-body dispersion method [1]. Density-driven errors can be corrected using the partition DFT scheme [2]. In this work, we evaluate the role played by both corrections in the relative stability of alkanes. We also delineate the role of medium-range correlation through protobranching energy calculations with range-separated DFAs.


*J.N. and A.V. thank Conacyt for grant Fronteras 867.
4:42PM H31.00008: Gapping of MnO, FeO, CoO, and NiO Mott insulators by SCAN without U* YUBO ZHANG, Tulane University, ZHI WANG, ALEX ZUNGER, RASEI, University of Colorado, Boulder, JIANWEI SUN (Presenter), Tulane University — Mott insulation is generally enabled by the physics of symmetry conserving on-site interelectronic repulsion U on single 3d sites via the celebrated Hubbard Model. DFT, exact for the ground state properties in principle, can not consistently open band gaps for MnO, FeO, CoO, and NiO Mott insulators if one uses symmetry conserving structures along with conventional semi local approximations to its exchange correlation functional. It has been recently shown [1] that using energy-lowering symmetry breaking mechanisms, DFT+U which distinguishes occupied and empty orbitals, opens band gaps for the monoxides. Here we show that even without invoking U, the semi local SCAN density functional [2] whose potentials are orbital dependent via the kinetic energy density dependence, opens band gaps for the monoxides in their AFM and PM (modeled with SQS) phases. The mechanism of gapping is analyzed. This success revives DFT for d electron materials and encourages the development of more sophisticated density functionals.


*Work supported by DOE under grants DE-SC0012575 (DOE EFRC CCM) at Tulane and DE-SC0010467 (DOE BES DM) at CU

4:54PM H31.00009: The Jahn-Teller effect in density functional theory* MARK PALENIK (Presenter), BRETT IGOR DUNLAP, DANIEL GUNLYCKE, United States Naval Research Laboratory — Using degenerate perturbation theory, Jahn and Teller proved that open-shell molecules with symmetry distort into lower symmetry configurations. Extending this proof to Kohn-Sham (KS) density functional theory (DFT) is not straightforward because of the nonlinear Coulomb and exchange-correlation potentials. These potentials affect the relationship between nuclear symmetry and electronic degeneracy, altering degenerate perturbation theory itself. Using our recently developed degenerate density functional perturbation theory, we define a perturbative approach to Jahn-Teller distortions for KS DFT. We use fractional occupation numbers to symmetrize the initial electron density, artificially stabilizing the nuclei in the highest possible symmetry. Using second-order perturbation theory, we find the changes in geometry that occur when the symmetry of the electron density is broken to form a state with integer occupation numbers. This methodology allows us to retain many of the computational benefits of working in higher symmetry. We demonstrate the resulting equations in a system of ten electrons in a superatom-like harmonic oscillator potential.

*This work has been supported by the Office of Naval Research, directly and through the U.S. Naval Research Laboratory.

5:06PM H31.00010: Self-interaction corrected dipole polarizabilites of free atoms and their ions* KUSHANTHA PRADEEP KUMARA WITHANAGE (Presenter), Central Michigan University, SHARMIN AKTER, Physics, University of Texas, El Paso, CHANDRA SHAHI, Physics, Temple University, TUNNA BARUAH, RAJENDRA R ZOPE, Physics, University of Texas, El Paso, JOHN P PERDEW, Physics, Temple University, JUAN PERALTA, KOBLAR JACKSON, Central Michigan University — Conventional density functional theory (DFT) suffers from electron self-interaction error (SIE) and hence tends to underbind the electrons. As a consequence, within DFT the electrons’ density in free atoms and their ions tends to be too responsive to an external electric field. Self-interaction corrected density functional theory (SIC-DFT) calculations improve the description of electron binding, because the unphysical SIE is removed. We apply Fermi-Löwdin orbital self-interaction correction (FLO-SIC) to calculate static dipole polarizabilites of free neutral atoms, their cations and their anions. We compare FLO-SIC-DFT polarizabilites of these systems against results from parent DFT functionals. We find FLO-SIC-DFT polarizabilites agree better with experimental and accurate quantum chemistry calculation result

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0018331.
5:18PM H31.00011: Performance of the Fermi-Lowdin Self-Interaction Correction Method in Combination with meta-GGA Functionals* YOH YAMAMOTO (Presenter), CARLOS MANUEL DIAZ, RAJENDRA ZOPE, TUNNA BARUAH, Physics, University of Texas at El Paso — Despite the success of DFT in describing the electronic properties of many electrons systems, the most widely used density functional approximations (DFA) suffer from self-interaction errors which limit their predictive power. We have recently implemented the meta-GGA functionals including the recent SCAN functional [1] that satisfies all 17 known exact constraints and is appropriately normed in the Fermi-Lowdin Self-Interaction Correction (FLOSIC) code [2,3]. The FLOSIC is a size-extensive implementation of the self-interaction-free DFA. In this talk, we present the results of FLOSIC calculations using the meta-GGA functionals. We present the performance of FLOSIC in combination with meta-GGA functionals in total energies, ionization potential, and atomization energies of various atoms and molecules.


*This work was supported by the Office of Basic Energy Sciences, US Department of Energy, DE-SC0002168 and DE-SC0018331

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H32 DCP: The Journal of Chemical Physics Editors’ Choice Lectures BCEC 204A - Laura Gagliardi, University of Minnesota - Tag(s): Invited

2:30PM H32.00001: Revisiting Glassy Behavior in Polystyrene with Single Molecule Approaches* [Invited] LAURA KAUFMAN (Presenter), ALYSSA MANZ, KEEWOOK PAENG, NICOLE MANDEL, Columbia University — Polystyrene in the rubbery regime displays phenomenology also seen in small molecule supercooled liquids, and dynamic heterogeneity in this system has been well studied. We have revisited several aspects of glassy behavior and dynamic heterogeneity in polystyrene using single molecule approaches. In particular, we have characterized exchange time (τex, the timescale a particular dynamical environment maintains a given dynamics) at a number of temperatures down to and including the glass transition temperature. These studies reveal that the ratio of τex to the alpha relaxation time (τex/τα) is independent of temperature in the range probed. More recently, we have characterized dynamic heterogeneity in polystyrene as a function of fragility as controlled by molecular weight. Over a broad range of molecular weights, we find a similar degree of dynamic heterogeneity and ratio of τex to the alpha relaxation time in polystyrene. Finally, aiming to resolve long-standing questions regarding the origins of rotational-translational decoupling, we have combined rotational and translational measurements of single molecule probes in polystyrene. Initial results suggest slowly rotating molecules are typically also slowly translating molecules but continue to suggest overall translational diffusion is faster than would be expected given system viscosity.

*This work was supported by the National Science Foundation under Grant Nos. DGE 16-44869, CHE 1213242, and CHE 1660392.
3:06PM H32.00002: Nucleation of the short-chain n-alkanes from the vapor phase: Experiments and Monte Carlo simulations* [Invited] BARBARA WYSLOUZIL (Presenter), KEHINDE OGUNRONBI, Ohio State University, ALIASGHAR SEPEHRI, BIN CHEN, Chemistry, Louisiana State University — The n-alkanes do not nucleate easily from the vapor phase, and, when rapidly cooled in a supersonic expansion, saturation levels on the order of 10,000 are typical. [1, 2] The nucleation rates measured for n-pentane through n-heptane, at temperatures ranging from ~109 K to 168 K, are on the order of 10^{17} cm^{-3}s^{-1}, increasing slightly with decreasing temperature. Despite the high degree of supercooling, Monte Carlo (MC) simulations suggest that for n-pentane through n-heptane the critical clusters remain liquid like under experimental conditions, whereas n-octane and n-nonane adopt more ordered structures. For all three alkanes, the scaled experimental and simulated nucleation rates are offset by ~3 orders of magnitude. Explicitly accounting for the surface tension difference between the real and model substances, however, increases the offset to ~ 6 orders of magnitude, equivalent to a a formation free energy difference of ~13k_BT . This difference could be reduced by changing the cutoff criterion or by using model potentials that better describe n-alkane behavior.


Funding provided by NSF Grant Nos. CHE-1464924, CHE-1052015, and EPS-1003897. We thank the Louisiana State High Powered Computing Center (LSU-HPC) for providing computational resources and Ilja Siepmann for helpful discussions. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

3:42PM H32.00003: Inferring properties of intrinsically disordered proteins from single-molecule FRET and small-angle X-ray scattering data* [Invited] ROBERT BEST (Presenter), Laboratory of Chemical Physics, NIDDK, National Institutes of Health — Intrinsically disordered proteins are a class of polypeptides in which a significant portion of the chain is not folded into a specific three-dimensional structure. Because of their abundance and importance in many biological contexts, it is important to characterize the extent of structure formation in these proteins. However, as a result of their extensive disorder, conventional structure-determination methods used for folded proteins are not appropriate, and the broad distribution of structures in such a disordered system needs to be considered. I will describe methods for using molecular simulations to account for the diversity of structures in intrinsically disordered proteins while fitting to the experimental data, which help to reconcile differences between different experimental methods. Methods based on molecular simulation are more computationally demanding, but also the most general approach. I will show how in many cases, if the IDP is sufficiently disordered, it is also possible to use simpler approximations which we have developed.

*This work was supported by the Intramural Research Program of the NIDDK, NIH

4:18PM H32.00004: Accurate modeling of liquid water and proton transfer in water* [Invited] XIFAN WU (Presenter), Temple University — Water is of the utmost importance for life and proton transfer via hydronium and hydroxide ions in water is also ubiquitous. A genuinely predictive ab initio model of water is the key to understanding the proton transfer effect in water. However, accurate prediction of water requires to climb up the Jacob’s ladder within density functional theory to include the treatment of van der Waals interactions and the mitigation of self-interaction error. We demonstrate that a fully ab initio approach, relying on the strongly constrained and appropriately normed (SCAN) density functional, provides such a description of water. SCAN accurately describes the balance among covalent bonds, hydrogen bonds, and van der Waals interactions that dictates the structure and dynamics of liquid water. At the similar level of theory, we then show that structural diffusion of hydronium preserves the previously recognized concerted behavior. However, by contrast, proton transfer via hydroxide is dominated by stepwise events, arising from a stabilized hyper-coordination solvation structure that discourages proton transfer. Specifically, the latter exhibits non-planar geometry, which agrees with neutron scattering results. Asymmetry in the temporal correlation of proton transfer enables hydronium to diffuse faster than hydroxide and may underlie observed isotope anomalies.

*US Department of Energy SciDAC under grant numbers DE-SC0008726 and DE-SC0008626 Divison of Materials Research (DMR) of National Science Foundation under Award DMR-1552287
4:54PM H32.00005: Imaging excited states of nanomaterials* [Invited] DUC NGUYEN (Presenter), Northwestern University, JOSHUA J. GOINGS, University of Washington, Seattle, HUY A. NGUYEN, JOSEPH W LYDING, University of Illinois at Urbana-Champaign, XIAOSONG LI, University of Washington, Seattle, MARTIN GRUEBELE, University of Illinois at Urbana-Champaign — Nanomaterials are promising for applications in photocatalysis, photosensitization, photodetection, photovoltaics and optoelectronics. In these applications, nanomaterials are first photoexcited, then the generated energy or charge is either used to break chemical bonds or transferred to nearby electrodes, particles or molecules of interest. Understanding photoexcited nanomaterials at their characteristic length scale is critical for performance optimization, however, is challenging given their small size and fast relaxation. We develop and use single-molecule adsorption scanning tunneling microscopy (SMA-STM), a powerful technique capable of imaging photoexcited nanomaterials with sub-nanometer spatial resolution, to investigate photoexcited quantum dots (QDs), carbon nanotubes (CNTs) and their interactions. Images of individual photoexcited QDs (absorption images) vary significantly from dot-to-dot. For a single QD, different excited states are probed by changing the applied electric field. Using the STM tip to nudge and roll the QDs on the surface, different images of the excited state at different angles are obtained. Energy transfer in arrays of QDs, QD-CNT interactions are also imaged and manipulated at individual nanoparticle level. Finally, I will discuss my recent work on probing molecular-scale catalytic interactions of oxygen with an oxygen reduction molecular catalyst using another optical STM technique, STM tip-enhanced Raman spectroscopy (STM-TERS).

*The experimental work at UIUC was supported by the National Science Foundation grant NSF CHE and DMR Directorates (D. N., H. A. N, J. L and M. G), and the computational work at UW was supported by a US National Science Foundation Graduate Research Fellowship (DGE 1256082 to J.J.G.) and grants from the National Science Foundation, NSF CHE 1464497 and CHE 1565520 (J.J.G. and X.L.). D. N. thanks the Beckman Institute for a Beckman Graduate Fellowship while this work was carried out.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H33 FLAP: Functional Oxides BCEC 204B - Turan Birol, University of Minnesota - Tag(s): Focus

2:30PM H33.00001: Enhancement of Thermal Conductivity Across the Metal-Insulator Transition in Vanadium Dioxide* LU CHEN (Presenter), ZIJI XIANG, COLIN TINSMAN, TOMOYA ASABA, Department of Physics, University of Michigan, QING HUANG, HAIDONG ZHOU, Department of Physics and Astronomy, The University of Tennessee, Knoxville, LU LI, Department of Physics, University of Michigan — The metal-to-insulator transition (MIT) in vanadium dioxide (VO2) is investigated by electrical and thermal transport measurements. We report an order-of-magnitude enhancement of thermal conductivity across the MIT region in the VO2 single crystal. Magnetic field dependent measurements reveal that the thermal conductivity peak doesn't show an obvious dependence on the magnetic field, which indicates that the enhancement of thermal conductivity could come from neutral heat carriers such as phonons. Our experiment explores a potential direction for achieving thermal management in phase-change materials.

*This work is mainly supported by the Office of Naval Research through the Young Investigator Prize under Award No. N00014-15-1-2382 (thermal transport and electrical transport measurements). The sample growth in UTK is supported by NSF-DMR-1350002 (sample growth). The measurement instrument benefit from the National Science Foundation Major Research Instrumentation award under No. DMR-1428226 (supports the purchase of the PPMS). Q.H. thanks for the support from the Go students program of ORNL.

2:42PM H33.00002: Structural and Electronic properties of Copper Doped amorphous Alumina* KASHI SUBEDI (Presenter), Ohio University, KIRAN PRASAI, Applied Physics, Stanford University, DAVID A DRABOLD, Ohio University — To understand the atomic properties of Conducting Bridge Random Access Memory(CBRAM) devices based on Alumina with Copper as one of the active electrodes, we offer new models of amorphous Alumina with varying concentrations of Cu having general form (a-Al2O3)1-nCun with n = 0, 0.10, 0.20 and 0.30. We study the structural properties of these models. It turns out that Cu atoms cluster because of its less proclivity to diffuse in the highly ionic host a-Al2O3. The clustering produces a narrow conducting path for electrical current. To elucidate the electric conduction path, we employ the Kubo-Greenwood formula in a novel space-projected form[1]. We show that the conduction-active component of the network is an interconnected Cu cluster.


*Work supported by NSF grants under DMR awards 1507670, 1507166 and 1506836
Phase transitions and optical properties of Sr$_2$SnO$_4$  

NIKOLAOS MEMMOS (Presenter), TURAN BIROL, Department of Chemical Engineering and Materials Science, University of Minnesota — Layered perovskite Ruddlesden Popper (RP) transition metal oxides are interesting because of the effects of their 2 dimensional crystal structure on their lattice response, as well as electronic and optical properties. The Stannate Sr$_2$SnO$_4$ has the K$_2$NiF$_4$ type RP structure at high temperatures, but undergo multiple structural phase transitions as the temperature is lowered. In this talk, we present our first principles Density Functional Theory results that elucidate the mechanism behind these phase transitions. We discuss the details of the octahedral tilting and examine its effects on the electronic and optical properties of Sr$_2$SnO$_4$.

*NSF DMREF Grant No. DMR-1629260

Formulation and characterization of sinterless Barium Strontium Titanate (BST) nanocomposite dielectric inks for flexible RF and Microwave electronics applications  

OSHADHA RANASINGHA (Presenter), MAHDI HAGHZADEH, CRAIG ARMIENTO, ALKIM AKYURTLU, Department of Electrical and Computer Engineering, University of Massachusetts-Lowell — The demand for printable electronics over conventional electronics is rising exponentially due to various reasons. Tunable radio frequency (RF) and microwave (MW) devices make a high impact on the size, cost and the overall performance of flexible electronics. The dielectric constant of BST can be tailored by an applied electric field, which allows BST to be used in varactors for tunable RF and MW applications such as tunable filters and conformal antennas.

The Curie temperature ($T_C$) of (Ba$_x$Sr$_{1-x}$TiO$_3$) can be tailored by adjusting the molar fraction of barium. BST has a paraelectric phase above the Curie temperature and below the Curie temperature, BST has a ferroelectric phase. BST shows highest dielectric properties such as tunability, high dielectric constant and low loss tangent in the paraelectric phase.

These inks can be processed below 150 0C and a high performance can be achieved without sintering the BST nanoparticles. Also, these inks are compatible with different types of printing technologies, such as dispensing and ink jet and aerosol jet. These BST-polymer inks showed 44.29 ± 1.85 as the highest dielectric constant and 0.02 ± 0.01 as the lowest loss tangent at 10 GHz. The maximum tunability achieved was 15% at 10 GHz with an applied electric field of 10 V/µm.

Chromium Pairs in Combustion Synthesized α-Alumina  

JOHN KREBS (Presenter), SARAH ROBITAILLE, NED STEPHEN DIXON, LINDA S FRITZ, Franklin & Marshall College — High surface area alumina has gained much attention as a support structure for a number of possible biological and biomedical applications. Combustion synthesis provides a simple route to produce large quantities of alumina with optically active impurities after liquid phase mixing. In this report, we present results on chromium ion separation in combustion-synthesized highly-doped ruby. Aluminium and chromium nitrates are dissolved in water/urea solutions. The solutions are then heated above 500 degrees, at which point they undergo a self-propagating combustion reaction transforming them into high-surface area solids. X-ray diffraction confirms the single phase a-alumina structure. Optically excited fluorescence (excited at 473 nm) spectra are used to measure the ratio of the fourth nearest neighbour emission peak to that of the single ion peak to quantify impurity pair formation as a function of chromium concentration. The ratio increases linearly over the concentration range up to four atomic percent. Time-resolved decay dynamics of the pairs will be presented.

Producing p-ZnO via rf magnetron sputtering onto a thin evaporated layer of Zn$_3$As$_2$  

JOHN COLTON (Presenter), JAMES ERIKSON, MICAH N SHELLEY, JAMES COLTER STEWART, CARRIE EMMA MCCLURE, SPENCER KING, NATHAN SCHWARTZ, DAVID D ALLRED, GARY RENLUND, Brigham Young University — Zinc oxide (ZnO) is a wide band gap semiconductor with many potential applications, including UV lasers, transparent circuits, and radiation resistant devices. The native defects in ZnO cause it to be n-type, and stable high quality p-type ZnO has proven hard to create. We report on a technique whereby As-doped p-ZnO is created using rf magnetron sputtering onto a thin evaporated layer of Zn$_3$As$_2$. The optical characteristics and thickness of the Zn$_3$As$_2$ layer have been determined by spectroscopic ellipsometry. ZnO quality and doping has been studied with photoluminescence, X-ray diffraction, Hall effect, and other techniques. Annealing in a vacuum leads to better sample quality, although the p-type characteristics have not always been reproducible.
4:06PM H33.00009: Structurally triggered metal-insulator transition in rare-earth nickelates and related $e_g^1$ perovskites PHILIPPE GHOSEZ (Presenter), Theoretical Materials Physics, Q-MAT, CESAM, University of Liege — Rare-earth nickelates (RNiO₃), apart from LaNiO₃, exhibit on cooling a metal-insulator transition (MIT), a concurrent structural phase transition and a magnetic phase transition. Here, I first assess the ability of first-principles calculations within the DFT+U formalism to describe the properties of rare-earth nickelates. Then, using such a formalism, I show that the MIT in nickelates can be seen as a structurally triggered phase transition [1] highlighting so a first concrete example of such a kind of phase transition in simple perovskites. The origin of this unusual mechanism is then traced back in the electronic and magnetic properties, revealing a Peierls-type instability, structurally triggered by oxygen rotation motions and eventually assisted by magnetic ordering. This knowledge helps rationalizing the evolution of the MIT in thin films and heterostructures [2] and is also relevant to other $e_g^1$ perovskites like alkaline-earth ferrites and rare-earth manganites [3].

**4:30PM H33.00011: Enhancement of Young's modulus in freestanding SrTiO$_3$ thin films** VARUN HARBOLA (Presenter), Physics, Stanford University, SAMUEL CROSSLEY, SEUNG SAE HONG, Applied Physics, Stanford University, YORICK BIRKHOLZER, Institute for nanotechnology, University of Twente, DI LU, Physics, Stanford University, YASUYUKI HIKITA, Stanford Institute for Material and Energy Sciences, SLAC National Accelerator Laboratory, HAROLD HWANG, Applied Physics, Stanford University — Recent developments in thin film growth provide a powerful route to free-standing single-crystal films of perovskite oxides by water etching of a sacrificial underlayer (Di Lu et al., Nature Materials 15, 1255 (2016)). We have used atomic force microscopy to systematically probe the elastic properties of suspended SrTiO$_3$ films, in a thickness series from 4-98 nm, which has been previously inaccessible and unexplored. We observe the thickness dependence of elastic modulus of SrTiO$_3$ to be non-monotonic, with a strong enhancement of stiffness for thicknesses below 30 nm. We provide evidence that the nature of this elastic stiffening lies in an effective flexoelectric coupling. This study provides the basis for studying strain manipulation and strain control of oxides at the nanoscale. In particular, oxide membranes can be designed to mimic stiffnesses of 2d materials like graphene and transition metal dichalcogenides.

**4:42PM H33.00012: Examination of the high-temperature optical properties of HfO$_2$ thin films for metamaterial selective-emitter applications** MINSU OH (Presenter), NICOLE PFIESTER, MARGARET STEVENS, KEVIN GROSSKLAUS, THOMAS VAN DER VEEL, Tufts University — Metamaterial selective-emitters can enhance the efficiency of thermophotovoltaic (TPV) energy conversion systems by selecting the wavelengths of light emitted towards the TPV photodiodes. As such, the optical properties of any material used as part of a metamaterial selective-emitter must be known and controlled. As one of the highest melting point dielectric materials, hafnium dioxide (HfO$_2$, melting point of ~2760°C) has attracted researchers’ attention for use in high-temperature applications; such as metamaterial selective-emitters. In this work, HfO$_2$ was deposited on a Si substrate by atomic layer deposition (ALD) and then diced into smaller pieces. The frequency-dependent complex permittivity of the HfO$_2$ films was measured via ellipsometry during annealing at temperatures from room temperature (RT) up to 600°C and then again at RT after annealing. The ellipsometric measurements were conducted over a wavelength range of 200 – 500 nm. The degree of crystallization and film density is correlated with the measured permittivity of HfO$_2$ by X-ray reflectivity (XRR) and X-ray diffraction (XRD).

*The authors would like to thank the Office of Naval Research for funding this work: N00014–15–1–2946

**4:54PM H33.00013: phonoRam: A workflow tool for predicting Raman activity with DFT** ANDREW MISKOWIEC (Presenter), JENNIFER NIEDZIELA, Oak Ridge National Laboratory — The Raman activity tensor is a fundamental property describing the coupling of light with matter. As polarized Raman spectroscopy becomes more routine, detailed knowledge of the tensor components is necessary to interpret spectra, in addition to the powder-averaged value measured in unpolarized experiments. We present phonoRam, a python-based workflow tool based on the phonopy phonon analysis package, that simplifies and manages the calculation of the Raman activity tensor using DFT. We present an overview of the package, convergence of the macroscopic dielectric tensor values, and a set of test cases. We present an investigation of U$_3$O$_8$, a material with 68 Raman active modes and polarization dependence, using polarized Raman and phonoRam to analyze the crystallite structure.

**5:06PM H33.00014: Optical Bandgap and Electric Transportation of Co- and Al-co-doped ZnO with Low Defect Concentration** HSUHUNG CHOU (Presenter), H. C. LIN, National Sun Yat-sen University, I. EDELMAN, Institute of Physics, Krasnoyarsk, 660036, Russia, SHIH-JYE SUN, Department of Physics National University of Kaohsiung, Kaohsiung City, Taiwan — The defects in Co- and Al-co-doped ZnO, Co$_{0.05}$Al$_{0.02}$Zn$_{0.93}$ (CAZO), films were generated during sputtering growth by mixing low percentage of hydrogen, 0.1–1% denoted as CAZO-H2%, along with argon gas at 450°C. For comparison, an extremely low defect film, except the native oxygen vacancies, was grown under a mixture of oxygen with argon gas, which is denoted as CAZO-O2. The optical band gaps and electric resistivities were measured as a function of the H$_2$%. We found the CAZO-O2 is insulating while the resistance drops to a single digit (less than 10 Ω) with the addition of a very small amount of H$_2$, 0.1%, in the growth atmosphere and reaches the minimum for CAZO-1%. Combining previous data with higher defect concentrations, the lowest resistance was observed for the CAZO-1% sample. The optical bandgap, E$_{opt}$, however, shows the opposite trend that increases smoothly with the defect concentration from E$_{opt}$=3.4eV for CAZO-O2 sample, similar to the bandgap of pure ZnO, to 3.61eV for CAZO-1.1%. The role of defects on the bandgap and resistance will be presented.

*The authors acknowledge the financial support from the Ministry of Science and Technology (MOST), Taiwan through Grant No. MOST-107-2112-M-110-012 and MOST-107-2811-M-110-013.
In this work, we demonstrate how the electron-counting model (ECM) can be used in understanding the phases, particularly in explaining the stability of the oxygen-vacancy channels (OVCs), and in examining the Co valance problem in SCO2.5 and HSCO2.5. Using density-functional theoretical (DFT) methods, we analyze the crystalline, electronic, and magnetic structures of BM- and H-Sco. We discovered stable phases with large bandgaps (> 1 eV) for both BM-Sco and H-Sco, with reasonable agreement with experiments. Our calculation also indicates limited charge transfer from H to O that may explain the special stability of the H-Sco phase and the reversibility of H incorporation observed in experiments. In contrary to the initial study, our calculation also suggests intrinsic antiferromagnetism (AFM) of H-Sco, showing how the measured ferromagnetism (FM) has possible roots in hole doping.

*We acknowledge the University Grants Committee of Hong Kong for ECS (numbered 24300814), GRF(14319416) and GRF (14307018) and the CUHK for their direct grant (numbered 4053084).
4:18PM H34.00004: Optimal Sound Absorption Metastructures: Practical Solutions from Fundamental Physics

[invited] PING SHENG (Presenter), The Hong Kong University of Science and Technology — Even in the 21st century, noise still constitutes a major environmental problem, with the low frequency noise being especially pernicious. While resonance-based acoustic metamaterials can display many novel wave manipulation capabilities, they have the Achilles' heel of being narrow-frequency in character. It would be most desirable if a sound absorber can be designed to fit the noise spectrum, with a minimum allowed thickness. Such sound absorbing structures can now be realized through a design recipe that incorporates the causality constraint on the acoustic response\(^1\). We use the causality constraint to delineate what is ultimately possible for sound absorbing structures, and denote those which can attain near-equality for the causality constraint to be "optimal." Anchored by the causality relation, an integration strategy can be formulated for realizing structures with target-set absorption spectra and a sample thickness close to the minimum value as dictated by the causality constraint. By using this approach, we have realized a 10.86 cm-thick structure that exhibits a broadband, near-perfect flat absorption spectrum starting at around 400 Hz, while the minimum sample thickness from the causality constraint is 10.36 cm. To illustrate the versatility of the approach, two additional optimal structures with different target absorption spectra are presented. This "absorption by design" strategy would enable the tailoring of customized solutions to difficult room acoustic and noise remediation problems.

References

*Work done in collaboration with Min Yang, Shuyu Chen, and Caixing Fu.

4:54PM H34.00005: Pore-scale study of multiphase flow in porous media

[invited] DAVE WEITZ (Presenter), Harvard University — TBD

Tuesday, March 5, 2019 2:30 PM - 5:06 PM

Session H35 DQI: Semiconducting Qubits: Characterization of Electron and Hole Spin Qubits BCEC 205B - Andrew Pan, HRL Laboratories, LLC - Tag(s): Focus

2:30PM H35.00001: Four-qubit quantum processor in isotopically enriched silicon\(^*\) ANTHONY SIGILLITO (Presenter), JAMES LOY, DAVID ZAJAC, FELIX BORJANS, MICHAEL GULLANS, JASON R PETTA, Physics, Princeton University — Quantum processors based on spins in semiconductors are rapidly becoming a strong contender in the race to build a quantum computer. When coupled with micromagnets, these devices offer high fidelity single-qubit [1] and two-qubit [2,3] control while maintaining long coherence times. Until now, silicon spin qubit devices incorporating micromagnets have been limited to one and two qubit demonstrations, even though a one-dimensional extended array of silicon quantum dots has been demonstrated [4]. In this presentation, we will present a four-spin-qubit device architecture. This device is fabricated on an isotopically enriched \(^{28}\text{Si}/\text{SiGe}\) quantum well and offers four individually addressable spin qubits. Multi-qubit gates can be implemented by gating nearest-neighbor exchange interactions. Preliminary data demonstrating single- and multi-qubit operation will be presented.


*Research sponsored by ARO grant No. W911NF-15-1-0149 and the Moore Foundation's EPIQS Initiative through grant GBMF4535. We thank Lisa Edge for providing the \(^{28}\text{Si}\) heterostructure. Devices were fabricated in the Princeton University QDNL.
Characterization of gate fidelities in a Si/SiGe two-qubit device

XIAO XUE (Presenter), THOMAS F WATSON, QuTech & Kavli Institute of Nanoscience, Delft University of Technology, JONAS HELSEN, QuTech, Delft University of Technology, DANIEL WARD, DONALD E SAVAGE, MAX G LAGALLY, SUSAN COPPERSMITH, MARK ALAN ERIKSSON, University of Wisconsin-Madison, STEPHANIE WEHNER, QuTech, Delft University of Technology, LIEVEN VANDERSYPEN, QuTech & Kavli Institute of Nanoscience, Delft University of Technology — Various candidate implementations for future quantum computers have been investigated over the past twenty years. Silicon spin qubits show great promise [1] for their long coherence times and integration using semiconductor technology but there have been very few quantitative studies of the fidelities of two-qubit gates. Here we characterize the gate fidelities of a C-Phase gate using randomized benchmarking. For single-qubit gates, we perform randomized benchmarking on each spin by itself and also on both spins simultaneously, to probe cross-talk effects. Furthermore, we developed and experimentally verified a new method called character randomized benchmarking [2,3], which combines the advantages of simultaneous and interleaved randomized benchmarking. With this new method, we characterized the fidelity of a C-Phase gate with tighter bounds than those in the traditional approach.


Benchmarking of two-qubit gates for singlet-triplet qubits

CHENGXIAN ZHANG (Presenter), City University of Hong Kong and South China Normal University, XIN WANG, City University of Hong Kong — We perform benchmarking to evaluate the performance of two-qubit dynamically corrected gates (DCGs) in the singlet-triplet spin qubit system. We execute two types of circuits, i.e. the Deutsch-Jozsa algorithm and Grover algorithm, each of which is carried out with DCGs and gates not immune to noise. The benchmarking process is performed by repeating 100 times of the respective circuit under 1/f noises with different noise exponents (α). The average error per execution of one algorithm is compared between DCGs and non-noise-correcting ones, and whether DCGs offer improvement depends on the noise exponent, α. We have found that when α < 0.8 the DCGs would not offer improvements, but DCGs can outperform the non-correcting ones otherwise. The fact that DCGs can offer improvement for a wide range of α, on one hand, suggests using DCGs on two-qubit gates can reduce the error, but on the other hand also indicates that quantum algorithms involving two-qubit gates suffer more heavily from noises than those only involving single-qubit gates if no correction to noise is performed.

*This work is supported by the Research Grants Council of the Hong Kong Special Administrative Region, China (No. CityU 21300116, CityU 11303617).

Noise correlations in a two-qubit Si/SiGe quantum dot device

JELMER BOTER (Presenter), XIAO XUE, THOMAS F WATSON, TOBIAS KRAHENMANN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, VICKRAM PREMAKUMAR, DANIEL WARD, DONALD E SAVAGE, MAX G LAGALLY, MARK G FRIESEN, SUSAN COPPERSMITH, MARK ALAN ERIKSSON, ROBERT JAMES JOYNT, University of Wisconsin-Madison, LIEVEN VANDERSYPEN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Qubits are affected by noise in their environment, but conversely can also be used to probe this noise and study properties such as spectral density and correlations. We use a two-qubit device in a Si/SiGe heterostructure [1] to investigate noise correlations by studying the decay of two Bell states. These Bell states are insensitive to either correlated or anti-correlated noise, resembling the concept of decoherence-free subspaces, which allows us to extract the uncorrelated, correlated and anti-correlated contributions to the noise affecting the qubits from the decay times for the different initial states. Knowledge about the noise properties makes it possible to design operations that are less sensitive to this noise, and yields information on the noise source, which potentially makes it possible to reduce the noise. We demonstrate this method by artificially adding (anti-) correlated noise and use it characterize the noise in our system.


*Army Research Office (ARO) under grant numbers W911NF-17-1-0274 and W911NF-12-1-0607. Growth facilities used for fabricating samples is supported by DOE (DEFG02-03ER46028). Facilities supported by NSF through the University of Wisconsin-Madison MRSEC (DMR-1121288).
Magnetic-Field Effects on Error and Leakage in Randomized Benchmarking of a Si/SiGe Triple-dot Qubit  
CODY JONES (Presenter), HRL Laboratories, LLC — The exchange-only, triple-dot qubit is fully controllable through voltage-based modulation of the exchange interaction between neighboring dot pairs, requiring no magnetic gradients or magnetic resonance. Nevertheless, several magnetic effects play important roles in errors and leakage of the qubit under operation, whether by dephasing for an idle qubit or during a multi-pulse experiment such as randomized benchmarking. This talk discusses the magnetic-field-dependent impacts of three types of magnetic gradients: magnetic screening gradients due to the Meissner effect in superconducting gates, interface-spin-orbit effects, and contact hyperfine interactions including the full vector of nuclear magnetization. While Meissner and spin-orbit gradients are suppressed by operating near zero magnetic field, we find that gradients oriented in directions transverse to the field, in particular the flip-flop terms of the hyperfine component, play a more dominant role. Isolating the effects of magnetic gradients on qubit performance is aided by modifications to the randomized benchmarking protocol that allow reliable extraction of the proportion of total error due to leakage, which is a signature of magnetic gradient effects in exchange-only qubits.

Analyzing the fidelity of a singlet-triplet spin-orbit qubit in silicon using gate set tomography  
CHLOE BUREAU-OXTON (Presenter), Universite de Sherbrooke, KENNETH RUDINGER, NOAH T JACOBSON, DANIEL WARD, JOHN ANDERSON, RONALD P. MANGINELL, JOEL R. WENDT, TAMMY PLUYM, MICHAEL P LILLY, Sandia Natl Labs, MICHEL PIORO-LADRIERE, Universite de Sherbrooke, DWIGHT R LUHMAN, MALCOLM S. CARROLL, Sandia Natl Labs — It has been recently demonstrated that spin-orbit effects observed in silicon quantum dots are much larger than what is expected for bulk silicon [1-3]. These spin-orbit effects can be used to achieve all-electrical universal control of a double quantum dot singlet-triplet qubit without the need for any external components, such as micromagnets or microwave resonators, to produce a magnetic field gradient [4]. In this work, we use gate set tomography to analyze the fidelity of these gates. We also explore the possibility of using AC control, both in the weak and strong driving regimes, to improve the fidelity of qubit operations.

Measurements of capacitive coupling in two double dots in Si/SiGe for application in two qubit gates  
SAMUEL NEYENS (Presenter), EVAN R MACQUARRIE, JOHN DODSON, NATHAN HOLMAN, BRANDUR THORGRIIMSSON, THOMAS McJUNKIN, JOELLE CORRIGAN, MARIO PALMA, Department of Physics, University of Wisconsin-Madison, LISA EDGE, HRL Laboratories, LLC, MARK G FRIESEN, SUSAN COPPERSMITH, MARK ALAN ERIKSSON, Department of Physics, University of Wisconsin-Madison — We present measurements of a Si/SiGe quantum dot device made with overlapping self-oxidized Al gates. The device includes a linear array of four quantum dots and two auxiliary dots for charge sensing. The dots have a lithographic pitch of 130 nm and are separated from the gates by a 30 nm SiGe spacer and 5 nm of aluminum oxide deposited by ALD. We measure the charge noise in all six dots and observe a power spectral density that is approximately 1/f in the 1-200 Hz range with a chemical potential noise amplitude of 1-2 μeV/Hz^{1/2} at 1 Hz. We tune the device to form two tunnel-coupled double dots and observe the capacitive coupling with both double dots at the (0,1)-(1,0) polarization line. We measure a detuning shift of ~8 GHz due to the change in polarization of the adjacent double dot, demonstrating the potential of the system for coherent two-qubit coupling via capacitive interaction.
3:54PM H35.00008: Detuning dependence of capacitive coupling for quantum dot hybrid qubits* ARMAN SETSER

Implementation of robust two-qubit entangling gates is necessary in order to form a universal set of multi-qubit operations. We derive the coupling form between two capacitively coupled qubits, each consisting of three electrons in a double quantum dot (i.e., two hybrid qubits), and show how the effective coupling behaves as a function of detuning. By pulsing the detuning adiabatically, we show how two-qubit entangling operations can be performed on relatively fast 100ns timescales. The entangling operations are then simulated in the presence of experimentally measured quasistatic noise. The fidelities are typically only around 90%, pointing to the need for further improvement via shaped-pulse optimization.

* This work by was supported by the National Science Foundation under Grant No. 1620740 and by the Army Research Office under Grant No. W911NF-17-1-0287

4:06PM H35.00009: Induced quantum dot probe for qubit and material characterization CHARLES TAHAN (Presenter), YUN-PIL SHIM, RUSKO RUSKOV, HILARY HURST, Laboratory for Physical Sciences — We propose a non-destructive means of characterizing quantum dot parameters across a semiconductor wafer by inducing a quantum dot on the material system of interest with a separate probe chip that can also house the measurement circuitry. We show that a single wire can create the dot, determine if an electron is present, and be used to measure critical device parameters. Adding more wires enables more complicated setup and measurements. As one application for this concept we consider silicon metal-oxide-semiconductor and silicon/silicon-germanium quantum dot qubits relevant to quantum computing and show how to measure low-lying excited states (so-called `valley' states) in a novel way. The approach provides a simple and flexible method for characterization applicable to various quantum systems.

4:18PM H35.00010: Device-level modeling of hole quantum dot qubits in germanium* MITCHELL BRICKSON (Presenter), ANDREW BACZEWSKI, WILL HARDY, NOAH T JACOBSON, TZU-MING LU, LEON MAURER, DWIGHT R LUHMAN, Sandia National Laboratories — Holes in Ge quantum wells in Ge/SiGe heterostructures have a number of promising properties that have made them the target of growing interest for qubit applications. These include strong intrinsic spin-orbit coupling, the absence of valley degeneracy, and small effective masses. In this talk, we will describe ongoing work towards developing comprehensive models of these systems to facilitate the design and optimization of devices and the rationalization of experiments. We make use of electrostatic/strain modeling to compute the potential landscape and capacitances of a given device structure. The potential landscape is fed into a multi-band effective mass theory, with other parameters drawn from first principles models, to extract a qubit Hamiltonian. We will report on work describing ongoing quantum dot experiments and make projections pertaining to qubit tunability and performance.

*This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences, user facility. Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525.

4:30PM H35.00011: EDSR of a single heavy hole in a lateral GaAs/AlGaAs quantum dot qubit SERGEI STUDENIKIN (Presenter), MOTOI TAKAHASHI, GUY AUSTING, ALEX BOGAN, LOUIS GAUDREAU, MAREK J KORKUSINSKI, PIOTR ZAWADZKI, ANDREW SACHRAJDA, National Research Council of Canada, LISA A TRACY, JOHN RENO, TERRY HARGETT, Sandia National Laboratories — Single holes are attractive as spin qubits due to their advantageous properties which include a reduced hyperfine interaction, a strong spin-orbit coupling for sub-nanosecond spin rotations, and the absence of valley complications. Here we report single hole electric dipole spin resonance (EDSR) measurements over the 20-50 GHz range taking advantage of the strong spin-orbit coupling. The experiment was performed in a GaAs double quantum dot device described in [1] tuned in such way that only one of the dots contained a single heavy hole with the Fermi level of the adjacent lead positioned in between Zeeman split spin states. In this situation one hole is initialized in the lowest spin level and the current is blocked. A small microwave voltage is applied to a plunger gate to mediate EDSR rotating the hole spin from the lower to the upper spin level allowing the hole to tunnel to the lead. The spin resonance is detected as an increase in current when the resonant condition is fulfilled. The second dot is used as an auxiliary tool to tune the g-factor via a strong spin-dependent tunnel coupling[1]. We show that g-factor can be tuned in the range of 30% by a small change of the voltage applied to the auxiliary dot plunger gate.

Origins and enhancement of hole spin-mixing in InAs quantum dot molecules

ARTHUR LIN (Presenter), Joint Quantum Institute, University of Maryland and NIST, MATTHEW F DOTY, Department of Materials Science and Engineering, University of Delaware, GARNETT BRYANT, National Institute of Standards and Technology — Hole spins in self-assembled InAs quantum dots molecules (QDMs) are a strong candidate for qubit architecture due to their all-optical operation and enhanced tunability via voltage bias across the two dots. In order to capitalize on the all-optical operation and the enhanced tunability, we exploit the spin-mixing provided by the “molecule-like” coupled hole states. Through an atomistic tight-binding model and perturbative field analysis, we discuss the origin of spin-mixing and compare it with previous models using effective Hamiltonians. We then apply our understanding to the case where the GaAs inter-dot region is alloyed with a dilute amount of Bi. Replacing As atoms with the heavier Bi atoms enhances spin-orbit effects and, in turn, increases spin-mixing. However, it complicates the model, as atomistic alloying effects have to be considered, something not explored by prior models. Finally, we briefly discuss the practical operation of InAs/GaBiAs QDM qubits with the enhanced spin-mixing.

Controlling hole spin in quantum dots: Rashba or not Rashba

GARNETT BRYANT (Presenter), National Institute of Standards and Technology, ARTHUR LIN, Physics, University of Maryland — Hole spins in semiconductor quantum dots (QD) are promising qubits. Zeeman-split states form two-level systems with splitting determined by the physical spin of the hole. Due to strong spin-orbit coupling, hole spin orientation is locked to the QD axis for magnetic fields B away from the Voigt configuration. However, in Voigt configuration, the hole spin displays significant texture across the dot but is weakly polarized. Application of an electric field parallel or antiparallel to B in the Voigt configuration restores the hole spin. This spin control can be related to the QD geometry. The question remains whether this can be explained as a Rashba effect originating from interface fields or is inherent to an atomistic description of hole spins in QDs. Tight-binding theory is used to study GaAs/AlAs QDs with a graded alloy describing the QD interface to minimize Rashba effects of sharp interfaces. The results are compared with results for QDs with sharp interfaces. Several examples illustrate how a graded interface influences the spin locking seen for QDs with sharp interfaces and how this changes spin texture and spin polarization in the Voigt configuration. The results are used to assess the contribution of Rashba effects.

Session H36 DCOMP: Real-Space Methods for Large Scale Electronic Structure Problems

BCEC 205C - Leeor Kronik, Weizmann Institute of Science - Tag(s): Invited

Real-space numerical grid methods: The next generation of electronic structure codes

JAMES CHELIKOWSKY (Presenter), University of Texas at Austin — Two physical ingredients, pseudopotentials and density functional theory, are widely used in electronic structure computations for a variety of materials applications. If we wish to address large, complex systems, the implementation of these ingredients on high performance computational platforms is vital. Real space grid methods offer a compelling vehicle for such computations. These methods are mathematically robust, very accurate and well suited for modern, massively parallel computing resources [1]. I will illustrate the utility of these methods as implemented in the PARSEC code [2]. Key algorithms in this code include subspace filtering based on Chebyshev polynomials for an accelerated eigenvalue solution, spectrum slicing for an added level of parallelism, Cholesky QR algorithms to improve the performance of orthogonalization, and a 2D partition of the wave functions for efficient matrix-vector operations. Applications will be illustrated for nanostructures containing tens of thousands of atoms.


*Supported by a subaward from the Center for Computational Study of Excited-State Phenomena in Energy Materials at the Lawrence Berkeley National Laboratory, which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DEAC02-05CH11231.
3:06PM H36.00002: Large-scale density-functional calculations in real space and its application to bilayer graphene and semiconductor epitaxial growth [Invited] ATSUSHI OSHIYAMA (Presenter), Institute of Materials and Systems for Sustainability, Nagoya University — Facing current and future massively parallel architecture of supercomputers, we need to make close collaboration between the fields of physical science and computer science. Such collaboration we name COMPUTICS is already in progress (http://computics-material.jp/index-e.html). I here explain an example of such collaboration which allows us to perform total-energy electronic-structure calculations based on the density-functional theory (DFT) in the real-space scheme for tens-of-thousands-atom systems and also the real-space Car-Parrinello Molecular Dynamics simulations for thousands-of-atom systems. I first explain how we are able to perform such large-scale computations efficiently in our code named RSDFT. Recent development of the device simulation combined with the non-equilibrium Green's function (NEGF) method and its application to Si nanowire MOSFETs are also reported. As examples of the application to materials science, I will discuss (1) the localization of Dirac electrons induced by moire pattern in twisted bilayer graphene, (2) ammonia decomposition and N incorporation on epitaxially grown GaN films, (3) intrinsic carrier traps near SiC/SiO2 interfaces, and possibly (4) the formation of amorphous systems with thousands of atoms.

In collaboration with J.-I Iwata (Advance Soft), D. Takahashi (U Tsukuba), G. Milnikov (Osaka U), N. Mori (Osaka U), K. Uchida (Kyoto Inst Tech), Y.-i. Matsushita (Tokyo Inst Tech), K. M. Bui (Nagoya U), M. Boero (Strasbourg U), and K. Shiraishi (Nagoya U).

3:42PM H36.00003: Discontinuous projection method for large, accurate electronic structure calculations in real space* [Invited] JOHN PASK (Presenter), Lawrence Livermore Natl Lab — For decades, the planewave (PW) pseudopotential method has been the method of choice for large, accurate Kohn-Sham calculations of condensed matter systems, in ab initio molecular dynamics simulations in particular. However, due to its reliance on a Fourier basis, the method has proven notoriously difficult to parallelize at scale, thus limiting the length and time scales accessible. In this talk, we discuss new developments aimed at increasing the scales accessible substantially, while retaining the fundamental simplicity, systematic convergence, and generality instrumental to the PW method's success in practice. The key idea is to release the constraint of continuity in the basis set, and with the freedom so obtained, employ a basis of local Kohn-Sham eigenfunctions to solve the global Kohn-Sham problem. In so doing, the basis obtained is highly efficient, requiring just a few tens of basis functions per atom to attain chemical accuracy, while simultaneously strictly local, orthonormal, and systemically improvable. We show how this basis can be employed to accelerate current state-of-the-art real-space methods substantially by reducing the dimension of the real-space Hamiltonian by up to three orders of magnitude. Results for metallic and insulating systems of up to 27,000 atoms using up to 38,000 processors demonstrate the scalability of the methodology in a discontinuous Galerkin formulation. Proceeding via projection of the real-space Hamiltonian instead promises to reach larger scales still.

*This work was performed, in part, under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Support for this work was provided through the Scientific Discovery through Advanced Computing (SciDAC) program funded by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences.
AMIR NATAN (Presenter), Physical Electronics, Tel-Aviv University — The use of hybrid and screened hybrid functionals in Density Functional Theory (DFT) became popular as they allow to reduce the error between the calculated and experimentally measured properties. The calculation of the Fock exchange operator, required for those methods, is becoming a computationally prohibitive task with system size. An efficient approach, is to replace the explicit calculation of the Fock operator with its projection on the Hilbert sub-space that is spanned by the previous self-consistent field (SCF) occupied eigenvectors. It is possible to extend the method by projecting also on low lying empty eigenvectors to calculate also the empty eigenvalues. We have implemented this method1 within the PARSEC2,3 real-space code and combined it with efficient Poisson solvers4 and further hardware acceleration by Graphical Processing Units (GPUs) to achieve affordable hybrid calculations of atomistic structures with 1000 atoms on a single workstation5. We demonstrate the efficiency of this method by calculating the electronic properties of silicon quantum dots (QD) and graphene nano-ribbons with hybrid and screened hybrid functionals (e.g. PBE0 and HSE)5. We show how the formalism can be equally applied in real-space to 3D6 and 2D periodic systems.

References:


* A.N. thanks ISF grant 1722/13 for funding.
2:30PM H37.00001: Thermodynamic properties of the Shastry-Sutherland model from quantum Monte Carlo simulations  
ANNA HONECKER (Presenter), Laboratoire de Physique Théorique et Modélisation, Cergy-Pontoise University, IDO NIESEN, Institute for Theoretical Physics, University of Amsterdam, JONAS STAPMANN, Institut für Theoretische Festkörperphysik, RWTH Aachen University, BRUCE NORMAND, Neutrons and Muons Research Division, Paul Scherrer Institute, FREDERIC MILA, Institute of Theoretical Physics, Ecole Polytechnique Fédérale Lausanne (EPFL), PHILIPPE CORBOZ, Institute for Theoretical Physics, University of Amsterdam, STEFAN WESSEL, Institut für Theoretische Festkörperphysik, RWTH Aachen University — We investigate the minus-sign problem that afflicts quantum Monte Carlo (QMC) simulations of frustrated quantum spin systems, focusing on spin S=1/2, two spatial dimensions, and the extended Shastry-Sutherland model. We show that formulating the Hamiltonian in the diagonal dimer basis leads to a sign problem that becomes negligible at low temperatures for small and intermediate values of the ratio of the inter- and intra-dimer couplings. This is a consequence of the fact that the product state of dimer singlets is the exact ground state both of the extended Shastry-Sutherland model and of a corresponding sign-problem-free model. We map the sign problem throughout the extended parameter space from the Shastry-Sutherland to the fully frustrated bilayer model and compare it with the phase diagram computed by tensor-network methods. We use QMC to compute with high accuracy the temperature dependence of the magnetic specific heat and susceptibility of the Shastry-Sutherland model for large systems up to a coupling ratio of 0.526(1) and down to low temperature.

2:42PM H37.00002: Thermal Critical Points and Quantum Critical End Point in the Frustrated Bilayer Heisenberg Antiferromagnet  
JONAS STAPMANN, RWTH Aachen University, PHILIPPE CORBOZ, University of Amsterdam, FREDERIC MILA, EPFL Lausanne, ANDRAES HONECKER, Universite de Cergy-Pontoise, BRUCE NORMAND, Paul Scherer Institute, Villingen, STEFAN WESSEL (Presenter), RWTH Aachen University — We present a quantum Monte Carlo scheme for the simulation of frustrated quantum magnets that allows us to reduce or even eliminate the spin-problem for several dimerized quantum spin systems. We discuss in particular its application to the thermal properties of the spin-1/2 Heisenberg model on a frustrated square lattice bilayer. At zero temperature for the later model, a discontinuous quantum phase transition separates an interlayer singlet phase from an antiferromagnetic ground state formed by interlayer triplets. We show that this discontinuous transition extends up to finite temperatures and terminates in a quantum critical point. We identify this critical point as belonging to the Ising universality class, alert long-range order being absent at finite temperatures. We furthermore trace the discontinuous quantum phase transitions between the fully frustrated and the unfrustrated bilayer model using iPEPS tensor network methods. In particular, we identify a quantum critical end point that terminates the quantum critical line originating from the critical point of the unfrustrated bilayer system on the discontinuous transition line.

2:54PM H37.00003: Dimers on the checkerboard: model, partition sum, and correlations*  
ALEXANDER SEIDEL (Presenter), Department of Physics, Washington University in St. Louis, JULIA WILDEBOER, Department of Physics, Arizona State University — We present analytic results on a special dimer model on the (sem non-bipartite) checkerboard that does not allow for parallel dimers surrounding diagonal links. We report exact results on the enumeration of closed packed dimer coverings on finite checkerboard lattices under periodic boundary conditions. Further, we comment on the behavior of the dimer-dimer correlations and find that the correlations between any two dimers vanishes identically if the distance between them is larger than two unit cells.

*JW thanks NSF DMR 1306897 and NSF DMR 1056536 for partial support.

3:06PM H37.00004: Semiclassical Analysis of Quantum Dimer Models*  
GARRY GOLDSTEIN (Presenter), Physics, Rutgers University, CLAUDIO CASTELNOVO, Physics, Cambridge University, GABRIEL KOTLIAR, Physics, Rutgers University, ALEXEI TSVELIK, Physics, Brook Haven National Laboratory — We use the slave boson approach to develop the semiclassical description of the Rokshar Kivelson square lattice quantum dimer model, which allows a 1/S expansion. The action reproduces a generalized height representation. We extend these results to the dimer model on the cubic lattice, where we obtain emergent quantum electrodynamics description. The estimated speed of light: c = S/2*Sqrt([[J − V ]]/4)). We confirm aspects of the height mapping such as the correlation between the sign of the terms in the height action and the sign of the potential term in the RK Hamiltonian. In dimensions D = 2, 3 the QED emerges at wave vectors (π,π) and (π,π,π) respectively. Our estimate of the RK parameter is 1/16 which is within a 20 to 30 percent of the exact value of 1/4π. We extend our analysis to the hexagonal and diamond lattices, and we find that the speed of light for the diamond lattice is given by c^2 = 8^4*(J − V )/64.

*A.M.T. is supported by the Condensed Matter Physics and Materials Science Division, in turn funded by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DESC0012704. This work was supported by the Engineering and Physical Sciences Research Council (EPSRC) Grant No. EP/M007065/1 (C.C. and G.G.) and by NSF grant No. DMR-1733071 (G.G.)
3:18PM H37.00005: Quantum Order-By-Disorder in Frustrated Spin Nanotube Models* PREMALA CHANDRA (Presenter), PIERS COLEMAN, Rutgers University, Piscataway NJ, PETER P. ORTH, Iowa State University, Ames IA, SHIVAJI SONDHI, Princeton University, Princeton NJ — Thermally driven order-by-disorder has been extensively studied in two-dimesional frustrated Heisenberg magnets where it gives rise to long-range discrete order. Here we discuss the quantum analogue in frustrated magnets wrapped around one-dimensional nanotubes that we call "wrapped magnets". We show that as a function of the ratio of the frustrated bond couplings, wrapped magnets develop quantum phase transitions into states with nematic spin orders. For the simplest J1-J2 wrapped magnet, the emergent order parameter has Z2 symmetry and thus can undergo a transition from disordered to ordered at T=0 (D = 1+ 1). The quantum critical point is in the Ising universality class, and has gapless Ising excitations. In more complex models, such as the wrapped windmill model, there is the interesting possibility of an intermediate spin Luttinger liquid phase.

*This work is partially supported by DOE Basic Energy Science grant DE-FG02-99ER45790 (P. Coleman).

3:30PM H37.00006: Magnetization Process of the Triangular- and Kagome-Lattice Antiferromagnets TORU SAKAI (Presenter), HIROKI NAKANO, Graduate School of Material Science, University of Hyogo — The S = 1/2 kagome- and triangular-lattice Heisenberg antiferromagnets are investigated under a magnetic field using the numerical-diagonalization method[1]. A procedure is proposed to extract data points with very small finite-size deviations using the numerical-diagonalization results for capturing the magnetization curve. For the triangular-lattice antiferromagnet, the plateau edges at one-third the height of the saturation and the saturation field are successfully estimated. This study additionally presents results of magnetization process for a 45-site cluster of the kagome-lattice antiferromagnet; the present analysis suggests that the plateau does not open at one-ninth the height of the saturation.In addition the quantum phase transition of the triangular-lattice antiferromagnet at the 1/3 magnetization with respect to the next-nearest-neighbor interaction[2].


3:42PM H37.00007: Identifying Hidden Spin Nematic Order with Interpretable Machine* KE LIU (Presenter), JONAS GREITEMANN, LODE C POLLET, Ludwig Maximilian University of Munich — Frustrated magnetism is one of the central topics in modern condensed matter physics, as frustration often acts as a firm source of unconventional states of matter. Canonical examples include various spin liquids and spin nematics. However, distinguishing these states and identifying their characterization are usually challenging. In this talk, we present a machine learning protocol to detect and discern general spin-orientation orders. This method may be used as an alternative tool in studying phase transitions in frustrated spin and orbital systems, and may prove useful for identifying hidden spin nematics and ruling out spurious spin liquid candidates.

*This work is supported by FP7/ERC Consolidator grant No. 771891 (Lode Pollet).

3:54PM H37.00008: Uncovering anisotropic magnetic phases via fast dimensionality analysis* MANOHAR KARIGERASI (Presenter), Materials Science and Engineering, University of Illinois Urbana-Champaign, LUCAS WAGNER, Physics, University of Illinois Urbana-Champaign, DANIEL P SHOEMAKER, Materials Science and Engineering, University of Illinois Urbana-Champaign — A quantitative geometric predictor for the dimensionality of magnetic interactions is presented. This predictor is based on networks of superexchange interactions and can be quickly calculated for crystalline compounds of arbitrary chemistry, occupancy, or symmetry. The resulting data are useful for classifying structural families of magnetic compounds. We have examined compounds from a demonstration set of 42 520 materials with 3d transition metal cations. The predictor reveals trends in magnetic interactions that are often not apparent from the space group of the compounds, such as triclinic or monoclinic compounds that are strongly 2D. It can be used to identify quantum spin liquids, cuprate superconductors and other quasi-dimensional systems. We present specific cases where the predictor identifies compounds that should exhibit competition between 1D and 2D interactions, and how the predictor can be used to identify sparsely populated regions of chemical space with as-yet-unexplored topologies of specific 3d magnetic cations.1


*This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the United States Department of Energy, Office of Basic Energy Sciences.
We present our \( ^{23}\text{Na} \) and \( ^{75}\text{As} \) NMR study of the over-doped pnictide \( \text{NaFe}_{1-x}\text{Cu}_x\text{As} \), which has been demonstrated to be a possible Mott insulator near \( x \approx 0.5 \) [1,2]. Our NMR spectral-weight and linewidth analysis of the \( ^{23}\text{Na} \) quadrupolar spectrum reveals inequivalent Na sites and indicates a progressive formation of real space Cu and Fe stripe ordering as the Cu concentration approaches 0.5. Our spin-lattice relaxation data shows an antiferromagnetic transition at 190 K for \( x = 0.48 \). At lower Cu concentration there is a spin-glass transition evident from both susceptibility and spin-lattice relaxation data that appears at 80 K for \( x = 0.39 \). We have performed numerical simulation of our \( ^{75}\text{As} \) lineshape by testing a Cu-induced staggered magnetization model and discuss these in the context of the \( ^{23}\text{Na} \) NMR data. [1] Song, Yu, et al., Nat. Commun. 7, 13879 (2016). [2] C.E. Matt et al. Phys. Rev. Lett. 117, 097001 (2016)

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**4:18PM H37.00010: Tuning Magnetic Order with Iron Intercalation in Transition Metal Dichalcogenides**

CAOLAN JOHN (Presenter), SPENCER DOYLE, ERAN MANIV, Physics, University of California, Berkeley — The transition metal dichalcogenides are a class of two-dimensional materials currently under intense research due to their attractive electronic properties. Through the process of intercalation, magnetic atoms can be inserted between the layers of these materials to introduce long range magnetic order, enabling the exploration of magnetism in these systems. I will present magnetization and thermodynamic measurements that indicate precise control of this introduced magnetic order in iron intercalated \( \text{NbS}_2 \), with antiferromagnetic order being established at iron intercalation values above \( x = 1/3 \) in \( \text{Fe}_x\text{NbS}_2 \). In addition, I will discuss evidence of a new frustrated magnetic order emerging below critical intercalation values.

*Caolan John is supported by the Haas Scholars Program and by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4374.

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**4:30PM H37.00011: Magnetization plateaus in \( \text{Tb}_2\text{SrFe}_2\text{O}_7 \)**

HUIBO CAO (Presenter), YAN WU, WEI TIAN, Neutron Scattering Division, Oak Ridge National Laboratory, JAE-WOOK KIM, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University — Discovery of emergent magnetic states has drawn a lot of interest in studying geometrically frustrated magnets. We recently studied magnetization plateaus in a layered perovskite \( \text{Tb}_2\text{SrFe}_2\text{O}_7 \). \( \text{Tb}_2\text{SrFe}_2\text{O}_7 \) has a bilayer perovskite structure (\( \text{A}_3\text{B}_2\text{O}_7 \)) with Tb and Sr both at A-sites alternately ordered along the c-axis. Different from the multiferroic \( \text{Ca}_2\text{SrFe}_2\text{O}_7 \) that hosts the polar crystal structure and the magnetic ordered state with canted Fe moments, \( \text{Tb}_2\text{SrFe}_2\text{O}_7 \) has the non-polar structure symmetry of \( \text{P}42/mnm \) and the antiferromagnetic structure for the Fe-sublattice below 600 K. The magnetization plateaus were observed below the second transition at 15 K. With the field applied along c-axis, three plateaus were observed. Single crystal neutron diffraction revealed that the magnetic transition at 15 K is from magnetic order of Tb-sublattice accompanied with the spin reorientation of Fe-sublattice. It was also proved that the order of 2-in-2-out spin structure is due to magnetic coupling with the Fe-sublattice. In this presentation, I will show the evolution of the spin structure with temperature and magnetic field and disclose the nature of the magnetization plateaus in \( \text{Tb}_2\text{SrFe}_2\text{O}_7 \).

*This research used resources at SNS and HFIR, DOE Office of Science User Facilities operated by the ORNL.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H38 GMAG DMP: Monolayer Magnets
2:30PM H38.00001: First-principles approach to novel 2D ferromagnets  
SILVIA PICOZZI (Presenter), HRISHIT BANERJEE, CNR-SPIN Chieti (IT), Consiglio Nazionale delle Ricerche — There is currently an increasing enthusiasm towards long-range magnetic order in two-dimensional materials (such as CrI3 and Cr2Ge2Te6), from the fundamental and from the applicative point of view, from theory and from experiments. In this work, we carry out an extensive investigation based on density functional theory on an extended class of such materials, starting from the database of exfoliable materials reported in N. Mounet et al., Nature Nano. 13, 26 (2018). In the aim of optimizing the properties of 2D-ferromagnets, in particular focusing on an increase of the Curie temperature, our analysis ranges from semiconducting chalcohalides (with formula M-VI-VI, where M is a transition metal, VI and VII are chalcogen and halogen elements) to di-halides (with formula M-(VII)2). In addition to structural and electronic properties, we analyse magnetic properties, in terms of magnetic moments, Heisenberg exchange coupling constants and magnetic anisotropy energy. Some of the considered materials (such as CrSBr or NiBr2) show exchange coupling constants significantly larger than the prototypical CrI3, so they might be promising candidates for larger transition temperatures.

2:42PM H38.00002: Anisotropic magnetic interactions in CrI3  
IGOR MAZIN (Presenter), United States Naval Research Laboratory, SERGEY STRELTSOV, Ural Federal University, Ekaterinburg, Russia, DANIEL KHOMSKII, University of Cologne, Germany — CrI3 is famous among van-der-Waals materials because it displays ferromagnetism in the bulk form, and also in the monolayer form, with an only slightly reduced Curie temperature. Since Heisenberg and XY models do not allow long-range ordering in 2D, it was initially assumed that the magnetic Hamiltonian in CrI3 is of the Ising symmetry. However, it was later shown that it is not the single-site anisotropy, but exchange interaction anisotropy (driven by the spin-orbit coupling on I) that ensures the high Curie temperature. It was assumed, however, without any theoretical justification, that this interaction is of the simplest, pseudo-Ising, form, namely $S^z S^z$, $z$ being the global hexagonal axis. In this talk, we will present first principle calculations showing that not only this pseudo-Ising interaction is present in the system, but all three nearest-neighbor anisotropic terms allowed by symmetry ($S^x S^y S^y$ and $S^y S^z S^z$, plus proper rotations for two other bonds) are of similar order.

2:54PM H38.00003: Interlayer magnetic coupling in bilayer CrI3: A first-principles study  
SANG-HOON LEE (Presenter), CHANUL KIM, YOUNG-WOO SON, School of Computational Sciences, Korea Institute for Advanced Study — Recent discoveries of two-dimensional van der Waals (vdW) magnetic materials, especially CrI3, has accelerated various experimental and theoretical investigations. It has been shown that CrI3 has the intriguing interlayer magnetic orderings: In contrast to the ferromagnetic bulk crystal, a bilayer CrI3 shows an antiferromagnetic coupling between the layers that is hardly computed as magnetic ground states within conventional first-principles computational methods. In this talk, we show that the spin-dependent vdW interactions and the extended on-site correlation are of vital importance in describing the magnetism in a bilayer CrI3 within ab initio computation schemes.

3:06PM H38.00004: Tuning Magnetism in Atomically Thin CrI3 by Hydrostatic Pressure  
TINGXIN LI (Presenter), SHENGWEI JIANG, JIE SHAN, KIN FAI MAK, Cornell University — Atomically thin CrI3 has recently been discovered as a two-dimensional magnetic semiconductor. Remarkably, while monolayer CrI3 is ferromagnetic, antiferromagnetic inter-layer coupling is favored in few-layer CrI3. Because the interlayer exchange coupling is relatively weak, it is expected to be sensitive to external perturbations. Indeed, control of the interlayer magnetic order in atomically thin CrI3 by an electric field and electrostatic doping has recently been demonstrated. Here we report an experimental study of the magnetic order in few-layer CrI3 under hydrostatic pressure. We utilized the giant tunneling magnetoresistance observed in CrI3 spin-filter devices to probe the interlayer magnetic order. We found that the magnetic properties of atomically thin CrI3 can be tuned by applying a moderate pressure.

3:18PM H38.00005: Criticality, anisotropy and dimensionality in the van der Waals ferromagnet CrI3  
EFRÉN NAVARRO-MORATALLA (Presenter), Instituto de Ciencia Molecular, Universitat de Valencia, MATHIAS AUGUSTIN, DINA ABDUL WAHAB, School of Mathematics and Physics, Queen's University Belfast, IVAN JESUS VERA MARUN, KOSTYA NOVOSELOV, School of Physics and Astronomy, University of Manchester, RICHARD F. L. EVANS, Department of Physics, The University of York, ELTON J. G. SANTOS, School of Mathematics and Physics, Queen's University Belfast — Magnetic order is prohibited in the 2D Heisenberg isotropic model at finite temperatures by the long-established theorem put forward by Mermin and Wagner. Indeed, the recent studies on true 2D magnets have nothing but confirmed that magnetic anisotropy is pivotal for eliminating this restriction and allowing, for example, the onset of 2D ferromagnetism in a bilayer of chromium germanium telluride, or in a single layer of chromium triiodide (CrI3). These materials happen to be two identical uniaxial systems from the point of view of their magnetic anisotropy. However, the critical behavior of these 2D magnets is still a matter of debate amidst contradictory reports of the critical exponents. By modelling magnetometry experiments on bulk crystals and magneto-optic data of the monolayer we will shed new light on the universality class of these van der Waals magnets.
Distinct spin-lattice and spin-phonon interactions in monolayer magnetic CrI₃*

LUCAS G. WEBSTER, Department of Physics, Astronomy, and Geosciences, Towson University, 8000 York Road, Towson, MD 21252, USA., Towson University, LIANGBO LIANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, Oak Ridge National Lab, JIA-AN YAN (Presenter), Department of Physics, Astronomy, and Geosciences, Towson University, 8000 York Road, Towson, MD 21252, USA., Towson University — We apply the density-functional theory to study various phases (including non-magnetic (NM), anti-ferromagnetic (AFM), and ferromagnetic (FM)) in monolayer magnetic chromium triiodide (CrI₃). We found that (1) the introduction of magnetism in monolayer CrI₃ gives rise to metal-to-semiconductor transition; (2) the electronic band topologies as well as the nature of direct and indirect band gaps in either AFM or FM phases exhibit delicate dependence on the magnetic ordering and spin-orbit coupling; and (3) the phonon modes involving Cr atoms are particularly sensitive to the magnetic ordering, highlighting distinct spin-lattice and spin-phonon coupling in this magnet. First-principles simulations of the Raman spectra demonstrate that both frequencies and intensities of the Raman peaks strongly depend on the magnetic ordering. The polarization dependent A₁g modes at 77 cm⁻¹ and 130 cm⁻¹ along with the E₂g mode at about 50 cm⁻¹ in the FM phase may offer a useful fingerprint to characterize this material. Our results not only provide a detailed guiding map for experimental characterization of CrI₃, but also reveal how the evolution of magnetism can be tracked by its lattice dynamics and Raman response.

*Work supported by the NSF grant DMR 1709781.

Nature of the Magnetic Anisotropy in the Two-Dimensional Honeycomb Ferromagnet CrI₃*

FRANZ UTERMOHLEN (Presenter), INHEE LEE, KYUSUNG HWANG, Department of Physics, The Ohio State University, DANIEL WEBER, Department of Chemistry and Biochemistry, The Ohio State University, CHI ZHANG, Department of Physics, The Ohio State University, JOHAN VAN TOL, STEPHEN HILL, National High Magnetic Field Laboratory, JOSHUA E. GOLDBERGER, Department of Chemistry and Biochemistry, The Ohio State University, NANDINI TRIVEDI, P CHRIS HAMMEL, Department of Physics, The Ohio State University — The recent discovery of intrinsic ferromagnetism in two-dimensional (2D) van der Waals crystals, such as CrI₃, has drawn much interest due to its potential for future 2D spintronic applications; however, the nature of the anisotropic magnetic interactions that allow 2D ferromagnetic order in this system remains poorly understood. In this work, we provide a detailed description of the anisotropic spin interactions in monolayer CrI₃ using a microscopic spin Hamiltonian constructed from the symmetries of the system. We present the results of our mean field theory and linear spin-wave theory calculations for this model and explain which interaction is responsible for stabilizing 2D ferromagnetic order in this system. Finally, we provide estimates for the strength of each interaction by comparing these results to our experimental data from angle-dependent ferromagnetic resonance on bulk CrI₃ single crystals.

*NT acknowledges the support of the Center for Emergent Materials: an NSF MRSEC, under award number DMR-1420451. FU acknowledges support from the DOE-BES grant DE-FG02-07ER46423.

Origin of magneto-crystalline anisotropy underlying 2D ferromagnetism in CrI₃ single crystals from ferromagnetic resonance

INHEE LEE (Presenter), KYUSUNG HWANG, UTERMOHLEN G. FRANZ, DANIEL WEBER, CHI ZHANG, Ohio State University, JOHAN VAN TOL, STEPHEN HILL, National High Magnetic Field Laboratory, JOSHUA E. GOLDBERGER, NANDINI TRIVEDI, P CHRIS HAMMEL, Ohio State University — We provide the detailed magnetic anisotropy structure of a CrI₃ single crystal obtained through the measurement of the angle dependence of ferromagnetic resonance. We present a microscopic spin model describing the anisotropic interactions in a monolayer in terms of the experimentally measured Heisenberg, Kitaev, symmetric-anisotropic and quadrupole interactions that incorporate the material’s crystal symmetries. Comparison of Tc calculated using spin wave theory with the experimentally known values reveals that CrI₃ is dominantly a Kitaev ferromagnet rather than Heisenberg. We also find that symmetric-anisotropic interaction stabilizes 2D ferromagnetic order by opening the magnon gap ~ 0.4 meV at the center of the Brillouin zone and we predict a Kitaev-interaction-induced ~ 5 meV magnon gap opening at the Dirac point. This work clarifies the complex anisotropic behaviour of spins in CrI₃, opening a route to develop 2D ferromagnets with higher Tc and explore novel 2D spin orders arising from Kitaev physics in van der Waals materials.
magnetic properties make the ScCl monolayer a promising candidate for spintronic applications. In addition, the ScCl monolayer possesses excellent thermal and dynamical stabilities and great feasibility of experimental exfoliation from its layered bulk. These intriguing electronic and ferromagnetism can also be extended to ScCl bilayers. Moreover, a small amount of hole doping can turn the ScCl monolayer into a half-metal and further improves the magnetic moment and Curie temperature. The novel monolayer (45 K) and the boiling point of liquid nitrogen (77 K). Moreover, a small amount of hole doping can turn the ScCl monolayer into a half-metal and further improves the magnetic moment and Curie temperature. The novel monolayer (45 K) and the boiling point of liquid nitrogen (77 K).

4:06PM H38.00009: Stacking-dependent magnetism in bilayer CrI3+ NIKHIL SIVADAS (Presenter), Cornell University, SATOSHI OKAMOTO, Oak Ridge National Lab, XIAODONG XU, University of Washington, CRAIG J FENNIE, Cornell University, DI XIAO, Carnegie Mellon University — We report the connection between the stacking order and magnetic properties of bilayer CrI3 using first-principles calculations. We show that the stacking order defines the magnetic ground state. By changing the interlayer stacking order one can tune the interlayer magnetism between antiferromagnetism and ferromagnetism. To measure the predicted stacking-dependent magnetism, we propose using a linear magnetoelectric effect. Our results not only gives a possible explanation for the observed antiferromagnetism in bilayer CrI3 but also have direct implications in heterostructures made of two-dimensional magnets.

*NS and CJF are supported by NSF through the Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM) (DMR-1539918), SO is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, DX and XX acknowledge the support from DOE BES Pro-QM EFRC (DE-SC0019443).

4:18PM H38.00010: Spectroscopic studies of magnetic ordering in two-dimensional trihalides and chromium-based compounds QIAN SONG (Presenter), Massachusetts Institute of Technology, YUFEI LIU, Physics, Peking University, ZHIHAI ZHU, JIARUI LI, CONNOR A OCCHIALINI, ABRAHAM LEVITAN, MIN GU KANG, JONATHAN PELLICARI, Massachusetts Institute of Technology, LI YUE, Physics, Peking University, RICCARDO COMIN, Massachusetts Institute of Technology — Since the discovery of layer-dependent ferromagnetism in chromium triiodide(CrI3), the two-dimensional(2-D) crystals with intrinsic magnetism persisting even into monolayer attract widespread concern. This kind of 2-D magnets provide us a totally new platform for further development of spintronics, magnetoelectronics etc. Even though the details of the magnetic coupling between layers have not been fully understood, such ferromagnetism in CrI3 give us hint that other 2-D trihalides and chromium-based compounds may also show remarkable magnetic properties down to thin layers. Here we will present our work on looking for new 2-D magnets and the understanding of the magnetic ordering in these materials.

*This work is supported by the National Key Research and Development Program of China (2017YFA0204800), the Natural Science Foundation of China (21525311, 21773027), the Scientific Research Foundation of Graduate School of Southeast University (YBJj1773),

4:30PM H38.00011: High Curie-temperature intrinsic ferromagnetism and hole doping-induced half-metallicity in two-dimensional scandium chlorine monolayers+ BING WANG (Presenter), Southeast University — High Curie-temperature ferromagnetic two-dimensional (2D) materials with large spin polarization have been a long-sought goal due to their potential in spintronics applications. Here we report a promising 2D scandium chloride (ScCl) monolayer with intrinsic ferromagnetism and high Curie temperature up to 185 K, which is much higher than that of the reported CrI3 monolayer (45 K) and the boiling point of liquid nitrogen (77 K). Moreover, a small amount of hole doping can turn the ScCl monolayer into a half-metal and further improves the magnetic moment and Curie temperature. The novel ferromagnetism can also be extended to ScCl bilayers. In addition, the ScCl monolayer possesses excellent thermal and dynamical stabilities and great feasibility of experimental exfoliation from its layered bulk. These intriguing electronic and magnetic properties make the ScCl monolayer a promising candidate for spintronic applications.

*This work is supported by the National Key Research and Development Program of China (2017YFA0204800), the Natural Science Foundation of China (21525311, 21773027), the Scientific Research Foundation of Graduate School of Southeast University (YBJj1773),

4:42PM H38.00012: Probing magnetism of a 2D magnet with Pt through magnetoresistance+ TANG SU (Presenter), International Center for Quantum Materials, Peking University, MARK LOHMANN, JUNXUE LI, MOHAMMED ALGHAMDI, MOHAMMED ALDOSARY, YADONG XU, YAWEN LIU, VICTOR ORTIZ, WEI YUAN, University of California, Riverside, KENJI WATANABE, TAKASHI TANIGUCHI, 1-1 Namiki, Tsukuba, National Institute for Materials Science, JING SHI, University of California, Riverside — 2D magnetic materials have lately attracted tremendous research interest in condensed matter physics. Very interestingly, chromium triiodide (CrI3), an insulating member of the 2D magnet family, has been discovered to possess antiferromagnetic coupling between layers, as demonstrated by magneto-optic Kerr effect and tunneling measurements in ultra-thin samples. In our work, we place a CrI3 flake in direct contact with a pre-patterned Pt Hall bar which serves as a sensing layer. We observe a sharp increase in magnetoresistance (MR) at H(along c-axis) ~ 2T. This feature coincides with a major magnetization switching previously reported in CrI3 flakes with thickness above 3 layers. Temperature and field direction dependent MR measurements have also been conducted and the results reveal further information about the nature of the magnetic interactions. Our approach offers a unique platform to study magnetic ordering in CrI3 and other highly resistive 2D magnetic materials through electrical transport measurements. It also provides an interesting perspective for studying the intriguing physics of exchange proximity coupling and spin current effect at 2D van der Waals interfaces.

*This work was supported by DOE BES Award No. DE-FG02-07ER46351 and NSF-ECCS under Award No. 1610447.
4:54PM H38.00013: Dipolar interaction and exchange anisotropy in two-dimensional ferromagnetic quantum Heisenberg spin lattices.*

JOREN VANHERCK (Presenter), Physics Department, University of Antwerp, BART SORREE, Department of Electrical Engineering (ESAT), KU Leuven, WIM MAGNUS, Physics Department, University of Antwerp — Spin wave majority gates are considered as a viable beyond CMOS technology [1], if sufficiently scaled down. Although quantum effects are important when considering such scaled-down devices with thin ferromagnets, these are not sufficiently taken into account in today’s device simulations. Similarly, the effect of magnetic dipolar interaction on both the direction and magnitude of magnetization is poorly understood.

We present results [2] on the magnetization in two-dimensional ferromagnets with exchange anisotropy in an external magnetic field applied in an arbitrary direction. Using double-time temperature-dependent Green's functions, we take into account quantum and thermal effects and we show the existence of a magnetic reorientation transition in anisotropic Heisenberg ferromagnets. Additionally, the framework can be extended to fully take into account magnetic dipole-dipole interaction, including its effect on the magnetization direction.


*We acknowledge funding from IMEC.

5:06PM H38.00014: Checkerboard Antiferromagnetic Order in FeSe Monolayer

SHUANG QIAO (Presenter), Tsinghua University — Although the paramagnetic state has been confirmed in FeSe bulk via inelastic neutron-scattering (INS), the magnetic states in FeSe monolayer and thin films remain mysterious due to the difficulties in both experimental and theoretical approaches. Experimentally, current magnetic measurement techniques are extremely difficult to be applied to thin film structures. Theoretically, first principle calculation can not deal with paramagnetic system with strong spin fluctuations. Here we report a systematic approach based on surface defects and in-plane strain, and utilizing scanning tunneling measurements (STM) combining with first-principles calculations, to identify the magnetic states in FeSe monolayer and thin films. We provide a strong evidence of the existence of checkerboard antiferromagnetic order in FeSe monolayer by measuring and computing scanning tunneling microscopy images of two typical surface defects. The checkerboard antiferromagnetic order in FeSe monolayer is further verified by estimating the magnetic property of surface defect experimentally and theoretically. Moreover, we confirm the checkerboard antiferromagnetic order exists also in FeSe thin films by studying the electronic band structure evolution with in-plane strain.

5:18PM H38.00015: High Temperature Half-metallicity in Two-Dimensional CoGa2X4 (X=S, Se, Te)*

SHUQING ZHANG (Presenter), XIAOLONG ZOU, Tsinghua-Berkeley Shenzhen Institute — The recent discoveries of intrinsic ferromagnets CrI3 and Gr2Ge2Te6 with critical temperatures lower than 45 K create huge potential for spintronic applications of two-dimensional (2D) van der Waals crystals. Here, we discover a family of 2D half-metallic ferromagnets CoGa2X4 (X=S, Se or Te), which exhibit high critical temperature, fully polarized spin state and strain-dependent magnetization direction simultaneously. The Magnetocrystalline anisotropy energy calculation with spin-orbital coupling indicate that CoGa2X4 favor easy plane magnetizations, which are expected to have BKT transitions. According to the 2D XY model, the critical temperatures \( T_c \) of transitions for CoGa2X4 are much higher than room temperature. Further, under experimentally achievable biaxial tensile strain (2%~6%), the magnetization directions of CoGa2X4 could change from in-plane to out-of-plane, providing a route to control the efficiency of spin injection/detection. The proposed half-metallic CoGa2X4 system belong to the big family of layered AB2X4 compounds, and these materials would enrich the available 2D candidates for various applications.

*China Postdoctoral Science Foundation (No. 2018M631458)
**History-Dependent Dynamic Nuclear Polarization in Gallium Arsenide in the Resonant Spin Amplification Regime**

JOSEPH IAFRATE (Presenter), MICHAEL MACMAHON, MICHAEL J DOMINGUEZ, HUA-WEI HSU, VANESSA SIH, University of Michigan — Dynamic nuclear polarization (DNP) arises through the interaction of atomic nuclei in a material with spin-polarized electrons. An optically-driven electron system transfers spin polarization to the nuclei. In turn, nuclear spins produce a magnetic field that affects electron spin precession frequency. We use a pulsed laser to excite and measure electron spin polarization in a gallium arsenide epilayer, in the regime of resonant spin amplification. By measuring Kerr rotation as a function of applied magnetic field, we can detect the influence of the nuclear spins. We report an unexpected dependence of DNP on both magnetic field history and transverse electron spin polarization [1]. Variations of the applied field sequence and duration reveal a minutes-long precise memory of the particular field history of the system.


**Spin Dynamics in the Thermoelectric Li:MnTe Antiferromagnetic Semiconductor**

RAPHAEL HERMANN (Presenter), MICHAEL MANLEY, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge TN-37831-6064, USA, VASILE O GARLEA, DOUGLAS L ABERNATHY, Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6475, USA, HUAIZHOU ZHAO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People's Republic of China, JOSEPH P C HEREMANS, Department of Mechanical and Aerospace Engineering, Department of Physics, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH 43210, USA — We report the magnetic structure and excitation spectrum of Li0.03:MnTe, a material related to the MnTe antiferromagnetic semiconductor with a Néel temperature of ~307 K. MnTe was proposed to exhibits a strong contribution of magnon drag to the thermopower[1]. Neutron scattering reveals the magnetic structure and spin-spin correlations in the ordered and disordered phases of Li0.03:MnTe. Above the magnetic ordering temperature, strong quasielastic paramagnon scattering is observed. The characteristic energy width of the scattering is temperature independent and provides evidence for slow, ~30 fs, magnetic fluctuations. These data provide necessary input for modelling of the transport properties.


**Dependence of dynamic nuclear polarization on resonant spin amplification and external field history under periodic optical electron spin pumping**

MICHAEL MACMAHON (Presenter), JOSEPH IAFRATE, MICHAEL J DOMINGUEZ, HUA-WEI HSU, VANESSA SIH, University of Michigan — Greater control of nuclear spin polarization could provide breakthroughs in both classical and quantum information storage and processing. We use optical pump-probe techniques in a gallium arsenide epilayer to manipulate an electron spin polarization that persists over several pulse cycles1. The interference of spins excited from different pulses in a swept external magnetic field results in resonant spin amplification (RSA), and we demonstrate a dynamic nuclear polarization perpendicular to the electron spin polarization that actively responds to the external field sweep direction and magnitude of RSA. We also show that the electron-nuclear spin system retains memory of the external field history, including interruptions and reversals in magnetic field sweeps, and present a model that explains key features of these results.


*This work was supported in part by NSF and by the U.S. Department of Defense NDSEG program*
For spin-based quantum computation in semiconductors, dephasing of electron spins by a fluctuating background of nuclear spins is a main obstacle. It has been shown that in self-assembled InAs quantum dots, this nuclear background can be precisely controlled by periodically exciting single electron spins using optical laser pulses. A feedback mechanism between the electron spin polarization and the nuclear system focuses the electron spin precession frequency into discrete modes that are commensurate with the laser repetition rate. In such a spin-mode-locked system, the electron spin lifetime within individual dots can surpass the limit given by nuclear background fluctuations. Here we show that spin mode-locking is a universal phenomenon that also occurs in ensembles of lithographically-defined many-electron GaAs/AlGaAs dots [1]. This opens the door to achieve long electron spin coherence times also in systems that can be controlled in shape, size and position. We discuss possible mechanisms of spin mode-locking and show experiments that suggest that the optical Stark effect plays an important role in the nuclear focusing of our many-electron dots.


We have studied the dynamics of previously reported spin-dependent charge carrier recombination transitions in Tris(8-hydroxyquinolinato) aluminium (Alq3) thin films with both continuous wave [2] as well as pulsed [3] electrically detected magnetic resonance (EDMR) spectroscopy under bipolar injection conditions. The measurements revealed transverse charge carrier spin relaxation times, $T_2$, shorter, but of the same order of magnitude to those previously observed in other organic semiconductors thin films such as various π-conjugated polymers, spin-orbit induced $g$-strain of the charge carrier magnetic resonances, as well as the local hyperfine field distribution magnitudes of both the electrons and the holes. Our measurements show that, qualitatively, the nature of spin-dependent recombination transitions in Alq3 film is similar to that of the polymer materials and metal-organic complex Zinc phthalocyanine(ZnPc) [4].


This work has been supported by the National Science Foundation, NSF-DMR #1701427.

In this talk, we will show that the spin lifetime in OSECs can be further prolonged by improving the charge delocalization. HFI, originating from the coupling between electron spins and nuclei, has been demonstrated to strongly influence the spin dynamics in OSECs. Nevertheless, the role of charge localization on the HFI strength in organic thin films has not yet been experimentally investigated. In our PRL (120, 086602, 2018), the statistical relation hypothesis that the effective HFI of holes in regioregular poly(3-hexylthiophene) (P3HT) is proportional to $1/N^{0.5}$ has been examined, where $N$ is the number of the random nuclear spins within the envelope of the hole wave function. First, we verify that HFI is the dominant spin interaction in P3HT. Second, assuming that holes delocalize fully over the P3HT polycrystalline domain, the strength of HFI is experimentally demonstrated to be proportional to $1/N^{0.52}$ in excellent agreement with the statistical relation. Finally, the HFI of electrons in P3HT is about 3 times stronger than that of holes due to the stronger localization of the electrons.
4:06PM H39.00007: Two-electron-spin ratchets as a platform for microwave-free dynamic nuclear polarization of arbitrary material targets  PABLO ZANGARA, JACOB HENSHAW (Presenter), DANIELA PAGLIERO, Department of Physics, City College of New York, ASHOK AJAY, Department of Chemistry, University of California Berkeley, JEFFREY A REIMER, Department of Chemical and Biomolecular Engineering, University of California Berkeley, ALEXANDER PINES, Department of Chemistry, University of California Berkeley, CARLOS MERILES, Department of Physics, City College of New York — Recently, several schemes centered around the negatively charged Nitrogen Vacancy(NV) color center in diamond as means to hyperpolarize nuclei have been realized1–2. Here we theoretically consider the case of the NV and the substitutional nitrogen (P1) centers in diamond to show that outside protons spin-polarize efficiently upon a magnetic field sweep across the NV–P1 level anti-crossing. In particular, the nuclear polarization buildup during the low-to-high and high-to-low stages of the sweep cycle adds constructively regardless the relative sweep velocities. The system dynamics can be interpreted in terms of an NV–P1 spin ratchet whose sign depends on the relative timing of an accompanying optical excitation pulse. Our calculations indicate that the polarization transfer process is insensitive to the NV axis orientation, and efficient over a broad range of electron-electron and electron-nuclear spin couplings, even if the proxy spins suffers from short relaxation times.


4:18PM H39.00008: Spin-orbit coupling in antiferromagnetic MnTe*  GEN YIN (Presenter), Electrical and Computer Engineering, University of California, Los Angeles, JIE-XIANG YU, Physics, University of New Hampshire, YIZHOU LIU, ROGER LAKE, Electrical and Computer Engineering, University of California, Riverside, JIADONG ZANG, Physics, University of New Hampshire, KANG WANG, Electrical and Computer Engineering, University of California, Los Angeles — We show that the spin-orbit coupling (SOC) in α-MnTe impacts the transport behavior by generating an anisotropic valence-band splitting, resulting in four spin-polarized pockets near Gamma. A minimal k-dot-p model is constructed to capture this splitting by group theory analysis, a tight-binding model and ab initio calculations. The model is shown to describe the rotation symmetry of the zero-field planer Hall effect (PHE). The PHE percentage is determined by the SOC induced band shape, and is quantitatively estimated to be 25% ~ 31% for an ideal thin film with a single antiferromagnetic domain. The k-dot-p Hamiltonian given by this research is not only effective, but also minimal. The quartic spin-orbit coupling terms in the model is necessary, in the absence of which, the extra C4T symmetry rules out any Hall effect. The predicted value of PHE percentage is an order of magnitude greater than previous experimental observations, suggesting a vast space to optimize the material for device applications.

*This research is partially supported by SHINES, an EFRC funded by the US-DOE, BES under award #SC0012670, J.X.Y. and J.Z. were supported by the DOE of US, BES Award No. DE-SC0016424. G.Y. and K.W. are also supported by US NSF (DMR-1411085), and the ARO contract W911NF-15-1-10561.

4:30PM H39.00009: Paramagnon drag yields a high thermoelectric figure of merit in Li-doped MnTe*  YUANHUA ZHENG (Presenter), Ohio State University, TIANQI LU, Institute of Physics, Chinese Academy of Sciences, MD MOBARAK HOSSAIN POLASH, MORTEZA RASOULIANBOROUJENI, North Carolina State University, NING LIU, Institute of Physics, Chinese Academy of Sciences, MICHAEL MANLEY, Oak Ridge National Laboratory, YUAN DENG, Beihang University, PEIJIE SUN, XIAOLONG CHEN, Institute of Physics, Chinese Academy of Sciences, RAPHAEL HERMANN, Oak Ridge National Laboratory, DARYOOSH VASHAEE, North Carolina State University, JOSEPH P C HEREMANS, Ohio State University, HUAIZHOU ZHAO, Institute of Physics, Chinese Academy of Sciences — MnTe is an antiferromagnetic semiconductor with a Neel temperature of 307 K. In the antiferromagnet phase, the magnon-electron interaction gives rise to a magnon-drag contribution to thermopower. Surprisingly this magnon-drag thermopower extends to the paramagnetic phase. Experimental results provide evidence for the effect of locally ordered thermal fluctuations of magnetization with finite lifetime (paramagnons). When the lifetime of the paramagnons is longer than the electron-paramagnon scattering time, the paramagnons can effectively push the electrons and contributes to thermoelectric power. By analyzing the measured thermopower, resistivity, Hall coefficient, specific heat and magnetization, a quantitative explanation is given for thermopower of both the AFM and PM regime based upon the hydrodynamic theory [1]. As a result, the ZT of the best sample exceeds 1 at 950 K.

*YZ and JPH acknowledge the ARO MURI under grant number W911NF-14-1-0016. DV acknowledges partial support by Air Force Office of Scientific Research (AFOSR) under contract number FA9550-12-1-0225 and the National Science Foundation (NSF) under grant numbers ECCS-1351533, and CMMI-1363485.
4:42PM H39.00010: Modification of the Heavy Hole Wave-function in Multiply Occupied Magnetic Quantum Dots

James Piętka (Presenter), St. Bonaventure University, Peiyao Zhang, Tenzin Norden, Arman Najafi, Physics, State Univ of NY - Buffalo, Biplob Barman, Physics, University of Michigan-Flint, Yutsung Tsaí, Physics, Univ of Texas, Bruce Mccomboe, Jong E Han, Igor Zutic, Athos Petrou, Physics, State Univ of NY - Buffalo, Rafal M Oszwalowski, Physics, South Dakota School of Mines and Technology, Wen-Chung Fan, Wu-Ching Chou, National Chiao Tung University — We compare the magnetic field PL peak energy red shift of ZnTe Quantum Dots (QDs) embedded in a ZnMnSe matrix using two types of laser excitation: (a) Excitation at 405 nm (3.06 eV) with photon energy above the ZnMnSe matrix gap. This leads to electron-hole pair generation mainly in the matrix. (b) Excitation at 488 nm (2.54 eV) with photon energy below the ZnMnSe matrix gap but above the bandgap of the ZnTe QDs. In the latter case, carriers are excited directly into the ZnTe QDs.

The PL peak energy magnetic red shift is up to 3 times larger with 488 nm excitation compared to excitation using 405 nm excitation. Under 488 nm excitation an additional PL feature associated with the e_1l_1 shell is observed indicating multiple hole occupancy of the QDs. Using exact diagonalization, we study the doubly occupied quantum dot. We find that in our system, the enhanced exchange interaction between the hole and the Mn ion spins causes the triplet state to be the ground state. Furthermore, the hole-hole repulsion results in the extension of the hole wavefunction further into the ZnMnSe matrix which leads to enhanced magnetic PL red shift.

*NSF DMR 1305770

4:54PM H39.00011: Ferromagnetic Contacts to InSb nanowires

Yifan Jiang (Presenter), Department of Physics and Astronomy, University of Pittsburgh, Zedong Yang, School of Physics and Astronomy, University of Minnesota Twin Cities, Diana Car, Sasa Gazibegovic, Badaowy Ghada, Roy L. M. OP Hét Veld, TU Eindhoven, Sébastien Plissard, LAAS Toulouse, Erik P. A. M. Bakkers, TU Eindhoven, Vlad S Pribiag, School of Physics and Astronomy, University of Minnesota Twin Cities, Sergey M Frolov, Department of Physics and Astronomy, University of Pittsburgh — InSb nanowires are versatile platforms for a variety of quantum transport experiments. Here we develop ferromagnetic contacts onto InSb nanowires. We fabricate four terminal devices (spin-valve geometry) using both Ti/Au and CoFe contacts. At low temperature, both local and non-local experiments demonstrate hysteretic spin-valve like signals. Besides spin injection, we are considering other explanations, for example, the magneto-Coulomb effect. In addition, magnetized ferromagnetic contacts themselves create local magnetic fields, which may affect conductance in high g-factor InSb nanowires.

5:06PM H39.00012: Electrical Spin Injection into Silicon Nanowires with Axial Doping Gradient

Konstantinos Kountouriotis, Jorge L Barreda, Timothy Keiper, Department of Physics, Florida State University, Mei Zhang, Department of Industrial and Manufacturing Engineering, FAMU/FSU College of Engineering, Peng Xiong (Presenter), Department of Physics, Florida State University — For nanoscopic semiconductor spintronic devices, the all-important issue of the ferromagnet/semiconductor (FM/SC) interface becomes even more critical. Here we elucidate the effects of the FM/SC nano interface on electrical spin injection and detection, utilizing a unique type of Si nanowires (NWs) with an inherent axial doping gradient. Two-terminal and nonlocal four-terminal lateral spin-valve measurements were performed using different combinations from a series of FM contacts positioned along the same NW. The data are analyzed with a general model of spin accumulation in a normal channel under electrical spin injection from a FM, which reveals a distinct correlation of decreasing spin-valve signal with increasing injector junction resistance. The observation is attributed to the diminishing contribution of the d-electrons in the FM to the injected current spin polarization with increasing Schottky barrier width. The results demonstrate that there is a window of interface parameters for optimal spin injection efficiency and current spin polarization, which provides important design guidelines for nano-spintronic devices with quasi-1D semiconductor channels.

1K. Kountouriotis et al., Nano Lett. 18, 4386 (2018)

** Work supported by NSF grant DMR-1308613.

Tuesday, March 5, 2019 2:30 PM - 5:18 PM

Session H40 GMAG DMP DCOMP: Complex Oxide Films and Heterostructures II: Iridates and Multiferroics BCEC 208 - Yayoi Takamura, University of California, Davis - Tag(s): Focus
Controllable emergent 2D quantum antiferromagnetism realized in iridate-based heterostructures [Invited] JIAN LIU (Presenter), University of Tennessee — The physics of a square lattice of pseudospin-half electrons in layered iridates has been shown to be particularly rich, giving rise to a novel playground for some of the most outstanding and challenging problems in condensed matter physics, such as metal-insulator transition and quantum magnetism. Significant interests have been focused on the analogy with high-$T_c$ cuprates due to the appealing electronic and magnetic similarities with the CuO$_2$ plane despite the much larger spin-orbit coupling (SOC) of Ir. However, unlike the large material family of cuprates, studies on the layered iridates have been limited to a few Ruddlesden-Popper compounds. This talk will discuss our recent work on overcoming this bottleneck by constructing different artificial variants of the two-dimensional (2D) lattice with heteroepitaxial growth of perovskite iridate. By tuning the layer dimension and the quantum confinement structure, our results show that the magnetic order and exchange interactions of the pseudospin are highly sensitive to the lattice degrees of freedom. By leveraging this structural control, we demonstrate a giant response of the 2D antiferromagnetic order to a sub-Tesla external field. This effect manifests a hidden spin rotational symmetry, which was originally proposed for the CuO$_2$ plane but never observed due to the lack of SOC, illustrating the power of atomic layering in exploring and revealing the intriguing SOC-driven emergent behavior beyond the cuprate phenomenology.

Tuning electronic and magnetic states of pseudospin-$\frac{1}{2}$ square lattice in artificial iridate superlattice JUNYI YANG (Presenter), LIN HAO, Physics and Astronomy, Univ of Tennessee, Knoxville, DEREK MEYERS, Materials Science and Engineering, University of California, Berkeley, HAN ZHANG, Physics and Astronomy, Univ of Tennessee, Knoxville, HAIXUAN XU, Materials Science and Engineering, Univ of Tennessee, Knoxville, MARK DEAN, Brookhaven National Laboratory, JIAN LIU, Physics and Astronomy, Univ of Tennessee, Knoxville — The discovery of $J_{\text{eff}}=1/2$ Mott insulating state in the Sr$_2$IrO$_4$ has drawn a lot of attention since this 2D pseudospin-$1/2$ square lattice is analogous to high-$T_c$ cuprates. On the other hand, the emergent phenomena exhibited by the pseudospin-$1/2$ electrons could be highly susceptible to small changes in the structural degrees of freedom due to the cooperation between electronic correlation and spin-orbit coupling (SOC). Engineering a layered structure of pseudospin-$1/2$ square lattice in artificial superlattices can afford extra tunability of the electronic and magnetic interactions for stabilizing novel collective quantum states. Through controlling dimensionality, spacing layer and epitaxial strain in perovskite iridate-based superlattices, we have investigated the evolution of the spin-orbit-entangled electronic and magnetic ground state under different control parameters. The results from a suite of characterizations, including transport measurements, magnetometry, and synchrotron-based x-ray spectroscopy and scattering, reveal new routes to drive the collective behavior of the interacting pseudospin-$1/2$ electrons, which is not achievable in the bulk.

Metal insulator transition in SrIrO$_3$ Ultra-Thin Films examined by ionic liquid gating* FERNANDO GALLEGO, JAVIER TORNOS, FABIAN CUELLAR, MARIONA CABERO, ALBERTO RIVERA-CALZADA, JUAN I. BELTRAN, Universidad Complutense de Madrid. Spain, M. CARMEN MUÑOZ, F.J. MOMPEÁN, MAR GARCÍA-HERNÁNDEZ, Instituto de Ciencia de Materiales de Madrid ICM-CSIC, CARLOS LEON, JACOBO SANTAMARIA (Presenter), Universidad Complutense de Madrid. Spain — Perovskite SrIrO$_3$ (SIO) is a narrow-band semimetal, which combines strong spin-orbit coupling and electron correlations. This system has attracted much attention because it is at the verge of a Mott transition. Epitaxial SIO ultrathin-layers show a thickness dependent metal-insulator transition (MIT) which is controlled by strain. The insulating state exhibits a strong temperature dependence of the resistance, hysteretic-magnetoresistance and anomalous Hall effect at low temperature, indicating ferromagnetic order. We have explored MIT in SIO ultrathin-layers by using Electric Double Layer (EDL) techniques, that employ ionic liquid as gate dielectric. We have simultaneously measured longitudinal (magneto) resistance and Hall effect across this transition to address whether the MIT is band-width or carrier-density-controlled.

*Funding by spanish AEI grant MAT 2017 87134 C02
3:30PM H40.00004: Probing Skyrmion Phases in SrIrO3/SrRuO3 thin film by Topological Hall Minor Loops* KENG-YUAN MENG (Presenter), ADAM AHMED, BRYAN D. ESSER, JOSE FLORES, DAVID W. MCCOMB, FENGYUAN YANG, Ohio State University — Skyrmions are topological quasi-particles promising for next generation magnetic storage devices. Fundamental understanding of how field history affects skyrmion formation in host materials is vital in regards to technological application. Topological Hall effect is one of major techniques in probing the skyrmion formation. Magnetization and Hall minor hysteresis loops could reveal critical information in addition to traditional full loops. Here we show Hall minor loops of a SrIrO3/SrRuO3 bilayer, which host nanoscale skyrmions as revealed by pronounced topological Hall effect. At low temperature Hall minor loops track the magnetization reversal process, indicating that the skyrmion formation is closely related to magnetization reversal. However, at high temperatures, the Hall resistivity switches before reaching zero field induced by the dominant topological Hall effect; furthermore, the Hall minor loops reveal truly novel behavior that significantly deviates from the magnetization minor loops. We propose such behaviors could due to stabilization of skyrmions even when applied field is larger than magnetization coercive field.

*This work was supported by DARPA (D18AP00008) and OSU MRSEC (DMR-1420451).

3:42PM H40.00005: Giant magnetic response of a two-dimensional antiferromagnetic iridate* LIN HAO (Presenter), Department of Physics and Astronomy, University of Tennessee, DEREK MEYERS, Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, HIDE MARO SUWA, JUNJI YANG, Department of Physics and Astronomy, University of Tennessee, TAMENE R. DASA, HAIXUAN XU, Department of Materials Science and Engineering, University of Tennessee, CRISTIAN BATISTA, Department of Physics and Astronomy, University of Tennessee, MARK DEAN, Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, JIAN LIU, Department of Physics and Astronomy, University of Tennessee — Layered iridates are featured of preserving a hidden SU(2) symmetry such that anisotropic exchange interactions have no contribution to spin anisotropy. Achieving this symmetry, however, is highly challenging because it's necessary to incorporate strong spin-orbit coupling, control the 2D lattice structure, and minimize the interlayer coupling. We solved this issue through top-down design and bottom-up synthesis of SrIrO3 and SrTiO3 superlattices [1] to realize a pseudospin-half antiferromagnetic (AFM) square lattice. We observed giant AFM responses to sub-tesla external fields by exploiting the strong 2D critical fluctuations preserved under the symmetry-invariant exchange anisotropy. The observed field-induced logarithmic increase of the ordering demonstrates a new pathway for the highly efficient control of AFM order [2]. Further investigation on the transport properties suggests a novel coupling between AFM fluctuations and charge fluctuations, highlights the application potential in semiconductor devices.


*J.L. acknowledges support by the Organized Research Unit Program at the University of Tennessee and support by the DOD-DARPA under grant no. HR0011-16-1-0005.

3:54PM H40.00006: Interfacial symmetry control of the chiral magnetism in iridate-manganite superlattices* ELIZABETH SKOROPATA (Presenter), JOHN A NICHOLS, ANKUR RASTOGI, CHANGHEE SOHN, Materials Sciences and Technology Division, Oak Ridge National Laboratory, RYAN DESAUTELS, Large Scale Structures Division, Oak Ridge National Laboratory, XIANG GAO, SATOSHI OKAMOTO, MATTHEW BAHLEK, HO NYUNG LEE, Materials Sciences and Technology Division, Oak Ridge National Laboratory — Correlated oxides have been extensively studied due to the diverse physical properties arising from strong 3d electron correlations combined with lattice and orbital degrees of freedom. Recently, progress toward the creation of exotic quantum and topological properties has been led by the synthesis of 5d oxides with strong spin-orbit coupling. We will present our recent work examining the physical properties of high-quality epitaxially grown LaMnO3/SrIrO3 superlattices. By creating large inversion symmetry breaking with different A- and B-sites in LaMnO3/SrIrO3, we obtain an “topological” Hall effect (THE) that results from interface-induced chiral magnetism resulting from interfacial Dzyaloshinskii-Moriya interactions (DMI). We explore the role of interface symmetry to drive the emergence of the THE at 3d/5d oxides by altering DMI at single interfaces. Furthermore, we compare the effects of (atomic) interfacial DMI and extended superlattice symmetry which together are responsible for the total effective DMI that drive the THE.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
4:06PM H40.00007: Dynamical multiferroicity*  DOMINIK JURASCHEK (Presenter), Department of Materials, ETH Zurich — In this talk, I present how circularly polarized optical phonons create magnetic moments, reminiscent of atomistic electromagnetic coils. An appealing mechanism for inducing multiferroicity in materials is the generation of electric polarization by a spatially varying magnetization that is coupled to the lattice through the spin-orbit interaction. Here, I describe the reciprocal effect, in which a time-dependent electric polarization induces magnetization even in materials with no existing spin structure. I present a formalism for this dynamical multiferroic effect in the case for which the polarization derives from optical phonons, and estimate the strength of the phonon Zeeman effect, which is the solid-state equivalent of the well-established vibrational Zeeman effect in molecules, using density functional theory. I further show that a recently observed behavior—the resonant excitation of a magnon by optically driven phonons—is described by the formalism.

*This work was supported by the ETH Zürich. Calculations were performed at the Swiss National Supercomputing Centre (CSCS) supported by the project IDs s624 and p504.

4:18PM H40.00008: Coupling of single atom magnetic anisotropy to the neighboring electric polarization  JOSE MARTÍNEZ CASTRO, MARTEN PIANTEK, Instituto de Nanociencia de Aragón, University of Zaragoza, MATS PERSSON, Department of Chemistry, University of Liverpool, CYRUS F. HIRJIBEHEDIN, London Centre for Nanotechnology, University College London, DAVID SERRATE (Presenter), Instituto de Ciencia de Materiales de Aragón, CSIC-University of Zaragoza — Multiferroic coupling arises when two ferroic order parameters influence each other. The most popular case is the coupling of magnetization and electric polarization, arising from the interaction of magnetic moments with the surrounding localized electrical charges. In this work we address such interaction at the atomic scale. More specifically, we have recently reported that it is possible to use the abrupt compositional discontinuity occurring at a surface to induce bistable electric polarization in ultrathin ionic insulators [Nature Nanotech. 13, 19-23 (2018)]. Scanning Probe Methods are capable to manipulate matter at the atomic scale while probing simultaneously its electronic and magnetic properties. In this way, using ultrathin films of binary rock-salts, we have built the specific structural and compositional environment that provides a bistable electric polarization controlled by an external electric field. We have deposited individual Co atoms onto the rock-salt films and measured their magnetocrystalline anisotropy by means of inelastic electron tunneling spectra. We show that the uniaxial anisotropy can reversibly tuned to two stable values following the electric polarization switching as a consequence of the crystal electric field experienced by the Co atom.

4:30PM H40.00009: Strain-Induced Anisotropy in NiCo2O4 Epitaxial Films*  CORBYN MELLINGER (Presenter), University of Nebraska - Lincoln, JACE C WAYBRIGHT, South Dakota State University, XIAOZHE ZHANG, XIAOSHAN XU, University of Nebraska - Lincoln — The room temperature ferrimagnetic spinel structured NiCo2O4 (NCO) has garnered interest due to its potential applications in high-capacity supercapacitors. Additional applications in spintronics necessitate studies on its magnetic behavior, which comes about from the magnetic Co tetrahedral and mixed Ni/Co octahedral sites.

We present SQUID measurements on pulsed laser deposited NCO thin films. Measurements show NCO grown on (001)-oriented MgAl2O4 (MAO) single-crystal substrates display an unconventional out-of-plane magnetic easy axis, overcoming shape anisotropy effects of the thin film. NCO/MAO(110) and NCO/MAO(111) films show in-plane easy axes defined by the crystallographic orientation of the substrate. The anisotropy comes about due to distortion of the local environments around the magnetic cations. Observations are explained using single-ion anisotropy and crystal field theory considerations. Research presented opens possibilities for dynamic control of magnetism based on applied strain.

*This work was supported by the Nebraska Public Power District through the Nebraska Center for Energy Sciences Research at the University of Nebraska-Lincoln.
response upon strain is strongly dependent on the material. For LaTiO₃, the interaction parameters are determined by the degree of localization of the orbitals, and grow with increasing tensile strain. In contrast, LaCrO₃ shows the opposite trend: the interaction parameters shrink upon tensile strain. This is caused by the enhanced screening due to the larger electron filling. LaVO₃ shows an intermediate behavior.

*Research sponsored by the Estonian Ministry of Education and Research (IUT23-3) and Estonian Ministry of Education and Research and the European Regional Development Fund project TK134.

5:06PM H40.00012: Effects of strain on the dynamic magnetic properties of europium iron garnet* VICTOR ORTIZ (Presenter), BASSIM ARKOOK, JUNXUE LI, WEI YUAN, TANG SU, IGOR BARSUKOV, JING SHI, Physics and Astronomy, University of California, Riverside — Ferrimagnetic insulators (FMI) have attracted the interest of the spintronic community as a source of pure spin currents and as a medium for long-range magnon spin transport. Among FMI, rare earth iron garnet (REIG) have a plethora of attributes desirable for practical applications. Epitaxial growth of REIG thin films offers an opportunity to control the magnetic properties; in the case of europium iron garnet (EuIG), the role of Eu for tuning magnetic properties remains elusive. In this work, we present an experimental study on the effect of strain in EuIG thin films on the dynamic magnetic properties. EuIG films of varying thickness (10-100 nm) were grown on various (111) garnet substrates by pulsed laser deposition. The strain was controlled by film thickness and substrate used, as characterized by X-ray diffraction. We performed angular and frequency dependent ferromagnetic resonance measurements on the samples and found a systematic increase in the values of Gilbert damping $\alpha$ and inhomogeneous linewidth $\Delta H_0$ and the appearance of higher order anisotropies when a large strain is exerted in the films.

*This work is supported as part of SHINES, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences under Award SC0012670.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H41 GMAG DMP: Skyrmion Crystals BCEC 209 - Lisa DeBeer-Schmitt, Oak Ridge National Laboratory - Tag(s): Focus
2:30PM H41.00001: Various topological spin textures and their dynamics in helimagnets* [Invited] XIUZHEN YU (Presenter), CEMS, RIKEN — The ability to manipulate topological spin textures such as skyrmions is a key to the development of electronic devices that are very low in power consumption. Recently, hexagonal skyrmion lattice (hex-SkL) have been discovered in several systems, such as chiral/polar magnets and ferromagnets with uniaxial anisotropy. In addition to the hex-SkL, we have observed the first for a square lattice of merons and antimerons (sq-ML)—topologically distinguish with skyrmions in a thin plate of the helimagnet Co8Zn9Mn3. By finely varying the magnetic field applied perpendicularly to the plate, the transformation between the sq-ML and hex-SkL has been obtained. We found that the skyrmions were very robust, lasting even as we lowered the temperature of the plate, but the merons and antimerons were much more sensitive, and relaxed into spin helices as the temperature fell.

The transition between a hex-SkL and non-topological spin textures, helical or conical structure, have been also demonstrated by the in-situ Lorentz transformation electron microscopy observations with current excitation or field cooling in a helimagnet FeGe. The skyrmion dynamics, such as the collective transformation of sparsely-populated skyrmions to microcrystals of skyrmions, and the current-driven skyrmion motion have been observed. This work has been done in collaboration with Profs. Yoshinori Tokura, Naoto Nagaosa, Taka-hisa Arima, Yusuke Tokunaga and Fumitaka Kagawa, and with Drs. Wataru Koshibae, Yasujiro Taguchi, Daisuke Morikawa, Naoya Kanazawa, Tomoyuki Yokouchi and Kiyou Shibata.


*This work was supported in part by Japan Science and Technology Agency (JST) CREST program (Grant Number JPMJCR1874), Japan.

3:06PM H41.00002: Field-tuned skyrmion crystals: anomalous quantum oscillations induced by Zeeman fields*

SOPHEAK SORN (Presenter), STEFAN DIVIC, ARUN PARAMEKANTI, University of Toronto — Recent experiments on chiral magnets have observed skyrmion crystal phases which are stable in the presence of Dzyaloshinsky-Moriya interactions and Zeeman fields. Skyrmion crystal coupled to itinerant electrons manifests itself in electronic transport as the anomalous “topological Hall effect” caused by a real-space Berry-phase mechanism. This also leads a formation of Chern bands which depend on the properties of the skyrmion crystal unit cell. Our study has shown that incorporating quartic spin interactions into a system which hosts a skyrmion crystal results in a field-tunable skyrmion lattice constant. Itinerant electrons coupled to such skyrmion crystals can then be described by a Hofstadter-type model whose Chern bands depend strongly on the Zeeman field coupled to the local moments. Such metallic magnets serve as candidates for observing Zeeman-field-induced anomalous quantum oscillations.

*This research was funded by the Natural Sciences and Engineering Research Council of Canada and the Canadian Institute for Advanced Research.

3:18PM H41.00003: Unpinning the skyrmion lattice in MnSi*

CHETAN DHITAL (Presenter), Physics, Kennesaw State University/Louisiana State University, LISA DEBEER-SCHMITT, Oak Ridge National Laboratory, DAVID P YOUNG, JOHN DITUSA, Louisiana State University — Materials hosting magnetic skyrmion lattices are promising materials for future spintronic applications. Given their potential technological use, it is important to understand the response of these magnetic textures under different physical and chemical environments. We have investigated the behavior of the skyrmion lattice in MnSi1-xGa2 single crystals with variations in the temperature and the magnitude and direction of a magnetic field using small angle neutron scattering and magnetization measurements. Our results indicate that the disorder caused by the inclusion of even of small amount of a heavier element such as Ga can substantially change the pinning of the skyrmion lattice when compared to pure MnSi.

*This material is based upon the work supported by the U.S. Department of Energy under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents. C. Dhital also acknowledges Department of Physics Kennesaw State University.
3:00PM H41.00004: Magnetic Hysteresis of the Skyrmion Lattice in MnSi

ALLAN LEISHMAN (Presenter), MORTEN ESKILDSEN, University of Notre Dame, MARC JANOSCHEK, ERIC BAUER, Los Alamos National Laboratory, DIRK HONECKER, Institut Laue-Langevin, LISA DEEBER-SCHMITT, Oak Ridge National Laboratory, JONATHAN S WHITE, Paul Scherrer Institute — Understanding the complex dynamics of skyrmion formation and destruction is key to developing new technologies which make use of them. Here we report the observation of a hysteresis effect associated with forming and destroying the SkL in the chiral magnet MnSi using small angle neutron scattering (SANS). This effect is very small when compared to the applied field of the cryomagnet (~ 1 mT vs 200 mT), but is observable and reproducible by the added precision of a custom built solenoid supplementing the cryomagnet. This hysteresis effect is due to an intrinsic energy barrier associated with forming and destroying the SkL. We have explored the time dependence and magnetic history dependence of the phenomenon to better understand its origin, which we believe to be related to the intrinsic topological energy barrier associated with forming the skyrmions.

*This work is supported by the US DOE, Office of Basic Energy Sciences Award No. DE-SC0005051. Work at Los Alamos Natl. Lab. was performed under the auspices of the US DOE. A portion of this research used resources at the High Flux Isotope Reactor, a US DOE Office of Science User Facility operated by Oak Ridge Natl. Lab., at Institut Laue-Langevin, and at the Swiss spallation neutron source SINQ, Paul Scherrer Institute.

3:42PM H41.00005: Transitions between skyrmion- and hedgehog-lattice states in cubic chiral magnets MnSi$_{1-x}$Ge$_x$

YUKAKO FUJISHIRO (Presenter), NAOYA KANAZAWA, University of Tokyo, TARO NAKAJIMA, XIUZHEN YU, RIKEN Center for Emergent Matter Science, KAZUKI OHISHI, YUKIHIKO KAWAMURA, KAZUHISA KAKURAI, Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, TAKAHISA ARIMA, HIROYUKI MITAMURA, ATSUSHI MIYAKE, University of Tokyo, KAZUTO AKIBA, Okayama University, MASASHI TUKUNAGA, AKIRA MATSUO, KOICHI KINDO, University of Tokyo, TAKASHI KORETSUNE, Tohoku University, RYOTARO ARITA, YOSHINORI TOKURA, University of Tokyo — Topological spin textures such as magnetic skyrmions and spin hedgehogs show novel emergent phenomena, which can be exploited for spintronic functionalities. Whereas the formation or deletion of them has been intensively studied so far, switching of spin textures among different topologically-nontrivial classes remains largely unexplored.

We report on transitions between skyrmion- and hedgehog-lattice states in cubic chiral magnets MnSi$_{1-x}$Ge$_x$ with variation of lattice constant controlled by Si/Ge substitution. By combining neutron scattering, Lorentz transmission electron microscopy and high-field transport measurements, we observe three different topological spin textures: skyrmion lattice in $x = 0-0.25$ as well as two distinct hedgehog lattices in $x = 0.3-0.7$ and $x = 0.8-1$, as respectively characterized by large topological Hall effects.

The emergence of various topological spin states in the chemical-pressure-controlled materials suggests a new route for direct manipulation of the spin-texture topology by a simple mechanical method such as pressure.

3:54PM H41.00006: First-principles study of oxide skyrmion crystal Chern insulator

FUMIYUKI ISHIH (Presenter), Nanomaterials Research Institute, Kanazawa University, YO PIERRE MIZUTA, HIKAURO SAWAHATA, NAOYA YAMAGUCHI, Graduate School of Natural Science and Technology, Kanazawa University — The magnetic skyrmion crystal (SkX), formed by a topological vortex-like spin in condensed matter, has attracted considerable attention in last decade. We performed density functional calculations for SkX in electron-doped EuO monolayer and found Chern insulating ground state where Chern number $C=2$[1]. Calculated large anomalous Nernst effect [1,2] and electric-field effect will be discussed.


4:06PM H41.00007: Collective antiskyrmion-mediated phase transition and defect-induced melting in chiral magnetic films

LEONARDO PIEROBON, Department of Materials, ETH Zurich, CHRISTOFOROS MOUTAFIS, YU LI, School of Computer Science, University of Manchester, JÖRG F. LÖFFLER, Department of Materials, ETH Zurich, MICHALIS CHARILAOU (Presenter), Department of Physics, University of Louisiana at Lafayette — The topological stability of skyrmions goes beyond the energetics of materials and strongly depends on the dynamics of magnetization textures, and the combined effects of energetics, topology, and magnetization dynamics, lead to wildly rich phenomena. Based on detailed high-resolution micromagnetic simulations, we have found a new first-order field-induced phase transition in which a skyrmion lattice inverts its polarity through a metastable creation and annihilation of an antiskyrmion lattice. Importantly, we have observed that in the presence of even a single defect in the material, the phase transition becomes second-order and progresses through a gradual melting of the skyrmion lattice. Our analysis suggests that in a perfect skyrmion lattice the response to an external magnetic field is an abrupt collective phenomenon due to topological constraints, whereas a single defect disrupts the constraint and facilitates topological charge melting, consequently leading to the gradual response of the material to an external field. This provides a basis for a much wider scope of experiments on skyrmion lattices, with emphasis on the interplay between topological constraints and material defects.
4:18PM H41.00008: Skyrmion Crystals in Decorated Transition Metal Dichalcogenides.*

ALDO RAELIARJAONA (Presenter), KIRILL BELASHCHENKO, ALEXEY KOVALEV, University of Nebraska - Lincoln — We investigate the existence of skyrmion crystal phases in decorated transition metal dichalcogenides (TMDs) such as X/MoS2, for (X=Co,Ni,Fe). We model the system using a frustrated triangular lattice, in the presence of in-plane and out-of-plane Dzyaloshinskii-Moriya interaction. We study the phase diagram by varying the strength of the Heisenberg exchange, Dzyaloshinskii-Moriya interaction, and anisotropy. We also perform Monte Carlo simulations to study the H-T (magnetic field - temperature) phase diagram. We study the appearance of the antiferromagnetic skyrmion crystals residing on the three sublattices of the decorated TMDs. The phase transitions and characteristics of the phases are obtained by computing the specific heat C and the spin structure factor $S_k$.

*U.S. DOE, under Award No. DE-SC0014189

4:30PM H41.00009: Chiral domain topology, Moiré patterns, and magnetism in M1/3Nb(Ta)S(Se)2 (M=transition metals)

SANG-WOOK CHEONG (Presenter), FEI-TING HUANG, KAI DU, SEONG JOON LIM, JAE-WOOK KIM, Rutgers University, New Brunswick, KASUN GAMAGE, JUNJIE YANG, Department of Physics, Central Michigan University, MYUNG-GEUN HAN, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — Transition metal dichalcogenides (TMDs) have been extensively investigated as 2D materials last decade. A large amount of transition metals can be intercalated into the van der Waals gaps of a wider range of TMD materials, but a limited studies have been recently reported in intercalated TMDs. The limited examples include Fe$_x$TaS$_2$ crystals with $x=1/4$ and 1/3, which exhibit intriguing configurations of antiphase and/or chiral domains related to ordering of intercalated M ions with 2a×2a and $\sqrt{3}$a×$\sqrt{3}$a superstructures, respectively. In addition, Cr$_{1/3}$NbS$_2$ undergoes helical spin order below 133 K, and shows an interesting solitonic behavior when in-plane magnetic fields are applied in the helical spin state. We have explored a series of chiral M1/3Ta(Nb)S(Se)$_2$ (M=transition metals) to investigate the correlation among crystallographic and magnetic domain topologies and their physical properties. These results as well as Moiré patterns with self-twisted TMDs induced by intercalation will be discussed.

4:42PM H41.00010: Monte Carlo studies of the phases and phase diagram of quasi 2D Skyrmion systems*

PO-KUAN WU (Presenter), JAMES ROWLAND, Ohio State University, YING-JER KAO, Physics, National Taiwan University, MOHIT RANDERIA, Ohio State University — We present results for large-scale Monte Carlo simulations of the field-temperature phase diagram of thin-film chiral magnets with ferromagnetic exchange and Dzyaloshinskii-Moriya interaction. Using spin structure factors, skyrmion density structure factors, magnetization and specific heat, we show that there are five interesting regions of the phase diagram: (1) a skyrmion solid phase, (2) a skyrmion liquid regime, (3) a helical phase, (4) a fluctuating helical regime, and (5) a field-polarized regime. Using orientational order parameters we identify the phase boundaries for the skyrmion melting transition and the helical melting transition. We also investigate the phase diagram as a function of film thickness $L$, showing how that the interlayer correlations and the maximum transition temperature for the skyrmion solid evolves as a function of $L/L_D$, where $L_D$ is the helical pitch length.

*PKW, JR and MR are supported by DARPA Grant No. D18AP00008.

4:54PM H41.00011: Computational-Guided Search for Ultrasmall Skyrmions in Ferrimagnets*

CHUNG MA (Presenter), Department of Physics, University of Virginia, YUNKUN XIE, JIANHUA MA, Department of Electrical and Computer Engineering, University of Virginia, WEI ZHOU, JIE QI, HAMED VAKILITALEGHANI, Department of Physics, University of Virginia, AVIK GHOSH, Department of Electrical and Computer Engineering, University of Virginia, JOSEPH POON, Department of Physics, University of Virginia — Magnetic skyrmions are topologically protected spin textures. They can potentially improve density and energy efficiency in memory and logic devices. With the immense material's space, it could take years to experimentally explore all the possible materials for skyrmions' device application. To guide experiments, we employ computational models to identify several materials for stabilizing ultrasmall skyrmions at room temperature. One of the more promising candidates is amorphous rare-earth-transition-metal ferrimagnet. Our atomistic stochastic Landau-Lifshitz-Gilbert (LLG) model has revealed that Néel skyrmions, with a diameter of 10 nm or less, are stable in 5 nm thick GdFe and GdCo at room temperature. Following this guidance, we have fabricated GdCo samples and controlled the Dzyaloshinskii-Moriya interaction (DMI) through tuning the interfacial layers. Results from these samples are used as feedbacks to refine our computational models. Using this computational-guided approach, the time needed to explore promising materials for skyrmions-based devices will be vastly reduced.

*This work is supported by the DARPA TEE program.
5:06PM H41.00012: Imaging Skyrmion Magnetization Dynamics in Time-Resolved Lorentz Electron Microscopy
GABRIELE BERRUUTO (Presenter), IVAN MADAN, YOSHIE MUROOKA, GIOVANNI MARIA VANACORE, THOMAS LAGRANGE, Institute of Physics, EPFL, DAMIEN MCGROUTHER, YOSHIHIKO TOGAWA, SUPA, University of Glasgow, FABRIZIO CARBONE, Institute of Physics, EPFL — The creation, annihilation, movement, and control of magnetic skyrmions with different tools has been the subject of intensive research in recent years. So far, little attention has been given to the use of light as (yet another) external knob to trigger magnetic changes in skyrmion-hosting materials.

With a combination of camera-rate and ultrafast pump-probe Lorentz Transmission Electron Microscopy we directly resolve the spatio-temporal evolution of the skyrmion magnetization ensuing (fs and ns) optical excitation. The laser-induced creation and annihilation of skyrmions in bulk (Bloch) and interfacial (Néel) systems is reported, and the ultimate speed of such writing and erasing is discussed. In a 60-nm thick slab of the prototypical chiral magnet FeGe, we study how the extreme cooling rates of the crystal ( > 10⁷ K/s) following the photoexcitation can quench the magnetization into a disordered metastable skyrmion lattice.

5:18PM H41.00013: Dynamics in Multiferroic Skyrmion GaV₄S₈
WILLIAM RATCLIFF (Presenter), JEFFREY W LYNN, MARKUS BLEUEL, National Institute of Standards and Technology, LUNYONG ZHANG, Laboratory for Pohang Emergent Materials and Max Plank POSTECH Center for Complex Phase Materials, Pohang University of Science and Technology, SANG-WOOK CHEONG, Physics, Rutgers University — GaV₄S₈ is a rare example of a material hosting a multiferroic Neel-type Skyrmion [1]. We have grown 91 mg single crystals of this material and explored the field/temperature phase diagram using Small Angle Neutron Scattering (SANS) as a probe. We have also investigated the dynamics of the skyrmion phase. In this study, we apply a static field along the [111] crystallographic direction. We also apply a modulated magnetic field along this direction and observe time tagged events on our detector to observe the time dependence. In this talk, we will discuss our results in the context of recent AC susceptibility measurements [2].


*The work at Rutgers University was supported by the NSF under Grant No. DMR-1629059.
The work at Postech was supported by the National Research Foundation of Korea(NRF) funded by the Ministry of Science and ICT(No. 016K1A4A4A01922028).
Access to NG7SANS was provided by the Center for High Resolution Neutron Scattering, a partnership between NIST and the National Science Foundation under Agreement No. DMR-1508249.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM
Session H42 DPOLY: Dillon Medal Symposium BCEC 210A - Mark Ediger, University of Wisconsin - Madison - Tag(s): Focus
2:30PM H42.00001: John H. Dillon Medal Talk: Probing Glass Physics Through Measurements of Polymer Dynamics in Thin films and in Strongly Confined Systems*  
[invited] ZAHRA FAKHRAAI (Presenter), Chemistry, University of Pennsylvania  
— Extensive research in the past two decades has shown that the free surfaces of glasses have dramatically faster dynamics compared to the bulk dynamics with much lower activation energies for rearrangement. In ultrathin films of polymers and molecular glasses, the enhanced surface mobility results in large changes in the value of the glass transition temperature (T_g), enhanced overall dynamics, as well as other property changes such as elasticity, mechanical response, and aging rate.

In this presentation, I will discuss how as the film thickness is reduced below ~30 nm, the dynamics at the two interfaces strongly correlate such that the bulk-like dynamics disappear, and the free surface dynamics are influenced by the substrate dynamics and vice versa. In molecular glasses, supported on weakly interacting substrates these effects can cause a sharp transition from bulk dynamics to liquid-like behavior resulting in dewetting of 30nm films at temperatures well below T_g. These long-range dynamical correlations cannot be simply explained by changes in local interaction potentials. Furthermore, the thickness of this transition remains independent of chemical structure or substrate interactions and appears to be set by the bulk glass properties. As such, the strong perturbation at the free surface can be used as a probe of fundamental aspects of dynamics in bulk super-cooled liquids close or below their T_g.

In contrast, in highly confined systems such as polymers infiltrated into dense nanoparticle packings, while strong changes in T_g and viscosity are still observed, the geometric confinement effect is only significant when the pore sizes are a few nanometers. This is a much shorter length scale than what is observed in systems with free surfaces, suggesting that geometric confinement and free surfaces can have distinctly different effects on the dynamics.

*NSF-DMREF DMR-1628407, NSF-PIRE OISE-1545884, NSF-MRSEC DMR-1720530

3:06PM H42.00002: The glass transition in polydisperse polymers: contribution of mixing entropy  
VALENTIN RUFFINE, ADAM RAEGEN, JAMES FORREST (Presenter), University of Waterloo — All polymerization processes give rise to polydisperse samples where the molecules exhibit a distribution of polymerization index, N. Due to the strong dependence of glass transition temperature, T_g, on N for small N, such polydispersity can potentially have a strong impact on the measured T_g values. Gibbs and DiMarzio 60 years ago (J. Chem. Phys. 28, 373 1958) suggested that the T_g value of polydisperse samples is determined by the number average N of the sample “except for an ordinarily small correction” due to the excess mixing entropy. By considering mixtures of near oligomeric polystyrene with different compositions but the same number average molecular weight we can separate the entropic contribution due to chain ends from that of the chain mixing. We find that the measured T_g values of these mixtures has a significant composition dependence. We quantify this difference by considering the extra mixing entropy of the small chains. This analysis is also able to explain previously measured anomalies in bimodal mixtures of PS.

3:18PM H42.00003: Investigation of deformation mechanism of impact polypropylene  
YUE ZHANG (Presenter), Product Fundamentals, ExxonMobil Asia Pacific Research and Development Company, Ltd., LI QIAN, YING LU, Changchun Institute of Applied Chemistry, YINGYING SUN, ExxonMobil Chemical Company, YONGFENG MEN, Changchun Institute of Applied Chemistry — Polypropylene (PP) is one of the most important plastics widely used due to its heat resistance, high stiffness and good processability. However, the application of PP is often limited by its poor impact resistance. In industry, in reactor copolymerization of ethylene-propylene (EP) following PP homo polymerization is an economic and efficient way of toughening PP where the product is impact copolymer of polypropylene (ICP). Yet the mechanism of PP toughening is still elusive which may involve several energy adsorbing mechanism upon deformation. Here we investigate the cavitation formation process upon deformation in ICP using ultra-small angle X-ray scattering (USAXS), where cavity size and shape evolution were monitored upon deformation. Different ICP systems with varying EP fraction and compositions were studied, aiming to correlate the micro-structure developed upon deformation with the molecular attributes of different ICP systems.
3:30PM H42.00004: Fragility and the Glass Transition of Geometrically Confined Polynorbornenes  
LAURA GRAY (Presenter), RODNEY PRIESTLEY, Chemical & Biological Engineering, Princeton University — Over the past twenty years many studies have shown a reduction in the glass transition temperature (Tg) of thin polymer films confined on the nanoscale when supported on non-attractive substrates or free-standing. These results have been explained by the propagation of enhanced mobility from the free-surface into the polymer film. Many questions remain as to the varying length scale over which Tg decreases, the magnitude of the Tg perturbation observed for different polymers as well as the role cooperatively rearranging regions play in Tg. In this study we measure the dynamic fragility, cooperative length scale, and confined Tg for a series of chemically similar polynorbornenes. We do not see a clear trend in bulk fragility, cooperative length scale, and the magnitude of the Tg perturbation over a wide range of fragilities. Utilizing the unique capabilities of flash differential scanning calorimetry we are also able to quantify the influence of confinement on the fragility and cooperative motion of polynorbornenes.

3:42PM H42.00005: Polymerization Thermodynamics under Nanoconfinement*  
QIAN TIAN, HAOYU ZHAO, SINDEE SIMON (Presenter), Texas Tech University — The behavior of materials confined at the nanoscale has been of considerable interest over the past several decades, especially changes in the glass transition temperature (Tg) and/or melting point (Tm). Less well studied are the effects of nanoconfinement on polymerization kinetics and thermodynamics. Our recent focus has been on understanding how nanoconfinement influences the polymer/monomer equilibrium in the free radical reaction of poly(alkyl methacrylates). We find that nanoconfinement shifts the monomer/polymer equilibrium back towards monomer, and this effect can be exploited to determine the entropy loss on confining a chain. We find that the entropy loss is as high as 10 J/mol/K, approximately 10 % of the change going from monomer to polymer. The results seem to indicate that as the n-alkyl group increases from methyl to ethyl to butyl, the entropy of confinement decreases. Interestingly, the magnitude of the Tg depression in ultrathin films of poly(n-alkyl methacrylate)s also decreases as the length of the alkyl group increases in work by Vogt et al.; whether the origin is linked to the change in chain confinement entropy is an open question.

*Funding from NSF DMR 1610614 is gratefully acknowledged.

3:54PM H42.00006: Shear modulus and shear-stress relaxation in simulated free-standing polymer films  
JORG BASCHNAGEL (Presenter), GEEVARGHESE GEORGE, Institut Charles Sadron, IVAN KRIUCHEVSKYI, LAMCOS, INSA, Villeurbanne, HENDRIK MEYER, JOACHIM WITTMER, Institut Charles Sadron — Using molecular dynamics simulations of a coarse-grained model for polymer glasses we examine viscoelastic properties of free-standing (nonentangled) polymer films. We focus on the (in-plane) shear relaxation modulus G(t) and the (in-plane) shear modulus μ, which we analyze as a function of film thickness (h) for temperatures (T) above and below the glass transition temperature Tg(h). The shear modulus is determined via the stress-fluctuation formalism and found to depend, in addition to h and T, also on the time window (Δt) employed for data sampling. This dependence on Δt can related quantitatively to the time dependence of G(t), provided time-translational invariance holds. Therefore, G(t) is the important underlying quantity, which obeys, in good approximation, a time-temperature superposition principle. We determine the viscosity of the films. For a given T the viscosity decreases with film thickness. This effect can be mainly traced back to the decrease of Tg with decreasing h. The presence of the free interfaces also weakens the shear rigidity of the polymer glass relative to the bulk, which can be understood via the relation between μ and G(t) mentioned before.

4:06PM H42.00007: Mobility Gradients in Supported Glass-Forming Polymer Films Do Not Imply Gradients in Cooperative Motion  
JACK DOUGLAS (Presenter), WENGANG ZHANG, Materials Science and Engineering Division, NIST, FRANCIS STARR, Department of of Physics, Wesleyan University — We investigate the extent of collective motion in the interfacial regions of a thin supported polymer film and within the film interior by molecular dynamics simulations to understand the role of collective motion in the often large changes in interfacial molecular mobility observed in polymer films. Contrary to commonly stated expectations, we find that the extent of collective motion determining the temperature dependence of the structural relaxation time does not vary significantly within the film, a finding consistent with Adam-Gibbs proposal that the extent of collective motion in glass-forming liquids is related to the configurational entropy, a thermodynamic property that cannot vary with position within the film.
4:18PM H42.00008: Dynamic Phase Transitions in Confined Polymer Glasses  ROBERT RIGGLEMAN (Presenter), ROBERT IVANCIC, University of Pennsylvania — Despite more than two decades of effort, several qualitative features regarding the segmental dynamics of thin films of glass-forming materials remain poorly understood. This challenge is of paramount importance in thin film membranes, organic electronic devices, and critical steps of semiconductor manufacturing. Recent simulations and experiments have provided compelling evidence that the dynamics near surfaces are qualitatively different from those of a bulk supercooled liquid, and in this talk I will describe our efforts at characterizing those dynamics by investigating a non-equilibrium phase transition associated with glass-forming materials. This transition is associated with a supercooled liquid that undergoes a sharp transition from a mobile dynamic phase to a phase with reduced mobility, and it provides a clear signal in the dynamics of the glass-forming polymer under confinement. I will describe our characterization of this transition in free-standing thin films of supercooled liquids, where we find that only the bulk of the film is able to undergo this transition. This suggests that the dynamics at the free surface are not glassy in nature, at least not at the temperatures accessible to our simulations.

4:30PM H42.00009: Coarse-Grained Models for Predicting Structure and Thermodynamics in Polymer Systems with Specific and Directional Intermolecular Interactions  ARTHI JAYARAMAN (Presenter), University of Delaware — Recent work in my research group has been aimed at developing predictive coarse-grained (CG) models for investigating structure and dynamics in soft materials with chemistries that have specific and directional molecular interactions. Although computational studies have been tremendously useful in understanding molecular phenomena and guiding synthesis and engineering of new macromolecular soft materials for a wide variety of applications, the inability to capture small scale specific and directional interactions (e.g., hydrogen bonds) alongside macromolecular length and time scales represents a key limitation of most studies to date. We address this limitation by developing coarse-grained models that capture the anisotropic, directional and specific interactions (e.g., hydrogen bonding interaction) governing the structure and thermodynamics in many polymer systems of interest. We have been using molecular dynamics simulations with these new coarse-grained models for studies of biomaterials and polymer nanocomposites. In this talk, I will discuss one example of how the development of these CG models is enabled by synergistic feedback from concurrent/past experiments which I will highlight alongside the computational results from my group.

4:42PM H42.00010: Heterogeneous polymer degradation due to photothermal heating*  LAURA CLARKE (Presenter), HONGLU HUANG, GABRIEL FIRESTONE, RUSSELL E GORGA, JASON BOCHINSKI, North Carolina State University — We are interested in observing the effects of thermally-driven chemical reactions occurring in small volumes within a solid material, where diffusion of reactants and products is limited. Such experiments can be achieved by photothermally heating metal nanoparticles incorporated within the polymer which results in significant heat generation at the particles and an inhomogeneous steady state temperature distribution within the solid material, where regions far from any particle are cool, whereas those in a particle's immediate vicinity experience temperatures of 100-200 deg. C. Polyethylcyanoacrylate (PECA) degrades by depolymerizing and in confinement, the monomer will repolymerize to form oligomers. In principle, such a process might enable internal conversion of polymer to oligomer without significant loss of mechanical properties, and thus potentially address issues such as microfragmentation of plastics in the environment. We characterize degradation of PECA:starch:nanoparticle composites via GPC, dilute solution viscometry, electron and optical microscopy, and mechanical property measurements, and compare and contrast degradation obtained via photothermal heating with that obtained by conventional means.

*National Science Foundation CMMI-1069108 and CMMI-1462966

4:54PM H42.00011: Charge Density- and Hydrophobicity-Dependent Dynamics of Polyelectrolyte Complex Coacervates  JENNIFER LAASER (Presenter), JUN HUANG, University of Pittsburgh — We use a library of polyacrylamide-based polymers to investigate the roles of charge density and hydrophobicity in determining the phase behavior and viscoelasticity of polyelectrolyte complex coacervates. The polymers, which are made by post-polymerization functionalization of poly(N-acryloxy succinimide), have charged monomer fractions between 60 and 100%, with the balance comprised of either hydrophilic (acrylamide) or hydrophobic (butyl acrylamide) comonomers. We identify the critical salt concentration of the coacervates by optical turbidity, and characterize their degree of swelling and viscoelasticity via thermogravimetric analysis and small amplitude oscillatory shear rheology, respectively. We find that as the charge density of the polymers is decreased, the critical salt concentration and volume fraction of polymer in the coacervates also decrease, and the relaxation dynamics speed up. Interestingly, these properties depend only on the charge density, and not on the hydrophobicity of the comonomer. This suggests that hydrophobic interactions are much weaker than the entropic forces driving coacervate formation, and may provide a new window into understanding the extent to which polymer concentration and electrostatic interactions determine coacervate dynamics.
Rearrangement of 2D aggregates of droplets under compression: signatures of the energy landscape from crystal to glass*

KARI DALNOKI-VERESS (Presenter), JEAN-CHRISTOPHE ONO-DIT-BIOT, McMaster University, PIERRE SOULARD, ESPCI Paris, SOLOMON BARKLEY, McMaster University, ERIC WEEKS, Emory Univ, THOMAS SALEZ, Univ. Bordeaux, ELIE RAPHAEL, ESPCI Paris — We study a signature of the energy landscape through the crystal-to-glass transition by compressing 2D finite aggregates of emulsion droplets. Oil droplets of two distinct sizes are used to compose small aggregates in an aqueous environment. Aggregates range from perfectly ordered monodisperse crystals to disordered bidisperse glasses. The aggregates are compressed between two parallel boundaries; crucially, one of the boundaries acts as a force sensor. The compression forces provide a signature of the aggregate composition and give insight into the energy landscape. In particular, crystals dissipate all the stored energy through single catastrophic fracture events whereas the glassy aggregates break step-by-step. Remarkably, the yielding properties of the 2D aggregates are strongly impacted by even a small amount of disorder.

*Funding: NSERC (Canada); Joliot chair from ESPCI Paris; Global Station for Soft Matter, Hokkaido University; NSF (CBET-1804186).

Photo-Induced Order-Disorder Transitions in Block Copolymer Solutions*

TIMOTHY LODGE (Presenter), CECILIA C HALL, CECELIA RIVERA, CLAIRE SEITZINGER, YUKI HIROSE, University of Minnesota — Photo-stimuli responsive materials are of interest for a broad range of applications, and take advantage of the inherently non-invasive, spatially resolved, and species-selective optical response. We demonstrate here a photo-reversible order-disorder transition in a block copolymer/ionic liquid system. The copolymer is a symmetric poly(methyl methacrylate)-b-poly(benzyl methacrylate-stat-azomethacrylate) diblock, with $M \approx 45 \text{kDa}$, and 5% azomethacrylate in the second block. Poly(benzyl methacrylate) exhibits LCST behavior in the common ionic liquid ethyl methyl imidazolium bistrifluoromethylsulfonimide (EMI TFSI). Under UV irradiation, the trans to cis photoisomerization of azobenzene significantly increases the solubility of the thermoresponsive block, leading to an order-to-disorder transition at appropriate concentrations and temperatures. Under visible light, the cis to trans recovery causes the sample to re-order. The progress of the transition is monitored by in situ photo-rheology, and the morphologies are confirmed by SAXS.

*NSF-DMR-1707578

Tuesday, March 5, 2019 2:30 PM - 4:54 PM

Session H43 DCMP: DCMP Prize Session I BCEC 210B - Daniel Arovas, University of California, San Diego - Tag(s): Invited

2:30PM H43.00001: Oliver E. Buckley Condensed Matter Prize talk: Elihu Abrahams: pioneer in the physics of disordered electronic systems [Invited] PATRICK LEE (Presenter), Massachusetts Institute of Technology — Elihu Abrahams (1927-2018) was recognized by the Buckley Prize for his early and key contributions to the theory of transport in doped semiconductors and disordered electronic systems. In a seminal work with his student Miller, he introduced the network model for hopping conductivity. Later he co-authored with Anderson, Licciardello and Ramakrishnan an influential paper (6169 citations) on the scaling theory of localization. I shall review these accomplishments and share memory of a life well lived.

3:06PM H43.00002: Oliver E. Buckley Condensed Matter Prize Talk: Coulomb gap here, there, and everywhere [Invited] BORIS SHKLOVSKI (Presenter), University of Minnesota — In 1975 Alexei Efros and myself discovered that due to electron-electron interactions the density of localized electron states vanishes near the Fermi level as a quadratic function of the energy distance to the Fermi level. We named this phenomenon the Coulomb gap and showed that it leads to the variable range hopping conductivity which depends on the temperature $T$ as $\exp[-(T_E/T)^{1/2}]$. This Efros-Shklovskii law was confirmed in hundreds of experimental papers, where in many cases it describes $10^6$ times dynamic range of conductivity. After going through the history and physics of this discovery I will review many new applications of Efros-Shklovskii law beyond lightly doped semiconductors among which the Quantum Hall Effect is the most prominent. I will also dwell on the McMillan-Shklovskii theory of the Coulomb gap emergence across a Metal-Insulator transition and the related question of screening of the Coulomb gap.
3:42PM H43.00003: APS Medal for Exceptional Achievement in Research: Topology and Other Tools in Condensed Matter Physics* [Invited] BERTRAND I. HALPERIN (Presenter), Harvard University — Notions from topology have played a big role in our current understanding of both classical and quantum systems, and much of my work has been related, in one way or another, to topological ideas. However, topology has only been one tool in my research, sometimes as a starting point and sometimes an afterthought. Other ingredients have included ideas from statistics and quantum mechanics, and analyses of interaction energies and the effects of topological defects on other variables of a system. One portion of my work has focused on phase transitions that could be understood in terms of a proliferation of topological defects, and on dynamic properties that could be understood by the motion of such defects. Other portions of my work have made important use of notions of percolation. My work on quantum Hall systems, at least in retrospect, has always been related to notions of topology in Hilbert space. In my talk, I will present some examples of these applications.

*My research has been supported over the years by Harvard University and Bell Laboratories and by grants from the National Science Foundation and other government agencies, Microsoft Corporation, and Schlumberger Research.

4:18PM H43.00004: Aneesur Rahman Prize for Computational Physics Talk: Digital Alchemy, Machine Learning and Inverse Design for Self Assembly [Invited] SHARON GLOTZER (Presenter), University of Michigan — From the Stone Age to the Silicon Age, the materials available to humankind define the world in which we live. The materials of tomorrow will be designed and engineered on demand, where and when they are needed, with precision and personalization. Computer simulation and machine learning both have critical roles to play in creating this future. Already, they allow — from a nearly infinite number of possibilities — the inverse design of nanoparticle building blocks optimized for self assembly into colloidal crystal structures with targeted properties. In this talk, we present a new thermodynamic computational approach to the inverse design of colloidal matter, and demonstrate its use in obtaining colloidal crystals with arbitrary complexity, engineered phase transitions, and target photonic properties. We show how machine learning can be used to autonomously identify crystal structures in hundreds of thousands of simulations, as well as to identify key alchemical attributes of particles that correlate with colloidal crystal structure.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H44 DCMP: Demise of Superconductivity in Overdoped Cuprates BSEC 210C - Tag(s): Invited

2:30PM H44.00001: Starfish-shaped Cooper pairs with ultrashort antinodal length scales across all doping levels in cuprate superconductors.* [Invited] DANIEL DESSAU (Presenter), University of Colorado, Boulder — We access the fully causal electronic self-energy utilizing a brand new 2-dimensional method of ARPES analysis [1], which removes the critical limitations of the previous one-dimensional MDC (Momentum Distribution Curve) and EDC (Energy Distribution Curve) methods. This new method, which utilizes orders-of-magnitude fewer parameters than the MDC and EDC methods, brings in the energy, momentum, and temperature -dependence of the self energies and is fully consistent with the already-successful studies showing the gap filling-in behavior [2,3]. The full set of parameters we access allows us to make the first direct measurements of the shape and size of the pairs [4]. This is all critical information for explaining how coherence between the pairs (the superconducting state) evolves as a function of doping and temperature.


*We acknowledge generous support from the US Department of Energy
The key findings are as follows. (i) The superconducting phase stiffness is extremely low, comparable to $T_c$. (ii) The superfluid density $N_s(T)$ decreases linearly with $T$, up to $T_c$. (iii) $T_c$ scales with $N_{S0}$ linearly but with an offset, except very close to the dome edges where it scales as $\sqrt{N_{S0}}$. (iv) The superconducting state develops from an electronic nematic state that breaks the $C_4$ symmetry of the underlying crystal lattice. (v) The electron fluid behaves as if it were comprised of two components, one Fermi-liquid (FL) like and the other showing resistivity linear in $B$, diminishing with increased doping, and tracking the nematicity, $N_{S0}$, and $T_c$.

The related results of other groups show that the above appears to be typical of high-$T_c$ cuprates and independent on the details of the Fermi surface, the number of CuO$_2$ planes in the unit cell, the presence or absence of CuO chains, the density and the nature of dopants, the superconducting gap size, etc.

We conclude that high-$T_c$ superconductivity in cuprates involves some new physics that entails strong pairing, strong electron correlations, strong thermal phase fluctuations, and strong pair-breaking, intrinsic but $T$- and doping-dependent.

References

*Supported by U.S. DOE, Basic Energy Sciences, Materials Sciences and Engineering Division and Gordon and Betty Moore Foundation's EPiQS Initiative Grant GBMF4410.

Developing a complete description of the ground state evolution is crucial to decoding the complex phase diagram. Here we use the structure of broken translational symmetry, namely d-form factor charge modulations in (Bi,Pb)$_2$(Sr,La)$_2$CuO$_{6+\delta}$, as a probe of the ground state reorganization which occurs at the transition from truncated Fermi arcs to a large Fermi surface. We use real space imaging of local electronic inhomogeneity as a tool to access a range of dopings within each sample, and we firmly establish the spectral gap $\Delta$ as a proxy for local hole doping. From the $\Delta$-dependence of the charge modulation wavevector, we discover a commensurate to incommensurate transition that is coincident with the Fermi surface transition from arcs to large hole pocket, demonstrating the qualitatively distinct nature of the electronic correlations governing the two sides of this quantum phase transition. Furthermore, the doping dependence of the incommensurate wavevector on the overdoped side is at odds with a simple Fermi surface driven instability.

*This work was supported by the Gordon and Betty Moore Foundation's EPiQS Initiative grant GBMF4536 and the National Science Foundation grant DMR-1341286.

This is accompanied by an unexpected scaling of the zero-temperature superfluid density with $T_c$, which should be constant within a conventional BCS picture. By considering lifetime effects I show that these observations can be explained by temperature-dependent scattering in the presence of a $d$-wave energy gap, and a decreasing pairing interaction strength with doping.

*The author gratefully acknowledges financial support from Victoria University of Wellington and the MacDiarmid Institute for Advanced Materials and Nanotechnology.
In a superconductor there exist two different types of scattering processes, depending on their action on the Cooper pairs: pair-conserving and pair-breaking. Making use of the microscopic coherent potential approximation, we have developed a phenomenological description of the so-called Dynes superconductors in which both processes are characterized by separate lifetimes [1]. Our theory solves the long-standing puzzle about the origin of the ubiquitous Dynes formula [2] for the tunneling density of states. It also predicts how the electron spectral functions change in presence of both types of scattering, correcting the previously used phenomenological two-lifetime expressions. In this talk, after introducing the concept of the Dynes superconductors, I will discuss its applicability to the d-wave cuprate superconductors, in which the two types of scattering processes correspond to small- and large-angle scattering. I will start by showing that, along fixed tomographic cuts, the Dynes phenomenology provides good fits of the electron spectral functions [3]. Then I will turn to a discussion of the recent electrodynamic experiments on overdoped cuprates [4,5]. I will show that the breakdown of the Homes law at extreme overdoping [4] is a generic property of the Dynes superconductors and I will discuss the relation between the dirty d-wave picture [6] and the Dynes phenomenology. The role of the Fermi liquid corrections and of the inelastic processes will also be discussed.


* Work supported by the Slovak Research and Development Agency under Contract No. APVV-15-0496.
2:42PM H45.00002: Valley-dependent impurity scattering in α-T₃ ααlattices and specific role of Lorentz forces
Danhong Huang (Presenter), Air Force Research Lab · Kirtland, Andrii Iurov, Center for High Technology Materials, University of New Mexico, Ying-Cheng Lai, Hongya Xu, School of Electrical, Computer and Energy Engineering, Arizona State University, Godfrey Gumbs, Department of Physics and Astronomy, Hunter College of the City University of New York — We have obtained the angular distribution of extrinsic skew-scattering currents related to a set of randomly-distributed impurities in α-T₃ lattices using the Boltzmann moment equations. With the help of the screened second-order Born approximation, we have calculated the inverse momentum-relaxation-time tensor and revealed the anisotropy which appears to be the source of the angle-dependent currents. The static dielectric function was obtained under the random-phase approximation (RPA). The scattering is also modified by Berry-phase variation and local asymmetry in impurity potentials next to the two inequivalent K and K′ valleys. The resulting skew current depends on the electron doping level and is determined by the ratio of energy to momentum relaxation times.

2:54PM H45.00003: Tuning the opto electronic properties of ultrasmooth large area rGO films grown via Pulsed laser deposition (PLD) technique
Muhammad Juvaid (Presenter), IIT Madras and National University of Singapore — We present the growth of large area ultra-smooth reduced graphene oxide (rGO) thin films on a four inch wafer via beam scanning mode of Pulsed laser deposition technique. With the versatility of the PLD technique, the easy tuning of optoelectronic properties is achieved on rGO thin films without employing any buffer layers. The conventional growth mechanism of rGO films involves hazardous chemicals, whereas this physical vapour deposition technique gives high quality rGO films with tunable optoelectronic properties. This wafer-scale growth mechanism of rGO thin films can potentially employ in various optoelectronic applications due to its high transparency and p-type conductivity. We illustrate the optoelectronic tunability of large area rGO films and its use through the evaluation of transparent conducting films, where our rGO films show highest performance as compared to existing p-type transparent conducting films.

3:06PM H45.00004: Intercalation of Cu and Ru beneath the top graphene layer of graphite surfaces
Yong Han (Presenter), Ann Lil-Rosasales, Michael C. Tringides, James William Evans, Patricia A. Thiel, Iowa State University — STM experiments show that Cu forms encapsulated islands under the top graphene layers of graphite, as a result of vapor deposition of Cu on a sputtered graphite surface [JPCC 122, 4454]. Deposition at 800 K is optimal for formation of encapsulated multilayer Cu islands. Deposition below 600 K favors Cu clusters adsorbed on top of graphite, while deposition above 800 K favors single-layer intercalated Cu islands. To form Ru nanoislands below the top graphene layer requires deposition at 1000 K to 1180 K [Nanotechnology 29, 505601]. We present an extensive study of energetics using density functional theory to compare stabilities of a wide variety of configurations of atoms, clusters, and layers of Cu and Ru on/under the graphite surface. For Cu-graphite systems, the only configuration that is significantly more stable under the graphite surface than on top of it, is a single Cu atom. This analysis leads us to conclude that formation of encapsulated Cu islands is kinetically driven, rather than thermodynamically driven. On the contrary, the embedded Ru islands are thermodynamically favored over on-top clusters.

3:18PM H45.00005: Electrical and mechanical properties of h-BN nanoplates on Ir(111) studied by STM and NC-AFM
Mengxi Liu (Presenter), Xiaohui Qiu, National Center for Nanoscience and Technology — Hexagonal boron nitride (h-BN) on metal surfaces is subjected to substrate interactions as well as in-plane strains resulted from the lattice mismatch between h-BN and the underlying substrate. Here, we investigate the electrical and mechanical properties of h-BN nanoplate grown on Ir(111) using a combined approach of scanning tunneling microscopy (STM), noncontact atomic force microscopy (nc-AFM) and density functional theory (DFT) calculations. The in situ synthesized h-BN nanoplates have a characteristic triangular shape with zigzag-type edges. Boron and nitrogen atoms can be identified by distinct chemical interaction with metallic tip. The nc-AFM images show a strong tip-dependent contrast, which transforms from honeycomb lattices to hexagonal spots by switching W-tip to Cl-tip. Based on DFT calculations, we interpret the contrast conversion in terms of a combination of tip dipole and charge transfer from Ir(111) surface to BN nanoplates bound to Ir(111). In addition, the elastic deformation of h-BN nanoplates was measured by nc-AFM force map and lateral stiffness of h-BN nanoplates dramatically depend on their size.

*The work was supported mainly by U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
3:30PM H45.00006: Scanning tunneling spectroscopy study of incorporated Al atoms in Si(100) substrate

HYUNSOO KIM (Presenter), University of Maryland, College Park, ARUNA RAMANAYAKA, Joint quantum institute, KE TANG, University of Maryland, College Park, JOSHUA POMEROY, National Institute of Standards and Technology — We have studied the structures and electrical properties of incorporated Al atoms in Si(100) using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) at room temperature in ultra-high vacuum. Our recent work shows that, in Si/Al/Si heterostructures, a hole is a dominant charge carrier and we have achieved a comparable mobilities to previous reports on similar two-dimensional hole gas systems at high charge carrier densities. [1,2] However, the electronic states of Al have not been studied well as dopants in Si. STS can provide the local density of states to understand the electrical properties of incorporated Al atoms in Si(100) similar to the Si/Al/Si heterostructure in our recent work. [1] We will discuss the local density of states measured by STS of incorporated Al atoms in a clean (2x1) reconstructed Si(100) substrate at various densities prepared by thermal Al evaporation and annealing in situ at 550 °C.


3:42PM H45.00007: Discovery of a New Layered Crystal, Hexagonal Beryllium Oxide

LIFEN WANG (Presenter), Institute of Physics, LEI LIU, Department of Materials Science and Engineering, College of Engineering, Peking University, JI CHEN, Electronic structure theory, Max Plank Institute, SHANG-PENG GAO, Department of Materials Science, Fudan University, GONG GU, Department of Electrical Engineering and Computer Science, University of Tennessee — The reported work was prompted by the intriguing question whether sp²-coordinated, layered polymorphs of octet compounds other than BN can exist. While such polymorphs with thicknesses within a thermodynamic limit are predicted, the possibility of their thicker layered crystals has long been dismissed. Here, using high-resolution transmission electron microscopy and electron energy loss spectroscopy, we show that BeO crystallizes in the sp²-coordinated, layered structure in liquid cells formed by sheets of graphene. We further reveal that the layered crystals can be thicker than the thermodynamically determined ultra-thin limit, beyond which the layered phase is energetically unfavored. The discovery counters a long-held dismissal and calls for a reevaluation of the possible existence of sp²-coordinated, layered polymorphs of octet compounds beyond the ultra-thin limit.

*This work was supported by DARPA HR0011-13-2-0016, by NSF DMR-1410940 and ECCS-1231808, by the National Program for Thousand Young Talents of China. By office of Science user facility supported by the U. S. Department of Energy, under Contract No. DE-AC02-06CH11357.

3:54PM H45.00008: A Study of Vertical Transport in Silicon-Graphene Junction

SIDONG LEI, XIAODAN ZHU, SHINHUNG TSAI (Presenter), University of California, Los Angeles, XIAODAN ZHU, SHINHUNG TSAI, University of California, Los Angeles, XING ZHANG, Rice University, GEN YIN, CARLOS TORRES, ARYAN NAVABI, University of California, Los Angeles, ZEHUA JIN, Rice University, HUSSAM QASEM, University of California, Los Angeles, ROBERT VAJTAI, Rice University, ROGER LAKE, University of California, Riverside, PULICKEL M AJAYAN, Rice University, KANG WANG, University of California, Los Angeles — In this report, we explore the important roles of single layer graphene in the vertical tunneling process as a tunneling barrier. Although being a semimetal in the lateral lattice plane, the graphene together with the vdW gap acts as a tunneling barrier, that is nearly transparent to vertically tunneling electrons, due to its atomic thickness and the transverse momenta mismatch between the injected electrons and the graphene band structure. This is accentuated using electron tunneling spectroscopy (ETS) showing a lack of features corresponding to the Dirac cone band structure. Meanwhile, the graphene acts as a lateral conductor through which the potential and charge distribution across the tunneling barrier can be tuned. These unique properties make graphene an excellent 2D atomic grid, transparent to charge carriers, and yet offer the control of the carrier flux via the electrical potential.

*We would like to acknowledge the support of National Science Foundation (EFMA-1433541). We would also like to acknowledge the collaboration of this research with King Abdul-Aziz City for Science and Technology (KACST) via The Centre of Excellence for Green Nanotechnologies (CEGN).
4:06PM H45.00009: Construction of graphene/silicene heterostructure by Si intercalation  GENG LI (Presenter),
Institute of Physics, Chinese Academy of Sciences — Geng Li

Institute of Physics & University of Chinese Academy of Sciences, Chinese Academy of Sciences, Beijing 100190, China

Silicene-based van der Waals heterostructures have been theoretically predicted to have interesting physical properties, but their experimental fabrication has remained a challenge because of the easy oxidation of silicene in air. Here we report the fabrication of graphene/silicene van der Waals heterostructures by silicon intercalation. Density-functional-theory calculations show weak interactions between graphene and silicene layers, confirming the formation of van der Waals heterostructures. The heterostructures show no observable damage after air exposure for extended periods, indicating good air stability. The I-V characteristics of the vertical graphene/silicene/Ru heterostructures show rectification behavior.


4:18PM H45.00010: The mechanism for the stabilization and surfactant properties of epitaxial silicene  ALBERTO CURCELLA, ROMAIN BERNARD, YVES BORENSZTEIN, MICHELE LAZZERI (Presenter), GEOFFROY PREVOT, Sorbonne Universite — Using real-time in situ scanning tunneling microscopy and density functional theory simulations, we have studied the growth of Si films on Ag(111) for coverages above the silicene monolayer, evidencing the existence of metastable phases and an original growth mechanism. Above monolayer Si coverage, an initial sqrt(3)Xsqrt(3) structure forms, which is identified as an Ag-free Si bilayer with additional Si adatoms. With further deposition, this structure is replaced by a distinct bilayer structure covered by Si trimers and Ag atoms. The formation of these bilayers follows counterintuitive dynamics: they are partially inserted within the Ag substrate and form by expelling, from the underlying substrate, the atoms that reinsert below the adjacent silicene layer. The growth is therefore characterized by an unexpected “surfactant competition” between Ag and silicene: while silicene is a metastable surfactant for the Ag(111) surface, Ag plays the role of a surfactant for thicker diamond-like Si islands. In spite of being thermodynamically unfavoured, the silicene monolayer is, thus, a remarkably stable structure because of the high kinetic barrier for the growth of thicker layers.

4:30PM H45.00011: Ab initio study of 2D plasmon enhancement in alkali intercalated graphene on metallic substrates  VITO DESPOJA (Presenter), Institute of Physics, Zagreb, LEONARDO MARUSIC, Maritime Department, University of Zadar — Alkali metal (AM) atoms, (e.g. in LiC2 or CsC8) donate electrons to the graphene π band causing the appearance of another Dirac plasmon (DP) in the EEL spectra. At the same time, the AM σ band remains partially filled and supports a strong Dirac plasmon (DP) in the EEL spectra. The same time, the AM σ band remains partially filled and supports another Dirac plasmon, which hybridizes with the Dirac plasmon causing appearance of the weak linearly dispersive plasmon, known as the acoustic plasmon (AP) [1,2]. We present the results of a theoretical simulation of alkali atoms intercalated between the graphene and a metallic substrate (e.g. Ir(111) or Al(111)) and forming a periodic superlattice, which causes a huge enhancement of DP and AP. Moreover the AP intensity and Fermi velocity strongly depend on graphene/substrate separations. This enhancement mechanism, in addition to its very interesting fundamental aspect, suggests many possibilities for plasmonic applications. The theoretical simulation is performed using a state of the art DFT (ground state) + RPA (excited state) technique, adapted for the study of the dielectric properties in large multilayer heterostructures, which completely exclude inter-supercell Coulomb interaction.


4:42PM H45.00012: First-Principles investigation of Epitaxial Pt Layer on Graphene  JI IL CHOI, FAISAL ALAMGIR,
SEUNG SOON JANG (Presenter), School of Materials Science and Engineering, Georgia Institute of Technology — Platinum is a face centered cubic structured crystal that has been widely known as a superior catalyst for various chemical reactions, while low-dimensional structures, such as mono- or bi-layer platinum, have attracted less attention due to experimental difficulties in synthesizing such 2D structures. In this study, we present a computational research on the unique architecture of epitaxial platinum (mono/multi) layers grown on graphene (Pt_ML/GR), in support of remarkable recent progress in the synthesis of these architectures in simple cubic-like (SC-L) and face-centered cubic-like (FCC-L) phases on the graphene. Recently proposed strongly constrained and appropriately normed (SCAN) density function study (DFT) is employed to investigate the structural and electronic properties of the epitaxial SC-L Pt layered graphene. In these architectures, Pt exhibits registry with the C-C bridge sites along the armchair and zigzag directions. Here, the details of the atomistic/electronic structures and binding energies are discussed. Further, the detailed band structure and the partial/total densities of state (DOS) of the Pt_ML/GR architectures, with Pt in an SC-L registry, are presented.
Two dimensional phases of Ag on Ge(111): insights from first-principles calculations

SHREE RAM ACHARYA (Presenter), DUY LE, University of Central Florida, SHIRLEY CHIANG, CHING FONG, Physics, University of California, Davis, TALAT S. RAHMAN, University of Central Florida — Experimental observations using low-energy electron diffraction (LEED) of deposited Ag on the Ge(111) surface have revealed a number of two-dimensional Ag structures which depend on Ag coverage and sample temperature[1]. We have applied density functional theory based calculations to explore the Ag/Ge(111) phase diagram and to obtain insights into the electronic and geometric structures and the vibrational dynamics. In this comparative study of clean Ge(111) with (1x1), reconstructed c(2x8) and (2x1) geometries, and of sub-monolayer Ag covered Ge(111) with (4x4), (v3xv3)R30 and (1x1) overlayers, we find that Ge atoms on the surface prefer three-fold hollow sites and Ag adatoms prefer to form triangular structures. Furthermore, temperature-coverage dependent surface phase diagram constructed by minimizing the surface free energies shows that up to 37% Ag coverage, (4x4) is the stable phase beyond which up to 90% coverage, the phase coexists with (v3xv3)R30 and (1x1) phases at temperature below 600K and higher respectively. Beyond 90% coverage, isolated (v3xv3)R30 and (1x1) phase are the most stable with the same temperature boundary of 600K.


Work supported by NSF DMR-1710306; NSF DMR-1710748.

Study of the surface properties of Tin ultrathin film on superconducting substrate

DANDAN GUAN (Presenter), Shanghai Jiao Tong University — Two dimensional (2D) topological insulators (TIs) are 2D materials that possess a pair of topological edge states connecting the bulk band gap. Later, Kane and Fu predicted that the superconductivity (cooper pairs) of superconductors (SC) would be introduced into TIs to form TI/SC heterostructures, in which majorana fermions could be found [1]. And 2D tin film (stanene) is theoretically predicted as quantum spin Hall (QSH) insulators by Shou-Cheng Zhang’s group [2], many experimental efforts have been devoted to confirming the topological properties of tin film. Here for the Sn/ sSC system, the pure Face-centered cubic (FCC) structure of Sn surface has been obtained for the first time. Superconductivity has also been detected on the FCC-Sn(111) surface, but no topological edge states exist. Furthermore, phase transition occurs from FCC-Sn(111) to β-Sn(001) by keeping the sample at room temperature for a certain time. Due to the strain relaxation on the β-Sn islands, both the in-plane unit cell and out-of-plane structures distort, and the height of surface atoms varies periodically to form a universal ripple structure.

References:

Liquid crystal (5CB) adsorption on two-dimensional materials

PAUL BROWN (Presenter), ASEE Fellow for the United States Naval Research Laboratory, SEAN A FISCHER, United States Naval Research Lab, JAKUB KOLACZ, ASEE Fellow for the United States Naval Research Laboratory, CHRISTOPHER SPILLMANN, DANIEL GUNLYCKE, United States Naval Research Lab — Liquid crystals are widely used in display technologies. Their collective behavior and use ultimately hinges on single molecules interacting with a supporting surface. Since the isolation of graphene in 2004, the potential for combining two-dimensional nanosheets with liquid crystals has become an area of scientific interest. However, little attention has focused on the local interfacial interactions between the mesogen and two-dimensional materials. In this presentation, we discuss the local mesogenic interactions between the well-known nematic liquid crystal 5CB, and a series of monolayer crystals such as graphene, molybdenum disulfide, phosphorene, and h-BN. In particular, we present electronic ground state properties obtained using density functional theory with nonlocal van der Waals corrections that reveal subtle orientational, energetic, and electronic properties for the characterization of local mesogen-substrate interactions, whereby the anchoring of liquid crystal can be understood more generally across atomically flat surfaces.

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Tuesday, March 5, 2019 2:30 PM - 4:54 PM

Session H46 DMP GMAG: 4d/5d Transition Metal Systems -- Pyrochlores
Unconventional spin-phonon coupling in 4d and 5d transition metal oxides

The spin-phonon (SP) coupling has long been a central theme in condensed matter physics. To date, most of these phenomena have been understood by considering the Heisenberg interaction between spins. However, recent studies on 4d/5d transition metal oxides (TMOs) have revealed that strong spin-orbit coupling (SOC) plays the crucial role in their magnetism. Since the orbitals are generically coupled to the lattice, the strong SOC present in 4d/5d orbitals creates strong and inevitable interactions between spin and lattice.

Using optical spectroscopy, we carried out comparative studies on the 5d TMOs. From infrared (IR) phonon spectra, we discovered unconventional SP coupling in Cd$_2$Os$_2$O$_7$ and Y$_2$Ir$_2$O$_7$. For Cd$_2$Os$_2$O$_7$, we observed large phonon frequency shifts below $T_N$. This is due to the SP coupling arising from single-ion anisotropy [1,2]. We also identified frequency shifts of Y$_2$Ir$_2$O$_7$ near $T_N$. However, in this case, the Dzyaloshinskii-Moriya interaction plays a crucial role in the phonon renormalization [3]. Using near-IR pump-probe technique, we investigated coherent phonon oscillations of 4d TMO. Recently, Ca$_2$RuO$_4$ has been of particular interest due to its exotic magnetic ground state driven by strong SOC. We observed that a coherent $A_g$ phonon oscillation changes abruptly its amplitude and phase as the spin order develops.

Density functional theory calculations revealed that the structural deformation by the magnetic order can induce such variations in coherent phonons, which we suggest as a unique signature of SP coupling [4]. Our comprehensive studies on unconventional SP coupling may lead to scientific advancement in 4d/5d TMOs, and possibly endow opening new research fields come across.


This work was supported by the Institute for Basic Science in Korea (IBS-R009-D1).

AC magnetic susceptibility and heat capacity studies of the geometrically frustrated pyrochlores Ce$_2$Zr$_2$O$_7$ and Ce$_2$Hf$_2$O$_7$, as possible quantum spin liquids (QSL’s)

QSL’s are of great interest due to their unusual ground states; they do not exhibit spin freezing even at 0K, have no conventional order parameter associated with a broken symmetry, and can emerge in insulators containing localized spin degrees of freedom. In this work, single crystals of the low-spin geometrically frustrated 2D lattice pyrochlore compounds Ce$_2$Zr$_2$O$_7$ and Ce$_2$Hf$_2$O$_7$ prepared by the floating zone method, were investigated for a possible QSL state. Measurements of AC magnetic susceptibility from 100 Hz to 10 kHz and heat capacity up to 9T were performed down to 100 mK. Despite a well-ordered pyrochlore crystal structure and strong magnetic interactions between Ce$^{3+}$ ions in Ce$_2$Zr$_2$O$_7$ and Ce$_2$Hf$_2$O$_7$, no evidence for a transition to a long-range ordered state was found, possibly due to strong quantum fluctuations that prevent spin freezing and lead to QSL ground state. With increasing magnetic field, the Schottky heat capacity anomaly moves to higher temperatures, indicating the presence of a gap in the excitation spectrum, which increases monotonically with increasing field. The behavior for a two-level system with an excited level at energy $\Delta$ above the ground state is compared with the heat capacity data.

Research supported by US DOE BES, NSF DM, cQMS (EPIQS - GBMF6402)
3:18PM H46.00003: Time-resolved optical study of the metal-to-insulator transition in Cd2Os2O7  

CHEN LI (Presenter), XIANG LI, DANIEL SILEVITCH, ALON RON, YISHU WANG, Caltech, Physics, Math & Astronomy, JIAQIANG YAN, DAVID GEORGE MANDRUS, Materials Science and Technology, Materials Science and Technology, THOMAS F ROSENBAUM, DAVID HSIEH, Caltech, Physics, Math & Astronomy — The 5d transition metal oxide Cd2Os2O7 undergoes a continuous metal-to-insulator transition (MIT) with a concomitant magnetic transition into an all-in-all-out (AIAO) antiferromagnetic state below a critical temperature TMIT = 227 K. Here, we investigate the effects of this transition on its photo-carrier dynamics by performing temperature and wavelength dependent ultrafast optical reflectivity measurements. We show that the opening of a charge gap at TMIT causes a divergence like behavior of the photo-carrier relaxation time consistent with a Rothwarf-Taylor model. Our efforts to perform these experiments under high pressure environments will also be discussed, which is motivated by recent resonant x-ray diffraction results on Cd2Os2O7 showing a monotonic suppression of AIAO order with pressure.

3:30PM H46.00004: Tuning the ground state of a candidate Weyl semimetal Eu2Ir2O7 by Bi doping  

PRACHI TELANG (Presenter), KSHITI MISHRA, SURJEET SINGH, Indian Institute of Science Education and Research, Pune — The interplay of spin-orbit coupling (λ) and onsite coulomb interactions (U) in the pyrochlore iridates A2Ir2O7 has been predicted to give rise to a plethora of non-trivial topological phases. Here we investigate the pyrochlore series (Eu1-xBix)2Ir2O7 whose end members are located in two different regions of the λ-U phase space. Eu2Ir2O7 (EIO) shows a metal to insulator (MI) transition at 120 K concomitant with an antiferromagnetic ordering where the Ir moments order in an all-in-all-out(AIAO) structure. EIO is predicted to be a Weyl semimetal; whereas Bi2Ir2O7 (BIO) is a non-Fermi liquid metal with at least two magnetic transitions below 2 K. In this presentation, we show that Bi substitution as high as 3.5% dopes electrons in the system without altering the electronic structure and tunes the Fermi energy with little change in MI/AIAO transitions. However at higher doping levels both these transitions are very strongly suppressed. The sample prepared with 10% Bi doping showed an highly unconventional metallic behaviour and no signs of MI/AIAO ordering down to at least 2 K. For higher doping, the behaviour gradually evolved to that of BIO. Our study exemplifies the appearance of unusual behaviours at the boundary between Weyl semimetal and non-Fermi liquid of the λ-U phase space.

3:42PM H46.00005: Magnetic torque in spin-orbit coupled metal Cd2Re2O7  

SHINYA UJI (Presenter), National Institute for Materials Science, YASUHITO MATSUBAYASHI, KAORI SUGII, DAIGOROU HIRAI, ZENJI HIROI, Institute for Solid State Physics, University of Tokyo, TAKUMI HASEGAWA, Graduate School of Integrated Arts and Sciences, Graduate Hiroshima University, SHIORI SUGIURA, HISHIRO HIROSE, TAICHI TERASHIMA, National Institute for Materials Science — Spin-orbit (SO) interactions lead to peculiar symmetry-broken phases in highly correlated systems. Among various SO coupled metals, a metallic pyrochlore Cd2Re2O7 is known to show unique multipole orders associated with the inversion symmetry breaking below ~200 K, whose order parameter has Eu symmetry. We have measured the magnetic torque of Cd2Re2O7 in a wide temperature and field range. We find that a four-fold symmetry of the magnetic torque signal as well as a two-fold symmetry is significantly enhanced at low temperatures below ~200 K. The symmetry analysis of the torque signal strongly suggests the presence of the primary order parameter (OP) with the even parity Eu symmetry, which induces the four-fold term, whereas the two-fold arises from the odd parity Eu OP. It is very likely that the Eu symmetry OP is purely of electronic origin and the coexistence with the odd-parity Eu OP provides important insights into the origin of the multipole orders induced by the SO coupling.

3:54PM H46.00006: Electronic and magnetic ground states of the Kitaev material candidates A2CeIrO6 (A~ = Ba,Sr)  

ADAM ACZEL (Presenter), Oak Ridge National Laboratory, JAMES P.I. CLANCY, McMaster University, QIANG CHEN, HAI DONG ZHOU, University of Tennessee, DALMAU REIG-I-PLESSIS, GREG MACDOUGALL, University of Illinois at Urbana-Champaign, JACOB RUFF, CHESS, MARY UPTON, Argonne National Laboratory, TRAVIS J WILLIAMS, STUART CALDER, JIAQIANG YAN, Oak Ridge National Laboratory — Quantum magnets with significant bond-directional Ising interactions, so-called Kitaev materials, have attracted tremendous attention recently in the search for exotic spin liquid states. Here we present a comprehensive set of measurements that enables us to elucidate the crystal structures, Ir4+ single ion properties, and magnetic ground states of the double perovskite iridates A2CeIrO6 (A~ = Ba,Sr). The crystal structures of Ba2CeIrO6 and Sr2CeIrO6 are found to be cubic and monoclinic respectively, with a large nearest neighbor distance >~5\AA~between Ir4+ ions. X-ray absorption spectroscopy and resonant inelastic x-ray scattering were used to establish J_{eff}~ = ~1/2~ spin-orbit-assisted Mott insulating states, while bulk characterization and neutron powder diffraction identify A-type antiferromagnetic order. These electronic and magnetic ground states are both consistent with expectations for face-centered-cubic magnets with dominant Kitaev exchange, which indicates that spacing magnetic ions far apart may be a promising design principle for uncovering new Kitaev materials.
**4:06PM H46.00007: Global Metal-Insulator Transition in the Pyrochlore Iridates (Nd_{1-x}Ca_x)_{2}Ir_{2}O_{7}**
ZACH PORTER (Presenter), ELI ZOGHLIN, University of California, Santa Barbara, GENEVA LAURITA, Bates College, JACOB P.C. RUFF, CHESS, YONGSEONG CHOI, DANIEL HASKEL, Argonne National Lab, STEPHEN WILSON, University of California, Santa Barbara — We report on the suppression of the metal-insulator transition (MIT) in polycrystalline samples of Nd_{2}Ir_{2}O_{7} under substitution of Nd for Ca. Each calcium ion effectively dopes one hole on an Ir^{4+} (5d^{4}, j_{eff}=1/2) site, mediating a filling-controlled Mott-like transition. Ca substitution also changes bandwidth by modulating Ir-O bond lengths and angles, without altering site symmetry. Local structure and absorption spectroscopy confirm that Ca substitution does not result in phase separation or large changes to Ir electronic configuration. The MIT has a coincident antiferromagnetic transition on the Ir sublattice (T_N = T_{MIT}) for all measured samples, which both decrease with Ca content. Weak low-temperature upturns in susceptibility and resistivity for samples with high Ca content suggest that Nd sublattice magnetism couples to carriers in the metallic regime.

*This work was supported primarily by ARO Award No. W911NF-16-1-0361. The MRL Shared Experimental Facilities are supported by the MRSEC Program of the NSF under Award No. DMR 1720256, a member of the NSF-funded Materials Research Facilities Network. Research at CHESS is supported by the NSF under Award No. DMR-1332208. Use of the APS at ANL was supported by the U.S. DOE Office of Science under Contract DE-AC02-06CH11357.

**4:18PM H46.00008: Enhanced Thermopower in Hole-doped Pyrochlore Iridates: Correlated Metal with Quadratic Band Touching**
RYOMA KANEKO (Presenter), Department of Applied Physics and Quantum-Phase Electronics Center, University of Tokyo, MARIE-THERESE PHILIPP, Center for Emergent Matter Science, RIKEN, JUN FUJIOKA, Graduate School of Pure and Applied Sciences, University of Tsukuba, SHIRO SAKAI, Center for Emergent Matter Science, RIKEN, RYOTARO ARITA, Department of Applied Physics and Quantum-Phase Electronics Center, University of Tokyo, HIROSHI SHINAOKA, Department of Physics, Saitama University, KENTARO UEDA, YOSHINORI TAKURA, Department of Applied Physics and Quantum-Phase Electronics Center, University of Tokyo — Quadratic band touching (QBT) is a band structure in which the parabolic valence and conduction band touch at a point, protected by spatial and time inversion symmetry. The possibility that QBT becomes the source of exotic electronic phases such as Weyl semimetal has been discussed. The existence of QBT has been confirmed in Pr_{2}Ir_{2}O_{7} (PIO), which is a member of pyrochlore-type iridate R_{2}Ir_{2}O_{7} (RIO, R=Rare earth). Since QBT in PIO is stabilized by the crystal symmetry, we can consider the possibility of the universal existence of QBT in the paramagnetic metallic phase of RIO. Therefore, we made hole-doped samples of insulator Eu_{2}Ir_{2}O_{7} to compare its electronic properties with PIO.
Using the charge transport measurement and ab-initio calculation, we have explored the thermopower and electronic structure of correlated metal with QBT in hole-doped pyrochlore iridates. We found that the hole-doped QBT yields a thermopower peak, which can be enhanced exceeding 40 V/K below 50 K by tuning the band-filling and lattice distortion. The thermopower peak is observed even in the doping induced metallic phase created from Mott insulator, indicating that the QBT is robust against the strong electron correlation as well as the lattice distortion while keeping the cubic symmetry.

**4:30PM H46.00009: Stoichiometry Control, Electronic and Transport Studies of Pyrochlore Iridate Thin Films**
WENCAO YANG, Indiana University Bloomington, YUANTAO XIE, Shenzhen University, XING SUN, Purdue University, XIAOHANG ZHANG, University of Maryland, College Park, KYUNGWHA PARK, Virginia Tech, SICHIANG XUE, Purdue University, YANLONG LI, CHENGANG TAO, Virginia Tech, QUANXI JIA, University at Buffalo – The State University of New York, YAROSLAV LOZOVYY, Indiana University Bloomington, HIAYAN WANG, Purdue University, JEAN HEREMANS, Virginia Tech, SHIXIONG ZHANG (Presenter), Indiana University Bloomington — Pyrochlore iridate thin films are predicted to host a variety of exotic magnetic and topological states. Experimental probing of the emergent quantum states strongly relies on the synthesis of high-quality thin film samples. In this work, we demonstrate the epitaxial growth and stoichiometry control of pyrochlore Bi_{2}Ir_{2}O_{7} thin films via pulsed laser deposition followed by a post annealing process. The as-deposited films form a bilayer-like structure consisting of an Ir-deficient top-surface and an Ir metal layer at the bottom. Post annealing in iridium oxide atmosphere significantly improves the stoichiometry and homogeneity throughout the film thickness. Density functional theory calculation shows a fourfold degenerate Dirac node slightly below the Fermi energy at the X point, coexisting with some trivial bands around the Γ point. Transport studies revealed a transition from a weakly-metallic to weakly-insulating behavior at around 150 K, accompanied by positive magnetoresistance at low temperatures.

*Work supported in part by the College of Arts and Sciences in Indiana University, DOE DE-FG02-08ER46532, and NSF DMR-1565822.*
Mapping the magnetic and electronic structure of $(\text{Eu}_{1-x}\text{Ca}_{1-x})_2\text{Ir}_2\text{O}_7$ across a global metal-insulator transition* ELI ZOGHLIN (Presenter), ZACH PORTER, Materials, University of California, Santa Barbara, GENEVA LAURITA, Chemistry and Biochemistry, Bates College, DANIEL HASKEL, YONGSEONG CHOI, Advanced Photon Source, Argonne National Laboratory, STEPHEN WILSON, Materials, University of California, Santa Barbara — Motivated by the prediction of quantum critical behavior with the suppression of the temperature dependent metal-insulator transition in $\text{Ln}_2\text{Ir}_2\text{O}_7$ ($\text{Ln} = \text{Y, lanthanide}$), including the formation of a topological semi-metal phase$^{1,2}$, we present characterization of polycrystalline samples for the series $(\text{Eu}_{1-x}\text{Ca}_{1-x})_2\text{Ir}_2\text{O}_7$. Doping completely suppresses the MIT with only a weak decrease in the magnetic transition, leading to a fully metallic state that retains the bulk magnetism of the $x = 0$ compound. XRD and XAS suggest that the change of $T_{\text{MIT}}$ occurs due to an interplay between bandwidth tuning via a change in the Ir-O-Ir bond angle as well as filling control. X-ray PDF shows no changes in short-range order associated with either the MIT or the magnetic transition, additionally confirming that Ca-doping does not result in significant phase separation. Preliminary XMCD data probing the magnetic state across the MIT will be discussed.*


*This work was supported by ARO Grant W911NF-16-1-0361.

Tuesday, March 5, 2019 2:30 PM - 4:30 PM

Session H47 FOEP: From FunSized Physics to Escaping Labs; Adventures in Public Engagement BCEC 213 - James Kakalios, University of Minnesota - Tag(s): Outreach

2:30PM H47.00001: Lessons learned from outreach grant administration JAMES ROCHE (Presenter), American Physical Society — TBD

2:42PM H47.00002: Physics is for Everyone: How to Market Physics for The Masses* PHOEBE SHARP (Presenter), Rhodes College — Marketing science for the general public is challenging. As physics students, we understand the importance and need for science education, so reaching out to those outside of our physics and science communities is a great way to share our curiosity and excitement for how the world works. This summer, I worked on providing accessible and interesting content for patrons of the Physics Central website, a site that works to encourage curiosity in physics through comics, blog posts, and other media outlets. That included writing scientific articles about often overlooked concepts in physics, as well as researching ways to make the website more eye catching and relevant.*

*Society of Physics Students
APS Public Outreach Department
APS Education and Diversity Department
Rhodes College

2:54PM H47.00003: The US Physics Team: Training for competition and building community JIAJIA DONG (Presenter), Bucknell University / AAPT — Since the founding of the US Physics Team in the mid-1980s, the team coaches have had the mission of selecting and training the top US high school physics students to compete in the annual International Physics Olympiad. Over the decades, the coaches have worked hard to encourage participation from high schools around the nation, to design challenging training materials, and to build a growing community of students who share their curiosity and passion in physics. The bond built through learning physics together remains strong when the students later find their roles in the society such as physicists, engineers, lawyers, and doctors.

Recently celebrating its 30th anniversary, the Team continues to try to broaden its impact, by reaching more students who are not only interested in learning physics, but enthusiastically embrace the challenges of problem-solving, finding efficient, elegant, and insightful solutions, and discovering new physics. We share the story of the US Physics Team, and invite your contribution to the growth of the program.
3:06PM H47.00004: LabEscape, A Science-Based Escape Room: Where We Are, and How We Got Here*  PAUL KWIAT (Presenter), IAN CALL, ERIC HUDEC, REBECCA WILTFONG, University of Illinois at Urbana-Champaign — Based on APS seed money, we have set up what we believe is the world's first science-based escape room: LabEscape. By interacting with physics components in the room, participants uncover clues that allow them to solve the mystery of missing quantum physicist Professor Alberta Schrodenberg, and escape! Our goal is to show that science can be useful and accessible (no prior background is assumed), as well as beautiful and even fun! The room is operated by undergraduate STEM students, and most of the puzzles were created by them as well, all based on physics phenomena, including polarization, refraction, induction, lasers, etc. Along the way the Agents directly experience some key aspects of scientific research, and are exposed to basic themes in quantum information. To date we've had nearly 4000 participants, and received near perfect reviews. For more information, see LabEscape.org; to sign up at APS, visit LabEscape.org/APS/.

*This project was supported in part by the APS, NSF, and SPIE, as well as the UIUC College of Engineering.

3:18PM H47.00005: LabEscape, A Science-Based Escape Room: Now What*  IAN CALL (Presenter), ERIC HUDEC, PAUL G KWIAT, REBECCA WILTFONG, University of Illinois at Urbana-Champaign —

Our science-based escape room has been operating in our local mall for over two years, and although not it's primary goal, LabEscape has been an excellent laboratory for observing group dynamics (we've had ~800 groups go through), the impact of diversity, and the roles of curiosity, communication, and collaboration. We've developed several different scenarios with varying durations and varying degrees of success. We'll discuss what has and hasn't worked, and our efforts to expand to an even wider audience, e.g., in other cities, science centers, etc. One recent addition is the inclusion of a portable version, which we debuted at the August, 2018 AAPT conference, and have now brought to the APS March meeting.

For more information, see LabEscape.org; to sign up at APS, visit LabEscape.org/APS/.

*This project was supported in part by the APS, NSF, and SPIE, as well as the UIUC College of Engineering.

3:30PM H47.00006: What's been happening at FunSizePhysics?*  SHIREEN ADENWALLA (Presenter), JOCELYN BOSLEY, University of Nebraska - Lincoln, LEIGH SMITH, Physics, University of Cincinnati —

www.funsizephysics.com is a website created with the express purpose of advertizing exciting new developments in condensed matter physics to the tax paying public. In addition, the website was designed to be a convenient place in which to collaborate on and discuss a variety of outreach efforts. The website is unique in that it incorporates research descriptions written by the researchers themselves for a broad audience, unlike numerous science blogs and/or websites. We describe the ongoing efforts to present current and ongoing NSF-funded research to the public in ways that engage a broader audience of non-experts and to make the website a resource for NSF PIs to develop best practices for outreach activities to K-12 students and the general public. We have also embarked on an ambitious program to impact the ability of present and future scientists to communicate with the public, using professional science writers as teachers and modelers for science communication. The ambitious aim is to change how condensed matter physicists communicate with the public.

*Funding from NSF-DMR 1725823 is gratefully acknowledged.

3:42PM H47.00007: Electron Microscopy: Building Nanoscale Knowledge and Community Connections  SARAH GOODMAN (Presenter), Department of Materials Science and Engineering, Massachusetts Institute of Technology —

Electron microscopy (EM) is not only key to solving the greatest challenges we face in the energy sphere, but it can also be a powerful tool for establishing connections between current and aspiring scientists as well as the public. The work of scientists and engineers is often portrayed as complicated and inaccessible, which can alienate the general public and deter students from pursuing the STEM fields, particularly those who don't often see role models like themselves as scientists. Here, I will present the results of three types of community outreach events that used EM to provide both the public and K-12 students an opportunity to engage in the same type of work that researchers do. In two events, the general public was invited to experience EM demos and use the tools themselves, which allowed the process and tools of research become demystified. In another event, a group of middle school students used the transmission electron microscope to image gold nanoparticles at atomic resolution. By including the community in our everyday research activities, we can work towards building trust between scientists and the public to pave the way for stronger science policy in the future.
3:54PM H47.00008: Physics for all ages: Texas A&M Physics Show  TATIANA ERUKHIMOVA (Presenter), Texas A&M University — The Texas A&M Physics Show started in 2007 and has been attended by 22,000 people since then. We offer 40-50 Shows per year. The target audience for the Physics Show is preK-12. The Show lasts 90 min and consists of three parts: 45-60 min Show in the Auditorium, 20 min interactive Hands-on activities in the lobby, and the depth charge outside. Examples of demonstrations that we share with children include clouds, lightning, and magic bubbles, solid air and liquid oxygen, jet propulsion, levitating superconducting trains and flying toilet paper and many more. The presentation is tailored to groups of different ages and "attention spans". We'll discuss pros and cons of starting a similar program and what it takes to run it all year round.

4:06PM H47.00009: How to involve citizen scientists in your research*  JAMES FREERICKS (Presenter), Georgetown University — Citizen science is often viewed as crowd science where citizens are employed in labor intensive data collection or in other tedious activities required for complex research. But the advent of MOOCs makes it easy to identify, recruit, and collaborate with talented citizen scientists on any research problem. The MOOC audience provides a highly educated and motivated space to recruit research partners from. I will describe a number of different citizen science projects I have been involved in in the past year which have lead to three publications and a number of ongoing projects. I will illustrate how one can recruit research partners and examine how one can find appropriate projects to collaborate on. Whether you are in need of research collaborators or just assistance in your research projects, recruiting citizen scientists provides a new resource to advance your research agenda. I recommend it as a best practice to everyone. It is a wonderful way to give back to the community, provide broader impacts of your work, and get more research finished.

*This work was funded by the National Science Foundation under grant number PHY-1620555.

4:18PM H47.00010: Inventing the Future: How to Make Stuff that Can Change the World  RYAN BAUMBACH (Presenter), National High Magnetic Field Laboratory - Florida State University — Condensed matter physics and materials science topics that persistently defy efforts to engage the public imagination. This is despite the fact that modern society thrives due to the development of thousands of new materials that are routine and essential parts of most people's everyday lives. In this talk I will describe progress towards creating video content that is designed to educate and entertain as it tells the story of how a material is conceived, created and embedded into our lives. I will not only present the resulting video, but will also describe the unique collaboration that has led to its production, which involves scientists and science communicators at the National High Magnetic Field Laboratory and filmmakers, actors, and artists at the Florida State University College of Motion Picture Arts. I will present insights gained from this new paradigm for producing science content for public consumption.

Tuesday, March 5, 2019 2:30 PM - 5:18 PM

Session H48 DFD GSNP: Granular, Porous Media, Multiphase Flows & Bubbles  BCEC 251 - Fu-Ling Yang - Tag(s): Focus

2:30PM H48.00001: Dynamical model for nonlocal inertial-number rheology of dense granular flows*  KENG-LIN LEE (Presenter), FU-LING YANG, Mechanical Engineering, National Taiwan University — Dense granular materials present complicated fluid and solid behaviors. The materials flow above a yield stress which is greater than the magnitude when the flow stops, known as hysteresis. Nonlocal flow rheology emerges due to particle cooperative motions, resulting in flow-size dependence in quasistatic regime and long-range collision momentum transport in dense inertial regime. In this talk, we formulate a dynamical Ginzburg-Landau model of phase transition that can describe these features. We choose the inertial number I as a fluidization order parameter and derive the free energy functional using scaling arguments along with a yield-stress weakening mechanism. The model yields a nonmonotonic flow curve in a homogeneous flow environment, accounting for hysteresis and intermittency in the quasistatic regime. The model shows a generalized Bagnold stress revealing two nonlocal mechanisms: collisions among correlated structures within which fluidization spread. The model captures several salient features in inclined flow configuration including hysteretic starting and stopping heights, Pouliquen's inertial flow rule and flow-thickness dependent velocity shapes.

*This project was supported by the Ministry of Science and Technology of Taiwan through Grants No. 106-2628-E-002-012-MY3.
Boundary Condition for Dense Granular Flows on Smooth Boundary* FU-LING YANG, CHENG-CHUAN LIN (Presenter), Mechanical Engineering, National Taiwan University — When granular material moves relative to a smooth boundary, we often assign a Coulomb-type stress boundary condition with a constant effective wall friction coefficient $\mu_w$. Recent experimental and numerical (DEM) investigations on both steady and transient flows reveal a roubst trend that that $\mu_w$ decays monotonically with the distance from a moving boundary such as a free surface, a slip base, or an internal shear band. Individual grain rotation is found to be an internal mechanism to degrade bulk $\mu_w$. We discover that grain anular speed is correlated with granular temperature which has been reported to correlate with bulk slip velocity or shear rate. We integrate the findings to present a boundary condition for dense granular flows with non-zero velocity relative to its boundary.

*The authors acknowledge the financial support from Ministry of Science and Technology, Taiwan from both the grant MOST 106-2628-E-002-012-MY3 and the French-Taiwan Orchid Project 107-2911-I-002-536.

Cooperative and uncooperative motions in gravity-driven flows* KERSTIN NORDSTROM (Presenter), EMMA C THACKRAY, GRACE S CAI, Mount Holyoke College — We present results from experiments and complementary molecular dynamics simulations of 2D gravity driven granular flows. We specifically study silo flow: discharge through an aperture in a rectangular cell. We obtain particle-scale data in our experiments using high-speed, high-resolution video. We find the presence of cooperatively moving regions and characterize them by their sizes, speeds, and lifetimes. We also find the presence of regions of high nonaffine motion and characterize them similarly. In our analysis, we place particular emphasis on the role of initial packing structure on the resulting bulk flow behavior and microscopic deformations. Our results suggest that the transition from clogging behavior to free flow can be modified by changing the packing structure.

*Acknowledgement is made to the donors of the American Chemical Society Petroleum Research Fund (PRF# 56888-UNI9) for support of this research.

New concepts for modeling connectivity effects in capillary pressure hysteresis in porous media ZONGYU GU (Presenter), AMIN AMOOIE, MARTIN BAZANT, Massachusetts Institute of Technology — Continuum models of porous media often characterize microscopic features of the pore space using macroscopic parameters like porosity and tortuosity, and macroscopic state variables like fluid saturations. To account for the effects of pore-scale connectivity between different sized pores, we propose a new parameter, “pore-space accessivity” to contrast serial and parallel arrangements of different sized pores, and a new state variable, “radius-resolved saturation”, to describe the microscopic distribution of fluids. Based on a statistical branching process, we derive a new microscopic constitutive theory of capillary pressure hysteresis for arbitrary drainage-imbibition cycles. Expanding on the classical “capillary bundle” picture by means of providing a useful first approximation for connectivity effects in porous media, these concepts may have much broader utility in continuum modeling of porous media in a variety of applications.

Capillary filling of water in structural defects at fiber-matrix interface of unidirectional composite materials KALPANI GALPAYAGE DONA (Presenter), Department of Physics, Florida Atlantic University, SARAH E DU, LEIF CARLSSON, Ocean and Mechanical Engineering, Florida Atlantic University — Presence of internal structural defects and damages in a polymeric composite can affect its moisture absorption behavior. This study developed a mathematical model to evaluate the behavior of water uptake in the voids at fiber/matrix interface of unidirectional composite materials. The model considers moisture absorption via diffusion by the Fick’s law and water filling driven by capillary action in the voids at the fiber/matrix interface. The water wicking in the voids is modeled using a one-dimensional two-phase fluid flow, where capillary filling is influenced by the initially trapped air bubbles in the voids, permeation of air is enhanced by the pressure from water front of capillary flow. A material parameter, contact angle was introduced to measure the strength of capillary action in the voids. The model was verified experimentally with a carbon fiber reinforced vinyl ester material. The predicted water filling behavior agreed well with the experimentally measured content of absorbed water. Dependences of water absorption behavior on contact angle and void size were discussed.
3:30PM H48.00006: Instabilities of Vertical Time-Dependent Miscible Displacements in Homogeneous Porous Media
YOUSSEF ELGAHAWY (Presenter), JALEL AZAIEZ, Department of Chemical and Petroleum Engineering, University of Calgary — Buoyancy-driven instabilities develop at the interface between fluids in miscible flow displacements. Such instabilities significantly affect the efficiency of displacement processes encountered in many applications such as enhanced oil recovery and CO2 sequestration. Thus, it is imperative to control such instabilities. Most studies on vertical miscible displacements are limited to displacements involving a constant injection rate. However, in some practical processes the injection rate is in fact time-dependent. The objective of this study is to investigate the effects of time-dependent injection rates on the growth of fingering instabilities. The governing equations are solved numerically using the Hartley-Pseudo-spectral method. First, the dynamics of fingering instabilities were examined using nonlinear simulations, under constant injection rates, to determine the criteria for the instability which depends on the mobility ratio, density difference, and the critical injection velocity. Then, utilizing time-dependent injection schemes, it was found that the instability can be attenuated depending on the cycle period and velocity amplitude. Moreover, the flow is always less unstable when the displacement is initiated through an extraction stage rather than an injection one.

3:42PM H48.00007: Continuum-Scale Modeling of Multiphase Flow in Porous Media From a New Microscopic Theory of Hysteresis
AMIN AMOOIE (Presenter), ZONGYU GU, Department of Chemical Engineering, Massachusetts Institute of Technology, MARTIN BAZANT, Department of Chemical Engineering and Department of Mathematics, Massachusetts Institute of Technology — We present continuum modeling of multiphase flow in macroscopic porous media based on a new microscopic hysteresis theory that provides physics-based macroscopic parameters and state variables to capture essential pore-scale features. We propose accessivity to characterize the network connectivity of different-sized pores in a porous medium, and radius-resolved saturations to characterize the distribution of fluid phases within. Developing a statistical theory for quasistatic immiscible drainage-imbibition in arbitrary cycles, we arrive at simple models that naturally arrest hysteresis in capillary pressure and relative permeability. Existing models use empirical case-based modifications to capture hysteretic data and rectify the curvatures of their predictions, which fails to make a physical connection to the medium microstructure. Employing the proposed conceptual framework, here we then develop a novel multiphase flow simulator for macroscopic porous media, where the new constitutive relationships for both capillary pressure and relative permeability consistently link the continuum model to the microscopic state of fluid phases in a porous medium of a given microstructure.

3:54PM H48.00008: Non-orthogonal multiple-relaxation-time lattice Boltzmann method: theory and its application in multiphase flows*
LINLIN FEI (Presenter), Department of Energy and Power Engineering, Tsinghua University, KAI HONG LUO, Department of Mechanical Engineering, University College London — A three-dimensional multiple-relaxation-time lattice Boltzmann method (MRT-LBM) is constructed based on a series of non-orthogonal moments. Compared with the widely used orthogonal-moments-based MRT-LBM, the present formulation simplifies the mapping between the discrete velocity space and the moment space, and exhibits better flexibility across different lattices. The proposed method is then extended to simulate multiphase flows with large density ratio and tunable surface tension, and validated via benchmark cases. Finally, we present simulations of several practical and challenging problems using the non-orthogonal MRT-LBM to highlight its capability for simulating realistic multiphase flows.

*The research has received funding from the MOST National Key Research and Development Programme (Project No. 2016YFB0600805) and the UK Engineering and Physical Sciences Research Council (EPSRC) under the project "UK Consortium on Mesoscale Engineering Sciences (UKCOMES)" (Grant Nos. EP/L00030X/1 and EP/R029598/1).

4:06PM H48.00009: Cavitation in Boxing: A physical approach*
THIBAULT GUILLET (Presenter), JULIETTE AMAUGER, LadHyX, Ecole polytechnique, DAVID QUERE, PMMH, ESPCI, CAROLINE COHEN, CHRISTOPHE CLANET, LadHyX, Ecole polytechnique — When a closed container filled of water (model of the head) is accelerated by a shock, cavitation bubbles can form and eventually, at their collapse, cause the shattering of the container. Predicting the growth and collapse dynamics of a bubble is crucial in limiting its damages. By conducting simultaneous high-speed imaging of the motion and pressure measurements in the fluid, we show that Rayleigh-Plesset equation accurately predicts the time evolution of the bubble radius. Additionally, we both experimentally and theoretically prove that the pressure distribution in the fluid can be directly derived from the acceleration. Finally, the overall bubble dynamics is found to be governed by the maximal acceleration and the timespan of the shock.

*We thank Direction Générale de l'Armement (DGA) for their financial support.
JULIETTE AMAUGER (Presenter), THIBAULT GUILLET, LadHyX - Ecole Polytechnique, DAVID QUERE, PMMH - ESPCI, CHRISTOPHE CLANET, CAROLINE COHEN, LadHyX - Ecole Polytechnique — Traumatic Brain Injury (TBI) is a major healthcare problem, increasingly occurring in sports like rugby, boxing or football. The occurrence of TBI is dependent on the head acceleration and the duration of the shock, as expressed by the empirical Wayne State Tolerance Curve (WSTC). One of the possible causes of TBI is the formation of cavitation bubbles in the cerebro-spinal fluid. To investigate this hypothesis, we experimentally observe the formation of cavitation bubbles due to a shock on a water tank, and we quantify the influence of the acceleration and timespan of the shock on the bubbles dynamics. In the cranial cavity, the cerebro-spinal fluid can flow in and out through the spinal cord. Using a flexible membrane to mimic this phenomenon, we show that this motion is a prerequisite for bubble growth. From the prediction of the bubbles sizes, we build a phase diagram of the damaging capacity of the bubbles on the brain as a function of the acceleration profile, in good agreement with the prediction of the WSTC.

*Project funded by DGA

GARTH EGAN (Presenter), XAVIER LEPRO CHAVEZ, EDMOND LAU, ERIC R SCHWEGLER, Lawrence Livermore Natl Lab — In recent years, it has been suggested that micron and sub-micron scale cavitation can occur in the human brain during explosive pressure wave, blunt trauma, or sports collision type events and that the resulting bubble collapse could be the main cause of damage leading to traumatic brain injuries. However, the behavior of very small bubbles is not yet well understood because of the challenges associated with imaging on the necessary length and time scales. Here, we present the direct imaging of bubble collapse in a liquid cell using the Movie-Mode Dynamic Transmission Electron Microscope (MM-DTEM) at Lawrence Livermore National Laboratory. Bubbles were induced in ~1-3 µm of water using laser heating of 60 nm gold particles and typically found to collapse within 200 ns. Polymer coated on the liquid cell substrates served as witnesses to potential damage. The behavior of the system was further explored with molecular dynamic (MD) simulations.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

CHRISTOPHER BOYCE (Presenter), Department of Chemical Engineering, Columbia University, ALEXANDER PENN, MAXIM LEHNERT, Department of Mechanical and Process Engineering, ETH Zurich, AZIN PADASH, Department of Chemical Engineering, Columbia University, KLAAS P PRUESSMANN, Institute for Biomedical Engineering, ETH Zurich and University of Zurich, CHRISTOPHER MULLER, Department of Mechanical and Process Engineering, ETH Zurich — Rapid magnetic resonance imaging (MRI) is used to measure the dynamics of bubbles and jets of gas injected into 3D gas-fluidized beds of granular particles. When two bubbles initially of equal volume rise side-by-side, one bubble collapses while the other maintains its size. This phenomenon is attributed to channeling of gas flow through one bubble, leaving the collapsing bubble with insufficient gas flow to maintain its roof and rise velocity via drag force. When two jets of gas are injected side-by-side, bubbles pinch off from the two jets at alternating times, creating a zipper-like pattern. This phenomenon is attributed to the growth of one jet pushing particles toward the second jet, causing bubble pinch-off from the second jet. The second jet subsequently grows, pushing particles toward the first jet, causing a cyclical pattern to form. Different bubble and jet interaction patterns are seen depending on the size of the particles in the fluidized bed; these differences are attributed to the variation in gas permeability through assemblies of granular particles with particle size.

*This work was supported by the Swiss National Science Foundation under grant number 200021_153290.

IVO PETERS (Presenter), University of Southampton, YOSHIYUKI TAGAWA, Tokyo University of Agriculture and Technology — The collapse of a vapor bubble near a flat solid boundary results in the formation of a jet that is directed towards the boundary. In more complex geometries such as corners, predictions of the collapse cannot be made in a straightforward manner due to the loss of axial symmetry. We experimentally investigate the bubble collapse and jet formation in corners formed of two flat solid boundaries with different opening angles. Using potential flow analysis, we accurately predict the direction of the jet and bubble displacement. We further show that for a corner with an opening angle $\alpha$, there exist analytic solutions that predict the jet direction for all the cases $\alpha = \pi/n$, where $n$ is a natural number. These solutions cover, in discrete steps, the full range of corners from the limiting case of a bubble near a single wall ($n = 1$) up to a bubble in between parallel walls ($n \to \infty$).
5:06PM H48.00014: Give it a boost -- The shape of a traveling long bubble during the transition between two steady states

YINGXIAN ESTELLA YU (Presenter), LAILAI ZHU, SUIN SHIM, Department of Mechanical and Aerospace Engineering, Princeton University, JENS G EGGERS, School of Mathematics, University of Bristol, HOWARD A STONE, Department of Mechanical and Aerospace Engineering, Princeton University — When a confined long bubble translates steadily in a cylindrical capillary, with negligible gravity effects, a uniform thin film of fluid separates the bubble surface and the tube wall. Although a wide variety of investigations have been carried out analyzing the relationship between the film thickness profile and the bubble velocity, most of the literature considers the case where the translational velocity is a constant, thus the bubble profile is steady. Instead, in this work, we investigate how this steady state is established by considering the transitional motion of the bubble as it adjusts its film thickness profile between two steady states, characterized by two different bubble speeds. Different sections of the time-dependent film profile will be characterized, and we will further discuss how the “travel history” of the bubble is stored in the bubble shape. The theoretical results are further verified both by experiments and numerical simulations. The results can potentially be applied to a tunable in-situ particle separation process.

*We thank the NSF for support via grant CBET-1804863. JE acknowledges support from the Leverhulme Trust through International Academic Fellowship IAF2017010. YEY thanks the PEI for support via Mary and Randall Hack ’69 Research Fund.

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Session H49 DPOLY GSOFT DFD GSNP: 3D Printing of Functional Soft Materials and Devices

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2:30PM H49.00000: Dillon Prize Talk break —

3:06PM H49.00002: 3D Printing of NdFeB Nylon Polymer Bonded Magnets

MARIAPPAN PARANS PARANTHAMAN (Presenter), Oak Ridge National Laboratory — The main goal of this research is to print near-net shape NdFeB polymer bonded magnets and to minimize the generated waste. One of the ways in which we can achieve this goal is by using extrusion based big area additive manufacturing technique to create complex shapes and geometries of polymer bonded magnets from a computer aided design which requires no tooling but little post-field-annealing reducing the amount of waste generated. We have successfully demonstrated the fabrication of near-net shape magnets with complex geometries and high energy product using over 65vol% of NdFeB in nylon polymer composite magnets. Several configurations of magnetic fields were used for aligning the magnets during printing. A higher energy product of 11.3 MGOe have been obtained for 65 vol% anisotropic composite bonded magnets aligned in 20 kOe with post-annealing. It is also observed at certain conditions; the post-aligned printed magnets didn’t deform and hence the original shape is preserved. We will discuss in detail about the correlation of magnetic alignment with properties.

*This research was supported by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.

3:18PM H49.00003: Quantitative mechanical and electrical assessment by local probe methods of inkjet-printed PEDOT:PSS thin films

EDGAR GUTIERREZ-FERNANDEZ, IEM-CSIC, Serrano 121, 28006 Madrid, Spain, I.A. GABALDON-SAUCEDO, Departament d'Enginyeria Electrònica i Biomèdica, IN2UB-Universitat de Barcelona, 08028, Barcelona, Spain., M. C. GARCIA-GUTIERREZ, IEM-CSIC, Serrano 121, 28006 Madrid, Spain, A. VAREA, Departament d'Enginyeria Electrònica i Biomèdica, IN2UB-Universitat de Barcelona, 08028, Barcelona, Spain., A. NOGALES, IEM-CSIC, Serrano 121, 28006 Madrid, Spain, E. REBOLLAR, IQFR-CSIC, Serrano 119, Madrid 28006, Spain, A. VILA, A. CIRERA, Departament d'Enginyeria Electrònica i Biomèdica, IN2UB-Universitat de Barcelona, 08028, Barcelona, Spain., TIBERIO EZQUERRA (Presenter), IEM-CSIC, Serrano 121, 28006 Madrid, Spain — Among the different technologies implied in scalable additive manufacturing inkjet printing is very well-suited for processing polymers. Thin films of PEDOT:PSS on ITO can be prepared by inkjet printing technology. A relatively broad range of thicknesses can be obtained by addition of subsequent polymer layers resembling an additive manufacturing process. The resulting inkjet PEDOT:PSS films are homogeneous as regard both electrical and mechanical properties. In spite of line topography both the Quantitative Nanomechanical Mapping (QNM) and the Conductive-AFM (C-AFM) characterization reveal homogeneous values throughout the polymer surface regardless of the welding zones. The results discussed in this work provide the basis for the application of inkjet printing as deposition method for electrically conducting PEDOT:PSS into large area with mechanical stability.

*This work has been supported by Spanish MINECO under the projects MAT2014-59187-R, MAT2015-66443-C02-1-R and CTQ2016-75880-P.
3:30PM H49.00004: Understanding the Effect of Block Copolymer Micelles on the Nanostructure and Rheological Response of Inks for Direct Ink Writing  RISHABH EKBOTE, DEBORAH LIU, DANIEL KROGSTAD (Presenter), University of Illinois at Urbana-Champaign — Bioinspired, hierarchical materials are of interest due to their ability to create materials with unique combinations of mechanical properties. We are interested in using a combined top-down and bottom-up approach to create synthetic materials with hierarchical structures. Towards this goal, we are using block copolymers to create nanoscale ordering in inks that can be printed using direct ink writing. However, the inclusion of micelle forming block copolymers has significant impact on the rheology of the inks, and thus their printability. Here, we will discuss the progress made towards understanding the effects of the block copolymer structure and concentration on the rheological properties of block copolymer containing epoxy inks.

3:42PM H49.00005: Leveraging Jammed Microgels to Shape Complex Fluids: One Method for 3D Printing with Cells, Gels, Elastomers, and Colloids [Invited]  THOMAS ANGELINI (Presenter), University of Florida — 3D printing is generally a race against instabilities; the challenge is to prevent printed liquid features from flowing of breaking up once deposited. Printing directly into a support material made from jammed granular-scale gel particles mitigates the two nearly ubiquitous sources of instability encountered in 3D printing: surface tension and body forces. The yield stress of these jammed microgels can be tuned over a broad range, making them excellent media in which to create macroscopic structures with microscopic precision. While tracing out spatial paths with an injection tip, the microgels yield at the point of injection and then rapidly re-solidify, trapping injected material in place. In this talk, we demonstrate how this physical approach to creating 3D structures negates the effects of surface tension and gravity, allowing a wide breadth of materials to be structured. With this method we create complex 3D objects made from silicones, hydrogels, colloids, and living cells, including functional living cell constructs and fluidic devices made from silicone. Immediate application areas include tissue engineering, flexible electronics, particle engineering, smart materials, and encapsulation technologies.

4:18PM H49.00006: Utilization of Polymer-Nanoparticle Composite in Micro-Stereolithography 3D Printing  HONGXIA LI (Presenter), AIKIFA RAZA, AFRA ALKETBI, TIEJUN ZHANG, Mechanical Engineering Department, Masdar Institute, Khalifa University — Advances in micro-stereolithography (µ-SL) 3D printing enable the fabrication of complex microstructures for biomedical, energy and other applications. However, the narrow selection of optical-curable printing materials limits its wide deployment. 3D printed micromodels are used to mimic the morphology of natural rock and reveal the microfluidic flow physics for subsurface energy application, but the surface chemistry of the printed polymer micromodel are totally different from natural rock surface. Therefore, polymer-based composites are used to tailor intrinsic properties, such as mechanical strength and surface wettability. In this work, we utilize the composite of polymer and calcite nanoparticle in a high-resolution µ-SL 3D printing system. Light scattering induced by the nanoparticles and its influence on printing resolution are analyzed under various particle sizes and concentrations. The transparency of printed micromodels reduces accordingly, which would affect the microfluidic flow imaging performance. Surface wettability conditions, including the contact angle and its hysteresis, are also characterized. This study provides important guidance in the utilization of polymer/nanoparticle composite in µ-SL 3D printing for broad microfluidic applications.

4:30PM H49.00007: Morphology and Mechanical Properties of Stereolithography-Printed Polymer Networks  ANNA SMALLWOOD-ROONEY (Presenter), RYKELLE ADLEY, ADAM MERKLE, KEITH DENIVO, SUNGMIN PARK, CHANG YEOL RU, Rensselaer Polytechnic Institute — Stereolithography (SLA) is a method of 3D printing in which polymer network objects are formed through the repeated curing of photopolymer resin by a computer-controlled UV laser source. Objects that are 3D printed on a SLA platform show a layered morphology on the microscopic scale, and the resolution of the printed object is determined predominantly by the thickness of each layer, typically on the 100 um scale. Layer formation during printing is dependent on laser intensity and decay during the printing process. Printed layers are generally characterized by a strongly crosslinked region that decays gradually into a more loosely crosslinked domain which is adjacent to a highly crosslinked region of the next layer. This pattern of curing is a function of laser intensity and reflects decay of intensity throughout each curing cycle, or layer. The SLA-printed morphology is characterized on the microscopic scale as a function of laser intensity and decay during printing. High resolution optical microscopy techniques will offer a depiction of crosslinking density change across layered 3D printed structure. The layer curing process will also be investigated by real-time FTIR, DSC, and DMA.
4:42PM H49.00008: Self-Limiting Electrospray Deposition of Polymers and Polymer Composites  
LIN LEI (Presenter), DYLAN A. KOVACEVICH, CHRISTIANNA KUZNETSOVA, JONATHAN SINGER, Mechanical and Aerospace Engineering, Rutgers University — Electrospray deposition is widely used to create polymer microcoatings from dilute spray solutions. In a certain regime of experimental parameters, a limiting thickness emerges where the accumulation of charge repels further spray. This self-limiting electrospray deposition (SLED) can uniformly cover complex multiscale structures efficiently. Here we investigate the application of polymer blends to increasing the durability of the spray films for different mechanical applications. We use the addition of photo- or thermal-crosslinkers that can either maintain the hierarchical spray structure of hollow particles or result in a dense film to obtain stiffer coatings for protective barriers. The results show mechanically-tough coatings with tunable porosity which are resistant to decomposition by chemical reactions and mechanical damage. To make the films that are more flexible for compliant surfaces, polymer blends which consisting of plastic and elastomeric components are sprayed. The net result was a coating that could enhance adhesion and sustain ~17% strain in the underlying structure. Furthermore, we have applied SLED to coat 3D structures produced via additive manufacturing with these mechanically-tuned coatings.

4:54PM H49.00009: 3D Printable Soft Elastomers  
ZIHAO GONG (Presenter), SHIFENG NIAN, Materials Science and Engineering, University of Virginia, LIHENG CAI, Materials Science and Engineering and Chemical Engineering, University of Virginia — Existing feedstock for 3D printing is nearly all plastics. These materials are not only mechanically stiff but also fragile. These severely limit their applications where soft, elastic polymers are required to easily comply with the shapes of objects they contact. Here we develop a soft, 3D printable elastomer through molecular design. We synthesize a triblock copolymer, in which the two end-blocks are poly(styrene) (PS) with a high glass transition temperature, T_g, about 100°C, and the middle block is a poly(dimethylsiloxane) (PDMS) with a low T_g about 100°C. At room temperature, such copolymers self-assemble to a network, in which the effective network strands are the PDMS, and crosslinks are glassy plastic domains formed by PS. This network is extremely soft with Young's modulus below 100kPa, more than three orders of magnitude lower than that of plastics. At high temperature, the glassy domains dissociate, enabling a temperature triggered solid-to-liquid transition. Harnessing this feature, we use extrusion-based 3D printing to create a complex, hierarchical 3D structure with an exceptional combination of softness and deformability. Our studies provide a new strategy for the development of 3D printable soft elastomers.

5:06PM H49.00010: Embedded 3D Printing with Acoustic Focusing  
LEANNE FRIEDRICH (Presenter), MATTHEW BEGLEY, University of California, Santa Barbara — Intra-nozzle particle positioning methods enable the design of composite 3D printed components with structural and functional gradients. One method is acoustic focusing, wherein a piezoelectric actuator establishes a bulk acoustic wave in the nozzle which co-orient and moves particles to the wave nodes. Because acoustic focusing requires low viscosity inks (such as soft materials with functional particles), we use a granular hydrogel as support material. This study investigates how layer-by-layer deposition of support material and printing into a support bath each influence the maintenance of acoustically focused microstructures and the fidelity of printed structures. While layer-by-layer support prevents filaments from breaking into droplets, it can also destabilize filaments near liquid elbows and induce rotational flows that disrupt focused structures. Similarly, though writing into support material enables complex structures, it can also hinder inter-layer and intra-layer fusion and disrupt existing structures. Using digital image analysis and particle image velocimetry, we measure the effects of ink and support composition and printing parameters on maintenance of acoustically focused microstructures, stability of filaments and liquid elbows, and inter-filament fusion.

5:18PM H49.00011: Room Temperature Extrusion 3D Printing of Polyether Ether Ketone Using a Stimuli-Responsive Binder  
CHANG-UK LEE (Presenter), University of Wisconsin - Madison, JOHANNA VANDENBRANDE, ADAM GOETZ, MARK GANTER, DUANE STORTI, University of Washington, ANDREW BOYDSTON, University of Wisconsin - Madison — We report 3D printing of polyether ether ketone (PEEK) at room temperature by direct-ink write technology. The room-temperature extrusion printing method was enabled by a unique formulation comprised of commercial PEEK powder, soluble epoxy-functionalized PEEK (ePEEK), and fenchone. This combination formed a Bingham plastic that could be extruded using a readily available direct-write printer. After printing, thermal processing at 230 °C resulted in crosslinking of the ePEEK components to form a stabilizing network throughout the specimen. A final sintering stage was conducted at 380 °C. The T_g of product specimens was found to be 158 °C, which is 13 °C higher than commercial PEEK as measured by DSC. Moreover, the thermal decomposition temperature was found to be 528 °C, which compares well against commercial molded PEEK samples. Chemical resistance in trifluoroacetic acid and 8 common organic solvents were investigated, and no signs of degradation were observed from parts submerged for 1 week in each solvent. Test specimens also displayed desirable mechanical properties, such as a Young's modulus of 2.5 GPa, which corresponds to 63% of that of commercial PEEK.

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especially for visualizing polymer dynamics, visualizing nanostructures in life sciences, the application of this technique in polymer science is much more rare, universal, simplified labelling strategy and the ability to visualize polymer assembly and dynamics in situ. A major constraint is from the lack of suitable fluorophore chemistry and simple strategies to label polymer chains. In this talk, we will discuss a functional diarylethene-based photoswitchable fluorophore, which can be directly copolymerized with standard monomers such as styrene and methyl methacrylate with no further post-coupling reactions or purifications needed. The attachment of fluorophores onto polymer chains enables super-resolution imaging of model polymer blend systems (PS/PMMA) with different nanostructures. As each individual fluorophore can switch between its bright and dark state many times, multiple time-lapse images can be acquired to observe the dynamic nanostructural evolution of polymer blends during solvent vapor annealing. With the advantages of a high, localized electric field in the plane of the surface, and subjects that region to UV light. When wet, the electric field forces the polymers to align beneath the tip, and the UV light engenders insoluble PPV, preventing loss of alignment. We align a large rectangular region by scanning a probe using this technique, and use cross-polarization measurements to demonstrate alignment. The ability to fabricate ordered layers removes material variations from studies of conduction and interfacial phenomena, thus represents a significant step towards measuring the intrinsic properties of conducting polymers.
4:18PM H50.00006: Exploring Textures of a Nematic Liquid Crystal for Fourier Phase Contrast Microscopy
CHARLOTTE KYEREMAH (Presenter), JEFFREY LA, DEVULAPALLI RAO, MOHAMED AMINE GHARBI, CHANDRA S
YELLESWARAPU, University of Massachusetts Boston — Phase contrast microscope is used in teaching and research labs to
view transparent specimens such as live cell cultures. It enables to study dynamic biological processes. In the past we have
developed Fourier phase contrast microscopy technique using photoinduced birefringence in liquid crystals that constitute
a fascinating class of matter characterized by the counterintuitive combination of fluidity and long-range order. A low
power laser is passed through a commercial inverted microscope to facilitate the Fourier plane at the output of the video
port. When the liquid crystal cell is placed at the Fourier plane, low spatial frequencies at the center of the Fourier
spectrum are intense to transform the liquid crystal molecules into isotropic phase whereas high spatial frequencies are
not intense enough and remain in the anisotropic phase. This results π/2 phase difference between high and low spatial
frequencies, a basic requirement for phase contrast imaging. Liquid crystal materials are known for their exceptionally
successful applications in displays, smart windows, and biosensing applications. Here we exploit different textures of a
nematic liquid crystal 5CB: planar, perpendicular, hybrid and twisted, and investigate their abilities to improve the contrast
of phase images.

4:30PM H50.00007: Tractor beams for colloidal particles are not self-accelerating modes* ARGHA MONDAL
(Presenter), YISHUAI XU, LEWIS A WRAY, DAVID GRIER, New York University — We previously have demonstrated that
structured laser beam can act as a tractor beam for colloidal particles. In addition to their ability to pull objects upstream,
these modes of light have other remarkable properties. Due to the homology of the paraxial wave equation with
Schrödinger's equation, the wave function for a quantum mechanical particle in a circular box can be prepared in shape-
preserving wave packets that rotate at constant angular speed around the center of the box, similar to a tractor beam.
This apparent violation of Ehrenfest's theorem is resolved by considering the force exerted on the particle's wave packet
by the enclosing wall. Remarkably, the wave packet continues to rotate even after the wall potential is removed. We show
that this force-free finite-energy rotating state actually corresponds to classical motion with constant velocity, again in
agreement with Ehrenfest's theorem. Even so, the classical angular momentum carried by the rotating states poses a
conceptual challenge because it differs from its quantum mechanical angular momentum, and indeed can have the
opposite sign.

*This work was supported primarily by the National Science Foundation under award number DMR-1305875 and in part
by the MRSEC program of the NSF through award number DMR-1420073.

4:42PM H50.00008: High efficiency Fresnel lens design and fabrication in a two-stage photopolymer JOHN E
HERGERT (Presenter), DAVID J GLUGLA, AMY C SULLIVAN, MARVIN D ALIM, ROBERT R MCLEOD, Electrical, Computer, and
Energy Engineering, University of Colorado at Boulder — Diffractive optical elements (DOEs) assimilate optical functionality
within thin (≤100 µm), lightweight films. With the recent advent of high dynamic range two-stage photopolymers, gradient-
index volume DOEs can now achieve diffraction efficiencies competitive with conventional surface-relief DOEs, while also
offering the advantages of contact-free, self-processing optical recording into a flat film that can be laminated between
protective sheets. Here we design and fabricate Fresnel lenses with what we believe to be the highest reported diffraction
efficiencies achieved to date using this gradient-index DOE approach. Our analysis shows that these high diffraction
efficiencies are crucially enabled by the high index modulation of the photopolymer (n1 > 0.01) and the high pixel count of
the single-shot recording exposure (6400 × 6400 pixel chrome mask). The recorded lenses are 50 µm in thickness and up
to 16 mm in diameter, with f-numbers ranging from 16 – 24 and diffraction efficiencies up to 85%. This high performance
represents an important step toward practical applications, ranging through solar energy concentrators, customized vision
optics, integrated photonics, heads-up displays, and hybrid lenses.

4:54PM H50.00009: Quantitative index metrology for 3D voxelated structures in photopolymer DAVID J GLUGLA,
IZABELLA R BERMAN (Presenter), Electrical, Computer and Energy Engineering, University of Colorado at Boulder, MADELINE B
CHOSY, Carleton College, MARVIN D ALIM, Chemical and Biological Engineering, University of Colorado at Boulder, AMY C
SULLIVAN, ROBERT R MCLEOD, Electrical, Computer and Energy Engineering, University of Colorado at Boulder — Thanks to recent
advances in two-stage photopolymers, it is now possible to dictate arbitrary 3D voxelated refractive index structures
within a continuous volume of polymer, with dynamic range Δn in excess of 0.01 and with micron-scale spatial resolution.
However, quantitative metrology for such structures remains an under-explored challenge. Here we demonstrate that TIE-
based phase imaging, in conjunction with scanning confocal reflection microscopy, can achieve unambiguous quantitative
characterization of arbitrary voxelated index structures. This characterization then guides the design, fabrication, and
validation of novel optical components, including flexible gradient-index lenses for in situ medical imaging.
5:06PM H50.00010: Bio-inspired design of Mechanochromisms via surface engineering  
SONGSHAN ZENG, RUI LI, DIANYUN ZHANG, LUYI SUN (Presenter), University of Connecticut — A bilayer structure composed of polyvinyl alcohol composite thin film atop thick polydimethylsiloxane substrate was prepared. The bilayer structure shows dynamic strain-responsive optical properties. The transition between a transparent state to an opaque state can be easily achieved by uniaxially stretching and releasing the device. Also, a series of derivative mechanochromisms with capabilities of switch “on/off” fluorescence, change fluorescent color, reveal/hide information upon mechanical stimuli are prepared. These devices feature virtually no changes in optical/mechanical properties after being repeatedly stretched and released thousands of times, promising for widespread applications.

5:18PM H50.00011: Reversible Self-Focusing in Light-Responsive Spiropyran Functionalized Gels  
DEREK MORIM, Department of Chemistry and Chemical Biology, McMaster University, AMOS MEEKS (Presenter), ANKITA SHASTRI, John A. Paulson School of Engineering and Applied Sciences, Harvard University, ANDY TRAN, Department of Chemistry and Chemical Biology, McMaster University, ANNA SHNEIDMAN, John A. Paulson School of Engineering and Applied Sciences, Harvard University, FARIHA MAHMOOD, Department of Chemistry and Chemical Biology, McMaster University, JOANNA AIZENBERG, John A. Paulson School of Engineering and Applied Sciences, Harvard University, KALAICHELVI SARAVANAMUTTU, Department of Chemistry and Chemical Biology, McMaster University — Self-focusing, where interactions between a light beam and its medium creates a refractive index gradient that acts as a waveguide for the beam, has been observed at low powers (nW-mW) in a variety of soft-matter systems. This intensity dependent refractive index change is often created by the irreversible photopolymerization of monomers in solution. However, a reversible system would enable potential applications in soft all-optical computing based on dynamic interactions between self-focused beams. Here we show a fully reversible soft self-focusing medium based on stimuli-responsive hydrogels (poly(acrylamide-co-acrylic acid) and poly(N-isopropylacrylamide)) doped with photoresponsive spiropyran pendant groups. In this system the intensity-dependent contraction of the gel leads to a local increase in the refractive index, resulting in self-focusing of the incident beam. In addition to being reversible this system shows long-range interactions between beams separated by over 10 beam widths. To explain these experiments we have developed a numerical model coupling the spiropyran isomerization, gel dynamics, and the propagation of light. This model allows us to design more complex beam interactions and thus to create systems where light is dynamically controlled by light.
Sea Urchin Biomineralization – Formation of Intricate Single Calcite Crystals via Amorphous Precursors

[Invited]
YAELE POLITI (Presenter), MARIE ALBÉRIC, ZHAOYONG ZOU, ANDERS WESTERAARD JENSEN, WOUTER HABRAKEN, Max Planck Institute of Colloids and Interfaces, PUPA GILBERT, University of Wisconsin, Madison, EMIL ZLOTOYABKO, Technion-Israel Institute of Technology, PETER FRATZL, LUCA BERTINETTI, Max Planck Institute of Colloids and Interfaces —

Biomineralization of sea urchin skeletal elements results in complex structures with smooth, curved surfaces that diffract as single calcite crystals 1. This is achieved by a crystallization pathway involving amorphous precursor phases 2,3. Similar processes are now recognized in various other organisms. Yet, the dynamics of mineral rearrangement and the energetic landscape of this transformation are still poorly understood. We addressed these questions studying the crystallization of biogenic and synthetic ACCs by state-of-the-art calorimetric, spectroscopic and scattering methods. The skeletal elements of the sea urchin Paracentrotus lividus are composed of ACC, organics, a small amount of water and calcite 4. Insight into the interplay between these components is gained by HR-XRPD of skeletal elements annealed at elevated temperatures. Complementarily, by mapping the distribution of ACC, H2O, ACC and calcite in growing spines by X-PEEM we demonstrated variable transformation kinetics across the spine. In-vitro experiments show that the effect of water, as well as organic and inorganic additives, on the stability of synthetic ACC is primarily kinetic [5]. A key finding with relevant to biomineralization is that although water drastically changes the crystallization enthalpy, the overall ACC thermodynamic stability is independent of the hydration level due to enthalpy-entropy compensation. The rate of the transformation, on the other hand, is critically dependent on the water content; water increases ion mobility, resulting in higher kinetic instability [5].


Multistep Crystallization Pathways for Protein Crystals and Colloidal Assemblies

[Invited]
SHARON GLOTZER (Presenter), SANGMIN LEE, ERIN TEICH, MICHAEL ENGEL, JENS GLASER, University of Michigan — While much is now known about the extraordinary complexity and structural diversity possible for crystals of proteins, nanoparticles and colloids, far less is known about the process by which these crystals form. Simple “classical” models of nucleation and growth may hold for the self-assembly of simple crystal structures, but what of crystals with large unit cells? We present recent results from computer simulation demonstrating that crystallization pathways in protein solutions or entropic colloidal fluids may be as diverse and complex as the resulting crystals, with crystallization following a remarkable variety of multistep pathways that include fluid-fluid transitions. We explore the role of shape, entropy, and, in the case of proteins, both specific and nonspecific interactions in selecting the pathway.

Design of Functional Protein Membranes*

[Invited] MONICA OLVERA DE LA CRUZ (Presenter), BAOFU QIAO, TRUNG NGUYEN, Department of Materials Science and Engineering, Northwestern University — Protein surfaces are composed of sub-nanometer domains, with different degrees of hydrophilicity. These domains play a crucial role in protein assembly, ligand recognition, and drug docking. We explored here the surface domains to disperse enzymes in organic solvents where their activity can be enhanced using random heteropolymers that mimic unstructured proteins in membraneless organelles. The analysis of the correlations between polar domains with the polar components of amphiphilic random heteropolymers mediated by water elucidates the formation of protein-polymer complexes with a core (protein)-shell (polymer) morphology that help stabilize the proteins’ structures and preserve their enzymatic activities in unfavorable solvents as observed in recent experiments (1). At a more coarse-grained resolution, we find that the proteins selectively favor the binding of random copolymers with similar monomer sequences (2). The balance between the energetic and entropy gains in polymer adsorption is determined by the spatial distribution of the polar and non-polar domains and the average composition of the polymers.


*Acknowledgment: The work was supported by Department of Energy Award No. DE-FG02-08ER46539 and the Sherman Fairchild Foundation.
The Growth Mechanisms and Biomimetics of Tooth Enamel* [Invited] JANET MORADIAN-OLDAK (Presenter), Biomedical Sciences School of Dentistry, University of Southern California — A very fundamental part of biomineralization is the complex extracellular macromolecular framework in which mineralization occurs, such as the collagen fibrils in bone and dentin, polysaccharides in nacre and amelogenin and non-amelogenin proteins in dental enamel. Unlike other mineralized tissues, such as bone and dentin, mature enamel is acellular and cannot regenerate itself after substantial mineral loss. Biomimetic enamel regrowth is a significant topic in material science and dentistry as an alternative approach for the treatment of defects in dental enamel. We have developed protocols for superficial biomimetic enamel regrowth, based on a novel amelogenin-chitosan hydrogel. Amelogenin is a critical protein for controlling the organized growth of apatite crystals in enamel. We expanded upon the concept of biomineralization to design smaller amelogenin-inspired peptides with conserved functional domains for clinical translation. The synthetic peptides displayed a characteristic nanostructured scaffold reminiscent of ‘nanospheres’ seen in the enamel matrix and effectively controlled apatite nucleation in vitro. Following application of the peptides to sectioned human molar teeth, a robust, oriented, synthetic aprismatic enamel was observed in situ. There was a two-fold increase in the hardness and modulus of the regrown enamel-like apatite layers and an increase in the attachment of the tooth-regrown layer interface compared to control samples. Repeated peptide applications generated multiple enamel-like HAP layers of limited thickness produced by epitaxial growth in which c-axis oriented nanorods evolved on the surface of native enamel. We report that peptide analogues with active domains can effectively regulate the orientation of regenerated HAP layers to influence functional response.


Engineering materials inspired by nature* [Invited] JOANNA MCKITTRICK (Presenter), University of California, San Diego, MICHAEL FRANK, nanoComposix, San Diego, CA — Magnetic field aligned freeze casting is a novel method to fabricate porous, anisotropic ceramic scaffolds with a hierarchy of architectural alignment in multiple directions. This concept was inspired by the structure of trabecular bone and the spiraling nature of the narwhal tusk. A weak rotating magnetic field applied normal to the ice growth direction in a uniaxial freezing apparatus allowed the manipulation of magnetic nanoparticles to create different pore structures and channels with long-range order in directions parallel and perpendicular to the freezing direction. Porous scaffolds consisting of different host ceramics as particles or platelets (hydroxyapatite (HA), ZrO2, Al2O3, or TiO2) mixed with varying concentrations of Fe3O4 nanoparticles were fabricated by freeze casting under no magnetic field, a static or rotating magnetic field. In the magnetic field direction, the compressive strength and stiffness of the scaffolds containing was doubled.

*This work was supported by a Multi-University Research Initiative through the Air Force Office of Scientific Research (AFOSR-FA99550-15-1-009) and a National Science Foundation Biomaterials Grant (DMR-1507978).

Tuesday, March 5, 2019 2:30 PM - 5:18 PM

Session H52 GSOFT GSNP: Machine Learning in Nonlinear Physics and Mechanics BCEC 253B - Shmuel Rubinstein, Harvard University - Tag(s): Focus

2:30PM H52.00001: A case study in neural networks for scientific data: generating atomic structures [Invited] TESS SMIDT (Presenter), Computational Research Division, Lawrence Berkeley National Laboratory — Expertise in both the scientific domain of interest and deep learning techniques are essential in order to properly translate scientific problems into tasks amenable to deep learning. Scientific data has a lot of context; for example, the laws of physics obey certain symmetries. Can the network learn this context from the data or should we impose this context as constraints in our network or training procedures? Additionally, scientific data representations, neural network operations and appropriate loss functions desirable for scientific applications can be very different from those most prevalent in the deep learning literature; when is it appropriate to use existing methods and when is it necessary to develop new ones?

We present examples of these challenges when applying deep learning techniques to the generation of atomic systems (new atomic arrangements that may be crystals, molecules, nanoclusters, polymers, proteins, etc.). We present a novel rotation-equivariant convolutional neural network -- or tensor field network -- that has the ability to articulate, recognize and differentiate local and global features in any orientation in complex atomic systems. We discuss strategies for generating hypothetical atomic structures using the concepts of geometric motifs (the recurring patterns of atoms in materials) and neural networks that can manipulate discrete geometry. We present the use of toy models to test the expressiveness and accuracy of tensor field network operations.
3:06PM H52.00002: A computational model for crumpled thin sheets to complement data-driven machine learning* JOVANA ANDREJEVIC (Presenter), JORDAN HOFFMANN, YOHAI BAR-SINAI, LISA LEE, SHRUTI MISHRA, SHMUEL RUBINSTEIN, CHRISTOPHER RYCROFT, Harvard University — Crumpling is ubiquitous across length scales and diverse structures in nature, yet a complete theoretical description of the mechanisms underlying ridge formation remains elusive. To characterize the intricate damage networks of crumpled thin sheets, our recent work has shown that appropriate simulations can assist data-driven machine learning to overcome the scarcity of high-quality experimental data. Inspired by this data augmentation approach, here we detail a computational model for thin, viscoelastic sheets and demonstrate its ability to capture the properties and behavior of crumpled sheets. We validate the model's robustness through statistical comparison with high-quality experimental data, and discuss the prospects for its application in assisting data-driven machine learning.

*This work was supported by the National Science Foundation through the Harvard Materials Research Science and Engineering Center (DMR-1420570) and through the Graduate Research Fellowship Program (DGE-1745303).

3:18PM H52.00003: Machine Learning in a data-limited regime: Augmenting experiments with synthetic data uncovers order in crumpled sheets LISA LEE (Presenter), JORDAN HOFFMANN, YOHAI BAR-SINAI, JOVANA ANDREJEVIC, SHRUTI MISHRA, SHMUEL RUBINSTEIN, CHRISTOPHER RYCROFT, Harvard University — Machine learning is a powerful tool for uncovering structure in complex, high-dimensional data. However, a large amount of data is necessary in order to properly train a machine learning network, making it difficult to apply to experimental systems where data is limited. Here we resolve this difficulty by augmenting an experimental dataset with synthetically generated data from a simpler relevant system. Specifically, we study the local order in crease patterns of crumpled sheets, a paradigmatic example of spatial complexity. We supplement sparse crumpled experimental data with abundant simulated sheets of synthetic folds. This technique significantly improves the predictive power in a test problem of pattern completion, demonstrating the usefulness of machine learning in experiments where data may be scarce. Additionally, assessing the accuracy of networks trained with varying types of simulated data reveals the relevance of various physical rules to understanding crease patterns.

3:30PM H52.00004: Search and design of stretchable graphene kirigami using convolutional neural networks PAUL HANAKATA (Presenter), Boston University, EKIN DOGUS CUBUK, Google Brain, DAVID K CAMPBELL, HAROLD PARK, Boston University — Making kirigami-inspired cuts in a sheet has been shown to be an effective way to design stretchable materials with metamorphic properties where the 2D shape can transform into complex 3D shapes. However, a systematic understanding on how cutting patterns alter the mechanical properties of the resulting kirigami remains elusive. Here, we use machine learning (ML) to approximate the objective functions, such as yield stress and yield strain, as functions of the cutting pattern. Our approach enables the rapid discovery of graphene kirigami designs that yield extreme stretchability as verified by molecular dynamics (MD) simulations. We find that convolutional neural networks (CNN) can be applied for regression to achieve an accuracy close to the precision of the MD simulations. This approach can then be used to search for optimal designs that maximize elastic stretchability with only 1000 training samples in a large design space of roughly 4,000,000 candidate designs. This example demonstrates the power and potential of ML in finding optimal kirigami designs at a fraction of iterations that would be required of a purely MD- or experiment-based approach, where no prior knowledge of the governing physics is known or available.


3:42PM H52.00005: Clog prediction in granular hoppers using machine learning methods JESSE HANLAN (Presenter), DOUGLAS DURIAN, Department of Physics and Astronomy, University of Pennsylvania — Grains discharge from a hopper at constant rate, proceeding probabilistically until a stable arch forms. Thomas and Durian (PRL 2015) showed that recasting the characteristic measure of a flow event from the average mass discharged to the fraction of flow microstates that precede (i.e. cause) a clog explains why the former grows as an exponential function of hole diameter, rather than a critical power law. This makes clear that clogs form as the flow brings new microstates into the vicinity of the outlet, which are randomly sampled until a stable arch is found. Characterizing the flow microstates that cause clogs should then better inform a predictive framework. As a first step, Koivisto and Durian (PRE 2017) found that the same statistics governed hoppers in air or submerged in a viscous fluid. This implies that clog formation depends primarily on position degrees of freedom; however, the phase space of grain microstates in a hopper is extremely high-dimensional. Here, we apply deep learning to probe the function space of position microstates in a two-dimensional hopper, to identify and separate out characteristic structures responsible for clogging. Preliminary analysis of a small dataset gives a cross validation success rate of 90%.
MATTHEW PINSON, ARVIND MURUGAN, University of Chicago — Systems with multiple stable states have proven essential in physical knowledge from the high dimensional models implemented. Structure of droplets arising from a Rayleigh-Taylor instability and highlight several techniques to recover significant data-driven framework. We focus on the study of fluid-mediated instabilities. We show that one can predict the spatial accuracy of these models heavily relies on training with extensive dataset and scales accordingly to the number of samples are efficient since their computational complexity scales as a set of matrix-vector multiplications. However, the prediction ability to capture complex relationships and patterns in data. Further, predictions stemming from these trained networks details of the physics of those systems far from equilibrium remains elusive; prompting the need for the development of numerical simulations are computationally expensive and exponentially sensitive to initial conditions. As a result, the forecasting phenomenon arising from nonlinear dynamical systems is a daunting task. Formal models are rarely analytically tractable and numerical simulations are computationally expensive and exponentially sensitive to initial conditions. As a result, the implementation of learned multi-stability. In contrast, our learning framework considers sequential introduction of desired stable states so that material parameters must be incrementally updated to stabilize each additional state. We show that designed states are optimally stable within elastic networks with Hookean springs. However, incremental learning requires springs with strong non-linearity. We interpret such non-linearity as biasing the distribution of strain in these elastic networks to be localized in a sparse subset of springs, much like a Bayesian prior in sparse regression. In this way, we identify principles for practical implementations of learned multi-stability.

We acknowledge financial support from the NSF DMREF-1534890 and the microfluidics facility of the NSF MRSEC DMR-1420382.

TRISTAN A SHARP (Presenter), ANDREA J LIU, University of Pennsylvania — Cellular motion in dense tissues often consists of neighbor-swapping events or rearrangements. The rearrangements underlie the glassy dynamics and much of the collective dynamics of dense disordered cellular packings. Here we present a machine learning (ML) approach that links the local disordered structure surrounding a cell with the propensity of the cell to rearrange in a Voronoi cell vertex model. “Softness,” $S$, an ML-derived quantity originally introduced to quantify the link between local structure and rearrangements in inert glassy liquids, provides an effective proxy for a cell's probability to rearrange, $P_R$. The local structural features that determine the softness of a cell are quantified. Decreasing temperature lowers $P_R$ for a given value of $S$, but the distribution of $S$ also shifts up, opposing the change, leading to previously-observed sub-Arrhenius dynamics. This contrasts with the behavior of Lennard-Jones glassy liquids, where the distribution of $S$ shifts down with decreasing temperature, leading to super-Arrhenius dynamics.

We gratefully acknowledges funding from NSF-DMR-1506625 and No. U54 CA193417

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We gratefully acknowledges funding from NSF-DMR-1506625 and No. U54 CA193417

JOEL MARTHELOT, PIERRE-THOMAS BRUN, CBE, Princeton University — Forecasting phenomenon arising from nonlinear dynamical systems is a daunting task. Formal models are rarely analytically tractable and numerical simulations are computationally expensive and exponentially sensitive to initial conditions. As a result, the details of the physics of those systems far from equilibrium remains elusive; prompting the need for the development of new tools. Neural networks have been at the forefront of the machine learning community for their versatility and ability to capture complex relationships and patterns in data. Further, predictions stemming from these trained networks are efficient since their computational complexity scales as a set of matrix-vector multiplications. However, the prediction accuracy of these models heavily relies on training with extensive dataset and scales accordingly to the number of samples in the latter. Here we propose an approach to rethink the traditional experimental setting in applied physics in favour of a data-driven framework. We focus on the study of fluid-mediated instabilities. We show that one can predict the spatial structure of droplets arising from a Rayleigh-Taylor instability and highlight several techniques to recover significant physical knowledge from the high dimensional models implemented.

*We acknowledge NSF-MRSEC 1420709 for funding and the University of Chicago Research Computing Center for computing resources.
4:42PM H52.00010: Visualizing probabilistic models and data with Intensive Principal Component Analysis (InPCA)*
KATHERINE QUINN (Presenter), COLIN B CLEMENT, FRANCESCO DE BERNARDIS, MICHAEL D NIEMACK, JAMES PATARASP
SETHNA, Cornell University — Unsupervised learning makes manifest the underlying structure of data without curated
training and specific problem definitions. However, the inference of relationships between data points is frustrated by the
`curse of dimensionality' in high-dimensions. Inspired by replica theory from statistical mechanics, we consider replicas of
the system to tune the dimensionality and take the limit as the number of replicas goes to zero. The result is the intensive
embedding, which is not only isometric (preserving local distances) but allows global structure to be more transparently
visualized. We develop the Intensive Principal Component Analysis (InPCA) and demonstrate clear improvements in
visualizations of the Ising model of magnetic spins, a neural network, and the dark energy cold dark matter
((\Lambda)CDM) model as applied to the Cosmic Microwave Background.

*NSERC fellowship, NSF DMR-1312160, DMR1719490, AST1454881.

4:54PM H52.00011: Physical Symmetries Embedded in Neural Networks
MARIOS MATTHEAKIS (Presenter), DAVID
SONDAK, PAVLOS PROTOPAPAS, Harvard University — Artificial neural networks (ANNs) have become indispensable tools in
many machine learning applications and in recent years, ANNs have become an active area of research in the physical
sciences. An important consideration for building ANNs for scientific applications is how to incorporate non-negotiable
physical constraints. We propose ANNs with embedded physical symmetries including even-odd symmetry, time-
reversibility, positivity, energy-momentum conservation, and Galilean invariance. We constrain the weights of the NN so
that the physical properties are exactly satisfied by the neural network output. Furthermore, embedding constraints into
the NN can drastically reduce the search space thereby providing an efficient deep learning architecture.

5:06PM H52.00012: Maximizing thermal efficiency of heat engines using neuroevolutionary strategies for
reinforcement learning
CHRISTOPHER BEELER (Presenter), ULADZIMIR YAHORAU, RORY COLES, KYLE MILLS, University of
Ontario, Institute of Technology, ISAAC TAMBLYN, University of Ontario Institute of Technology, University of Ottawa, and National
Research Council of Canada — Classic control problems such as Mountain Car [1] and Acrobat [2] are based on simple
Newtonian physics. Both have been solved previously with reinforcement learning algorithms. Here, we show that
reinforcement learning can also be used to solve classical problems in thermodynamics. Using a reinforcement
learning method based on genetic algorithms, our software agent can learn to reproduce thermodynamic cycles
without prior knowledge of physical laws. We have created a simulated learning environment which models a
simple piston, where an agent can activate thermodynamic processes. With this method, we were able to
optimize an artificial neural network based policy to maximize the thermal efficiency for several different cases.
Depending on the actions available to the agent, different known cycles emerged, including the Carnot, Stirling,
and Otto cycles. Importantly, we show an example of how reinforcement learning can be used to aid scientists in
finding solutions to problems that have yet to be fully explored. In one of the heat engine environments, we
introduced a non-adiabatic process which caused the engine to lose energy. In this case, the agent produced, what
is to the best our knowledge, the best solution for the problem.


Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H53 GSOFT GSNP: Elasto-Active Instabilities
BCEC 253C - Corentin Coulais, University of Amsterdam - Tag(s):
Invited

2:30PM H53.00001: Soft Robots: Functionality via Instabilities [Invited]
KATIA BERTOLDI (Presenter), Harvard University — Soft robots made of compliant materials have drawn significant attention over the past few years because of their ability to produce complex and adaptive motions through nonlinear deformation. The simplicity of their design, ease of fabrication and low cost sparked the emergence of soft robots capable of walking, crawling, camouflaging and assisting humans in grasping. In this talk, I will show that the response of these soft machines can be further enhanced by embracing instabilities. While instabilities have traditionally been avoided as they often represent mechanical failure, here we exploit them to amplify the response of soft actuators, facilitate their motion and trigger instantaneous and significant changes in shape.
Fluttering and dancing elastic rods: the dynamics of the elastica subject to follower and configurational forces* [Invited] DAVIDE BIGONI (Presenter), University of Trento, Italy — Using the elastica theory, configurational or ‘Eshelby-like’ forces will be shown to arise in elastic structures when a change in configuration is possible, with a related release of energy. Configurational forces will be shown to influence the dynamics of a falling body connected through an elastic rod to a sliding sleeve, so that a damped nonlinear oscillator results, which generates a complex motion, nicknamed ‘dancing’. Finally, the dynamics of an elastic rod in a cantilever configuration and subject to a tangential follower load of the ‘Ziegler type’ at its end (the ‘Pfluger problem’) is addressed. This structure is subject to a Hopf bifurcation, corresponding to the initiation of the ‘flutter instability’. A new experimental set-up is presented as designed, produced and tested to realize the follower load. Experiments provide the evidence of flutter and divergence instability and result in the first proof that damping sources have a destabilizing effect on the system (the so-called ‘Ziegler paradox’).

*ERC-2013-ADG-340561-INSTABILITIES

From the onset of creasing as a Kosterlitz-Thouless transition to "buckling without bending" in morphogenesis [Invited] J. M. SCHWARZ (Presenter), Physics, Syracuse University — Cusped inward folds, known as creases, form on a free surface of a soft disordered solid under compression at critical strains below that of buckling. Harnessing a model for composite elastic materials, quasi-particle excitations termed ghost shear lag fibers serve as surface stress localizers to initiate this creasing transition. The mathematics of these stress localizers maps to charges on the free surface of the solid. This mapping, combined with the presence of fluctuations due to the underlying disordered material under compression, point to the creasing transition as a Kosterlitz-Thouless transition. For the sake of contrast, a new shape-changing mechanism, termed “buckling without bending”, involving not only solid material but a proliferating fluid layer under mechanical constraints will also be presented. The implications of creasing, buckling, and “buckling without bending” for the cerebrum, the cerebellum, and brain organoids will be addressed along the way.

Interplay between elasticity and activity: from vibrated elastic particles to penetration of active particles through elastic membranes* [Invited] HARTMUT LOEWEN (Presenter), Institute of Theoretical Physics II, Heinrich-Heine University Düsseldorf —

Here we first discuss the motion of self-propelled vibrated granulates with elastic legs leading to activity [1]. While inertia is usually neglected in standard models, the significance of inertia on macroscopic self-propelled particles is experimentally demonstrated. We observe a distinct inertial delay between orientation and velocity of particles, originating from the finite relaxation times in the system. This effect is fully explained by an underdamped generalisation of the Langevin model of active Brownian motion. In stark contrast to passive systems, the inertial delay profoundly influences the long-time dynamics and enables new fundamental strategies for controlling self-propulsion in active matter.

Second, analytical and simulational results for an active particle navigating against an elastic membrane are proposed [2]. Basically there are three states:

i) penetration of the active particle through the membrane and healing of the membrane,
ii) penetration of the active particle through the membrane and destruction of the membrane,
iii) trapping of the active particle by the membrane.


*This work was supported by the German Research Foundation (DFG).

TBD [Invited] L MAHADEVAN (Presenter), Harvard University — TBD
XUANJI YU (Presenter), Department of Physics, Division of Materials and Science Engineering, Boston University, Boston, MA, United States, FEI CHEN, Department of Physics, Boston University, Boston, MA, United States, CHI-HANG LAM, Department of Applied Physics, Hong Kong Polytechnic University, Hung Hom, Hong Kong, OPHELIA TSUI, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong — The dynamics of interfacial slippage of entangled polystyrene (PS) films on an adsorbed layer of polydimethylsiloxane (PDMS) on silicon was studied from the surface capillary dynamics of the films. By using PS with different molecular weights, we observed slippage of the films in the viscoelastic liquid and rubbery solid state respectively. Remarkably, all our data can be explained by the linear equation, \( J = -M \nabla P \) and a single friction coefficient, \( \xi \), where \( J \) is the unit-width current, \( M \) is mobility and \( P \) is Laplace pressure. For viscous films, \( M \) is accountable by using conventional formulism. For rubbery films, \( M \) takes on different expressions depending on whether the displacements associated with the slip velocity, \( v_s \), dominate or elastic deformations induced by \( \nabla P \) dominate. For viscoelastic liquid films, \( M \) is the sum of the mobility of the films in the viscous and rubbery states.

**We acknowledge funding supports from the Research Grant Council of Hong Kong (Award nos. 15301014, 16303418 and 15330516) and National Science Foundation (Award no. DMR-1310536).**

CATHERYN JACKSON (Presenter), Core R&D, Dow Chemical, DAVID MOSLEY, Electronics and Imaging, DuPont Co. — Chemical mechanical planarization (CMP) uses polyurethane polishing pads and highly engineered slurries to planarize, or polish, silicon wafers for semiconductor manufacturing. Friction is present as a critical aspect of this complex process, and is a function of \( \text{pH} \), isoelectric point of the slurry particles, particle concentration, pad design, and other variables. Despite the connection of friction with CMP outcomes, detailed studies of friction and polishing are lacking due to the expense and difficulty of modifying commercial equipment to make precise tribology measurements. A pin-on-disk tribology attachment for the Anton-Paar MCR-502 rheometer can simulate a commercial polisher, to condition the pad in-situ and then polish the Si wafer. We measure both friction and the z-displacement, or change in gap, at realistic downpressures (1-5 psi) and sliding velocities (up to 1 m/s), which allows careful study of lubrication mechanisms, pad wear and slurry performance. The friction and z-displacement results for water at different pH's are consistent with some mechanistic models used to represent surface and colloidal forces in these systems.

DANIEL GARCIA (Presenter), THOMAS ANGELINI, Mechanical and Aerospace Engineering, University of Florida — The material properties of soft matter systems are measured with rheometers and tensile testing instruments whenever there exist few limitations on sample volume and fixturing where samples can be prepared specifically to work with the hardware of a given instrument. By contrast, indentation methods are advantageous for measuring material properties when sample preparation and geometry are highly constrained, which is often the case with tissue samples, hydrogel coatings, or soft objects with defined shapes like contact lenses. However, many soft matter materials exhibit frequency-dependent moduli, which are challenging to account for using the simple models of Hertz and Winkler. In this talk I will review our recent work to developed a Fourier-analysis method that leverages the Kramers-Kronig relations to extract frequency dependent elastic and viscous moduli from Force-indentation curves, eliminating the challenges associated with physically oscillating contact instruments.
3:42PM H54.00005: Rate and State Dependent Friction Law Showing Convex Velocity Dependence and Vanishing Static Friction Force Derived from Microscopic Point of View.* HIROSHI MATSUKAWA (Presenter), Aoyama Gakuin University — Rate and state dependent friction law, which describe the behavior of the friction force in terms of the sliding velocity and the state variable, is well employed in the study of earthquake and so on. I derive new type of rate and state dependent friction law from microscopic point of view. It turns out that the static friction force vanishes in general. The kinetic friction force grows from zero with increasing sliding velocity. Under some condition the kinetic friction force shows maximum as a function of the sliding velocity in the steady state. The physical mechanism of these behavior of the friction force is explained. The relation with the earthquake is also discussed.

*This work was supported by JSPS KAKENHI Grant Number JP16H06478 in Scientific Research on Innovative Areas “Science of Slow Earthquakes” and JSPS KAKENHI for Scientific Research(C) Grant Number JP17K05586.

3:54PM H54.00006: Structure-Based Design of Anti-Fouling Polymer Nanocoating MAYA ENDOH (Presenter), DANIEL SALATTO, ZHIXING HUANG, MANI K SEN, Stony Brook University, YUMA MORIMITSU, Kyushu University, WEIYI LI, Stony Brook University, DAISUKE KAWAGUCHI, KEJI TANAKA, Kyushu University, YIZHI MENG, DAVID THANASSI, TADANORI KOGA, Stony Brook University — Fouling is the undesirable accumulation of a material on a wide variety of objects, such as medical devices, ship hulls, and membranes, and has now become a widespread global problem from land to ocean with both economic and environmental penalties. Here we report a radically new designed polymeric coating that is a few nanometers thick (“polymer nanocoating”) with an anti-fouling property. It is found that the anti-fouling property of this polymer nanocoating is generalizable to various homopolymer systems regardless of their hydrophilicity/hydrophobicity and their surface energy. This is attributed to the highly packed chain conformations via the self-organization process of the adsorbed polymer chains on the impenetrable solid surfaces. Furthermore, the preparation of the polymer nanocoating is a simple and versatile top-down approach based on good solvent rinsing. We hypothesized that the origin of the anti-fouling property is the highly packed conformation of polymer chains with a large number of segment/solid contacts within a two-dimensional space. This finding facilitates a simple and versatile structure-based design of an anti-fouling coating using common types of synthetic polymers.

4:06PM H54.00007: Mechanisms of Ultra-Low Wear Polymeric Solid Lubricants* [Invited] DAVID BURRIS (Presenter), Mechanical Engineering, University of Delaware — Polymeric solid lubricants can address the many limitations of more traditional lubrication systems including complexity, cost, maintenance requirements, vapor pressure, and sensitivity to environmental contamination, temperature, and composition. At present, commercially available materials have been designed based on the conventional wisdom that wear reductions require increased strength and toughness, and friction reductions require increased availability of soft/lamellar phases. Unfortunately, friction and wear reductions compete in this framework, which fundamentally limits overall tribological performance. The fundamental problem with the conventional wisdom is that it neglects to account for the transfer film, a layer of adhered debris that ultimately protects the solid lubricant from the counterface and vice versa. It is now understood that the friction and wear properties of these systems depend as much (and likely more) on the formation, properties, and stability of the transfer film as they do on the composition, structure, and properties of the solid lubricant itself. Unfortunately, the relevant transfer film properties have proven difficult to measure and the extent to which they contribute to friction and wear reduction remains unclear. In this talk, I will review some of the ultra-low wear polymeric solid lubricants we have developed and studied over the last decade, our efforts to understand the attributes of and specific roles played by the transfer film, and how we have applied these insights to a more useful materials design framework that prioritizes the properties and stability of the transfer film.

*The authors gratefully acknowledges support from the the Air Force Office of Scientific Research (FA9550-10-1–0295) and the National Science Foundation Graduate Research Fellowship (1247394)
Poroeleastic sliding of thin grafted hydrogel layers  JESSICA DELAVOIPiÈRE, YVETTE TRAN, SIMM, ESPCI, BERTRAND HERTEUFEU, Saint Gobain Research Paris, EMILIE VERNEUIL, SIMM, ESPCI, CHUNG YUEN HUI, School of Mechanical and Aerospace Engineering, Cornell University, ANTOINE CHATEAUMINOIS (Presenter), SIMM, ESPCI — We investigate the sliding friction of thin (µm), water swollen, hydrogel layers grafted onto glass substrate with an emphasis on the contribution to friction of stress-induced poroelastic drainage of the hydrogel network. Friction experiments using poly(dimethylacrylamide) hydrogels films are carried out with the contact immersed in water. In addition to friction force measurements, an optical set-up allows imaging the contact. The velocity-dependence of friction force $F_t$ and contact shape is found to be controlled by a Péclet number $Pe$ corresponding to the ratio of advective (sliding) to diffusive components (fluid drainage). When $Pe<1$, the equilibrium circular contact achieved under normal indentation remains unchanged during sliding. Conversely, for $Pe>1$, a decrease in the contact area is observed together with the development of a contact asymmetry when velocity is increased. These findings are discussed in the light of a poroelastic model based on a thin film approximation. This model indicates that changes in contact geometry are due to the development of a pore pressure imbalance when $Pe>1$. An order of magnitude estimate of $F_t$ and its dependence on normal load and velocity is provided under the assumption that most of frictional energy is dissipated by poroelastic flow.

Time-dependent friction and polymer dynamics in hydrogel surface contacts*  NICHOLAS L CUCCIA, SURAJ POTHINENI, JUSTIN BURTON (Presenter), Emory University — Hydrogels are composed of a sparse, crosslinked polymer matrix infused with water. They can be found in a multitude of biological settings, from cell nuclei to cartilage, and are used in many industrial applications. However, their material properties are not well-understood due to their heterogenous nature. Here we investigate the interfacial rheology of both polyacrylamide and agarose hydrogels using a custom, low-force pin-on-disc tribometer under a variety of environmental conditions. Under a constant normal load, these hydrogels exhibit a dynamic frictional transition characterized by a precipitous drop in the friction coefficient at a critical velocity. Within a range of speeds near this dynamic frictional transition, transient behavior can be observed. Upon increasing the speed, the coefficient of friction decreases exponentially, with a characteristic decay time of order 5-10 minutes. Surprisingly, a cessation of sliding results in a much more rapid recovery of the friction coefficient, suggesting that nonlinear processes control these timescales. We will show how this transition can be tuned by varying the liquid salt concentration, liquid viscosity, and sliding geometry.

Granular charging at a distance*  TROY SHINBROT (Presenter), Biomedical Engineering, Rutgers University, New Brunswick, BEHROOZ FERDOWSI, Geosciences, Princeton University, SANKARAN SUNDARESAN, Chemical and Biological Engineering, Princeton University, NUNO ARAUJO, Faculdade de Ciências, Universidade de Lisboa — Contact charging of granular materials can play a dominant role in effects as varied as lightning in sandstorms, the formation of extraterrestrial planetesimals, and segregation of pharmaceutical powders. Yet the physics underlying this charging is exceptionally poorly understood. For example we have no clear theory for how insulating grains recruit enough charge carriers to deposit charge but not enough to discharge. In this talk, we note that charging and discharging kinetics may be distinct, and from this observation we develop a mathematical model. The model surprisingly predicts that charging can decrease as contact frequency increases. We confirm this prediction experimentally in a vibrated bed and propose future steps.

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Session H55 GSNP: The Subtle Road to Equilibrium -- or Not?  BCEC 254B - David Campbell, Boston Univ -

Tag(s): Focus
2:30PM H55.00001: The subtle road to equilibrium - or not?* [Invited] CARLO DANIELI (Presenter), MITHUN THUDIYANGAL, YAGMUR KATI, Center for Theoretical Physics for Complex Systems, Institute for Basic Science, DAVID K CAMPBELL, Boston University, SERGEJ FLACH, Center for Theoretical Physics for Complex Systems, Institute for Basic Science — The influence that deviations from equilibrium have on the ergodic equipartitioned dynamics of classical and quantum systems has been widely investigated in the recent years. Classically, systems of many interacting bodies are typically chaotic, and their microcanonical dynamics ensures that time averages and phase space averages are identical, in agreement with the assumption of ergodicity. In proximity to an integrable limit the properties of the network of nonintegrable action space perturbations help decide whether i) ergodization time scales stay on the order of the Lyapunov times, or whether ii) the system fragments into regular regions - formed by coherent localized excitations with anomalously large lifetimes - and chaotic parts. In this latter case, the ergodization time scales overgrows the Lyapunov times, and the system enters a dynamical glass (DG) phase at a finite distance to the integrable limit. We use a set of observables which turn into conserved quantities in the integrable limit to quantify the properties of the DG phase. A sectioning of a typical trajectory by equilibrium Poincare manifolds detects the coherent excitations, whose statistics signals the onset of the DG phase since they control the ergodization time scales of the systems. We forecast that our studies may be successfully extended to quantum models, where the DG phase could consist into a prelude of the MBL phase.

*The author acknowledges financial support from IBS (Project Code No. IBS-R024-D1)

3:06PM H55.00002: Lyapunov exponents, ergodization time and out-of-time-order correlators in chaotic many-particle systems from Loschmidt echoes* ANDREI TARKHOV (Presenter), Center for Photonics and Quantum Materials, Skolkovo Institute of Science and Technology, SANDRO MARCEL WIMBERGER, Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, BORIS V. FINE, Center for Photonics and Quantum Materials, Skolkovo Institute of Science and Technology — We propose an experimentally realizable method to demonstrate Lyapunov instability and to estimate ergodization time in chaotic many-particle systems by monitoring equilibrium noise of virtually any observable quantity before and after time reversal of dynamics (Loschmidt echo). In the quantum regime, the quantity of interest for the method is a counterpart of out-of-time-order correlators (OTOCs). The ergodization time is defined as the characteristic time required to extract the largest Lyapunov exponent from a system's dynamics. The proposal focuses specifically on a lattice of coupled Bose-Einstein condensates in the classical regime describable by the discrete Gross-Pitaevskii equation. We support our theoretical analysis by direct numerical simulations demonstrating that the largest Lyapunov exponent and the ergodization time can indeed be extracted from the Loschmidt echo routine.


*This work was supported by a grant of the Russian Science Foundation (Project No. 17-12-01587).

3:18PM H55.00003: Quantum versus classical thermalization in many-body isolated systems* FELIX IZRAILEV (Presenter), Benemerita Universidad Autonoma de Puebla — In view of recent studies of the thermalization occurring in many-body isolated systems, we discuss the onset of relaxation towards a steady-state equilibrium, paying main attention to the systems with finite number of interacting particles. We have found that in the models of randomly interacting fermions and bosons, the effective number of components in the wave packets increases exponentially in time, provided the eigenstates are strongly chaotic in the Hilbert space defined by non-interacting particles. Our semi-analytical approach allows one to obtain the estimates for the rate of this increase and for the characteristic time of the saturation which can be considered as the time for a complete thermalization. Special interest has been payed to the correlations between occupation numbers, that increase in time during the scrambling of wave packets in Hilbert space. These correlations are responsible for the onset of the Bose-Einstein and Fermi-Dirac distributions. We discuss the relevance of the exponentially fast quantum dynamics to the Kolmogorov-Sinai entropy characterizing degree of chaos in the corresponding classical systems.

*CONACYT, Mexico, Proyecto no. 286633
3:30PM H55.00004: Behavior and Breakdown of Higher-Order Fermi-Pasta-Ulam-Tsingou Recurrences*  

SALVATORE PACE (Presenter), DAVID K CAMPBELL, Boston University — We investigate numerically the existence and stability of higher-order recurrences (HoRs), including super-recurrences, super-super-recurrences, etc., in the alpha and beta Fermi-Pasta-Ulam-Tsingou (FPUT) lattices for initial conditions in the fundamental normal mode. Our results represent a considerable extension of the pioneering work of Tuck and Menzel on super-recurrences. For fixed lattice sizes, we observe and study apparent singularities in the periods of these HoRs, speculated to be caused by nonlinear resonances. These singularities depend very sensitively on the initial energy. We compare the mechanisms by which the super-recurrences in the two model's breakdown as the initial energy and respective nonlinear parameters are increased. The breakdown of super-recurrences in the beta-FPUT lattice is associated with the destruction of the so-called metastable state and hence is associated with relaxation towards equilibrium. For the alpha-FPUT lattice, we find this is not the case and show that the super-recurrences break down while the lattice is still metastable. We close with comments on the generality of our results for different lattice sizes.

*We thank Boston University's Undergraduate Research Opportunities Program and Boston University's Research Computing Services.

3:42PM H55.00005: Aperiodically driven integrable systems and their emergent steady states  

DIPTIMAN SEN (Presenter), Indian Institute of Science, SOURAV NANDY, ARNAB SEN, Indian Association for the Cultivation of Science — For periodically driven closed quantum many-body systems, it is known that the local properties of the system eventually synchronize with the drive and can be described by an appropriate periodic Gibbs ensemble. We have studied what happens in a class of integrable systems if they are driven aperiodically. We show that the resulting unitary dynamics leads to new emergent steady states in at least three cases. A random noise causes eventual heating to an infinite temperature ensemble for all local properties. A driving which is self-similar in time leads to an entirely different steady state which we call the ´geometric generalized Gibbs ensemble'. Finally, a quasiperiodic driving which follows the Fibonacci sequence can lead to steady states which are not described by either a periodic Gibbs ensemble or an infinite temperature ensemble. To understand the approach to the steady state, we study the time evolution of certain coarse-grained quantities in momentum space that fully determine the reduced density matrices for subsystems whose sizes are much smaller than the full system. Such quantities provide a concise description for any drive protocol in integrable systems that are reducible to a free-fermion representation.

References:


3:54PM H55.00006: Dynamical Glass Phase and Ergodization Times in Josephson Junction Chains*  

MITHUN THUDIYANGAL (Presenter), CARLO DANIELI, YAGMUR KATI, SERGEJ FLACH, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon 34051, Korea — Models of Josephson junction chains turn integrable in the limit of large energy densities or small Josephson energies. Close to these limits the Josephson coupling between the superconducting grains induces a short range nonintegrable network. We compute distributions of finite time averages of grain charges and extract the ergodization time $T_E$ which controls their convergence to ergodic $\delta$-distributions. We relate $T_E$ to the statistics of fluctuation times of the charges, which are dominated by fat tails. $T_E$ is growing anomalously fast upon approaching the integrable limit, as compared to the Lyapunov time $T_\Lambda$ - the inverse of the largest Lyapunov exponent - reaching astonishing ratios $T_E/T_\Lambda \geq 10^8$. The microscopic reason for the observed dynamical glass phase is routed in a growing number of grains evolving over long times in a regular almost integrable fashion due to the low probability of resonant interactions with the nearest neighbors. We conjecture that the observed dynamical glass phase is a generic property of Josephson junction networks irrespective of their space dimensionality.

*The authors acknowledge financial support from Institute for Basic Science (Project Code No. IBS-R024-D1).
4:06PM H55.00007: Non-Gibbs states on a Bose-Hubbard Lattice*  ALEXANDER CHERNY, Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, THOMAS ENGL, SERGEI FLACH (Presenter), Center for Theoretical Physics of Complex Systems, Institute for Basic Science — We study the equilibrium properties of the repulsive quantum Bose-Hubbard model at high temperatures in arbitrary dimensions, with and without disorder. In its microcanonical setting the model conserves energy and particle number. The microcanonical dynamics is characterized by a pair of two densities: energy density $\varepsilon$ and particle number density $n$. The macrocanonical Gibbs distribution also depends on two parameters: the inverse nonnegative temperature $\beta$ and the chemical potential $\mu$. We prove the existence of non-Gibbs states, that is, pairs $(\varepsilon, n)$ which can not be mapped onto $(\beta, \mu)$. The separation line in the density control parameter space between Gibbs and non-Gibbs states $\varepsilon \sim n^2$ corresponds to infinite temperature $\beta = 0$. The non-Gibbs phase can not be cured into a Gibbs one within the standard Gibbs formalism using negative temperatures.

*This work was supported by the Institute for Basic Science, Project Code IBS-R024-D1. TE acknowledges financial support by the Alexander-von-Humboldt foundation through the Feodor-Lynen Research Fellowship program Nr. NZL-1007394-FLF-P.

4:18PM H55.00008: Probing the mobility edge in an interacting model using MPS* NICHOLAS POMATA (Presenter), Stony Brook University, SRIRAM GANESHAN, Physics, The City College of New York, TZU-CHIEH WEI, Stony Brook University — The quasiperiodic Generalized Aubry-André model is known to exhibit a mobility edge in the noninteracting limit for a certain range of disorder strengths. However, there is not much known about the interacting version of the model. We use the Shift-Invert Matrix Product State method of Yu, Pekker, and Clark to study this system with sizes from 32 to 128 sites, computing excited states for different disorder realizations (produced by varying the phase in the quasiperiodic potentials). Our goal is to determine where many-body localized states are absent or present, starting from the single-particle mobility edge.

*This work is partially supported by the National Science Foundation under Grant No. PHY 1620252.

4:30PM H55.00009: Effective ergodicity breaking phase transition in a driven-dissipative system* SAKIB MATIN (Presenter), HARVEY GOULD, W. KLEIN, Boston University — The growing interest in non-equilibrium systems has prompted question of what equilibrium methods can be extended to non-equilibrium systems. We discuss a non-equilibrium phase transition in the Olami-Feder-Christensen model that is characterized by critical exponents which obey scaling laws from equilibrium statistical mechanics. Below the critical noise, the sites are trapped in different limit cycles. The probability distributions of different trajectories are distinct and highlight the non-ergodic nature of the phase. Above the critical noise all sites converge to the same time average and the system is effectively ergodic. We use tools from the study of glassy systems and nonlinear dynamics to illuminate various properties of this non-equilibrium phase transition. Our results show a promising start to extending the methods of equilibrium statistical mechanics to a new class of non-equilibrium systems.

*UROP (Undergraduate Research Opportunities Program) and Boston University Shared Computing Cluster

4:42PM H55.00010: Investigating many-body mobility edges in isolated quantum systems* XING BO WEI, Department of Physics, Zhejiang Normal University, CHEN CHENG, Beijing Computational Science Research Center, GAO XIANLONG, Department of Physics, Zhejiang Normal University, RUBEM MONDAINI (Presenter), Beijing Computational Science Research Center — The existence of many-body mobility edges in closed quantum systems has been the focus of intense debate after the emergence of the description of the many-body localization phenomenon. Here we propose that this issue can be settled in experiments by investigating the time evolution of local degrees of freedom, tailored for specific energies and intial states. An interacting model of spinless fermions with exponentially long-ranged tunneling amplitudes, whose non-interacting version known to display single-particle mobility edges, is used as the starting point upon which nearest-neighbor interactions are included. We verify the manifestation of many-body mobility edges by using numerous probes, directly comparing it with the predictions of the Eigenstate Thermalization Hypothesis (ETH). Our results indicate the coexistence of regions with finite measure when approaching the thermodynamic limit where thermalization and localization are manifest, suggesting that one cannot explain their appearance as merely being a result of finite-size effects.

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Rogue Fluctuations in Fermi-Pasta-Ulam-Tsingou Systems

SURAJIT SEN (Presenter), RAHUL KASHYAP, University at Buffalo, The State University of New York — Rogue waves, also referred to as freak waves, are large, short lived waves in the oceans and have been the subject of intense research due to their destructive nature. We consider discrete strongly nonlinear systems with Fermi-Pasta-Ulam-Tsingou type potentials by means of extensive simulations. We define rogue fluctuations in these systems as large and persistent kinetic energy fluctuations with finite lifetimes in these systems at late enough times. Our simulations suggest that rogue fluctuations are generic to strongly nonlinear systems. We also observe from our simulations that rogue fluctuations show features which are reminiscent of rogue waves in the oceans, providing evidence that they are natural candidates for analogs of rogue waves in discrete systems [1]. Effects arising from the presence of phonons in these systems are also explored.


SS has benefited from support of the Fulbright Foundation during this work

Quantum coherence in the ergodic and many-body localized phase

SAYANDIP DHARA (Presenter), University of Central Florida, ALIOSCIA HAMMA, Physics, University of Massachusetts - Boston, EDUARDO R MUCCIOLO, University of Central Florida — We use quantum coherence as a tool to study the structure of the eigenstates of disordered and interacting quantum many body systems. In particular, we numerically calculate several different measures of quantum coherence for the excited eigenstates to be able to capture the signatures of the ergodic and the many-body localized phase in these finite systems. It is apparent that the different measures of coherence show different behaviour with the increasing disorder strength. We also investigate how the unitary evolution affects quantum coherence in several disordered spin chains. Starting from a maximal coherent state in the computational basis, we study the dynamics of decoherence in both the ergodic and the many-body localized phase. We show that coherence can capture many important features of quantum dynamical phases and offers important computational advantages.
Laboratory rivers*  [Invited]  OLIVIER DEVAUCHELLE (Presenter), ANAIS ABRAMIAN, Institut de physique du globe de Paris, GREGOIRE SEIZILLES, Nexicap Partners, PAULINE DELORME, Department of Geography and Environment, University of Southampton, ERIC LAJEUNESSE, FRANCOIS METIVIER, LAURIE BARRIER, Institut de physique du globe de Paris — Alluvial rivers transport sediment, and build their own bed out of it. The flow entrains superficial grains of sediment and deposit them downstream, thus deforming the channel that confines it. This fluid-structure coupling generates ripples, dunes, bars and meanders through various instabilities. It also selects a river's size and slope.

To entrain a sediment grain, the flow-induced shear stress must overcome its weight. This threshold, typical of granular materials, sets the characteristic size of alluvial rivers. Beyond this threshold, however, a river needs to balance the cross-stream fluxes of sediment to maintain its bed. Unfortunately, these fluxes are barely accessible to field measurements.

Creating small rivers in laboratory experiments is an old idea, but only now can we track thousands of individual grains, as they travel downstream, to reveal the statistics of sediment transport, and their consequences on a river's shape.

In a laminar flume, we find that the roughness of the bed causes the traveling particles to roam across its surface. This random walk induces a Fickian flux which tends to homogenize the transport of sediment. Meanwhile, the bed assumes a convex shape which brings the traveling grains near its center. As a result, the sediment flux distributes itself in this self-organized potential well according to Maxwell-Boltzman statistics.

The same mechanism allows laboratory rivers to adjust their cross-section and their width to the sediment discharge: they widen and shallow to accommodate a larger input. Beyond a critical sediment discharge, however, a river destabilizes into a braid of intertwined channels. We suggest that a new instability, driven by bedload diffusion, might explain this transition.

Finally, we look for the expression of these dynamics in large sedimentary structures deposited by rivers: alluvial fans.

*This work was funded by the Emergence(s) program of the City of Paris (OD), and the EC2CO program (EL).

Fluid-Fluid Displacement Patterns in Microfluidic Analogues of Rough Fractures with Controlled Roughness  YU QIU (Presenter), KE XU, AMIR PAHLAVAN, RUBEN JUANES, Civil and Environmental Engineering, Massachusetts Institute of Technology — We report results of immiscible fluid-fluid displacement experiments on 3D-printed artificial fractures with controlled roughness. Our fracture analogue consists of a microfluidic cell with an irregular post pattern and a "free gap" between the top of the posts and the flat surface. We inject a low-viscosity nonwetting fluid to displace a more viscous wetting fluid and observe a transition from porous media flow to flow between parallel plates as a function of free-gap height. When the free gap is smaller than or comparable to the post height, the drainage pattern is similar to that in a 2D porous micromodel. In contrast, when the free gap is significantly larger than the post height, drainage in the gap dominates, and the displacement pattern is controlled by the capillary number. At high Ca, a film of the defending phase is left on the rough surface behind the front; this film then redistributes and forms discrete wetting clusters. At low Ca, the invading fluid occupies the full height of the free gap, with little wetting phase trapped even under unfavorable viscosity ratio. Our observations point to the mechanistic interplay of roughness and capillarity on trapping of the wetting phase in a rough fracture, a process that significantly affects its multiphase-flow properties.

Erosion of unconsolidated beds by turbidity currents  THOMAS HALSEY (Presenter), ExxonMobil Upstream Research Co — Turbidity currents are gravity flows of fluids with suspended, denser sediment, which remains aloft due to turbulence generated by the current motion itself. To remain active, turbidity currents must have an ability to entrain material from their base to counteract the sedimentation of particles from the current to the base. A number of decades ago, Bagnold, Engelund, and Fredsøe proposed a physical picture for erosion as a function of the overall velocity of the turbidity current (bed stress). Recently, it has been argued that the high-velocity form of this law is critical in determining the overall mechanics of turbidity currents, particularly their predilection to erode or deposit sediment in different locations. I re-examine the Bagnold-Engelund-Fredsøe picture, and determines the corresponding erosion law in a way that is consistent with turbidity current mechanics, and has a high-velocity plateau that determines the qualitative features of turbidity current deposition and erosion. This overall picture implies that the mixing of sediment from the boundary layer near the underlying bed with the overall current-suspended sediment will be the rate-limiting step in erosion.
Characteristic lengths of stream networks in porous terrain

ERIC STANSIFER (Presenter), MIT, OLIVIER DEVAUCHELLE, IPGP, DANIEL ROTHMAN, MIT — The conditions for sediment transport of particles in streams has previously been found to give a relationship between the stream's slope and flux. Using this relationship, we establish a lower bound on the size of features in a stream network. Tributaries that violate this lower bound do not receive groundwater and dry up. This technique also gives bounds on a network's drainage density, which is its total length divided by the area it drains; this is the inverse of a characteristic length. These bounds obey scaling laws with respect to physical constants that describe the hydrological environment of the network, such as grain size, porosity, and water table depth, and we observe the effects of these scaling laws in a real-world network.

Channelling and branching in frangible porous media*

DAVID FRONK, NICHOLAS DERR, Harvard University, AMALA MAHADEVAN, Woods Hole Oceanographic Institution, CHRISTOPHER RYRCROFT, LAKSHMINARAYANAN MAHADEVAN (Presenter), Harvard University — Fluid flowing through a fragile porous medium can cause channels to form due to erosion. We write down an effective theory for the process in terms of a multiphase flow model that couples a Darcy equation with a dynamical permeability to a dynamical equation for the rate of erosion. Solving the problem numerically shows that the appearance of tree-like branches as well as channels depending on the boundary conditions, and the rate of flow change at the boundary. Adding deposition and evaporation to the model leads to patterns similar to vascularization in tissues and suggests ways to engineer soft materials to self organize into biomimetic patterns.

Fingering Instability in Granular Suspension Injected into Thin Fractures*

RAUSAN JEWEL (Presenter), RAM SUDHIR SHARMA, ARSHAD KUDROLLI, Clark University — We discuss observation of a fingering instability when granular beads suspended in a liquid, with the same mass density, are injected into a fracture in the form of a Hele-Shaw cell filled with a similar wetting fluid. When the suspension is injected from a point into the cell, with the same density fluid, we find that the suspension spreads uniformly with a smooth circular front, with an expansion rate proportional to the injection rate. In contrast, when the density of the injected fluid and the interstitial fluid are even slightly different, we find that fingers form when the granular suspension is injected, and as the front spreads above a critical radius. We demonstrate that only the density difference is important, and the patterns form with both higher and lower density interstitial fluid. We will discuss the evolution of the fingers as a function of injection rate and the volume fraction of the beads, and contrast with the Saffman-Taylor instability observed when a less viscous fluid is injected into a more viscous fluid.

Self-organized compaction fronts in cyclically-sheared sinking grains*

JIKAII WANG (Presenter), J. M. SCHWARZ, JOSEPH D PAULSEN, Syracuse University — Suspension that are sheared cyclically at small amplitude can enter an absorbing steady state where the particles return to their initial positions after each cycle. However, much less is known about the transient dynamics leading up to this reversible steady state. We perform simulations of sheared non-Brownian suspensions where the particles are also sinking under gravity at low speed. We observe a rising front between two regions of different particle area fractions that propagates at constant velocity. Although the suspension is relatively dilute, the front has a sigmoidal shape that is similar to the profile of a dynamic jamming front [1]. Surprisingly, the width of the front is independent of the effective diffusion constant for colliding particles, and depends only on the area fractions of the two regions. To understand our findings, we look for front-like solutions in a set of coupled nonlinear PDEs describing our simulations in the continuum limit. This approach should elucidate the potential for compaction front dynamics in related systems.


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**We gratefully acknowledge the Donors of the American Chemical Society Petroleum Research Fund and NSF-DMR-CMNT-1507938 for partial support of this research.
4:30PM H56.00009: Pattern formation in partially wet granular materials* ANDREAS ZIPPELIUS (Presenter), KAI HUANG, Experimentalphysik V, University of Bayreuth — From sand dunes to Faraday heaping, driven granular matter, i.e., large agglomeration of macroscopic particles, is rich pattern forming system. When a granular material is partially wet (e.g., wet sand on the beach), a different pattern forming scenario arises due to the cohesive particle-particle interactions: Kink-wave fronts were found to be the dominating pattern. Here, we focus on the formation of density-wave fronts in a driven wet granular layer undergoing intermittent gas-liquid-like transition. Fronts, which are curved into a spiral shape, propagate coherently along the circular rim of the container with leading edges. They are stable beyond a critical distance from the container center. Based on the measurement of the critical distance and the rotation frequency, we propose a model for the pattern formation by considering the competition between the time scale for the collapse of cohesive particles and that of the energy injection resisting this process. Possible connections of this pattern to galaxy formation as well as to traffic jam will be discussed.

*This work is supported by the German Research Foundation through Grant No. HU1939/2-1.

4:42PM H56.00010: DEM modeling of coupled multiphase flow and granular mechanics: wettability control on fracture patterns YUE MENG (Presenter), BAUYRZHAN PRIMKULOV, Civil and environmental engineering, Massachusetts Institute of Technology, ZHIBING YANG, School of water resources and hydropower engineering, Wuhan University, FIONA KWOK, Civil and environmental engineering, University of Hong Kong, RUBEN JUANES, Civil and environmental engineering, Massachusetts Institute of Technology — As one of the factors that influences multiphase flow in porous media, wettability has been studied for decades, yet many fundamental questions remain. In a recent experimental study, the impact of wettability on the fluid-fluid displacement pattern in a deformable granular pack was investigated. The experiments show the emergence of fracture of the granular pack under certain conditions of injection rate and confining stress. They also show that changes in wettability lead to striking differences in the fracture network morphology. Here we use discrete element modeling (DEM) to provide insight into the mechanisms underpinning these experimental results. We first develop a 2D model with single-phase flow, and validate it against results from fluid-driven deformation of a confined monolayer of hydrogel particles [MacMinn et al., PRX 2015]. To study two-phase flow, we couple a dynamic pore-scale network description of fluid-fluid displacement with a DEM model of the mechanical deformation of the skeleton of solid grains. This modeling approach allows us to capture the effects of varying wettability on the fracture pattern, thereby offering a grain-scale mechanistic understanding of the fracturing process.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H58 GSOFT: Emulsions and Foams BCEC 257A - Rodrigo Guerra, New York University

2:30PM H58.00001: Faceted liquid droplets: when colloids are attracted by topological defects* SHIR LIBER (Presenter), ALEXANDER V. BUTENKO, ELI SLOUTSKIN, Physics, Physics Department and Institute of Nanotechnology & Advanced Materials, Bar-Ilan University, Ramat-Gan 5290002, Israel — Particles at disordered droplet interfaces were extensively investigated, aiming both at their fundamental physics and at their applications in particle-stabilized pharmaceuticals and aerosols. Yet, particles residing at the ubiquitous ordered interfaces have never been studied.

We study the dynamics of tracer colloids, incorporated into a curved 2nm-thick crystal, forming at $T=T_s=26$ °C at the interface of liquid oil-in-water emulsion droplets. We demonstrate the particles to be spontaneously dragged to particular surface locations, identified with topological defects within the crystalline structure. At $T=T_d<T_s$ the droplets undergo an unprecedented sphere-to-icosahedron shape transformation, with their bulk remaining liquid. At $T_d$, the attractors self-position onto the vertices of the icosahedra and fix there the colloids’ positions. At an even lower temperature, the particles are spontaneously expelled from the droplets. These phenomena allow functional liquid “atoms” to be designed, with their “valency” fixed by precise temperature-tuned positioning of the interfacial ligands, en route to supra-“atomic” nano-structures. Our observations also impact upon the understanding of protein positioning on cell membranes, controlling essential biological functions.

*ISF #1779/17
2:42PM H58.00002: Adsorption of Anionic Nanoparticles at Oil-water Interfaces Driven by Ion Partitioning*  
ROBERT KEANE (Presenter), WEI HONG, WEI HE, ROBBIE BANCROFT, SAM TEALE, ANTHONY DINSMORE, Physics, University of Massachusetts, Amherst — Adsorption of particles at oil-water interfaces is the basis of Pickering emulsions, which are common in nature and industry. For anionic particles, however, the negative potential at the water-oil interface inhibits spontaneous adsorption, which limits the scope of useful materials. Here we address this problem by adding ions that selectively partition in the two phases, thereby changing the interfacial potential and driving anionic particle adsorption. We add oil-soluble tetrabutyl ammonium perchlorate (TBAP) to the nonpolar phase and Ludox silica nanoparticles to the aqueous phase. We find a threshold TBAP concentration, above which emulsions are stable for months. This threshold increases with particle concentration and with the oil's dielectric constant. Adding salt to the water raises the threshold and causes spontaneous coalescence. The results are consistent with a model based on Poisson-Boltzmann theory, which predicts that TBAP anions (ClO_4^-) migrate into the water phase and leave behind a net positive charge in the oil. Our results clarify the role of interfacial electrostatics and show how a large class of inorganic anionic nanoparticles can be used to stabilize emulsions.

*This work was supported by the National Science Foundation through CBET-1438425.

2:54PM H58.00003: Domain, nanoridge and mesa growth kinetics in stratifying foam films*  
VIVEK SHARMA (Presenter), YIRAN ZHANG, SUBINUER YILIXIATI, CHRYSTIAN OCHOA, CHENXIAN XU, University of Illinois at Chicago — Ultrathin films exhibit stratification due to confinement-induced structuring and layering of small molecules in simple fluids, and of supramolecular structures like micelles, lipid layers and nanoparticles in complex fluids. Stratification proceeds by the formation and growth of thinner domains at the expense of surrounding thicker film, and results in formation of nanoscopic terraces and mesas within a film. The detailed mechanisms underlying stratification are still under debate, and are resolved in this contribution by addressing long-standing experimental and theoretical challenges. Thickness variations in stratifying films are visualized and analyzed using interferometry, digital imaging and optical microscopy (IDIOM) protocols, with unprecedented high spatial (thickness < 100 nm, lateral ~500 nm) and temporal resolution (< 1 ms). Using IDIOM protocols we developed recently, we characterize the shape and the growth dynamics of nanoridges and mesas that flank the expanding domains in micellar thin films. We show that topographical changes including nanoridge & mesa growth, and the overall stratification dynamics, can be described quantitatively by nonlinear thin film equation, amended with supramolecular oscillatory surface forces.

*NSF CBET 1806011

3:06PM H58.00004: Iridescent clusters and marginal regeneration in vertical soap films*  
ERICA LI (Presenter), CHENXIAN XU, ELIZABETH JOHN, CHRYSTIAN OCHOA, VIVEK SHARMA, University of Illinois at Chicago — Liquid foams consist of bubbles separated by thin films. Individual films consist of two surfactant-laden surfaces that are ~ 5 nm - 10 micron apart. Sandwiched between these interfacial layers is a fluid that drains primarily under the influence of gravitational, viscous and interfacial forces, including disjoining pressure. Understanding and controlling the drainage kinetics of thin films is an important problem that underlies the stability, lifetime and rheology of foams and emulsions. We experimentally follow the drainage kinetics of foam films using imaging, color science and cluster imaging velocimetry. Interference between light reflected from two surfactant-laden surfaces that are ~ 100 nm - 10 micron apart leads to thickness-dependent iridescent colors in the visible region. Below 50 nm the thin films appear as black. In this study we characterize, track and analyze the motion of thick and thin regions that travel under combined influence of gravity, buoyancy and due to advection by capillary-driven flows. In particular, we study the origin of marginal regeneration, i.e. the complex flow patterns that originate near the borders of foam films.

*NSF CBET 1806011
3:30PM H58.00006: Phase behavior and structure of sodium naphthenate micelles  SHANG GAO (Presenter), Chemical and Biomolecular Engineering, University of California, Los Angeles, SAMANVAYA SRIVASTAVA, Chemical and Biomolecular Engineering, University of California at Los Angeles, VIVEK SHARMA, Chemical Engineering, University of Illinois at Chicago — The formation and stability of petroleum foams and emulsions can sometimes be attributed to sodium naphthenates surfactants. However, relatively little information is available about the sizes and shapes of self-assembled structures formed by sodium naphthenates, limiting our ability to control foam or emulsion stability and the success of sequestration or extraction processes. In this study, we develop a comprehensive understanding of the phase behavior of sodium naphthenate micelles (including size, shape and inter-micellar interactions) through a combination of static and dynamic scattering measurements. Small-angle X-ray scattering (SAXS) measurements revealed intriguing trends – micelle shape and size varied with increasing surfactant concentrations in the dilute (<5 wt%) limit. At higher concentrations (5 wt% – 40 wt%), while the micelle shapes and sizes remained largely invariant, inter-micellar interactions became increasingly significant, leading to stronger structure factor contributions to scattering intensities. These concentration-dependent trends are contrasted against trends in hydrodynamic size and zeta-potential of the micelles from dynamic light scattering measurements, as well as stratification kinetics of foams containing sodium naphthenate micelles.

3:42PM H58.00007: Rheology and structure of macro- and nano-emulsions with adhesive droplets*  NEDA SANATKARAN, REZA FOUDAHI (Presenter), Chemical and Materials Engineering, New Mexico State University — In this work, we investigate the viscoelastic and flow properties of oil-in-water nanoemulsions to verify rheological scaling models of macroemulsion systems. Emulsions were prepared using silicone oil with different average droplet sizes (ranging from 1 μm to below 100 nm) dispersed in sodium dodecyl sulfate solution above the critical micelle concentration. Droplet size distributions were narrow and remained unchanged for all the samples. Viscoelastic responses and yielding of emulsions were examined as a function of dispersed phase volume fractions (35 – 65 %) for each of the droplet sizes. The range of volume fractions for the samples was obtained via an evaporation-dilution technique. We elucidate the experimental result using the theoretical models for interdroplet interactions. The scaling of rheological properties with Laplace pressures becomes invalid in the nanoemulsion regime. The liquid, gel, and glass states are investigated based on the elastic modulus, yield stress and yield strain of studied adhesive emulsions.

*We would like to thank ACS PRF (55725-DNI7) for funding and NSF award #1438584 that made the purchase of the rheometer possible.

3:54PM H58.00008: Formation, growth and coalescence of nanoscopic mesas in stratifying foam films*  CHENXIAN XU (Presenter), SUBINUER YILXIATI, YIRAN ZHANG, VIVEK SHARMA, University of Illinois at Chicago — Ultrathin micellar foam films exhibit stratification due to confinement-induced structuring and layering of micelles. Stratification proceeds by the formation and growth of thinner domains at the expense of surrounding thicker film, and flows and instabilities drive the formation of nanoscopic terraces, ridges and mesas within a film. The detailed mechanisms underlying stratification are still under debate, and are resolved in this contribution by addressing long-standing experimental and theoretical challenges. Thickness variations in stratifying films are visualized and analyzed using interferometry, digital imaging and optical microscopy (IDIOM) protocols, with unprecedented high spatial (thickness < 100 nm, lateral ~500 nm) and temporal resolution (< 1 ms). Using IDIOM protocols we developed recently, we characterize the shape and the growth dynamics of mesas that flank the expanding domains in micellar thin films, and we track their evolution, as well as coalescence dynamics.

*NSF CBET 1806011
4:06PM H58.00009: Foam formation analysis during drainage of a surfactant solution* NICOLLE DE LIMA (Presenter), Mechanical Engineering, Pontificial Catholic University of Rio de Janeiro, SHIMA PARSA, Physics and Applied Physics, Harvard University, MARCIO CARVALHO, Mechanical Engineering, Pontifical Catholic University of Rio de Janeiro — Foam is widely used in oil recovery operations to maximize oil production, and solve problems caused by either a thief zone or gravity override. Foam, that can be pre-formed and injected in the reservoir or produced in-situ through the pore space, fills the high permeability areas known as thief zones and divert the displacing fluid into the direction of trapped oil, reducing the relative permeability of gas and leading to a more stable flood front. The presence of liquid lamellae between gas bubbles in the foam also reduces the gas mobility, by the increase of the gas apparent viscosity. The flow mobility is a function of the pore geometry and foam properties. However, the dynamics of foam in a porous media is not fully understood due to its complexity. The goal of this research is to study foam formation during drainage of a two-dimensional porous media glass model by visualizing the pore scale displacement flow of a surfactant solution by injected gas. A microfluidic setup composed of glass micromodel, syringe pump, pressure transducer, and a microscope is used to study the evolution of the phase distribution and foam characteristics as a function of pore space geometry and flow conditions through image processing.

*Fulbright, CNPq, Repsol Sinopec, PUC-Rio and Harvard.

4:18PM H58.00010: Capillary imbibition of emulsions in thin rectangular channels MASOUD NOROUZI DARABAD (Presenter), SAMIRA ABEDI, SIVA A VANAPALLI, MARK W VAUGHN, Chemical Engineering, Texas Tech University, Lubbock, TX — Emulsions imbibing in a capillary under transient surface-tension driven flow display an unexpected richness in droplet interactions, clustering and ordering. Droplet size and concentration effects on the droplet interactions of monodisperse oil-in-water emulsions are demonstrated by use of a thin channel to form a pseudo 2-dimensional flow. We categorize droplet-droplet and cluster-cluster interactions at the microscale and find markedly different behavior in ordering, relative phase velocity and droplet-induced interface perturbation depending on concentration and the relative size of the droplets compared to the channel height.

4:30PM H58.00011: Spinning and chaining emulsion droplets in ultrasonic standing waves* MOHAMMED ABDELAZIZ (Presenter), JAIRO A DIAZ, DAVID GRIER, Center for Soft Matter Research, New York University, MAURICIO HOYOS, Laboratoire de Physique et Mécanique des Milieux Hétérogènes, ESPCI Paris — We demonstrate experimentally that emulsion droplets of TPM (3-(trimethoxysilyl)propyl methacrylate) in water spin when levitated in ultrasound, and that the spinning droplets organize themselves into long spinning chains. When the same droplets are solidified into spheres by free-radical polymerization, they no longer spin, and they form crystals rather than chains. We explain these acoustokinetic phenomena through a dipole-order expansion of the incident and scattered waves, by analogy to the theory of optical trapping.

*This work was supported by the Materials Research Science and Engineering Center program of the National Science Foundation through award number DMR-1420073.

4:42PM H58.00012: Molecular Dynamics Simulations of Liquid-Liquid Phase Separation in Biology IAN SEIM (Presenter), AMY GLADFELTER, DAPHNE KLOTSA, University of North Carolina at Chapel Hill — A newly appreciated mechanism by which biochemistry is organized in cells without membrane barriers is liquid-liquid phase separation (LLPS). RNA and protein condense into liquid droplets through LLPS and are crucial for normal physiological function, but they are also implicated in the development of several neurological diseases as well as theories about the origins of life and cells themselves. Since the means by which droplets form, maintain shape, and achieve molecular specificity are poorly understood, a major challenge is to understand how nanometer scale molecules coalesce to produce cellular bodies of diverse material properties and distinct identities. Our aim is to model the process and properties of LLPS involving mRNAs and disordered proteins using molecular dynamics (MD). Specifically, by using both low and high-resolution representations of the system, we can map sequence-specific effects onto a low-resolution setting. In the coarse-grained space, the solvent is modeled implicitly using Brownian dynamics and the molecules as bead-spring polymers. These techniques provide access to space and time-scales that are critical to the phase separated state which involves the collective behavior of thousands of molecules.
In situ wrinkling during evaporative drying of a polymer solution drop on a soft swellable substrate is used to facilitate biochemical reactions, provide cellular compartmentalization, and sequester condition-specific factors. Whether biological LLPS events are active processes remains a difficult question to address because experiments that alter cellular ATP levels also affect the liquid properties of LLPS states. Understanding when different biological LLPS phenomena are active will provide insight into how the cell controls and drives their formation. The first instance of biological LLPS defined and one of the best characterized is the P granule of *C. elegans*. P granules exist in the cytosol of *C. elegans* germ-line cells and specify polarity during early embryonic development. To detect active processes in P granules, we measure interfacial tension in the positional trajectories of single-walled carbon nanotube probes targeted to the P granules of *C. elegans* embryos. These extremely bright, photostable, infrared fluorophores provide sufficiently long single-particle trajectories for irreversibility calculations. By measuring irreversibility in the fluctuations of P granules we hope to understand if and when P granules are active liquid states and to directly connect this to a cellular chemical energy input.

Self-swallowing droplets arise when water droplet moves through a partially miscible oil containing large amount of colloidal particles. The rapid mass transfer causes reduction of interfacial area, which leads to particles jamming and phase transition. As a result, an elastic film is generated and soon undergoes a buckling instability in response to the compressive stress due to volume shrinkage of the droplets. Therefore, a re-entrant cavity forms at the rear interface through which a jet of the outer fluid penetrates the droplet. The degree of the swallowing behavior and thus the shape of the droplets could be well adjusted by changing the experimental parameters, and the whole swallowing process could be reversibly regulated. This work not only provides indications for intriguing fundamental questions concerning hydrodynamic and interfacial effects, but also inspires technical innovations including in microfluidics, printing, soft materials processing, etc.

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**Tuesday, March 5, 2019 2:30 PM - 5:30 PM**

**Session H59 GSOFT DPOLY DBIO: Rheology of Gels II**

**2:30PM H59.00001: Viscoelasticity of gels with dynamic bonds: molecular kinetics and macroscopic mechanics**

*Invited* RONG LONG (Presenter), University of Colorado, Boulder — Incorporation of dynamic bonds into the polymer network of soft gels has been exploited as a strategy to enhance fracture toughness and to enable self-healing. Gels with dynamic bonds often exhibit macroscopic viscoelasticity which can be traced back to the kinetics of dynamic bonds undergoing dissociation and reformation. I will present our recent efforts to connect the molecular-level chemical kinetics to the continuum-level viscoelasticity. As a model system, I will focus on a hydrogel with two types of crosslinks: dynamic physical crosslinks and permanent chemical crosslinks, and describe two different approaches for modeling the relation between molecular kinetics and viscoelasticity. These two approaches are shown to capture experimental data of tensile tests with various strain histories and oscillatory torsion tests. I will also discuss how our modeling approach can potentially lead to a general theoretical framework of nonlinear viscoelasticity.
Electrolytes containing colloidal gels have been proposed as a possible alternative to overcome the mechanical strength and ionic conductivity trade-off in electrolytes. These results suggest that such open network colloidal gels may provide a means to consider the rheology and conductivity characteristics of open, equilibrium gels designed from an inverse design strategy on the interaction potentials. Using small amplitude oscillatory shear (SAOS) simulations, rheology of these samples also exhibited “dark curing”, the extent of which increased with [LiTf2N]. EPR spectroscopy demonstrates that Li+ can stabilize propagating radicals, leading to enhanced curing following UV exposure. Taken together, these results demonstrate that the rheological behavior of photopolymerized ILs can be tuned by varying the composition and UV dosage.

**3:42PM H59.00005: Selectively enhanced diffusion through polymer gels**

CARL GOODRICH (Presenter), MICHAEL PHILLIP BRENNER, Harvard University, KATHARINA RIBBECK, Massachusetts Institute of Technology — Designing selective hydrogels that passively filter particles based on their interactions is a fundamental goal of nanotechnology. While it is conceptually straightforward for a particle's interactions to facilitate its own retention (specific binding domains on the gel trap particles with complementary recognition sites), it is much more difficult for a particle to facilitate its own diffusion. This requires the binding interaction to locally reorganize the internal structure of the gel. We present a mechanism for this behavior and describe a theoretical model of the diffusion of interacting and non-interaction particles that is backed by numerical results. We also discuss how our results can lead to the design of artificial selective gels inspired by the Nuclear Pore Complex.
3:54PM H59.00006: Rheology of aluminosilicate hydrogels* DONATIEN GOMES-RODRIGUES, NICOLAS COURTOIS, JEAN-BAPTISTE CHAMPENOIS, ARNAUD POULESQUEN (Presenter), CEA Marcoule — Thanks to their environmental acceptability and their adaptability over a wide range of applications, alkali solutions of aluminosilicates are increasingly used in nuclear or building and construction industry. Although such solutions are increasingly used in the industry, there remain outstanding questions regarding the gelation process, that are driven by the composition of the solution, their stabilities and their aging. It is therefore crucial to provide a clear and realistic description of such fluids in order to tune and tailor macroscopic properties.

The aim of this work is to study the linear viscoelasticity properties of the gels throughout a variety of rheological tests, combining with time resolved Small Angle X-ray Scattering (SAXS) from liquid to gelling state. The aluminosilicate gels show a power law behavior that is well described by the Fractional Maxwell Model (FFM). The derived parameters of the FFM are well correlated to the fractal dimension that can be directly extracted from the SAXS measurements. Aging of these gels will also be discussed in relation to the results obtained at mesoscale by SAXS.

*French ANR DYNAMISTE (ANR-15-CE07-0013)

4:06PM H59.00007: Rheology of Gels [Invited] JAMES SWAN (Presenter), MIT — Gels, nonfluid networks of particles or polymers that are pervaded by fluid, appear ubiquitously within soft matter in practical applications as well as in living biological systems. The mechanical properties of gels are intermediate between those of fluids and solids, and depend sensitively on the structure of the gel constituents across multiple length scales. This focus session invites experimental, theoretical, and computational studies of the rheological properties of gels, including chemical and physical gels, hydrogels, colloidal gels, and biological gels, with particular interest and emphasis on connecting structural properties to flow properties. Contributions examining the effect of non-equilibrium activity (driven by molecular motors or by active particles) on gel mechanics are encouraged.

4:42PM H59.00008: Phase behavior of equilibrium linker gels MICHAEL HOWARD (Presenter), RYAN JADRICH, BETH LINDQUIST, THOMAS TRUSKETT, McKetta Department of Chemical Engineering, University of Texas at Austin — Gels made from networks of colloids linked by physical bonds are an important class of soft materials. A standard route to produce a gel is to rapidly cool a suspension of isotropically attractive colloids, with gelation resulting from kinetic arrest during spinodal decomposition. However, such gels are inherently nonequilibrium, and the gel's properties inevitably change as it ages. Alternatively, “equilibrium” gels with open, homogeneous structures that are resilient to aging can be created by restricting the number of bonds that form between particles. Here, we report on equilibrium gelation controlled by the addition of a secondary “linker” macromolecule that mediates bonding between colloids. The phase diagrams of such mixtures were predicted using Wertheim’s thermodynamic perturbation theory (TPT) and compared to molecular dynamics simulations. Good agreement was obtained between the predictions and simulations, with the spinodal region depressed to lower colloid densities by increased linker length at fixed linker-to-colloid number ratio. However, the presence of looping in the colloid–linker networks inhibited percolation compared to TPT predictions at low linker concentrations.

4:54PM H59.00009: Effect of Surface Stiffness on the Interfacial Dynamics of Dense Microgel Liquids KEHUA LIN (Presenter), YINGXI ELAINE ZHU, Wayne State University — Many biological and engineering processes involve highly soft and deformable surfaces, ranging from biolubrication between synovial joints to aquaplaning of rubbery tires. In this talk, I will present our recent study of the effect of surface stiffness on the glassy dynamics of dense microgel liquids. Specifically, we investigate the interfacial dynamics of poly(N-isopropylacrylamide) (PNIPAM) microgels, whose particle stiffness can be tuned by polymer crosslinking degree upon polymerization, at a solid surface coated with PNIPAM microgels of matched or mismatched stiffness. By using confocal laser scanning microscopy, we analyze the mean-squared-displacement (MSD) of PNIPAM particles in the first 1-2 confined layers near the coated surface. The MSD shows strong dependence on surface stiffness and particles tend to approach the Brownian motion at the softest surface even at the microgel volume fraction approaching the one for glass transition. The correlation between dynamic heterogeneity and friction of confined dense PNIPAM suspensions is further examined with varied particle volume fraction and particle-to-surface stiffness ratio.
5:06PM H59.00010: Non-equilibrium deformation and relaxation of giant floppy vesicles in a precisely controlled extensional flow*  DINESH KUMAR (Presenter), CHARLES SCHROEDER, University of Illinois at Urbana-Champaign — In this work, we study the non-equilibrium dynamics of single floppy vesicles under large strain rates (~15 s⁻¹) using a Stokes trap, which is a new technique developed in our lab for controlling the center-of-mass position of multiple particles or single molecules in a free solution. In this way, we directly observe the vesicle shape and conformations as a function of reduced volume, which is a measure of a vesicle's equilibrium shape departure from sphericity. We observe the formation of asymmetric dumbbell shapes, symmetric dumbbell, pearling, and wrinkling and buckling instabilities for vesicles depending upon the nature of flow and amount of membrane floppiness. We report the precise stability boundary of the flow-based phase diagram for vesicles in Capillary number (Ca)-reduced volume space, where Ca is the ratio of the bending time scale to the flow time-scale. We further probe the stability boundary at two different viscosity ratios to understand how the onset of instability in vesicles depends on viscosity ratio. We also present results on the long-time relaxation dynamics of vesicles from high deformation back to their equilibrium shapes after the cessation of flow.

*We thank NSF CBET PMP #1704668 for funding this project.

5:18PM H59.00011: Dependence of Hydrogel-Glass Energy of Adhesion and Kinetics of Delamination on Hydrogel Concentration  RICHARD PARG (Presenter), ERIN SHELTON, JOHN DUTCHER, Department of Physics, University of Guelph — Pseudomonas aeruginosa bacteria move collectively at viscous interfaces via twitching motility¹, which plays an important role in biofilm formation and subsequent infection. This phenomenon is studied by forcing the bacteria to twitch at the interface of a glass microscope slide and a hydrogel such as agar. The expanding bacterial colony needs to break the adhesive bond between the glass and the agar. Although the pulling force generated by the type-IV-pilus² and the stiffness of the agar hydrogel³ have been measured, the adhesive interaction between the glass and the agar is not well characterized. We have used micropipette deflection experiments to measure the increase in the adhesive shear strength with increasing agar concentration: 120 ± 60 N/m² for 1.0% w/v agar, and 260 ± 110 N/m² for 1.5% w/v agar. To more accurately mimic the breaking of the adhesive bond by the bacterial cells, we have developed a confined blister test that measures the energy of adhesion and the kinetics of delamination of agar-glass interfaces. I will describe the results of our measurements performed for different agar concentrations.

1 Semmler, Whitchurch, Mattick (1999) Microbiology 145:2863
3 Sharma, Bhattacharya (2014) Journal of Food Engineering 141:93

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H60 FED DCMP: Jonathan F. Reichert and Barbara Wolff-Reichert Award for Excellence in Advanced Laboratory Instruction: Incorporating State-of-the-Art Research into Advanced Labs  BCEC 258A - Peggy Cebe, Tufts University - Tag(s): Education, Invited, Undergraduate

2:30PM H60.00001: Laboratory courses and the professional preparation of physics majors* [Invited]  BENJAMIN ZWICKL (Presenter), Rochester Institute of Technology — Embracing career preparation as a goal of lab courses is one way to advocate for the maintenance and expansion of labs in the curriculum. If labs are seen as primarily supporting students' conceptual understanding they are in danger of being replaced by virtual simulations optimized for teaching concepts. If labs are viewed as training grounds for the professional preparation of students as they pursue a range of STEM careers, labs become indispensable in the education of physics majors. Drawing from multiple studies of practicing researchers and engineers as well as PER on laboratory courses, labs will be shown to support both the technical competencies (e.g., measurement, data analysis, troubleshooting, design, modeling) and the "soft" competencies (e.g., teamwork, oral communication, documentation, self-directed learning) that are important for professional success. I will suggest ways in which lab courses can best utilize the unique features of the lab environment to explicitly and visibly support students' professional preparation.

*NSF DUE-1624887, DGE-1432578, DGE-1561493

3:06PM H60.00002: Open-ended projects in undergraduate lasers and optics courses [Invited]  CHAD HOYT (Presenter), Honeywell — We describe an approach to undergraduate laboratories in two upper-level classes at Bethel University: Optics and Lasers. These courses integrate a standard lecture, lab exercises, and open-ended projects. The projects typically have a novel aspect. Examples include a lithium magnetooptical trap, plasmonics, digital and analog holography, ultrafast fiber laser optics, quantum optics and atomic and molecular spectroscopy.
3:42PM H60.00003: Designing (and re-designing) realistic research practices for undergraduate Advanced Labs

[Invited] SARA CALLORI (Presenter), Department of Physics, California State University, San Bernardino — Our institution is undergoing a quarter-to-semester transition, which has given our department the opportunity to assess and redesign how our instructional laboratories prepare students for futures within physics and other STEM fields. Currently, our one-quarter Advanced Lab course focuses on introducing students to contemporary scientific instrumentation and includes a relatively short independent research project. While both types of activities give students a taste of some facets of scientific research, they do not necessarily touch on other realistic research skills, such as oral and written communication and statistical and error analysis. Here I will discuss the “state of the lab” and reflect on the strengths and weaknesses of our current course and how this assessment is contributing to a course and curricular re-design. This scales from upgrading current Advanced Lab instructions to promote more open-ended analysis, to newly implemented activities designed to build writing and computation skills, to a longer-term overhaul of the entire instructional laboratory curriculum.

4:18PM H60.00004: Advancing the Advanced Lab: Opportunities and Challenges post-BFYIII

[Invited] JOSEPH KOZMINSKI (Presenter), Department of Physics, Lewis University — In the last five years, the American Association of Physics Teachers (AAPT) has approved recommendations for both the undergraduate laboratory curriculum and for computational physics in the undergraduate curriculum. These recommendations along with the Phys 21 report from the APS and AAPT Joint Task Force on Undergraduate Physics Programs emphasize the need for physics programs to help students develop a range of transferrable skills and knowledge that prepares them for diverse job and graduate school opportunities post-graduation. The undergraduate laboratory is a place where many of these experimental, technical, analytical, modeling, and communication skills are addressed. In July 2018, the Third Conference on Laboratory Instruction Beyond the First Year (BFY III) brought together advanced laboratory instructors for a three-day conference with the theme of developing laboratory experiences that integrate experimentation, computation, and theory. Through hands-on workshops, plenary sessions, poster sessions, and small group discussions, participants considered how to transform their upper-level laboratory curricula to include high-impact experiences through which students can build this desired skill-set, develop good laboratory practices, and enrich their understanding of physics and the applications of physics across disciplines. This talk will address the recommended outcomes of the laboratory curriculum, things learned at BFY III, and challenges and opportunities for the advanced lab community in fostering the development of critical skills and competencies through authentic and engaging laboratory experiences.

4:54PM H60.00005: Jonathan F. Reichert and Barbara Wolff-Reichert Award for Excellence in Advanced Laboratory Instruction Talk: Engaging Students in Authentic Scientific Practices in Physics Lab Courses

[Invited] HEATHER LEWANDOWSKI (Presenter), University of Colorado, Boulder — Physics is an empirical science. Therefore, learning physics must include learning how to design and conduct experiments, analyze and interpret data, and revise models and apparatus. Physics lab courses at the introductory and upper-division levels are one of only a few opportunities for students to engage in these authentic physics practices. For many students, instructional labs are the only opportunity. However, these courses do not always have the students reach the desired learning goals. Our work looks to improve lab experiences by improving students’ competency with modeling of physical and measurement systems, troubleshooting skills, documentation practices, and views of the nature of experimental physics.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H61 GSOFT DBIO GSNP: Active Matter IV BCEC 258B - Daniel Pearce, University of Geneva - Tag(s): Focus
2:30PM H61.00001: Dynamic instabilities of contractile acto-myosin rings* [Invited] KARSTEN KRUSE (Presenter), Biochemistry and Theoretical Physics, University of Geneva — The actin cytoskeleton is a prototypic example of active matter and shows a wealth of dynamic phenomena alien to conventionally studied materials. In living cells, actin filaments and myosin motors often organize into dynamic rings. This is notably the case during the late stages of cell division of animal cells, where such a ring contracts and thereby cleaves the mother cell into two daughters. Similar structures are observed in dividing fission yeast, where their functional role is less clear, though. Furthermore, rings spanning several cells appear upon closure of tissues. It has been found experimentally that myosin forms stationary or moving clusters in acto-myosin rings. The mechanism underlying their formation and their role in ring dynamics remain unclear. Based on the analysis of a phenomenological theory, we show that traveling and stationary clusters are generic features of contractile actin rings. Our numerical results indicate that there is a direct transition from homogenous actin and myosin densities to chaotic dynamics along rings. We then use a mesoscopic approach to study a possible molecular mechanism for the observed generic phenomena. It suggests that the transient formation of bipolar filaments provides a common mechanism underlying the experimentally observed patterns. The theory also shows that stationary myosin clusters are associated with elevated contractile stress, whereas traveling clusters are not. We compare these theoretical results to experimental observations in mammalian and fission yeast cells.

*This work is funded by SNF through grant 205321_175996.

3:06PM H61.00002: Tuning surface aggregation of active particles.* RAGHUNATH CHELAKKOT (Presenter), SUCHISMITA DAS, Physics, IIT Bombay — Collection of disk-like self-propelled particles, interacting via a short-range repulsive force is an effective model to understand the emergent properties in active matter. It is well known that for sufficiently high propulsion speed and density they aggregate to form clusters and at low density, they are in a homogeneous fluid state.

We study the aggregation properties of such particles on a rigid wall at a low density where they do not spontaneously form clusters in the bulk. Our numerical studies show that the cluster formation crucially depends on how the particles interact with the wall and the propulsion speed of the particles. We get two different type of clusters on the surface, as a function of the wall properties. For a range of wall parameters and particle mobility, the particles form a connected cluster all along the wall. For these parameters, we study the surface height fluctuations and compare with studies made on passive particle deposition. For a different range of wall parameters, we observe that the connected cluster becomes unstable and it breaks into smaller clusters. We study the growth dynamics of these clusters and their dependence on wall parameters and particle propulsion speed.

*SERB, DST (INDIA)

3:18PM H61.00003: Response of a system of passive or active particles to periodic forcing* MICHAEL WANG (Presenter), ALEXANDER GROSBERG, New York University — The presence of active, persistent forces in various biological and artificial systems changes how those systems behave when forced. We present a minimal model of a system of passive or active swimmers driven on the boundaries by a time-dependent forcing. We extract the linear response functions of the system and interpret them in terms of the storage and dissipation of energy through the particles within the system. We find that while a slowly driven active system responds similar to a passive system with a redefined diffusion constant, a rapidly driven active system exhibits a new behavior that may be related to a change in the motoring activity of the active particles due to the forcing.

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

3:30PM H61.00004: Diffusion of active matter with inertia* MARIO SANDOVAL-ESPINOZA (Presenter), Department of Physics, Metropolitan Autonomous University, JOHN F BRADY, Division of Chemistry and Chemical Engineering, Caltech — In this work we study the motion of active Brownian particles (ABPs) while keeping both translational and rotational inertia. Following a Langevin formalism, we theoretically find that whereas translational inertia does not play a role in the ABPs effective diffusion, rotational inertia is able to enhance the ABPs’ diffusion. To elucidate such a new effect, one has to properly take into account the rotational inertia contribution in the orientation correlations. The mean-square speed for this system is also studied and its dependence on translational and rotational inertias is determined theoretically. To validate our analytical results, Brownian dynamics simulations are performed.

*M. Sandoval thanks Consejo Nacional de Ciencia y Tecnologia, CONACYT Grant: CB 2014/237848.
3:42PM H61.00005: Critical motility-induced phase separation belongs to the Ising universality class  
BENJAMIN PARTRIDGE (Presenter), CHIU FAN LEE, Department of Bioengineering, Imperial College London — Active matter is an extreme kind of non-equilibrium system in that detailed balance is broken at the microscopic scale. A typical active system can be a collection of particles that continuously exert mechanical forces on their surrounding environment, and systems of interacting active particles can display novel phenomena, ranging from the emergence of collective motion in two dimensions when the active particles are aligning, to motility-induced phase separation (MIPS) when the particles interact solely via volume exclusion interactions. However, even though active matter breaks detailed balance in a fundamental way, it remains unclear whether the hydrodynamic, universal behavior of active matter necessarily differs from that of equilibrium systems. The investigation of universal behavior, besides being of central interest to physics, allows us to transfer knowledge of a well-known system to a different system of novel interest. Here, we do exactly that by demonstrating that the critical behaviour of MIPS belongs to the Ising universality class with conservative dynamics. We do so using three approaches: hydrodynamic argument, field-theoretic description of a microscopic model, and simulation of a lattice model.

3:54PM H61.00006: Topotaxis of Active Particles  
KOEN SCHAKENRAAD (Presenter), LINDA RAVAZZANO, JOERI WONDERGEM, ROELAND MERKS, LUCA GIOMI, Leiden University — Recent biophysical experiments have shown that the amoeba Dictyostelium Discoideum, while moving persistently in an environment filled with obstacles, can navigate away from more crowded areas towards regions with more space: an effect called topotaxis. We theoretically study active particles in a crowded environment and discuss whether or not persistent motion on itself, in the absence of any more complicated biological interactions, can drive this behavior.

4:06PM H61.00007: The Effect of Confinement on Active Brownian Particles  
CAMILLA M. KJELDBJERG (Presenter), JOHN F BRADY, Division of Chemistry & Chemical Engineering, California Institute of Technology — Active Brownian Particles (ABPs) are subject to confinement effects when their run or persistence length, $l = U_0 \tau_R$, is comparable to the characteristic size of the confining geometry. Here, $U_0$ is the intrinsic swim speed and $\tau_R$ is the reorientation time of the ABPs. Furthermore, ABPs accumulate at no-flux surfaces owing to their persistent swimming. These two effects can produce some unusual and startling effects. For example, it has been seen in simulations (Ray, et al. *PRE* 2014) that two parallel walls attract each other when placed in a dilute bath of ABPs. In this work, we provide a simple model based on the Smoluchowski equation for the ABPs and an overall macroscopic momentum balance to predict analytically this attractive force. We extend this simple modeling to predict the partitioning of ABPs between a confined channel of width $H$ and an infinite reservoir, showing that the concentration within the channel over that in the bulk increases as $l/H$. The theoretical results are compared to Brownian dynamics simulations.

4:18PM H61.00008: The universality class of Motility-Induced Phase Separation  
MATTEO PAOLUZZI (Presenter), Physics, Università Sapienza, CLAUDIO MAGGI, NANOTEC, CNR — Motility-Induced Phase Separation (MIPS) is a dynamical mechanism peculiar of Active Systems that brings to a gas/liquid phase separation even without any attraction force between the active agents. The resulting spinodal decomposition shares many similarities with its equilibrium counterpart. However, the properties of the active system close to the end point of the transition, corresponding to a critical point in equilibrium systems, remain still poorly investigated. In this work, driven by the analogy with gas/liquid phase transition, we investigate numerically the phase diagram of purely repulsive Active Ornstein-Uhlenbeck and Run-and-Tumble particles. We show that in both cases the phase coexistence ends with a critical point.

4:30PM H61.00009: Spatial Variation of Transport Properties of Active Brownian Particles*  
HYEONGJOO ROW (Presenter), JOHN F BRADY, Division of Chemistry and Chemical Engineering, California Institute of Technology — Self-propelling microswimmers such as motile bacteria and Janus particles can be modeled as Active Brownian Particles (ABPs) and characterized by their transport properties: swim speed, translational diffusivity, and rotational diffusivity. We have developed a general theory to describe suspensions of ABPs with spatially varying transport properties. We find that the number density distribution of ABPs is primarily governed by the swim speed and is always lower in the region with the faster swim speed as first shown by Tailleur & Cates (*PRL* 2008). We also show that the translational diffusivities of ABPs smooth out the effect of the variation of swim speed. The theory implies that spontaneous reverse-osmosis is achievable owing to the spatial variation of the swim speed of active matter.

*H.R. acknowledges support from Kwanjeong Educational Foundation in South Korea.
4:42PM H61.00010: Curvature-dependent tension and tangential flows at the interface of motility-induced phases*
ADAM PATCH (Presenter), Physics, Wilkes Honors College, Florida Atlantic University, DAVID YLLANES, BioHub, UC San Francisco, DANIEL SUSSMAN, Physics, Syracuse University, M. CRISTINA MARCHETTI, UC Santa Barbara — Purely repulsive active particles spontaneously undergo motility-induced phase separation (MIPS) into condensed and dilute phases. Remarkably, the mechanical tension measured along the interface between these phases is negative. In equilibrium, this would imply an unstable, expanding interface. However, these out-of-equilibrium systems display long-time stability and intrinsically stiff phase boundaries. In this work, we use active Brownian particle simulations and a novel frame of reference at the phase boundary to carefully study the emergent tangential currents at the interface, finding correlations between local interface curvature and measured values of interfacial tension. The combined observation of tangential currents in the gas and local "self-shearing" of the surface of the dense phase suggest a stiffening interface that redirects particles along itself to heal local fluctuations. In this way, the wildly fluctuating MIPS interface restores itself via an out-of-equilibrium Marangoni effect.


4:54PM H61.00011: Binary mixtures of hard sphere active Brownian particles*
THOMAS KOLB (Presenter), DAPHNE KLOTSA, University of North Carolina at Chapel Hill — We computationally study the phase behavior and dynamics of a binary mixture of active Brownian particles, where each 'species' is distinguished by its persistence of motion (effectively two species: fast, slow active particles). We find that our binary active system demonstrates motility-induced phase separation (analogous to monodisperse active systems) depending on the activity ratio, and concentration of each species. We observe a variety of steady states, which emerge as we vary the ratio of constituent particle activity, ranging from volatile partially segregated steady-state clusters, prone to fission, to a homogenously distributed, relatively stable, single cluster. We extend current theory for passive-active mixtures to account for active-active mixtures as well.

*NSF GRFP

5:06PM H61.00012: Non-equilibrium work and reversibility in active particles in disordered media
JOSHUA STEIMEL (Presenter), University of the Pacific, ALFREDO ALEXANDER-KATZ, MIT — Active particles can in principle extract/do work on the environment. Here we explore experimentally a single active spinning particle in an inclined plane sliding in a disordered array of obstacles. Our results show that there are several interesting features in this system depending on the reversibility of the system during a cycle of the time reversible protocols. In particular we observe the rectification of the activity which allows the spinner to drift faster than the reference drift in the absence of obstacles. Our results should be of interest to understand under what conditions non-equilibrium systems are able to extract work from their environment and connect it to the thermodynamic counterparts.

5:18PM H61.00013: Extreme Active Matter at High Densities*
CHANDAN DASGUPTA (Presenter), Physics, Indian Institute of Science, Bangalore, RITUPARNO MANDAL, Simons Centre for the Study of Living Machines, National Centre for Biological Sciences, Bangalore, PRANAB JYOTI BHUYAN, Physics, Indian Institute of Science, Bangalore, PINAKI CHAUDHURI, The Institute of Mathematical Sciences, Chennai, MADAN RAO, Simons Centre for the Study of Living Machines, National Centre for Biological Sciences, Bangalore — Extreme active matter, consisting of self-propelled particles characterized by large persistence time τp and high Péclet number, exhibits remarkable behavior at high densities. In the limit τp → ∞, the fluid jams as the self-propulsion force f is decreased below a critical value f*(∞). The system is stuck at a force-balanced configuration for f < f*(∞), with stresses concentrated along force chains. For large but finite τp, the approach to dynamical arrest at low f goes through a phase characterized by intermittency in kinetic and potential energy. This intermittency is a consequence of long periods of jamming separated by bursts of plastic yielding associated with Eshelby deformations akin to those found in the response of dense granular materials to an externally imposed shear. In the vicinity of the boundary between the intermittent and "normal" fluid phases, correlated plastic events result in large-scale vorticity and turbulent motion. Thus, dense extreme active matter brings together the physics of glass, jamming, plasticity and turbulence, in a new state of driven classical matter.

*This work was supported in part by the Department of Science and Technology, India and the Simons Centre for the Study of Living Machines, National Centre for Biological Sciences, Bangalore.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM
2:30PM H62.00001: Beyond the transmon: A new generation of superconducting qubits

[Invited] DAVID SCHUSTER (Presenter), University of Chicago — TBD

3:06PM H62.00002: Entanglement and complexity of interacting transmon qubits subject to asymmetric noise

[Invited] ELIOT KAPIT (Presenter), Physics, Colorado School of Mines — The simulation complexity of predicting the time evolution of delocalized many-body quantum systems has attracted much recent interest, and simulations of such systems in real quantum hardware are promising routes to demonstrating a quantum advantage over classical machines. In these proposals, random noise is an obstacle that must be overcome for a faithful simulation, and a single error event can be enough to drive the system to a classically trivial state. We argue that this need not always be the case, and consider a modification to a leading quantum sampling problem-- time evolution in an interacting Bose-Hubbard chain of transmon qubits [Neill et al, Science 360, 195 (2018)] -- where each site in the chain has a driven coupling to a lossy resonator and particle number is no longer conserved. The resulting quantum dynamics are complex and highly nontrivial. We show that this problem is likely to be harder to simulate than the isolated chain, and that it can achieve volume-law entanglement even in the strong noise limit (likely persisting up to system sizes beyond the scope of classical simulation). Further, we show that the metrics which suggest classical intractability for the isolated chain point to similar conclusions in the noisy case. These results suggest that quantum sampling problems including nontrivial noise could be good candidates for demonstrating a quantum advantage in near-term hardware.

*Eliot Kapit's research is supported by the National Science Foundation via grant PHY-1653820, and by Google, Inc.

3:42PM H62.00003: Superconducting Gatemon Qubit based on a Proximitized Two-Dimensional Electron Gas

[Invited] LUCAS CASPARIS (Presenter), MALCOLM R CONNOLLY, MORTEN KJÆRGAARD, Niels Bohr Institute, NATALIE PEARSON, Department of Physics, ETH Zurich, ANDERS KRINGHØJ, THORVALD W LARSEN, FERDINAND KUEMMETH, Niels Bohr Institute, TIAN WANG, CANDICE THOMAS, SERGEI GRONIN, GEOFFREY C. GARDNER, MICHAEL MANFRA, Department of Physics and Astronomy, Purdue University, CHARLES M MARCUS, KARL D PETERSSON, Niels Bohr Institute — The coherent tunnelling of Cooper pairs across Josephson junctions (JJs) generates a nonlinear inductance that is used extensively in quantum information processors based on superconducting circuits, from setting qubit transition frequencies and interqubit coupling strengths, to the gain of parametric amplifiers for quantum-limited readout. The inductance is either set by tailoring the metal-oxide dimensions of single JJs, or magnetically tuned by parallelizing multiple JJs in superconducting quantum interference devices (SQUIDs) with local current-biased flux lines. JJs based on superconductor-semiconductor hybrids represent a tantalizing all-electric alternative. The *gatemon* is a recently developed transmon variant which employs locally gated nanowire superconductor-semiconductor JJs for qubit control [1,2]. Here, we go beyond proof-of-concept and demonstrate that semiconducting channels etched from a wafer-scale two-dimensional electron gas (2DEG) are a suitable platform for building a scalable gatemon-based quantum computer [3]. We show 2DEG gatemons meet the requirements by performing voltage-controlled single qubit rotations and two-qubit swap operations. We measure qubit coherence times up to ~2 μs, limited by dielectric loss in the 2DEG host substrate.


*This work was supported by Microsoft Project Q, the U.S. Army Research Office, the Innovation Fund Denmark, the Danish National Research Foundation, and the Villum Foundation.

4:18PM H62.00004: Quantum computing with driven-dissipative Josephson circuits

[Invited] ZAKI LEGHTAS (Presenter), Mines ParisTech / ENS Paris — Superconducting qubits are one of the most promising platforms to implement quantum technologies. Quantum processors of tens of qubits are now available, and exciting applications with these intermediate size systems are in perspective. However, many algorithms, including all those with a proved quantum speed-up, require extremely low error rates. This will most likely require quantum error correction (QEC). Unfortunately, current QEC architectures require daunting overheads in physical qubits and control electronics. The goal of this research is to reduce this overhead, and our approach is based on two key ideas. First, we use high Q resonators to redundantly encode quantum information. Second, we engineer non-linear dissipation to protect and manipulate this information.
4:54PM H62.00005: A programmable superconducting quantum processor with three all-to-all coupled qubits*

[Invited] TANAY ROY (Presenter), SUMERU HAZRA, SUMAN KUNDU, MADHAVI CHAND, ANIRBAN BHATTACHARJEE, KISHOR SALUNKHE, MEGHAN P. PATANKAR, KEDAR DAMLE, RAJAMANI VIJAYARAGHAVAN, Department of Physics, TATA INSTITUTE OF FUNDAMENTAL RESEARCH — Quantum information processing (QIP) exploits the laws of quantum mechanics to enhance computational capabilities beyond the limits of classical algorithms. Among various platforms for realizing QIP, superconducting qubits are at the forefront as they offer an unparalleled combination of good coherence, fast gates, and design flexibility. A majority of recent experimental demonstrations in the superconducting architecture have utilized transmon-like qubits and transverse inter-qubit coupling for implementing small quantum algorithms. Nevertheless, efficient universal quantum computing has remained a challenge due to the limited connectivity and access to only two-qubit entangling gates. This results in reduced performance due to inefficient implementation of quantum algorithms. In this talk, I will introduce “trimon” [1], a three-qubit device based on a multi-mode superconducting circuit providing strong inter-qubit coupling and access to three-qubit native gates. I will discuss the basic working principles of the device, implementation of generalized controlled-controlled-NOT gates and universal programmability of the processor [2]. Next, I will demonstrate the high-fidelity preparation of various two- and three-qubit entangled states and implementation of a few quantum algorithms [3] like Deutsch-Jozsa, Grover’s search and the quantum Fourier transform. Finally, I will talk about the possibility of scaling to larger systems using the trimon as a building block to achieve improved qubit-qubit connectivity in medium-scale quantum processors.

References:

*Funding provided by Department of Atomic Energy, Govt. of India

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H63 DBIO: Physics of Microbiomes and Microbial Communities II BCEC 259A - Raghuveer Parthasarathy, University of Oregon - Tag(s): Focus

2:30PM H63.00001: Modeling the influence of metabolic trade-offs on microbiota diversity* [Invited] NED WINGREEN (Presenter), Princeton University — Metagenomics has revealed huge diversity in nature, with thousands of microbial species coexisting in microbiota. However, classical resource-competition models predict that the number of species in steady coexistence cannot exceed the number of resources. To investigate the role of environmental conditioning and trade-offs in promoting diversity, we physically modeled the population dynamics of microbes that compete for resources in a chemostat. The model reproduces several notable features of natural ecosystems, including high diversity, keystone species, and characteristics of neutral theory, despite an underlying non-neutral competition for resources. Do metabolic trade-offs still promote diversity if nutrient supplies vary in time or if populations are spatially structured? The answer is yes in both cases. Serial dilutions preserve diversity, but with a surprising non-monotonic dependence on nutrient supply. Spatial structure selects one diverse solution, rather than a degenerate set. Importantly, we find that temporal or spatial variation permit diversity even when trade-offs are only approximate.

*This work was supported in part by the National Institutes of Health Grant R01 GM082938 and in part by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030).
3:06PM H63.00002: The motility can drive spatial exclusion and promote coexistence in bacterial populations
ERCAG PINCE (Presenter), Department of Living Matter, AMOLF, SEBASTIAN GÜDE, Quantitative Biology, UC Berkeley, KATJA M. TAUTE, Rowland Institute at Harvard, TOM S SHIMIZU, SANDER J TANS, Department of Living Matter, AMOLF — Bacterial cells encountered in nature rarely live in isolation, they share and compete for space and nutrients with cohabitant microbial communities. They are also known to explore their surroundings and exhibit motility. Despite the ubiquity of motile phenotypes, the fundamental role of bacterial dispersal in the formation of diverse microbial communities and coexistence in spatial habitats have not been elucidated. In this study, we investigated the motility-driven competition for resources between two strains resulting in strong negative frequency-dependent-selection, i.e. each strain becomes fitter than the other when low in frequency. The observed lack of competitive exclusion is a direct consequence of the active segregation: few fast movers can forage and rapidly colonize in virgin territories of the habitat whereas few fast-grower cells can proliferate at the initial contact position. We showed that the coexistence breaks down when the initial contact area is as large as the habitat size or the nutrients become available homogeneously. Our findings demonstrate that motility can foster coexistence between bacterial populations displaying growth-dispersal trade-off in competition for nutrients and space.

3:18PM H63.00003: Single cell segmentation in microbiome imaging* HAO SHI (Presenter), Department of Physics, Cornell University, IWJN DE VLAMINCK, Meining School of Biomedical Engineering, Cornell University — Microbes in nature often live in communities with intricate spatial organization. Recent developments in molecular barcoding strategies and confocal spectral imaging have enabled spatially resolved and highly multiplexed phylogenetic measurements in these communities. However, quantitative analysis of these information-rich imaging dataset remains difficult, primarily due to bottlenecks in accurate single cell segmentation. Here, we present our approach to segment spectral images of environmental microbiome using information contained in the neighborhood of each voxel. We will discuss preliminary segmentation results and quantitative analysis of the spatial organization of microbial communities at the single cell level.

*This work is funded by the Noyce Foundation and a National Institute of Health Director's New Innovator Award.

3:30PM H63.00004: Community coexistence and stability: insights from a mediator-explicit model of microbial interactions* SANDRA DEDRICK, SAMANTHA DYCKMAN, BABAK MOMENI (Presenter), Boston College — Communities of interacting microbes impact our health and environment. For example, microbes in our gut microbiota can collectively (but not as individual species) confer resistance against pathogen colonization. How species form a community is thus an important question for maintaining or manipulating human-associated communities for improved health outcomes.

We formulate and experimentally constrain a model that explicitly incorporates chemical compounds (e.g. metabolites or waste-products) that can mediate microbial interactions. In a continuous-growth setting where resources are supplied (similar to a bioreactor or gut microbiota), our model highlights facilitation and self-restraint as interactions that contribute to coexistence. We show that when interactions are strong, coexistence and stability are determined primarily by the topology of facilitation and inhibition influences and not the strengths of influences. Importantly, we show that consumption of chemical mediators moderates interaction strengths and promotes coexistence. Our results offer insights into how to build or restructure microbial communities of interest.

*This work is supported by an Award for Excellence in Biomedical Research from the Smith Family Foundation.

3:42PM H63.00005: Examining Pairwise and Multi-Species Interactions in Larval Zebrafish* EDOUARD HAY (Presenter), DEEPIKA SUNDARRAMAN, Physics, University of Oregon, DYLAN MARTINS, DREW SHIELDS, KAREN GUILLEMIN, University of Oregon, RAGHUVEER PARTHASARATHY, Physics, University of Oregon — The microbial communities resident in animal intestines are composed of dozens to hundreds of species and play important roles in host health and disease. The determinants of microbial composition, which may include physical characteristics or biochemical interactions, remain largely unknown. Further, it is unclear for many multi-species consortia whether their species-level makeup can be predicted based on an understanding of pairwise species interactions, or whether higher-order interactions are needed to explain community assembly. It is also unclear how spatial organization plays a role in determining the make up of these complex communities.

To address this, we consider commensal intestinal microbes in larval zebrafish, initially raised germ-free to allow introduction of controlled combinations of bacterial species. Using a combination of dissection and plating assays and 3-dimensional live imaging, we demonstrate the construction of communities of 1 to 5 species and test whether outcomes from 2-species competitions contain enough information to predict the abundances in more complex communities. We also quantify changes in species' spatial distributions induced by the presence of other species, which may explain correlations in their abundances.

*NSF, NIH, Kavli Foundation.
RACHEL MOK, BOYA SONG, DOMINIC SKINNER, Massachusetts Institute of Technology, JEFFREY OISHI, Bates College, JORN 4:18PM H63.00008: Nonlinear rheological behaviour of bacterial biofilms*

In this study, we focus on the rheological properties of bacterial biofilms at multiple scales in determining the architectures of biofilms in flow. This is achieved by examining the interactions that generate Vibrio cholerae biofilm morphologies. Our results demonstrate the importance of dynamics at the intersections between biofilm architectures and mechanical processes including cell growth, cell-cell interactions within the embedded matrix. Biofilm architectures are sculpted by mechanical processes including cell growth, cell-cell interactions and external forces. Using single-cell live imaging in combination with simulations we characterize the cell-cell and cell-flow interactions that generate Vibrio cholerae biofilm morphologies. Our results demonstrate the importance of dynamics at multiple scales in determining the architectures of biofilms in flow.

*The work is supported by Engineering and Physical Sciences Research Council (UK) award EP/K039083/1 to Newcastle University.

4:06PM H63.00007: Emergence of order and structure in biofilms growing in fluid shear PHILIP PEARCE (Presenter), Massachusetts Institute of Technology, RAIMO HARTMANN, PRAVEEN SINGH, Max Planck Institute for Terrestrial Microbiology, RACHEL MOK, BOYA SONG, DOMINIC SKINNER, Massachusetts Institute of Technology, JEFFREY OISHI, Bates College, JORN DUNKEL, Massachusetts Institute of Technology, KNUT DRESCHER, Max Planck Institute for Terrestrial Microbiology — In many situations bacteria aggregate to form biofilms: dense, surface-associated, three-dimensional structures inhabited by cells. Situations bacteria aggregate to form biofilms. We present a physical model to a phenomenon prone to misinterpretation by invoking chemotaxis or quorum sensing.

THOMAS P. CURTIS, JINJU CHEN, School of Engineering, Newcastle University — Mechanical robustness is a hallmark of many bacterial biofilms. Traditionally, these have been characterised in the small strain limit. Rheological studies in the large strain limit are extremely rare and are presumably of interest in various industrial and biomedical scenarios. We perform Large amplitude oscillatory shear (LAOS) on three species of bacterial biofilms: Bacillus subtilis, Comamonas denitrificans and Pseudomonas fluorescens. Our results show a distinct variation in intra-cycle strain stiffening/shear thickening indices and the yield characteristics of the Pipkin space for each of the individual species. Furthermore, mixing two strains of microbes; we study the variation in rheological measures (in Pipkin space) of dual species biofilms and compare them with the single species biofilms. This study builds towards an understanding of the rheological characteristics of multi-species biofilms: starting from a single species perspective, followed by mixtures of microbial species and in the future by using an artificial community which is representative of a microbiome (e.g. wastewater treatment plant).

4:18PM H63.00008: Nonlinear rheological behaviour of bacterial biofilms* SAIKAT JANA (Presenter), SAM CHARLTON, THOMAS P. CURTIS, JINJU CHEN, School of Engineering, Newcastle University — Mechanical robustness is a hallmark of many bacterial biofilms. Traditionally, they have been characterised in the small strain limit. Rheological studies in the large strain limit are extremely rare and are presumably of interest in various industrial and biomedical scenarios. We perform Large amplitude oscillatory shear (LAOS) on three species of bacterial biofilms: Bacillus subtilis, Comamonas denitrificans and Pseudomonas fluorescens. Our results show a distinct variation in intra-cycle strain stiffening/shear thickening indices and the yield characteristics of the Pipkin space for each of the individual species. Furthermore, by mixing two strains of microbes; we study the variation in rheological measures (in Pipkin space) of dual species biofilms and compare them with the single species biofilms. This study builds towards an understanding of the rheological characteristics of multi-species biofilms: starting from a single species perspective, followed by mixtures of microbial species and in the future by using an artificial community which is representative of a microbiome (e.g. wastewater treatment plant).

4:30PM H63.00009: Role of confinement in growing bacterial colonies ZHIHONG YOU (Presenter), Leiden University, DANIEL PEARCE, University of Geneva, LUCA GIOMI, Leiden University — Bacterial colonies are abundant in biological and artificial environments, and they are frequently subject to various types of confinement. Yet, the role of confinement, especially from the mechanical perspective, is still not clear. Here, using molecular dynamics simulations and continuum modelling, we demonstrate that the combination of confinement and growth gives rise to strongly anisotropic stress, resulting in the emergence of global nematic order.

4:42PM H63.00010: Mechanical interactions in growing yeast colonies ANDREA GIOMETTO (Presenter), DAVID R. NELSON, ANDREW MURRAY, Harvard University — Microbial populations often assemble in dense populations in which proliferating individuals exert mechanical forces on the nearby cells. Here, we use yeast strains whose doubling times depend differently on temperature to show that physical interactions among cells affect the competition between different genotypes in growing yeast colonies. Our experiments demonstrate that these physical interactions have two related effects: they cause the prolonged survival of slower-growing strains at the actively-growing frontier of the colony and cause faster-growing strains to increase their frequency more slowly than expected in the absence of physical interactions. These effects also promote the survival of slower-growing strains and the maintenance of genetic diversity in colonies grown in time-varying environments. The three-dimensional structure of these colonies reflects the history of the environments experienced by the colonies, and the survival of strains depends on the geometry of the colony perimeter. A continuum model inspired by overdamped hydrodynamics reproduces the experiments and predicts that the strength of natural selection depends on the width of the actively growing layer at the colony frontier. We verify these predictions experimentally.
**4:54PM H63.00011: Dynamic self-organization of microorganisms far from equilibrium**  
ROUJIN GHAFFARI (Presenter), SEZIN GALIGOLU, UNAM, Bilkent University, EVREN DORUK ENGIN, Institute of Biotechnology, Ankara University, SERIM ILDAY, UNAM, Bilkent University — We report ultrafast laser-induced dynamic self-organization of quasi-2D confined solutions of *e.coli, m.luteus, s.cerevisiae*, and *p.aeruginosa* far from equilibrium. The laser beam has no interaction with the microorganisms; it only creates thermal gradient-induced convective flows in their growth medium. By precisely controlling these flows, we have been able to form aggregates with predetermined sizes and geometries, and manipulate the adaptive behavior of microorganisms under ‘noisy’ environments. We further demonstrate if and how these microorganisms can withstand harsh physical conditions. Last, we showcase separation of gram positive and gram negative bacteria from an initially homogenous mix.

**5:06PM H63.00012: Effect of cellular and environmental conditions on bacterial collective oscillation**  
SONG LIU (Presenter), YILIN WU, The Chinese University of Hong Kong — Collective oscillation in biology is ubiquitous and often arises from coupling between individual oscillators in phase space. Previously, we discovered a novel type of collective oscillatory motion in bacterial suspensions, which arises from weak synchronization and diffusive coupling between random trajectories but does not require individual oscillators. However, it is unclear what determines the intrinsic oscillation frequency in the system. Here we manipulate the cellular and environmental conditions to systematically to identify potential factors controlling the oscillation frequency. Our results will provide necessary information to fully understand the collective oscillatory motion and suggest new directions for active matter engineering.

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**Tuesday, March 5, 2019 2:30 PM - 5:30 PM**

**Session H64 DBIO GSOFT: Physics of the Cytoskeleton Across Scales III**

**2:30PM H64.00001: Nonlinear microscale mechanics and macromolecular mobility of tunable cytoskeleton composites**  
RAE ROBERTSON-ANDERSON (Presenter), Physics and Biophysics, University of San Diego — Actin and microtubules are two key protein filaments that comprise the cytoskeleton, enabling cells to exhibit multifunctional nonlinear mechanics. However, it remains an open question as to how the structure, interactions, and dynamics of these proteins map to the nonlinear and non-equilibrium mechanics that the cytoskeleton exhibits. We address this open problem by using a robust approach that combines: tunable in vitro cytoskeleton networks, rheology that spans from molecular to mesoscopic scales, and single-molecule transport and mobility measurements. Specifically, we use optical tweezers microrheology to characterize the nonlinear mechanics of cytoskeleton networks while simultaneously using fluorescence microscopy and particle-tracking to determine macromolecular mobility and network stress propagation. To directly map network properties to stress response, we perform measurements using custom-designed in vitro networks of actin and microtubules with structural properties and interactions that can be precisely tuned. I will describe these methods as well as our recent intriguing results that demonstrate the elegant couplings that can emerge between network structure, stress response, and macromolecular mobility in cytoskeleton networks.

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*This work was supported by: a Scialog Collaborative Innovation Award #24192 from Research Corporation and Gordon & Betty Moore Foundation, an NSF CAREER Award #1255446; an NIH NNIGMS Award #R15GM123420; and a W.M. Keck Foundation Research Award.*
3:06PM H64.00002: Reconstitution of basic mitotic spindles in cell-like confinement  [Invited]  MARILEEN DOGTEROM (Presenter), Bionanoscience, TU Delft — Bipolar organization of the mitotic spindle is the result of forces generated by dynamic microtubules and associated proteins in interaction with chromosomes and the cell boundary. Biophysical experiments on isolated spindle components have provided important insights into the force-generating properties of different components, but a quantitative understanding of the force balance that results from their concerted action is lacking. Here we present an experimental platform based on water-in-oil emulsion droplets that allows for the bottom-up reconstitution of basic spindles. We find a typical metaphase organization, where two microtubule asters position symmetrically at moderate distance from the mid-zone, is readily obtained even in the absence of chromosomes. Consistent with simulations, we observe an intrinsic repulsive force between two asters that can be counterbalanced alternatively by cortical pulling forces, anti-parallel microtubule crosslinking, or adjustment of microtubule dynamics, emphasizing the robustness of the system. Adding motor proteins that slide anti-parallel microtubules apart drives the asters to maximum separation, as observed in cells during anaphase. Our platform offers a valuable complementary approach to in vivo experiments where essential mitotic components are typically removed, instead of added, one by one.

3:42PM H64.00003: Revealing Cytoskeletal Dynamics and Avalanches via Active Micropost Arrays*  YU SHI (Presenter), KATHERINE XIAN, SHANKAR SIVARAJAN, Department of Physics and Astronomy, Johns Hopkins University, CHRISTOPHER L PORTER, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, DANIEL H REICH, Department of Physics and Astronomy, Johns Hopkins University, JOHN CROCKER, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — The cytoskeleton is critical for a wide range of cellular behavior, including motility, morphology, and mechanotransduction. However, understanding of the connections between molecular-scale processes and cell-scale dynamics is not complete. Here we present results using poly(dimethylsiloxane) active micropost array detectors (AMPADs) with embedded magnetic actuators to measure the fluctuations and local rheology of cells’ actomyosin stress fiber network and cortex in detail. We find that both structures display consistent power law rheology, along with highly heterogeneous and intermittent fluctuations. Notably, the fluctuating motion is dominated by large step-like displacements, resembling the dynamics observed in avalanches and earthquakes. The effects of substrate stiffness and geometry will also be discussed. Our results imply that actomyosin contractile units act in a highly collective manner and that cellular actomyosin networks self-organize into marginally stable plastic networks whose properties influence the biomechanical behavior of cells.

*Supported in part by NIH grant 1R01HL127087

3:54PM H64.00004: A model of sliding and stalling in microtubule bundles  SHANE FIORENZA (Presenter), MATT GLASER, M. BETTERTON, University of Colorado, Boulder — Microtubules, motor proteins, and crosslinkers self-assemble a variety of cytoskeletal networks within the cell. Minimal systems of two antiparallel microtubules, kinesin-4 motors, and PRC1 crosslinkers reconstitute controlled sliding and stalling, leading to stable antiparallel overlaps like those seen in the mitotic spindle. Experiments show that the final overlap length and initial sliding velocity are both linearly proportional to the two microtubules’ initial overlap length. However, the mechanisms behind this length-sensing are not fully understood. We develop a model to show how crosslinker-motor interactions produce these regulated microtubule overlaps. We observe sliding even when motors exert no direct forces on neighboring microtubules due to purely steric interactions. Direct binding interactions between crosslinkers and motors can significantly increase the lifetime of the final overlap.
How actin dynamics affect membrane nanotube mechanics

ANTOINE ALLARD (Presenter), FLAVIEN BRETTE, ALEXANDRE DESLYS, Curie Institute, GUILLAUME LAMOUR, Université d'Évry Val d'Essonne, FABRICE VALENTINO, Curie Institute, TIMO BETZ, Münster University, CLÉMENT CAMPILLO, Université d'Évry Val d'Essonne, CÉCILE SYKES, Curie Institute — The living cell is an out-of-equilibrium system that constantly remodels its architecture to ensure biological functions such as division or intracellular transport. The latter involves the formation of intermediate cylindrical membrane nanotubes. These nanotubes are then split into membrane compartments transported in other areas of the cell. Whereas mechanics of pure membrane nanotubes are now well understood, the role of the actin cytoskeleton on tube stability remains unclear.

To address this question, we develop a bottom-up approach based on model lipid membranes on which we reconstitute actin assembly with a minimal number of proteins. Two distinct methods allow us to reproduce the in vivo cylindrical membrane geometry. First, nanotubes are pulled from vesicles with optical tweezers. Second, lipid deposits are brushed and characterized by atomic force microscopy. We finally observe the formation of an actin muff that proves successful activation of actin network growth around the tube.

Both methods allow us to derive the viscoelastic properties of the muff. For example, tubes surrounded by the muff retract slowly (3.5 s) compared to pure membranes (< 0.5 s). A striking observation is that tube radius decreases in the presence of actin and may initiate further scission.

Tuning Migratory and Cytoskeletal Response of Cells to Texture with Collagen-IV Coating*

MATT J. HOURWITZ (Presenter), JOHN T FOURKAS, Department of Chemistry and Biochemistry, University of Maryland-College Park, WOLFGANG LOSERT, Department of Physics, University of Maryland-College Park — Cell migration is vital for many physiological processes, both beneficial and detrimental. Actin is a cytoskeletal protein scaffold that assembles and disassembles to accomplish cell motion in a specific region and direction. A stimulus must be provided to influence guided cellular motion. In addition to biochemical signals, physical cues such as the texture of the environment also provide a guiding stimulus. To better understand how cytoskeletal and migratory processes integrate biochemical information with texture information, we studied actin dynamics and migration of MCF10A cells, an immortalized human breast epithelial cell line, on 3D nanotopographical surfaces. We systematically varied the coating with collagen IV, a basement membrane protein representing key biochemistry of the local ECM. Preliminary studies show that the response of actin to surface texture significantly depends on collagen coating concentration.

Acknowledgements: This work was performed in collaboration with Carole Parent, Stan Lipkowitz, and Christina Stuelten.

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Microrheology of Microtubule-Actin-Vimentin Composite Cytoskeletal Networks*

YINAN SHEN (Presenter), MARJAN SHAYEGAN, Department of Physics & SEAS, Harvard University, ARTURO MONCHO, Department of Applied Physics & Institute Carlos I for Theoretical and Computational Physics, University of Granada, HUI LI, Institute of Physics, Chinese Academy of Sciences, HUAYIN WU, WEICHAO SHI, Department of Physics & SEAS, Harvard University, SONGLEI LIU, Harvard Medical School, Harvard University, JING XIA, DIANZHUO WANG, LIHENG CAI, MENG ZHANG, RUIHUA DING, Department of Physics & SEAS, Harvard University, FREDERICK MACKINTOSH, Chemistry, Physics and Astronomy & Chemical and Biomolecular Engineering, Rice University, DAVID A WEITZ, Department of Physics & SEAS, Harvard University — Mechanics of the cytoskeleton is known to be responsible for maintaining cell mechanical integrity and determining cellular functions. We develop a method that enables us to reconstruct a three-component in-vitro network composed of intermediate filaments (vimentin filaments), microtubules and F-actin filaments, which are three fundamental cytoskeletal components. This composition is more physiologically relevant compared with any of the previously reconstituted cytoskeletal networks, which are composed of one or two components only. We investigate the structure and mechanical properties of this multicomponent cytoskeletal network using a combination of several microscopies and microrheology. We show that vimentin filaments couple the other cytoskeletal filaments together by introducing steric constraints between cytoskeletal polymers; these inter-network interactions extend the composite network elastic behavior to a longer time scale, prolong the network relaxation time, and facilitate the stress propagation within the network. These findings are helpful to deepen our understanding of the mechanical role vimentin plays in regulating cellular activities.

*NIH grant 2P01GM096971
4:42PM H64.00008: Maximal entropy production rates in non-contractile actomyosin* DANIEL S. SEARA (Presenter), VIKRANT YADAV, IAN LINSMEIER, PASHA TABATABAI, Yale Univ, PATRICK W. OAKES, University of Rochester, ALI TABELI, University of Northern Iowa, SHILADITYA BANERJEE, University College London, MICHAEL MURRELL, Yale Univ — The actin cytoskeleton is an active semi-flexible polymer network whose non-equilibrium properties coordinate both stable and contractile behaviors to maintain or change cell shape. While myosin motors drive the actin cytoskeleton out-of-equilibrium, the role of myosin-driven active stresses in stable states of actomyosin is unclear. To investigate this, we synthesize an actomyosin material in vitro whose active stress content can tune the network from stable to contractile and analyze the resulting filament dynamics using the framework of stochastic thermodynamics. We find that the entropy production rate does not increase monotonically with myosin content, but instead is maximized in a non-contractile, stable state. Our study provides evidence that the origins of system entropy production and activity-dependent dissipation relate to disorder in the molecular interactions between actin and myosin.

*DSS acknowledges support from NSF Fellowship grant # DGE1122492. MM acknowledges funding from NSF CMMI-1525316, ARO MURI W911NF-14-1-0403, NIH RO1 GM126256, and NIH U54 CA209992. SB acknowledges Strategic Fellowship support from the University College London, and funding from Royal Society and Tata grant # URF/R1/180187.

4:54PM H64.00009: Actively crosslinked microtubule networks: mechanics, dynamics and filament sliding SEBASTIAN FUERTHAUER (Presenter), CCB, Flatiron Institute, BEZIA LEMMA, UCSB, PETER FOSTER, MIT, STEPHANIE C EMS-MCCLUNG, CLAIRE E WALCZAK, Indiana University, ZVONIMIR DOGIC, UCSB, DANIEL NEEDLEMAN, Harvard University, MICHAEL JOHN SHELLEY, CCB, Flatiron Institute — Cellular components such as cytoskeletal filaments and motors are the essential constituents of a new class of materials: so called active fluids. While much progress has been made in understanding these systems using experiments and phenomenological theories, deriving rigorous theoretical description from microscopic considerations remains a challenge. We present experiments and theory on a system of stabilized microtubules driven by the molecular motor protein XCTK2. Through photobleaching experiments, we demonstrate that in this system microtubules are aligned along the long direction of the system and travel through the gel at a velocity independent of the local average polarity. We show that this result is most naturally understood in the frameworks of an active gel theory that goes beyond pairwise microtubule interactions and treats the gel as highly cross-linked. Our theory bridges the length scales from the microscopic mechanical behavior of motor-filament interactions to the large scale behavior of the active gel and generalizes to describe different kinds of cytoskeletal assemblies.

5:06PM H64.00010: Particle delivery using bead-loading gives insight into heterogeneity of the cellular cytoplasm* WENLONG XU (Presenter), ASHOK PRASAD, Chem & Bio Engr, Colorado State University — Microrheology is an important technique for probing the properties of the cytoplasm, but requires particle delivery inside cells. Here we report a particle delivery method based on a method of protein delivery called bead-loading, requiring no specialized instruments. Bead loading is able to deliver 100nm fluorescent particles that are widely dispersed into the cellular cytoplasm. Particle tracking reveals that the fluorescent particles probe two very different regions of the cytoplasm. One set of beads are significantly confined, and treatment by drugs indicate that the confinement is due to the actin cytoskeleton. The second set of beads seemingly display free diffusion, but ATP depletion experiments show that the motion has an actively driven component. Most strikingly, the main effect of most drug treatments is through changing the relative distribution of these two populations. Our analysis suggests that the specific mode of particle delivery may be strongly affecting the measured properties of cells, underlining the importance of intracellular heterogeneity. The general applicability of our particle delivery technique and the distribution of intracellular movement were confirmed in three different cell lines.

*We acknowledge support from NSF CAREER grant (PHY-1151454)
strengths and degrees of shape frustration for which these behaviors are possible. We also show how depolymerization can be prevented or even arrested in-progress (the latter allowing rescue and regrowth) by the presence of even very few GTP-tubulin dimers, and explore the ranges of binding interaction hypothesized as a part of microtubule dynamics, drive depolymerization via the unpeeling "ram's horns" consistent with tubulin, we demonstrate that conformational changes in subunits that frustrate tubulin binding, which have long been understood. Using molecular dynamics simulations of whole microtubules built from a new coarse-grained model of GTP-tubulin dimers (tubulin bound to GTP), but hydrolysis of GTP- to GDP-tubulin within the tubules eventually destabilizes them toward catastrophically-fast depolymerization, if the leading cap of GTP-tubulin is lost. The molecular mechanisms and features of the individual tubulin proteins that drive such apparently contradictory behavior are still not well-understood. Using molecular dynamics simulations of whole microtubules built from a new coarse-grained model of tubulin, we demonstrate that conformational changes in subunits that frustrate tubulin binding, which have long been hypothesized as a part of microtubule dynamics, drive depolymerization via the unpeeling "ram's horns" consistent with experiments. We also show how depolymerization can be prevented or even arrested in-progress (the latter allowing rescue and regrowth) by the presence of even very few GTP-tubulin dimers, and explore the ranges of binding interaction strengths and degrees of shape frustration for which these behaviors are possible.

**Tuesday, March 5, 2019 2:30 PM - 5:30 PM**

**Session H65 DBIO: Controlling Cells with Electric Fields**

**BCEC 260 - Wolfgang Losert, University of Maryland, College Park**

Tag(s): Focus

**2:30PM H65.00001: Controlling the intracellular dynamics of neuronal model systems**

KATE M O’NEILL (Presenter), University of Maryland, College Park — Excitable tissues in the body have unique properties that allow for the transfer of information between individual cells and across larger scales. For example, recent work has investigated the spatiotemporal dynamics of electrical activity propagation in neural and cardiac tissues in both in vivo and in vitro settings. In the present work, we study how the intracellular behavior of in vitro cultures of primary rat cortical neurons can be tuned and controlled with electric fields. However, in addition to the effects on electrical signal propagation that are traditionally studied, we are also interested in the morphological responses of neurons to these electric fields with the goal of understanding the interaction between electrical activity propagation and cytoskeletal dynamics, particularly of actin. To accomplish this goal, we do the following: 1) apply electric field stimulation to the in vitro neuronal culture, 2) image changes in transmembrane potential or intracellular actin, and 3) quantify the intracellular response. We show that the dynamics of actin change significantly over time as the structural components of neurons (axons and dendrites) mature and become more stable. Moreover, we show that neurons can be electrically activated by direct current (DC) electric fields, but the degree and complexity of the response to the field strongly depends on the age of the cells with a more prevalent response observed as the neurons (and therefore, synapses) have matured. In sum, we have found that we can tune neuronal cell behavior with electric fields, and in future work, we hope to apply these same perturbations to other cells and make inferences about the intracellular behavior of other electrically excitable cell types.

*K Kate O’Neill was funded by a MURI grant (#FA9550-16-1-0052) to Dr. Wolfgang Losert.

**3:06PM H65.00002: Precisely regulate ERK signaling pathway with local electric fields**

QUAN QING (Presenter), Arizona State University — Our main research interest is to understand how artificial electronics can interact with biological systems. Live cells rely on a big network of signaling pathways that sense and respond to biochemical, electrical and mechanical (BEM) stimuli. We want to explore if we can modulate this BEM network, particularly with external electric field, and investigate the mechanism at the molecular level.

In this presentation I will talk about our recent discovery of modulation of extracellular-signal-regulated kinase (ERK) pathway using alternative current (AC) electric fields (EFs). The amplitude, duration, and frequency of activation of the ERK pathway code diverse spectrum of information at cell, tissue and organism levels to instruct cells to migrate, proliferate, or differentiate. Synchronized control of ERK activation would provide a powerful approach to regulate cell behaviors. Here we show for the first time that AC EFs in a new frequency range can reproducibly activate ERK activities through patterned local microelectrodes with single-cell resolution. Both the amplitude and frequency of ERK activation can be precisely synchronized and modulated. We pinpointed a new mechanism of AC EF induced highly specific phosphorylation of epidermal growth factor (EGF) receptor (EGFR) to activate the EGFR-ERK pathway, which may serve as a powerful platform for control of cell behaviors with implications in wide range of biomedical applications.

*We acknowledge the support by the Air Force Office of Scientific Research under award number FA9550-16-1-0052, and the support by the National Institute of Biomedical Imaging and Bioengineering of the National Institutes of Health under award number R21EB020822.
The complete understanding of contact guidance, chemotaxis and electrotaxis may be obtained. By investigating and analyzing the actin cytoskeleton as an excitable system, a more controlled manner, to understand better immune responses. Specifically, we are studying in the cells' intracellular scaffolding, chemical gradients and endogenous electric fields guides cells to the site of inflammation. However, mimicking this system in vitro has not been previously explored. In this work, we combine the above guidance cues artificially, and in a temporally scaled fashion, to understand the emergence of various, driven phenomena, from schooling behavior in fish to electrical network dynamics in neurons and cardiomyocytes. On a tissue scale, these collective dynamics often arise in response to changes in the extracellular and intracellular environment. In this talk, we describe the collective signaling of HEK293T/17 cells modified to express sodium and potassium ion channels that form electrically-active monolayers. We investigate the collective firing dynamics across multiple spatio-temporal scales in these cell sheets in a highly-controlled fashion in order to understand the emergence of various, driven electrical wave morphologies and propagation dynamics. To accomplish this goal, we apply electrical and optical perturbations utilizing a novel optical system—a Multi-Scale Microscope—that allows for simultaneous imaging across two different spatial scales using epifluorescence and rescan confocal imaging techniques.

*This material is based on work supported by MURI grant AFOSR MURI FA9550-16-1-0052 and student funding by the National Science Foundation COMBINE-NRT Program under Grant No. DGE-1632976.

3:54PM H65.00004: Investigating wave morphodynamics in electrically active cell sheets

PHILLIP ALVAREZ (Presenter), Biophysics, University of Maryland, College Park, SYLVESTER J GATES III, Institute for Physical Science and Technology, University of Maryland, College Park, SAMIRA AGHAYEE, Biophysics, University of Maryland, College Park, KATE M O'NEILL, Institute for Physical Science and Technology, University of Maryland, College Park, GABRIEL FRANK, Life Sciences, Ben-Gurion University of the Negev, WOLFGANG LOSERT, Physics, University of Maryland, College Park — Biological systems exhibit many emergent phenomena, from schooling behavior in fish to electrical network dynamics in neurons and cardiomyocytes. On a tissue scale, these collective dynamics often arise in response to changes in the extracellular and intracellular environment. In this talk, we describe the collective signaling of HEK293T/17 cells modified to express sodium and potassium ion channels such that they form electrically-active monolayers. We investigate the collective firing dynamics across multiple spatio-temporal scales in these cell sheets in a highly-controlled fashion in order to understand the emergence of various, driven electrical wave morphologies and propagation dynamics. To accomplish this goal, we apply electrical and optical perturbations utilizing a novel optical system—a Multi-Scale Microscope—that allows for simultaneous imaging across two different spatial scales using epifluorescence and rescan confocal imaging techniques.

*AFOSR grant number FA9550-16-1-0052

4:06PM H65.00005: Electric-Field Manipulation of a Cell-Free Gene Expression Reaction

ALEXANDRA TAYAR (Presenter), Physics, University of California Santa Barbara, YUVAL EFRAT, SHIRLEY SHULMAN DAUBE, MICHAEL LEVY, ROY H BAR-ZIV, Weizmann Institute of Science — Biological systems are regulated dynamically to respond to external environmental perturbations, and change their internal state as a result. Introducing controlled dynamical perturbations in minimal systems can provide insight into these processes. Currently, small biomolecular inducers are commonly used, yet applying these inducers locally and dynamically to compartmentalized micron-scaled reactions remains challenging. Here, we report on a DNA compartment fabricated in silicon and connected to thin electrodes, capable of external control of cell-free protein synthesis under steady-state conditions. We demonstrate manipulation of RNA polymerase, ribosomes and GFP in a nonuniform electrical field, using dielectrophoresis (DEP). We show local depletion of nutrients and machinery in an active gene expression reaction at physiologically relevant conditions. The response to the applied field is rapid at the scale of expression dynamics, and spatially confined thereby establishing spatiotemporal resolution of electric field control of gene expression.

*This work was supported by grants from the Israel Science Foundation, The Minerva Foundation, Office of Naval Research. A.M. Tayar thanks the Clore Foundation for a doctoral fellowship.

4:18PM H65.00006: Characterizing electrotaxis for control of cellular migration

TOM ZAJDEL (Presenter), DANIEL COHEN, Princeton University — It is well established that bioelectric fields arise during morphogenetic processes across many cell types, influencing development, metastasis, and wound healing. Many cell types use endogenous electric fields as a cue to guide cell migration in a process known as electrotaxis. While electrotaxis presents a tremendous opportunity for remote electronic control of cell migration, a formal physical approach exploring the limits and plasticity of this guided migration has not been conducted. In this work, we examine the input/output dynamics of electrotaxis in MDCK epithelial cell sheets, using rapid prototyping techniques to produce a versatile, reconfigurable platform capable of applying a programmable electric field to tissues. We modulate stimulation current density and duty cycle to probe the electrotaxis impulse and step responses. We also use live fluorescence imaging in labeled cell lines to characterize the biophysical response of the cytoskeleton during electrotaxis, which generates force during cell migration. Because collective cell migration is crucial to multicellular form and function, tools for reliable control would be invaluable for further studies of the biophysical processes underlying tissue development, wound healing, and other multicellular programs.
4:30PM H65.00007: Design considerations for high-performance dielectrophoretic devices  ZACHARY KOBOS (Presenter), SHARI YOSINSKI, AYASKA FERNANDO, MARK A REED, Yale Univ — Dielectrophoresis (DEP) uses electric field gradients to trap and manipulate the position of particles in solution. The DEP force does not require direct contact with the particle nor the use of any form of labelling mechanism, making it an attractive candidate for manipulation of cells for biological applications. Performing dielectrophoresis in high-conductivity solutions, such as physiological samples, presents significant challenges for the force magnitude, power delivery, and device integrity. We present a coherent set of circuit-level design principles for optimizing electrode geometry for enhanced performance in high-conductivity environments. Investigations of the influence of various design parameters on the DEP force are performed by monitoring changes in the equilibrium velocity, as DEP competes with the Stokes force during fluid flow.

4:42PM H65.00008: Large-scale Actin Wave Patterns Perturbed by Electric and Mechanical Cues in Giant Dictyostelium discoideum* QIXIN YANG (Presenter), Department of Physics, University of Maryland, College Park, MATT J. HOURWITZ, Department of Chemistry, University of Maryland, College Park, LEONARD CAMPANELLO, Department of Physics, University of Maryland, College Park, BEDRI SHARIF, PETER DEVROUTES, Department of Cell Biology, Johns Hopkins, School of Medicine, JOHN T FOURKAS, Department of Chemistry, University of Maryland, College Park, WOLFGANG LOSERT, Department of Physics, University of Maryland, College Park — Dictyostelium discoideum(Dd) provides a good system to study actin dynamics guided by extracellular cues such as electric field, mechanical cues and chemical gradients. However, waves in normal Dd extinguish at the boundary and only show confined sections of wave patterns. Here we apply electrofusion to produce giant Dd, a polykaryotic cell which is up to ten times the size of normal Dd. In those cells F-actin waves travel freely across plasma membrane and show large-scale wave patterns independent of boundary effects. We use this system to explore how nanoridges and DC electric fields perturb actin waves on a scale as large as 50 microns.

*This work is funded by the Air Force Office of Scientific Research grant FA9550-16-1-0052

4:54PM H65.00009: Propagation of electrical activity coupled to actin dynamics in electrically active neuron-like cells* SYLVESTER GATES (Presenter), KATE M O'NEILL, PHILLIP ALVAREZ, SAMIRA AGHAYEE, WOLFGANG LOSERT, Institute of Physical Sciences, University of Maryland, College Park — Coupling between excitable systems is a well-known phenomenon. Recent work focused on the excitability of neural and cardiovascular systems has illuminated the dynamics behind electrical signal propagation in these tissues through the use of recording microelectrodes. Other studies have shown that dendritic spines are enriched with dynamic actin at the synapses of electrically-coupled neurons. Here we investigate both electrical activity propagation and actin dynamics in a simple, excitable system: in vitro cultures of human embryonic kidney (HEK-293) cells. This cell line (NK-HEKs) has been engineered to be electrically excitable through the expression of sodium (Na+) and potassium (K+) channels. We electrically stimulate the cells to induce changes in transmembrane potential monitored noninvasively through new, fast-acting voltage sensitive dyes. We simultaneously image actin sodium (Na+) and potassium (K+) channels. We electrically stimulate the cells to induce changes in transmembrane potential monitored noninvasively through new, fast-acting voltage sensitive dyes. We simultaneously image actin dynamics in the same cells using internal fluorophores with the goal of understanding how changes in actin dynamics may drive or be driven by changes in transmembrane potential. Our results suggest that actin fluctuates in response to stimulation in these electrically active cells.

*This work is funded by an AFOSR MURI grant to WL(PI).

5:06PM H65.00010: Escherichia coli's physiology can turn membrane voltage dyes into actuators LEONARDO MANCINI (Presenter), Centre for Synthetic and Systems Biology, University of Edinburgh, Edinburgh, UK, TIANYAN, Biomedical Pioneering Innovation Center (BIOPIC), Peking University, Beijing 100871, China, GUILLAUME TERRADOT, Centre for Synthetic and Systems Biology, University of Edinburgh, Edinburgh, UK, YINGYING PU, YINGXING LI, Biomedical Pioneering Innovation Center (BIOPIC), Peking University, Beijing 100871, China, CHIEN-JUNG LO, Department of Physics and Graduate Institute of Biophysics, National Central University, Jhongli, Taiwan 32001, ROC, FAN BAI, Biomedical Pioneering Innovation Center (BIOPIC), Peking University, Beijing 100871, China, TEUTA PILIZOTA, Centre for Synthetic and Systems Biology, University of Edinburgh, Edinburgh, UK — Bacteria tend to maintain an energy-costly electric potential across the biological membrane. The voltage thus stored can then be reinvested to fuel essential reactions, such as those required for feeding, movement and anabolism. Assays of Nernstian membrane voltage dyes accumulation are arguably the most widespread techniques to quantify such potential. However, interactions of such molecules with the complex cellular environment and physiology are often poorly understood. Here, we characterize the parametrical landscape in which these molecules behave like sensors and where they actually take the role of actuators. We recommend an experimental framework that can be used to characterize Nernstian dyes and we apply it to the characterization of the dye Thioflavin T in E. coli.
CONNER HERNDON (Presenter), FLAVIO FENTON, Georgia Institute of Technology — Proper contraction of cardiac muscle relies on the coordinated propagation of transmembrane voltage. Disturbances of this propagation can result in deadly cardiac arrhythmias such as fibrillation, the manifestation of chaos in the heart. Even in healthy tissue, high heart rates can drive the system to a dynamical instability known as alternans, a period doubling bifurcation in action potential duration (APD) which is strongly correlated with the onset of fibrillation and sudden cardiac death. Much theoretical effort based on the relationship between the APD and preceding diastolic interval (DI) has aimed to suppress the onset of alternans. Results from simulation and theory claim the suppression of alternans under stimulation at a constant DI; however, few experiments have addressed these predictions. In this talk, I will discuss comparative cardiac dynamics in the hearts of species including rabbit, dog, cat, pig, frog, zebrafish, snake, lizard, and alligator through the use of microelectrode recordings and high spatiotemporal resolution optical mapping of fluorescent voltage and calcium signals across the surfaces of hearts. Furthermore, I will discuss my closed-loop control system for performing constant DI stimulation and the highly unexpected results.

*NSF#1446675, NIH#143450

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H66 DBIO GSNP: Inference, Information, and Learning in Biophysics II

Benjamin Machta

2:30PM H66.00001: Reconstructing biological dictionaries: How does neural code translate into behavior?*

DAMIAN HERNANDEZ, Centro Atómico Bariloche, SAMUEL SOBER, ILYA NEMENMAN (Presenter), Emory University — The problem of deciphering how low-level patterns (action potentials in the brain, amino acids in a protein, etc.) drive high-level biological features (sensorimotor behavior, enzymatic function) represents the central challenge of modern biology. There are no general methods for reconstructing such dictionaries from small data sets, and for building vocabularies of statistically significant, independent words in them. Here we derive a method for solving this class of problems, which we call the unsupervised Bayesian Ising Approximation (uBIA) and demonstrate its utility in deciphering the motor code in the pre-motor neurons of a songbird. From small data sets, we detect codewords that predict behavior. These words contains arbitrary number of precisely timed spikes, confirming that the motor code in this system is build from precisely timed multi-spike patterns. We show that distinct classes of such words are used preferentially in codes responsible for motor exploration versus exploitation, opening a window on how motor behaviors are controlled by the brain.

*This work was supported in part by NIH Grants 1R01-EB022872 and 5R01-NS099375.

2:42PM H66.00002: Learning to Crawl

SHRUTI MISHRA (Presenter), Harvard University, WILLEM VAN REES, Massachusetts Institute of Technology, LAKSHMINARAYANAN MAHADEVAN, Harvard University — We combine a mechanical model for a segmented, soft-bodied crawler (Paoletti and Mahadevan, 2014) with a reinforcement learning algorithm for choosing the neuronal excitations. The crawler chooses the neuronal excitations based on a minimal description of the state of its own body, with the goal of moving forward in 1-D. The gait achieved by learning neuronal excitations in this manner depends on the mechanical properties of the crawler. For a regime of properties, the crawler achieves forward locomotion by means of a peristaltic wave, qualitatively similar to what is observed in D. melanogaster larvae. This provides a mechanism for how organisms may learn to achieve locomotion in the absence of a central pattern generator, or recover from injury. This work also suggests a way to explore actuation patterns for soft-robots in cases where the optimal actuation patterns may not be intuitive and provides a means for online learning while exploring an unfamiliar terrain.
2:54PM H66.00003: Non-Gaussian Bayesian theory of sensorimotor learning with multiple timescales*  
BAOHUA ZHOU (Presenter), DAVID HOFMANN, SAMUEL SOBER, ILYA NEMENMAN, Emory University — Various experimental studies have documented that sensorimotor learning phenomena occur on multiple timescales. Many theoretical models have been proposed to explain these experimental observations. However, while successful in certain aspects, these models only focus on average learning behaviors, and they cannot explain some crucial features of learning. For example, they cannot account for the dynamics of the whole distributions of the motor outputs and cannot explain why learning speed and magnitude negatively correlate with the perturbation size. Here we propose a model that includes multiple hidden dynamical variables, which collectively generate the desired motor command. The model is a multi-dimensional Bayesian filter that deals with the dynamics of non-Gaussian joint distributions of those hidden variables. Our model explains simultaneously the dynamics of distributions of the songbird vocal behaviors in various experiments, including: (i) adaptations after step changes or ramps in the error signal, and (ii) dynamics of relaxation following removal of the perturbation. We expect this model can be applied to data from other species and sensorimotor behaviors.

*This work was supported partially by NIH Grant # 1 R01 EB022872, and NIH Grant # NS084844.

3:06PM H66.00004: Structure from noise: Mental errors yield abstract representations of events*  
CHRISTOPHER LYNN (Presenter), ARI E KAHN, DANIELLE BASSETT, University of Pennsylvania — Humans are adept at uncovering complex associations in the world around them, yet the underlying mechanisms remain poorly understood. Intuitively, learning the higher-order structure of statistical relationships should involve sophisticated mental processes, expending valuable computational resources. Here we propose a competing perspective: that higher-order associations actually arise from natural errors in learning. Combining ideas from information theory and reinforcement learning, we derive a novel maximum entropy model of people’s internal expectations about the transition structures underlying sequences of ordered events. Importantly, our model analytically accounts for previously unexplained network effects on human expectations and quantitatively describes human reaction times in probabilistic sequential motor tasks. Additionally, our model asserts that human expectations should depend critically on the different topological scales in a transition network, a prediction that we subsequently test and validate in a novel experiment. Generally, our results highlight the important role of mental errors in shaping abstract representations, and directly inspire new physically-motivated models of human behavior.

*MacArthur, Sloan, ISI, and Allen Foundations and ARL, ARO, ONR, NSF.

EVE ARMSTRONG (Presenter), CLELIA DE MULATIER, University of Pennsylvania, DAVID WHITE, Wilfred Laurier University, MARC SCHMIDT, VIJAY BALASUBRAMANIAN, University of Pennsylvania — During mating season, most species of songbird engage in a societal evolution wherein monogamous pairs “freeze out”. Presumably, these bonds are a recipe for successful procreation. The means by which all individuals “agree” on this structure is unknown. The role of song is significant\(^1\), but its mechanism of orchestrating bonding is obscure. Moreover, a dynamical systems modeling approach would be premature, as it is not clear how to define the variables.

We tackle this problem with a maximum-entropy Ising model. This approach has been applied to an eclectic set of contexts\(^2,3,4\), but – to our knowledge – not to acoustic signaling. Our inferred model, trained on instances of song, is a stronger predictor of mating pairs than are the statistical correlations: it finds monogamous pairs and also instances of polygamy. Minima on the energy landscape align with particular pairs. The Ising model fails to capture all of the structure in the data, suggesting that triadic interactions matter. Moreover, the language of statistical physics offers a framework for examining the biological motivations for songbird social structure. Refs: 1) Perkes et al., Behavioural processes 2018; 2) Schneidman et al., Nature 2006; 3) Lee, Broedersz, Bialek, J Stat Phys 2015; 4) Louie et al. PNAS 2018.

3:30PM H66.00006: Analytical corrections to entropy for under-sampled discrete distributions.  
DAMIAN HERNANDEZ, AHMED ROMAN (Presenter), ILYA NEMENMAN, Physics, Emory University — Estimating entropy of probability distributions of various data sets is a common question in modern data analysis. A common problem is that the number of independent samples obtained in experiments is limited, so that many states are under-sampled and naive entropy estimators are inaccurate. Previous studies found that the statistics of states that occur in data sets multiple times (coincidences) provide useful corrections to entropy estimates in the extremely under-sampled regime. These corrections are largely numerical in nature and so provide little insight to which features of the dataset cause them. Here, we present analytical approximations to a coincidence-based entropy estimators, which shed some light on this question.
3:42PM H66.00007: Inferring geometric embeddings for single cell data MOR NITZAN (Presenter), Harvard University, NIKOS KARAISKOS, Max Delbruck Center for Molecular Medicine, NIR FRIEDMAN, The Hebrew University of Jerusalem, NIROLAUS RAJEWSKY, Max Delbruck Center for Molecular Medicine — Massively multiplexed sequencing of RNA in individual cells is transforming basic and clinical life sciences. However, in standard experiments sequenced cells do not retain information about their original spatial context although it is crucial for understanding cellular function. Recent attempts to overcome this fundamental problem rely on employing additional imaging data which can guide spatial mapping. Here we present a conceptually different approach that allows to reconstruct spatial positions of cells in a variety of tissues without using reference imaging data. We first show for several complex biological systems that distances of single cells in expression space monotonically increase with their distances across tissues. We therefore seek to map cells to tissue space such that this principle is optimally preserved, while incorporating imaging data when available. We show that this optimization problem can be cast as an optimal transport problem and solved efficiently. We apply our approach successfully to reconstruct the mammalian liver and intestinal epithelium as well as the fly embryo. Our results demonstrate a simple spatial expression organization principle that can be used to infer meaningful spatial position probabilities from the sequencing data alone.

3:54PM H66.00008: Interpreting time series data from dynamic signaling pathways in single cells* WEERAPAT PITTAYAKANCHIT (Presenter), KABIR HUSAIN, ARVIND MURUGAN, University of Chicago — A growing body of evidence suggests that cells encode information in the dynamics of signaling molecules. For instance, both the identity and dose of different external ligands may be encoded in the temporal dynamics of a single transcription factor. Understanding which aspects of experimental time-series are informative, and which can plausibly be decoded by cells given biochemical constraints, remains an open problem. Here, we combine modified versions of interpretable machine learning techniques, such as InfoGAN, with domain knowledge of the NF-kB pathway to obtain insights on how experimental time-series data of NF-kB encodes information about the ligands TNFa and IL-2.

*AM and WP thanks the Simon Foundation for the funding support. KH thanks the James S McDonnell Foundation for the support via a postdoctoral fellowship.

4:06PM H66.00009: Learning image models for optimal information extraction: image registration from first principles* COLIN B CLEMENT (Presenter), MATTHEW BIERBAUM, JAMES PATARASP SETHNA, Cornell University — We demonstrate an unbiased method of image registration which has errors consistent with the Cramer-Rao bound (CRB) by using Super Registration: learning an optimal model for the underlying image and shifting that to match the data. Image registration is the inference of transformations relating noisy and distorted images. Fundamental in computer vision, experimental physics, and medical imaging, even in the simplest case of translation, known methods are biased and none achieve the CRB. Cutting edge experiments operate at extreme limits of signal-to-noise, for example, low-dose TEM imaging of sensitive biological materials. It is in these high-noise scenarios when existing registration techniques fail to correctly infer shifts. Following Bayesian inference, we prove that the standard method of shifting one image to match another cannot reach the CRB. We reach the theoretical lower bound in shift resolution and extract a higher resolution, de-noised model of the latent image. Finally, while sub-pixel errors in shift inference do not dramatically change the reconstructed image for oversampled data, we show that using our new registration method can lead to 10× more precise particle tracking.

*This work was supported by the NSF Center for Bright Beams, award #1549132.
In many biological phenomena, cells migrate through confining environments. To study such confined migration, we place migrating cells in two-state micropatterns, in which the cells stochastically migrate back and forth between two square adhesion sites connected by a thin bridge. We adopt a data-driven approach where we learn an equation of motion directly from the experimentally determined short time-scale dynamics, decomposing the migration into deterministic and stochastic contributions. This equation captures the dynamics of the confined cell and accurately predicts the transition rates between the sites. We thereby derive the emergent non-linear dynamics that governs the migration directly from experimental data. In particular, we find that the deterministic dynamics is poised near a bifurcation between a limit cycle and bistable behaviour. As a result, we find that cells are deterministically driven into the thin constriction; a process that is sped up by noise. Our approach yields a conceptual framework that may be extended to describe cell migration in more complex confining environments.

*This work was supported by the DFG via SFB1032 (Projects B01 and B12). D.B. is supported by the Graduate School of Quantitative Biosciences Munich (QBM) and the Joachim Herz Stiftung.

Single-molecule field-effect transistors (smFET) have been recently exploited to probe molecular dynamic events occurring at the single-molecule scale. Hidden Markov models (HMMs) are commonly used to model single-molecule kinetic trajectories, but they require restrictive assumptions and a priori knowledge of the likely kinetic model, both rarely met in real experiments. In particular, a major challenge in extracting kinetics from smFET data relies on the non-stationarity of the recorded signals due to noise and drifts. Here, we propose a new approach based on machine learning to retrieve the hidden trajectory between molecular states. Our method is a two-step algorithm based on compression of the raw data using a minimum description length cost function, followed by a k-medoid clustering of the compression patterns. A decision-aid tool automatically selects the multi-state model providing the best-fitting trajectory. Based on tests on synthetic and experimental data, we found that this entropy-based method allows to extract a robust idealized trajectory, without requiring any prior or supervision. We also found that using this idealized trajectory as a prior for HMM analysis provides better performances for the detection and modeling of non-stationary molecular dynamics.

Mutations play a critical role in molecular evolution and the development of many diseases, such as cancer and neurodegenerative diseases. A growing body of evidence shows that rates of mutation in DNA are not only highly variable, but also influenced by the specific sites and nearby sequences. We have found that the physics of electron hole localization, most pronounced at or near guanine sites, plays a significant role in influencing sequence-specific mutation rates [M.Y. Suárez-Villagrán, R. B. R. Azevedo, & J. H Miller, Jr., Genome Biology & Evolution, 10, 1039 (2018)]. Most recently we have been applying the predictive capability of Deep Neural Network architectures, among other machine learning approaches, to predict and validate genetic mutation rates in human mitochondrial DNA. Given a segment of a sequence from the neighborhood of a specific base pair, we are able to predict mutation rates with much greater accuracy than that of a random predictor. We are currently testing the limits of automatic predictors for similar tasks, with an aim towards better understanding of both evolution and the emergence of somatic disease states, such as cancer.

*Texas Center for Superconductivity at the University of Houston and NIH
The Effects of Non-Specific Binding Kinetics on Fluorescence Activated Cell Sorting (FACS)*

BHAVEN MISTRY (Presenter), Biomathematics, UCLA, THOMAS CHOU, Mathematics, UCLA — Fluorescence activated cell sorting (FACS) is extensively used in biological studies to differentiate cells of interest (mutants) from control cells (wild-types). For mutant cells characterized by expression of a distinct membrane surface structure, fluorescent marker probes can be designed to bind specifically to those structures, resulting in a sufficiently high fluorescence intensity that indicates a mutant cell. However, endogenous membrane structures on wild-type cells may nonspecifically bind to the probes, resulting in false positive results. These same endogenous membrane structures would also be present on mutant cells, allowing both specific and non-specific binding to a single cell. We create a kinetic model of fluorescent probe binding dynamics by tracking populations of mutant and wild-type cells with differing numbers of probes bound specifically and non-specifically. By assuming the suspension is in equilibrium prior to cytometry, we analytically derive a likelihood function of the FACS output in order to infer the total number of mutant cells while accounting for the non-specific binding of probes. We further show how our model can be used to infer unknown binding rates of fluorescent markers if cell counts are a priori known.

*NSF DMS-1516675 and NSF DMS-1814364

Reverse-time inference of targeted biological dynamics

NICOLAS LENNER (Presenter), STEPHAN EULE, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — Mesoscopic bio-systems typically evolve towards functionally important target-states, such as cell cycle checkpoints or decision boundaries for the release of complex behavior. To infer the underlying directional out-of-equilibrium dynamics from such data, we develop a theory of target-state-aligned ensembles that reveals whether and when the system can be represented by a single, effective stochastic equation of motion. We show how, in this equation, genuine biological forces can be separated from spurious forces, which, invariably arise from target-state-alignment. We apply our inference scheme to canonical biological examples such as cell division and morphogenesis.

Information flow and the accuracy of concentration measurements in a genetic network*

MARIANNE BAUER (Presenter), WILLIAM BIALEK, THOMAS GREGOR, Princeton University, MARIELA D PETKOVA, Biophysics, Harvard University, ERIC WIESCHAUS, Princeton University — Many genes are regulated by transcription factor (TF) proteins which bind to DNA and control the synthesis of messenger RNA (mRNA). The information which output mRNA or protein levels carry about input TF concentrations is a measure of regulatory power. All this information passes through a bottleneck, the occupancy of the relevant binding sites along the DNA, and random arrival of TFs at these sites sets an irreducible noise level, which in turn limits the information capacity. We explore these issues in the gap gene network of the early fly embryo, where recent work shows that the concentrations of these transcription factors carry enough information to specific cellular position to 1% precision along the length of the embryo. But how accurately would the system need to “measure” these concentrations in order to extract this information? We show that these measurements need to be more accurate than is plausible given the physical limits at a single binding site, suggesting that the complex array of multiple binding sites provides a solution to the problem of efficient information transmission.

*Supported in part by the NSF Center for the Physics of Biological Function (PHY-1734030), and grant PHY-1607612; by NIH grants P50GM071508, R01GM077599, and R01GM097275; and by HHMI.

Tuesday, March 5, 2019 2:30 PM - 5:30 PM

Session H69 DLS: Optical Frequency Comb Spectroscopy

BCEC 052A - Kristan Corwin, Kansas State University -

Tag(s): Invited
2:30PM H69.00001: Tri-comb Spectroscopy* [Invited] STEVEN CUNDIFF (Presenter), BACHANA LOMSADZE, BRAD C SMITH, Department of Physics, University of Michigan — Optical multidimensional coherent spectroscopy (MDCS) has been developed over the last 20 years and proven very powerful at unfolding congested spectra, identifying coupling between resonances, making size-resolved measurements of nanoparticles and revealing many-body interactions [1]. However, MDCS has required a complex apparatus and has suffered from limited spectral resolution.

Inspired by developments in dual-comb spectroscopy, we developed comb-based MDCS, improving the spectral resolution by over an order of magnitude, which we demonstrated by resolving the hyperfine split transitions in a rubidium vapor [2]. With the addition of third frequency comb, which we call "tri-comb spectroscopy," we are able to eliminate all moving parts and further improve the resolution with a data record of less than 0.5 seconds long [3]. These results also demonstrate the separation of the two isotopies of rubidium, showing the promise of MDCS for chemical sensing where the separation of species is a critical challenge.

These results open a path towards an implementation of MDCS that can rapidly produce spectra using a compact and robust apparatus that can be used outside a laboratory.


*The research is based on work supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via contract 18020600001.

3:06PM H69.00002: Widely tunable cavity-enhanced ultrafast spectroscopy and the dynamics of hydrogen bond networks.* [Invited] THOMAS ALLISON (Presenter), MYLES SILFIES, JOSE MIGUEL BAUTISTA, Departments of Chemistry and Physics, Stony Brook University, GRZEGORZ KOWZAN, Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Poland, YUNING CHEN, Departments of Chemistry and Physics, Stony Brook University — Ultrafast optical spectroscopy methods, such as transient absorption spectroscopy and 2D spectroscopy, are widely used across many disciplines. However, these techniques are typically restricted to optically thick samples, such as solids and liquid solutions. In previous work (Reber et al. Optica 3, 311 (2016)), using frequency comb lasers and resonant optical cavities, we have demonstrated the extension of all-optical ultrafast spectroscopy methods to dilute molecular beams and recorded transient absorption signals with detection limits as low as ΔOD = 2×10^{-10}. In this talk I will discuss our progress in developing widely tunable cavity-enhanced ultrafast spectrometers operating from the ultraviolet to the mid-infrared and their application to the ultrafast dynamics of elementary hydrogen bond networks.

*National Science Foundation award number 1708743

3:42PM H69.00003: Multi-comb coherent control for material studies* [Invited] KAORU MINOSHIMA (Presenter), AKIFUMI ASAHARA, The University of Electro-Communications, JST ERATO-IOS — Dual-comb spectroscopy (DCS), which uses two frequency combs with slightly different repetition frequencies, has become a powerful tool for high-precision spectroscopy because of its capability for rapid, broadband, high-resolution, and high-sensitivity measurement. Recently, the applicability of the DCS has greatly expanded to such as nonlinear spectroscopy and solid-state study. By utilizing the DCS as the tool to retrieve the dynamical response of the electric field of the optical wave in the sub-PHz frequency domain, we can directly obtain the complex optical properties of the materials as the response function, which provides an attractive tool for direct characterization of new materials without model assumption. We have applied the technique for direct characterization of the complex optical properties of solid materials [1] and studying ultrafast phenomena [2]. In this study, we focused on the coherent controllability with multi-comb and realized generation and coherent detection of the raid polarization modulation of ultrashort pulse train. The technique was applied to the dynamical characterization of complex optical tensor of material. Moreover, we realized the spatio-temporal phase control of ultrashort pulse train by combining the optical frequency comb and optical vortex, i.e., optical vortex comb, and applied to the DCS for azimuth sensitive spectroscopy with all the advantages of the standard DCS. Such technique is useful for coherent excitation and control of orbital angular momentum related phenomena, such as topological physics, spintronics, and chiral material.


*This work was supported by Japan Science and Technology Agency (JST) through the Exploratory Research for Advanced Technology (ERATO) MINOSHIMA Intelligent Optical Synthesizer (IOS) Project (JPMJER1304).
Soliton microresonator frequency combs* [Invited] TOBIAS KIPPENBERG (Presenter), Ecole polytechnique federale de Lausanne — Optical frequency combs\(^1\)\(^2\) provide equidistant markers in the IR, visible and UV and have become a pivotal tool for frequency metrology and are the underlying principle of optical atomic clocks, but are also finding use in other areas, such as broadband spectroscopy or low noise microwave generation. Development are underway to create chip-scale frequency comb sources\(^1\) that are low power, compatible with wafer scale processing, exhibit microwave repetition rates, for applications that are airborne or in space. Such "micro-combs" are based on parametric frequency conversion of a continuous wave laser, and make use of dissipative Kerr soliton formation\(^2\)\(^3\) \(^4\) (DKS). Such dissipative Kerr solitons provide access to fully coherent and broadband combs with tailorable bandwidth. In this talk the Physics of dissipative solitons is reviewed, as discovered in crystalline resonators. Microcombs, give rise to a host of nonlinear dynamical phenomena, including Soliton Cherenkov radiation\(^5\), breather solitons\(^6\), soliton switching\(^7\), to soliton crystals\(^8\), and multi-soliton complexes. In addition soliton microcombs have been applied in massively parallel coherent communication\(^9\), dual comb distance measurements\(^10\), with record acquisition rate, and exhibit a bandwidth that can be extended to the biological imaging window. Soliton microcombs have the potential to advance timekeeping, and make frequency metrology ubiquitous.

*We acknowledge funding by the AFOSR, DARPA DODOS, DARPA SCOUT and Swiss National Science Foundation (SNF), as well as Microsoft and ZEISS AG.

Dual Comb Spectroscopy for Emissions Measurements+ [Invited] ELEANOR WAXMAN (Presenter), KEVIN COSSEL, FABRIZIO GIORGETTA, WILLIAM SWANN, National Institute of Standards and Technology Boulder, GAR-WING TRUONG, Crystalline Mirror Solutions, MICHAEL CERMACK, National Institute of Standards and Technology Boulder, DANIEL HESSELIUS, IRISS, University of Colorado, IAN CODDINGTON, NATHAN NEWBURY, National Institute of Standards and Technology Boulder — Trace gas measurements are critical for understanding city contributions to greenhouse gas emissions and for identifying and quantifying natural gas leaks from oil and gas wells. Here we present a near-infrared dual comb spectroscopy system that we use for trace gas measurements. Our system is comprised of a dual comb spectroscopy instrument, a telescope and co-located detector, and a retroreflector located at the far end of our measurement path. This enables us to measure over path lengths of several hundred meters to several kilometers. We have compared this system against a near-identical system over the open atmosphere with excellent agreement of retrieved trace gas concentrations. We then deployed this system at NIST to measure the carbon dioxide enhancement over the city of Boulder, Colorado which we primarily attribute to vehicle exhaust. This is coupled with Gaussian plume modeling to estimate the emissions from the city and we have good agreement with the city estimate of vehicle emissions. Finally, we deploy the system in the field in a van to measure emissions from a simulated natural gas leak using a mobile UAS-mounted retroreflector. This work shows the promise of using horizontal column-integrated open-path measurements for emissions quantification.

*We acknowledge funding from DARPA DSO SCOUT program, NRC fellowship program, and the NIST Special Projects office.

Tuesday, March 5, 2019 4:00 PM - 6:00 PM

Session H29A APS: Planned Giving Session BCEC 162A

4:00PM H29A.00001: Planned Giving Session — tbd

Tuesday, March 5, 2019 4:30 PM - 6:30 PM

Session J72 APS: Meet the Physical Review Journal Editors Reception BCEC East Registration

4:30PM J72.00001: Meet the Physical Review Journal Editors Reception — Learn about the exciting new journal from APS, which begins accepting submissions in 2019. Also take this opportunity to meet the editors and discuss the Physical Review family of journals.

All are welcome. Light refreshments will be served.

Tuesday, March 5, 2019 5:30 PM - 6:30 PM
Session J34 APS: Town Hall: Guide to Effective Practices for Physics Departments: Implications for Program Review and Accreditation BCEC 205A - Tag(s): Education

5:30PM J34.00001: Town Hall: Guide to Effective Practices for Physics Departments: Implications for Program Review and Accreditation — ABET, the accrediting body for nearly every engineering program in the U.S., recently announced that they were actively pursuing accreditation of physics and other undergraduate science programs. APS is concerned that accreditation may stifle educational innovation or lead us into a “check the box” mentality of program review. On the positive side, many chairs have indicated the need for a helpful set of resources that will enable them to run a department more effectively, and address areas of need. As a response to these concerns the APS Council approved the formation of a task force to: “Develop a guide for self-assessment of undergraduate physics programs founded on documented best practices linked to measurable outcomes.” The task force has been working on developing a community-based, living-document that will serve as a guide on how to improve the health of a physics department, tackle common problems, and prepare for external review. We will discuss progress on developing this guide, and solicit input on how to make these materials useful and accessible to the physics community.

Tuesday, March 5, 2019 5:30 PM - 7:00 PM

Session J73 APS/SPS: Student Reception BCEC Ballroom East/West - Tag(s): Undergraduate

5:30PM J73.00001: Student Reception — Graduate and undergraduate students can mingle with working physicists at the special student reception with light fare until 7:00 p.m. Immediately following, all students who presented at the March Meeting in the Undergraduate Research Sessions will be recognized, and students with outstanding presentations will also receive a special prize.

Tuesday, March 5, 2019 5:30 PM - 7:00 PM

Session J80 DCMP DMP: DCMP/DMP Joint Fellows Reception Westin Grand Ballroom B

5:30PM J80.00001: DCMP/DMP Joint Fellows Reception — DCMP/DMP Joint Fellows Reception

Tuesday, March 5, 2019 5:45 PM - 6:45 PM

Session J26 GIMS: GIMS Business Meeting BCEC 160B

5:45PM J26.00001: GIMS Business Meeting — GIMS Business Meeting

Tuesday, March 5, 2019 5:45 PM - 6:45 PM

Session J31 DCP: DCP Business Meeting BCEC 203

5:45PM J31.00001: DCP Business Meeting — DCP Business Meeting

Tuesday, March 5, 2019 5:45 PM - 6:45 PM

Session J36 GMAG: GMAG Business Meeting BCEC 205C

5:45PM J36.00001: GMAG Business Meeting — GMAG Business Meeting

Tuesday, March 5, 2019 5:45 PM - 6:45 PM

Session J45 GPC: GPC Business Meeting BCEC 211

5:45PM J45.00001: GPC Business Meeting — GPC Business Meeting
Tuesday, March 5, 2019 5:45 PM - 6:45 PM
Session J46 GERA: GERA Business Meeting BCEC 212
5:45PM J46.00001: GERA Business Meeting — GERA Business Meeting

Tuesday, March 5, 2019 5:45 PM - 6:45 PM
Session J47 FOEP: FOEP Business Meeting Coppersmith Restaurant - Tag(s): Outreach
5:45PM J47.00001: FOEP Business Meeting — FOEP Business Meeting

Tuesday, March 5, 2019 5:45 PM - 6:45 PM
Session J51A DPOLY: DPOLY Business Meeting BCEC 253A
5:45PM J51A.00001: DPOLY Business Meeting — DPOLY Business Meeting

Tuesday, March 5, 2019 5:45 PM - 6:45 PM
Session J60 DBIO: DBIO Business Meeting BCEC 258A
5:45PM J60.00001: DBIO Business Meeting — DBIO Business Meeting

Tuesday, March 5, 2019 5:45 PM - 6:45 PM
Session J61 DQI: DQI Business Meeting BCEC 258B
5:45PM J61.00001: DQI Business Meeting — DQI Business Meeting

Tuesday, March 5, 2019 5:45 PM - 6:45 PM
Session J62 GSNP: GSNP Business Meeting BCEC 258C
5:45PM J62.00001: GSNP Business Meeting — GSNP Business Meeting

Tuesday, March 5, 2019 6:45 PM - 7:45 PM
Session J51B DPOLY: NSF Question and Answer Session on Polymers and Soft Matter BCEC 253A - Tag(s): Invited
6:45PM J51B.00001: NSF Question and Answer Session on Polymers and Soft Matter —

Tuesday, March 5, 2019 7:00 PM - 8:00 PM
Session J52 DCMP: DCMP Business Meeting BCEC 253B
7:00PM J52.00001: DCMP Business Meeting — DCMP Business Meeting

Tuesday, March 5, 2019 7:30 PM - 8:30 PM
Session J53 DMP: DMP Business Meeting BCEC 253C
Session J81 APS: Reviews of Modern Physics: The First Ninety Years

Session J81.00001: 2D Materials: Science and Technology

7:30PM J81.00001: 2D Materials: Science and Technology [invited] ANTONIO HELIO CASTRO NETO (Presenter), Centre for Advanced 2D Materials, National University of Singapore — The surprising isolation of graphene in 2004 has created a new field of research, namely, 2D Crystals. Nowadays we know that there are thousands of different types of 2D crystals with electronic properties that range from metals and semiconductors to magnets and superconductors. These new materials have had not only an impact in modern science but they are already having a technological impact in the industry. In this seminar I will review the field and its evolution in the last few years.

8:00PM J81.00002: Previews of Modern Physics [invited] NIGEL DAVID GOLDENFELD (Presenter), University of Illinois at Urbana-Champaign — The Reviews of Modern Physics (RMP) is certainly the most well-cited review journal in the world of physics. Its stellar reputation reflects the depth and detail of its reviews of fields that have reached sufficient maturity for a review to be warranted. In this talk, I will argue that there is another factor that has perhaps made an outsize contribution to its impact: some of the most influential articles have been reviews about fields that in some sense do not yet exist, or are still in their formative stages. I will focus on several examples drawn from the world of condensed matter and statistical physics, including: (1) Leo Kadanoff’s RMP on critical phenomena (1967); (2) Ken Wilson’s RMP on the Kondo problem (1975); (3) Jim Langer’s RMP on the field of non-equilibrium pattern formation (1981); (4) Stephen Wolfram’s RMP on cellular automata (1983); (5) Albert and Barabasi’s RMP on the statistical mechanics of networks (2002). I would contend that these review articles owe their success not simply to the traditional metrics of comprehensiveness of scope, timeliness and quality of exposition, but to the fact that they catalyzed the evolution of their respective fields, by inspiring receptive scientists to see possibilities that would not otherwise have been so apparent. I will try to draw some recommendations that could guide future authors who wish to write a “preview” of an emerging field.

8:30PM J81.00003: Interface-induced phenomena in magnetism: writing a review article in an important topical subject with 27 leading scientists as co-authors [invited] FRANCES HELLMAN (Presenter), University of California, Berkeley — This article reviews static and dynamic interfacial effects in magnetism, focusing on interfacially driven magnetic effects and phenomena associated with spin-orbit coupling and intrinsic symmetry breaking at interfaces. It provides a historical background and literature survey, but focuses on recent progress, identifying the most exciting new scientific results and pointing to promising future research directions. It starts with an introduction and overview of how basic magnetic properties are affected by interfaces, then turns to a discussion of charge and spin transport through and near interfaces and how these can be used to control the properties of the magnetic layer. Important concepts include spin accumulation, spin currents, spin-transfer torque, and spin pumping. An overview is provided to the current state of knowledge and existing review literature on interfacial effects such as exchange bias, exchange-spring magnets, the spin Hall effect, oxide heterostructures, and topological insulators. The article highlights recent discoveries of interface-induced magnetism and noncollinear spin textures, nonlinear dynamics including spin-transfer torque and magnetization reversal induced by interfaces, and interfacial effects in ultrafast magnetization processes.

Session K01 DCMP: Floquet Systems

Wednesday, March 6, 2019 8:00 AM - 10:36 AM

Session K01.00003: Interface-induced phenomena in magnetism: writing a review article in an important topical subject with 27 leading scientists as co-authors [invited] FRANCES HELLMAN (Presenter), University of California, Berkeley — This article reviews static and dynamic interfacial effects in magnetism, focusing on interfacially driven magnetic effects and phenomena associated with spin-orbit coupling and intrinsic symmetry breaking at interfaces. It provides a historical background and literature survey, but focuses on recent progress, identifying the most exciting new scientific results and pointing to promising future research directions. It starts with an introduction and overview of how basic magnetic properties are affected by interfaces, then turns to a discussion of charge and spin transport through and near interfaces and how these can be used to control the properties of the magnetic layer. Important concepts include spin accumulation, spin currents, spin-transfer torque, and spin pumping. An overview is provided to the current state of knowledge and existing review literature on interfacial effects such as exchange bias, exchange-spring magnets, the spin Hall effect, oxide heterostructures, and topological insulators. The article highlights recent discoveries of interface-induced magnetism and noncollinear spin textures, nonlinear dynamics including spin-transfer torque and magnetization reversal induced by interfaces, and interfacial effects in ultrafast magnetization processes.
8:00AM K01.00001: Central Charge of Periodically Driven Critical Kitaev Chains* DANIEL YATES (Presenter), YONAH S LEMONIK, ADITI MITRA, New York University — Periodically driven Kitaev chains show a rich phase diagram as the amplitude and frequency of the drive is varied, with topological phase transitions separating regions with different number of Majorana zero and π modes. We explore whether the critical point separating different phases of the periodically driven chain may be characterized by a universal central charge. We affirmatively answer this question by studying the entanglement entropy (EE) numerically, and analytically for the lowest entangled many particle eigenstate at arbitrary non-stroboscopic and stroboscopic times. We find that the EE at the critical point scales logarithmically with a time-independent central charge, and that the Floquet micro-motion gives only sub-leading corrections to the EE. This result also generalizes to multi-critical points where the EE is found to have a central charge which is the sum of the central charges of the intersecting critical lines.

*This work was supported by the US Department of Energy, Office of Science, Basic Energy Sciences, under Award No.–DE-SC0010821.

8:12AM K01.00002: Signatures of Floquet Majorana Fermions in Planar Josephson Junctions* DILLON LIU (Presenter), JAVAD SHABANI, ADITI MITRA, Center for Quantum Phenomena, New York University — We show how Floquet Majorana fermions may be experimentally realized in a periodically driven solid state platform. We consider a planar Josephson junction formed via a superconducting-proximitized 2D electron gas (2DEG) with Rashba spin-orbit coupling and in-plane Zeeman field. Using bulk Floquet topological invariants we analyze the number of zero and π Majorana modes for experimentally realistic parameters. Then we describe several experimental signatures of these exotic modes in finite wires, including differential conductance and local density of states. Notably, features in these quantities exhibit sub-harmonic responses to the drive.

*DTL and AM were supported by the US Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0010821. J.S. was supported by the US Army Office of Research, ARO: W911NF-18-1-0067, and US Air Force Office of Scientific Research Young Investigator Award, FA9550-16-1-0348.

8:24AM K01.00003: Time-Crystalline Topological Superconductors* AARON CHEW (Presenter), California Institute of Technology, DAVID MROSS, Weizmann Institute of Science, JASON ALICEA, California Institute of Technology — Time crystals form when arbitrary physical states of a periodically driven system spontaneously break discrete time-translation symmetry. We introduce the notion of 1D time-crystalline topological superconductors, for which time-translation symmetry breaking and Majorana physics nontrivially intertwine. In the simplest realization, such a phase exhibits a bulk magnetization that returns to its original form after two drive periods, together with unconventional Floquet Majorana end modes that recover their initial form only after four drive periods. We also propose experimental implementations and detection schemes for this new phase.

*Grants DMR-1341822 and DMR-1723367 (A. C. and J. A.); the Minerva foundation with funding from the Federal German Ministry for Education and Research (D.F.M.); Grant Award W911NF-17-1-0323 (A. C. and J. A.); BSF Grant No. 2016258; Caltech's IQIM with support of Grant GBMF1250; and the Walter Burke Institute for Theoretical Physics at Caltech.

8:36AM K01.00004: Three-dimensional Chiral Lattice Fermion in Floquet Systems XIAO-QI SUN (Presenter), MENG XIAO, TOMAS BZDUSEK, SHOUCHENG ZHANG, SHANHUI FAN, Stanford University — We show that the Nielsen-Ninomiya no-go theorem still holds on Floquet lattice: there is an equal number of right-handed and left-handed Weyl points in three-dimensional Floquet lattice. However, in the adiabatic limit, where the time evolution of low-energy subspace is decoupled from the high-energy subspace, we show that the bulk dynamics in the low-energy subspace can be described by Floquet bands with extra left/right-handed Weyl points, despite the no-go theorem. Assuming adiabatic evolution of two bands, we show that the difference of the number of right-handed and left-handed Weyl points equals twice the winding number of the adiabatic Floquet operator over the Brillouin zone. Based on these findings, we propose a realization of purely left- or right-handed Weyl particles on a 3D lattice using a Hamiltonian obtained through dimensional reduction of a four-dimensional quantum Hall system. We argue that the breakdown of the adiabatic approximation on the surface facilitates unusual closed orbits of wave packets in applied magnetic field, which traverse alternatively through the low-energy and high-energy sector of the spectrum.
8:48AM K01.00005: Disentangling beyond-cohomology symmetry protected topological phases*  
JEONGWAN HAAH, Microsoft, LUKASZ FIDKOWSKI (Presenter), University of Washington, MATTHEW HASTINGS, Microsoft — We construct a three-dimensional locality preserving unitary operator which disentangles the ground state of the Walker-Wang three fermion model. We show that this locality preserving unitary operator cannot be a quantum circuit, or otherwise one could construct a commuting projector model which realizes a phase with nonzero chiral central charge, which is widely believed to be impossible. We comment on the relation to Many-body localized Floquet topological phases.

*NSF DMR-1519579, Microsoft Research

9:00AM K01.00006: Transport signatures of symmetry protection in one-dimensional topological insulators  
OLEKSANDR BALABANOV (Presenter), HENRIK JOHANNESSON, Department of Physics, University of Gothenburg — The unique feature of any topological insulator is presence of gapless states on its boundaries. In one dimension these states live on the edges and are protected against symmetry-preserving local perturbations. Here we describe a scheme for probing the robustness of the edge states by calculating the transport characteristics of an array of dimers attached to external leads. Numerical results obtained from non-equilibrium Green's function theory will be presented. It will be shown that there is a drop in the differential conductance as the dimer array is perturbed by a local symmetry-breaking perturbation, while the drop is strongly suppressed if the symmetries are maintained. A brief analytic description will be provided in support of the numerics. Both types of 1D topological insulators, conventional time-independent and periodically-driven (Floquet), are considered.

9:12AM K01.00007: Topologically protected braiding in a single wire using Floquet Majorana modes*  
TORSTEN KARZIG (Presenter), BELA BAUER, Station Q, Microsoft, TAMÍ PEREG-BARNEA, Department of Physics, McGill University, MARIA-THERESA RIEDER, Department of Condensed Matter Physics, Weizmann Institute, GIL REFAEL, Department of Physics, Caltech, EREZ BERG, Department of Physics, University of Chicago, YUVAL OREG, Department of Condensed Matter Physics, Weizmann Institute — The non-Abelian nature of Majorana zero modes is most prominently exhibited through braiding. While originally formulated for 2D systems, it has been shown that braiding can also be realized using 1D wires by forming an essentially 2D network. Here, we show that in driven systems far from equilibrium, one can do away with the second spatial dimension altogether by instead using quasienegy as the second dimension. To realize this, we use a Floquet topological superconductor which can exhibit Majorana modes at two special eigenvalues of the evolution operator, 0 and Pi, and thus can realize four Majorana modes in a single, driven quantum wire. We describe and numerically evaluate a protocol that realizes non-local braiding of two Majorana zero modes in a single wire by adiabatically modulating the Floquet drive and using the Pi modes as auxiliary degrees of freedom.

*This work was supported by NSERC DG (TPB), the BSF and ISF grants and by the ERC under the European Community's Seventh Framework Program (FP7/2007–2013)/ERC - Grant agreement MUNATOP-340210. YO and EB acknowledge support from CRC 183 of the Deutsche Forschungsgemeinschaft. We are also grateful for the hospitality of the Aspen Center for Physics, which is supported by National Science Foundation grant PHY-1607761.

9:24AM K01.00008: Metal to insulator phase transitions in Floquet-Bloch systems*  
ILIYA ESIN (Presenter), Technion - Israel Institute of Technology, MARK RUDNER, Niels Bohr Institute, Copenhagen University, NETANEL LINDNER, Technion - Israel Institute of Technology — Time-periodic drives provide a versatile tool for inducing topological phenomena in quantum many body systems. In this work, we study steady-states of low-dimensional semiconductors subjected to strong resonant periodic drives. Stable steady-states in these systems arise from the balance between phonon-assisted relaxation processes, electron-hole recombination via photo-emission and electron-electron scattering. We show that tuning the parameters of the phonon bath drives the system through a critical point, which separates an electron-hole metal phase from a Floquet insulator phase. Our results may help guide future studies towards inducing novel non-equilibrium phases of matter by periodic driving.

*This work was supported by European Research Council (ERC) under the European Union Horizon 2020 Research and Innovation Programme (Grant Agreement No. 678862 and 639172), the Israeli Science Foundation and the Villum Foundation.
Motivated by recent experimental realizations of topological charge pumping in cold atoms, we theoretically study the Rice-Mele model with spatiotemporal disorder coupled to two leads using the Floquet Keldysh green’s function approach. The temporal disorder characterizes random motion of electrons due to a bath, with diffusive, sub-diffusive, or white noise as special cases. We obtain the pumped charge in the full range of drive frequency away from the adiabatic limit for different strengths of disorder, and for different temporal disorders. We quantify and discuss localization-delocalization transitions in the Floquet spectrum and their effect on the topological pumped charge.

*Work supported by the NSF CAREER grant DMR-1350663, BSF grant No. 2014345, and the College of Arts and Sciences at Indiana University.

This work is supported by the NSF CAREER grant DMR-1350663, BSF grant No. 2014345, the College of Arts and Sciences at Indiana University, and the NSERC of Canada

*This work is supported by the NSF CAREER grant DMR-1350663, BSF grant No. 2014345, the College of Arts and Sciences at Indiana University, and NSF Materials Research Science and Engineering Center Grant No. DMR-1720595

*This material is based upon work supported by NSF Graduate Research Fellowship Program Grant No. 1122374, Grant No. DMR-1506475, and NSFC 11274192.
**Floquet Topological Semimetal with Nodal Helix**

KWON PARK (Presenter), KUN WOO KIM, HYUNWOONG KWON, Korea Institute for Advanced Study — Topological semimetal with nodal line is a novel class of topological matter extending the concept of topological matter beyond topological insulators and Weyl/Dirac semimetals. Here, we show that a Floquet topological semimetal with nodal helix can be generated by irradiating graphene or the surface of a topological insulator with circularly polarized light. Nodal helix is a form of nodal line running across the Brillouin zone with helical winding. Specifically, it is shown that the dynamics of irradiated graphene is described by the time Stark Hamiltonian, which can host a Floquet topological insulator and a weakly driven Floquet topological semimetal with nodal helix in the high and low frequency limits, respectively. One of the most striking features of the Floquet topological semimetal at low frequency is that the Berry phase accumulated along the time direction, also known as the Zak phase, has a topological discontinuity of $\pi$ across the projected nodal helix. It is predicted that such a topological discontinuity of the Berry phase manifests itself as the topological discontinuity of the Floquet states. At intermediate frequency, this topological discontinuity can create an interesting change of patterns in the quasienergy dispersion of the Floquet states.

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**Wednesday, March 6, 2019 8:00 AM - 11:00 AM**

**Session K02 DMP: Topological Metamaterials** BCEC 107A - Che-Ting Chan, Hong Kong University of Science and Technology - Tag(s): Focus

**8:00AM K02.00001: Exceptional Nanophotonics** [Invited] LIANG FENG (Presenter), University of Pennsylvania — Integrated nanophotonics promises next-generation computing platforms. In this talk, I will present our work on exceptional nanophotonics, creating “quantum” exceptional points on-a-chip and utilizing their associated topology. Based on the exceptional point-induced unidirectionality, we harness optical losses to enable unique photonics functionalities, in particular, an orbital angular momentum (OAM) microcavity that structures and twists lasing radiations at the micro/nano-scale and a low-power all-optical switch, which may address the growing demand for information capacity. Additionally, I will discuss non-Hermitian topological photonics where optical non-Hermiticity and topological physics are coupled to produce robust photonic integrated circuits and laser sources and novel microscopic thermal sensors.

**8:36AM K02.00002: Definite photon deflections of topological defects in metasurfaces and symmetry-breaking phase transitions with material loss**

HUI LIU (Presenter), CHONG SHENG, Department of Physics, Nanjing University, HUANYANG CHEN, Department of Electronic Science, Xiamen University, SHINING ZHU, Department of Physics, Nanjing University — In this work [1], by using an artificial waveguide bounded with rotational metasurface, the nontrivial effects of a topological defect of spacetime are experimentally emulated. The photon deflection in the topological waveguide has a robust definite angle that does not depend on the location and momentum of incident photons. This is remarkably different from the random optical scattering in trivial space. By including material loss such a topological effect can be well understood from the symmetry breaking of photonic modes. Our technique provides a platform to investigate topological gravity in optical systems. This method can also be extended to obtain many other novel topological photonic devices.


*This work was financially supported by the National Natural Science Foundation of China (Nos. 11690033, 61425018, 11621091, and 11704181), National Key R&D Program of China (2017YFA0303702), and National Key Research and Development Program of China (No. 2017YFA0205700).

**8:48AM K02.00003: Loss induced high efficient Lorentz nonreciprocal metasurfaces**

WANG TAT YAU (Presenter), WENYAN WANG, KIN HUNG FUNG, Hong Kong Polytechnic University — Lorentz nonreciprocal metasurfaces rely on breaking all symmetries related to energy flow reciprocity. We numerically design a metasurface made of dimer unit cell to achieve nonreciprocity. The dimer consists of a gyromagnetic and lossy dielectric cylinder. Under the biased magnetic field, the TE (nonzero electric field out of plane) polarized plane wave at normal incident in different direction exhibit nonreciprocal transmission. We successfully employ the multiple scattering theory (MST) up to the dominant resonant modes of cylinders to describe the numerical nonreciprocal feature. The nonreciprocal mechanism can be revealed by the eigenresponse theory that different direction incidence comprises of different portion of lossy mode which will favour to excite the lossy dielectric cylinder, leading to nonreciprocal transmission.

*Hong Kong Research Grant Council (grant nos. 15301917 & AoE/P-02/12)
9:00AM K02.00004: Topological pumping in a maGneto-mechanical system* INBAR GRINBERG (Presenter), MAO LIN, CAMERON HARRIS, WLADIMIR BENALCAZAR, CHRISTOPHER PETERSON, TAYLOR HUGHES, GAURAV BAHL, University of Illinois at Urbana-Champaign — A topological charge pump conveys quanta of charge across a gapped system while being robust against array disorder, external noise, and disorder in the pumping protocol. The implementation of topological insulators in both optical and acoustic coupled resonator systems has opened exciting paths towards new control over light and sound, however an equivalent temporal topological pump has yet to be demonstrated. In this work, we demonstrate that a 1D classical system that is adiabatically spatio-temporally modulated can produce an equivalent topological pump for bosons. Our experimental demonstration consists of an array of magneto-mechanical resonators, where the inter-resonator coupling rates are controlled by the distance over which the magnetic interaction takes place. We modulate both the coupling rates and the on-site potentials using a mechanical apparatus, and demonstrate that mechanical energy can be pumped from one edge mode of the array to the other edge mode while the system remains gapped. We show that this 1D array is the equivalent of a Chern insulator in one real dimension and one synthetic dimension.

*N.We acknowledge the supported of the US National Science Foundation and the US Office of Naval Research.

9:12AM K02.00005: Unidirectional excitation of surface plasmon polaritons in a grating system with Parity-Time symmetry YIHAO XU (Presenter), Mechanical Engineering, Northeastern University, LIN LI, YONGMIN LIU, Electrical and Computer Engineering, Northeastern University — Over the past years, there has been rapidly growing interest in non-Hermitian photonic systems. A Hamiltonian with Parity-Time (PT) symmetry can show real spectrum below a certain threshold, known as the exceptional point (EP), accompanied with novel phenomena above the EP. Here we propose a plasmonic grating system with PT symmetry to excite unidirectional surface plasmon polaritons (SPPs). We have designed realistic grating array only consisting of passive rectangular gratings (i.e., without gain materials), which can significantly reduce the challenges in fabrication and optical experiments. In addition, instead of using ideal sinusoidal permittivity modulation in simulation in former paper(2), here we demonstrate in both simulation and experiment that using discrete grating array can also achieve excellent contrast between SPPs in opposite directions. In summary, we have demonstrated a sub-wavelength scale plasmonic grating structure with PT symmetry that can realize high performance for unidirectional excitation of SPPs. These results can be employed as a new approach to designing nanoscale optical devices, such as low-loss plasmonic routers and isolators for optical computation, communication, and information processing.


9:24AM K02.00006: Atomic-scale nanophotonics and quantum optics through 2D phonon polaritons* NICHOLAS RIVERA (Presenter), Applied Physics, Harvard University, THOMAS CHRISTENSEN, Massachusetts Institute of Technology, PRINEHA NARANG, Applied Physics, Harvard University — Recent developments have demonstrated extreme confinement of electromagnetic energy in the mid-infrared via phonon polaritons in polar insulators. Phonon polaritons hold promise for low-loss nanophotonics, as well as realizing extreme interactions with quantum emitters at the single-photon level. To bring these materials to the ultimate limit of optical nano-confinement, it is critical to consider phonon polaritons in low-dimensional polar materials, where the physics of optical phonons is fundamentally different due to the lack of LO-TO splitting. In this talk, we find universal forms for the properties of phonon-polaritons in one- and two-dimensions which result from the unique character of Coulomb interactions in low-dimensional systems. Leveraging first-principles calculations of optical phonons in 2D, we calculate the polaritonic properties of polar insulator monolayers, presenting specific results for hexagonal boron nitride. We find regimes of low-loss and high-confinement of electromagnetic energy, and show how these regimes can be probed with EELS. We then show how nanostructuring can be used to develop ultrafast quantum emitters of phonon polaritons in the mid-IR.

*N.R. is supported by the DOE Computational Science Graduate Fellowship.
**9:36AM K02.00007: Zak phase of 1-D electrostatically gated graphene grating and optical properties of plasmonic edge state**

ZHIYUAN FAN (Presenter), GENNADY SHVETS, Cornell University — We design periodic metal gates on top of a hBN/Graphene/hBN sandwich heterostructure to modulate local graphene conductivity. We investigated properties of graphene surface plasmon (GSP) of a doubly gated graphene. Stop bands due to GSP modes mixing can be controlled by electrostatic doping. Topology of each plasmon band can be characterized by a Zak phase. When two insulators of a same bandgap but distinct Zak phases are joined together, an edge state in the bandgap has been observed in many physical systems. The edge state observed on our graphene grating platform presents an anisotropic dipole moment. While it radiating into the left or right in the forward direction offers an interrogation approach for band topologies of component graphene gratings, the angle of radiation remains a tunable property that depends on an interplay of the mode's resonant frequency, the bandgap width, its mid-gap frequency and the dimensions of metal gates. Due to its capability of active tuning, this may serve as a stepping stone on the way toward active control of surface plasmon band structures for optical communication, wavefront steering or sensing applications.

*Z.F. and G.S. acknowledge support from ONR Grant #N00014-17-1-2161 and UDRI Grant #RSC17004.

**9:48AM K02.00008: Broadside Coupled Resonators for Real-time Tunable Metamaterials**

XIAOGUANG ZHAO (Presenter), Boston University, JINGDI ZHANG, Department of Physics, University of California San Diego, GUANGWU DUAN, Boston University, JACOB SCHALCH, RICHARD DOUGLAS AVERITT, Department of Physics, University of California San Diego, XIN ZHANG, Boston University — Metamaterials based on broadside coupled split ring resonators (BC-SRRs) exhibit large tunability induced by modulating the coupling that arises from mutual capacitance and inductance. We design and fabricate a real-time tunable terahertz metamaterial by integrating BC-SRRs with comb-drive actuators, and characterize the dynamic response using terahertz time domain spectroscopy. The experimental results reveal that we can control the amplitude and phase of the transmission coefficient dynamically by driving the comb-drive actuators. We also observe remarkable modulation in the group delay. A two-port resonator model, derived from coupled mode theory, can analytically explain the experimental results and unveils the critical role of coupling between BC-SRRs. The results demonstrate that the propagation of electromagnetic waves can be dynamically controlled through modulating coupled resonators in metamaterials.

*Research supported by National Science Foundation under Grant No. ECCS-1309835 and ECCS-1810252.

**10:00AM K02.00009: Ultrahigh Numerical Aperture Silicon Metalens at Visible Wavelengths**

JUNTAO LI (Presenter), HAOWEN LIANG, School of Physics, Sun Yat-sen University, China, THOMAS F KRAUSS, Department of Physics, University of York, UK — High Numerical Aperture (NA) Metalens is among the promising optical elements for ultrathin microscope objective [1, 2]. Meanwhile, crystalline silicon (c-Si) has been shown to be used in the high transmission metasurfaces at visible wavelength because of its low loss and low cost [3, 4]. Here, we demonstrate an oil front-immersion metalens with NA = 1.48, a bandwidth of 211 nm and a focusing efficiency of 48% at 532 nm wavelength, base on a 500 nm thick c-Si on sapphire [2] (compared with 50% for back-immersion TiO2 metalenses with NA = 1.1 [1]). Thereby demonstrating the highest NA of any metalens at visible wavelengths reported to the best of our knowledge. We further implement our metalens onto the laser scanning confocal microscopy as the immersion objective to demonstrate the imaging quality. We note that this fabrication process is fully compatible with mature CMOS technologies. We envision this design also to be beneficial for immersion metalens doublets, thereby pushing metasurfaces into practical applications such as confocal microscopy and achromatic lenses.

References
[2] H. Liang, et. al., Nano Letters, 18, 4460, 2018
By using the dyadic Green's matrix spectral method, we demonstrate that aperiodic deterministic Vogel spirals made of electric dipoles support light localization in three dimensions, an effect that does not occur in traditional uniform random media. We discover a transition from an extended to a localized regime by evaluating the Thouless conductance and by performing a finite-size scaling. Vogel spirals are suitable photonic platforms to localize light thanks to their distinctive structural correlation properties that enable collective electromagnetic excitations with strong light-matter coupling. By decomposing the dyadic field propagator in its different components we show that light localization in Vogel arrays originates from collective electromagnetic coupling involving the contributions of multiple length scales. Our results unveil the importance of structural correlations in deterministic aperiodic photonic media for the design of localized states with strongly enhanced light-matter interactions. In addition, our findings may open new vistas for the engineering of mesoscopic transport and localization phenomena and should encourage deeper investigations of photonic devices based on deterministic aperiodic architectures.

Selected by Focus Topic Organizer Xiaobo Yin, Natalia Litchinister, Nanfang Yu

**Wednesday, March 6, 2019 8:00 AM - 11:00 AM**

**K03.00001: Classification and construction of higher-order symmetry protected topological phases of interacting bosons***

**ALEXANDER RASMUSSEN** (Presenter), **YUANMING LU**, Ohio State University — Motivated by the recent discovery of higher-order topological insulators, we study their counterparts in strongly interacting bosons: `higher-order symmetry protected topological (HOSPT) phases'. While the usual (1st-order) SPT phases in d spatial dimensions support anomalous (d-1)-dimensional surface states, HOSPT phases in d dimensions are characterized by topological boundary states of dimension (d-2) or smaller, protected by certain global symmetries and robust against disorders. Based on a dimensional reduction analysis, we show that HOSPT phases can be built from lower-dimensional SPT phases in a way that preserves the associated crystalline symmetries. When the total symmetry is a direct product of global and crystalline symmetry groups, we are able to classify the HOSPT phases using the Künneth formula of group cohomology. Based on a decorated domain wall picture of the Künneth formula, we show how to systematically construct the HOSPT phases, and demonstrate our construction with many examples in two and three dimensions.

*NSF under award number DMR-1653769 (AR,YML) and in part by NSF grant PHY-1607611 (YML).

**K03.00002: Intrinsically interacting topological crystalline insulators and superconductor***

**ALEXANDER RASMUSSEN** (Presenter), **YUANMING LU**, Ohio State University — Motivated by recent progress in crystalline symmetry protected topological (SPT) phases of interacting bosons, we study topological crystalline insulators/superconductors (TCIs) of strongly interacting fermions. We construct a class of intrinsically interacting fermionic TCIs, and show that they are beyond both free-fermion TCIs and bosonic crystalline SPT phases. We also show how these phases can be characterized by symmetry protected gapless corner/hinge states.

*NSF under award number DMR-1653769 (AR,YML) and in part by NSF grant PHY-1607611 (YML).
8:24AM K03.00003: Disorder-induced helical phase in magnetic topological insulators*

ARBEL HAIM (Presenter), Caltech, RONI ILAN, Tel Aviv University, JASON ALICEA, Caltech — In magnetically doped thin-film topological insulators, aligning the magnetic moments generates a quantum anomalous Hall phase with a single chiral edge state. We study the de-magnetization process and show that disorder from randomly oriented magnetic moments can produce a quantum-spin-Hall-like phase with counter-propagating helical edge modes protected by a unitary reflection symmetry. This phase is analogous to the quantum spin Hall effect observed in the zeroth Landau level of graphene, which is also protected by a unitary symmetry (spin rotation). We show that introducing superconductivity, combined with selective breaking of reflection symmetry by a gate, allows for creation and manipulation of Majorana zero modes via purely electrical means.

*We acknowledge support from the Army Research Office under Grant Award W911NF-17-1-0323 (J.A.); the NSF through grants DMR-1723367 (J.A.); an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation through Grant GBMF1250 (J.A.); the Caltech Institute for Quantum Information and Matter, and the Walter Burke Institute for Theoretical Physics at Caltech (A.H. and J.A.).

8:36AM K03.00004: Topological states from topological crystals*

ZHIDA SONG, Chinese Academy of Sciences, SHENG-JIE HUANG (Presenter), University of Colorado, Boulder, YANG QI, Fudan University, CHEN FANG, Chinese Academy of Sciences, MICHAEL A HERMELE, University of Colorado, Boulder — We show that crystalline symmetry protected topological states is adiabatically connected to a real-space crystalline pattern of lower-dimensional topological states, which we refer to as a topological crystal. As a demonstration of principle, we explicitly enumerate all inequivalent topological crystals for non-interacting time-reversal symmetric electronic insulators with significant spin-orbit coupling and any one of the 230 space groups in three dimensions. Because every topological crystalline insulator can be deformed into a topological crystal, the enumeration of the latter gives topological crystalline insulators a full classification and for each class an explicit real-space construction.

*SZD and CF acknowledge support from Ministry of Science and Technology of China under Ministry of Science and Technology of China under grant numbers 2016YFA0302400, 2016YFA0300600, from National Science Foundation of China under grant number 11674370, and from Chinese Academy of Sciences under grant number XXH13506-202. The research of SJH and MH is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences (BES) under Award number DE-SC0014415.

8:48AM K03.00005: Landau levels of topological surface states probed by quantum capacitance*

SU KONG CHONG (Presenter), RYUICHI TSUCHIKAWA, JARED HARMER, Department of Physics and Astronomy, University of Utah, TAYLOR D. SPARKS, Department of Materials Science and Engineering, University of Utah, VIKRAM V. DESHPANDE, Department of Physics and Astronomy, University of Utah — Three-dimensional topological insulator (3D TI) is known by its unique Dirac dispersion surface states arising from band inversion of its bulk. Development of discrete Landau levels (LLs) in strong perpendicular magnetic field provides strong evidence of quantization from two-dimensional nature of the topological surface states. Density of states of the surface states' LLs can be quantitatively determined through a quantum capacitance measurement. However, quantum capacitance in 3D TI is relatively less explored primarily due to mixing signals from the bulk or narrow bulk bandgap such as strained HgTe. In this work, we study the quantum capacitance of a truly bulk insulating 3D TI via a TI-based van der Waals heterostructures configuration. The quantum capacitance data are compared to the quantum Hall conductance in transport. By controlling the dual-gate voltages, we access the LLs from each surface states. The chemical potentials as function of charge density are extracted to quantify the LL spacings.

*A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1644779* and the State of Florida.
9:00AM K03.00006: Band structure and superconductivity in In-doped topological insulator (Pb_{0.5}Sn_{0.5})_{1-x}In_xTe probed by NMR spectroscopy∗ BEN-LI YOUNG (Presenter), PING-CHUN TSAI, Department of Electrophysics, National Chiao Tung University, GENDA GU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory — The bulk band structure and superconductivity in the In-doped topological crystalline insulators (Pb_{0.5}Sn_{0.5})_{1-x}In_xTe, for x = 0, 0.1, 0.2, and 0.3, have been investigated by nuclear magnetic resonance (NMR) techniques. We found that the NMR frequency shifts of $^{117}$Sn, and $^{207}$Pb are dominated by the spins of free charge carriers, whereas the $^{125}$Te frequency shift is determined by the magnetic orbital moments of the binding electrons. By analyzing these shifts, we conclude that In substitution for 0 ≤ x ≤ 0.3 provides not just hole carriers but also lifts the chemical potential from the valence bands to the conduction bands, in consistent with the results from the electric transport measurements. The superconductivity in the x = 0.3 sample is investigated by the nuclear spin-lattice relaxation rate (1/T_1) as a function of temperature, where a Hebel-Slichter coherence peak is observed near the critical temperature. This suggests that the superconducting gap in the bulk is fully opened and this feature may favor that (Pb_{0.5}Sn_{0.5})_{0.7}In_{0.3}Te is a conventional superconductor rather than a chiral p-wave topological superconductor.

∗This work was supported by Ministry of Science and Technology, Taiwan (Grants No. MOST 104-2112-M-009-013).

9:12AM K03.00007: Disorder-driven phase transitions in chiral-symmetric topological insulators JAHAN CLAES (Presenter), TAYLOR HUGHES, University of Illinois at Urbana-Champaign — Chiral-symmetric topological insulators exhibit properties, such as polarization, that are robust to translation-symmetric perturbations provided the perturbations do not close the energy gap. However, it's unclear to what extent these topologically protected properties are robust to disorder, as disorder breaks the translation symmetry. Here we study a collection of 2D chiral-symmetric models with disorder using a covariant real space formula for the topological invariant. Generically, we find that the topological invariants remain precisely quantized until a critical value of disorder, at which point it smoothly decreases to zero. Furthermore, we find that the critical disorder occurs exactly when states at the Fermi energy become delocalized. We therefore demonstrate that the topological characteristics are robust, and that in the presence of disorder the topology is protected by a mobility gap in place of an energy gap.

9:24AM K03.00008: Low Temperature Terahertz Nano Imaging of WTe2 Thin Film RAN JING (Presenter), YINMING SHAO, Department of Physics, Columbia University, ZAIYAO FEI, XIAODONG XU, Department of Physics, University of Washington, DIMITRI BASOV, Department of Physics, Columbia University — We discuss the development of cryogenic scanning near-field microscope suitable for nano-scale imaging and spectroscopy at terahertz frequency range with the spatial resolution below 130 nm[1]. We report terahertz near-field measurement of WTe2 thin film of 1 to 3 layers[2] above and below the metal-insulator transition. Clear contrast in near-field signal can be observed among regions with different layer numbers and between metallic and insulating state.


9:36AM K03.00009: Detection of higher order topological phase in a disordered breathing Kagome model by using machine learning HIROMU ARAKI (Presenter), TOMONARI MIZOGUCHI, YASUHIRO HATSUGAI, University of Tsukuba — A higher order topological insulator is a new concept of topological states of matter, which is characterized by the emergent boundary states whose dimensionality is lower by more than two compared with that of the bulk, and draws a considerable interest. Yet, its robustness against disorders is still unclear. Here we investigate a phase diagram of higher order topological insulator phases in a breathing Kagome model in the presence of disorders, by using a state-of-the-art machine learning technique. We find that the corner states survive against the finite strength of disorder potential as long as the energy gap is not closed, indicating the stability of the higher order topological phases against the disorders. We also discuss the relation between the higher order topological phase and the Z_3 Berry phase, which is a bulk topological invariant.
9:48AM K03.00010: Double-frequency Aharonov-Bohm effect and non-Abelian braiding property of Jackiw-Rebbi zero-mode * YIJIA WU (Presenter), International Center for Quantum Materials, School of Physics, Peking University, Beijing, China, JIE LIU, Department of Applied Physics, School of Science, Xian Jiaotong University, Xian, China, HAIWEN LIU, Center for Advanced Quantum Studies, Department of Physics, Beijing Normal University, Beijing, China, HUA JIANG, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou, China, XINCHENG XIE, International Center for Quantum Materials, School of Physics, Peking University, Beijing, China — Ever since its first proposal in 1976, Jackiw-Rebbi zero-mode has been drawing extensive attention for its charming properties including charge fractional quantization, topologically protected zero-energy and possible non-Abelian statistics. We numerically investigate the Jackiw-Rebbi zero-mode in a quantum spin Hall insulator heterostructure and show that its zero-energy nature leads to a double-frequency Aharonov-Bohm effect in electronic transport. Such observation suggests that Majorana zero-mode could be viewed as a special case of Jackiw-Rebbi zero-mode. Moreover, similar to the Majorana zero-modes, Jackiw-Rebbi zero-modes also show non-Abelian braiding properties in a cross-shaped junction. However, such non-Abelian property can be destroyed by infinitesimal disorder breaking charge-conjugation symmetry, implying the presence of charge-conjugation symmetry is of equal importance as the topological gap in the topological quantum computation.

*The work was funded by NSFC (11534001), National Key R and D Program of China (2017YFA0303301), NBRP of China (2015CB921102).

10:00AM K03.00011: Quasi-particle Interference on the Step Edges of Epitaxial Stanene on InSb (111) * JIANFENG ZHANG (Presenter), XIAOHU ZHENG, RUI-RUI DU, Peking University — Stanene (single-layer of tin), having an atomic structure similar to graphene, offers a promising platform for achieving room-temperature quantum spin Hall effect with a gap of 0.3 eV [1-3]. We have performed the in-situ scanning tunneling microscopy experiments on stanene which was epitaxially grown on the InSb (111). Several types of step edges have been observed in the atomic-resolution STM topographic image. The quasi-particle interference near the steps has been detected by STS, allowing us to study the electron scattering behavior along the edge in relation to the topological property of the edge state.

Reference:

*The work is supported by NBRPC (No.2014CB920901) and National Key R and D Program of China (No.2017YFA0303301).

10:12AM K03.00012: Experimental demonstration of the robustness of topological surface states on a PbTaSe2 superconductor HAO ZHENG (Presenter), Shanghai Jiao Tong University, SHUANG JIA, Peking University, China, HSIN LIN, Academia Sinica, ZAHID HASAN, Princeton University — Conventional semiconductor electronic surface states are determined by the details of its surface geometry, and the chemical nature of the surface atoms. Conversely, topological surface states arise entirely from the non-trivial bulk band topology. In topological insulators, the bulk electronic structure is always gapped while the surface is metallic everywhere independent of surface details. This bulk-boundary correspondence is the key manifestation of topology in a condensed matter system.

Unfortunately, there has yet to be solid experimental demonstrated in a real material. Here, on superconducting Z2 topological insulator PbTaSe2(001), we uncover two types of surfaces with distinct surface geometry and chemistry, namely 1 × 1-Se and 2 × 2-Pb surfaces. By means of scanning tunneling microscopy, we find metallic surface states on both types of surfaces. Moreover, we discern the superconducting gap to be uniform on both surfaces. Our research serves as the first experimental proof that the topological surface state is robust against surface geometry reconstruction, variation in chemical termination of the surface, and superconducting interactions, possibly opening new pathways for research in topological materials.

10:24AM K03.00013: Study of the topological surface state quantum Hall effect in the bulk-insulating topological insulator devices FENGQI SONG (Presenter), Nanjing University — In the topological insulator BiSbTeSe2 devices, which allowing an optimized surface transport, we observe the well-developed quantum Hall effect. By depositing the Co clusters on the top surface, the quantum Hall plateaus were modulated. We find an anomalous quantization trajectory for the top surface, as well as a quasi-half-integer plateau. This is due to the sizeable Zeeman gap induced by the Co clusters on the top surface through antiferromagnetic exchange coupling, which delays the Landau level hybridization for a moderate magnetic field.

Also, in the high quality Sn-Bi1.1Sb0.9Te2S devices, the quantum Hall plateau show a more precious value, which allows the study of the plateau to plateaua transition. We find the scaling exponent is nearly half of that in the traditional two dimensional electron gas, which may be originate from the electron interactions.
**10:36 AM K03.00014: Chiral Phonon Transport Induced by Topological Magnons**

EVEN THINGSTAD (Presenter), AKASHDEEP KAMRA, ARNE BRATAAS, ASLE SUDBO, Norwegian University of Science and Technology — The plethora of recent discoveries in the field of topological electronic insulators has inspired a search for boson systems with similar properties. There are predictions that ferromagnets on a two-dimensional honeycomb lattice may host chiral edge magnons. In such systems, we theoretically study how magnons and phonons couple. We find topological magneto-polarons around the avoided crossings between phonons and topological magnons. Exploiting this feature along with our finding of Rayleigh edge phonons in armchair ribbons, we demonstrate the existence of chiral edge modes with a phononic character. We predict that these modes mediate a chirality in the coherent phonon response and suggest to measure this effect via elastic transducers. These findings reveal a possible approach towards heat management in future devices.

*We acknowledge financial support from the Research Council of Norway Grant No. 262633 Center of Excellence on Quantum Spintronics*. A. S. also acknowledges financial support from the Research Council of Norway Grant No. 250985, Fundamentals of Low-dissipative Topological Matter*.

**10:48 AM K03.00015: First-order topological quantum phase transitions in strongly correlated one-dimensional systems**

SIMONE BARBARINO (Presenter), TU Dresden — Topological quantum phase transitions, such as the transition between a topological insulator and a trivial gapped phase, are hallmarked by the change of a topological invariant [1]. For non-interacting fermions, such transitions between insulating phases are continuous since they are accompanied by the closing of the band gap as long as the symmetries of the system are maintained. For interacting fermions, by contrast, this paradigm is altered and first-order topological quantum transitions can occur [2].

In my talk I discuss the first example of a first-order topological quantum phase transition in a strongly correlated one-dimensional system [3]. Specifically, I consider a four-leg ladder which supports a symmetry protected topological phase in the presence of an on-site repulsive interaction, but is driven towards a trivial phase by a nearest-neighbor interaction. Employing a DMRG approach, I investigate at a numerically exact level the first-order nature of the transition.

References

**Wednesday, March 6, 2019 8:00 AM - 11:00 AM**

Session K04 DMP: Dirac/Weyl Semimetals -- Transport I

**8:00 AM K04.00001: Transport Properties in Dirac semimetal ZrTe5**

QIANG LI (Presenter), Brookhaven National Laboratory — We report transport measurements of Dirac semimetal ZrTe5 single crystals. We found the anomalous peak in the temperature dependence of resistivity is the result of the Lifshitz transition, which also leads to a sign change in thermopower. Large negative longitudinal magneto-resistance is the result of the chiral magnetic effect. Magnetic field effectively transforms Dirac semimetals into Weyl semimetals by breaking time reversal symmetry. Large anomalous Hall effect observed in ZrTe5 is the result of the Berry curvature generated by the Weyl nodes.

*Work at Brookhaven is supported by the Office of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy (DOE) under Contract No. DE-SC0012704.*
8:12AM K04.00002: Magnetic field induced Weyl points and anomalous transport in Bi$_{89}$Sb$_{11}$* WENJUAN ZHANG (Presenter), Department of Physics, The Ohio State University, DUNG VU, Department of Mechanical and Aerospace Engineering, The Ohio State University, CUNEYT SAHIN, MICHAEL FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, NANDINI TRIVEDI, Department of Physics, The Ohio State University, JOSEPH P C HEREMANS, Department of Mechanical and Aerospace Engineering, The Ohio State University — A significant enhancement of magneto thermal conductivity in semimetal Bi$_{1-x}$Sb$_x$ alloy for a particular Sb concentration x=11% was discovered. As shown in a previous theoretical work on Weyl semimetals [1], Fermi arcs provide efficient ‘conveyor belt’ for magneto thermal transport. In this talk, we argue that Bi$_{1-x}$Sb$_x$ becomes a Weyl semimetal under magnetic field and the enhancement of magneto thermal conductivity is due to the resulting Fermi arcs, based on the tight binding parameterization calculated by a modified virtual crystal approximation. By calculating Chern numbers on two-dimensional slices of the three-dimensional Brillouin zone, we show that a pair of Weyl points appear near L points above a critical field strength, and that the separation between those Weyl points increases with the field strength which explains the anomalous angular dependence of magneto thermal conductivity on magnetic field.


*This research is supported by the Center for Emergent Materials, an NSF MRSEC, under Award Number DMR-1420451.

8:24AM K04.00003: Experimental evidence for the presence of Fermi-arc driven entropy transport in the field-induced Weyl semimetal Bi$_{89}$Sb$_{11}$* DUNG VU (Presenter), Department of Mechanical Engineering, The Ohio State University, CUNEYT SAHIN, Department of Physics and Astronomy, University of Iowa, WENJUAN ZHANG, Department of Physics, Ohio State University, MICHAEL FLATTÉ, Department of Physics and Astronomy, University of Iowa, NANDINI TRIVEDI, Department of Physics, Ohio State University, JOSEPH P C HEREMANS, Department of Mechanical Engineering, The Ohio State University — Topologically protected Fermi arc surface states in Weyl semimetals have been predicted to produce a conveyor-belt entropy transport [1]. Related theory talks [2][3] show that Bi$_{89}$Sb$_{11}$ alloys become Weyl semimetals in a magnetic field applied along the trigonal direction above a critical value $H_C$. Here, we report a strong field-induced increase in electronic thermal conductivity of Bi$_{89}$Sb$_{11}$ single crystals along the trigonal direction in longitudinal magnetic fields $H>H_C$. The Lorenz ratio increases up to 80-fold at $H=9$T. We report the temperature, length, and angular dependence of the effect in 5 different samples of Bi-Sb alloys with mobilities up to 2x10$^6$ cm$^2$V$^{-1}$s$^{-1}$. The effect is absent in fields not oriented along the trigonal direction; when the samples are doped n-type and $E_F$ s not at the Weyl point; and in the ordinary semimetal Bi$_{95}$Sb$_{5}$. We posit that the large positive magnetothermal conductivity is a unique signature of topologically protected surface states.


*Funding: NSF DMR-1420451.

8:36AM K04.00004: Supercurrent oscillations in Weyl Semimetal MoTe$_2$* WUDI WANG (Presenter), STEPHAN KIM, MINHAO LIU, ROBERT CAVA, NAI-PHUAN ONG, Princeton University — MoTe$_2$ is a type-II Weyl semimetal with intrinsic superconductivity and pressure-induced superconductivity. Our interest is in the superconducting state at ambient pressure, with $T_c$ around 100mK. We fabricated microscale MoTe$_2$ flakes with Au contacts by mechanical exfoliation and nanofabrication and measured their transport properties. We observed multiple peaks in the differential resistance (dV/dI) vs. bias current curves, and the positions of these peaks change periodically with magnetic field. Most samples show two kinds of oscillations, one is Fraunhofer Pattern (single slit diffraction) type with oscillation amplitude decreasing at high magnetic field, the other one is Young's Interference Pattern (double-slit interference) type with oscillation amplitude not decreasing. The latter one (Young's type) always has period corresponding to about 60% of the physical area of samples. We conclude that the latter one come from the edge of the crystals and indicating the existence of superconducting edge state in MoTe$_2$

*The research was supported by the U.S. Army Research Office (W911NF-16-1-0116) and a MURI award for topological insulators (ARO W911NF- 12-1-0461).
8:48AM K04.00005: General aspects of the anomaly-related magneto-conductance in Weyl semimetals  HIROAKI ISHIZUKA (Presenter), Department of Applied Physics, University of Tokyo, NAOTO NAGAOSA, Center for Emergent Matter Science, RIKEN — Magneto-conductance (MC) in Weyl semimetals is intensively studied as it is presumably related to the chiral magnetic effect. While the theory of anomaly contribution is widely accepted, its relation to the experimentally-observed MC remains controversial, because there are many other mechanisms for MC. For this purpose, the understanding on the general property of the MC is favorable, e.g., the effects of tilting, warping, and other details. However, studies on such effects are still limited, and no general understanding is reached so far. One challenge here is the lack of general and concise formalism, which is convenient for intuitive discussions.

In this work, we discuss the general behavior of anomaly-related MC by introducing a concise formalism. Using this formalism, we explicitly show that the MC in type-II Weyl semimetals is dominated by the electrons around the Weyl nodes [1]. We also show an intuitive explanation of the tilting dependence of the MC [1]. Our formalism also implies that the MC in type-I Weyl semimetals remains robust even when multiple Weyl nodes are enclosed in a Fermi surface [2].


9:00AM K04.00006: Ultra-high surface conductivity in Weyl semimetal NbAs  CHENG ZHANG (Presenter), ZHUOLIANG NI, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China, JINGLEI ZHANG, Anhui Province Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory of the Chinese Academy of Sciences, Hefei 230031, China, XIANG YUAN, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China, XIANGANG WAN, National Laboratory of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, China, SERGEY Y. SAVRASOV, Department of Physics, University of California, Davis, California 95616, USA, FAXIAN XIU, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China — In two-dimensional (2D) systems, high mobility is typically achieved in low-carrier-density semiconductors and semimetals. Increasing the carrier density in these systems to be comparable to typical metals usually degrades the mobility value, owing to an enhanced scattering probability from the large Fermi wave vector and possible charged impurities from the doping process. Here, we discover that the surface state of Weyl semimetal NbAs can overcome such a limit and maintain a high mobility even in the presence of a high carrier density. To study its surface transport properties, we first develop a new growth scheme to synthesize high-quality nanostructures of NbAs with tunable Fermi levels. Owing to the large surface-to-bulk ratio, the 2D surface state exhibits dominant quantum oscillations with a high carrier density. Combined with the high mobility value, a record-high surface sheet conductance among non-superconducting 2D systems is achieved up to 5-100 S. Corroborated by theory, we attribute the origin of the ultra-high surface conductance to the disorder-tolerant nature of Fermi arcs. Our results present the first transport evidence for the low-dissipation property of NbAs surface state and establish it as an excellent 2D metal with supreme conductivity.

9:12AM K04.00007: Current at a distance in the Dirac semimetal ZrTe5*  NICHOLAS QUIRK (Presenter), SIHANG LIANG, NAI-PHUAN ONG, Princeton University — Non-local electronic conductivity in Dirac and Weyl semimetals has been predicted to arise from charge pumping in the bulk due to the chiral anomaly, and from cyclotron-like orbits of surface Fermi arcs weaving together with bulk states. We used focused ion beam (FIB) milling to thin samples of the Dirac semimetal ZrTe5 to sub-μm thicknesses, and we created electrical devices with these samples to probe these two non-local conductivity mechanisms. We will discuss difficulties we encountered using FIB and methods we tried in order to overcome them, and we will describe experiments we undertook to detect non-local conduction.

*Gordon and Betty Moore Foundation
9:24AM K04.00008: Anisotropic Giant Planar Hall Effect in type-II Weyl Semimetals* PENG LI (Presenter), Institute for Quantum Computing, Department of Electrical and Computer Engineering, University of Waterloo, CHENHUI ZHANG, Physical Science and Engineering, King Abdullah University of Science and Technology, GEORGE NICHOLS, LONG CHEN, GUOXING MIAO, Institute for Quantum Computing, Department of Electrical and Computer Engineering, University of Waterloo, XIXIANG ZHANG, Physical Science and Engineering, King Abdullah University of Science and Technology — Recently, giant planar Hall effect originating from chiral anomaly, which is related to the chiral Landau levels, has been predicted and realized in nonmagnetic Dirac/Weyl semimetals. WTe$_2$ is considered to be an intriguing type-II Weyl semimetal with its Weyl cone tilted due to its broken inversion symmetry. Here, we report the observation in WTe$_2$ of the giant planar Hall resistivity that shows a $B^2$ magnetic-field dependences as predicted by theory. Most importantly, we observed a highly anisotropic planar Hall resistivity when the current flows along $a$- and $b$-axis of WTe$_2$. The planar Hall resistivity at low temperatures with current flowing along $b$-axis is almost twice of that along $a$-axis, because the chiral Landau levels and chiral anomaly are well-defined (or absent) when the magnetic field is parallel (or perpendicular) to the tilting direction ($b$-axis) of Weyl cone in WTe$_2$.

*It is funded by Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery grant RGPIN-04178, and Ontario Early Researcher Award. This work is also funded by King Abdullah University of Science and Technology (KAUST), Office of Sponsored Research (OSR) under the Award No. CRF-2015-SENSORS-2709 (KAUST) and CRF-2015-2626-RG4.

9:36AM K04.00009: Fermi surface study of the Weyl type-II semimetal candidate NbIrTe$_4$* RICO SCHOENEMANN (Presenter), National High Magnetic Field Laboratory, SHOUVIK SUR, Northwestern University, VICTOR QUITO, Iowa State University, YU-CHE CHIU, WENKAI ZHENG, National High Magnetic Field Laboratory, GREGORY T. MCCANDLESS, JULIA Y. CHAN, University of Texas at Dallas, LUIS BALICAS, National High Magnetic Field Laboratory — Here we present a study of the Shubnikov-de Haas (SdH) effect in the type-II Weyl semimetal candidate NbIrTe$_4$. Quantum oscillations were obtained at temperatures down to 0.3 K and in high magnetic fields up to 35 T. The angular dependence of the SdH frequencies is in good agreement with results from DFT calculations, although we are not able to detect every orbit. We observe an unusual butterfly shaped magnetoresistance as a function of the sample orientation with respect to the magnetic field, which is likely to originate from the shape and anisotropy of the Fermi surface. Furthermore, we measured a large non-saturating magnetoresistance up to fields 35 T which suggests charge carrier compensation. On the other hand Hall measurements indicate significantly different electron and hole densities, which implies that the non-saturating magnetoresistance is not driven by charge carrier compensation.

*This work was supported by DOE-BES through Award No. DE-SC0002613. The NHMFL is supported by NSF through NSF-DMR-1157490 and the State of Florida.

9:48AM K04.00010: Weyl fermion-phonon coupling and magnetic-field-induced large thermopower in TaP FEI HAN (Presenter), THANH NGUYEN, Nuclear Science and Engineering, Massachusetts Institute of Technology, NINA ANDREJEVIC, Materials Science and Engineering, Massachusetts Institute of Technology, RICARDO PABLO PEDRO, MINGDA LI, Nuclear Science and Engineering, Massachusetts Institute of Technology — Weyl semimetals (WSM) have massless chiral fermions, the so-called Weyl Fermions. The chiral anomaly in its magneto-transport is one of the signatures for the existence of the plus and minus Weyl nodes which always appear in a pair. Recent theoretical predictions discussed the possibility to detect chiral anomaly based on phonon spectra, where the exotic electronic degrees of freedom in a WSM are playing an increasingly important role to influence the phonon structure. We measured the phonons via inelastic X-ray scattering (IXS) on the TaP crystals near the Weyl points, where an ambipolar behavior is observed when moving away from the Weyl points. This is a reliable indicator of the existence and the strength of Weyl fermion-phonon coupling. We are further using the magnetic field to break the time-reversal-symmetry for observing the central phenomenon of chiral anomaly. We also observed an unexpected magnetic-field-induced large thermopower in TaP. We consider the large thermopower of the Weyl semimetal induced by magnetic field subjected to a quantizing magnetic field. The thermopower of the Weyl semimetal grows linearly with the field without saturation and can reach extremely high values. This sheds lights on the achievement of a record-high thermoelectric figure-of-merit.
10:00AM K04.00011: Observation of Magic Angle Effect in Angular Dependence of Magnetoresistance of ZrTe5 in the Quantum Limit* 

JOSHUA Mutch (Presenter), MINHAO HE, XINGHAN CAI, PAUL MALINOWSKI, XIAODONG XU, JIUN-HAW CHU, University of Washington — We report the discovery of sharp, anomalous dips in the angular dependence of magnetoresistance in ZrTe5 single crystals. These dips occur at fixed "magic angles" once the magnetic field passes the quantum limit. The magic angles correspond to commensurate angles where the field direction connecting neighboring atoms in the lattice, reminiscent of “Lebed's Magic Angles” found in the organic Bechgaard salts (TMTSF)2X. Unlike the Bechgaard salts, a quasi-1D open fermi surface is absent in ZrTe5. In contrast, it has a closed ellipsoidal Fermi surface well contained within a small fraction of the Brillouin zone. We discuss how the effect of commensurability may arise in a 3D Dirac system in high magnetic field.

*NSF MRSEC at UW (DMR1719797)
Gordon and Betty Moore Foundation's EPIQS Initiative, Grant GBMF6759

10:12AM K04.00012: Engineering Spin Hall Conductivity and Topological Character in Group-IV Tellurides and a Family of Weyl Semimetals* 

HAIHANG WANG (Presenter), JAGODA SLAWINSKA, University of North Texas, SILVIA PICOZZI, CNR-SPIN, Chieti, Italy, MARCO BUONGIORNO NARDELLI, University of North Texas — The discovery of topological insulators and topological semimetals has become one of the leading fields of research in condensed matter physics. The origin of these emerging quantum properties can be traced to the topology of the bulk band structure and the interplay with spin-orbit coupling. In particular, the ability to engineer band topologies would open the way to the design of materials with novel functionalities. In this work, we focus on the spin-Hall current as the main physical property emerging from the topology of the bands: through the interplay of strain and ferroelectricity, we demonstrate the emergence of giant spin-Hall effect in Group-IV Tellurides. Finally, we will also discuss the results of a recent investigation on a family of Weyl semimetals that was isolated through a high-throughput screening of materials in the AFLOW database. All the results, including the searching and characterization of topological materials, have been obtained using the PAOFLOW package, which is integrated into the AFLOWπ framework.

*This work is supported by DOD-ONR (N00014-13-1-0635, N00014-11-1-0136, N00014-15-1-2863). The calculations were performed on Talon3 at the University of North Texas, TACC at the University of Texas, Austin and the HPC Center at Department of Defense.

10:24AM K04.00013: Quantum limit properties of Weyl semimetals* [Invited] 

BRAD RAMSHAW (Presenter), Cornell University, KIMBERLY MODIC, Max Planck Institute for Chemical Physics of Solids, ROSS MCDONALD, ARKADY SHEKHTER, ERIC BAUER, FILIP RONNING, Los Alamos National Labs, TOBIAS MENG, TU Dresden, YI ZHANG, EUN-AH KIM, Cornell University, MUN CHAN, FEDOR BALAKIREV, ALBERT MIGLIORI, Los Alamos National Labs, PHILIP MOLL, Ecole polytechnique federale de Lausanne, MAJA BACHMANN, Max Planck Institute for Chemical Physics of Solids, NIRMAL GHIMIRE, Argonne National Laboratory —

Electrons confined to their 0th Landau level by extreme magnetic fields—a regime known as the quantum limit—experience strong electron-electron interactions, making them unstable to the formation of new states of matter. The discovery of monopnictide Weyl semimetals has renewed interest in the high-field properties of 3D electrons, with the added twist of linear electronic dispersions. We use magnetic fields up to 95 Tesla to take the Weyl semimetals NbP and TaAs into their quantum limit. In electrical transport and torque magnetometry, we identify signatures of the 0th Landau levels that are unique to Weyl fermions. In NbP, we show that Weyl fermions can be accessed in high fields, even when the zero-field chemical potential lies far from the nodes. In TaAs, we find that the left and right Weyl nodes are mixed by magnetic field, which opens a gap and suppresses the anomalous "ABJ"-induced conductivity. At the very highest fields in TaAs, we observe a thermodynamic phase transition to an as-yet unidentified state, indicating that Weyl semimetals are unstable to the formation of new states of matter.


Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K05 DMP: Topological Superconductivity: Fe-based Materials BCEC 108 - Qimin Yan, Temple Univ - Tag(s): Focus
8:00AM K05.00001: Majorana bound state observed in Fe-based superconductors [Invited] LINGYUAN KONG
(Presenter), Institute of Physics, Chinese Academy of Sciences — Iron-base superconductor (FeSC) is nontrivial on both
topological band structure and exotic quasiparticle excitations. Recently, Majorana bound state (MBS) was observed as
non-split zero-bias conductance peak across a vortex core of Fe(Te, Se). Due to a small Fermi energy, a large energy gap
separates the MBS with other trivial bound states, which makes FeSC a promising high-Tc platform for advance study of
MBS and topological quantum qubit. In this talk, I will focus on the properties of MBS shown in our STM experiments. We
found the observed MBS is most probably contributed by surface “Dirac fermions”. The “unavoidable” bulk of Fe(Se, Te)
plays as quasiparticle bath, which destroys MBS in a lifting temperature. I will also discuss some new Majorana evidences
of FeSC identified in recent tunneling experiments.

Reference


8:36AM K05.00002: Probing the Superconducting State of FeTe0.55Se0.55 with Point-Contact Spectroscopy* MASON
GRAY (Presenter), RYAN O’CONNOR, SAMUEL JENKINS, JOSEF FREUDENSTEIN, Boston College, RUIDAN ZHONG, GENDA GU,
Brookhaven National Lab, KENNETH BURCH, Boston College — The material FeTe1-xSex provides an easy platform to study the
Iron-based superconductors due to its simple crystal structure and relatively high superconducting transition temperature.
In addition, some recent ARPES and STM studies suggest that FeTe0.55Se0.45 may be topologically non-trivial. With this in
mind, we use Point-Contact Differential Conductance studies to further investigate this material. We find a “Cusp-like” Zero
Bias Conductance Peak (ZBCP) emerges below Tc. The magnetic field dependence of this ZBCP is investigated as a function
of field angle and temperature in order to determine its physical origin.

*NSF DMR-1709987

8:48AM K05.00003: Fragile zero-energy vortex bound state in the topological superconductor candidate
FeTe0.6Se0.4* TADASHI MACHIDA (Presenter), Center for Emergent Matter Science, RIKEN, YUE SUN, Department of Physics and
Mathematics, Aoyama Gakuin University, SUNSENG PYON, Department of Applied Physics, The University of Tokyo, SHUN TAKEDA,
Materials and Structures Laboratory, Tokyo Institute of Technology, YUHIKO KOHSAKA, TETSUO HANAGURI, Center for Emergent
Matter Science, RIKEN, TAKAO SASAGAWA, Materials and Structures Laboratory, Tokyo Institute of Technology, TSUYOSHI TAMEGAI,
Department of Applied Physics, The University of Tokyo — Majorana fermions are predicted to emerge in vortex cores of
topological superconductors. Although the presence of a zero-energy bound state (ZEBS) is a hallmark of the Majorana
fermions, it is still controversial due to the limited energy resolution and statistics [1-4]. Using a dilution-refrigerator
scanning tunneling microscope [5], we performed high-energy-resolution tunneling spectroscopy on quantum-limit vortex
cores in the topological superconductor candidate FeTe0.6Se0.4. We have found that some vortices host ZEBS and others
do not. The proportion of the vortices with the ZEBS decreases with the field strength, from > 80 % at 1 T to < 10 % at 6 T.
This apparent fragility of the ZEBS sheds light on the relation between the ZEBS and Majorana fermions.


*This work was partly supported by CREST Project No. JPMJCR16F2 from JST.
9:00AM K05.00004: Topological Vortex Phase Transitions in Iron-Based Superconductors  
SHENGSHAN QIN, Kavli Institute of Theoretical Sciences, LUNHUI HU (Presenter), University of California, San Diego, XIANXIN WU, Institute for Theoretical Physics and Astrophysics, Julius-Maximilians University of Wurzburg, Am Hubland, D-97074 Wurzburg, Germany, XIA DAI, Key Laboratory of Aperture Array and Space Application, Hefei, 230088, China, CONGCONG LE, Kavli Institute of Theoretical Sciences, CHEN FANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, FU-CHUN ZHANG, Kavli Institute of Theoretical Sciences, JIANGPING HU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We study topological vortex phases in iron-based superconductors. Besides previously known Majorana zero mode (MZM) phase protected by the existence of a three dimensional (3D) strong topological insulator (TI), we show that there are two additional phases as iron-based superconductors can be doped superconducting 3D weak topological insulators (3DWTI), a series of two dimensional (2D) topological insulators stuck along the third direction weakly. The vortex bound states of a superconducting 3DWTI, unlike in a 3D strong topological insulator, exhibit two different types of quantum states: (1) a robust nodal superconducting phase with pairs of bulk Majorana zero modes; (2) a full-gap topologically nontrivial superconducting phase, which has single vortex end MZM in a certain range of doping level. The recently observed zero bias peak in the vortex of (Li$_{0.8}$Fe$_{0.2}$)OHOFeSe belongs to the second case. We predict that some iron-based superconductors can be 3DWTIs of the first case, namely, their vortex states are quasi one-dimensional topological nodal superconductors.

9:12AM K05.00005: Mixed phase of iron based Dirac superconductors*  
ELIO KOENIG (Presenter), PIERS COLEMAN, Rutgers University, New Brunswick — Recently, bulk 3D Dirac semimetallic touching points were observed via ARPES in Li(Fe$_{1-x}$Co$_x$)As.[1] Separately, zero-bias vortex-core Majorana subgap states were reported using STM on the surface of the topological iron based superconductor FeTe$_{0.55}$Se$_{0.45}$.[2] Crucially, close to the topologically relevant Γ-Z line, this second material has a very similar band structure as Li(Fe$_{1-x}$Co$_x$)As. The Majorana modes are attributed to emergent topological 2D Dirac surface states with proximity induced superconductivity, i.e. via a Fu-Kane like mechanism which is independent from the 3D Dirac bulk states. Yet, we show that, in certain parameter regimes, the 3D Dirac semimetallic touching points also provide Majorana subgap states which disperse along the vortex tube. Here, we investigate experimental signatures of the latter and thereby demonstrate a route to unveil the rich topological structure of iron based superconductors.


*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award DE-FG02-99ER45790 (Elio Koenig and Piers Coleman).

9:24AM K05.00006: Quantum anomalous vortex and Majorana zero mode in iron-based superconductor Fe(Fe,S)  
ZIQIANG WANG (Presenter), KUN JIANG, Boston College, XI DAI, Hong Kong University of Science and Technology — In conventional spin-singlet s-wave superconductors, a time-reversal symmetry breaking magnetic impurity creates a vortex-free defect hosting the Yu-Shiba-Rusinov (YSR) states inside the superconducting (SC) gap. We show that this folklore changes in s-wave superconductors with strong spin-orbit coupling (SOC). In this case, topological defect excitations can nucleate through a quantized phase winding of the SC order parameter around the magnetic ion without applying an external magnetic field. The role of the magnetic field is played by the exchange field and SOC as in the anomalous Hall effect. Such vortices, dubbed quantum anomalous vortices (QAVs), support robust Majorana zero-energy modes (MZMs) when superconductivity is induced in the topological surface states. We demonstrate that the zero-energy bound states observed in Fe(Fe,S) superconductors are possible realizations of the MZMs localized at the QAVs produced by the interstitial magnetic Fe. The quantum anomalous vortex matter can provide an advantageous platform for manipulating MZMs in quantum computing.

*This work is supported by the U.S. Department of Energy, Basic Energy Sciences Grant No. DE-FG02-99ER45747.
In this work, we present angle-resolved photoemission spectroscopy study for 122* type TlCo2-xNi_xSe2 (x=0, 0.6, 1.2, 1.6, 1.9, 2.0) samples. The parent TlCo2Se2 (x=0) sample has an incommensurate spiral spin structure. With the increase of Ni doping content, the Néel temperature increase firstly and then decrease above x_c, in conjunction with the variation of lattice parameters. The AFM ordering disappears at x~1.7 eventually after which superconductivity occurs with maximum Tc~4 K for x=2. The superconducting temperature becomes higher with the doping concentration increases. ARPES results show a Dirac cone band along Z-M momentum path. It shifts down rigidly with doping which should be owing to the change of chemical potential. The photoemission circular dichroism suggests the chirality of the orbital angular momentum. Our results thus strongly suggest their possible topological origin. We also shown that the change of effective bandwidth, which is closely related to the iternerant and electron correlation. The study of Fermi surfaces evolution can clarify the carrier-doping-induced phase transition in this system. Our results facilitate to figure out the electronic structure for deep understanding on the complex phase diagram in the system.

**9:48AM K05.00008: Prediction of CoSb as a new layered superconductor**

WENJUN DING (Presenter), M. USMAN MUZAFFAR, WEI QIN, PING CUI, ZHENYU ZHANG, ICQD, University of Science and Technology of China — FeSe-based superconductors have been actively studied in the field of high temperature superconductivity due to their relatively simple structures and exotic superconducting phenomena. Bulk FeSe possesses a superconducting transition temperature (T_c) of ~8 K, while substantially enhanced T_c of ~65 K has been reported in one-unit-cell FeSe films on the SrTiO3(001) substrate. To date, the underlying superconducting and enhancement mechanisms are still under active debate. Here we employ first-principles calculations to predict a new layered superconductor of CoSb, which is isovalent to, and shares the same planar crystal structure with the single-layer FeSe. The electronic structures of the two systems are also very similar. In contrast, the magnetic properties of CoSb are distinctly different from that of FeSe, thereby offering new opportunities for exploiting high-T_c superconductivity and the underlying pairing mechanisms.

**10:00AM K05.00009: Observation of concurrent mass enhancement and superconductivity in a topological state**

NADER ZAKI (Presenter), JONATHAN DAVID RAMEAU, GENDA GU, PETER JOHNSON, Brookhaven National Laboratory — Low energy, laser-based ARPES is used to examine the temperature dependence of a topological state previously reported1,2 for the Fe-based superconductors, FeSe_xTe_1-x. In the present study of the same system at temperatures below the superconducting transition we observe the concurrent onset of mass enhancement at the Dirac point, suggestive of time reversal symmetry breaking, and the appearance of the superconducting gap at the Fermi level crossing. We discuss possible explanations for the coincident presence of these two gaps below T_c. At the same time, focusing on the Dirac state provides some evidence for increased robustness of superconductivity in the surface layer.

1Zhang et al., Science 360, 182 (2018)
2J.D. Rameau et al., (submitted)

*The work carried out at Brookhaven was supported in part by the U.S. DOE under Contract No. DE-SC0012704 and in part by the Center of Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy.

**10:12AM K05.00010: Topological Excitations in Three-band Anisotropic Superconductors**

ANDREA BENFENATI (Presenter), EGOR BABAEV, Royal Institute of Technology — In the recent experimental paper [1] it was reported a disordered-driven transition from the s_± to s_++ states in Ba(Fe_{1-x}Rh_x)2 As2. Theoretically this effect was studied in [2] and the field-induced coexistence of superconducting states in dirty multiband superconductors was investigated in [3]. In [4] a structural change in the morphology of vortex cores was found at the impurity-scattering-driven crossover in two-band superconductors.

We report a study of vortex matter in a three-band model near the s_± to s_++ state crossover where the vortex morphology is unusually sensitive to anisotropies, yielding various structural phase transitions in vortex matter. The work was supported by the Swedish Research Council Grant No. 642-2013-7837 and by Göran Gustafsson Foundation for Research in Natural Sciences and Medicine.

10:24 AM K05.00011: Non-local electrostatic gating in Majorana nanowires  
Jouri Bommer (Presenter), Hao Zhang, Michiel de Moor, Di Xu, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Sasja Gazibegovic, Roy L. M. Op Het Veld, Erik P. A. M. Bakkers, Department of Applied Physics, Eindhoven University of Technology, Mihir Pendharkar, Electrical and Computer Engineering, University of California, Santa Barbara, Chris Palmstrom, Materials Engineering, University of California, Santa Barbara, Leo P. Kouwenhoven, Station Q Delft, Microsoft — Ever since the predicted existence of Majorana Zero-Modes (MZMs), the building blocks of topological quantum computation in hybrid semiconductor-superconductor wires, experimental efforts to detect signatures of MZMs have mainly focused on tunneling experiments, culminating in the recent observation of quantized Majorana conductance. However, the local probes used in previous studies cannot unambiguously reveal the non-local separation of MZMs, the hallmark of topological superconductivity. Here we study non-local properties of MZMs in tunneling spectroscopy on InSb nanowires covered with epitaxial aluminium by using two separate gates underneath the superconductor, one to tune part of the wire into the topological phase and an additional remote gate to tune the potential at the far end of the topological section. By tuning the remote gate we observe zero-bias peak splitting in the local tunneling measurement, presumably due to variation in the overlap between MZMs at the two ends. In contrast, trivial Andreev Bounds States, identified by instability with respect to the local gates, are completely insensitive to the remote gate.

10:36 AM K05.00012: Spectroscopic evidence of chiral Majorana modes in a quantum anomalous Hall insulator/superconductor heterostructure  
Jian Lyu (Presenter), Physics, Hong Kong University of Science and Technology — Topological superconductors are considered the key to realize topological quantum computation. With the discovery of quantum anomalous Hall insulator (QAHI), it has been proposed that heterostructure of QAHI with conventional superconductor can be an ideal platform for obtaining Majorana fermion. By introducing superconductivity into dissipationless edge state of QAHI, two chiral Majorana edge modes with different Chern number $N$ of 1 and 2, respectively, can be generated. Recently, He et al. discovered the signature of integer and half-integer quantized conductance plateaus in QAHI/SC heterostructure. However, few arguments have indicated that there may be other mechanism to explain the phenomenon. Here we show spectroscopic evidence to support the existence of superconducting QAHI state at the edge of QAHI/SC heterostructure by using nano-point contact technique. Two different topological non-trivial phases are observed when the QAHI is gradually driven through its magnetization reversal. The $N = \pm 1$ phase with a conductance near $2e^2/h$ occurs in a narrow field regime just before the QAHI enters a trivial insulating state. Our results are consistent with theoretical predictions and will help to confirm the previous result of half-integer quantization due to Majorana fermion.

10:48 AM K05.00013: Topological vortex chain realized in type-II superconductors*  
Wei Qin (Presenter), Zhenyu Zhang, University of Science and Technology of China — In type-II superconductors, the Caroli-de Gennes-Matricon (CdGM) states were predicted as the low-energy quasiparticle excitations around a single Abrikosov vortex. For a periodic vortex lattice, the quantum tunneling effect between intersite CdGM states leads to the formation of Bloch-like bands inside the superconducting gap. In contrast to normal solids, such type of Bloch band describes the behaviors of Bogoliubov quasiparticles with the particle-hole symmetry naturally preserved. Here, we carry out theoretical studies on the potential topological properties harbored by these exotic Bloch bands. First, we investigate the quasiparticle excitations around an isolated magnetic vortex in the presence of Rashba spin-orbit coupling (SOC), which is demonstrated to lift the doubly degenerate CdGM states. Next, we construct a one-dimensional (1D) vortex chain and explore the SOC-induced band gap opening around the Fermi level. Based on symmetry analysis, the opened band gap possesses odd parity, indicating that the vortex chain essentially mimic a Kitaev chain, which is characterized by Majorana end modes. These findings can be naturally extended to 2D vortex lattice, thus providing generic appealing platforms for realizing and manipulating Majorana fermions.

*Supported by NSF of China

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K06 DCMP: Hidden Order in URu2Si2 and Other Compounds
BCEC 109A - Ryan Baumbach, National High Magnetic Field Laboratory
8:00AM K06.00001: Field-induced ferrohastatic order in cubic and tetragonal heavy fermion materials*  
REBECCA FLINT (Presenter), JOHN VAN DYKE, MILAN KORNJACA, Physics and Astronomy, Iowa State University — Heavy fermion compounds with non-Kramers doublet ground states can realize a novel heavy Fermi liquid with spinorial hybridization ('hastatic' order) that breaks both single- and double-time reversal. Hastatic order was initially proposed to explain the hidden order in the tetragonal URu2Si2, which is stable in magnetic field up to 35T. Now several cubic Pr-"1-2-20" materials exhibit a suggestive heavy Fermi liquid stabilized in intermediate magnetic fields. In this talk, we develop a simple, yet realistic model of ferrohastatic order in both cubic and tetragonal symmetries, and elaborate its experimental signatures and behavior in field, where it is a good candidate to explain the observed heavy Fermi liquids.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0015891.

8:12AM K06.00002: Kondo hybridization and enigmatic f-quasiparticles emerging from deep within the antiferromagnetic phase of USb2*  
IOANNIS GIANNAKIS (Presenter), JUSTIN LESHEN, MARIAM KAVAI, Department of Physics, Applied Physics and Astronomy, Binghamton University, Binghamton, SHENG RAN, SHANTA SAHA, NICHOLAS BUTCH, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, PEGOR AYNAJIAN, Department of Physics, Applied Physics and Astronomy, Binghamton University, Binghamton — Novel electronic phenomena frequently form in heavy fermion systems because of the f-electrons' localized and itinerant nature. When magnetically ordered, the f moments are expected to be frozen and localized, decoupled from the Fermi surface. It remains ambiguous whether a Kondo-lattice can emerge from deep inside the magnetic phase or simply breaks down below TN. Using spectroscopic imaging with the scanning tunneling microscope complemented by neutron scattering, we probe the electronic states in the antiferromagnetic USb2 as a function of temperature. We visualize an antiferromagnetic gap at high temperatures (T<TN~200K) in which Kondo hybridization gradually develops below Tcoh~80K near the Fermi energy. At T*=45K we find an electronic transition through the abrupt emergence of non-trivial sharp 5f quasiparticles, whose appearance agrees with the sudden release of entropy seen in specific heat. Our findings demonstrate the emergence of Kondo physics from inside USb2's antiferromagnetic phase, spectroscopically establishing the dual nature of f-electrons, and reveal an enigmatic electronic transition, which may share connection with the ‘hidden order’ phase of URu2Si2.

*We acknowledge support from the U.S. National Science Foundation (NSF) CAREER under award No. DMR-1654482.

8:24AM K06.00003: ARPES/STM study of the surface terminations and 5 f-electron character in URu2Si2*  
WEN ZHANG (Presenter), Science and Technology on Surface Physics and Chemistry Laboratory — Hidden order in URu2Si2 has remained a mystery that is now entering its fourth decade. The importance of resolving the nature of the hidden order has stimulated extensive research. Here we present a detailed characterization of different surface terminations in URu2Si2 by angle-resolved photoemission spectroscopy, in conjunction with scanning tunneling spectroscopy and dynamical mean-field theory calculations that may unveil a piece of this puzzle. The U-terminated surface is characterized by an electronlike band around the X point, while a holelike band characterizes the Si-terminated surface. We also investigate the temperature evolution of the electronic structure around the X point from 11 up to 70 K, and do not observe any abrupt change of the electronic structure around the coherence temperature (55 K). Our results suggest that surface terminations in URu2Si2 are an important issue to be taken into account in future work.

*the National Natural Science Foundation of China (Grants No. 11874330, No. 11504342, No. 11504341, No. 11774320, and No. 11704347), Science Challenge Project (Grant No. TZ2016004), and National Key Research and Development Program of China (Grant No. 2017YFA0303104)
8:36AM K06.00004: Gaussian fluctuation corrections to a mean-field theory of complex hidden order in URu$_2$Si$_2$\textsuperscript{*}

PENGTAO SHEN (Presenter), MAXIM DZERO, Kent State University — Hidden-order phase transition in the heavy-fermion superconductor URu$_2$Si$_2$ exhibits the mean-field-like anomaly in temperature dependence of heat capacity. Motivated by this observation, here we explore the impact of the complex order parameter fluctuations on the thermodynamic properties of the hidden order phase. Specifically, we employ the mean-field theory for the hidden order which describes the hidden order parameter by an average of the hexadecapole operator. We compute the gaussian fluctuation corrections to the mean-field theory equations including both the fluctuations due to “hidden order” as well as antiferromagnetic order parameters. We find that the gaussian fluctuations lead to the smearing of the second-order transition rendering it to become the first-order one. The strength of the first-order transition is weakly dependent on the strength of underlying antiferromagnetic exchange interactions.

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*NSF-DMR-1506547

DE-SC0016481

8:48AM K06.00005: Pressure-Induced Rotational Symmetry Breaking in URu$_2$Si$_2$

JAEWON CHOI (Presenter), OLEH IVASHKO, NIK DENNLER, Physik-Institut, Universität Zürich, MARKUS HUECKER, Department of Condensed Matter Physics, Weizmann Institute of Science, DAI AOKI, Institute of Material Research, Tohoku University, KARIN VON ARX, Physik-Institut, Universität Zürich, SIMON GEBER, Laboratory for Micro and Nanotechnology, Paul Scherrer Institut, OLOT GUTOWSKI, Deutsches Elektronen-Synchrotron DESY, MARK H FISCHER, Institute for Theoretical Physics, ETH Zürich, JOERG STREMPFER, MARTIN V. ZIMMERMANN, Deutsches Elektronen-Synchrotron DESY, JOHAN CHANG, Physik-Institut, Universität Zürich — The heavy-fermion compound URu$_2$Si$_2$ has provided an excellent arena to study phase transition and related symmetry breaking in correlated electron system. Despite of relentless efforts for several decades, elucidating the nature of hidden order (HO) phase at 17.5 K still remains enigmatic. Even though the experimental evidences for both broken rotational [1] and chiral symmetry [2] were found recently, little is known about crystal structure of the system. Here, we report a hard x-ray diffraction study of the single crystal URu$_2$Si$_2$ under hydrostatic pressure. For pressure above 3.4 kbar, we found a rotational symmetry breaking from tetragonal to orthorhombic crystal structure with onset temperatures near 100 K. Contrast to recent x-ray diffraction study [3], the pressure-induced orthorhomicity is not coincided with the HO transition. Instead, its temperature-dependence suggests possible relevance with the antiferromagnetic (AF) order. This observation has not yet been predicted by theories describing an adiabatic continuity of a complex order parameter. Therefore, our findings provide new perspectives to the long-standing conundrum.


9:00AM K06.00006: Temperature T vs Os concentration x phase diagram for URu$_{2-x}$Os$_x$Si$_2$ single crystals\textsuperscript{*}

ALEXANDER BREINDEL (Presenter), KALYAN SASMAL, NAVEEN POUSE, CHRISTIAN WOLOWIEC, SHENG RAN, M BRIAN MAPLE, University of California, San Diego — The compound URu$_2$Si$_2$ has attracted much interest due to its “hidden order” (HO) phase, whose order parameter has not been definitively determined after more than three decades of research on this compound. The substitution of isoelectronic Fe for Ru in URu2Si2 produces a transition from the HO phase to a large moment antiferromagnetic (LMAFM) phase, similar to what occurs under the application of pressure. This has been attributed to the “chemical pressure” associated with the substitution of the smaller Fe atom for Ru, which increases with Fe concentration. The substitution of isoelectronic Os for Ru also produces a transition from the HO to the LMAFM phase with increasing Os concentration. Since the substitution of Os, which is larger than Ru, generates a negative chemical pressure, this suggests other factors must be involved in the case of Os (e.g., spin-orbit coupling, increased hybridization due to increased spatial extent from Os d-orbitals). In this talk, we present the T vs x phase diagram, based on electrical resistivity, specific heat, magnetization, and thermal expansion measurements as a function of temperature and pressure, for Czochralski grown URu$_{2-x}$Os$_x$Si$_2$ single crystals.

*This research was supported by US DOE DE-FG02-04ER46105 and NSF DMR-1810310.
**9:12AM K06.00007: Pressure tuning in URu$_2$Si$_{2-x}$P$_x$**  
GRETA CHAPPELL (Presenter), DAVID E GRAF, KEVIN HUANG, ANDREW GALLAGHER, RYAN BAUMBACH, Florida State University — In an effort to elucidate the unknown hidden ordered state at $T_0 \sim 17.5$ K in the heavy fermion compound URu$_2$Si$_2$, temperature dependent electrical resistivity measurements were performed on the electron doping chemical substitution series Si $\rightarrow$ P under quasi-hydrostatic pressures up to 21 kbar. Previous studies show that electron doping causes the HO to be rapidly suppressed towards zero temperature over a small $x$-range, after which there is a broad paramagnetic (PM) region that is eventually replaced by antiferromagnetic (AFM1) order at large $x$\cite{1,2}. Our results indicate that, like $x = 0$, HO transforms to AFM2 at critical pressures that decrease with increasing $x$, while the PM and AFM1 states are robust against pressure. We will present the resulting $T - x - P$ phase diagram and discuss the ordered states in the electronic phase space surrounding URu$_2$Si$_2$.


*This work was performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation Cooperative Agreements Nos. DMR-1644779 and 1157490 and the State of Florida.

**9:24AM K06.00008: Observation of the hybridization gap in different ground states of URu$_2$Fe$_x$Si$_2$ and URu$_2$Si$_2$-xP$_x$**  
SHENZHI ZHANG (Presenter), GRETA CHAPPELL, RYAN BAUMBACH, Florida State University, NADEVEN POUSE, M BRIAN MAPLE, Physics, University of California, San Diego, LAURA H GREENE, WAN KYU PARK, Florida State University — Quasiparticle scattering spectroscopy (QPS) applied to heavy fermions utilizes a ballistic junction to probe how electrons scatter off strongly energy-dependent density of states in the bulk\cite{1}. Our previous QPS study on URu$_2$Si$_{2-x}$P$_x$\cite{2} found that a hybridization gap opens regardless of the ground state ordering as it was also observed in the no-order region, consistent with earlier reports where a hybridization gap was observed to open well above the hidden order transition temperature in URu$_2$Si$_2$\cite{1}. Fe substitution acts like the application of chemical pressure\cite{3} and the resulting phase diagram closely resembles the case of hydrostatic pressure, providing a new opportunity to probe the coexistent/competing region. We will present conductance spectra as a function of temperature and chemical substitution and discuss the correlation between hybridization process and emergent ground states.

\[1\] W. K. Park et al. PRL 108, 246403 (2012) 
\[2\] A. Gallagher et al. Nat. Commun. 7, 10712 (2016) 
\[3\] S. Ran et al. PNAS 113,13348(2016).

*NHMFL and GC is supported by NSF/DMR-1644779,1157490 and the State of Florida. SZ by the CES, a DOE EFRC under Award DE-AC0298CH1088 and the NSF/DMR 17-04712.WKP and LHG by the NSF DMR 17-04712.RB by the NSF/DMR 11-57490.NP and MBM by DOE DE-FG02-04ER46105

**9:36AM K06.00009: Optical conductivity of URu$_2$Si$_{2-x}$P$_x$ from the hidden-order to the antiferromagnetic phase**  
ALEXANDRE ZIMMERS (Presenter), RICARDO LOBO, LPEM, ESPCI, PSL University, CNRS, Sorbonne University, Paris-France, RYAN BAUMBACH, National High Magnetic Field Laboratory, Florida State University — We report the optical spectroscopy of the URu$_2$Si$_{2-x}$P$_x$ heavy fermion chemical substitution series. For $x=0$, this material is the now well-studied URu$_2$Si$_2$ compound with a Kondo temperature of 370K. In this material, the hybridization between heavy f electrons with conduction electrons creates a crossover to a Kondo liquid state having coherent transport properties below 70K. At 17.5K, a second-order mean-field transition creates an electronically ordered state whose origin remains unknown, commonly called the hidden order (HO) phase. Finally below 1.5K an unconventional superconducting phase emerges. The HO phase disappears for $x>0.035$ and, at much higher doping $x>0.25$, an antiferromagnetic phase (AFM) emerges at low temperature ($T_N\sim40K$ for $x=0.28$).

Here we investigated the passing between the HO and AFM phase by measuring the optical conductivity from 300K to 5K for $x=0.02, 0.23$ and 0.28 samples. Distinct optical signatures are observed. For $x=0.02$ (HO), a 6.5meV gap opens at low temperature in accordance with values observed in undoped samples. For the $x=0.28$ (AFM) a distinct higher energy gap is seen for $T<T_N$. At intermediate doping $x=0.23$, no particular spectral feature has been found. The spectral weight transfer of these various gap openings will be presented and discussed.
For strongly correlated f-electron metals it is commonplace for exotic ordered states to occur at temperatures well below the Kondo coherence temperature. More unusual is for phase transitions to emerge from the incoherent f-electron lattice at elevated temperatures, where single ion Kondo physics and strong thermal fluctuations would naively be presumed to be dominant terms. This is despite the prevalence of structural/electronic instabilities in the isolated f-electron elements, where a leading example is plutonium which undergoes six structure changes and features novel behavior including negative thermal expansion in the delta phase. In this talk we will discuss results for two examples: UPt$_2$Si$_2$ and UCr$_2$Si$_2$. Both systems exhibit phase transitions near room temperature that may involve modulation of the lattice or charge density wave order. In addition, UCr$_2$Si$_2$ undergoes a structural phase transition near 210 K. We will focus on efforts to identify the order parameters for these phases.

*This work was performed at the NHMFL, which is supported by the NSF Cooperative Agreement Nos. DMR-1644779 and 1157490 and the State of FL. Research of R.E.B., Y.L., D.G. was supported in part by the US DOE, BES, under Award No. DE-SC0016568 (EFRC-CAST).

UCh$_2-x$Ru$_x$Si$_2$ is an unusual Kondo lattice metal that shows antiferromagnetism at $T_N = 27$ K, a structural phase transition from tetragonal (I4/mmm) to triclinic (P) near $T_s = 210$ K, and a so-far unidentified phase transition near $T_M = 275$ K. Cr $\rightarrow$ Ru substitution results both in expansion of the unit cell volume and filling of the d-shell, causes $T_N$ and $T_S$ to be suppressed to zero temperature near $x_{cr} \approx 0.075$ and 0.13, respectively. In contrast, $T_M$ disappears immediately with small amount of Ru. In the critical region, there is evidence for non-Fermi liquid behavior, (i) a weak logarithmic divergence in the electronic component of the heat capacity divided by temperature and (ii) a sub-quadratic temperature dependence of the electrical resistivity. Thus, we suggest that this may be a model system for studying a lattice instability at zero temperature, its relationship to a nearby antiferromagnetic quantum phase transition, and the resulting impact on electronic properties and lattice modes in a strongly correlated electron metal.

*This work is supported by NSF under No. DMR-1644779 and the State of Florida, and DOE under Award No. DE-SC0016568.

Symmetry broken phases involving higher order multipolar degrees of freedom are historically referred to as so-called "hidden orders", due to the formidable task of detecting them with conventional probes. In this talk, we theoretically propose a novel and powerful means to directly probe higher-order symmetry breaking: magnetostriction. To that end, we focus on the family of Pr-based cage compounds with strongly correlated f-electrons, Pr(Ti,V,Ir)$_2$(Al,Zn)$_{20}$, whose low energy degrees of freedom are composed of purely higher-order multipoles. Employing a symmetry-constructed Landau theory of multipolar moments, we provide key scaling behaviours of the magnetostriction in a range of temperature regimes. These findings provide a way to have clear access to higher order multipolar moments.
10:24AM K06.00013: Sequential Localization and Strange-metal Behavior in a Multipolar Kondo System* SILKE PASCHEN (Presenter), Vienna University of Technology, ANG CAI, Rice University, EMILIAN NICA, Arizona State University, CHIA-CHUAN LIU, Rice University, RONG YU, Renmin University of China, KEVIN INGERSENT, University of Florida, QIMIAO SI, Rice University — Quantum criticality and beyond-Landau physics of Kondo destruction [1,2] in heavy fermion systems with multipolar degrees of freedom is attracting considerable interest. Recent experiments on the heavy fermion compound Ce₃Pd₂₀Si₆ show evidence of two consecutive Fermi surface collapsing quantum critical points (QCP) as it is tuned from a paramagnetic to an antiferroquadrupolar (AFQ) and then to an antiferromagnetic (AFM) state [3]. We are able to understand this behavior by advancing a theory of sequential destruction of an SU(4) spin-orbital-coupled Kondo entanglement in an SU(4) Bose-Fermi Kondo model, which represents an effective model for a multipolar Kondo lattice system with Kugel–Khomskii interaction. As a function of coupling strength to the bosonic bath, we find that a generic trajectory in the parameter space contains two QCPs associated with the Kondo destruction of the orbital and spin degrees of freedom, respectively. For a Kondo lattice, this corresponds to two stages of Fermi surface jump, thus providing a natural understanding of the experimental findings.


*NSF Grant No. DMR-1611392 & Robert A. Welch Foundation Grant No. C-1411.

10:36AM K06.00014: Switching the propagation vector of hidden-order phases in Ce₃Pd₂₀Si₆ with a magnetic field DMYTRO INOSOV (Presenter), PAVLO PORTNICHENKO, STANISLAV NIKITIN, TU Dresden, ANDREY PROKOFIEV, SILKE BUEHLER-PASCHEN, Vienna University of Technology — Hidden-order phases that occur in a number of correlated f-electron systems are among the most elusive states of electronic matter. Their investigations are hindered by the insensitivity of standard physical probes, such as neutron diffraction, to the order parameter that is usually associated with higher-order multipoles of the f-orbitals. The heavy-fermion compound Ce₃Pd₂₀Si₆ exhibits magnetically hidden order at subkelvin temperatures, known as phase II. Additionally, for magnetic field applied along the [001] cubic axis, another phase II' was detected, but the nature of the II-II' phase transition remained unclear. Here we use inelastic neutron scattering to demonstrate that this transition is associated with a switching in the propagation vector of the antiferroquadrupolar order from (111) to (100). Despite the absence of magnetic Bragg scattering in phase II', its ordering vector is revealed by the location of an intense magnetic soft mode at the (100) wave vector, orthogonal to the applied field. At the II-II' transition, this mode softens and transforms into quasielastic and nearly Q-independent incoherent scattering. Our experiment also reveals sharp collective excitations in the field-polarized paramagnetic phase, after phase II' is suppressed in fields above 4 T.

10:48AM K06.00015: Theoretical X-ray spectroscopic study of 5f-electron signatures in actinide materials* WEI-TING CHIU (Presenter), Physics Department, University of California, Davis, JIAN-XIN ZHU, CINT, Los Alamos National Laboratory — Actinide materials are not only important for power generation nowadays, but also exhibit interesting physical properties from the condensed matter physics perspective. The valence 5f electrons in early actinides are considered to be delocalized, while in the late actinides the 5f electrons show localized behavior. Studying the local moment and 5f-electron occupations will shed insight into the electronic behavior in these materials. X-ray absorption spectroscopy (XAS) and X-ray photoemission spectroscopy (XPS) have been powerful tools to reveal the valence electronic structure with the assistance from theoretical calculations. In this work, we build a single-impurity Anderson model for the materials, and use exact diagonalization method to calculate its eigenenergies and eigenstates. The X-ray spectra are obtained by employing Fermi's golden rule. Comparing the theoretical spectra with the experimental results provides a way to determine the 5f electronic signatures of the actinide materials, helping us understand the 5f electronic correlation effects.

*We gratefully acknowledge the support of the U.S. DOE through the LANL LDRD Program and the G. T. Seaborg Institute, and the U.S. DOE under Grant No. DE-SC0014671.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K07 DCMP GMAG: Spin Liquids and Ices BCEC 109B - Randy Fishman, Oak Ridge National Laboratory
8:00AM K07.00001: Discovery of chiral-spin order in purported Kitaev spin-liquids
CHANDRA VARMA (Presenter), University of California, Riverside, KIMBERLY MODIC, Max Planck Institute for Chemical Physics, BRAD RAMSHAW, Physics, Cornell University, ARKADY SHEKHTER, National High Field magnet Lab — We examine recent magnetic torque measurements in two compounds, γ-LiIrO$_3$ and RuCl$_3$, which have been discussed as possible realizations of the Kitaev model. The analysis of the reported discontinuity in torque, as an external magnetic field is rotated across the c-axis in both crystals, suggests that they have a translationally-invariant chiral spin-order of the form $< S_j \times S_k > \neq 0$ in the ground state and persisting over a very wide range of magnetic field and temperature. An extra-ordinary $|B|B^2$ dependence of the torque for small fields, beside the usual $B^2$ part, is predicted due to the chiral spin-order. Data for small fields is available for γ-LiIrO$_3$ and is found to be consistent with the prediction upon further analysis. Other experiments such as inelastic scattering and thermal Hall effect and several questions raised by the discovery of chiral spin-order, including its topological consequences are discussed.

8:12AM K07.00002: Characteristics of the intermediate-field ordered phase of alpha-RuCl$_3$ revealed by magnetic diffraction
ARNAB BANERJEE (Presenter), CHRISTIAN BALZ, Oak Ridge National Laboratory, PAIGE LAMPEN-KELLEY, Material Science and Engineering, University of Tennessee, JIAQIANG YAN, Oak Ridge National Laboratory, DAVID GEORGE MANDRUS, Material Science and Engineering, University of Tennessee, YAOHUA LIU, STEPHEN NAGLER, Oak Ridge National Laboratory — There has been great interest in alpha-RuCl$_3$ as a material that manifests Kitaev terms in the spin Hamiltonian and a possible field-induced quantum spin liquid (QSL) phase by 8 T [1]. Bulk Measurements show that in the in-plane magnetic field causes a transition to an intermediate ordered phase around 6 Tesla [1, 2], preceding the total suppression of magnetic order around 7.3 T. Here we use time-of-flight neutron diffraction to elucidate the nature of intermediate phase and its magnetic order. Our results provide new insights into the dimensionality of the magnetic order and the effective spin-Hamiltonian of the material.


*The work performed at ORNL used the Spallation Neutron Source, is sponsored in part by the DOE Office of Science, Basic Energy Sciences, Division of Scientific User Facilities.

8:24AM K07.00003: Magnon thermal Hall effect in the candidate Kitaev spin-liquid α-RuCl$_3$
JONATHAN COOKMEYER (Presenter), JOEL MOORE, Physics, University of California, Berkeley — Motivated by recent experiments measuring the thermal Hall conductivity of α-RuCl$_3$ and using spin-wave theory and model effective Hamiltonians from the literature, the magnon Thermal Hall coefficient in the magnetically ordered phase is computed. Comparing directly with the experiment, no previously proposed model well matches the data. A model is determined which can explain the data demonstrating that the magnon Berry curvature could be responsible. The discrepancy could also be explained by phonons but not by Kitaev-like excitations.

*We acknowledge support from the Quantum Materials Program at LBNL, funded by the US Department of Energy under Contract No. DE-AC02-05CH11231.

8:36AM K07.00004: Effective dimension, level statistics, and integrability of Sachdev-Ye-Kitaev-like models
EIKI IYODA (Presenter), HOSHO KATSURA, TAKAHIRO SAGAWA, University of Tokyo — Recently, quantum many-body systems exhibiting fast scrambling (delocalization of quantum information) have attracted much attention. A well-known example is the Sachdev-Ye-Kitaev (SYK) model, describing random all-to-all four-body interactions among fermions. Here, we introduce a variant of the SYK model, which we refer to as the Wishart SYK model [1]. The model includes the original SYK model without quenched disorder as a special case.
We investigate the Wishart SYK model for complex fermions and that for hard-core bosons. In both cases, the ground state of the model is massively degenerate. We numerically study the out-of-time-ordered correlators (OTOC) and level statistics. Then we find that the OTOC in the fermionic case exhibits large temporal fluctuations at late times, which is attributed to a small effective dimension of the initial state. We also show that the level statistics of the fermionic (bosonic) Wishart SYK model obeys the Poisson (GOE or GUE) distribution. This is consistent with the integrability of the fermionic model, which can be proved by mapping it to a known integrable model.


*This work is supported by JSPS KAKENHI Grant Number JP15K20944, JP16H02211, JP18K03445 and JP18H04478.
8:48AM K07.00005: A candidate Theory for the "Strange Metal" phase based on the Sachdev-Ye-Kitaev physics
XIAOCHUAN WU (Presenter), Department of Physics, UC Santa Barbara, XIAO CHEN, Kavli Institute of Theoretical Physics, CHAO-MING JIAN, Station Q, Microsoft Research, YIZHUANG YOU, Department of Physics, Harvard University, CENKE XU, Department of Physics, UC Santa Barbara — We propose a lattice model for strongly interacting electrons with the potential to explain the main phenomenology of the strange metal phase in the cuprate high-temperature superconductors. Our model is motivated by the recently developed "tetrahedron" rank-3 tensor model that mimics much of the physics of the better-known Sachdev-Ye-Kitaev (SYK) model. Our electron model has the following advantageous properties: (1) it needs only one orbital per site on the square lattice. (2) It does not require any quenched random interaction. (3) It has local interactions and respects all the symmetries of the system. (4) The soluble limit of this model has a longitudinal dc resistivity that scales linearly with temperature within a finite temperature window. (5) Again, the soluble limit of this model has a fermion pairing instability in the infrared, which can lead to either superconductivity or a "pseudogap" phase. The linear-T longitudinal resistivity and the pairing instability originate from the generic scaling feature of the SYK model and the tetrahedron tensor model.

9:00AM K07.00006: Charge transport in graphene-based mesoscopic realizations of Sachdev-Ye-Kitaev models*
OGUZHVAN CAN (Presenter), EMILIAN NICA, MARCEL FRANZ, Department of Physics and Astronomy, University of British Columbia — We address transport properties of a mesoscopic realization of the Sachdev-Ye-Kitaev (SYK) model which is an exactly soluble system of interacting spinless fermions connected to the black hole physics through the holographic principle. Starting with a recent proposal for simulating the SYK model in a graphene flake in an external magnetic field and extending it by considering leads attached to it, we model a realistic transport experiment and calculate directly measurable quantities featuring non-Fermi liquid signatures of the SYK physics. We show that the graphene flake realization is robust in the presence of leads and that measuring the tunneling current across the leads one can experimentally observe a non-Fermi liquid - Fermi liquid transition by tuning the external magnetic field threading the flake. After establishing the transport signatures of the SYK model near equilibrium using linear response framework, we then derive a formula to extend our results for tunneling current using Keldysh formalism to explore the effects of finite bias voltage across the leads, going beyond equilibrium.

*Research reported in this article was supported by NSERC, CIfAR and QuEST program of the SBQMI, UBC. Final stages of the work were completed at the Aspen Center for Physics (Marcel Franz)

9:12AM K07.00007: Characterization of quantum many-body chaos with quantum Lyapunov exponents and by two-point correlations: application to a generalized Sachdev-Ye-Kitaev model
HRANT GHARIBYAN, Stanford Institute for Theoretical Physics, Stanford University, MASANORI HANADA, School of Physics and Astronomy, and STAG Research Centre, University of Southampton, BRIAN SWINGLE, Condensed Matter Theory Center, Maryland Center for Fundamental Physics, Joint Center for Quantum Information and Computer Science, and Department of Physics, University of M, MASAKI TEZUKA (Presenter), Department of Physics, Kyoto University — We propose two quantities for characterization of quantum many-body chaos. Firstly, we define a simple quantum generalization of the spectrum of finite-time classical Lyapunov exponents. [1] We study its statistical features for the SYK model and find random matrix behavior, which is lost when the model is deformed away from chaos towards integrability [2] by a random two-fermion term. Secondly, we propose that two-point correlation functions can also characterize quantum many-body chaos, with numerical evidences for the SYK model as well as for the XXZ spin chain with random field, and discuss the plausibility of laboratory experiments.

9:24AM K07.00008: Chiral spin liquid phase of the triangular lattice Hubbard model*
AARON SZASZ (Presenter), JOHANNES MOTRUK, MICHAEL ZALETEL, JOEL MOORE, Physics, University of California, Berkeley — Motivated by experimental studies that have found signatures of a quantum spin liquid phase in organic crystals whose structure is well described by the two-dimensional triangular lattice, we study the Hubbard model on this lattice at half filling using the infinite-system density matrix renormalization group (iDMRG) method. On infinite cylinders with finite circumference, we identify an intermediate phase between observed metallic behavior at low interaction strength and Mott insulating spin-ordered behavior at strong interactions. Chiral ordering from spontaneous breaking of time-reversal symmetry, a fractionally quantized spin Hall response, and characteristic level statistics in the entanglement spectrum in the intermediate phase provide strong evidence for the existence of a chiral spin liquid in the full two-dimensional limit of the model. [arXiv: 1808.00463]

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program and by the Theory Institute for Materials and Energy Spectroscopies (TIMES).
Monopoles in Dirac spin liquids I: from spinon band topology to monopole quantum numbers

XUEYANG SONG (Presenter), Harvard University, CHONG WANG, YIN-CHEN HE, Perimeter Institute, ASHVIN VISHWANATH, Harvard University — We explore a low-energy theory for 2D quantum magnets, the Dirac spin liquid (DSL), a version of Quantum Electrodynamics (QED$_2$) with four flavors of Dirac fermions coupled to photons. We study the spatial/time-reversal symmetry properties of the magnetic monopoles, an important class of excitations that drive confinement. We show that the underlying band topology of spinon insulators, e.g., quantum spin hall phase/wannier insulator protected by rotation provides crucial information on the tricky Berry phase of monopole (under time-reversal / rotations, respectively). We also prove the existence of a trivial monopole on bipartite lattices by invoking its ascension to a QCD with SU(2) gauge structure.

Monopoles in Dirac spin liquids II: towards a unifying description of 2D quantum magnetism

CHONG WANG (Presenter), Perimeter Institute for Theoretical Physics, XUEYANG SONG, Harvard University, YIN-CHEN HE, Perimeter Institute for Theoretical Physics, ASHVIN VISHWANATH, Harvard University — The understanding of monopole quantum numbers in Dirac spin liquids provides a unified description of 2D quantum magnetism. In particular, it allows us to naturally account for various orders on both bipartite lattices such as the square and honeycomb lattice as well as the non-bipartite triangular and Kagome lattices. A dichotomy in behavior between the bipartite and non bipartite lattices is traced to the difference in monopole symmetry properties on these two lattices. We characterize universal signatures of the Dirac spin liquid state, including those that result from monopole excitations, which serve as a guide to numerics and to experiments on existing materials. Even when unstable, the Dirac spin liquid unifies multiple seemingly unrelated ordered states, which could help organize the plethora of phases observed in strongly correlated two dimensional materials.

Interplay of uniform U (1) quantum spin liquid and magnetic phases in rare earth pyrochlore magnets: a fermionic parton approach*

SAMBUDDHA SANYAL (Presenter), Chemistry, Columbia University, KUSUM DHOCHAK, Physics, Indian Institute of Science Education and Research, Bhopal, SUBHRO BHATTACHARJEE, International Centre for Theoretical Science (ICTS), Bengaluru — We study the uniform time reversal invariant quantum spin liquid (QSL) with low energy fermionic quasi-particles for rare earth pyrochlore magnets and explore its magnetic instability employing an augmented fermionic parton mean field theory approach. Self consistent calculations stabilise an uniform QSL with both gapped and gapless parton excitations as well as fractionalised magnetically ordered phases in an experimentally relevant part of the phase diagram near the classical phase boundaries of the magnetically ordered phases. The gapped QSL has a band-structure with a non-zero topological invariant. The fractionalised magnetic ordered phases bears signature of both QSL through fermionic excitations as well as magnetic order. Thus this provides a possible way to understand the unconventional diffuse neutron scattering in rare-earth pyrochlores such as Yb Ti O , Er Sn O and Er Pt O at low/zero external magnetic fields. We calculate the dynamic spin structure factor to understand the nature of the diffuse two-particle continuum.

*S.B. acknowledges MPG for funding through the partner group at ICTS and support of the SERB-DST (India) grant (ECR/2017/000504). S. S. acknowledge funding through SERB-DST (India), Indo-US Science and Technology Forum, Indo-US post-doctoral fellowship.

Microscopic model for Tb-based pyrochlore magnets

WEN JIN (Presenter), DANIEL WONG, MICHEL J P GINGRAS, Department of Physics and Astronomy, University of Waterloo, University of Waterloo — There have been extensive experimental investigations of the magnetic structures and excitations of Tb-based pyrochlores, Tb2B2O7 (B=Ti, Sn, Ge). Tb2Ti2O7 is a candidate for quantum spin ice, while Tb2Sn2O7 and Tb2Ge2O7 have long-range ordered spin ice state coexistent with strong spin fluctuations. However, a microscopic model of these materials is still lacking. In this talk, I will discuss our efforts to derive a pseudo spin-1/2 model of Tb-based pyrochlores via a projection operator approach. We find the virtual crystal field excitations between the two lower doublets result in significant renormalization of the classical Ising interactions and generate symmetry-allowed three-body interactions that play a crucial role in the selection of ground state. We find the electric quadrupole-quadrupole interactions also give rise significant quantum fluctuations.
Magnetic critical dynamics and monopole clustering of pyrochlore spin ice  

PUHAN ZHANG (Presenter), JING LUO, GIA-WEI CHERN, University of Virginia — Spin-ice materials such as Ho2Ti2O7 and Dy2Ti2O7 are a class of geometrically frustrated ferromagnets that retain an extensive residual entropy even at very low temperatures. Importantly, the elementary dipole excitations fractionalize into magnetic monopoles in these compounds. Indeed, the field-induced first-order transition in spin-ice compounds can be understood as a monopole liquid-gas transition. Despite extensive studies on magnetic monopole dynamics at low magnetic field, the kinetics of the liquid-gas transition and the particular role played by monopoles have not been thoroughly investigated. Here we present extensive numerical simulations to investigate the structural as well as dynamical properties of monopoles in the vicinity of the field-induced first-order transition. Our results relate the critical magnetic dynamics to the percolation of magnetic monopoles in the monopole gas phase. Interestingly, we show that similar percolating clusters consisting of bound monopole hole pairs also appear in the dense monopole liquid phase.

Quantum Anomalous Hall Phase Stabilized via Realistic Interactions on a Kagome Lattice*  

YAFEI REN (Presenter), Department of Physics, University of Science and Technology of China, TIANSHENG ZENG, Department of Physics, The University of Texas at Dallas, WEI ZHU, Los Alamos National Laboratory, DONNA SHENG, California State University, Northridge — Spontaneous topological phases driven by interactions have been proposed in various lattice models, which, however, have not been observed in experiments. In this work, we report an experimentally feasible scheme of realizing spontaneous quantum anomalous Hall effect (QAHE) driven by spatially decaying interactions between spinless Fermions on a topologically trivial kagome lattice with a quadratic band touching Fermi point. In the presence of weak first and second nearest-neighbor repulsive interactions (V1 and V2), the presence of QAHE is demonstrated by employing exact diagonalization and density-matrix renormalization group methods. The time-reversal symmetry is broken spontaneously by forming loop currents with long-range correlation. Quantized Hall conductance is obtained by measuring the pumped charge through inserting flux in a cylinder geometry. We find that the topologically nontrivial energy gap can be enhanced remarkably by a moderate V2 < V1 via calculating the spectrum and charge excitation gaps.

Probing The Spin-Spin Correlator Of Kagome Lattice Heisenberg Antiferromagnets Through Non-linear Optical Harmonic Generation  

NICHOLAS LAURITA (Presenter), ALON RON, Caltech, JEONG WOO HAN, JONGSEOK LEE, Department of Physics and Photon Science, Gwangju Institute of Science and Technology, JOHN P SHECKELTON, REBECCA W. SMAHA, WEI HE, JIAJIA WEN, YOUNG SANG LEE, Department of Applied Physics, Stanford University, MICHAEL NORMAN, Argonne National Laboratory, DAVID HSIEH, Caltech — Antiferromagnetically coupled quantum spins on the Kagome lattice are proposed to realize a spin-liquid ground state where short-range spin correlations exist but symmetry breaking is avoided through frustration and quantum fluctuations. The temperature dependence of the short-range spin-spin correlator is important for understanding the underlying spin Hamiltonian of candidate materials but is typically difficult to measure. Here we show that the non-linear optical response embeds the spin-spin correlator in spin-liquid candidates by performing high harmonic generation experiments on Herbertsmithite and Zn-Barlowite. We find the temperature evolution of the spin correlations of these materials to be in very good agreement with the theoretical prediction for the S = 1/2 Heisenberg Kagome antiferromagnet. These results provide a new route to probing the governing spin Hamiltonian of spin-liquid candidates.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K08 DCMP DMP: Non-equilibrium Superconductivity  

BCEC 150 - Dirk Van Der Marel, University of Geneva
superconductivity has attracted much attention in the past decade, due to the possibility of dramatically enhancing the transition temperature and finally creating a room-temperature superconductor. One promising realization of nonequilibrium superconducting states is achieved via pumping mid-infrared phonons. In this work, we perform a numerical study of an electron-phonon system after dynamically squeezing the phonons, which mimics the leading impact of the infrared pump. Using a variational non-Gaussian wavefunction, we are able to evaluate not only the superconducting order parameter, but also the time-resolved optical and ARPES spectroscopies. By comparing with optical probes, we identify the physical order parameter as a pair of dressed quasiparticles. Driving the system at different frequencies we observe that superconductivity can be either persistently enhanced or suppressed, depending on the resonant characteristic excitations. Revealing the dynamics of the parametric phonon pump, this work enables the design of conventional non-equilibrium superconductors.

The authors acknowledge the Max Planck/Harvard Research Center for Quantum Optics, AFOSR-MURI Quantum Phases of Matter (Grant FA9550-14-1-0035), and Harvard-MIT CUA, NSF Grant No. DMR-1308435.

8:12AM K08.00002: Allowing for real coherent phonon bursts to defend and actuate the superconducting state in YBCO

JOHN JAMES (Presenter), Saint Louis University — Assuming that BCS superconductivity is unstable for high transition temperatures, what would be required if real coherent phonon bursts formed to prevent (defend against) the complete collapse of this state when the superconducting gap fell to resonance with the low energy optical soft phonon mode? Could the resonant phonon bursts also establish (actuate) the high energy of the gap by requiring the gap formation energy at very low superconducting state density to be the soft optical phonon energy? For this treatment of the BCS gap as a population inversion to produce coherent phonons, the formation times would usually be enormous compared to the electron-defect scattering times. All defect interactions would need to be eliminated because they would be resonant with the phonon energy but differing in momentum. A model is presented in which chain site, out of CuO2 plane, oxygen atoms tend to mutually repel for nearest neighbor sites while attracting at second nearest neighbor, causes the depletion of chain oxygen in the vicinity of all defects. This forces the fermi level into the band gap near all defects and surfaces and allows the slow coherent phonon emission and superconducting ground state formation to occur.

8:24AM K08.00003: Light-induced d-wave superconductivity through Floquet-engineered Fermi surfaces in cuprates

DANTE KENNES (Presenter), Physics, Freie Universität Berlin, MARTIN CLAASSEN, Center for Computational Quantum Physics, The Flatiron Institute, MICHAEL SENTE, Center for Free Electron Laser Science, Max Planck Institute for the Structure and Dynamics of Matter, CHRISTOPH KARRASCH, Physics, Freie Universität Berlin — We introduce a mechanism for light-induced Floquet engineering of the Fermi surface to dynamically tip the balance between competing instabilities in correlated condensed matter systems in the vicinity of a van-Hove singularity. We first calculate how the Fermi surface is deformed by an off-resonant, high-frequency light field and then determine the impact of this deformation on the ordering tendencies using an unbiased functional renormalization group approach. As a testbed, we investigate Floquet engineering in cuprates driven by light. We find that the d-wave superconducting ordering tendency in this system can be strongly enhanced over the Mott insulating one. This gives rise to extended regions of induced d-wave superconductivity in the effective phase diagram in the presence of a light field.

D.M.K. and C.K. acknowledge support by the Deutsche Forschungsgemeinschaft through the Emmy Noether program (KA 3360/2-1). M.C. acknowledges support from the Flatiron Institute, a division of the Simons Foundation. M.A.S. acknowledges financial support by the DFG through the Emmy Noether program (SE 2558/2-1). Simulations were performed with computing resources granted by RWTH Aachen University under projects rwth0013 and prep0010.

8:36AM K08.00004: Wavelength Dependence of Pumping a Superconductor

TA TANG (Presenter), Applied Physics, Stanford, THOMAS DEVEREAUX, BRIAN MORITZ, Institute for Materials and Energy Science, Stanford — Experiment [E. Casandruc et al] has shown transient enhanced superconductivity in LBCO when pumped by ultrafast pulses. This provides a new way to control the properties of high Tc superconductors and explore non-equilibrium phenomenon. Here we explore the effects of pumping the cuprates at different wavelengths. The model is a multi-band Hubbard model (including apical oxygen sites), which we pump with an ultrafast gaussian-pulse to study its time evolution using exact diagonalization (ED). The results show that holes are pumped from the CuO2 plane into the apical oxygens at characteristic optical wavelengths.
**8:48AM K08.00005: Transient superconductivity without superconductivity**  
GIULIANO CHIRIACO (Presenter), ANDREW MILLIS, IGOR L ALEINER, Columbia University — Recent experiments on K$_3$C$_60$ and layered copper-oxide materials have reported substantial changes in the optical response following application of an intense THz pulse. These data have been interpreted as the stimulation of a transient superconducting state even at temperatures well above the equilibrium transition temperature. We propose an alternative phenomenology based on the assumption that the pulse creates a non-superconducting, though non-equilibrium situation in which the linear response conductivity is negative. The negative conductivity implies that the spatially uniform pre-pulse state is unstable and evolves to a new state with a spontaneous electric polarization. This state exhibits coupled oscillations of entropy and electric charge whose coupling to incident probe radiation modifies the reflectivity, leading to an apparently superconducting-like response that resembles the data. Dependencies of the reflectivity on polarization and angle of incidence of the probe are predicted and other experimental consequences are discussed.

*Basic Energy Sciences Division of the U.S. DOE grant DE-SC0018218  
Simons Foundation

**9:00AM K08.00006: Time-dependent McMillan-Ginzburg-Landau models for light-induced ultrafast phase transitions in cuprates and other complex materials**  
ROLAND ALLEN (Presenter), JIAN WENG, ROSS TAGARAS, Texas A&M University — Earlier we found that a very simple time-dependent Ginzburg-Landau model [1] described several features of the light-induced superconductivity in La$_{1.675}$Eu$_{0.2}$Sr$_{0.125}$CuO$_4$ (LESCO1/8) discovered by Cavalleri and coworkers [2]. But for a more detailed description of complex materials -- cuprate and other high-temperature superconductors, layered transition-metal dichalcogenides, colossal magnetoresistive manganites, ... -- more detailed models are needed, which should properly be called McMillan-Ginzburg-Landau models [3]. The description of both static phase diagrams and ultrafast dynamics with such models will be discussed, with a few examples.


**9:12AM K08.00007: Impact of damping on superconducting gap dynamics induced by intense terahertz pulses**  
TIANBAI CUI (Presenter), School of Physics and Astronomy, University of Minnesota, XU YANG, CHIRAG VASWANI, JIGANG WANG, Department of Physics and Astronomy, Iowa State University, RAFAEL M FERNANDES, School of Physics and Astronomy, University of Minnesota, PETER P. ORTH, Department of Physics and Astronomy, Iowa State University — Recent advances in terahertz pump-probe spectroscopy opened a new route to investigate non-equilibrium superconductivity and gap dynamics. The time-dependent BCS theory predicts 2Δ gap oscillations after an ultrafast non-adiabatic perturbation is turned off, a consequence of the excitation of the Anderson-Higgs mode. Because gap relaxation due to the coupling to the phonons happens usually at longer time scales, the average gap is expected to be constant after the pump is off. This is at odds with recent experiments using intense THz pulses with subgap frequencies in NbN, where the gap is seen to be suppressed already at the tens of ps time scale, after the pump is turned off. We show that this behavior arises from damping within the electronic subsystem due to effects beyond BCS theory, such as interactions between Bogoliubov quasiparticles and decay of the Higgs mode. We develop a semi-phenomenological model where these relaxation processes are conveniently expressed as T$_1$ and T$_2$ relaxation times in the pseudospin formalism. We discuss the impact of each relaxation process to the gap dynamics and show the quantitative agreement with the experiments.
Control of Non-equilibrium Quantum Phases and Collective Modes in Superconductors by Terahertz Light-Driven Supercurrents*  

MARTIN MOOTZ (Presenter), ILIAS PERAKIS, Physics, University of Alabama at Birmingham, JIGANG WANG, Physics and Astronomy, Ames Laboratory, Iowa State University — In superconductors several non-equilibrium phases exist ranging from quenched states to gapless superconducting phases with gapless excitation spectrum but unchanged macroscopic coherence and infinite conductivity. The dynamics of such non-equilibrium phases is associated with observation of collective modes which provide details about the underlying nature of superconductivity. Although recent advances in THz laser spectroscopy make the excitation of collective modes and gapless superconducting phases possible, their observations in ultrafast spectroscopy remain challenging. Here we demonstrate control of the non-equilibrium dynamics in superconductors by THz light-driven supercurrents. By applying a microscopic gauge-invariant theory we show that selective non-equilibrium phases can be excited and amplitude Higgs mode can be detected in the nonlinear response by inducing supercurrents via THz pulse shaping. THz light-control of supercurrents also allows for generation of a comb of odd or odd and even harmonics in emission.

*The work at the University of Alabama, Birmingham acknowledges support by the U.S. Department of Energy, Office of Science, Basic Energy Sciences DoE under award DE-SC0019137. JW acknowledges support from the Army Research Office under award W911NF15-1-0135.

Collective modes in superconductors and their coupling to near field THz probes*  

ZHIYUAN SUN (Presenter), Physics, Columbia University, MICHAEL FOGLER, Physics, University of California, San Diego, ANDREW MILLIS, Physics, Columbia University — We theoretically investigate methods to observe the phase (Anderson-Bogoliubov-Goldstone), amplitude (Higgs) and Carlson-Goldman modes using THz near field techniques. In a quasi-two-dimensional superconductor, we show that the Carlson-Goldman mode appears in the near field reflection coefficient as a weak feature in the sub-Terahertz frequency range. In a system of two superconductor layers separated by nanometer scale, the gapless phase mode reappears due to the mutual screening between the layers, as the antisymmetric plasmon mode of the system. This mode leads to a well defined resonance peak in the near-field THz response. Close to zero temperature, its speed contains the information of the original Goldstone mode. The amplitude mode could appear in the near field third harmonic generation for particle-hole asymmetric superconductors and we also discuss its observability in the linear response.

*This work is supported by the DOE under Grant DE-SC0018218.

The Higgs Amplifier  

DANIEL PODOLSKY (Presenter), Technion - Israel Institute of Technology, YAO WANG, EUGENE DEMLER, Physics, Harvard University — A sudden quench into a superconducting state results in strong Higgs oscillations in the amplitude of the superconducting order parameter. We study theoretically the optical response of a quenched superconductor and find that Higgs modulations lead to a marked enhancement of the reflectance. For strong enough modulations, the reflectance can even exceed unity, corresponding to signal amplification. We discuss possible implications to experiments on light-induced superconductivity in K₃C₆₀.

Collective modes in non-equilibrium in unconventional superconductors with competing ground states  

MARVIN ALEXANDER MÜLLER (Presenter), Institute for Theoretical Physics III, Ruhr-University Bochum, PAVEL VOLKOV, Ruhr-University Bochum and Rutgers University, ILYA EREMIN, Institute for Theoretical Physics III, Ruhr-University Bochum —

Motivated by the recent development of terahertz pump-probe spectroscopy, we investigate the short-time dynamics and collective modes in superconductors with multiple attractive pairing channels. We consider a single-band square lattice model with nearest neighbor attraction. This interaction decouples into s-, d- and p-wave channels leading to strong competition between them for various band fillings. Driving the system out of equilibrium, we find signatures of collective modes of symmetries different from the ground state (so-called Bardasis-Schrieffer modes) for the s-wave ground state. We show that polarization can be used to excite Bradsis-Schrieffer modes of a particular symmetry in a controlled way and discuss implications for the future pump probe experiments.
10:12AM K08.00012: Control of Competing Superconductivity and Charge Order By Non-equilibrium Currents* 
ANNE MATTHIES (Presenter), JIAJUN LI, MARTIN ECKSTEIN, Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — Strongly correlated materials often have rich phase diagrams. However, in many cases potentially interesting states are suppressed by competing phases which are thermodynamically in close proximity, e.g. superconductivity (SC) and charge-density-wave (CDW) order. How to control and distinguish competing phases arises as a very interesting and relevant question which is currently under intense research. In this work we study the competing CDW and SC order in the attractive Hubbard model under a voltage bias, using non-equilibrium steady-state (NESS) dynamical mean-field theory. We show that the CDW is suppressed in a current-carrying NESS by an effect beyond a simple Joule-heating mechanism. A “supercooled” metallic state is stabilized at a NE temperature lower than the equilibrium SC Tc. Since a current-carrying SC state is dissipation-less and thus not subject to the same non-thermal suppression, it can nucleate out of the supercooled metal. Hence, an electric current can change the relative stability of different phases compared to thermal equilibrium, even when a system appears locally thermal due to electron-electron scattering. This provides a general perspective to control intertwined orders out of equilibrium.

[arXiv:1804.09608]
*ERC starting grant No. 716648

10:24AM K08.00013: Efficient Prediction of Time-and Angle-Resolved Photoemission Spectroscopy Measurements on a Non-Equilibrium BCS Superconductor*  
TIANRUI XU (Presenter), TAKAHIRO MORIMOTO, ALESSANDRA LANZARA, JOEL MOORE, Physics, University of California, Berkeley — We study how time-and angle-resolved photoemission (tr-ARPES) reveals the dynamics of BCS-type, s-wave superconducting systems with time-varying order parameters. Approximate methods are discussed, based on previous approaches to either optical conductivity or quantum dot transport, in order to enable computationally efficient prediction of photoemission spectra. One use of such predictions is to enable extraction of the underlying order parameter dynamics from experimental data, which is topical given the rapidly growing use of tr-ARPES in studying unconventional superconductivity. The methods considered model the two-time lesser Green's functions with an approximated lesser self-energy that describes relaxation by coupling of the system to two types of baths. The approach primarily used here also takes into consideration the relaxation of the excited states into equilibrium by explicitly including the level-broadening of the retarded and advanced Green's functions. We present equilibrium and non-equilibrium calculations of tr-ARPES spectrum from our model and discuss the signatures of different types of superconducting dynamics.

*U.S. Department of Energy, Gordon and Betty Moore Foundation

10:36AM K08.00014: Probing Out-of-Equilibrium Spin Modes in a Mesoscopic Superconductor  
MARKO KUZMANOVIĆ (Presenter), Laboratoire de Physique des Solides (CNRS UMR 8502), Bâtiment 510, Université Paris-Sud, Université Paris-Saclay, F-91405 Orsay, France, BIYI WU, National Taiwan University, MAXIMILIAN WEIDENEDER, CHARIS H.L. QUAY, MARCO APRILI, Laboratoire de Physique des Solides (CNRS UMR 8502), Bâtiment 510, Université Paris-Sud, Université Paris-Saclay, F-91405 Orsay, France — While energy and charge-mode excitations in a superconductor (associated to out-of-equilibrium Bogoliubov quasiparticles) are well known, spin modes have been addressed only recently. If spins are injected into a spin-split superconducting Al nanowire, a long-range out-of-equilibrium magnetization can be observed [1], and both the spin accumulation [2] and spin relaxation [3] times have been measured, being ~10-20 ns and ~50 ps respectively. However a key question still remains: can the system be described by a truly spin dependent distribution function? In this work we studied the diffusion of quasiparticles injected into a spin-split superconducting Al nanowire, and performed a spectroscopic study of the quasiparticle population using spin sensitive detectors located at different distances from the injection point. We will present evidence for a spin-mode non-equilibrium distribution at time / length scales shorter that the spin-flip one (about 250 nm) as well as an energy-mode spin accumulation above it.

Maxwell's Demon. can be used as a resource for optimal work extraction even in the absence of feedback, as opposed to a traditional cycle. Our results are explained in the framework of nonequilibrium fluctuation relations. We thus show that irreversibility thermal/charging energy or with probabilities substantially greater than 1/2, despite zero free energy difference over the cycles featuring kicks of the control parameter, we demonstrate work extraction up to large fractions of the electron transistor at the single thermodynamic trajectory level. With two carefully designed out-of-equilibrium driving cycles featuring kicks of the control parameter, we demonstrate work extraction up to large fractions of the

**Wednesday, March 6, 2019 8:00 AM - 11:00 AM**

**Session K09 DCMP: Superconducting Critical Current and Vortex Dynamics**

**BCEC 151A - Timir**

Datta, University of South Carolina

**8:00AM K09.00001: Correlations in the strong pinning theory for vortices in type-II superconductors**

MARTIN BUCHACEK (Presenter), GIANNI BLATTER, VADIM B GESHKENBEIN, ETH Zurich — Vortex pinning in type-II superconductors is usually described within two frameworks, weak and strong pinning theory. Within weak pinning, vortices are pinned due to the collective action of defects while the latter framework assumes strong defects of low density, each of them capable of pinning the vortex lattice independently. By investigating the pairwise action of strong defects, we estimate corrections to the strong pinning theory due to correlations. In the limit of very strong defects, pinning force is determined through jumps in the elastic energy during the vortex depinning. We show that by taking into account the presence of other strong defects, the average size of the jump is reduced, leading to the reduction of the pinning force density. In the opposite limit with only moderately strong defects and on approaching the crossover to weak pinning, the strong pinning contribution would vanish but the pairwise action of defects enhances the pinning. In this case, we recover the result from the weak pinning theory with pinning force density being proportional to the squared density of defects.

**8:12AM K09.00002: Tuning vortex fluctuations and the resistive transition in superconducting films with a thin overlayer**

ALEXANDER GUREVICH (Presenter), Department of Physics, Old Dominion University — It is shown that the temperature of the resistive transition $T_r$ of a superconducting film can be increased by a thin superconducting or normal overlayer due to an “anti-proximity effect” which manifests itself in an initial increase of $T_r(d_2)$ with the overlayer thickness $d_2$ followed by a decrease of $T_r(d_2)$ at larger $d_2$. The nonmonotonic dependence of $T_r(d_2)$ resulting from the interplay of vortex fluctuations and the conventional proximity effect, was obtained by solving the Usadel equations to calculate the BKT transition temperature and the temperature of the resistive transition due to thermally-activated hopping of vortices. The model may explain the nonmonotonic dependence of $T_r(d_2)$ observed on (Ag, Au, Mg, Zn)-coated Bi films, Ag-coated Ga and Pb films or NbN and NbTiN films on AlN buffer layers. The transition temperature can be optimized by tuning the overlayer parameters, which can significantly weaken vortex fluctuations and nearly restore the mean-field $T_c$. These results suggest that bilayers can be used as model systems for systematic investigations of optimization of fluctuations in superconductors.

*This work was supported by AFOSR under grant FA9550-17-1-0196

**8:24AM K09.00003: Superconductivity in a disordered vortex lattice**

AMIT GHOSAL (Presenter), ANUSHREE DATTA, ANURAG BANERJEE, Indian Institute of Science Education and Research, Kolkata, NANDINI TRIVEDI, Ohio State University — Orbital magnetic field, as well as disorder, weaken superconductivity of a type-II superconducting film when acting individually. The Abrikosov vortex lattice, resulting from magnetic field, melts with the increasing field strength turning the superconductor into a metal. On the other hand, disorder causes a two-dimensional superconducting film to undergo a transition to an insulating state beyond a critical strength of disorder. Here we show that the simultaneous presence of these perturbations leads to an interesting evolution of superconductivity. We demonstrate that the local superconductivity strengthen due to a self-consistent spatial reorganization of order parameters. At weak disorder strengths, the same critical field that collapses the superconducting energy gap which is also responsible for the vanishing of the superfluid density. However, these two critical fields diverge from one another at large disorder strengths. In addition, disorder is found to distort the Caroli-de Gennes-Matricon bound state, which in the clean system features a strong zero-bias peak in the local density of states (LDOS) at the vortex-core. This peak disappears featuring a dip in LDOS at core, even for weak disorders. We comprehend such behavior and discuss possible experimental signatures.
9:00AM K09.00006: Imaging individual superconducting vortices in amorphous Mo$_{0.8}$Si$_{0.2}$ by scanning SQUID-on-tip* LORENZO CECCARELLI (Presenter), DENIS VASYUKOV, MARCUS WYSS, GIULIO ROMAGNOLI, MARTINO POGGIO, University of Basel — Understanding vortex pinning and dynamics in superconductors is crucial for the design of devices carrying non-dissipative currents. Here, we use a scanning nanometer-scale superconducting quantum interference device (nanoSQUID) [1,2] to image individual vortices in a Mo$_{0.8}$Si$_{0.2}$ amorphous thin film. MoSi$_{1-x}$ has recently gained prominence in sensitive superconducting single-photon detectors due to its ease of growth, homogeneity, and high critical temperature (~7 K) [3]. The high flux sensitivity and spatial resolution of our scanning nanoSQUID-on-tip allow us to study the behaviour of individual vortices in the presence of applied field and current. In particular, we investigate flux pinning by driving vortices through Lorentz forces exerted by applied currents [4,5], hopping between pinning sites, and the expulsion of magnetic flux upon lowering the applied magnetic field.


*Swiss NSF (No. 200020-178863); Kanton Aargau; Swiss Nanoscience Institute; NCCR QSIT; ERC Starting Grant NWScan (No. 334767).
9:36AM K09.00009: Time analysis of the voltage response created by a critical current pulse of superconducting NbTi nanowires*  
KHALIL HARRABI (Presenter), ABDELKARIM MEKKI, King Fahd University of Petroleum and Minerals, JEAN PAUL MANEVAL, Physics Department, ENS Paris France, LPA — We have investigated in time domain the voltage response of superconducting NbTi filaments with different thickness to a supercritical (>Ic) step-pulse of electrical current. The resistive state is created in the filament for exceeding the critical current, where a hot spot is found far below to the critical temperature and a permanent phase-slip center close to Tc. In both cases, the resistive response appears after a certain delay time t delay depending upon the temperature and the ratio I/Ic(T) which can been analyzed through a Time-Dependent Ginzburg-Landau equation. We found that the experimental data can be fitted by using a gap relaxation time, independently of the sample widths. However, it depends strongly on the filament thickness. Assuming proportionality to sample thickness, this indicates a phonon escape time of about 80 ps/nm for a NbTi film sputtered on polished crystalline Al2O3.

*KFUPM DSR_161052

9:48AM K09.00010: Critical current and persistent supercurrent in asymmetric superconducting rings  
JACOB HUDIS (Presenter), IRINEL CHIORESCU, PENG XIONG, Florida State University — Magnetic flux quantization through superconducting rings dictate that they contain a persistent supercurrent which switches direction at half-integer external flux quanta. The oscillatory persistent supercurrent manifests in critical current and resistance (Little–Parks) oscillations. Recently, it was shown theoretically and experimentally [1] that in an asymmetrically connected superconducting ring, the critical current may exhibit anomalous periodic behavior with external magnetic flux, including discontinuous jumps. Significant inconsistencies exist between experimental and simulation results [1]. We have performed modeling of the critical current in a superconducting ring as a function of geometrical asymmetries. Our simulations indicate that persistent current might not switch direction at the most energetically favorable locations; and the geometric asymmetry could be used to control the switching. Experimentally, asymmetric superconducting rings have been fabricated by electron-beam lithography, and the critical current will be measured and compared with the simulations. The results may find implications in novel superconducting electronics relying on flux quantization such as superconducting qubits and nano SQUIDs.


10:00AM K09.00011: Rotational transition, dislocations and domain formation in vortex systems with combined six- and 12-fold anisotropic interactions*  
MACIEJ OLSZEWSKI (Presenter), MORTEN ESKILDSEN, University of Notre Dame, CHARLES REICHHARDT, CYNTHIA REICHHARDT, Los Alamos National Laboratory — We introduce a model of vortices in type-II superconductors with a combined 6- and 12-fold anisotropy in the interaction potential, motivated by the vortex lattice (VL) phase diagram in MgB2 and UPt3. Using numerical simulations we show that the VL undergoes a continuous rotational transition as the ratio of the 6- and 12-fold anisotropy is changed, causing the VL to fracture into domains. We explore the structure of domain boundaries, and isolated dislocations present with single VL domains. Furthermore, we calculate the stress field associated with both dislocations and domain boundaries. The simulations provide a real space complement to results obtained from small-angle neutron scattering studies. We discuss how our simulations may be extended to model metastable VL phases observed experimentally, and the kinetics of the metastable-to-equilibrium transition. Finally we compare our numerical results to similar work on graphene lattices, skyrmions and colloids.

*This research was supported in part by the Notre Dame Center for Research Computing. MWO and MRE was supported by the US DOE, Office of Basic Energy Sciences, under Award No. DE-SC0005051. Part of this work was carried out under the auspices of the NNSA of the US DOE at LANL under Contract No. DE-AC52-06NA25396.
10:12AM K09.00012: Structural transition kinetics and activated behavior in the superconducting vortex lattice*

MORTEN ESKILDSEN (Presenter), ELIZABETH R LOUDEN, CATHERINE RASTOVSKI, STEPHEN J KUHN, ALLAN LEISHMAN, University of Notre Dame, LISA DEBEER-SCHMITT, Oak Ridge National Laboratory, CHARLES D DEWHURST, Institut Laue-Langevin, NIKOLAI D ZHIGADLO, University of Bern — Structural phase transformations are ubiquitous in solids, exhibiting common features independent of the microscopic properties of a particular material. We show that this commonality extends to phase transition kinetics associated with the superconducting vortex lattice. Using small-angle neutron scattering, we investigated the behavior of a metastable vortex lattice (VL) state in MgB2 as it is driven towards equilibrium by an AC magnetic field. This shows an activated behavior, where the AC field amplitude and cycle count are equivalent to, respectively, an effective “temperature” and “time”. The activation barrier increases as the metastable state is suppressed, corresponding to an aging of the VL. Furthermore, we find a cross-over from a partial to a complete suppression of metastable domains depending on the AC field amplitude, which may empirically be described by a single free parameter. This represents a novel kind of collective vortex behavior, most likely governed by the nucleation and growth of equilibrium VL domains.

*Supported by the US DOE, Office of Basic Energy Sciences, under Award No. DE-SC0005051. A portion of this research used resources at the High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

10:24AM K09.00013: Numerical approach for vortex dynamics in the presence of mesoscopic pining centers

IVAN SADOVSKYY (Presenter), ROMAN LUTCHYN, Station Q, Microsoft — The efficient and accurate description of superconducting vortex dynamics is required for a number of technological applications extending from microelectronics to dissipationless power transmission lines and powerful magnets.

In the limit of low magnetic fields, it is reasonable to use the Langevin approach for the vortex dynamics, which does not take into account vortex-vortex interaction and therefore is extremely effective from numerical point of view.

In the limit of high fields, the dynamics of vortices is largely determined by their interaction, and a model that correctly describes this interaction is required. In the vicinity of the critical temperature, Ginzburg-Landau (GL) approach is suitable to acquire the statistics of vortex dynamics. However, since the data for the statistical analysis is roughly proportional the number of vortices, the GL approach becomes numerically inefficient in low field limit.

In the present work we propose the efficient and accurate method for vortex dynamics description in low field limit. We combine (i) GL solver to extract effective energy potential for single vortex and (ii) Langevin approach to acquire statistical data for vortex dynamics. We check the applicability of the combined method by comparison results with time-dependent GL solver.

10:36AM K09.00014: Superconducting Nanostructures Grown by Ga+- and He+- Focused Ion Beam Induced Deposition (FIBID)

ROSA CÓRDOBA, PABLO ORÚS, Instituto de Ciencia de Materiales de Aragón (ICMA), Universidad de Zaragoza-CSIC, ALFONSO IBARRA, Laboratorio de Microscopías Avanzadas (LMA), Universidad de Zaragoza, DOMINIQUE MAILLY, Centre de Nanosciences et de Nanotechnologies, CNRS, JOSE MARIA DE TERESA NOGUERAS (Presenter), Instituto de Ciencia de Materiales de Aragón (ICMA), Universidad de Zaragoza-CSIC — Since the discovery of superconductivity in W-C deposits grown by Ga+ - Focused Ion Beam Induced Deposition (FIBID) [1], this material has been used as a model system to investigate the interplay of the vortex lattice with geometrical restrictions [2] or with periodic thickness modulations [3, 4]. We have recently carried out experiments for the investigation of non-local transport of vortices in Ga+ - FIBID nanowires [5]. These experiments indicate that long-distance (at least ten microns) propagation of vortices is sustained in such nanowires, with application in information technologies.

On the other hand, the limitations in resolution observed in Ga+ - FIBID nanostructures are overcome by the use of He+ - FIBID [6]. Results will be shown that highlight the potential of He+ - FIBID for the growth of superconducting nanowires and nanotubes with superb resolution. Applications of such nanostructures will be discussed.

References:

10:48AM K09.00015: Suppression of dissipation in superconducting nanostraps by parallel magnetic field*
ANDREAS GLATZ (Presenter), YONG-LEI WANG, Materials Science Division, Argonne National Laboratory, IGOR S ARONSON, Department of Chemistry, Penn State University, ZHILI XIAO, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory — Common wisdom dictates that an increase in the magnetic field escalates the loss of energy since the number of vortices increases. Here we show that this is no longer true if the magnetic field and the current are applied parallel to each other. Experimental studies on superconducting MoGe nanostraps reveal that the initial dissipative state with increasing magnetic field is followed by a pronounced resistance drop, signifying a reentrance of the superconducting state. Large-scale simulations of the 3D time-dependent Ginzburg–Landau model indicate that the intermediate resistive state is due to an unwinding of twisted vortices. When the magnetic field increases, this instability is suppressed due to a better accommodation of the vortex lattice to the pinning configuration. Our findings show that magnetic field and geometrical confinement can suppress the dissipation induced by vortex motion. [PNAS 114, E10274 (2017)]

*Work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K10 DMP DCOMP: Fe-based Superconductors -- FeSe Intercalates and Interfaces
BCEC 151B - Timur Kim - Tag(s): Focus

8:00AM K10.00001: Light induced non-volatile switching of superconductivity in single layer FeSe/SrTiO₃ heterostructures*  MING YANG, CHENHUI YAN, YANJUN MA, LIAN LI, CHENG CEN (Presenter), West Virginia University — The capability of using light to control the superconducting state is highly desirable for active quantum device applications. Since superconducting materials rarely exhibit strong photoresponses, and vice versa, optically sensitive materials are often not superconducting, the efficient coupling of these two characters in a single material can be a challenging task. Here we show that, in FeSe/SrTiO₃ heterostructures, the superconducting transition temperature in FeSe monolayer can be effectively raised by the interband photoexcitations in the SrTiO₃ substrate, attributed to a light induced metastable polar distortion uniquely enabled by the FeSe/SrTiO₃ interface, this effect only requires a less than 50 µW/cm² continuous-wave light field. The fast optical generation of superconducting zero resistance state is non-volatile but can be rapidly reversed by applying voltage pulses to the back of SrTiO₃ substrate. The capability of switching FeSe repeatedly and reliably between normal and superconducting states demonstrate the great potential of making energy-efficient quantum optoelectronics at designed correlated interfaces.

*This work is supported by Department of Energy Grant No. DE-SC-0010399, No. DE-SC-0017632 and National Science Foundation Grant No. NSF-1454950.

8:12AM K10.00002: Collective excitations and the superconductivity enhancement of FeSe/SrTiO₃* [Invited]  XUETAO ZHU (Presenter), Institute of Physics, Chinese Academy of Sciences — The observation of substantially enhanced superconducting transition temperatures of single layer FeSe films on SrTiO₃ (STO) substrates has stimulated intensive research to identify the underlying microscopic mechanism. At present, the significant role of interfacial coupling has been widely recognized, but the precise nature of the superconductivity enhancement remains open. By employing high resolution electron energy loss spectroscopy, collective excitations in FeSe/STO system, including the Fuchs-Kliewer (F-K) phonons of STO and the polaronic plasmon originating from collective oscillation of polarons, were measured and studied. With FeSe growth, two dramatic contrasts were observed comparing with bare STO. First, the F-K phonons show indispensable correlation with the polaronic plasmon, indicating F-K phonons participate into the collective oscillation of polarons. Second, the linewidth broadening of the F-K phonons after FeSe growth indicates significant coupling between F-K phonons of STO and electrons in FeSe. It is evidenced that the electrons in FeSe/STO systems are dressed by the strongly polarized local lattice distortions associated with the F-K phonons across the interface. Furthermore, such an interfacial electron-phonon interaction is non-adiabatic in nature, leading to the formation of dynamic interfacial polarons that form the observed polaronic plasmon. The corresponding theoretical model shows that the interfacial polaron-polaron interaction can induce additional attraction between electrons in the systems, resulting in enhanced electron pairing strength and, accordingly, superconductivity.

*The work was supported by the National Key R&D Program of China (No. 2017YFA0303600), and the National Natural Science Foundation of China (No. 11634016).
8:48AM K10.00003: Low-Temperature Gated Raman Spectroscopy and Quantitative EELS of FeSe/STO* NINA ANDREJEVIC (Presenter), Department of Materials Science and Engineering, Massachusetts Institute of Technology, SHENGXI HUANG, Department of Electrical Engineering, Pennsylvania State University, QINGPING MENG, Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, ALEXANDER PURETZKY, DAVID GEOHEGAN, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CUI-ZU CHANG, WEIWEI ZHAO, Department of Physics, Pennsylvania State University, YIMEI ZHU, LIJUN WU, Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, FEI HAN, MINGDA LI, Department of Nuclear Science and Engineering, Massachusetts Institute of Technology — We characterize the phonon dynamics and interfacial charge transfer in FeTe-capped monolayer (ML) and few-layer FeSe films on SrTiO3 using low-temperature gated Raman spectroscopy and electron energy loss spectroscopy (EELS). In FeTe/ML FeSe/STO, we observe emergence of a silent STO mode at 264 cm⁻¹ and slight hardening of STO phonons with an applied back-gate potential, consistent with the bare STO Raman response under electric field. Interestingly, we observe attenuation of the FeSe B₃g peak accompanied by mild softening of both FeSe and FeTe modes, in sharp contrast to the STO dynamics. Notably, this behavior is absent in our measurement of the few-layer sample, suggesting an interplay between the STO and FeTe layer when the FeSe film is sufficiently thin. This is further corroborated by slight hardening of FeTe phonons as the FeSe film thickness is reduced, which we attribute to a non-local effect by the STO. Finally, the intrinsic charge transfer at the FeSe/STO interface is quantified through comparison of experimental and calculated EELS spectra and contrasted between the ML and few-layer samples.

*N.A. acknowledges National Science Foundation GRFP support under Grant No. 1122374 and experimental support from user facilities at Oak Ridge and Brookhaven National Laboratories.

9:00AM K10.00004: Observation of discrete CdGM states in the vortex core of single layer FeSe/SrTiO₃ CHEN CHEN (Presenter), Department of Physics, Fudan University — For conventional type-II superconductors, confined quasi-particles in the vortex cores will give rise to Caroli-de Gennes-Matricon (CdGM) bound states with energies of \( E = \mu \Delta^2 / E_F \) (where \( \mu \) is a half integer, ±1/2, ±3/2...). However, discrete CdGM states were seldom identified due to the small value of \( \Delta^2 / E_F \), which is usually in the micro-eV range. Here we report a clear observation of multiple discrete CdGM states in single layer FeSe film on SrTiO₃, through high energy resolved tunneling spectrum. We found that the energy of these CdGM states can be well described by \( E = \mu \Delta^2 / E_F \) with \( \mu \) equal to half integers (no zero-bias conductance peak observed). Therefore our results support a simple s-wave pairing scenario for this high Tc system. Besides, we studied magnetic impurity (Fe) induced in-gap state with high energy resolution (\( T = 0.4K \)). We found that all the in-gap state are off zero bias and split at high field, despite their intensity and location may vary for different impurities. Our results would help to further unveil the mechanism underlying the high Tc single layer FeSe/SrTiO₃ superconductor.

9:12AM K10.00005: Cavity-enhanced electron-phonon coupling in monolayer FeSe/SrTiO₃* MICHAEL SENTEF (Presenter), MICHAEL RUGENTHALER, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter — We propose a quantum-electrodynamic setting to address the coupling of a low-dimensional quantum material to quantized electromagnetic fields in quantum cavities. Using a prototypical model system describing FeSe/SrTiO with electron-phonon long-range forward scattering, we study how the formation of phonon polaritons at the 2D interface of the material modifies effective couplings and superconducting properties in a Migdal-Eliashberg simulation. We find that through highly polarizable dipolar phonons, large cavity-enhanced electron-phonon couplings are possible but superconductivity is not enhanced for the forward-scattering pairing mechanism due to the interplay between coupling enhancement and mode softening. Our results demonstrate that quantum cavities enable the engineering of fundamental couplings in solids paving the way to unprecedented control of material properties.


*M.A.S. acknowledges financial support by the DFG through the Emmy Noether programme (SE 2558/2-1). A. R. acknowledges financial support by the European Research Council (ERC-2015-AdG-694097), Grupos Consolidados (IT578-13), and European Union's H2020 program under GA no. 676580 (NOMAD).
9:24AM K10.00006: On the Tc enhancement mechanism at the FeSe/SrTiO3 interface* TIANLUN YU (Presenter), QI SONG, XIA LOU, Physics, Fudan University, BINPING XIE, Laboratory of Advanced Materials, Fudan University, HAI CHAO XU, CHENHAOPING WEN, QI YAO, Physics, Fudan University, SHUYUAN ZHANG, XUETAO ZHU, LIANDONG GUO, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, RUI PENG, DONGLAI FENG, Physics, Fudan University — At the interface between monolayer FeSe films and STO substrate the superconducting transition temperature (Tc) is unexpectedly high. The mechanism for the Tc enhancement has been the central question, as it may present a new strategy for seeking out higher Tc materials.

To reveal the mechanism, by combining advances in high quality interface growth, 16O-18O isotope substitution, and extensive data from angle resolved photoemission spectroscopy, we provide striking evidence that the high Tc in FeSe/STO is the cooperative effect of the intrinsic pairing mechanism in the FeSe and interactions between the FeSe electrons and STO phonons.

Furthermore, our results point to the promising prospect that similar cooperation between different Cooper pairing channels may be a general framework to understand and design HTSCs.

*The National Key R&D Program of the MOST of China (Grant Nos. 2016YFA0300200, 2017YFA0303004); The National Science Foundation of China (Grant Nos. 11704073, 11504342).

Discussions with:
Profs. Dragan Mihailovic, Hugo Keller, Annette Bussmann-Holder, Frederick Walker, and Victor E. Henrich on the isotope effects;
Guangming Zhang, Qianghua Wang, and Steve Johnston on EPI.
Dr. Darren Peets for help with the editing.
Dr. Qiuyun Chen for help with the SIMS measurements.

9:36AM K10.00007: Effect of Mn substitution on superconductivity in iron selenide (Li, Fe)OHFeSe single crystals* HUAXUE ZHOU (Presenter), YIYUAN MAO, ZIAN LI, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, CHAI KE, School of Physics, Beijing Institute of Technology, Beijing 100081, China, SHUNLI NI, MINGWEI MA, SHAOBO LIU, JINPENG TIAN, YU LONG HUANG, JIE YUAN, FANG ZHOU, JIANQI LI, KUI JIN, XIAOLI DONG, ZHONGXIAN ZHAO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We synthesize a series of Mn substituted (Li, Fe)OHFeSe superconductor single crystals via a modified ion-exchange method, with the Mn dopant concentration z (the atomic ratio of Mn:Se) ranging from zero to 0.07. Interestingly, we find that the superconducting transition temperature Tc and unit cell parameter c of the Mn-doped (Li, Fe)OHFeSe samples display similar V-shaped evolutions with the dopant concentration z. The Mn dopant may be accommodated in the tetrahedral sites of both the (Li, Fe)OH- and FeSe-layers depending on the doping level, leading to a reduced or enhanced interlayer separation of (Li, Fe)OHFeSe. The observed positive correlation between the Tc and lattice parameter c, regardless of the Mn doping level z, indicates that a larger interlayer separation, or a weaker interlayer coupling, is essential for the high-Tc superconductivity in (Li, Fe)OHFeSe.

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References

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9:48AM K10.00008: Substrate Engineering of Monolayer FeSe Films* TAO JIA (Presenter), ZHUOYU CHEN, SLAVKO REBEC, Stanford University, DANDAN GUAN, Shanghai jiaotong University, MAKOTO HASHIMOTO, DONGHUI LU, ROBERT G MOORE, SLAC, ZHIXUN SHEN, Stanford University — Monolayer FeSe films will exhibit various properties on different substrates: the superconducting transition temperature (Tc) is suppressed if we choose graphene as the substrate, while SrTiO3 and TiO2 substrates can boost the Tc to ~60 K. In this talk, we present the systematic tuning of the substrate structure, and the resulting change in the properties of FeSe, using a combined in-situ system of oxide MBE, chalcogenide MBE, STM and ARPES.

*This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.
**10:00AM K10.00009:** ARPES and MBE studies on the role of the interface in Monolayer FeSe on SrTiO3

*SLAVKO REBEC (Presenter), TAO JIA, ZHUOYU CHEN, Stanford University, ROBERT G MOORE, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, ZHI-XUN SHEN, Stanford University — Monolayer FeSe on SrTiO3 (STO) has been heavily studied in recent years due to the discovery of a large enhancement in its superconducting Tc compared to bulk FeSe, which is attributed to interfacial coupling between the film and substrate. To better understand this interface and how it leads to such a Tc enhancement, we reexamine this system by using MBE grown FeSe and STO coupled with in-situ synchrotron based angle-resolved photoemission spectroscopy (ARPES). Here we present the influence of different STO surface terminations and photon energy dependent ARPES results which help to clarify the role of the substrate in the monolayer FeSe system.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under contract DE-AC02-76SF00515.*

**10:12AM K10.00010:** Ultrafast quasiparticle dynamics and electron-phonon coupling in (Li0.84Fe0.16)OHFe0.98Se

QIONG WU, HUAXUE ZHOU, YANLING WU, LILI HU, SHUNLI NI, YICHAO TIAN, FEI SUN, FANG ZHOU, XIAOLI DONG, ZHONGXIAN ZHAO, JIMIN ZHAO (Presenter), Chinese Academy of Sciences — Distinctive superconducting behaviors between bulk and monolayer FeSe make it challenging to obtain a unified picture of all FeSe-based superconductors. Here, we investigate the ultrafast quasiparticle (QP) dynamics of an intercalated superconductor (Li1-xFex)OHFe1-ySe, which is a bulk crystal but shares a similar electronic structure with single-layer FeSe on SrTiO3. We obtain the electron-phonon coupling (EPC) constant $\lambda_{A1g} (0.23 \pm 0.04)$, which well bridges that of bulk FeSe crystal and single-layer FeSe on SrTiO3. Moreover, we find that such a positive correlation between $\lambda_{A1g}$ and superconducting $T_c$ holds among all known FeSe-based superconductors, even in line with reported FeAs-based superconductors. Our observation indicates possible universal role of EPC in the superconductivity of all known categories of iron-based superconductors, which is a critical step towards achieving a unified superconducting mechanism for all iron-based superconductors.

*Supported by the National Key Research and Development Program of China (2017YFA0303603, 2016YFA0300300), the National NSF of China (11574383, 11774408, and 11574370), the Frontier Program of the CAS (QYZDY-SSW-SLH001), the International Partnership Program of CAS (GJHZ1826), and the CAS Interdisciplinary Innovation Team.*

**10:24AM K10.00011:** Electronic structure of high-Tc topological superconductor monolayer FeTe1-xSex/SrTiO3(001)

XILIANG PENG (Presenter), Institute of Physics, Chinese Academy of Sciences — Topological superconductors are promising platforms for finding Majorana bound states, which are expected to be used in robust quantum computation. However, transition temperature of conventional superconductors is relatively low and single materials combined with high-temperature superconductivity ($T_c$) and topological nontrivial states are scarce in reality. Here, we performed angle-resolved photoemission spectroscopy studies on a series of FeTe1-xSex monolayer films grown on SrTiO3(STO). The superconductivity of the films is robust and rather insensitive to the variations of the band position. However, the band gap between the electron- and hole-like bands at the Brillouin zone center decreases towards band inversion and parity exchange, which drive the system to a nontrivial topological state predicted by theoretical calculations. Our results provide a clear experimental indication that the FeTe1-xSex monolayer materials are high-temperature conrate topological superconductors in which band topology and superconductivity are integrated intrinsically.

**10:36AM K10.00012:** BCS-BEC Crossover of the FeSe/SrTiO3 Interface

SHUYUAN ZHANG (Presenter), XUETAO ZHU, JIANDONG GUO, Institute of Physics, Chinese Academy of Sciences — Superconductivity can be described either in the Bardeen-Cooper-Schrieffer (BCS) limit or in the Bose-Einstein condensation (BEC) limit. Unlike the superconductivity in the BCS limit where the involved electron-boson interaction (EBI) is adiabatic, in the BEC limit, the low superfluid density and short coherence length are expected in the non-adiabatic EBI picture. Our previous studies have shown that the EBI in FeSe/SrTiO3 systems exhibits an indispensable non-adiabatic nature, which leads to the superconductivity beyond the BCS limit. Here, through the analysis of BCS-BEC phase diagram, we find the superconductivity of single-layer FeSe on SrTiO3 substrate locates close to the BCS-BEC crossover unitary. Moreover, the superconductivity can be tuned toward to the BEC limit by surface hole doping. Indeed the potential pseudogap was observed in our scanning tunneling spectroscopy study. These findings provide a rare platform to explore the many-body interactions in superconductors.
The discovery of greatly increased superconducting Tc in FeSe/STO monolayer films (>60 K vs 8 K in bulk) has drawn enormous interest to the prospect of interfacial high-Tc materials. The presence of the STO substrate has been shown to induce heavy electron doping and lattice strain on the adjacent FeSe layer, and is widely proposed to contribute additional enhancement via interfacial phonon coupling. In order to effectively decouple the contributions of these effects to the resultant high-Tc state, we systematically explore the evolution of superconductivity as measured unambiguously by \textit{in situ} electrical resistivity under varied conditions of strain, surface doping concentration, and substrate interface condition. We show that the potassium surface dosing produces a heavily electron doped superconducting layer constrained to the film-vacuum interface, analogous to the monolayer FeSe/STO interface but lacking any STO phonon contribution. In contrast to observations from spectroscopic probes, we observe only modest discrepancies in the zero-resistance Tc for surface doped layers in comparison to monolayer films. We discuss possible explanations for this discrepancy and the implications of these results on the broader understanding of the FeSe/STO enhancement phenomenology.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K11 DMP DCOMP FIAP: Defects in Semiconductors -- Wide Band Gap

8:00AM K11.00001: Vibrational spectroscopy of O-H centers in Ga₂O₃*  

MICHAEL STAVOLA (Presenter), W FOWLER, YING QIN, Lehigh University — Hydrogen has a strong influence on the electrical properties of transparent conducting oxides where it can give rise to shallow donors and can passivate deep compensating defects. The ultra-wide bandgap semiconducting oxide Ga₂O₃ is no exception [1,2]. Vibrational spectroscopy shows that the introduction of H into Ga₂O₃ produces several O-H centers with strongly polarized vibrational lines and different thermal stabilities. Some of these defects appear to be shallow donors and others to be V_{Ga}^{nH} centers. Measurements made for samples that contain both H and D provide clues about the number of H atoms each of these defects contains. Our results suggest different O-H centers that contain a single H atom, two equivalent H atoms, and three or more H atoms. The polarization properties and mode coupling effects for these O-H centers provide structure-sensitive information for complementary theory that suggests specific defect structures [3].


*Supported by NSF grant DMR-1160756.

8:12AM K11.00002: Multiple O-H centers in β-Ga₂O₃*  

W FOWLER (Presenter), MICHAEL STAVOLA, YING QIN, Lehigh University — Hydrogen impurities play a crucial role in the electrical conductivity of β-Ga₂O₃ by acting as shallow donors and by passivating deep acceptors [1,2]. Polarized IR spectroscopy in conjunction with heat treatments of β-Ga₂O₃ single crystals treated in an H₂ (D₂) ambient reveals a number of vibrational lines originating from defects containing one or more O-H(D) species [3,4]. Theoretical calculations using the CRYSTAL06 code [5] with hybridized DFT Hamiltonian and the polarization properties of these vibrational lines are used to suggest structures involving one, two, or three O-H(D) species for these defects. We find strong evidence for one or more O-H(D) associated with Ga(1) vacancies and no evidence for any O-H(D) associated with Ga(2) vacancies in the crystals studied.


*Supported by NSF grant DMR 1160756.
LEONARD BRILLSON (Presenter), Ohio State University — Nanoscale optical and electrostatic techniques can now directly measure the movement of native point defects inside oxide semiconductors and how they control space charge regions, tunneling, and contact rectification. Depth-resolved cathodoluminescence spectroscopy (DRCLS) with hyperspectral imaging measures 3-dimensional defect redistribution on a nanoscale for ZnO, Ga2O3, SrTiO3, and BaSrTiO3, revealing how intrinsic and applied electric fields drive defect movement. Defects at metal-ZnO diodes change carrier densities, tunneling, and trap-assisted hopping, altering Zn- vs. O-polar Schottky barriers. Native point defects are present inside, not only on the surfaces of ZnO nano- and microwires as commonly thought.1,2 Nanoscale 3D measurement and imaging reveal electrically-active defects that extend deep inside wires, introducing new donors or acceptors that alter depletion widths, conducting channel volumes, and metal-ZnO nano-contact rectification. Using electron and ion beams, we altered defect distributions to create rectifying, ohmic, or blocking contacts with the same metal on the same nanowire, demonstrating the interplay between the nature of native point defects, the intrinsic doping, and the physical dimensions of the nanostructure itself in determining the electronic properties of the oxide interface.3 DRCLS also enabled us to correlate the dominant luminescence features of Ga2O3 with the most thermodynamically stable O vacancy, Ga vacancy, and Ga vacancy-hydrogen defect states in the band gap predicted theoretically.4 As with ZnO, the combined depth-resolved detection and processing of Ga2O3 suggests new avenues for identifying and controlling native point defects in semiconductors.


*Supported by NSF Grant DMR-1800130 and AFOSR Grant FA9550-18-1-0066.

**Deep acceptors in Ga2O3**

HARTWIN PEELAERS (Presenter), University of Kansas, JOHN LYONS, Center for Computational Materials Science, JOEL BASILE VARLEY, Lawrence Livermore National Laboratory, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — β-Ga2O3 is a wide-band-gap semiconductor with promising applications in high-power electronics. While n-type doping is straightforward, p-type doping is elusive, with only deep acceptors available. We use hybrid density functional theory to explore the properties of possible acceptors, and discuss the viability of obtaining semi-insulating material. All dopants we considered lead to deep acceptor levels that are more than 1.3 eV above the valence-band maximum. N and Mg were identified as the most promising deep acceptors. We evaluated incorporation in different configurations, and also considered the effect of native defects as well as complexes. We find that both dopants will lead to Fermi-level positions that are at least 1.3 eV away from the band edges. We also predict diffusion activation energies, finding that Mg is significantly more mobile. The information obtained in this study can be used to analyze and explain ion implantation experiments, and to guide design of semi-insulating Ga2O3 layers.

*Work supported by AFOSR, ONR, and DOE.

**A study of deep level defects in β-Ga2O3 using thermal admittance spectroscopy**

J HENDRICKS, Air Force Institute of Technology, Wright-Patterson AFB, MO AHOUJJA (Presenter), Physics, The University of Dayton, SHIN MOU, ADAM T NEAL, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH — The β-Ga2O3 semiconductor is receiving great interest due to its potential applications for high power and deep-ultraviolet devices. However, in spite of a promising future of β-Ga2O3 device technology, its electronic properties, in particular deep level defects, are still not well understood. In this paper we investigated deep level defects in unintentionally doped β-Ga2O3 Schottky diodes, edge-defined film fed grown, using thermal admittance spectroscopy (TAS). An Arrhenius analysis of the TAS measurements shows two deep levels with energies of E1=0.428 eV and E2=1.07 eV and cross sections of σ1=1.83x10^-13 cm^2 and σ2=4.64x10^-13 cm^2, respectively.
9:24AM K11.00006: QSGW calculation of the band structure of Ga2O3-Al2O3 alloys* AMOL RATNAPARKHE (Presenter), WALTER R L LAMBRECHT, Case Western Reserve University — β-Ga2O3 has recently drawn attention as an ultra-wide bandgap semiconductor. The alloys between Ga2O3 and Al2O3 are of interest to obtain even higher band gap materials. The two materials have different ground state structures, monoclinic β-Ga2O3, and corundum α-Al2O3 respectively. We study the Ga2O3-Al2O3 alloys in both the structures using the linearized muffin-tin orbital approach and ABINIT pseudopotential approach for the relaxation of the structural parameters. We consider all possible mixed structures within the common 10 atom primitive unit cells, with compositions $x = 0, 0.25, 0.5, 0.75, 1.0$ in $(\text{Ga2O3})_{1-x} \text{(Al2O3)}_x$. We find the relative ordering of the two structures in the end compounds in agreement with experiment and energy differences in good agreement with previous computational work. We find the Al atoms tend to preferentially occupy the octahedral site when substituting for Ga. The band structure of the alloy models in the two structures is evaluated using the QSGW method.

*This work is supported by NSF under Grant No. DMR-1755479.

9:36AM K11.00007: Enabling p-type doping in In2O3 by a band engineering through alloying† FERNANDO SABINO (Presenter), ANDERSON JANOTTI, Materials Science and Engineering, University of Delaware, SUHUAI WEI, Beijing Computational Science Research Center, — In2O3 is a wide-band gap semiconductor of great importance to the optoelectronic industry. It is often used as transparent contact for solar cells, LEDs, and liquid crystal displays. It has a highly dispersive conduction band, composed of the In s orbitals, that lie relatively low with respect to the vacuum level, making it easy to dope n-type, while the low-energy valence band, composed mostly of O p orbitals, making it difficult to achieve p-type doping because acceptor impurities introduce deep levels in the gap. One way to overcome this limitation is to raise its valence band. Using first-principles calculations we explore different approaches to lift the valence band in In2O3 by alloying. We discuss different alloying elements, both on oxygen and metal sites. We compute the formation enthalpy of these alloys, and their stability with respect to phase separation. We calculate band gaps, and analyze the effects of alloying on the position of the valence and conduction bands, determining the band alignment between the alloys and the parent compounds. Finally, we address their optical properties by calculating absorption coefficients as a function of alloy composition.

*This work was supported by the National Science Foundation Faculty Early Career Development Program DMR-1652994.

9:48AM K11.00008: Non-exponential decay of persistent photocarriers in an AlGaN/AlN/GaN heterostructure DAVID DAUGHTON (Presenter), BOKUAI LAI, JEFFREY LINDEMUTH, Lake Shore Cryotronics (United States) — We report on the kinetics of persistent photoconductivity (PPC) in AlGaN/AlN/GaN heterostructures grown on silicon substrates. Under sub-bandgap illumination (1.91, 2.10, and 2.73 eV), photocarriers from ionized, deep-level defects increase the 2DEG conductivity which persists for hours to days after the illumination has been removed. Using a novel Hall Effect characterization protocol, a logarithmic decay of the persistent carrier concentration, independent of carrier scattering, was observed. The measured logarithmic decay is consistent with a physical separation of defects from the conducting channel and is thought to result from a recombination front propagating through the heterostructure. Persistent photocarrier concentration kinetics were studied as a function of photon dose, wavelength, and temperature. At the shortest wavelength, temperature-dependent studies show the coexistence of two logarithmic decay channels and could indicate PPC in this heterostructure arises from multiple defect species or, perhaps, the defects have different spatial proximity to the conducting channel.

10:00AM K11.00009: Incorporation of Boron in Gallium Nitride† MARK E. TURIANSKY (Presenter), JIMMY SHEN, Department of Physics, University of California, Santa Barbara, DARSHANA WICKRAMARATNE, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — Ternary alloys of the group-III nitrides are integral in the design of electronic and optoelectronic devices. To extend the capabilities of these alloys, boron-containing nitride alloys, such as B$_x$Ga$_{1-x}$N (BGN), are being considered. Boron nitride, however, is most stable in the hexagonal phase, unlike GaN which is stable in the wurtzite phase. As such, there is a lack of experimental information on the properties of wurtzite-phase boron-containing alloys. Using first-principles calculations with a hybrid functional, we explore the nature of boron incorporation in GaN. In the dilute limit, we consider substitutional and interstitial incorporation of boron. We also study the change in the electronic structure of GaN with increasing boron concentration. Wurtzite BN has an indirect band gap, while GaN has a direct band gap. We investigate the direct and indirect nature of the alloy band gap using a projection scheme and by calculating dipole matrix elements. We find that the fundamental band gap of BGN is direct for boron concentrations below 50%. The large band-gap bowing results in a fundamental band gap that is effectively unchanged from the GaN band gap for a wide range of B concentrations.

*This work is supported by NSF.
Identifying Defects and their Electronic Signatures in Regrown GaN Heterostructures

JIAHENG HE (Presenter), GUANJIE CHENG, DAVIDE DEL GAUDIO, JORDAN M OCCENA, Department of Materials Science and Engineering, University of Michigan, FABIAN NAAB, Michigan Ion Beam Laboratory, University of Michigan, RACHEL GOLDMAN, Department of Materials Science and Engineering, University of Michigan, MOHSEN NAMI, BINGJUN LI, JUNG HAN, Department of Electrical Engineering, Yale University — Although silicon-based electronics are used to power light-emitting diodes and electric vehicles, their utility in high power applications is limited by a low breakdown voltage. The most promising alternative power devices consist of vertical GaN devices, which often require regrown active regions. Thus, advances in high power device performance require a detailed understanding of the influence of regrowth processing steps on interfacial defects and their electronic signatures. In this work, we examine a series of GaN p-i-n structures prepared with and without ex-situ ambient exposure and/or chemical etching. To quantify the concentration of various native and extrinsic point defects, we utilize a combination of ion beam analyses in conjunction with x-ray diffraction. For all samples, channeling Rutherford backscattering spectroscopy data reveals minimum yield values < 2%, with displaced atom densities ranging from 1 to 3 x 10^{20}/cm^3. For all samples, cathodoluminescence spectroscopy reveals the GaN near-bandedge and donor-acceptor pair luminescence. We discuss the influence of interface regrowth on variations in the intensity of yellow and infrared luminescence.

*JH gratefully acknowledges the support of ARPA-E AWD0000191.

Spectrally resolved dynamics of energy transfer in GaN:Eu

RUOQIAO WEI (Presenter), Lehigh University, BRANDON MITCHELL, West Chester University, DOLF TIMMERMAN, Osaka University, TOM GREGORKIEWICZ, University of Amsterdam, WAXINZHU, YASUFUMI FUJIIWARA, Osaka University, VOLKMAR R G DIEROLF, Lehigh University — Europium(Eu) doped Gallium Nitride has demonstrated great potential as the red-emitting active layer in nitride-based light emitting diodes(LEDs). External quantum efficiency of up to 9.2% have been achieved. In such optimized layers, we performed a systematic series of temperature dependent, spectrally and time resolved photoluminescence measurements with goal to understand the energy transfer processes between the host material and the various energy levels of the Eu ions. Eu ions are affected by their local environment resulting in at least eight different centers that can be spectrally distinguished. For the most dominant centers, we find that the energy transfer to the Eu ion takes place on a time scale faster than 5 ns. Depending on incorporation site, the energy transfer leads to the population of the {5}D_{0} and/or the {5}D_{2} state. Direct energy transfer to the {5}D_{1} states is negligible. We further show that Eu ions in their long-lived {5}D_{0} state can be excited further leading the creation of electron hole pairs which subsequently relax and transfer their energy back to the Eu ions. This leads to a change in the color of the total emitted light and enables color tunability of the LEDs.

Photoluminescence quantum efficiency of Nd optical centers in GaN epilayers

YIFEI WANG (Presenter), HO VINH, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — We report the photoluminescence quantum efficiency of Nd optical centers as well as the thermal quenching mechanism in GaN epilayers prepared by plasma-assisted molecular beam epitaxy. High resolution infrared spectroscopy, quantum yield and temperature dependence measurements of photoluminescence intensity from Er ions in GaN under resonant and non-resonant excitations were performed. The data provide a picture of the thermal quenching processes and activation energy levels of Nd optical centers in GaN epilayers. The results provide an important step in the realization of GaN:Nd epilayers as an optical gain medium at the infrared region.

Interface chemistry and electrical characteristics of 4H-SiC/SiO_{2} after nitridation in varying atmospheres

ANNA REGOUTZ (Presenter), Imperial College London — SiC/SiO_{2} is a prototypical wide-bandgap semiconductor/dielectric interface, which represents the challenges faced by many such material systems. A multitude of different defects leads to unacceptably large defect densities near the SiC conduction band and management of interfacial defects still remains a topic of lively discussion and current interest. Advanced X-ray spectroscopy methods can probe chemical states at interfaces, and X-ray Photoelectron Spectroscopy (XPS) in particular can deliver great insight into interfaces as it combines both qualitative and quantitative information on elemental distributions, chemical environments, and valence states. Here, we present a systematic study of the 4H-SiC/SiO_{2} interface in industrially manufactured samples with a particular focus on the effects of nitridation in a variety of atmospheres, to reduce interface defect states. Clear differences are found in both spectroscopy and electrical behaviour after high temperature treatments in N_{2}, NO, NH_{3} and NO+NH_{3} atmospheres. Core level spectra give a complete picture of chemical environments present in the oxide and carbide layers as well as at the interface providing insight into defect states and how they are compensated by nitridation.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM
Atomically thin, single crystalline 2D electronic materials have recently emerged, offering a remarkably wide range of building blocks of nanostructures, ranging from metals (e.g. graphene), large gap insulators (BN), to semiconductors (transition metal dichalcogenides and black phosphorous). One key advantage of these van der Waals materials lies in the flexibility of stacking different types of materials to form heterostructures, providing a design platform for achieving novel device functionality. In vdW hetero-bilayers, the interface encompasses the whole heterostructure and interlalyer interactions become the controlling parameter for the electronic structure.

In this talk I will first discuss directly probing the inter-layer interactions through the “lens” of moiré patterns using scanning tunneling microscopy and spectroscopy (STM/S). I will show that the interlayer coupling is strongly dependent on the inter-atomic alignment of the constituent layers. Moreover, as a consequence of moiré pattern formation, the energy band structure of the hetero-bilayer also shows lateral modulation, forming a 2D electronic superlattice. The moiré pattern “lens” also provides us with a means to measure the 2D strain tensor with high precision and high spatial resolution. In addition, the strain profile shows a direct correlation with the band gap modification. As the periodic potential modulation also provides lateral confinement for excitons, an intriguing scenario occurs – the 2D lateral superlattices also form 2D exciton quantum dot arrays. Recent reports of ultra-sharp atomic like spectra provide a direct confirmation of such a scenario. Finally, I will add another control knob and show evidence for valley spin mediated interlayer couplings, and their effect on excitonic states of the hetero-bilayer.

*This work was supported by NSF DMR-1808751, DMR-1720595, EFMA-1542747, and the US Airforce (FA2386-18-1-4097)

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8:36AM K12.00002: Insulating Bulk State in Monolayer WTe2*

**BOSONG SUN (Presenter), TAUNO PALOMAKI, PAUL MALINOWSKI, JIUN-HAW CHU, DAVID HENRY COBDEN, University of Washington** — The layered semimetal WTe2 displays a diverse set of properties in the two-dimensional limit. For example, using an electrostatic gate, one can control the carrier density and change the state of monolayer WTe2 from a 2D topological insulator a 2D superconductor. We will discuss our recent work to better understand the properties of the insulating bulk state seen in monolayer WTe2 near charge neutrality. Using graphene as a probe of the transverse penetrating electric field, we determine the chemical potential as a function of charge density, finding a thermodynamic gap of $45\pm5$ meV at low temperatures. We relate the measurements to transport and angle-resolved photoemission measurements.

*NSF MRSEC award 1719797

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8:48AM K12.00003: Evidence of Metal-Insulator Transition in 2D Van der Waals layers of Copper Indium Selenide (Culn$_7$Se$_{11}$)*

**PRASANNA DNYANESHWAR PATIL, SUJOY GHOSH, MILINDA WASALA, Department of Physics, Southern Illinois University Carbondale, IL-62901, USA., SIDONG LEI, ROBERT VAJTAI, PULICKEL M AJAYAN, Department of Materials Science and Nano Engineering, Rice University, Houston, TX-77005, USA., SAIKAT TALAPATRA (Presenter), Department of Physics, Southern Illinois University Carbondale, IL-62901, USA.** — Several recent reports have indicated the possibility of metal-insulator transition (MIT) in two-dimensional electron systems (2DES), which also includes atomically thick van der Waals layers of two-dimensional (2D) materials such as MoS$_2$, MoSe$_2$, ReS$_2$ etc. In general it appears that alteration of external control parameters such as pressure, charge carrier density etc. can give rise to such phenomenon in these materials. In this regard, this study will demonstrate the possibility of MIT in 2D van der Waals layers of Copper Indium Selenide (Culn$_7$Se$_{11}$). A study of conductivity ($\sigma$) of 2D Culn$_7$Se$_{11}$ FET devices (fabricated using flakes exfoliated from crystals grown using chemical vapor transport technique) as a function of temperature (T) and charge carrier density ($n_{2D}$) (modulated via electrostatic doping through SiO$_2$ gate) show strong features of MIT. The observed phenomenon will be discussed in light of existing theoretical models.

*This work was supported by the U.S. Army Research Office MURI grant # W911NF-11-1-0362.
dichalcogenides MX2 have recently attracted significant attention for their novel electronic properties in monolayer form. Crystals of MX2 materials have a quasi-two-dimensional character reflected in their electronic structure, the coupling between the layers dilutes the many exotic effects appearing in monolayer systems. Here, we report the synthesis of bulk single crystal superlattice materials that physically separate the MX2 layers in the 2H-MX2 structure resulting in enhancements of the 2D nature of their electronic properties observable in their transport behavior.

9:12AM K12.00005: Synthesis and characterization of transition metal chalcogenide superlattice compounds
ARAVIND DEVARAKONDA (Presenter), Department of Physics, Massachusetts Institute of Technology, CIGDEM OZSOY-KESKINBORA, Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, TAKEHITO SUZUKI, Department of Physics, Massachusetts Institute of Technology, MANABU KAMITANI, MARKUS KRIENER, YOSHINORI TOKURA, RIKEN Center for Emergent Matter Science (CEMS), DAVID BELL, Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, JOSEPH CHECKELSKY, Department of Physics, Massachusetts Institute of Technology — The transition metal dichalcogenides MX2 have recently attracted significant attention for their novel electronic properties in monolayer form. These include optical control of valley polarization, the valley Hall effect, and novel forms of superconductivity. While bulk crystals of MX2 materials have a quasi-two-dimensional character reflected in their electronic structure, the coupling between the layers dilutes the many exotic effects appearing in monolayer systems. Here, we report the synthesis of bulk single crystal superlattice materials that physically separate the MX2 layers in the 2H-MX2 structure resulting in enhancements of the 2D nature of their electronic properties observable in their transport behavior.

9:24AM K12.00006: Transport study of quasi-one dimensional transition metal trichalcogenides down to single-chain limit
KYUNGHOON LEE (Presenter), THANG PHAM, ALEX K ZETTL, Physics, University of California, Berkeley — With the successful isolation of few-to-single layer of graphene and transition metal dichalcogenides (TMDs), two-dimensional van der Waals (vdW) materials have been a central focus in condensed matter physics and materials science. In addition to 2D vdWs, a different class of 1D vdW materials, transition metal trichalcogenides (TMTs) such as NbSe3, is emerging with recent advances in isolation and structural characterization of their few-to-single chain encapsulated within carbon and boron nitride nanotubes. The single chain limit of TMTs may exhibit novel physical phenomena, including unusual ground state and collective-mode electronic transport, for instance sliding charge density wave and superconductivity, as found in their bulk counterparts. However, the experimental investigation of these potential properties has been hindered by the challenge of nanodevice fabricating on such small samples. Here, we propose a new approach, correlating the structure-property of the few-to-single chain vdW materials by transmission electron microscopy and device fabrication on the same individual chain-tube sample on a thin SiN membrane. Our work will open up new opportunities for study and application of 1D TMTs based electronics.

*U.S. Department of Energy, sp2-Bonded Materials Program

9:36AM K12.00007: Pump-probe spectroscopy of ultrathin 1T'-MoTe2
TINA DEKKER (Presenter), Electrical and Computer Engineering, University of Waterloo, NICOLAS RIVAS, ARIEL PETRUK, Chemistry, University of Waterloo, SHAZHOU ZHONG, Physics, University of Waterloo, FANGCHU CHEN, XUAN LU, YUPING SUN, Institute of Solid State Physics, Chinese Academy of Sciences, ADAM TSEN, ALBERTO GERMAN SCIAINI, Chemistry, University of Waterloo — Type II Weyl semimetal candidate MoTe2 in bulk form undergoes a transition at ~250 K from the monoclinic phase (1T'-MoTe2) to the inversion-symmetry breaking, orthorhombic phase (Td-MoTe2). Previous transport and Raman measurements on thin MoTe2 flakes have shown a dimensionally driven transition to the orthorhombic phase at room temperature for flakes less than ~12 nm. Using femtosecond broadband pump-probe spectroscopy, we impulsively excited MoTe2 flakes of varying thickness that are protected from oxidation. The temporal evolution of the vibrational wave packet causes spectral modulations of electronic transitions. A probe pulse following the pump reveals any pump-induced time dependence of these signals, including oscillations of the initially excited coherent nuclear motion. Using some novel data analysis tools, and after background subtraction, we were able to follow characteristic phonon modes of each phase resolved in time and frequency domains.
Local Probe Studies of the Orbital Texture of a Single-Layer Mott Insulator

YI CHEN (Presenter), WEI RUAN, MENG WU, University of California, Berkeley, SHUJIE TANG, Stanford University, HYEJIN RYU, Lawrence Berkeley Nat. Lab, HSIN-ZON TSAI, RYAN LEE, SALMAN ABDUL GAFFAR KAHN, FRANKLIN LIOU, CAIHONG JIA, University of California, Berkeley, OLIVER R ALBERTINI, Georgetown University, HONGYU XIONG, TAO JIA, Stanford University, ZHI LIIU, Shanghai Institute of Microsystem and Information Technology, JONATHAN SOBOTA, Stanford University, AMY LIU, Georgetown University, JOEL MOORE, University of California, Berkeley, ZHI-XUN SHEN, Stanford University, STEVEN G. LOUIE, University of California, Berkeley — Mott insulators are insulating phases induced by strong electron correlation that can lead to exotic states such as high-temperature superconductivity and quantum spin liquids. Recent advances in van der Waals material synthesis enable the exploration of novel Mott systems in the two-dimensional limit. Here we present the characterization of the single-layer Mott insulator 1T-TaSe2 via energy-, spatial-, and momentum-resolved measurement of its electronic structure by scanning tunneling microscopy/spectroscopy and angle-resolved photoemission spectroscopy. Our study establishes single-layer 1T-TaSe2 as a novel Mott insulator, thus providing an ideal experimental platform for investigating strong correlation physics in two-dimensional materials.

Electronic structure of 3d transition-metal dichalcogenide thin films grown by molecular-beam epitaxy

SATOSHI YOSHIDA (Presenter), MASAKI NAKANO, HIDEKI MATSUOKA, YUKI MAJIMA, YUE WANG, YUTA OHIGASHI, MASATO SAKANO, YOSHIHIRO IWASA, KYOKO ISHIZAKA, Department of Applied Physics, The University of Tokyo — There has been increasing interest in atomically-thin transition-metal dichalcogenides (TMDs) hosting intriguing properties absent in their bulk form. For example, in 4d and 5d transition-metal TMDs such as MoS2, WSe2, and NbSe2, valley degree of freedom plays an important role on novel two-dimensional properties. 3d TMDs, on the other hand, are expected to exhibit more varieties of phenomena involving excitonic physics, charge density wave, and magnetism, due to stronger electron-electron, electron-lattice and exchange interactions. Recently, emergent ferromagnetism in monolayer VSe2 was reported, although the situation is still controversial. To unambiguously characterize physical properties of atomically thin TMDs and further understand the origin of the emergent two-dimensional phenomena, the direct observation of electronic structures is crucial. We have fabricated atomically thin films of 3d TMDs by molecular-beam epitaxy with our growth recipe [1] and clarified electronic structures by angle-resolved photoemission spectroscopy (ARPES). In this presentation, we will discuss the physical properties appearing in two-dimensional 3d TMDs by comparison with the ARPES results and band calculations. [1] M. Nakano, et al., Nano Lett. 17, 5595 (2017).

Scanning tunnelling microscopy of ultrathin 1T-TaS2*

SEAN WALKER (Presenter), TARUN M PATEL, DELER LANGENBERG, University of Waterloo, YUPING SUN, Chinese Academy of Sciences, ADAM TSEN, JONATHAN D BAUGH, University of Waterloo — 1T-TaS2 is a two-dimensional transition metal dichalcogenide that shows multiple charge density wave (CDW) transitions. Scanning tunnelling microscopy (STM) has been used to extensively study these transitions in bulk 1T-TaS2. We utilize a device geometry that allows for in-plane transport measurements of ultrathin 1T-TaS2 samples (less than 30 nm thick) prepared via mechanical exfoliation in an inert environment, in conjunction with imaging the CDW at the atomic scale. We also investigate the effects of current-driven transitions on the CDW.

*This research was undertaken in part thanks to funding from the Canada First Research Excellence Fund. The authors would like to acknowledge funding from NSERC.

Exciton Condensation in Electron-hole Doped Hubbard Bilayers -- A Sign-problem-free Quantum Monte Carlo Study

XUXIN HUANG (Presenter), Stanford University, MARTIN CLAASSEN, Simons Foundation Flatiron Institute, EDWIN HUANG, Stanford University, BRIAN MORITZ, THOMAS DEVEREAUX, SLAC and Stanford University — A long-sought state of matter, exciton condensation, recently has been realized experimentally in several systems. We develop a sign-problem-free Determinant Quantum Monte Carlo (DQMC) algorithm for bilayer Hubbard model with electron-hole doping, which is an ideal platform to study exciton condensation due to the suppression of electron-hole recombination. In square lattice systems, we demonstrate a tendency for exciton condensation at momentum (∏, ∏), and this excitonic order appears to compete with a charge ordered state in the parameter regime we study. Exciton condensation on hexagonal lattices, presumably more pertinent to systems used in previous experimental realizations, has also been investigated and the results will be shown in comparison with square lattice results.
A monolayer transition metal dichalcogenide as a topological excitonic insulator

DANIELE VARSANO, Istituto Nanoscienze, Modena, Italy, CNR, MAURIZIA PALUMMO, Dept of Physics, University of Rome Tor Vergata, ELISA MOLINARI, FIM, Modena, Italy, University of Modena, MASSIMO RONTANI (Presenter), Istituto Nanoscienze, Modena, Italy, CNR —

Monolayer transition metal dichalcogenides in the $T'$ phase might realize the quantum spin Hall effect at room temperature, since they have a large bulk hybridization gap between the inverted valence bands that provides topological order with robustness. Here we demonstrate that $T'$-MoS$_2$ is unstable against the spontaneous generation of excitons by using first-principles many-body perturbation theory, as the computed exciton binding energy is larger than the quasiparticle gap. We predict that the true ground state of $T'$-MoS$_2$ is a novel correlated insulator in which both excitonic and topological orders coexist by reducing the spatial point group symmetry, whereas typically interactions tend to disrupt the topological order. A self-consistent calculation provides us with clear-cut signatures of this excitonic topological insulator, such as an enhanced bulk quasiparticle gap (and hence increased topological robustness), spontaneous inversion symmetry breaking, spin-splitting of quasiparticle bands. The phase diagram, in the space whose axes are temperature and strain, includes a second—topologically trivial—excitonic phase that spontaneously breaks mirror symmetry while changing discontinuously the quasiparticle gap, which surprisingly never closes.

Suppression of Exciton Condensation in Copper-Doped TiSe$_2$ Measured with M-EELS

MELINDA RAK (Presenter), SAMANTHA RUBECK, MATTEO MITRANO, ALI HUSAIN, University of Illinois at Urbana-Champaign, ANSHUL KOGAR, Massachusetts Institute of Technology, SEAN VIG, University of Illinois at Urbana-Champaign, JASPER VAN WEZEL, University of Amsterdam, GORAN KARAPETROV, Drexel University, EMILIA MOROSAN, Rice University, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — Excitons were predicted to form a Bose condensate, but for many years there was no direct experimental verification of this condensation in a solid. Using momentum-resolved electron energy-loss spectroscopy (M-EELS), we demonstrated the presence of an exciton condensate in $1T$-TiSe$_2$ by observing a soft electronic collective mode at the charge density wave (CDW) transition temperature, $T_C = 190$ K. As TiSe$_2$ is doped with copper to form Cu$_x$TiSe$_2$, the CDW transition temperature is suppressed and a superconducting dome emerges around $x = 0.04$. Using M-EELS, we found that the electronic collective mode softens partially near $T_C$ for very low dopings ($x < 0.004$), but does not soften above $x \sim 0.01$. Our results indicate that the exciton condensate is rapidly destroyed in Cu$_x$TiSe$_2$ by screening from the Cu atoms and that a conventional Peierls CDW persists above $x \sim 0.01$. We conclude that the excitonic state is not directly related to the superconductivity in Cu$_x$TiSe$_2$.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K13 DMP: 2D Materials (General) -- Topology and Exotic Phenomena

Growth and Transport Characterization of Epitaxial Graphene on Non-polar SiC Facets

YIRAN HU (Presenter), School of Physics, Georgia Institute of Technology, VLADIMIR PRUDKOVSKII, Institut Neel/CNRS-Univ. Grenoble Alpes, ANTONIO TEJEDA, Univ. Paris-Sud, ÂMINA TALEB IBRAHIMI, SOLEIL Synchrotron, YUE HU, School of Physics, Georgia Institute of Technology, CLEMENS B. WINKELMANN, Institut Neel/CNRS-Univ. Grenoble Alpes, LEI MA, TICNN, Tianjin University, CLAIRE BERGER, Institut Neel/CNRS-Univ. Grenoble Alpes, WALT A. DE HEER, School of Physics, Georgia Institute of Technology —

The ballistic transport and quantized conductance of $e^2/h$ observed in epitaxial graphene side wall nanoribbons at room temperature still lacks full explanation [1]. In an effort to solve this question, we produced graphene samples on specific SiC facets that host the side wall nanoribbons and fabricated standard transport measurement devices. Pre-growth patterning has been demonstrated to direct the graphene growth and improve growth uniformity. We did a variety of measurements, including AFM, Raman spectroscopy, ARPES, STS and transport measurements. These results indicate a charge-neutral graphene material, showing properties consistent with the observation of ballistic transport in side wall nanoribbons.

8:12AM K13.00002: Strain fields in graphene induced by nanopillars* SLAVISA MILOVANOVIC (Presenter), LUCIAN COVACI, FRANCOIS M PEETERS, University of Antwerp — The mechanical and electronic properties of a graphene membrane placed on top of a superlattice of nanopillars are investigated. We use molecular dynamics simulations to access the deformation fields and the tight-binding approaches to calculate the electronic properties. The system of interest consists of a triangular lattice of nanopillars with a period of $a=750$ nm over which the graphene layer is deposited. Ripples form in the graphene layer that span across the unit cell, connecting neighboring pillars, in agreement with recent experiments. We investigate the dependence of the pseudo-magnetic field (PMF) on unit cell parameters and the van der Waals interaction between graphene and the substrate. We find direct correspondence with typical experiments on pillars, showing intrinsic “slack” in the graphene membrane. PMF values are confirmed by the LDOS calculations at different positions of the unit cell showing pseudo-Landau levels at varying spacings. Our findings can be applied to other 2D materials (hBN, TMDs). Such systems are of interest as single-photon emitters where charge carriers are confined by the strain potential. Our study can be used as a guide to optimize parameters of the system for the improvement of the efficiency of the emitter.

*SPM is supported by FWO.

8:24AM K13.00003: Charged topological solitons in zigzag graphene nanoribbons. LUIS BREY (Presenter), M.P. LOPEZ-SANCHO, ICMM-CSIC — Zigzag graphene nanoribbons (ZZGN) have a magnetic ground state (GS) characterized by edge ferromagnetism with antiferromagnetic coupling between opposite edges. This GS appears because of a broken symmetry in the spin sector. Therefore, by inverting the spin polarization of the full system there is another energy degenerate GS. The band structures of the degenerate GS’s are inverted. When connecting two domains with opposite mass i.e. spin orientation, a symmetry protected zero energy topological state appears at the interface between the degenerate GS's. These topological states are soliton-like excitations that carry charge $\pm e$ with half electron localized at each edge of the nanoribbon. The connection between topological defects and electric charge suggests that solitons can be the relevant charge excitation in ZZGN's. Then whenever adding charge to the system an array of solitons can be formed, creating a solitonic phase. By performing numerical calculations, we find that at low doping, charge added to the system creates magnetic domains and becomes localized at the domain walls separating opposite degenerate ground states. Our results show that the topological properties of ZZGNR's are generated by electron-electron interactions rather than by spin orbit coupling.

8:36AM K13.00004: Topological Effects in 1D and 2D Materials: Topological Band Engineering, Optical Selection Rules, and Excitonic Shift Currents* [Invited] STEVEN G. LOUIE (Presenter), University of California at Berkeley and Lawrence Berkeley National Lab — In this talk, I present several fascinating manifestations of topological effects in the electronic and optical properties of atomically thin one-dimensional (1D) and two-dimensional (2D) materials. First, we find that symmetry-protected topological phases exist in graphene nanoribbons (GNRs) [1]. Semiconducting GNRs of different width, edge shape, and terminating unit cells can belong to different electronic topological classes, characterized by a $Z_2$ invariant. Junctions between segments of topologically distinct GNRs are predicted to support robust in-gap topological junction states which can be used for band engineering. Experimental realizations of these predictions have been achieved [2]. Second, we show that the conventional optical selection rules for excitons must be replaced in 2D by a novel, simpler formula, owing to a topological characteristic inherent to the photoexcitation of excitons in 2D [3]. The new selection rule is dictated by a winding number of the interband optical transition matrix elements (a heretofore unrecognized topological invariant). This appealingly simple and general new rule is applied to elucidate the optical spectra of gapped graphene systems. Third, I present some recent work on the effects of electron-hole interactions on shift currents in non-centrosymmetric 2D crystals (so-called bulk photovoltaic effect), in which we show excitonic effects lead to an enormous enhancement and, more interestingly, gives rise to DC conduction with sub-bandgap-frequency excitations.[4]

References:

*This work was supported by U. S. Department of Energy, National Science Foundation, and Office of Naval Research. I would like to acknowledge collaborations with members of the Louie group.
9:12AM K13.00005: Topological Vortices vs. discommensuration dislocations in charge-density-wave 2H-TaSe$_2$

SEONG JOON LIM (Presenter), Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, CHOOJAE WON, Laboratory for Pohang Emergent Materials, Pohang Accelerator Laboratory and Max Planck POSTECH Center for Complex Phase Materials, Pohang University of Science and Technology., SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, NJ — Charge density wave (CDW) discommensuration (DC) refers to a boundary between two different CDW phases and is a key to understand the phase transition from commensurate to incommensurate CDW. The phase transition can be rendered as a process of creating or eliminating DCs that results in change of incommensurability, and the place of such process, where DCs merge to each other, has been known as CDW dislocation. The idea of CDW DC dislocation has been primarily studied in 2H-TaSe$_2$, which shows a clear phase transition from incommensurate to commensurate CDW. Although there have been several experimental and theoretical results supporting the idea, it has nevertheless not been verified at the atomic scale using, for example, scanning tunneling microscopy (STM). We present an observation of such entangled points of multiple DCs in 2H-TaSe$_2$ by STM. The observation showed no phase slip which is against the idea of CDW dislocation, but the result instead unveiled the formation of topological vortices. In this talk an atomic scale comparison among the CDW DC dislocation model, the experimental results as well as a complicated vortex-like domain topology of 2H-TaSe$_2$ will be presented.

9:24AM K13.00006: Quantum paraelastic two-dimensional materials

TYLER BISHOP (Presenter), ERIN FARMER, AFSANA SHARMIN, University of Arkansas, ALEJANDRO PACHECO-SANJUAN, Mechanical Engineering, Universidad Tecnica Federico Santa Maria, PIERRE DARANCET, Center for Nanoscale Materials, Argonne National Laboratory, SALVADOR BARRAZA-LOPEZ, University of Arkansas — We study the elastic energy landscape of two-dimensional tin oxide (SnO) monolayers and discover a transition temperature using ab-initio molecular dynamics (MD), that is close to the value of the elastic energy barrier $J$ derived from $T = 0$ K density functional theory calculations. The power spectra of the MD evolution permits identifying soft phonon modes likely responsible for the observed structural transformation. The mean atomic displacements obtained from a Bose-Einstein occupation of the phonon modes suggest the existence of a quantum paraelastic phase, that could be tuned charge doping, implying that SnO monolayers could be two-dimensional quantum paraelastic material with a charge-tunable quantum phase transition.

*T. B. was funded by the NSF (Grant No. DMR1610126) and S.B.L. by an Early Career Grant from the DOE (DE-SC0016139). Part of this work was performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, under Contract No. DE-AC02-06CH11357. P.D. is funded by the Director, Office of Science, of the U.S. Department of Energy under contract DEAC02-06CH11357. Calculations were performed at Cori (NERSC), Carbon (ANL), and Trestles (Arkansas).

9:36AM K13.00007: Dependence of the hBN Layer Thickness on the Band Structure and Exciton Properties of Encapsulated WSe$_2$ Monolayers

IANN GERBER (Presenter), XAVIER MARIE, LPCNO, Institut National des Sciences Appliquées de Toulouse — The optical properties of two-dimensional transition metal dichalcogenide monolayers such as MoS$_2$ or WSe$_2$ are dominated by excitons, Coulomb bound electron-hole pairs. Screening effects due the presence of hexagonal-BN surrounding layers have been investigated by solving the Bethe Salpeter Equation on top of $GW$ wave functions in density functional theory calculations. We have calculated the dependence of both the quasi-particle gap and the binding energy of the neutral exciton ground state $E_b$ as a function of the hBN layer thickness. This study demonstrates that the effects of screening at this level of theory are more short-ranged that it is widely believed. The encapsulation of a WSe$_2$ monolayer by three sheets of hBN (~1 nm) already yields a 20 % decrease of $E_b$ whereas the maximal reduction is 27% for thick hBN. We have performed similar calculations in the case of a WSe$_2$ monolayer deposited on stacked hBN layers. These results are compared to the recently proposed Quantum Electrostatic Heterostructure approach.

*I. C. Gerber thanks the CALMIP initiative for the generous allocation of computational times, through the project p0812, as well as the GENCI-CINES and GENCI-IDRIS for the grant A004096649. X. Marie acknowledges the Institut Universitaire de France.
9:48AM K13.00008: Revealing of Dark Exciton States by Twisted Light in Two Dimensional Transition Metal Dichalcogenides  KRISTAN BRYAN C SIMBULAN, TENG-DE HUANG, Department of Physics, National Taiwan Normal University, FENG LI, JUNJIE QI, School of Materials Science and Engineering, University of Science and Technology Beijing, TING-HUA LU, YANNWEN LAN (Presenter), Department of Physics, National Taiwan Normal University — Brightening spin- and momentum-forbidden dark exciton in two-dimensional (2D) transition metal dichalcogenides (TMDs) is nontrivial to further advances in optoelectronics applications. In this study, we demonstrate the effects of the interaction between twisted light (light possessing orbital angular momentum) and atomically thin TMD material in the optical measurements. Our results show a reproducible blue shift in the photoluminescence (PL) spectra of both monolayer and bilayer TMD material as the topological charge of the illuminating twisted light is incremented along positive and negative values. This phenomenon is attributed to the transfer of orbital angular momentum from twisted light onto the center-of-mass momentum of excitons which consequently brightens momentum-forbidden dark exciton states. Further, based on the observation on power-dependence of PL spectra, we found a red shift with increasing laser power across different topological charge values of the incident light. It reveals that there is another factor such as heat or strain induced by twisted light, which can replace the dominant mechanism. This study uncovers a new selection rule in 2D TMD materials that can potentially be a useful control mechanism for future optoelectronic device applications.

10:00AM K13.00009: The influence of disorder in the external environment of 2D semiconductors on their electronic and optical properties  ARCHANA RAJA ( Presenter ), University of California, Berkeley, LUTZ WALDECKER, Stanford University and SLAC National Laboratory, JONAS ZIPFEL, University of Regensburg, YEONGSU CHO, University of Chicago, SAMUEL BREM, Chalmers University of Technology, JONAS ZIEGLER, University of Regensburg, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Tsukuba, ERMIN MALIC, Chalmers University of Technology, TIMOTHY BERKELBACH, University of Chicago, TONY F HEINZ, Stanford University and SLAC National Laboratory, ALEXEY CHERNIKOV, University of Regensburg — Disorder in solids typically stems from local fluctuations of material structure itself like composition, strain, and size. Here, we highlight a new source of disorder in atomically thin, two-dimensional (2D) materials: The variation in the effective strength of Coulomb interactions in the 2D material resulting from fluctuations in the dielectric screening of the adjoining environment. We experimentally monitor the influence of dielectric disorder for monolayer WS₂ and WSe₂ on SiO₂, PDMS and h-BN by probing correlations between ground and excited state exciton resonances, which exhibit different sensitivities to the external dielectric environment. Our observations are described in a theoretical framework that considers variation in external dielectric screening and intrinsic phonon scattering channels as contributing to the ground and excited-state exciton linewidths. Even moderate fluctuations in the external dielectric permittivity are shown to induce inhomogeneous variations of the bandgap and exciton binding energies on the order of 100’s of meV, constituting the major source of disorder in the studied samples. We identify elimination of dielectric disorder as key to achieving high material quality through encapsulation of 2D semiconductors in other van der Waals materials.

10:12AM K13.00010: Theory-assisted detection of nano-rippling and impurities in STEM images of angle-mismatched bilayer graphene*  ANDREW O’HARA (Presenter), OLEG S OVCHINNIKOV, JORDAN A. HACHTEL, Department of Physics and Astronomy, Vanderbilt University, STEPHEN JESSE, Center for Nanophase Materials Science, Oak Ridge National Laboratory, SERGEI KALININ, Institute for Functional Imaging of Materials, Oak Ridge National Laboratory, ALBINA Y BORISEVICH, Materials Science and Technology Division, Oak Ridge National Laboratory, SOKRATES T PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — Two-dimensional (2D) materials commonly contain ripples and impurity atoms that limit carrier mobilities, create pseudo-magnetic fields, and affect other electronic and magnetic properties. While scanning transmission electron microscopy (STEM) provides high-accuracy determination of the atomic positions and columns in the image plane, it is difficult to obtain precise atomic positions in the perpendicular direction. Detection of impurities with similar atomic numbers can also be difficult in Z-contrast imaging. In the case of multilayer 2D materials such as bilayer graphene, misalignment of the layers results in a moiré pattern that further compounds the problem of atomic identification. In this work, we introduce a combined approach utilizing STEM imaging and density-functional-theory calculations to recover this information from the experimentally accessible xy-coordinates in twisted bilayer graphene. We find that the strain-induced rippling obeys the continuum model of elasticity and that the moiré-pattern-induced undulations are approximately an order of magnitude smaller. Additionally, using the presented methodology, we are able to establish the presence of a substitutional nitrogen impurity.

*Supported by DOE Grant DE-FG-02-09ER46554 and NSF Grant DMR-1508433.
Strain enhancement of the Kondo effect in graphene

KEVIN INGERSENT (Presenter), Department of Physics, University of Florida, DWAEI ZHAI, SERGIO E ULLOA, NANCY PATRICIA SANDLER, Department of Physics and Astronomy, Ohio University — The Kondo physics of screening of an impurity's magnetic moment by electrons in doped graphene has been predicted to exhibit peculiar features. However, conclusive experimental observation of the phenomenon remains elusive. One possible obstacle to its identification is a very small Kondo temperature $T_K$ in situations where the chemical potential lies near the Dirac point. Here, we propose to use mechanical deformations in graphene to recognize the unique fingerprints that the Kondo regime exhibits [1]. Inhomogeneous deformations are known to produce specific alternating changes in the local density of states that indicate sublattice symmetry breaking effects. These patterns can be magnified to produce significant enhancement or depression of $T_K$ for magnetic impurities positioned at different lattice sites. The deformation-induced changes, particularly the strong increase of $T_K$ expected at certain impurity locations, may lift the Kondo scale into the experimentally relevant range and are suitable for detection using local probes such as scanning tunneling microscopy.


*We acknowledge support from NSF Grant Nos. DMR-1508325 (Ohio) and DMR-1508122 (Florida).

Nano-optical imaging of 2D TMD alloys

DMITRI VORONINE (Presenter), University of South Florida — Two-dimensional transition metal dichalcogenides (2D TMDs) are the materials of recent interest due to many promising applications. Novel materials and devices are based on the heterostructures formed by 2D TMDs. Alloys formed at TMD heterojunctions may enhance or limit the applications. It is important to characterize their optoelectronic properties with nanoscale spatial resolution. Tip-enhanced photoluminescence (TEPL) and tip-enhanced Raman scattering (TERS) techniques were used to image various TMD (MoS$_2$, WS$_2$, MoSe$_2$, WSe$_2$) alloys and heterostructures revealing detailed nanoscale features. Conventional far-field photoluminescence (PL) and Raman imaging provides highly averaged information with spectral congestion. In contrast, the TEPL and TERS methods, not limited by diffraction, provide substantial information related to nanoscale optical properties of 2D materials with resolution down to a few nanometers. The variations in the nanoscale optical properties correlating with the structural variation can provide a better understanding of the 2D TMD materials for the future development of highly efficient, flexible, lightweight optoelectronic devices.

Stacking-dependent interlayer phonons in 3R and 2H MoS$_2$

JEREMIAH VAN BAREN (Presenter), Department of Physics and Astronomy, University of California, Riverside, GAIHUA YE, ZHIPENG YE, POUYAN REZAIE, Department of Electrical and Computer Engineering, Texas Tech University, JIA-AN YAN, Department of Physics, Astronomy, and Geosciences, Towson University, YU PENG, ZHENG LIU, Centre for Programmed Materials, School of Materials Science and Engineering, Nanyang Technological University, RUI HE, Department of Electrical and Computer Engineering, Texas Tech University, CHUN HUNG LUI, Department of Physics and Astronomy, University of California, Riverside — Atomically thin MoS$_2$, a prototype two-dimensional semiconductor, commonly exhibits the 2H stacking order. In even layer numbers, 2H MoS$_2$ restores the inversion symmetry and hence loses many attractive properties, such as second harmonic generation, piezoelectricity and spin-valley coupling. But researchers have recently grown MoS$_2$ crystals with 3R stacking order, which in all layer numbers breaks the inversion symmetry and retains the valleytronic, piezoelectric and nonlinear optical properties as in the monolayer. We have directly probed the stacking-dependent interlayer coupling in the pure 2H and 3R structure of MoS$_2$ by ultralow-frequency Raman spectroscopy. We observe up to three shear branches and four breathing branches in MoS$_2$ samples with thickness from 2 to 13 layers. Our results show distinct behavior of the shear modes between 2H and 3R MoS$_2$, and also suggest a slightly enhanced interlayer coupling in 2H MoS$_2$ compared to 3R MoS$_2$. Through a combination first-principles calculations, group theory, and an effective bond-polarizability model, we account for all the major observations in our experiment.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K14 DCMP: Graphene: Electronic Transport and Characterization

BCEC 153C - Ivan Borzenets
Atomic-Resolution Visualization of Complex Structures in Intercalated Bilayer Graphene*

JASON BONACUM (Presenter), ANDREW O’HARA, Department of Physics and Astronomy, Vanderbilt University, OLEG SOVCHEK, Institute for Functional Imaging of Materials, Oak Ridge National Laboratory, GEORGE GORDEEV, SONAKSHI ARORA, STEPHANIE REICH, Fachbereich Physik, Institut für Experimentalphysik, Freie Universität Berlin, JUAN CARLOS IDROBO, Institute for Functional Imaging of Materials, Oak Ridge National Laboratory, RICHARD F HAGLUND, SOKRATES T PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, KIRILL BOLOTIN, Fachbereich Physik, Institut für Experimentalphysik, Freie Universität Berlin — Intercalation in two-dimensional materials has been widely investigated using spectroscopic, diffraction, and electrical measurements. However, these techniques generate spatially averaged data and provide information about the local atomic structure only inferentially. In this work, we deploy aberration-corrected scanning transmission electron microscopy to directly visualize the local atomic structure of FeCl3-intercalated bilayer (BLG) and few-layer graphene (FLG). The data exhibit a crystalline monolayer of FeCl3 inside BLG, atomically sharp intercalation boundaries, a variety of orientations for FeCl3 monolayers in FLG, and regions where the iron is reduced to form monolayer FeCl2. Our density-functional-theory calculations predict a low energy barrier of 0.04 meV/nm2 between different orientations of FeCl3, supporting the observation of multiple orientations. Furthermore, resonant-Raman spectroscopy yields evidence of two distinct graphene doping levels of $E_F=0.98\text{eV}$ and $E_F=1.06\text{eV}$ in intercalated bilayer graphene, which may be attributed to the coexistence of FeCl3 and FeCl2. These results highlight the critical need for atomic-resolution studies of FeCl3 and similar intercalants to understand the dynamics of doping in multilayer graphene and graphene superlattices.

*NSF DMR

Chiral symmetry breaking in rhombohedral multilayer graphene

NARJES KHEIRABADI, ANDREW HALLWOOD, JONATHAN F P ROGERS, EDWARD MCCANN (Presenter), Physics Department, Lancaster University, Lancaster, UK, MIKITO KOSHINO, Department of Physics, Osaka University, Japan — We model the single-particle electronic properties of rhombohedral multilayer graphene focusing on the topological surface states that yield two flat degenerate bands in the vicinity of the Fermi level. We show that chiral-symmetry breaking tight-binding parameters produce a finite dispersion of the two low-energy bands, but do not lift their degeneracy owing to the conservation of PT symmetry. We model PT symmetry breaking due to external fields, including interlayer asymmetry due to an external gate or substrate (broken space inversion) or an external magnetic field (broken time reversal symmetry).

Direct chemical potential measurements of fractional quantum Hall states in bilayer graphene

ALEXANDER ZIBROV (Presenter), FANGYUAN YANG, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki, Japan, ANDREA YOUNG, University of California, Santa Barbara — We report measurements of the chemical potential in high quality bilayer graphene (BLG) in the quantum Hall regime as a function of magnetic field, interlayer bias, and charge carrier density. To maintain sample quality while also enabling quantitative determination of the chemical potential of the BLG flake, we use a four plate capacitor heterostructure consisting of graphite top and bottom gates, BLG, and an integrated charge sensing graphene monolayer. The resulting devices show fractional quantum Hall states at odd-denominator filling fractions as large as 11 as well as even-denominator states at fillings $\nu=-5/2$, -1/2, 3/2 and 7/2. Changes in the chemical potential of the BLG flake generate modulations of the charge density in the monolayer graphene sensor layer, which we detect capacitively. These modulations form the error signal for a feedback loop whose control voltage is the BLG chemical potential. We demonstrate chemical potential sensitivity better than 10uV/√Hz, allowing determination of fractional quantum Hall energy gaps in this system. We then use the measured temperature dependence of the chemical potential to estimate the entropy of the electron system, and compare our results to predictions for abelian and nonabelian quasiparticles near fractional filling factors.
Large tunable intrinsic gap in rhombohedral-stacked tetralayer graphene at half filling

SHI CHE (Presenter), Department of Physics, The Ohio State University, KEVIN S MYHRO, YANMENG SHI, YONGJIN LEE, KEVIN THILAHAR, KEVIN BLEICH, Department of Physics and Astronomy, University of California, Riverside, DMITRY SMIRNOV, National High Magnetic Field Laboratory, CHUN NING LAU, Department of Physics, The Ohio State University — Rhombohedral-stacked tetralayer (r-4LG) has a highly unusual energy dispersion, which can be approximated as $E \sim k^4$, where $k$ is the wave vector. At half filling, the very flat energy bands in r-4LG are unstable to electronic interactions, giving rise to electronic states with spontaneous broken symmetries. Using transport measurements on suspended dual-gated devices, we observe an insulating ground state with a large interaction-induced transport gap up to 80 meV at the charge neutrality point. The energy gap is enhanced further with a perpendicular magnetic field, but closed or suppressed upon the application of an out-of-plane electric field of either polarity, increasing charge density or a critical temperature of ~40 K. This insulating gapped state is consistent to that observed in bilayer graphene (BLG) and rhombohedral-stacked trilayer graphene (r-TLG), and therefore proposed to be a layer antiferromagnet with broken time reversal symmetry. The large magnitude of the gap also suggests that, at least in r-4LG, the band flattening effect prevails over the increasing screening and charge de-confinement in thicker graphene, in agreement with a first principle calculation.

Energetics of complex phase diagram in a tunable bilayer graphene probed by quantum capacitance

MANABENDRA KUIRI (Presenter), ANINDYA DAS, Indian Institute of Science — Bilayer graphene provides a unique platform to explore the rich physics in quantum Hall effect. The unusual combination of spin, valley and orbital degeneracy leads to interesting symmetry broken states with electric and magnetic field. Conventional transport measurements like resistance measurements have been performed to probe the different ordered states in bilayer graphene. However, not much work has been done to directly map the energetics of those states in bilayer graphene. Here, we have carried out the magneto capacitance measurements with electric and magnetic field in a hexagonal boron nitride encapsulated dual gated bilayer graphene device. In presence of perpendicular magnetic field, we observe Landau level crossing in our magneto-capacitance measurements with electric field. The gap closing and reopening of the lowest Landau level with electric and magnetic field shows the transition from one ordered state to another one. Further more we observe the collapsing of the Landau levels near the band edge at higher electric field ($D > 0.5 \, V/nm$), which was predicted theoretically. The complete energetics of the Landau levels of bilayer graphene with electric and magnetic field in our experiment paves the way to unravel the nature of ground states of the system.

Quantitative Measurement of Valley Polarization in a Multicomponent Fractional Quantum Hall System

FANGYUAN YANG (Presenter), ALEXANDER ZIBROV, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, MICHAEL ZALETEL, University of California, Berkeley, ANDREA YOUNG, University of California, Santa Barbara — In bilayer graphene, the electronic structure at high magnetic fields are enhanced by spin, valley and orbital degrees of freedom. In particular, the valley quantum number can be directly mapped onto layer polarization, allowing for direct capacitive probes. In this talk, I will present quantitative measurements of valley polarization in high quality bilayer graphene quantum Hall system. The valley polarization is obtained by measuring antisymmetric combinations of top- and bottom- gate capacitances to the graphene bilayer. We improve on past approaches by using a multilayer heterostructure in which the bilayer is encapsulated in successive layers of hexagonal boron nitride (hBN), monolayer graphene, hBN, and graphite, allowing full control of density and layer polarization in both the bilayer and in the monolayer graphene gates. Our layer resolved measurements provide new quantitative insight into the ground states and excitations of both integer and fractional quantum Hall phases in bilayer graphene.
Time-resolved spectroscopies have significantly contributed to the study of the dynamical properties of conventional and quantum materials. By following the dynamics of excited electrons, one can follow the dominant scattering processes and discern the flow of energy from the electronic system to other degrees of freedom. Time and angle-resolved photoemission spectroscopy (TR-ARPES) allow one to access electron dynamics in a momentum resolved way. In this work, a balance of energy and time resolution revealed a peak associated with optical excitation. In addition, we observe quantized energy-loss scattering processes, which comes from the emission of an optical phonon from electrons in the direct-transition peak (DTP). The characteristic time scale associated with the transfer of spectral weight from the DTP to the phonon-scattering-peak can then be directly related to the mode-projected electron-phonon matrix element.

*This research is funded by the Max Planck-UBC-UTokyo Centre for Quantum Materials and the Canada First Research Excellence Fund, Gordon and Betty Moore Foundation’s EPiQS Initiative, NSERC, Canada Foundation for Innovation, and the CIFAR Quantum Materials Program.

Magnetic field shifts the channel away from our electric interface in a way that is inconsistent with the semiclassical expectation from the Lorentz force. Moreover, the magnetic field causes an imbalanced layer occupation preference to the chiral channels. These behaviors can be understood in the limits that either the electric or the magnetic field dominates. We numerically show in the general case that the system can be well-approximated as a weighted sum of the two limits.

There has recently been a wave of interest in the hydrodynamical behavior of quantum many-body systems. Using ‘Coulomb drag’ physics as a guide, we discuss analogues of shear viscosity in quantum systems on discrete lattices. We argue that, although particle-hole symmetric materials have zero Coulomb drag, they nevertheless show a thermal equivalent in the form of drag between energy currents. Using a combination of perturbation theory and techniques from integrability, we give analytical predictions for this effect in coupled one-dimensional wires and compare them to DMRG studies on the Hubbard model. We comment on the generalization of these results to higher dimensional systems.

The study of electric current, dominated by electron-electron interactions, has recently gained interest owing to a new generation of ultra clean materials. In this regime, the flow behaves as viscous hydrodynamics fluid, in contrast to non-interacting flow types such as diffusive and ballistic. In this work, we use a scanning single electron transistor (SET) to image the local potential landscape produced by flowing electrons in an expanding channel of graphene. This geometry is ideal to reveal the spatial manifestation of the quantum contact resistance as well as non-local aspects of ballistic and hydrodynamic flows. In this talk we will present our recent scanning measurements that shed new light on all the above aspects of electron flow.
10:00AM K14.00011: Probing exciton condensates in double layer graphene using the corbino geometry  
YIHANG ZENG (Presenter), J.I.A. LI, OLIVIA GHOSH, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, CORY DEAN, JAMES HONE, Columbia University — Double layer graphene system with a thin tunnel barrier was recently reported to host exciton condensates and novel interlayer fractional quantum hall (FQH) states in the presence of a high magnetic field. The corbino geometry, consisting normally of two concentric rings, provides a direct transport probe of the bulk response, without the contribution of sample edges. In such geometry, combing the parallel flow and counter flow experimental setup, we observe the perfect drag phenomenon, namely the current in each of the two layers has exactly the same intensity but opposite direction. It demonstrates that all the current in the system is carried by excitons and provides an important evidence of the existence of exciton condensate. For the first time, we demonstrate with perfect drag that the exciton coupling remains robust at high landau level where the enhanced screening effect between electrons reduces the interlayer coupling. We study the exciton coupling as a function of interlayer bias, temperature, magnetic field and dc bias. Evidence of a fractional exciton condensate, occurring at total filling fraction of 1/3, is discussed.

10:12AM K14.00012: Direct visualization of electrostatic gating on the band structure of two-dimensional materials via Angled Resolved Photo Emission Spectroscopy (ARPES)  
FREDERIC JOUCKEN (Presenter), Physics, University of California, Santa Cruz, JOSE AVILA, Antares beamline, Synchrotron Soleil, Paris, France, ZHEHAO GE, EBERTHER QUEZADA, Physics, University of California, Santa Cruz, HEMIAN YI, Antares beamline, Synchrotron Soleil, Paris, France, JOHN L DAVENPORT, Physics, University of California, Santa Cruz, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan, MARIA C. ASENSIO, Antares beamline, Synchrotron Soleil, Paris, France, JAIRO VELASCO JR., Physics, University of California, Santa Cruz — The ability to manipulate the band structure of two-dimensional (2D) materials via electrostatic gating is crucial for the realization of technological applications and study of fundamental physics with these materials. ARPES is the standard experimental technique for band structure visualization, however, to this date, the direct visualization of electrostatic gating on the band structure of 2D materials is lacking. Several obstacles have precluded the incorporation of electrostatic gating with ARPES measurements such as sample size, surface uniformity, and a working gate electrode. To address these obstacles, we performed ARPES experiments with submicron spatial resolution on a heterostructure of bilayer graphene (BLG) and hexagonal boron nitride (hBN) that is back gated with an underlying graphite flake. We found that such a device geometry enabled direct visualization of the BLG bands in conjunction with their shift via electrostatic gating. We will discuss the latest experimental progress towards the direct visualization of electrostatic gate modulation of BLG bands.

10:24AM K14.00013: RKKY Interaction in Graphene Landau Levels*  
JINLYU CAO (Presenter), HERBERT FERTIG, SHIXIONG ZHANG, Indiana University Bloomington — We consider the problem of RKKY coupling of classical magnetic moments on graphene when the conduction electrons are in Landau level states. This can be due to a real applied field, or to non-uniform strain. The problem cannot be fully handled in the usual perturbative approach due to the large degeneracy of the Landau levels. For zero chemical potential and two impurities, we demonstrate that four bound states break away from zero energy, with energies dependent of the relative orientations of the spins, two of which are below the Fermi energy. In strained graphene, these two filled states create an effective spin-spin interaction (\( -J_{SD} \)) in addition to the standard RKKY (\( J_{2sd} \)). Moreover, this contribution is active on only one of the graphene sublattices. At the mean-field level, this sublattice has stronger ferromagnetic coupling than the other, while the two sublattices are anti-ferromagnetically coupled. This can potentially give rise to a ferrimagnetic phase with a broken O(3) symmetry. By comparison, the RKKY interaction of dilute impurities in unstrained graphene in a real magnetic field (perpendicular to sample) allows for a canted antiferromagnetic state with broken U(1) symmetry, and an accompanying Kosterlitz-Thouless transition.

*Supported by NSF and BSF.

10:36AM K14.00014: Texture Transitions of Quantum Hall Skryme Crystals Near Charge Neutrality in Graphene*  
BRADEN FESHAMI (Presenter), HERBERT FERTIG, Indiana University Bloomington — How does the quantum Hall canted antiferromagnetic (CAF) groundstate of graphene transition into the ferromagnet when the system is doped away from zero filling factor? We study this question within a self-consistent Hartree-Fock theory, in which regular Skryme crystals are stabilized by long range Coulomb interactions. In addition to this we include a Hubbard on-site term in the Hamiltonian which breaks the symmetry in the valley degree of freedom, and stabilizes a CAF state when the Zeeman energy is not too large. The full set of possible symmetry-breaking terms in the interactions are realized by incorporating an active window of non-zero Landau levels in our Hartree-Fock state. We explore how textures in the various discrete degrees of freedom evolve with the system parameters, and discuss the consequences of this for the phase diagram within the space of the on-site Hubbard parameter, Zeeman strength, and filling factor.

*Supported by the NSF and the BSF.
Equilibrium-state currents in Quantum Hall graphene quantum dots and pn junctions

CYPRIAN LEWANDOWSKI (Presenter), Department of Physics, Massachusetts Institute of Technology, AVIRAM URI, ELI ZELDOV, Department of Condensed Matter Physics, Weizmann Institute of Science — Charge carriers in a quantum Hall state, when subjected to a spatially dependent electrostatic confining potential, arrange themselves in a characteristic pattern of alternating compressible and incompressible regions. By delineating the individual contribution of each Landau level (LL) to electric currents in these regions, we elucidate the microscopic origin of the currents flowing in thermodynamic equilibrium. We focus on the case of a graphene quantum dot and a pn junction geometry. We find, both theoretically and experimentally, non-zero currents flowing in both compressible and incompressible regions, which alternate in sign between neighboring regions. Whilst all occupied Landau levels contribute to the incompressible currents equally, as expected, the compressible currents receive a contribution only from the last occupied LL with the contribution proportional to its energy. This peculiar dependence of compressible currents on the LL energy is best exemplified by the 0th LL, which due to graphene’s band structure, is expected to carry no current in the compressible region. This behavior is in agreement with experimental observations.

*We acknowledge support from the STC Center for Integrated Quantum Materials under NSF award 1231319 and the MISTI MIT-Israel Seed Fund.

Wednesday, March 6, 2019 8:00 AM - 10:48 AM

Session K15 DMP: 2D Materials (Semiconductors) -- Transport and Optical Phenomena in Bilayers and Heterostructures

Transport and optical measurement on twisted homo-bilayer WSe2/WSe2 structure

ZHIREN ZHENG (Presenter), THAO DINH, QIONG MA, SUYANG XU, EFREN A NAVARRO-MORATALLA, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, NUH GEDIK, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — The freedom of stacking different layers of 2D van der Waals (vdW) materials with an arbitrary twist angle opens up tremendous opportunities in studying emergent properties that are not accessible in the natural crystal form. In particular, recent measurements on magic-angle twisted bilayer graphene device show strongly correlated electronic properties, including correlated insulating behavior and unconventional superconductivity due to the formation of flat bands. Flat bands are expected in other small twist angle systems, including twisted bilayer transition-metal dichalcogenide (TMD), which could lead to new transport and optical properties. In this work, we fabricated encapsulated and dual-gated twisted homo-bilayer WSe2/WSe2 devices with precise angle control. We studied their electronic and optical properties as a function of charge density, electric/magnetic field, and temperature with an aim to understand how the twist angle can modify the electron behavior in this homo-bilayer TMD systems.

Magneto-reflectance study of Zeeman effect in MoS2 bilayer

TENZIN NORDEN (Presenter), PEIYAO ZHANG, ARMAN NAJAFI, ARINJOY BHATTACHARYA, University at Buffalo, The State University of New York, MAREK J KORKUSINSKI, National Research Council - Canada, ATHOS PETROU, University at Buffalo, The State University of New York — We studied Zeeman splitting $\Delta E$ of different recombination channels in Bilayer MoS2 using magneto-reflectance spectroscopy. The Zeeman splitting of both A and B excitons of bilayer MoS2 is linear in magnetic field with a slope of approximately -0.2 meV/T similar to that of single layer MoS2. In addition, we observed a new feature labeled N at 2.01 eV between A (1.93 eV) and B (2.13 eV) excitons. We note that feature N is not observed in MoS2 monolayers. This new feature shows a positive Zeeman slope of 0.37 meV/T as compared to A and B excitons. Theoretical and experimental studies show that bilayer MoS2 exhibits optical properties resulting from an interplay of the direct-bandgap of monolayer system, and the indirect bandgap of the bulk. A crucial property of the bilayer system appears to be its inversion symmetry and tuning of that symmetry translates into the interplay of contributions of different valleys in the photoluminescence spectra and possible appearance of additional emission. We hypothesize that feature 'N' results from these valley-mixing effects.

Gate controlled emission from hetero-bilayer of transition metal dichalcogenides

By changing the charge carrier density in the WSe2 monolayer, we observe a shift from charge to neutral density in the transition metal dichalcogenide monolayers which modifies the emission of the interlayer exciton at the electrons and holes results in interlayer excitons with large lifetime. In our FET geometry, we control the charge carrier density in the transition metal dichalcogenide monolayers which modifies the emission of the interlayer exciton at the hetero-bilayer. By changing the charge carrier density in the WSe2 monolayer, we observe a shift from charge to neutral exciton in MoSe2 monolayer and simultaneous enhancement of interlayer exciton photoluminescence. We also report observation of localized emission from the hetero-bilayer at a low temperature of 4 K.

*NSF EFRI NewLAW grant #EFMA-1741691

Twist, Slip, and Circular Dichroism in Van der Waals Bilayers

Stacking atomically thin 2D materials with a rotational misalignment between its layers produces a van der Waals bilayer in which all mirror symmetries can be broken. A fundamental experimental signature of a twisted multilayer is circular dichroism (CD): the conversion of a linearly polarized incident optical field to an elliptically polarized field in transmission. This work investigates the relation between CD, the twist angle and interlayer slip. In experiments where bilayers are formed by contacting one layer with another one has control of the relative rotation angle between the symmetry axes of each sheet, but not of lateral shifts between the layers. Accounting for the lateral shift the configuration space of the system introduces a phase degree of freedom which manifests in the CD and its frequency dependence. We demonstrate how the symmetry constraints in this expanded configuration space is manifest in CD in twisted bilayers as a function of rotation angle. We apply this approach to discuss twisted graphene bilayers and on bilayer transition metal dichalcogenides where the twist coherently couples the intralayer excitons of the two layers.

*DOE Office of Basic Energy Sciences: DE FG02 84ER45118

Valley Polarization and Coherence in WSe2-WTe2 Alloys

We study the valleytronic properties of monolayer WSe2(1-x)Te2x (x=0...1), an alloy system where the endpoints WSe2 and WTe2 occupy different structural phases (H and 1T', respectively). As the Te composition x is increased, the alloy undergoes a semiconductor-semimetal phase transition, which we explore with temperature-dependent Raman and photoluminescence (PL) measurements. We find that Te incorporation activates new Raman modes, while also leading to non-monotonic shifts in the neutral exciton and trion energies and linewidths. Temperature-dependent PL measurements show valley polarization and valley coherence survive when Te doping is less than ~23%, above which valley polarization disappears while valley coherence gradually decreases. These findings demonstrate that valleytronic properties can be robust against disorder and illustrate the potential of two-dimensional alloys for valleytronic technologies.

*This work is funded by NSF EAGER grant #1748650.
O₂-induced *in-situ* manipulation of exciton recombination pathways in 2D heterostructures: Submicron, intensity-programmable pixels with rapid write-read-erase capability, as well as 2D O₂-sensor applications

ZACHARIAH HENNIGHAUSEN (Presenter), ISMAIL BILGIN, COLIN CASEY, KEVIN MENDEZ, MONIKA L EGGENBERGER, SWASTIK KAR, Northeastern University — We present a novel oxygen-induced switching between “non-radiative” and “radiative” exciton recombination in a family of 2D heterostructures: monolayer Bi₂Se₃ grown on arbitrary monolayer transition metal dichalcogenides (TMDs), to include TMD alloys. It is believed to be the result of O₂ diffusing/intercalating between the layers and disrupting the interlayer interaction. The signature photoluminescence (PL) peaks of TMDs are quenched in all as-grown heterostructures, but can be controllably recovered by heating in the presence of oxygen, and then re-quenched by heating in the presence of N₂ or Ar. The intensity PL switching can also be accomplished using a low-power focused laser, while changing the environment from pure nitrogen to air, enabling high control with submicron resolution. This allows for site-programmable, color-selectable, atomically-thin, micron-scale 2D optical "Write-Read-Erase" light-emitting pixels (PLPs) with effective volumes of ~10⁻²¹ m³. The emission intensity can be precisely varied by a factor exceeding 200×, with a wide range of emission energy values in the visible (1.5eV<Eₚh<2eV).

*NSF
Dept. of Veterans Affairs

Electrostatic Traps of Interlayer Excitons in MoSe₂/WSe₂ Heterostructures

ANDREW JOE (Presenter), LUIS JAUREGUI, KATERINA PISTUNOVA, YOU ZHOU, KRISTIAAN DE GREVE, ANDREY SUSHKO, GIOVANNI SCURI, MIKHAIL LUKIN, HONGKUN PARK, PHILIP KIM, Harvard University — The two-dimensional (2D) nature and large excitonic binding energy of transition metal dichalcogenides (TMDs) allow for the exploration of novel quantum optical effects. Using type-II heterostructures formed by stacking MoSe₂ and WSe₂ monolayers, optical excitation generates interlayer excitons, bound electrons and holes residing in spatially separated layers. The out-of-plane, permanent dipole moment of interlayer excitons allows for the control of the emission energy by tuning the vertical electric field using dual-gated devices. By spatially varying the vertical electric field with patterned gates, we can generate potential profiles that can spatially control the interlayer exciton energy. We observe changes in the exciton cloud shape and emission brightness depending on a flat, trapping, or anti-trapping electric field profile. Finally, we estimate an upper-bound interlayer exciton density that can be tuned with the trap depth. With the ability to generate high densities of interlayer excitons, trapped interlayer excitons can serve as a platform for generating and exploring Bose-Einstein condensates at high temperatures.

Fowler-Nordheim tunneling through WSe₂ vertical junctions

DONG HOON SHIN (Presenter), Ewha Womans University, TAE YOUNG JUNG, Chungnam National University, HAKSEO NG KIM, Korea Research Institute of Standards and Science (KRISS), SANG WOOK LEE, Ewha Womans University, SUYONG JUNG, Korea Research Institute of Standards and Science (KRISS) — Van der Waals (vdW) materials consisting of 2D atomic layers have attracted lots of interest in the future electronic applications thanks to their superior electrical, optical and mechanical properties. Due to their weak interlayer coupling across physical vdW gaps, vertical charge transport through these vdW layered materials is fundamentally different from in-plane transport behaviors. In this study, we investigate detailed vertical charge transport mechanisms, especially in the regime of Fowler-Nordheim (FN) tunneling, through vertical WSe₂ junctions while controlling WSe₂-layer thickness from a monolayer to multilayers with a single atomic-thick resolution. We implement a simple but reliable device structure, graphite/WSe₂/graphite vertical heterojunctions, fabricated on a h-BN/SiO₂/Si substrate by mechanical transfer technique. We observe vertical charge transport through WSe₂ layers is governed by the FN tunneling even for a monolayer WSe₂ when the vertical junctions are applied by sufficiently high electric fields. Moreover, we find out that FN tunneling characteristics can be used for identifying not only the layer number but also characterizing key material properties of layered vdW materials such as effective mass and quasiparticle energy gap.
Creating and tuning of interlayer exciton gases in transition metal dichalcogenides heterostructures

ZEFANG WANG (Presenter), Penn State University & Cornell University, KIN FAI MAK, JIE SHAN, Cornell University — Stacking two-dimensional materials into van der Waals heterostructure offers a powerful approach toward creating artificial lattices with desired band structures and functionalities. In transition metal dichalcogenides heterostructures, interlayer exciton emerges due to band alignment of constituent layers and has been demonstrated to have long exciton lifetime [1] and valley lifetime [2], providing a platform to study degenerate Boson gases, rich valley physics, and possible optoelectronics applications. Here we report highly tunable interlayer excitons by an out-of-plane electric field in homobilayer WSe\textsubscript{2}. Electric field can tune the interlayer exciton dipole orientation from negative to positive and induce a Stark shift of up to 100meV in the exciton resonance energy. Moreover, with applied electric field, the exciton lifetime is greatly enhanced by more than two orders of magnitude (from ~200ps to >20ns), allowing the creation of interlayer exciton gas with density as high as 1.2x10\textsuperscript{11}cm\textsuperscript{-2} by moderate continuous-wave optical pumping. Furthermore, we can achieve high interlayer exciton density (~10\textsuperscript{12}cm\textsuperscript{-2}) with a trilayer heterostructure by both optical pumping and electrical injection.


A fresh look at interlayer emission from WSe\textsubscript{2}/MoS\textsubscript{2} heterostructures

ELYSE BARRÉ, TONY F HEINZ, Applied Physics, Stanford University — The recent two years have seen a rising interest in the study of interlayer excitons (ILX) in Van der Waals layered materials, where electron-hole pairs are bound together across the interlayer gap. Special attention was drawn to such ILX in heterostructures of semiconductor transition metal dichalcogenides with staggered band alignment such as MoSe\textsubscript{2} and WSe\textsubscript{2}. That includes the exploration of their optical properties, lifetime, optical selection rules, spin/valley properties, the influence of crystal alignment (a.k.a the moire pattern), the role of momentum-indirect transition, etc.. The latter subject was also studied for the ILX observed in WSe\textsubscript{2} and MoS\textsubscript{2} heterostructure (Kunstmann et al. Nature Physics, DOI: 10.1038/s41567-018-0123-y, 2018), where the reported ~1.6 eV emission is assigned to such indirect transition. In this talk, I will report on the observation of a different interlayer emission from the same system. Probing its response to different experimental conditions, I will discuss its properties and its origin.

*The Viterbi Fellowship nurturing young faculty from the Erna and Andrew Viterbi Department of Electrical Engineering, Technion - Israel Institute of Technology, Haifa, Israel.

Observation of Moiré Excitons in van der Waals Heterostructure

CHENHAO JIN (Presenter), EMMA C. REGAN, AIMING YAN, IQBAL B UTAMA, DANQING WANG, University of California at Berkeley, YING QIN, SIJIE YANG, Arizona State University, ZHIREN ZHENG, University of California at Berkeley, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, SEFAATTIN TONGAY, Arizona State University, ALEX K ZETTL, FENG WANG, University of California at Berkeley — Moiré superlattice in van der Waals systems provide a powerful tool to engineer the properties of two-dimensional materials through introducing a new energy and length scale. For example, correlated insulating states and superconductivity have been reported in graphene systems, where the moiré superlattice qualitatively change the behavior of electrons. The effects of moiré superlattice on excitons, on the other hand, is less studies experimentally. Here we report the observation of moiré excitons in heterostructure of two-dimensional semiconductors, and show that the properties of excitons can also be strongly modified by a moiré superlattice.

*Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division of the U.S. Department of Energy under contract no. DE-AC02-05-CH11231 (van der Waals heterostructures program, KCFW16) NSF EFRI program (EFMA-1542741)
US Army Research Office under MURI award W911NF-17-1-0312
Elemental Strategy Initiative conducted by the MEXT, Japan and JSPS KAKENHI Grant Numbers JP15K21722
NSF DMR 1552220 NSF CAREER award
Spin-charge coupled transport in topological-insulator-based heterostructures

ENRICO ROSSI (Presenter), Department of Physics, William & Mary., MARTIN RODRIGUEZ-VEGA, Department of Physics, Indiana University.; GEORG SCHWIETE, Department of Physics and Astronomy, Center for Materials for Information Technology (MINT), The University of Alabama. — Experimental advances have made possible the creation of heterostructures composed of two or more layers of two-dimensional systems that combine their individual properties to reach desired functionalities. In this talk, we present the spin-charge coupled diffusion equations for heterostructures with random interlayer tunneling and in which one of the layers has strong spin-orbit coupling. We consider two distinct regimes: the weak coupling regime, for which the disorder-induced scattering time is shorter than the tunneling-induced scattering time, and the strong coupling regime, for which random tunneling events are dominant. We then apply our formalism to the case in which a two-dimensional electron gas is placed in proximity to the surface of a three-dimensional topological insulator and discuss the relevance of our results for experiments.

*This work is supported by NSF, ONR, BSF, the College of Arts and Sciences at Indiana University, and the College of Arts and Sciences at the University of Alabama.

Quantum spin-wave dynamics and magneto-transport behaviour in 2D van der Waals heterostructure

SUSHANT KUMAR BEHERA (Presenter), PRITAM DEB, Tezpur University — Spin-wave ensembles in qunatum regime coupled together to offer an exciting prospect of observing complex behaviour interlinking the microscopic spin features with macroscopic spin ensembles [Phys. Rev. Lett. 121, 126401 (2018)]. This feature is quite evidence in two dimensional van der waals heterostructure systems [Phys. Rev. Lett. 121, 067701, 2018]. In those systems, spin-transfer torque plays a major role to explain the induced magneto-transport phenomenon. Here, we demonstrate the collective interactions in an ensemble of spin-waves to unravel the full quantum dynamics and transport studies. We model a time-adaptive variational renormalization group method that accurately captures the underlying spin-wave dynamics and magneto-transport equations with potential device applications [arXiv:1808.04418].

*Department of Science and Technology, Govt. of India for DST-INSPIRE Fellowship (IF150325).
Tezpur University for providing HPCC Facility to perform simulation work.

Wednesday, March 6, 2019 8:00 AM - 10:36 AM

Session K16 DCOMP DCP: Aqueous Solutions, Solvated Interfaces, and Ionic Polarization

Non-equilibrium effects at solvated interfaces under an applied external bias

ALEXANDRE ROCHA (Presenter), Instituto de Física Teórica, State University of Sao Paulo, Brazil, LUANA PEDROZA, Centro de Ciencias Naturais e Humanas, Universidade Federal do ABC, Brazil, PEDRO B. MENDONÇA, Centro de Física de Materiales, Donostia, Spain, MARIVI FERNANDEZ SERRA, Department of Physics and Astronomy, Stony Brook University, U.S.A. — Understanding the local structure of water at the interfaces of metallic electrodes is a key issue in aqueous-based electrochemistry. Nevertheless a realistic simulation of such a setup is challenging, particularly when the electrodes are maintained at different potentials. To correctly compute the effect of an external bias potential applied to truly semi-infinite surfaces, we combine Density Functional Theory and Non-Equilibrium Green's Function methods. This framework allows for the out-of-equilibrium calculation of forces and dynamics, and directly correlates to the chemical potential of the electrodes, which is introduced experimentally. In this work, I will discuss this frame work and some applications to water molecules at the interface with metallic surfaces.

*Funded by DOE Early Career Awards No. DE-SC0003871 and DE-FG02-09ER16052, ICTP-SAIFR (FAPESP project No. 2011/11973-4) and the ICTP-Simons Associate Scheme, FP7 FET-ICT “Planar Atomic and Molecular Scale devices” (PAMS) project (funded by the European Commission under contract No. 610446), the Spanish Agencia Estatal de Investigación (Grant No. MAT2016-78293-C6-4-R) and the Dep. de Educación of the Basque Government and UPV/EHU (Grant No. IT-756-13).
8:36 AM K16.00002: Toward first-principles modelling of charged solid-electrolyte interfaces  CHAO ZHANG (Presenter), Department of Chemistry - Ångström Laboratory, Uppsala University, MICHIEL SPRIK, Department of Chemistry, Cambridge University — Oxide-electrolyte interfaces are universally present in energy storage device, nanofluidic chemical processor, drug delivery nanoparticles and containments treatment in ground water. The surface charge of all these interfaces is controlled by the pH of the electrolyte solution and this leads to the formation of the electric double layer (EDL) by deprotonation of adsorbed water molecules or protonation of the oxide surfaces. Despite of the rapid development of experimental techniques, the missing of microscopic understanding imposes a knowledge gap. In this regard, modelling and simulation of EDL can provide complementary information of the structure, dynamics and energetics of charged interfaces. Here, I will report our current methodological progress on the atomistic modelling of dielectric properties of charged oxide-electrolyte interfaces.


8:48 AM K16.00003: First-principles modeling of electrochemical reactions at the metal-water interface under applied voltages  SUDARSAN SURENDRALAL (Presenter), MIRA TODOROVA, Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, MICHAEL W FINNIS, Thomas Young Center, Imperial College London, JÖRG NEUGEBAUER, Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH — Ab initio modelling using density functional theory (DFT) is a powerful technique to study reactivity at electrochemical interfaces. We have recently developed an approach that allows to describe electrochemical systems under applied voltages and that can be easily implemented in existing DFT codes [1]. We apply this method to study Mg aqueous corrosion at anodic conditions, for which unusually high H2 evolution rates are observed. The DFT based molecular dynamics simulations we perform for the Mg(0001)/H2O system under increasing anodic polarization show dissociation events, proton transfer as well as H2 evolution at the Mg-water interface. A detailed analysis of our calculations reveals a novel and hitherto unconsidered reaction mechanism for the H2 evolution reaction, caused by an unusual adsorption phenomenon triggering a reaction resembling the cathodic Heyrovsky reaction.


9:00 AM K16.00004: DFT Characterization of Solvated NaCl Potentials of Mean Force and Energetics*  ALEC WILLS (Presenter), SEBASTIAN DICK, MARIVI FERNANDEZ SERRA, Stony Brook University — Potentials of mean force have long been a standard of measurement to characterize the energetics of the ion solvation process. In particular, classical molecular dynamics simulations frequently predict deeper minima than DFT simulations for the different solvated states. Moreover, different exchange-correlation functionals often don’t yield consistent potentials within DFT, some even predicting more stable second minima (solvent-separated ion pairs) than the usual deepest first minimum (contact ion pair). In this work, we investigate the electronic structure of solvated NaCl and the effects the charge localization has on nearby water molecules. We further investigate the errors in the system arising from the functional approximations and from the self-consistent ground-state Kohn-Sham electron density, and how the errors contribute to different stability characteristics.

*This material is based upon work supported by the Department of Energy under award number DE-FG02-09ER16052.
9:12AM K16.00005: Energetics of the adsorption of iodide ion at the air-water interface  YANBIN WANG (Presenter), PARTH RAKESH DESAI, SIDDHARTHA DAS, University of Maryland, College Park — Ion adsorption at air-water (a/w) interfaces has been extensively probed due to its significance in a large number of phenomena in environmental science, chemical physics, biophysics, etc. Recently, our group has investigated the ion-capillary wave interaction and its impact on the energetics of ion adsorption at an a/w interface considering generic ion. However, the specific ion adsorption behavior is more important, especially for those ions having a favorable energy of adsorption at the air/water interface. Therefore, we employed molecular dynamics method to study the iodine ion-capillary wave interaction. We reconstruct the potential of mean force using the distance between ion and the Gibbs dividing surface as the reaction coordinate. Furthermore, by analyzing the response of the system to the presence of iodine at the interface, e.g., the energetic change, the change in the overall fluctuations of surface and interfacial water, etc. we shed light to the understanding of the iodine ion adsorption at air/water interface.

9:24AM K16.00006: First-principles based quantification of charged species redistribution at electrochemical interfaces: Model system of zirconium oxide  JING YANG (Presenter), MOSTAFA YOUSSEF, BILGE YILDIZ, Massachusetts Institute of Technology — Modeling local distribution of charged ions and ionic defects at electrochemical interfaces is key to understanding related electrochemical processes. Based on the grand canonical approach which defines the electrochemical potential of individual charged species, a unified treatment of defects in solid oxide and ions on water side can be established. In this work, we apply this framework to the system of ZrO2/water interface. Density functional theory calculations are performed to obtain defect formation energy in the oxide materials and *ab initio* molecular dynamics is used to assess the formation free energy of H+ and OH- ions in water at different distances from the ZrO2 surface. The results are fed into a continuum model which produces the equilibrated distribution of these charged species. The continuum model considers explicitly both ion adsorption and defect segregation in the vicinity of the interface, and the diffuse layer and space charge layer in the extended area. Such a unified description reveals the influence of interfacial chemistry on oxide defect chemistry, and vice versa. This framework based on the grand canonical approach allows easy inclusion of additional charged species into the system and offer a general tool for studying electrochemical interfaces.

9:36AM K16.00007: Polarization induced ion adsorption on aqueous interfaces: Solvent effect on image charge interactions  CHANG YUN SON (Presenter), ZHEN-GANG WANG, Caltech — Understanding electrostatic interactions near interfaces is of critical importance in broad fields of science. Continuum electrostatics expects ions to be attracted to metal electrodes but repelled from low dielectric surfaces, while recent studies found certain ‘chaotropic’ ions are adsorbed on both air/water and graphene/water interfaces. Here we systematically study the effect of polarization of electrode, solvent and solute molecules on the adsorption of ions near interfaces with molecular dynamics simulation. An efficient method is developed to treat an electrolyte system between two surfaces, exploiting the mirror-expanded symmetry of the exact image charge solution. With neutral surfaces, the image interaction induced by the solvent dipoles and ions largely cancel each other, resulting in no significant net differences in the ion adsorption profile regardless of the interface. Under external electric field, the adsorption of ions are enhanced by the polarizing electrode. Explicit polarization of the electrolyte is necessary to capture the increased propensity of big halide ions near the electrode seen in experiments. Our analysis shows inclusion of both electrode and electrolyte polarization is of critical importance to model the electrolyte behavior with interfaces.

9:48AM K16.00008: Intercalation behavior of MXenes from ab initio molecular dynamics*  PAUL KENT (Presenter), WEIWEI SUN, Oak Ridge National Laboratory — MXenes are a large family of two-dimensional materials, primarily transition metal carbides and highly conductive, displaying exceptional performance for supercapacitors, batteries, and water purification. MXenes can host a wide range of species between their layers. Predictions and understanding are complicated by the presence of surface functional groups, such as O, OH, and F. Intercalation with aqueous ions such as Li, K, or Mg results in distinct structural and electrochemical responses. Here we present density functional ab initio molecular dynamics calculations for the behavior of ions confined in wetted MXene Ti3C2 layers. In this confined aqueous environment, ions display distinct behavior relating to their size, preferred solvation shell, and interaction with the surface groups, consistent with recent scanning probe microscopy data. This suggests that, besides the choice of electrolyte, careful selection of the surface groups and choice of MXene surface metal atoms are routes to optimize supercapacitor and sensing performance.

*This work was supported as part of the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.
10:00AM K16.00009: Detection of Amino Acids and Other Biochemical Molecules with GaAs Schottky Diodes* T. ALKHIDIR (Presenter), ECE, KUST, C. ALPHA, CNF, Cornell, D. L. GATER, M. ABI-JAOUDE, Chemistry, KUST, A. F. ISAKOVIC, Physics, KUST, Cornell Univ. — The sensitivity of the GaAs surface makes it a good candidate for sensing various molecular species of interest in biochemistry. Simultaneously, the growth in nanofluidics applications calls for detailed understanding of liquid-solid interfaces for a variety of interfaces’ combinations. The 1V operation range for GaAs Schottky sensor is shown to be sufficient to detect H2O, D2O, -OH, as well as PBS solutions of various concentrations at 300K. We show how interfacial density of states changes with each compound probed, and how this density changes with the applied electric field. Inorganic bonds, such as Ga-H, Ga-O (and related As-based ones), are differentiated through correlation of transport and FTIR data of liquid-solid interfaced. The same GaAs Schottky diode can be used to distinguish between different types of amino acids (non-polar, polar, and basic) through the specific examples of Gly, His, and Cys, respectively. Finally, the built-in potential and the interfacial density of states are determined as a function of the pH factor of solutions tested (4 < pH < 9). These results offer perspective on developing GaAs based system for micro- and nanofluidics based detection and differentiation of peptides.

*We acknowledge the support from A2RE-ADEC, SRC, and Cornell CNF.

10:12AM K16.00010: Polarizability, Infrared and Raman Spectra of Water from First-Principles Simulations Using Recent Exchange-Correlation Functionals* MICHAEL D LACOUNT (Presenter), FRANCOIS GYGI, University of California, Davis — We present the results of a series of uncorrelated first-principles molecular dynamics simulations of liquid water obtained with the recently proposed SCAN density functional[1]. Results are compared with those obtained using the PBE density functional, and known experimental results. Estimates of the polarizability, infrared spectra, and Raman spectra are calculated. These results, in addition to previous structural analysis performed by us and others, are used to further evaluate the accuracy of the SCAN functional when applied to simulations of water.


*Supported by the Midwest Integrated Center for Computational Materials (MICCoM), as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences.

10:24AM K16.00011: Polarizable Classical Force Field to Describe the Water/Metal Interfaces in QM/MM Simulations of Electrochemical Interfaces ALINE OLIMPIO PEREIRA (Presenter), LUANA PEDROZA, Centro de Ciências Naturais e Humanas, Universidade Federal do ABC (UFABC), GUSTAVO TROIANO FELICIANO, Instituto de Quimica, câmpus de Araraquara, Universidade Estadual Paulista (UNESP), MAURICIO COUTINHO-NETO, Centro de Ciências Naturais e Humanas, Universidade Federal do ABC (UFABC) — The microscopic understanding and control of the kinetic behavior and reactions that occur in water/metal interfaces play a key role to the development of several technological applications. Atomistic simulations have shown to be a versatile tool to provide a detailed comprehension of such interfaces at the atomistic level. Concerning the quantum aspects and size of such systems, multiscale QM/MM simulations seems to be an efficient approach to describe the electrode interface. One of the key elements in QM/MM approaches is the classical force field. Particularly for metals, the accuracy of the simulation strongly relies in the ability of the force field to reproduce surface polarization effects. Based on this, we develop suitable polarizable force fields to describe the water/metal interface. Charged virtual sites are added to the molecular topology of a simple LJ model in order to create dipoles that reproduce the surface polarization. Two methods are considered: (i) the metallic system is composed of permanent dipoles created by rods and (ii) the metal-virtual site pair is a flexible dipole described by a harmonic oscillator, such as in a Drude model. Both models are tested and adjusted in order to reproduce the polarization and adsorption properties of the metallic surfaces.
8:00AM K17.00001: Physics of Ultra-light Materials Under Pressure: Quantum and isotope effects in lithium metal

[Invited] SHANTI DEEMYAD (Presenter), University of Utah — In this talk I will discuss the physics of ultra-light materials and evolution of quantum effects under extreme pressures. In periodic table lithium is the first element immediately after helium and the lightest metal. While fascinating quantum nature of condensed helium is suppressed at high densities, because of the presence of long range interactions in metallic systems, lithium is expected to adapt more quantum solid behavior under compression. Physics of dense lithium offers a rich playground to look for new quantum phenomena in condensed matter. I will discuss the presence of quantum contributions to the structural phase transitions of lithium at low temperature and will present our results on resolving the long lasting mystery of lithium ground state1,2.


*This research is supported by NSF Division of Materials Research award 1351986

8:36AM K17.00002: Electronic and Optical Properties of SnO2 at High Pressure

NATHAN DASEN BROCK-GAMMON (Presenter), Department of Physics and Astronomy, University of Rochester, RANGA P DIAS, Department of Mechanical Engineering, Department of Physics and Astronomy, University of Rochester, ELLIOT SNIDER, Department of Mechanical Engineering, University of Rochester — Tin oxide (SnO2) is one of the most widely used n-type transparent conducting oxide materials, which has attracted increasing interest due to its outstanding electrical and optical properties for potential applications. We present a detailed investigation on pressure-induced structural, electronic, and optical transitions of SnO2 to 60 GPa, using a diamond anvil cell, micro-confocal Raman spectroscopy, infrared absorption, reflectivity, and electrical resistance measurements. The results indicate that a wide band gap (Eg=3.6 eV) n-type semiconductor undergoes a semiconductor to insulator transition at ~18 GPa. Furthermore, we will present the temperature dependent resistance changes and photoconductivity with different power density at high pressures.

*The NSF grant DMR-1809649 supported this research.

8:48AM K17.00003: Pressure-induced metallization in MoS2

AZKAR SAEED AHMAD (Presenter), South University of Science and Technology of China — Molybdenum disulphide is a material of considerable interest due to its unique semiconducting and opto-electronic properties. There have been several theoretical studies suggesting an electronic phase transition in molybdenum disulphide but solid experimental evidence is still lacking. However, here we perform comprehensive studies on the pressure-dependent electronic, vibrational and structural properties of multilayered molybdenum disulphide up to 67 GPa. Our experimental results reveal that the press-induced metallization is associated with variation in local structure. The metallization happens from the overlap of the valance and conduction bands owing to sulphur-sulphur interactions upon the reduction in interlayer spacing under compression.

*The funding from Shenzhen City Government and Startup funding is greatly acknowledged. We also acknowledge the DESY, ALS, and BSRF, for allowing us to perform synchrotron experiments.
9:00AM K17.00004: Normal state electrical resistivity of thorium metal above a base temperature of 1.1 K and under applied pressure up to \(-100\) GPa* CHRISTIAN WOLOWIEC (Presenter), ZACKARY R REHFUSS, KALYAN SASMAL, Physics Department, University of California, San Diego, JASON R JEFFRIES, Physics Division, Lawrence Livermore National Laboratory, YOGESH KUMAR VOHRA, Physics Department, University of Alabama, Birmingham, SAMUEL T WEIR, Physics Division, Lawrence Livermore National Laboratory, M BRIAN MAPLE, Physics Department, University of California, San Diego — Measurements of electrical resistance were performed on thorium metal in a diamond anvil cell (DAC) under pressure from \(-5\) to \(100\) GPa and down to a temperature of \(-1.1\) K. Previous reports indicate that the ambient pressure superconducting transition temperature \(T_c = 1.4\) K is suppressed to \(-0.7\) K at a pressure of approximately \(15\) GPa. We did not observe any superconducting transition above a base temperature of \(1.1\) K over the pressure range from \(-5\) to \(100\) GPa. There is a sign change near \(15\) GPa in the pressure dependence of the normal state resistivity (from \(dR/dP < 0\) to \(dR/dP > 0\)). Above \(30\) GPa, there is little or no pressure dependence in the electrical resistance suggesting there is no change in carrier number as pressure is increased up to \(100\) GPa. Thorium remains metallic (\(dR/dT > 0\)) from \(300\) K down to \(-20\) K over the entire pressure range up to \(100\) GPa. However, at higher pressures above \(-50\) GPa, there is a reduction in the slope (\(dR/dT > 0\)), which remains constant up to \(100\) GPa, also suggesting there is little or no change in the carrier concentration. Below \(20\) K, \(dR/dT\) is zero.

*High pressure research at the University of California, San Diego was supported by the National Nuclear Security Administration through the U.S. Department of Energy (DOE) under Grant No. DE-NA0002909.

9:12AM K17.00005: Pressure-induced superconductivity in weak topological insulator Bi\(_2\)Te\(_I\) and topological metal Bi\(_3\)Tel* DERRICK VANGENNENP, Department of Physics, University of Florida, YOU LAI, National High Magnetic Field Laboratory, Florida State University, YOGESH KUMAR VOHRA, Department of Physics, University of Alabama at Birmingham, SAMUEL T WEIR, Physics Division, Lawrence Livermore National Laboratory, RYAN BAUMBACH, National High Magnetic Field Laboratory, Florida State University, JAMES J. HAMLIN (Presenter), Department of Physics, University of Florida — Using a newly developed system designed to rapidly screen materials for pressure-induced superconductivity we have performed a series of high pressure electrical transport and ac magnetic susceptibility measurements on single crystals of the weak topological insulator Bi\(_2\)Te\(_I\) and the topological metal Bi\(_3\)Tel. Upon compression at low temperature, we find that Bi\(_2\)Te\(_I\) becomes superconducting at \(-13\) GPa and Bi\(_3\)Tel begins to superconduct at pressures above \(-11.5\) GPa. The superconducting critical temperature \(T_c\) reaches maximum values of \(7\) K and \(7.5\) K for Bi\(_2\)Te\(_I\) and Bi\(_3\)Tel, respectively. We observe distinct anomalies in the resistivity of both samples as a function of pressure, which may arise due to structural transitions.

*Supported by National Science Foundation (NSF) CAREER award DMR-1453752. Equipment development was partially supported by the NSF NHMFL UCGP. A portion of this work was performed at the National High Magnetic Field Laboratory (NHMFL), which is supported by NSF Cooperative Agreements No. DMR-1157490 and No. DMR-1644779 and the state of Florida. Designer diamond anvils were supported by DOE-NNSA Grant No. DE-NA0002928 and under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344.

9:24AM K17.00006: High pressure, high magnetic fields fermiology studies of YBCO.* AUDREY GROCKOWIAK (Presenter), WILLIAM A CONIGLIO, STANLEY W TOZER, Florida State University — The pnictide, cuprate and molecular conductor families exhibit similar phase diagrams, leading to a great deal of interest in a common mechanism for a “universal phase diagram”. The typical ingredients for such phase diagrams include an antiferromagnetic phase, a superconducting dome, and possibly one, or several quantum critical points (QCP). Chemical doping is one traditional way to look at such materials, however thermodynamic variables such as magnetic field or hydrostatic pressure have proven to be powerful tools to explore this phase diagram, with very strong magnetic fields being used to suppress the superconducting dome, allowing one to investigate the QCP.

We report on our high pressure (up to \(25GPa\)) and high fields (up to \(85T\)) Quantum Oscillation measurements of the Fermi surface of YBCO6.5.

*The National High Magnetic Field Laboratory is supported by National Science Foundation through NSF/DMR-1157490 and DMR-1644779 and the State of Florida.
Pressure-Induced Structural Phase Transition and Magnetic Fluctuations in CeNi

ANDREI PODLESNYAK (Presenter), ALEXANDER I KOLESNIKOV, GEORG EHLERS, ANTONIO M. DOS SANTOS, ATHENA S. SEFAT, Oak Ridge National Laboratory, GREGORY J. HALDER, Argonne National Laboratory, ALEX MIRMELSTEIN, Russian Federal Nuclear Center

The pressure-induced structural phase transition and magnetic fluctuations in the intermediate-valence compound CeNi has been investigated by x-ray and neutron scattering techniques. The observed \( Cmcm \rightarrow Pnma \) structural transition is analyzed using density functional theory calculations, which successfully reproduce the ground state volume, the phase transition pressure, and the volume collapse associated with the phase transition. Equations of state for CeNi on both sides of the phase transition are derived and an approximate \( P-T \) phase diagram is suggested for \( P < 8 \) GPa and \( T < 300 \) K.

The inelastic neutron scattering study of the dynamic magnetic response of CeNi reveals that the structural transition increases the characteristic energy of magnetic fluctuations due to enhanced Ce 4f - Ni 3d hybridization. At the same time, the inelastic 4f magnetic form factor remains unchanged.

*Research at Oak Ridge National Laboratory's Spallation Neutron Source was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy. The work at ORNL was also partly supported by the US DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

High Pressure Behavior of Ternary H-C-S Compounds: Structural and Electronic Properties

ELLIOT SNIDER (Presenter), Mechanical Engineering, University of Rochester, NATHAN DASENBROCK-GAMMON, Physics and Astronomy, University of Rochester, RANGA P DIAS, Physics and Astronomy, Mechanical Engineering, University of Rochester

Efforts to identify and develop room temperature superconducting materials are an intensive area of research, motivated by both fundamental science and the prospect for applications. We present pressure-induced structural and electronic properties of ternary H-C-S compounds to 150 GPa, using a diamond anvil cell, micro-confocal Raman spectroscopy, infrared absorption, and electrical resistance measurements. The results indicate that the H-C-S compound undergoes two structural phase transitions and an insulator-metal transition above 55 GPa. The temperature dependent resistance changes further show a gradual electronic transition from an insulator to a metal, which is driven by the pressure induced band gap closing. Also, we will discuss further investigation of these compounds as potential superconductors with high transition temperatures.

*The NSF grant DMR-1809649 supported this research.

High pressure study on a giant magnetoelectric effect hexaferrite via neutron techniques

YAN WU (Presenter), Neutron Scattering Division, Oak Ridge National Laboratory, KUN ZHAI, Institute of Physics, Chinese Academy of Sciences, JAMIE MOLAISON, BIANCA HABERL, Neutron Scattering Division, Oak Ridge National Laboratory, YOUNG SUN, Institute of Physics, Chinese Academy of Sciences, HUIBO CAO, Neutron Scattering Division, Oak Ridge National Laboratory

Multiferroics have attracted tremendous research interests because of their potential in constructing next-generation multifunctional devices. Y-type hexaferrite \( Ba_2Mg_2Fe_{12}O_{22} \) has promising magnetoelectric (ME) properties as a multiferroics which is sensitive to small magnetic field. When doped with Sr, the material keeps its sensitivity to field while the ME coefficients are greatly enhanced with Sr level increasing. Our previous work has reported new records of ME coefficients in single phase materials shown on \( Ba_2Mg_2Fe_{12}O_{22} \) with Sr doping that changes its ground state spin cone symmetry. Temperature dependent neutron diffraction investigation shows pinning effect emerging at heavy Sr doped sample that also change to be an alternating longitudinal conical ground state. Applying hydrostatic pressure has different effects on these simultaneously occurred phenomena, indicating their relatively independent mechanisms. With recent progress of diamond anvil cell (DAC) at the HB-3A beamline, we are able to identify interesting pressure effect picture up 7.3 Gpa on the system magnetic states.

*This research used resources at High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

ABSTRACT WITHDRAWN

10:12AM K17.00010: ABSTRACT WITHDRAWN
10:24AM K17.00011: High Pressure Behaviors of Dense Planetary Mixtures* [Invited] CHOONG-SHIK YOO (Presenter), Washington State University — Hydrogen (H₂) and helium (He) are two most fundamental solids abundant in the Universe. Compression behaviors of H₂ and He are critical to understand many body effects of these quantum solids; develop new condensed matter theories; and get insights into the internal structure of the Giant planets. In contrast to a rapid progress in understanding the phase diagram of H₂ at high pressures, a little is known about the phase behavior of planetary mixtures including the most fundamental quantum solids, H₂ and He. In this talk, we will describe our recent studies on high pressure behaviors of several systems of planetary mixtures including H₂-He, H₂-N₂, He-N₂, and H₂-H₂O. The results underscore a significant level of mixing in these planetary mixtures and thereby strong chemical interactions of the interstitial-filled guest H₂ with the host lattices of He, N₂ and H₂O. Based on these results we will point out several fundamental principles governing the pressure-induced phase and chemical transformations in the planetary mixtures, which include strong repulsive interaction, entropically driven phase mixing, proton exchange and ordering, and kinetic-controlled metastable phases.

*This work was performed in support of the NNSA (DE-NA0003342), NSF (DMR-1203834) and ARO (W911NF-17-1-0468).

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K18 DCOMP: Machine Learning Material and Experimental Data BCEC 156B - Noam Bernstein, United States Naval Research Laboratory - Tag(s): Focus

8:00AM K18.00001: Machine learning interatomic potentials with and without (much) human labor [Invited] NOAM BERNSTEIN (Presenter), Naval Research Laboratory — In this talk I will show the state of the art in generating an interatomic potential using machine learning techniques (specifically, the Gaussian Approximation Potential (GAP) framework, with the Smooth Overlap of Atomic Positions (SOAP) representation of atomic geometry) that is capable of representing the Born-Oppenheimer potential energy surface of a material based on data (energies and forces) computed using density functional theory. First I will show that a careful and very human labor-intensive process of assembling a training database results in a potential with exquisite accuracy, far surpassing any empirical potential in the literature in predicting material properties. Then I will demonstrate, using several different elemental compounds with quite different bonding chemistry, that the database building process can be largely automated. A combination of iterative training and ab initio random search (AIRSS) can be used to simultaneously “discover and fit” a material without the need for any prior knowledge of what structures are relevant for a given material.

8:36AM K18.00002: Machine Learning for Ultrafast Electron Diffraction* [Invited] ARAVIND KRISHNAMOORTHY (Presenter), University of Southern California — Ultrafast electron diffraction (UED) experiments provide high-quality data about atomic structure and dynamics of functional materials down to fs-ps timescales. Imminent improvements in repetition rate of electron sources and experimental facilities will dramatically increase the size of this available data and will provide new capabilities for ultrafast science. These advances will require analysis techniques that can efficiently extract atomistic insights from raw diffraction images. In this talk, I will describe a deep generative model, trained on existing ultrafast electron diffraction data on photoexcited two-dimensional and layered materials obtained at SLAC, as well as trajectories from classical molecular dynamics and non-adiabatic quantum molecular dynamics simulations. The model is used to analyze lattice distortions, phonon modes and changes in local crystal structure due to photoexcitation and identify potential precursors to structural phase transformations in these materials. Extensions to the model to utilize streaming data for real-time analysis and the utility of the model in experimental design will also be discussed.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607.
9:12AM K18.00003: Prediction of Molecular Properties Using Graph Kernel and Active Learning* YU-HANG TANG (Presenter), WIBE A DE JONG, Lawrence Berkeley National Laboratory — In this talk, we present a new machine learning method for training predictive models of extensive molecular properties through the application of a similarity kernel on graphical representations of molecules, which is intuitive and can adapt to molecules of arbitrary size and topology. The pairwise similarity matrices between molecules as computed by the graph kernel can be used to construct Gaussian process regression models that can predict extensive properties with provable size scaling. Using an active learning procedure, we demonstrate that models created by our method can achieve a state-of-the-art accuracy of less than 1 kcal/mol on predicting atomization energies for molecules in the QM7 dataset without using any explicit energy decomposition/localization scheme. The method also uses a much smaller number of training samples as compared to other methods to achieve the same level of accuracy.

*This work was supported by the Luis W. Alvarez Postdoctoral Fellowship at Lawrence Berkeley National Laboratory.

9:24AM K18.00004: Tree Tensor Networks for Generative Modeling* SONG CHENG (Presenter), TAO XIANG, LEI WANG, Institute of Physics, PAN ZHANG, Institute of theoretical physics — Tensor Network States are widely used representations for many-body quantum states. They have close connections to the Graphical Models for high-dimensional data. In both research domains employing patterns such as locality or low information complexity are crucial for designing the model architecture. We employ Tree Tensor Network (TTN) for generative model. The TTN exhibits balanced performance in expressibility and efficient training and sampling. We apply TTN generative model on random binary patterns and the binary MNIST datasets and compare its performance with the matrix product states and other the popular generative models such as the Variational AutoEncoder and PixelCNN. Finally, we discuss about the future development of Tensor Network States in machine learning problems.

*T.X; S.C. is supported by the Grant No. 2017YFA0302901, Grants No. 11190024 and No. 11474331. L.W. is supported by the Grant No. 2016YFA0300603 and the Grant No. 11774398. P.Z. is supported by the Grant No. QYZDBSSW-SYS032 and Project 11747601 of National Natural Science Foundation of China.

9:36AM K18.00005: Learning from the Density to Correct Total Energy and Forces in First Principle Simulations* SEBASTIAN DICK (Presenter), MARIVI FERNANDEZ SERRA, Stony Brook University — We propose a new molecular simulation framework that combines the transferability, robustness and chemical flexibility of an ab initio method with the accuracy and efficiency of a machine learned force field. The key to achieve this mix is to use a standard density functional theory (DFT) simulation as a pre-processor for the atomic and molecular information, obtaining a good quality electronic density. General, symmetry preserving, atom-centered electronic descriptors are then built from this density to train a neural network to correct the baseline DFT energies and forces. These electronic descriptors encode much more information than local atomic environments, allowing a simple neural network to reach the accuracy required for the problem of study at a negligible cost. The balance between accuracy and efficiency is determined by the baseline simulation. This is shown in results where high level quantum chemical accuracy is obtained for simulations of liquid water at standard DFT cost, or where high level DFT-accuracy is achieved in simulations with a low-level baseline DFT calculation, at about one order of magnitude reduced cost.

*DOE grant DE-FG02-09ER16052

9:48AM K18.00006: Microscopic Particle Localization Under Low-Light Conditions SHAO RAN HUANG (Presenter), RASHID ZIA, Brown University — Microscopic localization of particles under low-light conditions is a challenging task in microscopy, e.g. in biological physics and quantum photonics. While there has been considerable research on developing novel computational techniques, relatively less attention has been paid to integrated computational-experimental approaches leveraging hardware binning. Hardware binning allows one to judiciously sacrifice resolution, which is often excessive in locating objects of several pixels wide, to enhance the signal-to-noise ratio. Our research questions the default choice of single pixel measurements and investigates potential gains by combining multiple frames with differently hardware-binned images. Given the recent success in deep learning microscopy, we also investigate the use of deep residual learning in computing the convolution of the image with a suitable kernel for localization.
10:00AM K18.00007: Computational screening of experimental structural repositories for novel Li-ion conductors
LEONID KAHLÉ (Presenter), Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, Switzerland, ARIS MARCOLONGO, Cognitive Computing and Computational Sciences Department, IBM Research 8803 Zürich, Switzerland, NICOLA MARZARI, Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, Switzerland — A comprehensive screening of structural databases for ionic conductors by means of atomistic simulations could identify novel candidates for next-generation solid-state lithium-ion batteries, and deepen our understanding of the microscopic processes and structural motifs governing ionic diffusion in the solid state. This task is challenging because no classical simulation potential is predictive for wide varieties of materials classes, and first-principles simulations struggle to reach the necessary timescales. To model ionic diffusion efficiently and accurately, we derive a novel hybrid quantum/empirical model that can be used for molecular dynamics simulations of solid-state diffusion [1], by applying simple and intuitive approximations to fully self-consistent density-functional theory. This models underpins our high-throughput screening efforts for Li-ion conductors, powered by the AiiDA materials informatics [2] platform. I will present the different screening stages, show how high-level workflows can be used to automate and optimize the calculation of transport coefficients, and provide early results on promising candidates.


10:12AM K18.00008: Insights on materials space*  
CHANDRAMOULI NYSHADHAM (Presenter), KENNEDY LINCOLN, GUS HART, Brigham Young University — Using a kernel-based machine learning surrogate model, we present insights on generating and choosing the training and testing data for optimal modeling of materials space. We introduce a tool that helps us build an “ideal” kernel, which predicts with high accuracy on small training sets. We also present a methodology for quantifying the accuracy of any kernel based surrogate model for interpolating materials space. Our insights (based on analyzing data from over 73,000 unrelaxed DFT calculations comprising 45 different materials) helped improve our model’s predictions by as much as 50% for some systems.

*Funding from ONR (MURI N00014-13-1-0635)

10:24AM K18.00009: Quantum Criticality and Possible Superconductivity in Z_n Anisotropic Quantum Rotor Model Coupled with Free Fermion  
JIANQIAO LIU (Presenter), RYUICHI SHINDOU, School of Physics, Peking University — Quantum rotor model with Zn clock term (Zn anisotropic quantum rotor model) is known to exhibit a U(1) symmetric quantum critical point between Z_n symmetry breaking phase and quantum disorder phase for n ≥ 4. Around such quantum critical point, gapped bosonic excitations in the two phases become massless. Thereby, a coupling between a local boson degree of freedom and a free fermion could lead a superconductivity near the critical point. Motivated by this anticipation, we mapped the model into an electric flux model with electric charge, and carried out a quantum Monte-Carlo simulation study with a global update. Based on a finite-size scaling analysis of a superfluid stiffness parameter and comparison with the critical exponent of the 3D XY universality class, we discuss the critical nature of the quantum critical point. If the time allows, we discuss the possible superconducting pairing instability in the fermion system.

10:36AM K18.00010: OMDB-GAP1: A new dataset for band gap predictions for large organic crystal structures*  
BART OLSTHOORN (Presenter), RICHARD GEILHUFE, NORDITA, STANISLAV BORYSOV, Technical University of Denmark, DTU, ALEXANDER BALATSKY, NORDITA — Large datasets of ab initio calculations have enabled many pioneering studies of machine learning applied to quantum-chemical systems. For example, the machine learning models achieved chemical accuracy on the popular QM9 dataset which contains small organic molecules. Here, we present a new, more challenging dataset of 12,500 large organic crystal structures and their corresponding DFT band gap, freely available at https://omdb.diracmaterials.org/dataset. The dataset is based on the Organic Materials Database (OMDB) which hosts electronic properties of previously synthesized organic crystal structures. With an average of 85 atoms per unit cell, this dataset provides a new challenge for machine learning applications. We also evaluate the performance of two recent machine learning models on this new dataset: Kernel Ridge Regression with the Smooth Overlap of Atomic Positions (SOAP) and the deep learning model SchNet.

*the Swedish Research Council (638-2013-9243), the Knut and Alice Wallenberg Foundation, the European Research Council (DM-321031), the Marie Skłodowska-Curie grant agreement no.713683 (COFUNDfellowsDTU), Swedish National Infrastructure for Computing (SNIC) at the Center for High Performance Computing (PDC) and the High Performance Computing Center North (HPC2N)
10:48AM K18.00011: Theory of band gaps in nano-porous SiC*  
BLAIR TUTTLE (Presenter), COLTON BARGER, Penn State Erie, ANDREW O’HARA, SOKRATES T PANTELIDES, Physics, Vanderbilt University — Nano-porous SiC is an insulator used as a back-end-of-the-line dielectric in scaled integrated circuits. In the present study, nano-porous SiC atomic models are created from cubic SiC supercells. First, pores of varying sizes are created and hydrogen passivated. Then, bond switching techniques are applied to create models with variable bond densities and bond types. Density functional theory calculations are used to determine the model's physical and electronic properties including band gaps. We apply linear regression and random forest techniques to explore the role of bonding on the bandgaps of nano-porous SiC alloys.

*Research supported by Vanderbilt’s Physics NSF REU 1560035 and by Tuttle’s NSF RUI-DMR 1506403. This research was conducted using Advanced Cyber Infrastructure computational resources provided by The Institute for Cyber Science at The Pennsylvania State University.

Wednesday, March 6, 2019 8:00 AM - 10:48 AM

Session K19 DAMOP DCMP: Precision Many Body Physics VII  
BCEC 156C - Ehsan Khatami, San Jose State University - Tag(s): Focus

8:00AM K19.00001: Monte Carlo Studies of Quantum Critical Metals [Invited]  
EREZ BERG (Presenter), Condensed Matter Physics, Weizmann Institute — Metallic quantum critical phenomena are believed to play a key role in many strongly correlated materials, including high temperature superconductors. Theoretically, the problem of quantum criticality in the presence of a Fermi surface has proven to be highly challenging. However, it has recently been realized that many models used to describe such systems are amenable to numerically exact solution by quantum Monte Carlo (QMC) techniques, without suffering from the fermion sign problem. I will review the status of the understanding of metallic quantum criticality, and the recent progress made by QMC simulations, focusing on the cases of spin density wave and Ising nematic criticality. The results obtained so far will be described, as well as their implications for superconductivity, non-Fermi liquid behavior, and transport in the vicinity of metallic quantum critical points. Some of the outstanding puzzles and future directions are highlighted.

8:36AM K19.00002: Real time Quantum Monte Carlo for out of equilibrium strongly correlated systems.  
CORENTIN BERTRAND, INAC, CEA, ANTOINE MAILLARD, Ecole Normale Supérieure, SERGE FLORENS, CNRS, OLIVIER PARCOLLET (Presenter), Flatiron Institute, Simons Foundation, XAVIER WAINTAL, INAC, CEA —  
We discuss a real time diagrammatic Quantum Monte Carlo for strongly correlated systems, which allows to reach long time steady states. The method yields the expansion of physical quantities in power in the interaction, with a scaling $2^n$ at order $n$, uniformly in time. We present a systematic method to sum this expansion using conformal transformations and some recent benchmarks on Green functions in quantum impurity models in equilibrium and out of equilibrium.

8:48AM K19.00003: Infinite boundary conditions as a current source for impurity conductance in a quantum wire*  
ADAM IAIZZI (Presenter), National Taiwan University, CHUNG-YU LO, POCHUNG CHEN, Physics, National Tsing Hua University, YING-JER KAO, National Taiwan University — Developing nanoelectronic devices requires a detailed understanding of conduction in quantum wires. Numerical methods based on the density matrix renormalization group (DMRG) are excellent tools for studying one-dimensional quantum systems, but studying finite biases and currents requires time-dependent simulations, which remain challenging. Here we consider the problem of conductance across an impurity (or quantum dot) connected to metallic leads. Previous studies$^1,2$ have used a finite wire with open boundary conditions, which suffers from strong finite-size effects. We use a powerful numerical method incorporating infinite boundary conditions$^3$ (obtained from infinite DMRG$^4$) to simulate semi-infinite leads. We extract linear conductance from static correlation functions within a finite-size window that contains the impurity. Building on that, we use a time-dependent method to extract conductance in the presence of finite bias.


*MOST of Taiwan Grants No. 105-2112-M-002-023-MY3, 104-2628-M-007-005-MY3, 104-2112-M-002-022-MY3
9:00AM K19.00004: Resonant Tunneling with Dissipation in a Spin-full Quantum Dot.† TREVYN LARSON (Presenter), GU ZHANG, CHUNG-TING KE, MING-TSO WEI, HAROLD U BARANGER, GLEB FINKELSTEIN, Department of Physics, Duke University — We study resonant tunneling through a nanotube quantum dot subject to a dissipative environment. It has been previously shown that in the spin-less case, a quantum critical point is realized when the system is tuned on-resonance with symmetric coupling to the leads. At that point, conductance at low temperatures reaches \( e^2/h \) and several scaling laws are observed. Here, we demonstrate a qualitatively different behavior in the case of a spin-full resonance. In particular, the positions of resonant peaks change in a non-trivial fashion as a function of temperature, which is attributed to the lack of the particle-hole symmetry; and the peak height is not quantized and varies with dissipation strength. We argue that these signatures indicate the presence of the intermediate fixed point.

†Experimental work (TL, CTK, MTW, GF) were supported by DOE Award DE-SC0002765. Theoretical work (GZ, HB) was supported by DOE DE-SC0005237

9:12AM K19.00005: Quench dynamics of superconducting fluctuations and optical conductivity in a disordered system* ADITI MITRA (Presenter), YOAH S LEMONIK, New York University — There has been significant interest in the generation of very short-lived superconducting states in solid-state films. Here we consider the role of non-equilibrium superconducting fluctuations in such systems, generated by an interaction quench, considering the limit of large static disorder. In particular, we argue that because of critical slowing down, the regime of the fluctuation dominated (normal state) is more important than might be na"ively thought. We show how such a state might appear in the optical conductivity, and give the appropriate non-equilibrium generalization of the Azlamazov-Larkin and Maki-Thompson fluctuation corrections to the optical conductivity.

*This work was supported by the US National Science Foundation Grant nsf-dmr 1607059.

9:24AM K19.00006: Many-body Dynamic Structure Factors with Phase Space methods† JONATHAN WURTZ (Presenter), ANATOLI S POLKOVNIKOV, Boston University — Recently there has been much interest in describing the behavior of strongly-interacting quantum systems, especially equilibrium relaxation and hydrodynamic response. Intuitively, such behavior is classical, and should have an effective description with polynomial complexity as opposed to the exponential complexity of full quantum dynamics. This talk will detail work on one such semi-classical description, the Cluster Truncated Wigner Approximation, which approximates dynamics in a high-dimensional classical phase space. Via sampling in this phase space, the method precisely reproduces both short-time far-from-equilibrium quantum dynamics and long-time thermal dynamics. In particular, we will show how using this method one can accurately compute the spin diffusion constant with the dynamic structure factor.

†NSF DMR-1813499 and AFOSR FA9550-16-1-0334

9:36AM K19.00007: Berry's ansatz in Fock space: beyond random matrix theory for many-body quantum chaos REMY DUBERTRAND (Presenter), JUAN-DIEGO URBINA, KLAUS RICHTER, Institute für Theoretische Physik, University of Regensburg — Berry's ansatz of random superposition of vector basis to mimic the statistical properties of quantum states in classically chaotic systems, has been highly successful for one-body systems. It is at the heart of the original justification for the eigenstate thermalisation hypothesis (ETH) for many-body quantum systems. We detail its use in many-body Fock space using recent developments in many-body semiclassical techniques for Bose Hubbard models. Quantitative predictions for 2-point correlations in Fock space are given, which agree very well with numerics. This study highlights how semiclassical techniques can be efficient for many-body chaos beyond the universal regime of random matrix theory.
Floquet behavior of correlated systems with light-matter coupling* MONA KALTHOFF (Presenter), Max Planck Institute for the Structure and Dynamics of Matter, JAMES FREERICKS, Georgetown University, GOETZ S UHRIG, TU Dortmund, DANTE KENNES, Freie Universität Berlin, ANGEL RUBIO, MICHAEL SENTEF, Max Planck Institute for the Structure and Dynamics of Matter — Periodically driven nonequilibrium many-body systems have a quasi-energy spectrum which can be tailored by external driving fields, known as Floquet engineering of desired system properties [Sentef et al., Nat. Comm. 6, 7047 (2015); Uhrig et al, arXiv:1808.10199 (2018)]. However, continuous periodic driving is not realizable in pump-probe experiments in solids. For instance it is not clear which criteria a pulse has to meet for a system exposed to a pulsed drive to approach the Floquet limit of a periodically driven system. However, there are analytical results for noninteracting band electrons in infinite dimensions [Kalthoff et al., Phys. Rev. B 98, 035138 (2018)]. Moreover we discuss t-DMRG results for interacting 1D chains in the charge density wave phase to study the emergence of Floquet behavior for realistic pulse shapes. This builds on the recently proposed Floquet engineering in quantum chains [Kennes et al., Phys. Rev. Lett. 120, 127601(2018)].

*DFG Emmy Noether program SE 2558/2-1
ERC-2015-AdG-694097
Department of Energy, Office of Basic Energy Sciences, DE-FG02-08ER46542

Ultrafast many-body correlations in an excitonic insulator out of equilibrium RIKU TUOVINEN (Presenter), Max Planck Institute for the Structure and Dynamics of Matter, DENIS GOLEZ, MICHAEL SCHÜLER, PHILIPP WERNER, Department of Physics, University of Fribourg, MARTIN ECKSTEIN, Department of Physics, Friedrich-Alexander University Erlangen-Nürnberg, MICHAEL SENTEF, Max Planck Institute for the Structure and Dynamics of Matter — A fast time propagation method for nonequilibrium Green’s functions [1] based on the generalized Kadanoff-Baym Ansatz (GKBA) [2] is applied to a lattice system with a symmetry-broken equilibrium phase, namely an excitonic insulator [3]. The adiabatic preparation of a correlated symmetry-broken initial state from a Hartree-Fock wave function within GKBA is assessed by comparing with a solution of the imaginary-time Dyson equation [4]. We find that it is possible to reach a symmetry-broken correlated initial state with nonzero excitonic order parameter by the adiabatic switching procedure. We discuss under which circumstances this is possible in practice within reasonably short switching times. We further investigate the out-of-equilibrium dynamics of competing orders and how the balance between them could be controlled by laser driving [5].


Real-time quantum Monte Carlo for the spin-boson model* OLGA GOULKO (Presenter), Boise State University, GUY COHEN, MOSHE GOLDSTEIN, Tel Aviv University — The spin–boson model consists of a two-state system coupled to a bath of non-interacting harmonic modes. This fundamental, yet non-trivial model describes dissipation in a quantum system and can be mapped to an impurity coupled to interacting electron leads. Using the inchworm Monte Carlo algorithm we are able to precisely compute various nonequilibrium properties of the spin-boson model, such as the real-time evolution of the population difference between the two states at different temperatures, different forms of the bosonic bath spectrum, and different values of the spin-bath coupling, including the strong coupling regime. We also discuss how to calculate the heat current through the system coupled to two baths at different temperatures using full counting statistics.

*US-Israel Binational Science Foundation (Grants No. 2014262 and No. 2016087), The Chaoul Center for Nanoscale Systems
10:24AM K19.00011: Heating Dynamics in a Periodically Driven SYK-Model* CLEMENS KUHLENKAMP (Presenter), SIMON WEIDINGER, MICHAEL KNAP, Technical University of Munich — Periodically driven quantum matter can realize exotic dynamical phases that do not even exist in equilibrium. In order to understand how ubiquitous and robust these phases are, it is important to understand the heating dynamics of generic interacting quantum systems. We study the thermalization and heating dynamics in a generalized SYK-model subjected to a periodic drive, which realize a Fermi-Liquid (FL) to Non-FL crossover at a certain energy scale. Using an exact field theoretic approach we determine two regimes in the heating dynamics. At energies above the crossover scale the system is efficiently thermalizing and heats up exponentially. This crossover in the heating dynamics may be experimentally studied by measuring the absorption of THz laser light that impinges an irregularly shaped graphene flake in a strong magnetic field, which has been proposed to realize exotic SYK physics.

*We acknowledge support from the DFG grant No. KN 1254/1-1 and DFG TRR80 (Project F8).

10:36AM K19.00012: Entropy of the (1+1)-dimensional directed percolation* KENJI HARADA (Presenter), Graduate School of Informatics, Kyoto University — We investigate the informational aspect of a (1+1)-dimensional directed percolation which can be regarded as a reaction-diffusion process in a one-dimensional system and is a canonical model of a non-equilibrium continuous phase transition into an absorbing state. Using a tensor network scheme based on a mapping between a state probability distribution and a wave function, we can numerically calculate a time evolution of a state probability distribution. Although the density of active sites has no singular behavior, there is a new singular point in the conventional active phase at which the dynamical behavior of the entanglement entropy changes. The Rényi entropy has a cusp at the same point. The Rényi entropy also shows a universal relaxation at the critical point of the conventional absorbing phase transition.

*This work was supported by JSPS KAKENHI Grants No. 17K05576, and by MEXT as Exploratory Challenge on Post-K computer (Frontiers of Basic Science: Challenging the Limits) and Priority Issue on the Post-K computer (Creation of New Functional Devices and High-Performance Materials to Support Next-Generation Industries).

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K20 DCOMP DMP: First-principles Modeling of Excited-state Phenomena in Materials VII: 2D Materials and Surfaces BCEC 157A - Ismaila Dabo, Pennsylvania State University - Tag(s): Focus

8:00AM K20.00001: Ab initio time-dependent optical spectroscopy applied to spin and valley dynamics in monolayer transition metal dichalcogenides [Invited] ALEJANDRO MOLINA-SANCHEZ (Presenter), Institute of Materials Science, University of Valencia — Monolayer transition metal dichalcogenides (TMDs) like MoS₂ or WSe₂ are promising semiconducting 2D materials. Not only they have a bandgap in the optical range and suitable transport properties, but also provide a stimulating arena to study fundamental physics. For instance, the valence and conduction bands are spin-split because of the strong spin-orbit interaction. Moreover, due to the lack of inversion symmetry, with circularly polarized light, one can create excitons at selected K valley. The resulting imbalance in the population of the K valleys is the basics of valleytronics.

Ultrafast pump-probe spectroscopy measures accurately the valley dynamics, starting at the photogeneration of excitons at one valley and following the subsequent valley depolarization via intervalley and intravalley scattering. For instance, exploiting the valley selective optical selection rules and using two-colour helicity resolved pump-probe lasers, one can directly measure spin and valley dynamics and to estimate the ratio between intravalley and intervalley scattering rates. In spite of the numerous experimental data, the mechanisms of photo-generation and relaxation of the spin-valley polarization in TMDs are still heavily debated. It is in this context where time-dependent ab initio calculations are helpful to understand and predict the dynamical properties of 2D materials and to reproduce ultrafast spectroscopy experiments.

In this talk I will present our predictive and parameter-free approach to calculating ultrafast carrier dynamics in 2D materials, combining density functional theory with non-equilibrium many-body perturbation theory and including spin-orbit interaction. We calculate the photo-generation of carriers by a laser pulse, taking into account relaxation mechanisms such as electron-phonon scattering or radiative recombination, and simulate time-dependent spectroscopies like Kerr rotation, transient absorption or photoluminescence.
8:36AM K20.00002: The origin of single photon emission in 2D WSe$_2$*  YU JIE ZHENG, Department of Physics, National University of Singapore, YIFENG CHEN (Presenter), Centre for Advanced 2D Materials, National University of Singapore, YU LI HUANG, Institute of Materials Research & Engineering (IMRE), A*STAR (Agency for Science, Technology and Research), PRANJAL KUMAR GOGOI, Department of Physics, National University of Singapore, MING-YANG LI, LAIN-JONG LI, Physical Sciences and Engineering, King Abdullah University of Science and Technology, PAOLO E TREVISANUTTO, Centre for Advanced 2D Materials, National University of Singapore, QIXING WANG, Department of Physics, National University of Singapore, STEPHEN J PENNYCOOK, Department of Materials Science & Engineering, National University of Singapore, ANDREW THYE SHEN WEE, Department of Physics, National University of Singapore, SU YING QUEK, Centre for Advanced 2D Materials, National University of Singapore — Several experimental groups have shown that defect structures in 2D WSe$_2$ result in single photon emission (SPE). However, the origin of SPE is still unknown. We present a first principles study of the nature and optical properties of point defects in 2D WSe$_2$, together with scanning tunneling microscopy (STM) and scanning transmission electron microscopy images. We predict that O$_2$ can dissociate easily at Se vacancies, resulting in O-passivated Se vacancies (O$_{\text{Se}}$) and O interstitials (O$_{\text{ins}}$), which give STM images in good agreement with experiment. Our GW-Bethe-Salpeter-equation calculations show that O$_{\text{ins}}$ defects give exciton peaks ~50-100 meV below the free exciton peak, in good agreement with the localized excitons observed in independent SPE experiments. No other point defect (O$_{\text{Se}}$, Se vacancies, W vacancies, and SeW antisite defects) gives excitons in the same energy range. We conclude that the O$_{\text{ins}}$ defect is a source for the SPE previously observed in 2D WSe$_2$.

*We acknowledge grant NRF-NRFF2013-07 from the National Research Foundation (NRF), Singapore; ASTAR Pharos grant R-144-000-359-305; and support from the Singapore NRF, Prime Minister's Office, under its medium-sized centre program. SJP and PKG acknowledge MOE grant number R-144-000-389-114.

8:48AM K20.00003: Moiré Patterns of Excitons in Twisted Bilayer Transition-Metal Dichalcogenides Heterostructure*  XIAOBO LU (Presenter), SHIYUAN GAO, Physics, Washington University, St. Louis, XIAOQIN (ELAINE) LI, Department of Physics and Center for Complex Quantum Systems, Univ of Texas, Austin, LI YANG, Physics, Washington University, St. Louis — Twisted van der Waals heterostructures and the corresponding superlattices, moiré patterns, have been regarded as remarkable platforms to modulate many-electron interactions and optical excitations of two-dimensional structures. We employ first-principles many-body perturbation theory to study excitons and their moiré patterns in twisted bilayer MoSe$_2$/WSe$_2$ heterostructures. Because of significant type-II band offsets of heterostructures, direct interlayer excitons are always the lowest-energy excitons. We find that the energy variation of interlayer excitons is more significant in the R-type twisting structures than that in the H-type ones. Moreover, although the electron-hole binding energy is nearly spatially homogenous, the optical oscillator strength and radiative lifetime of interlayer excitons are very sensitive to the local stacking style, and they can vary in a few orders of magnitude in different regions of twisted bilayer structures. As a result, optical moiré patterns of interlayer excitons with high contrasts of brightness and radiative lifetime are expected.

*We are supported by the NSF CAREER Grant No. DMR-1455346, NSF EFRI-2DARE-1542815 and the AFOSR grant No. FA9550-17-1-0304. The computational resources have been provided by the Stampede2 at the TACC through XSEDE

9:00AM K20.00004: Dimensionality Dependence of Radiative Recombination in Black Phosphorus from First-principles*  FENG WU (Presenter), University of California, Santa Cruz, DARIO ROCCA, University of Lorraine and CNRS, Nancy (France), YUAN PING, University of California, Santa Cruz — Monolayer black phosphorus is a unique anisotropic 2D material with a sizable direct band gap and high mobility that has promising optoelectronic applications. However, the origin of how excitonic effects and excited state lifetime change with dimensionality has not been well understood. In this work we studied the electronic excitations and the radiative recombination in black phosphorus monolayer, nanoribbons and quantum dots by employing GW approximation (GW) and solving Bethe-Salpeter Equation (BSE). We demonstrate that 1) the exciton wavefunctions in 0D, 1D and 2D nanostructures are similar, which extend more along the armchair direction than zigzag, and reducing the size of nanostructures along the armchair direction significantly affects the exciton energy while that along the zigzag direction does not. 2) The radiative lifetime increases dramatically when the dimension shrinks from 2D to 1D to 0D, because the constraint of energy and momentum conversation makes that the radiative lifetime increases approximately $10^3$ times for each dimension reduction. This study provides important insights on engineering excited state properties of nanostructure materials.

*We acknowledge financial support from the National Science Foundation under grant No. DMR-1760260 and Hellman Fellowship
Exciton funnels in BPNRs. The excitons are able to be accumulated in unstrained, tensile or compressed regions, which enriches the means of controlling excitons for photo-detecting or photo-emitting. We find the type of funnels (spatial distribution and motion of excitons) can be tuned by changing the intensity and sign of the strain field, thickness and periodicity (zigzag or armchair) of BPNRs. By forming different funnels, the excitons are able to be accumulated in unstrained, tensile or compressed regions. This work implies that 2D materials are effective atomically thin dielectrics, and uncovers new insights into the unusual physics of screening in reduced dimensions.

Impact of defects on the opto-electronic properties of monolayer GeSe; a many-body perturbation theory perspective

KIRK LEWIS (Presenter), SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University — An accurate and detailed knowledge of the influence of defects will be central to the design of promising new 2D materials. Due to their reduced dimensionality and screening, these materials are even more likely to be impacted by defects than their 3D counterparts. We employ first-principles many-body perturbation theory within the GW/BSE approximation to investigate the influence of point defects on the opto-electronic properties of a monolayer semiconductor composed of GeSe. We systematically study a series of charged vacancies, their trap state energies, and their impact on optical absorption. We determine that the excitonic properties of the material are significantly affected by the presence of defects, with implications for devices fabricated using this material system.

Impact of defects on the opto-electronic properties of monolayer GeSe; a many-body perturbation theory perspective

The authors acknowledge funding support from the Department of Energy (Award #DE-SC0018080) and computational resources from DoE NERSC, DoD HPCMP, MGHPCC and NSF-XSEDE.
10:00AM K20.00009: Realizing an excitonic insulator by decoupling exciton binding energy from the minimum band gap  JIANG ZEYU (Presenter), Physics, Tsinghua University, YUANCHANG LI, Advanced Research Institute of Multidisciplinary Science, Beijing Institute of Technology, DUAN WENHUI, Physics, Tsinghua University, SHENGBAI ZHANG, Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute — Realizing excitonic insulator state in real materials has long been an attractive subject of condensed matter physics, as motivated by both fundamental interest in many-body physics and the potential application in transport devices due to its bosonic nature. Direct-gap materials serve as promising candidates for excitonic insulators, where the difficulty to distinguish from a Peierls charge density wave is avoided. However, direct-gap materials still suffer from a divergence of polarizability when the band gap approaches zero, leading to a diminishing exciton binding energy. We propose that one can decouple the exciton binding energy from the band gap in materials where band-edge states have the same parity. As a concrete example, we show by first-principles calculations that two-dimensional GaAs and experimentally mechanically exfoliated single-layer TiS$_3$ support prefectly to this principle, thus hold the possibility for experimental realization of excitonic insulators.

10:12AM K20.00010: Linear response and nonlocal dielectric function of freestanding and substrate-supported borophene from first-principles*  ANUBHAB HALDAR (Presenter), SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University — Two dimensional boron, or borophene, is a metallic monolayer material that has been recently synthesized on metallic substrates. First principles studies on the mechanical, optical, and electronic properties of borophene have predicted novel applications of borophene in flexible and power electronics. Additionally, borophene is a flexible, transparent, metallic material with highly nonlocal and anisotropic permittivity, and is a candidate as a plasmonic material. Here, we utilized first-principles density functional theory to conduct a systematic investigation of the linear response in isolated and metal-supported borophene, in order to quantitatively describe plasmon resonances in the visible region in the presence of the substrate. We determine that the dielectric properties of borophene are significantly affected by a silver substrate. This has implications for monolayer and thin film plasmonic and optoelectronic devices based on this platform.

*The authors acknowledge funding support from the Department of Energy (Award #DE-SC0018080) and computational resources from MGHPCC and NSF-XSEDE.

10:24AM K20.00011: Charge dynamics in proton-irradiated aluminum sheets*  ALINA KONONOV (Presenter), ANEESH JONELAGADDA, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Materials capable of withstanding continual ion radiation are highly desirable in space and nuclear applications. A detailed understanding of the mechanisms leading to degradation of materials under ion bombardment would enable targeted development of radiation resistant materials. As an energetic charged particle penetrates a material's surface, it deposits energy and excites electrons, leading to secondary electron (SE) emission and localized charge within the material. Even when direct collisions with nuclei are rare, fs scale surface charge dynamics may cause Coulomb explosion, which would damage and erode the material surface. We use time-dependent density functional theory to characterize SE emission, surface charge dynamics, and atomic forces in few-layer aluminum sheets under proton irradiation. From first-principles, we compute exit-side and entrance-side SE yields, SE energy spectra, and time scales of charge equilibration within the material as the projectile velocity and material thickness are varied. We also estimate the momentum acquired by aluminum atoms near the impact point. These simulations provide unprecedented insight into the dynamical response of materials' surfaces to ion bombardment.

*NSF OAC 17-40219
10:36AM K20.00012: Level Alignment in Large-Scale Hybrid Organic-Inorganic Systems from Hybrid Density Functional Theory

SVENJA JANKE (Presenter), Mechanical Engineering and Materials Science, Duke University, MARIANA ROSSI, Theory Department, Fritz Haber Institute of the Max Planck Society, SERGEY V. LEVCHENKO, Skolkovo Institute of Science and Technology, MATTTHIAS SCHEFFLER, Theory Department, Fritz Haber Institute of the Max Planck Society, MANOJ KUMAR JANA, CHI LIU, DAVID B MITZI, VOLKER BLUM, Mechanical Engineering and Materials Science, Duke University — Hybrid organic-inorganic systems allow to combine the properties of organic and inorganic substances at the nanoscale and hence open up a wide area for design of new materials with tunable properties. The positions of carrier levels and their alignment determine electronic properties of hybrid materials. A key challenge is that the systems in question tend to be large, due to alignment of components with inherently different lattice parameters or due to complex crystal structure packing. We here use hybrid density functional theory (FHI-aims all-electron code) for systems comprising over 1,000 atoms to reliably predict level alignments in two types of systems. For the paradigmatic interface system tetracene and pentacene at H/Si(111), we demonstrate the necessity of choosing large cells of up to 1,200 atoms that reflect the coincidence pattern and find type II heterojunction behavior with potential separation of charge between organic and inorganic component. For a layered double perovskite we demonstrate how level alignment between organic and inorganic compound is affected when the metal ion is exchanged, and rationalize experimentally observed photoluminescence in these systems.

*Supported by DFG-projects SFB-951, JA 2843/1-1; NSF 1728921

10:48AM K20.00013: Ehrenfest molecular dynamics approach to a light-induced softening of aluminum slab based on time-dependent density functional theory

HIROKI KATOW (Presenter), YOSHIIUKI MIYAMOTO, National Institute of Advanced Industrial Science and Technology — Modulation in lattice kinetics of simple metals under the irradiation of an ultra-short laser pulse is of great interest to both industrial applications and fundamental physics. In our study we performed Ehrenfest molecular dynamics (Ehrenfest MD) simulation of a nine-atomic-layer-thick aluminum slab based on time-dependent density functional approach. In our simulation the slab has (111) surface of aluminum fcc structure. The slab is put in vacuum, and is exposed to a femtosecond laser pulse. To analyze the Ehrenfest MD results, we employed a quasi one-dimensional model that bounds neighboring layers by a quadratic potential. Model parameters are fitted so that they reproduce Ehrenfest MD trajectory. We found a significant and non-uniform reduction of the force constants with the increase of laser intensity suggesting lattice softening by electronic excitation. In this presentation, we compare the results with the case of Born-Oppenheimer MD under finite electron temperature and discuss the correspondence between these two distinct types of theoretical methods.

*This presentation is based on results obtained from a NEDO project “Development of advanced laser processing with intelligence based on high-brightness and high-efficiency laser technologies (TACMI project).

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K21 DCOMP: Emerging Trends in Molecular Dynamics Simulations and Data Analytics I

8:00AM K21.00001: Reactive molecular dynamics simulations and machine learning* [Invited] PRIYA VASISHHTA (Presenter), Collaboratory for Advanced Computing and Simulations, University of Southern California — Machine learning (ML) is revolutionizing scientific and engineering disciplines owing to its ability to capture hidden patterns in large amounts of data. The recent success of ML can be attributed to increasing amount of data, simulation resources, and improving understanding of statistical inference. For these reasons computational materials science is undergoing a paradigm shift. The main reason is that trial-and-error approach to materials design is inefficient: laboratory trials require a lot of time, and the results of previous trials are not utilized in a systematic fashion. A data-driven approach, which draws upon all relevant data from experiments, and reactive and quantum molecular dynamics simulations, can address these issues. The MAGICS (Materials Genome Innovation for Computational Software) Center develops to aid the synthesis of stacked layered materials by chemical vapor deposition, exfoliation, and intercalation. The identification of different phases can be formulated as a classification problem and can be solved using ML techniques. We have used feed-forward neural network with three hidden layers to identify the different phases present during computational synthesis of MoSe2. Work reported here was carried out in collaboration with Rajiv K. Kalia, Aiichiro Nakano, Lindsay Bassman, Sungwook Hong, Aravind Krishnamoorthy, Kuang Liu, Ankit Mishra, Ken-ichi Nomura, and Pankaj Rajak,

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607.
In recent years, machine learning potentials have become a promising new approach for the representation of high-dimensional reactive potential-energy surfaces [1]. After training to a set of reference energies and forces obtained from electronic structure calculations they allow to perform large-scale simulations with first-principles accuracy at a fraction of the computational costs. As they do not contain any system-specific terms, they are applicable to a wide range of problems in chemistry, physics and materials science.

In this talk the methodology of high-dimensional neural network potentials (HDNNPs) [2,3] will be briefly reviewed, and its current scope and limitations will be discussed. The applicability of HDNNPs will be illustrated by recent studies of solid-liquid interfaces using copper [4] and zinc oxide [5,6] as prototypical examples. Since HDNNPs allow to describe the making and breaking of bonds, they enable the detailed investigation of the dissociation and recombination of water molecules as well as proton transport processes at interfaces. While water molecules do not spontaneously dissociate at ideal low-index copper surfaces, the water - zinc oxide system is very dynamic with properties strongly depending on the specific surface termination.


*JB thanks the DFG for a Heisenberg professorship (Be3264/11-2).
9:36AM K21.00005: Machine Learning Polarizable Force Field Parameters* YING LI (Presenter), Argonne National Laboratory, HUI LI, University of Chicago, FRANK PICKARD, National Institutes of Health, BADRI NARAYANAN, SUBRAMANIAN SANKARANARAYANAN, MARIA CHAN, Argonne National Laboratory, BENARD BROOKS, National Institutes of Health, BENOIT ROUX, University of Chicago — Machine learning (ML) techniques with the genetic algorithm (GA) have been applied to determine a polarizable force field parameters using quantum mechanics (QM) data of molecular clusters at the MP2/6-31G(d,p), DFMP2(fc)/cc-pVDZ, and DFMP2(fc)/cc-pVTZ levels to predict experimental condensed phase properties (i.e., density and heat of vaporization). The performance of this ML/GA approach is demonstrated on 4943 electrostatic potentials and 1250 cluster interaction energies for methanol. Excellent agreement between the training data set from QM calculations and the optimized force field model was achieved. The present effort shows the possibility of using machine learning techniques to develop descriptive polarizable force field using only QM data. The ML/GA strategy to optimize force fields parameters described here could easily be extended to other molecular systems.

*This work was supported by the Margaret Butler Postdoctoral Fellowship at Argonne Leadership Computing Facility. The computation was done on the Laboratory Computing Resource Center at Argonne National Laboratory. This research used resources of a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.

9:48AM K21.00006: Hot spot formation and shock initiation of RDX* ANKIT MISHRA (Presenter), KEN-ICHI NOMURA, AIICHIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, University of Southern California — Hot spot formation mechanism in energetic materials (EM) is crucial to handling and design of safer explosives. Presence of defects such as cracks, voids and grain boundaries are mainly responsible for creation of extreme conditions leading to hot spots. Recent experimental studies have shown that the presence of filled and empty void in EMs are responsible for creation of these regions. Here, we present a million-atom reactive molecular dynamics study to investigate the nature of hot spots during shock compression of RDX in gas filled and empty voids. We observe higher and sustained temperature rise in gas filled voids as compared to empty voids at particle velocities ranging from 2-4 km/sec. Furthermore, we observe that the higher amount of heat release on account of high potential energy drop in gas-filled voids correlate positively to more stable fragment formation, hence validating its role in high impact shock initiation of RDX.

* This work was supported by the Air Force Office of Scientific Research Grant No. FA9550-16-1-0042.

10:00AM K21.00007: Towards Exact Molecular Dynamics Simulations with Machine-Learned Force Fields STEFAN CHMIELA (Presenter), Machine Learning/Intelligent Data Analysis, Technische Universität Berlin, HUZIEL SAUCEDA, Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, KLAUS-ROBERT MÜLLER, Machine Learning/Intelligent Data Analysis, Technische Universität Berlin, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, Université du Luxembourg — The predictive power of molecular dynamics (MD) simulations hinges on the accuracy of the underlying interatomic potential, however ubiquitous classical force fields are typically challenged by quantum effects. We demonstrate how to leverage symmetric gradient domain machine learning (sGDML) to reconstruct global molecular force fields from high-level ab initio calculations that faithfully represent the accuracy of the reference data. A key feature of our approach is its ability to exploit spatial and temporal physical symmetries in a fully data-driven way, which enables a detailed reconstruction even when the sampling is well below the Nyquist rate. By doing so, the sGDML model can be parametrized from only a few hundred reference calculations and then allows converged MD simulations that provide insights into the dynamical behavior of molecules. We demonstrate how to reconstruct force fields for small molecules at the quantum-chemical CCSD(T) level of accuracy and outline how this process can be scaled to molecular solids using a hierarchical approach where intramolecular cohesive forces within the solid are reconstructed successively.

10:12AM K21.00008: Atomic Scale Response of Electrochemical Systems Under Potential Bias JAMES GOFF (Presenter), Materials Science and Engineering, Pennsylvania State University — In the past decade, there has been considerable progress in the simulation of solid-solution interfaces. This presentation will highlight ongoing developments in the modeling of electrochemical systems at the classical molecular level using the charge-optimized many-body potentials (COMB), and at the electronic-structure level using the self-consistent continuum solvation method (SCCS). The COMB force field in the is a variable-charge potential that enables the description of solvated electrodes, under applied voltage with the eCOMB formalism, with parameterization already available for a range of transition metals. Employing eCOMB, it is possible to simulate an electrochemical cell consisting of a cathode and anode in contact with an aqueous electrolyte. SCCS is an implicit solvation method to model quantum systems embedded in continuum electrolytes. We present a critical assessment of predictions from both models in determining the size-dependent surface distribution and electrochemical stability of transition-metal nanoparticles under electrical bias.
Constructing Accurate Machine Learning Force Fields for Flexible Molecules

VALENTIN VASSILEV GALINDO (Presenter), IGOR POLTAVSKYI, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, University of Luxembourg — Machine learning (ML) models can reproduce potential energy surfaces (PES) for molecules containing up to a few tens of atoms with an accuracy comparable to the most exact \textit{ab initio} methods. This provides a tool for computing thermodynamic properties that would require millions of CPU years otherwise. For instance, a recently developed sGDML\textsuperscript{1} model predicts forces and energy with CCSD(T) accuracy using just a few hundreds of configurations for training. However, up to now ML has been mainly applied to rather rigid molecules. In this regard, our objective is to test ML models for flexible molecules and out-of-equilibrium configurations along transition paths. For this, we select molecules (e.g. azobenzene, stilbene) with relatively complex transition paths, which result from an interplay between long- and short-range interactions. Then, different paths connecting PES minima are tested using sGDML. This allows us to define optimal descriptors and the appropriate strategies for choosing the training sets, which is crucial for ML models relying on a limited number of training points. Our results open an avenue for calculating transport paths, transition rates and other “out-of-equilibrium” properties with previously unattained accuracy.


Machine Learning for Auto-tuning of Simulation Parameters in Car-Parrinello Molecular Dynamics\textsuperscript{*}

JAYANATH CHAMINDU KADUPITIGE (Presenter), GEOFFREY C FOX, VIKRAM JADHAO, Intelligent Systems Engineering, Indiana University Bloomington — Simulating the dynamics of ions near polarizable nanoparticles (NPs) is challenging due to the need to solve the Poisson equation at every simulation timestep. Car-Parrinello Molecular dynamics (CPMD) simulations based on a dynamical optimization framework can bypass this obstacle by representing the polarization charge density as virtual dynamic variables, and evolving them in parallel with the physical dynamics of ions. Using these CPMD simulations of ions near polarizable NPs, we demonstrate the computational gains accessible by integrating machine learning (ML) for parameter prediction in CPMD simulations. An artificial neural network based regression model was integrated with CPMD and it predicted the optimal simulation timestep and critical parameters characterizing the virtual system on-the-fly with 94.3\% accuracy. The ML-enhanced, hybrid OpenMP/MPI parallelized, CPMD simulations generated stable and accurate dynamics of thousands of ions in the presence of polarizable NPs for over 10 million steps (over 30 ns) with walltime reducing from thousands of hours to tens of hours yielding a maximum speedup of ~600.

\textsuperscript{*}This work is supported by the National Science Foundation through Award 1720625.

Parallel Trajectory Splicing and the Value of Information\textsuperscript{*}

ANDREW GARMON (Presenter), Physics, Clemson University, DANNY PEREZ, Los Alamos National Lab — A range of specialized Molecular Dynamics (MD) methods have been developed in order to overcome the challenge of reaching longer timescales in systems that evolve through sequences of rare events. In this talk, we consider Parallel Trajectory Splicing (ParSplice) which works by generating large number of trajectory segments in parallel in such a way that they can later be assembled into a single statistically correct state-to-state trajectory, enabling parallel speedups up to the number of parallel workers. In practice, the ability for ParSplice to scale significantly improves when it is possible to predict where the trajectory will be found in the future. With this insight in mind, we develop a maximum likelihood transition model that is updated on the fly and show how the value of the information gained from generating a segment can rigorously be taken into consideration in order to improve performance.

\textsuperscript{*}This work was supported by the U.S. Department of Energy Office of Science Graduate Student Research (SCGSR) program, administered by the Oak Ridge Institute for Science and Education under DE SC0014664 and by the Exascale Computing Project (17-SC-20-SC).

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K22 DCOMP DMP: Electrons, Phonons, Electron-Phonon Scattering and Phononics II BCEC 157C - Boris Kozinsky, Harvard University - Tag(s): Focus
measurements, we find that a commensurate $\sqrt{3} \times \sqrt{3} \times 1$ superlattice forms in both SnS$_2$ and SnSe$_2$ at elevated pressures.

We implement first-principles calculations based on density functional and many-body perturbation theory. I will discuss the computational methodology and results for phonon-assisted optical absorption in metals and in indirect-gap semiconductors such as silicon (Si), boron arsenide (BAs), and boron nitride (BN). I will also discuss calculations for phonon-assisted Auger recombination in wide-band-gap semiconductors, an important nonradiative mechanism that dominates carrier recombination at high free-carrier concentrations. The results shed light into the interaction of light with materials and the efficiency of light emitters. This work was performed in collaboration with Kyle Bushick, Kelsey Mengle, Guangsha Shi, Andrew McAllister, Dylan Bayerl, and Chris Van de Walle.

*This work was supported by NSF awards 1254314 (DMR/CMMT CAREER program) and 1534221 (DMREF program). Computational resources were provided by the DOE NERSC facility.

8:36AM K22.00002: Time-Resolved Second Harmonic Generation Polarimetry Study of Elemental Tellurium
HONGLIE NING (Presenter), OMAR MEHIO, Institute for Quantum Information and Matter, California Institute of Technology, ELI ZOGHLIN, Materials Department, University of California, Santa Barbara, NICHOLAS LAURITA, Institute for Quantum Information and Matter, California Institute of Technology, STEPHEN WILSON, Materials Department, University of California, Santa Barbara, DAVID HSIEH, Institute for Quantum Information and Matter, California Institute of Technology — Elemental tellurium (Te) is a chiral semiconductor that breaks inversion symmetry, which allows for strong optical second harmonic generation (SHG). We performed time-resolved SHG polarimetry measurements on Te single crystals to understand the effects of inter-band carrier excitations on its lattice structure. I will describe the contrasting temporal evolution of the structure and charge excitations as a function of both temperature and pump fluence.

8:48AM K22.00003: First-principles resonant Raman spectroscopy for 2D materials
YUE YU (Presenter), JUN JIANG, Department of Physics and the Quantum Theory Project, University of Florida, LIANGBO LIANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, GEORGIOS D BARMARIS, Crete Center for Quantum Complexity and Nanotechnology, Department of Physics, University of Crete, SOKRATES T PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, XIAOGUANG ZHANG, Department of Physics and the Quantum Theory Project, University of Florida — We implement first-principles method for resonant Raman spectroscopy of solids based on a second-order Feynman diagram and the Franck-Condon principle. The Raman Intensity is calculated using an expression in the form of the Kramers-Heisenberg-Dirac (KHD) formula. Sum over all phonon configurations is performed using the Fourier transform into the time domain and evaluated with the help of Feynman path integrals. The triple integration method offers a simple and fast numerical approach that accounts for all multiple phonon processes. The ground state and excited state phonon modes are calculated to provide frequencies and equilibrium atomic positions. The computed Raman intensities for MoS$_2$/WS$_2$ heterostructure is in agreement with experimental data. We also explore the resonance properties of the Raman spectrum, in particular its strong dependence on the energy of incident laser and on temperature.

9:00AM K22.00004: Pressure-induced destabilization and periodic lattice distortion in SnX$_2$ (X = S, Se)
GYANU PRASAD KAFLE (Presenter), Department of Physics, Applied Physics, and Astronomy, Binghamton University-SUNY, CHRISTOPH HEIL, Institute of Theoretical and Computational Physics, Graz University of Technology, HARI PAUDYAL, Department of Physics, Applied Physics, and Astronomy, Binghamton University-SUNY, JIANJUN YING, Geophysical Laboratory, Carnegie Institution of Washington, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research, VIKTOR V. STRUZHKIN, Geophysical Laboratory, Carnegie Institution of Washington, ELENA R MARGINE, Department of Physics, Applied Physics, and Astronomy, Binghamton University-SUNY — Using first-principles calculations we investigate the behavior of tin disulfide (SnS$_2$) and tin diselenide (SnSe$_2$) under compression. In agreement with single-crystal X-ray diffraction, Raman, and transport measurements, we find that a commensurate $\sqrt{3} \times \sqrt{3} \times 1$ superlattice forms in both SnS$_2$ and SnSe$_2$ at elevated pressures. We show that the pressure-induced transition to the commensurate periodic lattice distortion (PLD) phase is due to the combined effect of strong Fermi surface nesting and electron-phonon coupling at a certain wave vector $q = (1/3, 1/3, 0)$. We further compare our findings to similar PLD transitions associated with charge density wave orderings in transition metal dichalcogenides.

*G. P. K. and E. R. M. acknowledge the financial support by the National Science Foundation (Award No. OAC-1740263). C. H. acknowledges support by the Austrian Science Fund (FWF) Project No. J3806-N36 and the Vienna Science Cluster.
9:12AM K22.00005: Microscopic dynamics in the Holstein model at high-temperature: Absence of diffusion*
STUART TRUGMAN (Presenter), CHEN-YEN LAI, Los Alamos National Laboratory — A single itinerant electron in the Holstein model is known to have a large conductivity at low temperatures as the electron is scattered by dilute thermally-excited phonons. At high temperatures, some theories suggest the dynamics are described by simple Boltzmann diffusion since there are many thermally excited phonons. Here, we investigate the dynamics of an itinerant particle of the Holstein model at high temperature. Our results suggest that the microscopic dynamics is not diffusion in some parameter regimes. In one dimension, the particle travels in a constant direction over time, which suggests an infinite conductivity. In higher dimensions, the particle follows a closed trajectory, a type of localization, and the trajectories are fractal.

*We acknowledge support from the US DOE through the Center for Integrated Nanotechnologies.

VÉRONIQUE BROUSSEAU-COUTURE (Presenter), Université de Montréal and RQMP, Montréal, Québec, Canada, ANNA MIGLIO, MATTEO GIANTOMASSI, Université Catholique de Louvain, IMCN/NAPS, Louvain-la-Neuve, Belgium, GABRIEL ANTONIUS, Department of Physics, University of California at Berkeley, California 94720, USA, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 9, YANG-HAO CHAN, Department of Physics, University of California at Berkeley, California 94720, USA and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, MICHEL COTE, Université de Montréal and RQMP, Montréal, Québec, Canada, XAVIER GONZE, Université Catholique de Louvain, IMCN/NAPS, Louvain-la-Neuve, Belgium — Computing the zero-point renormalization (ZPR) of the electronic bandgap due to electron-phonon coupling from first principles (FP) is a computationally challenging task, especially for polar materials, for which a very fine phonon wavevector sampling is required [1]. By contrast, the well-known Fröhlich Hamiltonian gives in the perturbative regime a simple analytical formula for the polaron binding energy, based on a few parameters that can be obtained from experiments or from FP calculations.

We compute the ZPR from FP for more than 20 polar binary semiconductors and insulators, and compare these results to those from a generalized Fröhlich model, in which the needed parameters are computed from FP. Despite the lack of Debye-Waller (DW) and interband contributions, we find that the simple Fröhlich approach agrees with FP results within a factor of two for most materials. We analyze the cancellation between the DW and Fan contributions from acoustic modes, and discuss the size of interband contributions in terms of Eliashberg functions. We finally develop a method to estimate the converged ZPR from coarser phonon samplings.


*NSERC grants RGPIN2016-06666, Calcul Québec and Compute Canada.

9:36AM K22.00007: First-principles study of self-trapped polarons*
WENG HONG SIO (Presenter), Department of Chemistry, University of Oxford, CARLA VERDI, SAMUEL PONCE, FELICIANO GIUSTINO, Department of Materials, University of Oxford — The polaron is a quasiparticles consisting of an electron or hole dressed by a cloud of phonons. Self-trapped polarons are found when the electron-phonon interaction is so strong that the electron is bound by the potential of the lattice distortion that it induces. Here we investigate the mechanisms of polaron formation in wide-gap insulators, using Li2O2 as a prototypical example. We study self-trapping both via direct density-functional theory (DFT) calculations and using a perturbation theory approach. We analyze the binding energy in terms of the underlying band structure and phonon dispersions, and we compare our findings with previous calculations and with classic models of self-trapped polarons. We discuss open questions in the ab initio study of polarons and possible solutions.

*The work was supported by the UK EPSRC (EP/L015722/1and EP/M020517/1) and the Leverhulme Trust (RL-2012-001), the Graphene Flagship (Horizon 2020 Grant No. 785219 - GrapheneCore2), the University of Oxford ARC facility, PRACE-15 and PRACE-17 resources MareNostrum at BSC.
9:48AM K22.00008: Phonon Behaviors of Charged Nanocrystals: Effects of Free Charge Carriers*  SHUN WANG (Presenter), BUTIAN ZHANG, School of Physics, Huazhong University of Science and Technology — The precise knowledge of phonons is important to understand the electronic and photonic properties of nanocrystals (NCs) and NC-based devices. It is common to introduce free charge carriers into NCs for device applications, highlighting the significance of studying the free carrier effects on phonon behaviors. In this study, we introduced the free carriers into a series of NCs (ZnO, CdSe, PbSe) and investigated the carrier-dependent phonon behaviors by using Raman spectroscopy. For charged NCs, the change of phonon frequencies and the overtone to fundamental intensity ratios were explained by the screening and band-filling effects caused by the accumulated free carriers. By using a time-dependent model, the overtone to fundamental intensity ratios were further correlated with the electron-phonon coupling strength of the involved excited states. The effects of free carriers on phonon behaviors, usually neglected in previous studies, should be carefully considered when analyzing the properties of charged NCs. Moreover, the relationship between the free carrier densities and Raman frequencies/relative intensities are potentially useful for nondestructive characterization of free carriers in NCs.

*This work was supported by the China Postdoctoral Science Foundation (No. 2018M632840).

10:00AM K22.00009: Experimental demonstration of generalized Fourier’s Law for heat conduction at the nanoscale  CHENGYUN HUA (Presenter), LUCAS LINDSEY, Oak Ridge National Laboratory, AUSTIN MINNICH, California Institute of Technology — Heat conduction under large temperature gradients that occur over scales of mean free paths of the energy carriers in solids is a topic of intense interest. Although the failure of Fourier’s law is well understood, the appropriate replacement has been the topic of debate. A concise relation that links temperature gradient to heat flux based on a rigorous mathematical interpretation is not only necessary but crucial to advance our knowledge of nanoscale heat transport. Here, we derived a generalized Fourier’s law based on Peierls-Boltzmann transport equation. This generalized Fourier’s law contains two parts, nonlocality of thermal conductivity, which has been previously hypothesized, and nonlocality of external effects, i.e. volumetric heat generation, which has long been ignored in literatures. We demonstrated the validity of this generalized Fourier’s law through comparisons with a series of time-domain thermoreflectance (TDTR) measurements. Furthermore, we showed that misinterpreting the generalized Fourier’s law in the experimental observation of nanoscale heat conduction would lead to erroneous microscopic information of phonons. To map the macroscopic observations to intrinsic phonon properties, it is crucial to appropriately take account into the microscopic heat input.

10:12AM K22.00010: Computing Raman Spectra With Wavelets Using The BigDFT Code*  MAXIME MORINIÈRE (Presenter), MICHEL COTE, Université de Montréal and RQMP, THIERRY DEUTSCH, LUIGI GENOVESE, CEA Grenoble — We report the calculations of Raman spectra using the BigDFT code.

The normal modes of vibration (or phonons) and their associated energies were found by slightly displacing each atom of the system around their ground position (this was already part of the BigDFT suite). We then added the possibility of computing the Raman intensity of each normal mode via electronic polarizability tensor calculations (in practice, this only amounts to applying small electric fields to the system of interest). The Raman spectra thus obtained are compared to the literature. A further check of the quality of the normal modes thus found is done by computing vibrational polarizability tensors.

The main perspective of this work is to use the order N version of the BigDFT code (instead of the usual cubic scaling version used in this work) to perform similar computations on larger systems.

*This project is supported by CEA (France) and Canada NSERC grants RGPIN2016-06666. The computational aspect of this research was enabled in part by support provided by Calcul Québec (www.calculquebec.ca) and Compute Canada (www.computecanada.ca)
GIORGIA FUGALLO (Presenter), BENOIT ROUSSEAU, Heat Transfer and Energy Laboratory of Nantes, CNRS, MICHELE LAZZERI, IMPMC-Sorbonne Université, CRNS — Density functional theory (DFT) is considered a predictive approach to determine anharmonic phonon-phonon interactions in crystals. Such a computational tool is a necessary ingredient, for example, of the first principles computational methods recently developed to determine phonon thermal transport in real systems. In this context, finding measurable quantities that can provide an independent benchmark for theoretical approaches is of paramount importance. Surprisingly, DFT has been rarely used to interpret the anharmonic features observable in infrared (IR) reflectance, transmittance and emittance spectra even though they provide a relatively direct probe to anharmonic properties in heteropolar materials and can be used to directly determine the anharmonic phonon self-energy of the optically active mode. I will show the influence of anharmonic effects on IR spectra of MgO, which is chosen as a test material because of the availability of different kinds of radiative properties measured experimentally and I will explain the limit of validity of a perturbative (multi-phonon) approach.

JIN-JIAN ZHOU (Presenter), MARCO BERNARDI, Caltech — Strong electron-phonon (e-ph) interactions lead to the formation of polarons, quasiparticles consisting of an electron carrying a phonon cloud. Polaron formation lowers the mobility and greatly affects charge transport in transition metal oxides and other polar compounds. Here, we develop a many-body ab initio approach to compute charge transport including polaron effects. We apply our approach to the two perovskite oxides BaSnO₃ and SrTiO₃, and analyze in detail how and why polaron formation affects charge transport in these materials. The calculations are connected with our recent work on SrTiO₃, where, using the Boltzmann Transport equation with lowest-order e-ph scattering, we accurately predicted the temperature dependence of the mobility in SrTiO₃ [1], whose absolute value was however higher than experiment. We show how including polaron effects can correct the lowest-order result, improving agreement with experiment.


*This work was supported by the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award Number DE-SC0004993.

SUDEEP ADHIKARI (Presenter), KEVIN BEACH, University of Mississippi — We present a theoretical framework for determining the mass deposited on a mechanical resonator subject to a flux of incoming particles of a single species. We consider the specific example of a vibrating nanostring and infer the history of mass deposition events from the frequency shifts in real time using a numerical optimization algorithm that correctly compensates for the configurational entropy. Our approach is tested against simulated data and is shown to perform well. We comment on its applicability to common inverse problems in physics, such as the extraction of spectral functions from imaginary-time Green's functions, that also suffer from configurational entropy effects.

**Wednesday, March 6, 2019 8:00 AM - 10:48 AM**

**Session K23 GIMS: Advances in Scanned Probe Microscopy III: Scanning Probes Spectroscopic Techniques** BCEC 158 - Tag(s): Focus

**8:00AM K23.00001: Fast nanomechanical spectroscopy: From ions to living cells** [Invited]  RICARDO GARCIA (Presenter), CSIC, Madrid — tbd
8:36AM K23.00002: Quantifying Tip-Sample Interactions in Vacuum Using Cantilever-based Sensors: An Analysis
OMUR DAGDEVIREN, CHAO ZHOU, ERIC ALTMAN, UDO DIETMAR SCHWARZ (Presenter), Yale University — We theoretically and experimentally show that the force law obtained from data acquired under vacuum conditions with dynamic force microscopy may deviate more than previously assumed from the actual interaction when the oscillation amplitude of the probe is of the order of the decay length of the force near the surface, which may result in a non-negligible error if correct absolute values are of importance [1]. However, the related inaccuracies can be effectively suppressed by using oscillation amplitudes sufficiently larger than the decay length of the tip-sample interaction. We also propose a novel technique that includes modulating the drive amplitude at a constant height from the surface while monitoring the oscillation amplitude and phase. Ultimately, such amplitude sweep-based force spectroscopy enables shorter data acquisition times and increased accuracy for quantitative chemical characterization compared to standard approaches that vary the tip-sample distance [1, 2]. In addition, since no feedback loop is active while executing the amplitude sweep, the force can be consistently recovered deep into the repulsive regime.

8:48AM K23.00003: Single ion hydrates under the SPM tip* JINBO PENG (Presenter), DUANYUN CAO, ZHILI HE, JING GUO, Peking University, PROKOP HAPALA, Czech Academy of Sciences, RUNZE MA, BOWEI CHENG, Peking University, JI CHEN, University College London, WEN JUN XIE, XIN-ZHENG LI, Peking University, PAVEL JELINEK, Czech Academy of Sciences, LIMEI XU, YI QIN GAO, EN-GE WANG, YING JIANG, Peking University — Ion hydration and transport at interfaces are relevant to a wide range of applied fields and natural processes. To correlate atomic structure with the transport properties of hydrated ions, both the interfacial inhomogeneity and the complex competing interactions among ions, water and surfaces require detailed molecular-level characterization. Here we constructed individual sodium ion (Na+) hydrates on a NaCl(001) surface by progressively attaching single water molecules to the Na+ using a combined scanning tunnelling microscopy(STM) and atomic force microscopy(AFM) system. We found that the Na+ hydrated with three water molecules diffuses orders of magnitude more quickly than other ion hydrates. Ab initio calculations revealed that such high ion mobility arises from the existence of a metastable state, in which the three water molecules around the Na+ can rotate collectively with a rather small energy barrier. Our work suggests that anomalously high diffusion rates for specific hydration numbers of ions are generally determined by the degree of symmetry match between the hydrates and the surface lattice.

*We thank the supports of the National Key R&D Program under Grant No. 2016YFA0300901,etc.

9:00AM K23.00004: Visualizing mineral-solution interfaces using 3D atomic force microscopy* ELIAS NAKOUZI (Presenter), BENJAMIN A. LEGG, SHUAI ZHANG, GREGORY K SCHENTER, JAEHUN CHUN, CHRISTOPHER J MUNDY, MARCEL D. BAER, SEBASTIEN KERISIT, JAMES J DE YOREO, Physical Sciences Division, Pacific Northwest National Laboratory — Understanding processes at solid-liquid interfaces is a key challenge for multiple research fields ranging from surface chemistry and catalysis to bio-membranes and living cells. Recent advances in atomic force microscopy—specifically 3D fast force mapping in amplitude modulated mode—have allowed the direct observation of interfacial solution structure with sub-nanometer resolution. We use this capability to probe multiple mineral-solution systems, including layered silicates (phlogopite and muscovite mica) and aluminum (oxy)hydroxides (boehmite and gibbsite) exposed to salt solutions of different pH and ionic strength. Depending on the system, our data show 3-5 structured layers spaced 0.2–0.5 nm apart and extending ~1.5 nm from the surface, with lateral features templated by the underlying crystal lattice. We compare the results to molecular dynamics simulations and discuss the promises and limitations of this exciting technique.

*A portion of this research was conducted under the Laboratory Directed Research and Development Program at Pacific Northwest National Laboratory, a multiprogram national laboratory operated by Battelle for the U.S. Department of Energy. Elias Nakouzi is grateful for the support of the Linus Pauling Distinguished Postdoctoral Fellowship program.
Fast multifrequency measurement of nonlinear conductance*  

RICCARDO BORGANI (Presenter), DAVID HAVILAND, Nanostructure Physics, KTH Royal Institute of Technology — We demonstrate fast acquisition of nonlinear current-voltage characteristics (IVC) at every pixel of a high-resolution conductive AFM image [1]. The technique exploits phase-coherent multifrequency lock-in measurement to acquire IVCs on a 512x512 grid in under 9 minutes (trace and retrace), and the inverse Fourier transform to perform the analysis in real time. Our approach overcomes the high resistance of the nanometer-scale tip-surface junction and the stray capacitance of the measurement leads which impose speed limitations (tens of seconds) on the traditional methods of measuring IVCs, making maps of variation over a surface impractical. The measurement technique allows for easy cancellation of parasitic displacement current due to the measurement leads and for separation of the galvanic and displacement currents in the junction. This ultrafast (milliseconds) acquisition of IVCs enables the AFM to reveal nanometer-scale variations in the electrical transport properties of organic photovoltaic and semiconducting thin films.


*The authors acknowledge financial support from the Swedish Research Council (VR), and the Knut and Alice Wallenberg Foundation.

Sub resonance AFM imaging coupled with machine-learning to identify cancer*  

IGOR SOKOLOV (Presenter), MAXIM E DOKUKIN, VEVEKANAND KALAPARTHI, MILOS MILJKOVIC, Tufts University, ANDREW WANG, Phillips Academy, JOHN SEIGNE, Dartmouth-Hitchcock Medical Center, PETROS GRIVAS, University of Washington, EUGENE DEMIDENKO, Geisel School of Medicine — We report on a new approach in diagnostic imaging based on nanoscale-resolution scanning of surfaces of cells collected from body fluids using, sub-resonance AFM tapping, Ringing mode, and machine learning analysis. The surface parameters, which are typically used in engineering to describe surfaces, are used to classify cells. The method is applied to the detection of bladder cancer, which is one of the most common human malignancies and the most expensive cancer to treat. The method, which utilizes cells collected from urine, shows 94% diagnostic accuracy when examining five cells per patient's urine sample. It is a statistically significant improvement (p<0.05) in diagnostic accuracy compared to the currently used clinical standard, cystoscopy, as verified on 43 control and 25 bladder cancer patients. Furthermore, the described approach can be extended to detect cell abnormalities beyond cancer as well as to monitor cell reaction to various drugs (nanopharmacology). Thus, this approach may suggest a whole new direction of diagnostic imaging.

*This work was partially supported by NSF CMMI 1435655 (I.S.) grant, Prouty funds from Norris Cotton Cancer Center, Dartmouth College (E.D., I.S., J.D.S.)

Visualizing the Electrostatic Barrier of a Material Interface to Nanoscale Dimensions: Defects, Silicides, and Dielectrics  

WESTLY NOLTING, JACK ROGERS, STEVEN GASSNER, HYEOSEON CHOI, VINCENT LABELLA (Presenter), Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute — Electrostatic barriers at material interfaces are the foundation of current and futuristic electronic and optoelectronic devices. Direct visualizing of the electrostatic barrier of an interface with nanoscale resolution can be accomplished utilizing ballistic electron emission microscopy (BEEM), an STM-based technique [1]. Tens of thousands of BEEM spectra are acquired on a regularly spaced grid and then fit to extract the Schottky barrier height. Physical and chemical insight is provided by computational modeling, which simulates the distributions of barrier heights and includes effects from the interface and transport of the hot electrons in the metal. This presentation will give an overview of the technique and its ultimate spatial and energetic resolution. Measurements of defects, incomplete silicide formation, the presence of multiple metal species at the interface, monolayer thick dielectric layers, and the influence of ionized impurity scattering in the semiconductor will also be presented.

Mapped AFM force spectroscopy on gels: methodological and interpretive developments

GREG HAUGSTAD, Characterization Facility, University of Minnesota, GUICHUAN YU, Informatics Institute, University of Minnesota, YING CHEN, GUFA LIN, Stem Cell Institute, University of Minnesota, ALON MCCORMICK, Chemical Engineering and Materials Science, University of Minnesota, MAGGIE ZENG (Presenter), Boston Scientific Corporation — We present aqueous-immersion force-distance analysis on fibrin gels and polyvinyl pyrrolidone (PVP) gel-phase coatings. Initial applications were mechanical matching (fibrin to tissue) and lubricity/durability assessment (PVP). In both cases we discovered (a) a need for extensive mapping (tens or hundreds of microns) to survey spatial heterogeneities in both mechanics and topography as well as their correlations; and (b) widely ranging modulus values both among gel samples (~0.1-100 kPa) and across individual gels (one order of magnitude). On the softest PVP gel coatings colloid microprobes were used instead of sharp AFM tips to allow a shear contact (friction characterization).

In developing data analytics, we find that vendor algorithms for modulus mapping require modification (here in matlab) in order to: (1) demarcate solid body mechanics (Hertzian) from steric forces within each force curve as a function of distance, and/or treat Poissons ratio as variable with gel compression; (2) account for local surface curvature and thereby system radius of curvature (for colloid probe); (3) invoke criteria for rejecting anomalous force-distance measurements (e.g., sites of fibril adhesion) prior to compiling distribution functions of spatially surveyed modulus measurements.

Conductance spectroscopy of confined water in Montmorillonite clay nanoparticles

KELSEY YEE (Presenter), AYDIN WELLS, N. E. ISRAELOFF, Northeastern University — Montmorillonite (MNT) clay confines water and ions to few-monolayer sheets. We use an SPM-based nano-dielectric-spectroscopy (NDS) technique to study frequency-dependent (10Hz-10 kHz) electrical properties of individual MNT nanoparticles (NP) with variable water content. We study ionic conductivity in this 2D nano-confined geometry, and compare with bulk material with inter-particle contributions. We focus on the high-frequency (HF) power-law regime of the conductivity peak in the electric modulus, M(f) ~ f^1-α, related to a hopping-conductivity, σ = σdc + σacf^α. We apply a sinusoidal voltage to the conducting tip during non-contact portion of a double pass scan, using high-harmonic for feedback, and the fundamental mode to measure the phase and amplitude of the force-derivative (FD). For a range of relative humidity (RH), the FD phase, ϕ(f) exhibits a peak, similar to the peak in bulk M(f), but shifted to lower frequencies. We use finite-element-modelling to extract NP conductivity spectra from data (poster by A. Wells). Simulated ϕ(f) for anisotropically conducting NP have HF power-laws matching M(f). In bulk, for various RH we find exponents, α = 0.3 ±0.05. NP exhibited exponents of α = 0.6 ±0.1. This suggests a different conductivity mechanism in bulk and NP.

How Much Information is in an STM Image?

MITCHELL YOTHERS, SOUMYA BHATTACHARYA, LLOYD BUMM (Presenter), Homer L. Dodge Department of Physics & Astronomy, University of Oklahoma — Scanning tunneling microscope (STM) images contain a wealth of information. We are developing real-space post-processing image analysis tools to extract information that would otherwise be hidden. We use decanethiol self-assembled monolayers (SAMs) on Au(111) as our model system. We demonstrate measurements of the “molecule” locations that are in principle accurate to less than 1 pm in any direction. By creating an averaged unit cell image from many imaged unit cells, we also demonstrate that the unit cell image has no additional symmetry beyond its lattice symmetry. Average unit cell images from different structural domains of the same image demonstrate which image features are due to the surface and which are due to the tip. Time-lapse image series of SAMs allow for time averaging techniques to be used to track and study individual molecules.

*Financial support from the National Science Foundation (CHE-1710102), the Homer L. Dodge Department of Physics, and the OU College of Arts and Sciences, and NVIDIA Corporation (donation of a Tesla K-40 GPU) is gratefully acknowledged.
10:24AM K23.00011: Revealing tip-surface interaction with dynamic force curves
DANIEL FORCHHEIMER (Presenter), RICCARDO BORGANI, DAVID HAVILAND, Royal Institute of Technology — The force between the AFM tip and the surface is conventionally studied using quasi-static deflection-approach curves. These must be converted into force-position curves by a transformation of coordinates, to be compared with models of the interaction, such as the Derjaguin-Muller-Toporov (DMT) model. For the transformation to be valid the motion has to be slow, as to not excite the resonance of the cantilever.

We instead excite the cantilever a two frequencies near its resonance, creating a beat that effectively approaches and retracts from the surface in what is called Intermodulation AFM. By measuring amplitude and phase during this beat, and using a transformation similar to that done for quasi-static curves (but now taking the full dynamics of the cantilever into account) we obtain two dynamic force curves. One conservative, Fi and one disipative, Fq.

Comparing theoretical Fi and Fq curves for standard models, such as the DMT, to experimental result reveal severe limitations of these models. They are typically not sufficient to explain the observed interaction between the tip and the surface. We show how a proposed new tip-surface model, which allow a dynamic surface, can overcome some of these limitations.

10:36AM K23.00012: Scanning Tunneling Microscopy and Spectroscopy of Novel Silver-Containing DNA Molecules
NATALIE FARDIAN-MELAMED (Presenter), Physical Chemistry Department and Center for Nanoscience and Nanotechnology, Hebrew University of Jerusalem, GENNADY EIDELSHTEIN, Biochemistry Department and Center for Nanoscience and Nanotechnology, Tel Aviv University, DVIR ROTEM, Physical Chemistry Department and Center for Nanoscience and Nanotechnology, Hebrew University of Jerusalem, ALEXANDER KOTLYAR, Biochemistry Department and Center for Nanoscience and Nanotechnology, Tel Aviv University, DANNY PORATH, Physical Chemistry Department and Center for Nanoscience and Nanotechnology, Hebrew University of Jerusalem — The quest for a suitable molecule to pave the way to molecular nano-electronics¹ has been met with obstacles for over a decade², ³. Candidate molecules such as carbon nanotubes lack the appealing trait of self-assembly, while DNA seems to lack the desirable feature of conductivity⁴. Silver-containing poly(dG)-poly(dC) DNA (E-DNA) molecules were recently reported as promising candidates for molecular electronics⁵, owing to the selectivity of their metallization, their uniform structure, their resistance to deformation, and their most possible conductivity⁵, ⁶. Here we present an elaborate temperature dependent high-resolution morphology characterization of these unique molecules, alongside a detailed depiction of their electronic level structure. Our findings⁷ were acquired by use of an ultra-high vacuum (UHV) scanning tunneling microscope (STM). The temperature dependence of E-DNA's topographic features and density of states spurs intriguing insights. Moreover, the energy levels found for E-DNA indicate a novel, truly hybrid metal-molecule structure, potentially more conductive than its DNA-based peers.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K24 DAMOP DQI: Hybrid/Macroscopic Quantum Systems, Optomechanics, and Interfacing AMO with Solid State/Nano Systems II

8:00AM K24.00001: Entanglement of Two Remote Mechanical Resonators* RALF RIEDINGER (Presenter), Harvard University, ANDREAS WALLUCKS, IGOR MARINKOVIĆ, TU Delft, SUNGKUN HONG, MARKUS ASPELMEYER, Universität Wien, SIMON GROEBLACHER, TU Delft — Entanglement is a key feature of quantum mechanics and plays an important role in many quantum information processing protocols. Here we report on the entanglement of two massive mechanical oscillators located on separate chips. Intriguingly, the silicon photonics devices employed in this experiment can serve as long-lived quantum memories and are directly interfaced to photons in the telecom wavelength range around 1550nm. We further report on the observation of entanglement between a flying telecom photon and a pair of such quantum memories.

*Marie Curie Horizon 2020 initial training programme OMT 722923, FOM Projectruimte grants 15PR3210, 16PR1054, WWTF ICT12-049, ERC CoG QLev4G, ERC Stg Strong-Q, FWF F40 (SFBO FOQUS) and P28172, and NWO/OCW Vidi grant (680-47-541/994). R.R. was a recipient of a DOC fellowship of the Austrian Academy of Sciences at the University of Vienna.
Optical Backaction-Evading Measurement of a Mechanical Oscillator

ITAY SHOMRONI
(Presenter), LIU QIU, Ecole polytechnique federale de Lausanne, DANIEL MALZ, ANDREAS NUNNENKAMP, University of Cambridge, TOBIAS KIPPERBERG, Ecole polytechnique federale de Lausanne — Quantum mechanics imposes a limit on the precision of a continuous position measurement of a harmonic oscillator, as a result of quantum backaction arising from quantum fluctuations in the measurement field. A variety of techniques to surpass this standard quantum limit have been proposed, such as variational measurements, stroboscopic quantum non-demolition and two-tone backaction-evading (BAE) measurements. The latter proceed by monitoring only one of the two non-commuting quadratures of the motion. This technique, originally proposed in the context of gravitational wave detection, has not been implemented using optical interferometers to date. Here we demonstrate continuous two-tone BAE measurement in the optical domain of a localized GHz frequency mechanical mode of a photonic crystal nanobeam cryogenically and optomechanically cooled close to the ground state, employing quantum-limited detection. We observe up to 0.67dB (14%) reduction of total measurement noise, thereby demonstrating the viability of BAE measurements for optical ultrasensitive measurements of motion and force in nanomechanical resonators.

This work was supported by funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 709147 (GeNoSOS).

Cavity cooling of levitated nanospheres by coherent scattering

UROS DELIC (Presenter), MANUEL REISENBAUER, Faculty of Physics, University of Vienna, DAVID GRASS, Duke University, NIKOLAI KIESEL, MARKUS ASPELMEYER, Faculty of Physics, University of Vienna — Although cavity cooling of levitated nanospheres has been demonstrated in recent years, regime of strong optomechanical cooperativity C>1 is yet to be reached, leading to full quantum control of nanosphere motion. A common obstacle in many experiments is stable levitation of nanospheres in ultra-high vacuum (UHV). However, stable trapping has been achieved in an optical dipole trap in several experiments through the use of three-dimensional parametric feedback. We exploit this by combining such a trap with an optical cavity and demonstrate cavity optomechanics with a silica nanosphere in UHV. We confirm the trapping of nanospheres of nominal radius through a novel method using the variable coupling to a cavity mode. We achieve C=0.02, showing a five orders of magnitude improvement of cooperativity from our previous work. We then modify this setup to drive the cavity mode solely by scattered photons from tweezer laser. In addition, cavity enhanced scattered photons provide a more effective, three-dimensional cooling of the nanosphere motion, immediately allowing us to reach strong cooperativity in high vacuum.

A coherent nanomechanical oscillator driven by single-electron tunneling

YUTIAN WEN (Presenter), NATALIA ARES, FELIX SCHUPP, T. PEI, GEORGE ANDREW DAVIDSON BRIGGS, Department of Materials, University of Oxford, EDWARD LAIRD, Department of Physics, Lancaster University — We study the strong electromechanical coupling between a vibrating carbon nanotube and a single-electron transistor (SET) defined along its length. The current through the SET is both a sensitive transducer for the motion, and a source of strong feedback that leads to mechanical oscillations. Using a novel time-resolved measurement technique, we characterize the coherence of these oscillations, finding an auto-correlation time as long as 100 microseconds. This system resembles an electromechanical maser, with the pumping provided by the electrical bias and the phonon cavity provided by the mechanical resonance. While the linewidth of the free-running oscillator is limited by slow frequency fluctuations, we show two ways to stabilise it: by locking its frequency to an injection tone, and by adjusting the mechanical tension in a phase-locked loop. With feedback applied, the mechanical linewidth can be stabilised to within 2 Hz at a 230 MHz oscillation frequency.


This work was supported by EPSRC (EP/N014995/1, EP/R029229/1), DSTL, Templeton World Charity Foundation, and the Royal Academy of Engineering.
8:48AM K24.00005: Coupled Piezoelectric and Optomechanical Resonators for RF-to-optical Frequency Conversion* MARCELO WU (Presenter), BISWARUP GUHA, Chemistry, University of Maryland, NIST, KRISHNA COIMBATORE BALRAM, Electric and Electronic Engineering, Bristol University, KARTIK A SRINIVASAN, Physical Measurement Laboratory, National Institute of Standards and Technology — The development of quantum computing technologies currently faces interconnectivity barriers. A leading platform for quantum processors uses superconducting microwave or radio-frequency (RF) circuits encased inside dilution refrigerators at millikelvin temperatures. Long-range communication is thus a major challenge due to loss of signal outside cryogenic environment. Recently, RF-to-optical photon converters have attracted significant interest for their use in linking RF signals to an optical signal that can propagate in high-speed low-loss optical fiber networks. We propose an on-chip nanoscale converter that connects RF signals to mechanical degrees of freedom using a piezoelectric resonator and then bridges to the optical domain using an optomechanical resonator. This effective electro-mechano-optical modulator is built on a GaAs material platform which exhibits strong photoelastic effect for optomechanical coupling. We demonstrate new device designs that compensate for the inherently low piezoelectric effect in GaAs and progress in the fabrication of an integrated piezo-optomechanical device.

*We acknowledge the UMD-CNST cooperative research agreement, Award No. 70NANB10H193, the UMD-NIST PREP program, and the ARO/LPS CQTS program.

9:00AM K24.00006: Laser heating of a charged gold nanosphere levitated in an ion trap at high vacuum* JOYCE COPPOCK (Presenter), SAMUEL KLUETER, JOSÉ HANNAN, Physics, University of Maryland, College Park, BRUCE E KANE, Laboratory for Physical Sciences — Levitation of a nanoparticle in high vacuum decouples the particle from its environment and enables sensitive thermodynamic measurements; specifically, a levitated particle can be heated in a controlled manner via illumination with a laser. We confine an electrically charged gold nanosphere in a quadrupole electric field trap at pressures as low as 1x10^-8 Torr and illuminate it with a linearly polarized 532 nm laser. Accurate measurements of the particle's charge-to-mass ratio, combined with observations of single discharge events, give a precise determination of its mass. We observe that the particle begins to evaporate at sufficiently high laser powers; from the evaporation rate, we can deduce its internal temperature. In this talk, we present evidence of the heating of 250 nm gold spheres to temperatures in the range of 1000-1250 K, near the melting temperature of 1337 K. Further heating of the particle should enable trapping and observation of a molten droplet.

*This work was supported by the Laboratory for Physical Sciences.

9:12AM K24.00007: Engineering dissipation dilution of strained nanomechanical resonators* SERGEY FEDOROV (Presenter), NILS JOHAN ENGELSEN, MOHAMMADJAFAR BEREYHI, ALBERTO BECCARI, AMIR HOSSEIN GHADIMI, RYAN SCHILLING, DALZIEL WILSON, TOBIAS KIPPPENBERG, Ecole polytechnique federale de Lausanne — Dissipation dilution by tensile strain enables micro- and nano- mechanical resonators that have quality factors (Q) exceeding those of bulk vibrations in the same material by orders of magnitude. For a long time, uniform beam- and membrane- shape resonators made of high-stress stoichiometric silicon nitride have been the system of choice to attain high Q and low effective mass—key parameters in force sensing and cavity optomechanics. Recently it was discovered that dissipation dilution (and hence Q) can be increased substantially in non-uniform resonators through techniques such as “soft clamping”, engineering local strain and “tapered clamping”. We show that soft clamping combined with strain engineering can be applied to nanobeams to produce record-high quality factors up to 800 million at room temperature and Q × frequency exceeding 10^15 Hz. The complementary tapered clamping approach results in enhanced Q for the fundamental flexural mode, unachievable with soft clamping. Time permitting, we will also present results on dissipation dilution engineering of membranes and cavity optomechanics with engineered resonators.

*This work was supported by the EU Horizon 2020 Research and Innovation Program under grant agreement no.732894 (FET Proactive HOT) and DARPA grant HR0011181003.
Directional transmission or amplification of microwave signals is indispensable in various applications involving sensitive measurements. Using a device including two on-chip superconducting resonators and two metallic drumhead mechanical oscillators, we experimentally demonstrate how to use this generic cavity optomechanical system to non-reciprocally amplify microwave signals. Pumping this device at four distinct microwave frequencies allows to design applications including sensitive metrology, ground state cooling of mechanical motion, and slowing of light.

**This work is supported by DARPA/MTO's PRISM: AIMS program through a grant from SPAWAR (N66001-16-1-4026) and Air Force Office of Scientific Research (AFOSR) MURI grant (FA9550-15-1-0029).**

**9:36AM K24.00009: Radio-frequency optomechanical characterization of a silicon nitride drum**

**ANNA PEARSON (Presenter), Department of Materials, University of Oxford, KIRAN KHOSLA, Blackett Laboratory, Imperial College London, MATTHIAS MERGENTHALER, GEORGE ANDREW DAVIDSON BRIGGS, Department of Materials, University of Oxford, EDWARD LAIRD, Department of Physics, Lancaster University, NATALIA ARENS, Department of Materials, University of Oxford — On-chip actuation and readout of mechanical motion is key for characterizing mechanical resonators and exploiting them for new applications. We capacitively couple a silicon nitride membrane to an off-resonant radio-frequency cavity formed by a lumped element circuit. Despite a low cavity quality factor of about 7.4 and off-resonant, room temperature operation, we are able to parametrize several mechanical modes and estimate their optomechanical coupling strengths. This enables fast characterization of a device without requiring a superconducting cavity, thereby eliminating the need for cryogenic cooling. We also observe optomechanically induced transparency and absorption which is crucial for a number of applications including sensitive metrology, ground state cooling of mechanical motion, and slowing of light.

**This work was supported by the Academy of Finland (contracts 250280, 308290, 307757, 312296), by the European Research Council (615755-CAVITYQPD), and by the Aalto Centre for Quantum Engineering. We acknowledge funding from the European Union's Horizon 2020 research and innovation program under grant agreement No. 732894 (FETPRO HOT).**

**9:48AM K24.00010: Realization of directional amplification in a microwave optomechanical device**

**LAURE MERCIER DE LÉPINAY (Presenter), ERNO DAMSKÄGG, CASPAR OCKELOEN-KORPPI, MIKA SILLANPÄÄ, Applied Physics, Aalto University — Directional transmission or amplification of microwave signals is indispensable in various applications involving sensitive measurements. Using a device including two on-chip superconducting resonators and two metallic drumhead mechanical oscillators, we experimentally demonstrate how to use this generic cavity optomechanical system to non-reciprocally amplify microwave signals. Pumping this device at four distinct microwave frequencies allows to design two transmission paths for excitations from one microwave port of the device to another, that can be made to interfere constructively or destructively depending on the signal's propagation direction. As a result, we demonstrate amplification in one direction by 9 decibels and a simultaneous isolation in the opposite direction by 21 decibels.**

**This work was supported by the Academy of Finland (contracts 250280, 308290, 307757, 312296), by the European Research Council (615755-CAVITYQPD), and by the Aalto Centre for Quantum Engineering. We acknowledge funding from the European Union's Horizon 2020 research and innovation program under grant agreement No. 732894 (FETPRO HOT).**
10:12AM K24.00012: Coupling of single photon emitters in hBN to microcavities*  
NICHOLAS PROSCIA (Presenter), HARISHANKAR JAYAKUMAR, ZAV SHOTAN, GABRIEL LOPEZ-MORALES, Physics, City College of New York, XIAOCHEN GE, WEIDONG ZHOU, University of Texas, Arlington, CARLOS A. MERILES, VINOD M MENON, Physics, City College of New York —Hexagonal Boron Nitride (hBN) was recently found to be a source of single photon emitters (SPE) which exhibit desirable properties such as narrow room-temperature linewidths, spectral tunability and operation under ambient conditions. Despite these advantageous properties, scalable integration of these emitters into chip-based cavities has proven elusive. Here, we demonstrate coupling of hBN defect emission to Si3N4 microdisk cavities by exploiting the topography of the cavity structure to engineer strain and thereby activate SPEs which near field couple to the cavities. We find the cavity coupled emission to have a Purcell enhancement of 1.3, close to the cavity's theoretical Purcell factor of 1.6. The present work is a first step towards cavity enhanced SPEs in this material system and paves the way for deterministic cavity coupling of SPEs that operate at room temperature.

*This work is supported by the NSF CREST IDEALS center, NSF MRSEC program (DMR-1420634) and the NSF EFRI 2-DARE program (EFMA -1542863) and was partially carried out at the CUNY ASRC NanoFabrication Facility.

10:24AM K24.00013: Valley-Mechanical Coupling in a Monolayer Semiconductor  
HAOKUN LI (Presenter), KING YAN FONG, HANYU ZHU, QUANWEI LI, SIQI WANG, SUOI WANG, XIANG ZHANG, University of California, Berkeley — The interaction of macroscopic mechanical object with electron charge and spin plays a vital role in today's information technology and fundamental studies of the quantum-classical boundary. Recently emerged valleytronics encodes information to the valley degree-of-freedom and promises exciting applications in communication and computation. We realize valley-mechanical coupling in a monolayer MoS2 resonator and demonstrate transduction of valley information to the mechanical states. The valley and mechanical degrees-of-freedom are coupled through the magnetic moment of the valley carriers under a magnetic field gradient. We identify the valley-actuated mechanical motion by optical interferometry and attain a transduction confidence level near unity. Our experiment lays the foundation for a new class of valley-controlled mechanical devices and facilitates realization of hybrid quantum valley-mechanical systems

10:36AM K24.00014: Interference effects in cavity optomechanics with hybridized membranes  
ONDREJ CERNOTIK (Presenter), CLAUDIU GENES, Max Planck Institute for the Science of Light, AURELIEN DANTAN, Department of Physics and Astronomy, University of Aarhus — Radiation pressure forces in cavity optomechanics allow for efficient cooling of motion, the manipulation of photonic and phononic quantum states, as well as generation of optomechanical entanglement. The standard mechanism relies on the cavity photons directly modifying the mechanical state. Hybrid cavity optomechanics provides an alternative approach by coupling mechanical objects to quantum emitters, either directly or indirectly via the common interaction with a cavity field mode. In these systems, the interference between forces from the cavity field and the emitters can give rise to novel optomechanical phenomena. We analyze two such hybrid optomechanical systems where a vibrating membrane is doped by quantum emitters or patterned with a photonic crystal structure. In particular, we demonstrate that, in the former system, a three-body interaction between the cavity field, emitters, and mechanical motion can be used to improve cooling of the mechanical motion [1]. Second, we show that, when an esnemble of emitters or a photonic crystal structure in the membrane strongly modifies the membrane reflectivity, the cavity linewidth can be significantly reduced and the system can reach the sideband resolved regime.


10:48AM K24.00015: Trapping Ultracold Fermionic Atoms in a Ring Bowtie Cavity  
KEVIN WRIGHT (Presenter), YANPING CAI, DANIEL ALLMAN, Dartmouth College — We have trapped ultracold fermionic atoms (6Li) in a ring cavity for the first time. The cavity is in a symmetric ring bowtie configuration with all glass-construction for compatibility with UHV environments and experiments requiring large magnetic fields for tuning atomic interactions. The high finesse and excellent passive mechanical stability of the cavity facilitate the creation of smooth, stable trapping potentials, with depths of up to 1 mK. The atoms can also be placed in a crossed-beam dipole trap, a 1D optical lattice, or a 2D optical lattice by varying the configuration of the cavity pump fields. After reporting on the performance of this first cavity, we will describe plans to use cavities of this type to study coupled atom-cavity systems in previously unexplored configurations

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K25 DAMOP DCMP: Disorder and Localization in AMO Systems II: Many-body Localization  
BCEC 160A - Michael Kolodrubetz, University of Texas at Dallas - Tag(s): Focus
MICHAEL SCHECTER (Presenter), THOMAS IADECOLA, SANKAR DAS SARMA, University of Maryland, College Park — We uncover a new non-ergodic phase, distinct from the full MBL phase, in a disordered two-leg ladder of interacting hardcore bosons. The dynamics of this emergent phase is determined by the many-body configuration of the initial state and features the coexistence of localized and extended many-body states at fixed energy density. We show that eigenstates in this phase can be described in terms of interacting emergent Ising spin degrees of freedom suspended in a mixture with inert charge-like degrees of freedom (doublons), and thus dub it a mobility emulsion (ME). We argue that grouping eigenstates by their doublon density reveals a transition between localized and extended states that is invisible as a function of energy density. We further demonstrate that the dynamics of the system following a quench may exhibit either thermalizing or localized behavior depending on the doublon density of the initial product state. These results establish a new paradigm for using many-body configurations as a tool to study and control nonergodic dynamics which can be realized in existing disordered Bose-Hubbard ladders.


*This talk is supported by the Laboratory for Physical Sciences and Microsoft.

ULRICH SCHNEIDER (Presenter), Cavendish Laboratory, University of Cambridge — Quasiperiodic potentials, in particular Aubry-Andre-type models, have routinely been employed by us and others as substitutes for real random disorder in the study of many-body localization with ultracold atoms. Far away from the transition, the resulting localized phases are indeed expected to be essentially identical. However, quasiperiodic potentials are not random but long-range ordered. Hence their physics must ultimately be very different. For instance, they do not contain any rare region and, as a result, the nature of the localization transition could be entirely different.

I will briefly review our experimental realization of many-body localization of interacting fermions in the presence of quasiperiodic disorder in 1D and 2D, with a particular focus on slow relaxation close to the localization transition. Furthermore, I will discuss a recent extension to 2D quasicrystals with high rotational symmetries. Matter-wave diffraction experiments in our eightfold symmetric optical quasicrystal directly reveal the presence of a fractal structure in momentum space. I will close with first measurements of the localization transition in these potentials.

*European Commission (UQUAM, AQuS,QUASICRYSTAL)
EPSRC Programme Grant
DesOEQ (EP/P009565/1)
Nanosystems Initiative Munich (NIM)

DI LUO, XIONGJIE YU, BRYAN CLARK (Presenter), Physics, University of Illinois at Urbana Champaign — A prime characterization of many-body localized (MBL) systems is the entanglement of their eigenstates; in contrast to the typical ergodic phase whose eigenstates are volume law, MBL eigenstates obey an area law. In this work, we show that a spin-disordered Hubbard model has both a large number of area-law eigenstates as well as a large number of eigenstates whose entanglement scales logarithmically with system size (log-law). This model, then, is a microscopic Hamiltonian which is neither ergodic nor many-body localized. We establish these results through a combination of analytic arguments based on the eta-pairing operators combined with a numerical analysis of eigenstates. In addition, we describe and simulate a dynamic time evolution approach starting from product states through which one can separately probe the area law and log-law eigenstates in this system.

*Blue Waters is a joint effort of the University of Illinois at Urbana Champaign and its National Center for Supercomputing Applications. This material is based upon work supported by the U.S. Department of Energy, Office of Science under Award Number FG02-12ER46875.
9:00AM K25.00004: Probing Entanglement in a Many-Body-Localized System*  ROBERT SCHITTKO (Presenter), ALEXANDER LUKIN, MATTHEW RISPOLI, MING E TAI, Harvard University, ADAM KAUFMAN, JILA, University of Colorado and National Institute of Standards and Technology, SOONWON CHOI, VEDIKA KHEMANI, JULIAN LEONARD, MARKUS GREINER, Harvard University — An interacting quantum system that is subject to disorder may cease to thermalize due to localization of its constituents, thereby marking the breakdown of thermodynamics. The key to our understanding of this phenomenon lies in the system's entanglement, which is experimentally challenging to measure. We realize such a many-body-localized system in a disordered Bose-Hubbard chain and characterize its entanglement properties through particle fluctuations and correlations. We observe that the particles become localized, suppressing transport and preventing the thermalization of subsystems. Notably, we measure the development of non-local correlations, whose evolution is consistent with a logarithmic growth of entanglement entropy - the hallmark of many-body localization. Our work experimentally establishes many-body-localization as a qualitatively distinct phenomenon from localization in non-interacting, disordered systems.

*We are supported by grants from the National Science Foundation, the Gordon and Betty Moore Foundation's EPiQS Initiative, an Air Force Office of Scientific Research MURI program, an Army Research Office MURI program and the NSF Graduate Research Fellowship Program.

9:12AM K25.00005: Many-body localization as a large family of localized ground states  MAXIME DUPONT (Presenter), University of California, Berkeley, NICOLAS MACÉ, NICOLAS LAFLORENCIE, CNRS and University of Toulouse — It is well-known that Many-Body Localized (MBL) eigenstates are only area-law entangled, even at high energy, although it is the usual hallmark of ground states of short-range Hamiltonians. It is therefore legitimate to ask whether zero-temperature physics may have some connections with MBL states. Building on this simple idea, we ask whether an arbitrary MBL state could also be the ground state of another Hamiltonian? This question falls in the more general following problem: given a single eigenstate, does it uniquely encode the underlying Hamiltonian? Using large scale DMRG simulations [1], we show that in the presence of disorder, a localized ground state is a very good approximation for an MBL excited state of a different Hamiltonian that differs only by its local disorder configuration. Following similar ideas, we also investigate [2] the ergodic - MBL transition at high energy using standard shift-invert exact diagonalization techniques.


9:24AM K25.00006: Kosterlitz-Thouless scaling at many-body delocalization phase transitions  PHILIPP DUMITRESCU (Presenter), Center for Computational Quantum Physics, Flatiron Institute, SIDDHARTH A PARMESWARAN, Rudolf Peierls Centre for Theoretical Physics, University of Oxford, ANNA GOREMYKINA, Department of Theoretical Physics, University of Geneva, MAKSYM SERBYN, IST Austria, ROMAIN VASSEUR, Department of Physics, University of Massachusetts, Amherst — We propose a scaling theory for the many-body localization (MBL) phase transition in one dimension, building on the idea that the transition proceeds via a `quantum avalanche'. The critical properties are captured at a coarse-grained level by a Kosterlitz-Thouless renormalization group flow. Based on this scaling picture, there are different scenarios for the behavior of fractal rare thermal inclusions within the MBL phase. We propose that the near-critical MBL phase could host rare thermal regions that are power-law distributed in size. This points to the existence of a second transition within the MBL phase, at which these power-laws change to a stretched exponential form. Large scale numerical simulations of a phenomenological models capturing the critical properties near the MBL transition support this picture.

9:36AM K25.00007: Quantum coherence, phases of matter and many-body localization*  LORENZO CAMPOS VENUTI, PAOLO ZANARDI (Presenter), University of Southern California — Quantum coherence is one of the most fundamental traits of quantum mechanics. The coherence generating power (CGP) is the ability of a quantum unitary map of generating coherence. It is defined as the average coherence produced by the map applied to the set of incoherent states. In this talk I will report upon an unexpected link between these information theoretic concepts, and well known condensed matter quantities. Given two point in the phase diagram of a system one can ask about the CGP of the adiabatic intertwiner connecting the two points. The CGP turns out to be the inverse participation ratio, a quantity used to detect many-body localization (MBL) while for close-by points the CGP is exactly given by the d.c. dielectric polarizability. Using known results we are able to show that, in the thermodynamic limit, the CGP becomes maximal in the ergodic phase and submaximal in the MBL phase while the differential coherence diverges in the ergodic and subdiffusive phase while it tends to a constant in the MBL phase.

*The research is partially supported by the Air Force Research Laboratory award no. FA8750-18-1-0041 and ODNI, Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.
9:48AM K25.00008: Global and short-range entanglement properties in excited, many-body localized spin chains*
COLIN WEST (Presenter), Physics, University of Colorado at Boulder, TZU-CHIEH WEI, C.N. Yang Institute for Theoretical Physics, Stony Brook University — We explore the use of short-range entanglement measures, such as concurrence and negativity, and global entanglement measures such as geometric entanglement, as indicators of many-body localization (MBL) in the spectra of disordered spin systems. From the perspective of entanglement monogamy, the two types of entanglement behave oppositely in the thermalized and MBL phases. In a recent work, the concurrence of subsystems, a measure of local entanglement, was used in a study of many-body localization in a one-dimensional spin-1/2 system (Bera and Lakshminarayan, 2016). We show numerically that the negativity displays notably similar behavior for this system, with the advantage that it can also be extended to systems of higher local dimension. We then demonstrate this extension in practice by using it to predict the existence of an MBL phase in a disordered spin-1 system. In terms of global entanglement, the geometric entanglement of both spin-1/2 and spin-1 systems is also shown to behave as a complementary indicator of the MBL phenomenon.

* C.G.W and T.-C.W. are grateful for support from the National Science Foundation via Grants No. PHY 1333903 and No. PHY 1314748. T.-C.W. also acknowledges support from NSF grant No. PHY 1620252.

10:00AM K25.00009: Multiscale entanglement clusters at the many-body localization phase transition*
LOIC HERVIOU (Presenter), Department of Physics, KTH Royal Institute of Technology, SOUMYA BERA, Department of Physics, Indian institute of Technology Bombay, JENS BARDARSON, Department of Physics, KTH Royal Institute of Technology — We study numerically the formation of entanglement clusters across the many-body localization phase transition. We observe a crossover from strong many-body entanglement in the ergodic phase to weak local correlations in the localized phase, with contiguous clusters throughout the phase diagram. Critical states close to the transition have a structure compatible with fractal or multiscale-entangled Griffith states, characterized by entanglement at multiple levels: small strongly entangled clusters are weakly entangled together to form larger clusters. The critical point therefore features subthermal entanglement and a power-law distributed cluster size, while the localized phase present an exponentially decreasing distribution. These results are consistent with some of the recently proposed phenomenological renormalization-group schemes characterizing the many-body localized critical point, and may serve to constrain other such schemes.

*This work was supported by the ERC Starting Grant No. 679722 and the Knut and Alice Wallenberg Foundation 2013-0093. This research was supported in part by the National Science Foundation under Grant No. NSF PHY-1748958.

10:12AM K25.00010: Universality class of many-body localization transition on 1D system with both random and quasiperiodic potentials
SHIXIN ZHANG (Presenter), HONG YAO, Tsinghua University — Whether MBL transitions in quasiperiodic (QP) and random systems belong to the same universality class or two distinct ones has not been decisively resolved so far. Here we investigate MBL transitions in one-dimensional (d=1) QP systems as well as in random systems by state-of-the-art real-space renormalization group (RG) calculation. Our real-space RG shows that MBL transitions in 1D QP systems are characterized by the critical exponent \( \nu \approx 2.4 \), which respects the Harris-Luck bound (\( \nu > 1/d \)) for QP systems. Note that \( \nu \approx 2.4 \) for QP systems also satisfies the Harris-CCFS bound (\( \nu > 2/d \)) for random systems, which implies that MBL transitions in 1D QP systems are stable against weak quenched disorder since randomness is Harris irrelevant at the transition. By investigating the system with both QP and random potentials via real-space RG, we directly show that the QP-induced MBL criticality is robust against small randomness. Consequently, our real-space RG results imply that there are indeed two stable universality classes of MBL criticalities. We further discuss the possible scenario of the global phase diagram with both types of MBL transitions.

10:24AM K25.00011: Constructing local integrals of motion in the many-body localized phase*  
VIPIN KERALA VARMA (Presenter), VADIM OGANESYAN, College of Staten Island, DAVID PEKKER, University of Pittsburgh, ABHISHEK RAJ, SARANG GOPALAKRISHNAN, College of Staten Island — We consider a many-body localized spin system and its description by the so-called l-bit Hamiltonian. We outline a renormalization flow procedure to construct the extensive set of conserved quantities, and demonstrate that their locality results in exponentially decaying interactions in this effective model. The associated localization length of this decay is shown to manifest properties very similar to the noninteracting case of Anderson localization: normality of its distribution across samples, and its direct qualitative correspondence to the local spectral properties. A numerical simulation of a magnetic spin-echo protocol quantitatively reproduces these theoretically computed length scales. We therefore argue that these local integrals of motion help to practically identify the many-body localized phase.

*NSF DMR Grant No. 1508538 and US-Israel BSF Grant No. 2014265.

10:36AM K25.00012: Apparent slow dynamics in the ergodic phase of a driven many-body localized system without extensive conserved quantities  
TALÍA LEZAMA MERGOLD LOVE (Presenter), Condensed Matter, Max-Planck-Institut für Physik komplexer Systeme, SOUMYA BERA, Department of Physics, Indian Institute of Technology Bombay, JENS BARDARSON, Physics, KTH Royal Institute of Technology — We numerically study the dynamics on the ergodic side of the many-body localization transition in a Floquet model with no global conservation laws. We describe and employ a numerical technique based on the fast Walsh-Hadamard transform that allows us to perform an exact time evolution for large systems and long times. As in models with conserved quantities we observe a slowing down of the dynamics as the transition into the many-body localized phase is approached. More specifically, our data is consistent with a subballistic spread of entanglement and a stretched-exponential decay of the return probability, with the appropriately defined exponents, for a fixed system size, seeming to smoothly go to zero at the transition. However, with access to larger system sizes, we observe a clear flow of the exponents towards faster dynamics and can not rule out that the slow dynamics is a finite-size effect. Furthermore, we observe examples of non-monotonic dependence of the exponents with time, with dynamics initially slowing down but accelerating again at even larger times, reminiscent of what is observed in large scale simulations of random regular graphs and consistent with the slow dynamics being a crossover phenomena with a localized critical point.

10:48AM K25.00013: Phase diagram and observables of many-body localization in transmon circuit arrays  
TUURE ORELL (Presenter), University of Oulu, ALEXIOS MICHAILDIS, MAKSYM SERBYN, IST Austria, MATTI SILVERI, University of Oulu — Disordered interacting quantum systems can undergo a phase transition from ergodic to many-body localized phase. Most of the previous theoretical studies on this subject concentrate on spin systems, and this phenomenon has been observed e.g. in optical lattices with ultra-cold atoms. In this work, we investigate the potential use of superconducting transmon circuits as a platform for experimental studies of the many-body localization [1]. We study numerically one-dimensional disordered arrays of up to 14 transmons, and find that the phase transition occurs at experimentally realizable values of disordered on-site potentials and is robust against experimentally relevant perturbations such as weak next-nearest neighbor and higher-order Kerr interactions. Based on the simulations of the system dynamics, we find that the temporal fluctuations of transmon occupations could be used as an observable for probing the many-body localization in transmon circuits.


Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K26 DQI: Superconducting Qubits: Noise and Decoherence I  
BCEC 160B - David Pappas, National Institute of Standards and Technology Boulder
8:00AM K26.00001: Measuring charge and flux noise correlations with a superconducting qubit  
BRADLEY CHRISTENSEN (Presenter), CHRIS D WILEN, ALEXANDER OPREMCAN, University of Wisconsin - Madison, JJ NELSON, Syracuse University, FRANCISCO SCHLENKER, LARA FAORO, LEV B IOFFE, University of Wisconsin - Madison, BRITTON L PLOURDE, Syracuse University, JONATHAN L DUBOIS, Lawrence Livermore National Laboratory, ROBERT F MCDERMOTT, University of Wisconsin - Madison — Superconducting qubits are a promising approach towards scalable quantum computing. Coherence times in state-of-the-art devices are now in excess of 100 us. While these times are impressive, achieving the necessary fidelities for suitably scalable surface code algorithms requires better coherence times, and as such, a better understanding of the microscopic origin of the fluctuators that gives rise to different noise sources (e.g., flux noise, charge noise, and dielectric noise).

Recent evidence suggests that significant contribution to charge and flux noise arise from surface defects. Thus, a natural question to further understand the specific mechanism of the noise is if charge and flux noise originate from the same set of surface defects. To this end, we have designed and fabricated a charge-sensitive transmon device. Here we discuss the results of Ramsey-based power spectral density measurements on charge-parity noise (due to quasiparticle tunneling), charge noise, as well as a Ramsey-based cross power spectral density measurement between charge and flux noise. These results indicate valid microscopic models of the fluctuators that give rise to charge and flux noise.

8:12AM K26.00002: Piezoelectric loss in superconducting quantum circuits: Part 1*  
TAEKWAN YOON (Presenter), YIWEN CHU, PRASHANTA KHAREL, VIJAY JAIN, Yale Univ, WILLIAM RENNINGER, University of Rochester, LUIGI FRUNZIO, PETER RAKICH, ROBERT J SCHOELKOPF, Yale Univ — In recent studies, it has been shown that strong coupling between a superconducting qubit and phonons can be achieved. [1,2] These results imply that any unintended electromechanical coupling in the system could lead to loss in superconducting circuit systems. In my talk, I will present a highly sensitive technique for measuring electromechanical coupling in a material at cryogenic temperatures and in the GHz regime. The measurement is based on RF driving of phonons through electromechanical coupling and optical readout through Brillouin scattering. I will present measurements done on an inversion symmetric material, the progress on relevant materials for superconducting circuits, and discuss its implications for qubit coherence times.


*US Army Research Office grant W911NF-18-1-0212, DOE Office of Science grant DE-SC0019406, Max Planck Research Award from the Alexander von Humboldt Foundation, ONR YIP (N00014-17-1-2514), NSF MRSEC (DMR-1119826), AFOSR (FA9550-09-1-0484 and FA9550-15-1-0270), and the Packard Fellowship for Science and Engineering.

8:24AM K26.00003: Piezoelectric loss in superconducting quantum circuits: Part II*  
VIJAY JAIN (Presenter), YIWEN CHU, TAEKWAN YOON, LUIGI FRUNZIO, ROBERT J SCHOELKOPF, Applied Physics, Yale University — Recent demonstrations of strong coupling between a superconducting qubit and an acoustic wave resonator [1,2] implies the adoption of sound as a versatile quantum resource. The qubits used in these experiments exhibited reduced coherence times as compared with the state of the art in circuit-QED. While many factors contribute to determining a qubit’s coherence, unintentional electromechanical coupling between the circuit and piezoelectric material may be appreciable. In this talk, we will present a technique for measuring the microwave loss due to the presence of known piezoelectric materials. Since electromechanical coupling has an expected frequency dependence, we use the overtones of a stripline resonator to measure the intrinsic loss resulting from piezoelectric materials placed in the field of the resonator. The frequency dependence of this effect may enable us to distinguish it from microwave dielectric loss.


*We acknowledge support from US Army Research Office Grant Nr. W911NF-18-1-0212 and the Max Planck Research Award from the Alexander von Humboldt Foundation.
Observation of Low Thermal Excited State Population of Transmon Qubit

YIZHOU HUANG (Presenter), JEN-HAO YEH, RUI ZHANG, SHAVINDRA P PREMARATNE, FREDERICK C WELLSTOOD, Department of Physics, University of Maryland, College Park, BENJAMIN PALMER, Laboratory for Physical Sciences — We have measured the thermal excited-state population of a 3D Transmon qubit from 12 mK up to 150 mK. The Al/AlOx/Al qubit had a g-to-e transition frequency of 3.6 GHz, an e-to-f transition frequency of 3.4 GHz, and T1 of 17 microseconds. The device was mounted in a rectangular Al cavity with a transition frequency of 7.9 GHz and the cavity input line had custom-made attenuators ensuring that noise on the input line was well-filtered and thermalized[1]. The residual excited state population of the qubit was measured by measuring the response of the system when driving Rabi oscillations between the e and f states, with no initial preparation pulse applied to the qubit[2] for one of the pulse sequences. With the refrigerator at 12 mK, we found that the residual excited state population of the qubit in the e state was 0.17% with uncertainty of 0.02%, corresponding to a remarkably small effective qubit temperature of just 28 mK. For refrigerator temperatures T above 40 mK, the effective temperature Tn of the qubit was very close to T.


An analysis method for two superconducting resonators with common defects

NEDA FOROUZANI (Presenter), University of Maryland, Laboratory for Physical Sciences, BAHMAN SARABI, Laboratory for Physical Sciences, OMID NOROOZIAN, EDWARD WOLLACK, SAMUEL H MOSELEY, NASA Goddard Space Flight Center, KEVIN DANIEL OSBORN, Laboratory for Physical Sciences —

We report on a novel device consisting of a pair of superconducting circuit resonators with nearly degenerate resonances. The resonators share the same capacitor C which is engineered as an electrical capacitor bridge such that the capacitances for the resonators share the same defects. One of the resonators is made tunable using the nonlinearity of titanium nitride's kinetic inductance and is current biased, such that the detuning from degeneracy can be controlled. The design allows us to study virtually the same ensemble of atomic-sized two-level tunneling systems (TLSs) coupled to both resonators when degenerate. Slightly off resonance they should be affected by correlated noise but also allow measurement through separate readout lines. In this talk we analyze the device with a new 4 port, 2 resonator scattering theory. This will allow the extraction of two related TLS losses, many resonator couplings related by device symmetry, and an analysis of the noise.

Investigating superconducting qubit loss channels in a quantum acoustical device

BRADLEY MOORES (Presenter), LUCAS SLETTEN, K. W. LEHNERT, JILA, University of Colorado Boulder — The loss channels that limit superconducting qubit coherence times are presently not well understood. Mounting evidence shows that qubits couple to dissipative two-level system baths in dielectrics. In contrast, a less explored loss channel is from phonon radiation that is intrinsic to the Josephson junction superconductor-insulator boundary. Most dielectrics have a vanishing piezoelectric effect in the bulk from inversion symmetry, but this is not the case at surfaces. Theory predicts that the loss rate from this piezoelectric effect can be comparable to the lifetimes of state-of-the-art transmon qubits. Here we investigate phonon radiation from Josephson junctions to put an upper bound on its limitations on the transmon's coherence time.

Charge-parity dynamics in offset-charge-sensitive transmons: Part 1

SPENCER DIAMOND (Presenter), KYLE SERNIAK, MAX HAYS, VALLA FATEMI, GIJS DE LANGE, SHYAM SHANKAR, LUIGI FRUNZIO, ROBERT J SCHOELKOPF, LEONID GLAZMAN, Yale Univ, MANUEL HOUZET, CEA Grenoble, MICHEL H. DEVORET, Yale Univ —

Understanding and mitigating the effects of nonequilibrium quasiparticle excitations is an important step towards improving the performance of superconducting qubits. By designing transmon qubits in the offset-charge-sensitive regime, one can achieve direct dispersive detection of quasiparticle tunneling events. We utilize these devices to measure quasiparticle tunneling rates as a function of various experimental parameters such as RF filtering and qubit design. This talk will focus on experimental methods.

*Work supported by: ARO, ONR, NSF, AFOSR, and YINQE
9:24AM K26.00008: Charge-parity dynamics in offset-charge-sensitive transmons: Part 2*  
KYLE SERNIAK (Presenter), SPENCER DIAMOND, MAX HAYS, VALLA FATEMI, GIJS DE LANGE, SHYAM SHANKAR, LUIGI FRUNZIO, ROBERT J. SCHOLEKOPF, LEONID GLAZMAN, Yale Univ, MANUEL HOUZET, CEA Grenoble, MICHEL H. DEVORET, Yale Univ — Understanding and mitigating the effects of nonequilibrium quasiparticle excitations is an important step towards improving the performance of superconducting qubits. By designing transmon qubits in the offset-charge-sensitive regime, one can achieve direct dispersive detection of quasiparticle tunneling events. We utilize these devices to measure quasiparticle tunneling rates as a function of various experimental parameters such as RF filtering and qubit design. This talk will focus on experimental results.

*Work supported by: ARO, ONR, NSF, AFOSR, and YINQE

9:36AM K26.00009: Non-equilibrium quasiparticles in superconducting circuits: photons vs. phonons*  
GIANLUIGI CATELANI (Presenter), JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Germany, DENIS M. BASKO, Laboratoire de Physique et Modélisation des Milieux Condensés, CNRS Grenoble, France — We study the effect of non-equilibrium quasiparticles on the operation of a superconducting device (a qubit or a resonator), including heating of the quasiparticles by the device operation. Focusing on the competition between heating via low-frequency photon absorption and cooling via photon and phonon emission, we obtain a remarkably simple non-thermal stationary solution of the kinetic equation for the quasiparticle distribution function. We estimate the influence of quasiparticles on relaxation and excitation rates for transmon qubits, and relate our findings to recent experiments.

*This work was supported in part by the Internationalization Fund - Seed Money initiative of Forschungszentrum Jüllich.

9:48AM K26.00010: Superconducting quasiparticle traps for CPW resonators  
ASHISH ALEXANDER (Presenter), CHRISTOPHER WEDDLE, CHRISTOPHER RICHARDSON, Laboratory of Physical Sciences, University of Maryland, College Park, MD — Excess quasiparticles limit the quality factor of the superconducting resonators by presenting an ohmic path for energy dissipation. It has been shown that normal metal in contact with the superconductor can act as a quasiparticle trap by confining quasiparticles away from the superconductor. Similarly, a small band gap superconductor in contact with a larger band gap superconductor can also act as a quasiparticle trap by confining quasiparticles away from the larger bandgap superconductor into the smaller one. Here aluminum (Al) and titanium nitride (TiN) are used as two superconductors. Finite difference method (FDM) simulations of the coupled phonon and quasiparticle systems of both superconductors suggest that the quasiparticle traps on the ground plane may be effective for setback distances less than 200 µm away from TiN waveguide features. Experimentally, a thin layer of Al is grown in-situ on TiN using molecular beam epitaxy (MBE) with a negligible dielectric layer between the two superconductors to increase the trapping efficiency of the Al. Currently work focuses on fabricating quarter wavelength resonators in TiN with different setbacks of the Al trap. The optimum setback of Al from the active region of the TiN resonator will be explored.

10:00AM K26.00011: Resolving the Location of Parasitic Defects in Superconducting Qubits*  
ALEXANDER BILMES (Presenter), GEORG WEISS, Physikalisches Institut, Karlsruhe Institute of Technology, RAMI BAREND'S, JULIAN KELLY, ANTHONY E MEGRANT, JOHN M MARTINIS, Google - Santa Barbara, ALEXEY V. USTINOV, JÜRGEN LISEN Feld, Physikalisches Institut, Karlsruhe Institute of Technology — New techniques to identify the location of decoherence-inducing material defects known as Two-Level-Tunneling systems (TLS) in superconducting qubits are demonstrated. We expose a transmon qubit circuit to a DC-electric field generated by electrodes surrounding the sample chip, and study the TLS response by monitoring their resonance frequencies using qubit swap spectroscopy. We find that about 50% of all detectable TLS do not couple to the applied E-field, as it is expected from TLS hosted in the Josephson junction tunnel barrier, but unlikely for TLS residing in surface oxides or at substrate interfaces. In contrast, all TLS respond to the mechanical strain generated by a piezo actuator. This indicates that surface TLS contribute about equally to qubit decoherence as those in qubit junctions. Moreover, by comparing measured and simulated coupling strengths to each DC-electrode, we obtain information about the possible locations and hosting interfaces of the observed surface TLS. This analysis directly indicates which circuit interfaces must be improved in order to enhance qubit coherence.

*Deutsche Forschungsgemeinschaft (DFG) Grant LI2446/1 (recipient J. Lisenfeld), Google Faculty Research Award 2018 (recipient A. V. Ustinov).
Reducing dissipation for superconducting qubits

NASSER ALIDOUST (Presenter), ANI NERSISYAN, STEFANO POLETTI, RICCARDO MANENTI, RUSS RENZAS, EYOBB SETE, CATVU BUI, KIM VU, TYLER WHYLAND, YUVRAJ MOHAN, SAM STANWYCK, JAYSS MARSHALL, KAMAL YADAV, ANDREW BESTWICK, MATTHEW J REAGOR, Rigetti Computing — Extending qubit lifetimes ($T_1, T_2$) remains a core challenge in developing large-scale quantum computers with superconductors. In this talk, we discuss a variety of substrate cleaning and subtractive patterning techniques responsible for increasing $T_1$ for superconducting qubits. For these analyses, we have developed fabrication flows based on subtractively-patterned niobium that yield resonators with average internal quality factors of $Q_{int} \approx 1 \times 10^6$ across several wafers and chips. We show options for integrating Josephson junctions into these process flows to make functional qubits with high coherence times.

*Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Spurious mode suppression using micromachined pillars in superconducting quantum devices

PETER A SPRING (Presenter), JOSEPH RAHAMIM, BRIAN VLASTAKIS, ANDREW D PATTERTON, TAKAHIRO TSUNODA, SOPHIA SOSNINA, MARTINA ESPOSITO, SALHA JEBARI, KITTI RATTER, GIOVANNA TANCREDI, PETER LEEK, Condensed Matter Physics, University of Oxford — As quantum circuits scale in size, the enclosures used to house them will contain spurious resonant electromagnetic modes detrimental to the circuits unless preventative steps are taken. A standard solution in microwave circuits is the use of through-chip vias. Here we present an alternative that moves the through-chip electrical connection off the substrate and to the enclosure, which suppresses substrate and enclosure modes simultaneously. We achieve this by placing a substrate in a rectangular cavity incorporating an array of micromachined pillars, such that the minimum mode frequency is set by the pillar spacing and not the enclosure dimensions. To accommodate the pillars the substrate is machined. We investigate the compatibility of both CNC and laser machining of holes in silicon with superconducting qubit fabrication. We present proof of principle experiments on enclosures incorporating pillars, and produce simulations with more complex arrangements of pillars in larger-scale devices.

*We acknowledge financial support from the EPSRC (grants EP/M013243/1, EP/N015118/1, EP/R044538/1), Oxford Instruments Nanoscience, Oxford Quantum Circuits Ltd, the Oxford Centre for Applied Superconductivity, the Nakajima Foundation and the Masason Foundation.

Phononic Losses in Superconducting Coplanar Waveguide Resonators on Piezoelectric Substrates

MARCO SCIGLIUZZO (Presenter), LAURE BRUHAT, ANDREAS BENTGSSON, JONATHAN BURNETT, PER DELSING, Microtechnology and Nanoscience, MC2, Chalmers University of Technology — In recent years there has been an increasing number of experiments involving superconducting qubits on piezoelectric substrates to investigate quantum acoustics. In this context Coplanar Waveguide (CPW) resonators provide a well established way for qubit manipulation and readout. However CPW resonators on piezoelectric substrates perform poorly, with two orders of magnitude lower internal quality factor ($Q$) compared with similar devices on low loss dielectrics.

In this work we present an investigation of the phononic loss channel for CPW resonators fabricated on a piezoelectric substrate. With the help of finite element method (FEM) simulations, we calculate the energy loss due to electromechanical conversion, and derive an upper limit for the internal $Q$. We fabricate quarter wavelength CPW resonators on GaAs and measure their internal $Q$ as function of frequency, power and temperature. We obtain a linear increase of the internal $Q$ with respect to frequency as expected for a frequency independent electromechanical coupling. Moreover we find a weak power dependence and a negligible temperature dependence around 10mK, excluding two level systems and nonequilibrium quasiparticles as the main source of losses.

Tunable High-Q Photonic Bandgap Microwave Cavity

ANKUR AGRAWAL (Presenter), AKASH DIXIT, DAVID SCHUSTER, AARON CHOU, University of Chicago — A woodpile structure made out of dielectric rods exhibits an omnidirectional photonic bandgap (PBG) which forbids the propagation of electromagnetic wave with energy within a certain range in all directions. We designed an electromagnetic cavity by creating a defect inside the crystal, such that its frequency lies within the forbidden bandgap. Very high Q-factors can be achieved since the light has no way to escape because of the bandgap and is only limited by the dielectric loss in the material. We predict the quality factor of such a cavity to be close to $10^8$ near 10 GHz. The cavity frequency is tuned by sliding the rods in and out. One of the potential applications is in the axion dark matter search, which is currently limited by the use of low $Q$-factor copper cavities due to the presence of a strong magnetic field. We predict the $Q$-factor of a PBG cavity to increase in the presence of a large magnetic field due to the shift in the two-level system energies to a higher level.

*DOE Contract No. DE-AC02-07CH11359 and the Heising-Simons Foundation
Wednesday, March 6, 2019 8:00 AM - 10:24 AM

**Session K27 DQI: Quantum Machine Learning II** BCEC 160C - Maria Schuld, University of KwaZulu-Natal - Tag(s): Focus

**8:00AM K27.00001: The Impact of Quantum Noise in Neuromorphic Systems** GERASIMOS ANGELATOS (Presenter), HAKAN TURECI, Electrical Engineering, Princeton University — The quantum dynamics of driven-dissipative systems with a stable classical fixed-point are well understood, however dynamics far from equilibrium and in regimes without a fixed-point are less studied. Considerable theoretical challenges arise because such situations often involve strong transient excitation while the role of quantum fluctuations remains significant. This scenario is realized in neuromorphic optical systems which respond to a weak input above threshold with a robust large amplitude pulse. The quantum dynamics of neuromorphic systems can thus not be described by the standard small fluctuation expansion around a classical steady-state, and a full quantum modeling is out of question due to large transients. We present a general theoretical approach based on quantum stochastic differential equations which captures quantum noise about classical trajectories and apply it to two physical realizations of neuromorphic dynamics: an excitable laser and a superconducting circuit. Contrary to previous findings, fundamental quantum noise drives large fluctuations in pulse response times, while the amplitude response remains robust. In addition, quantum noise softens the bifurcation to a self-sustained pulsation regime by exciting the system in the absence of an input.

**8:12AM K27.00002: Performance of the Quantum Approximate Optimization Algorithm on the Maximum Cut Problem** GAVIN CROOKS (Presenter), NICHOLAS C RUBIN, Rigetti Quantum Computing — The Quantum Approximate Optimization Algorithm (QAOA) is a promising approach for programming a near-term gate-based hybrid quantum computer to find good approximate solutions of hard combinatorial problems. However, little is currently known about the capabilities of QAOA, or of the difficulty of the requisite parameters optimization. We explore these issues with the aid of QuantumFlow, a simulation of a gate based quantum computer that uses TensorFlow to rapidly optimize variational quantum circuits. Our investigations support the prospects that QAOA will be an effective method for solving interesting problems on near-term quantum computers.

**8:24AM K27.00003: Machine Learning Detection of Bell Nonlocality in Quantum Many-Body Systems** DONG-LING DENG (Presenter), Institute for Interdisciplinary Information Sciences, Tsinghua University — Machine learning, the core of artificial intelligence, is one of today's most rapidly growing interdisciplinary fields. Recently, its tools and techniques have been adopted to tackle intricate quantum many-body problems. In this talk, I will introduce machine learning techniques to the detection of quantum nonlocality in many-body systems, with a focus on the restricted-Boltzmann-machine (RBM) architecture. Using reinforcement learning, I will demonstrate that RBM is capable of finding the maximum quantum violations of multipartite Bell inequalities with given measurement settings. This result builds a novel bridge between computer-science-based machine learning and quantum many-body nonlocality, which will benefit future studies in both areas.


*This work is supported by Laboratory for Physical Sciences, Microsoft, and the start-up fund from Tsinghua University.

**8:36AM K27.00004: Benchmarking superconducting qubits with generative model learning** KATHLEEN HAMILTON (Presenter), EUGEN DUMITRESCU, Oak Ridge National Laboratory, HOLLY STEMP, University of Surrey, RAPHAEL POOSER, Oak Ridge National Laboratory — Our work is focused on the identification and development of simple machine learning tasks that can act as hardware benchmarks to compare the relative performance of NISQ devices. Using MMD training and stochastic optimization of circuit parameters, we show how a recently introduced class of generative models (the Quantum Circuit Born Machine [1]) can quantify the performance of noisy superconducting qubits. We identify three sources of error that limit the performance of these models on noisy qubits: decoherence, gate fidelities and measurement errors. We construct several shallow depth circuit ansatz and using metrics which are related to fidelity we demonstrate how different errors affect model performance. We also investigate the effect of applying error mitigation to the final trained circuit versus incorporating error mitigation into the circuit training workflow.


*This work was supported as part of the ASCR Testbed Pathfinder Program at Oak Ridge National Laboratory under FWP #ERKJ332
8:48AM K27.00005: Local-measurement-based quantum state tomography via neural networks  BEI ZENG (Presenter), University of Guelph — Quantum state tomography is a daunting challenge of experimental quantum computing even in moderate system size. One way to boost the efficiency of state tomography is via local measurements on reduced density matrices, but the reconstruction of the full state thereafter is hard. Here, we present a machine learning method to recover the full quantum state from its local information, where a fully-connected neural network is built to fulfill the task with up to seven qubits. In particular, we test the neural network model with a practical dataset, that in a 4-qubit nuclear magnetic resonance system our method yields global states via 2-local information with high accuracy. Our work paves the way towards scalable state tomography in large quantum systems.

9:00AM K27.00006: Variational Quantum Neural Programming  PIERRE-LUC DALLAIRE-DEMERS (Presenter), Zapata Computing — Variational algorithms used for quantum simulations are naturally resistant to some errors and are therefore well suited for NISQ devices. Their application in quantum machine learning has yielded methods for data classification, compression and generation such as the quantum autoencoder. Using inspiration from neural programming in classical machine learning, we show how a quantum program can be learned through gradient descent. Quantum programs are usually defined operationally over a variable number of qubits while variational quantum algorithms are typically meant to operate on fixed-size quantum registers. We define a class of differentiable ansatz that can operate on an arbitrary number of qubits and be used to reproduce algorithms such as the quantum Fourier transform and phase estimation using only a set of examples on few qubits. We generalize this class of ansatz to explore the space of shallow algorithms.

9:12AM K27.00007: Quantum machine learning: Challenges and Opportunities*  [Invited]  LEONARD WOSSNIG (Presenter), SIMONE SEVERINI, Computer Science, University College London — In this talk I will pose the general framework of learning and then introduce the different topics which jointly define the area of quantum machine learning. Since machine learning is an intrinsically data driven approach, dependencies and assumptions play a major role. I will therefore introduce different input and output assumptions and discuss corresponding data access models before giving a high level explanation of the different techniques which have been proposed. I will finally discuss current and future challenges and opportunities of the field.

*I thankfully acknowledge the support through a Research Fellows Enhancement Award grant of the Royal Society.

9:48AM K27.00008: A Universal Training Algorithm for Quantum Deep Learning*  GUILLAUME VERDON (Presenter), JASON PYE, Institute for Quantum Computing, MICHAEL BROUGHTON, School of Computer Science, University of Waterloo — Quantum variational algorithms have seen a recent surge of interest, yet their connection to classical deep neural networks has so far remained elusive. In this talk, we will establish how to port over classical neural networks as quantum parametric circuits, and we will further introduce a quantum-native backpropagation principle which can be leveraged to train any quantum parametric network. We will present two main quantum optimizers leveraging this quantum backpropagation principle: Quantum Dynamical Descent (QDD), which uses quantum-coherent dynamics to optimize network parameters, and Momentum Measurement Gradient Descent (MoMGrad), which is a quantum-classical analogue of QDD. We will briefly cover multiple applications of QDD/MoMGrad to various problems of quantum information learning, and how to use these optimizers to train classical neural networks in a quantum fashion. Furthermore, we will show how to efficiently train hybrid networks comprised of classical neural networks and quantum parametric circuits, running on classical and quantum processing units, respectively.

Talk based on [arXiv:1806.09729].

*The authors acknowledge financial support from NSERC. This research was supported in part by Perimeter Institute for Theoretical Physics.
Development of quantum algorithms for data analysis and machine learning has gained much attention recently. For practical applications of such algorithms in the big data era, the quantum advantage must be retained in noisy settings. One intriguing example in which the quantum algorithm outperforms the classical counterpart in the presence of noise is the problem of learning a parity function defined by a hidden bit string, known as learning parity with noise (LPN). However, a learner is most likely to receive noisy classical data, rather than noisy quantum data as considered in the original quantum LPN algorithm. Then, whether the quantum technique is still preferred remains an interesting open problem. Here, we present a quantum-classical reinforcement learning algorithm to solve the LPN problem efficiently for classical data. The algorithm uses classical training data to prepare an input quantum state suitable for the original quantum LPN algorithm. Based on the outcome of the quantum algorithm, a reward and an action are classically determined to update the input quantum state for the next learning cycle. Our method uses an exponentially smaller number of training samples than the direct application of the original quantum LPN algorithm to classical data.

We describe a Markov chain monte carlo simulation of quantum circuits based on decomposing the circuit in question as a sum of Clifford gates. The idea is to leverage the classical simulability of Clifford dynamics to cases where the circuit is no longer simulable. The runtime scales quadratically with the 1-norm of the vector of expansion, and the runtime is comparable with state-of-the-art simulators for an important class of circuits; the so-called Clifford+T circuits. The simulation method can be extended to two other problems: estimating transition probabilities and estimating the partition function of an n-qubit Hamiltonian. We give theoretical error and runtime estimates, and introduce a few sub-algorithms which can improve the performance in some cases.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K28 DQI: Quantum Measurement and Sensing I

8:00AM K28.00001: Quantum metrology in the presence of dissipation with superconducting qubits.* [Invited] KATER MURCH (Presenter), Physics, Washington University in St. Louis — While quantum systems can offer significant advantages over classical systems in metrology, often the quantum states that confer such advantages are degraded by decoherence. I will discuss experiments that explore strategies to mitigate this degradation through continuous quantum measurement and feedback. Furthermore, dissipation also yields potential for further metrological advantages that are associated with exceptional point degeneracies in non-Hermitian systems. I will discuss how such degeneracies can be realized in single dissipative qubits and present investigations of enhanced measurement sensitivity in single quantum systems.

*This work was supported the ONR Grant No. 12114811 and the NSF Grant No. PHY-1607156

8:36AM K28.00002: Non-Hermitian quantum sensing: exceptional point and non-reciprocal approaches HOI-KWAN LAU (Presenter), AASHISH CLERK, University of Chicago — Unconventional properties of non-Hermitian systems, such as the existence of exceptional points, have recently been suggested as a resource for sensing [1,2]. The impact of noise and utility in quantum regimes however remains unclear. We describe here a full analysis of quantum parametric sensing using coupled mode systems described by effective non-Hermitian Hamiltonians; our approach rigorously accounts for quantum noise effects [3]. Focusing on two-mode devices, we derive fundamental bounds on the signal power and signal-to-noise ratio for any such sensor. We use these to demonstrate that enhanced signal power requires gain, but not necessarily any proximity to an exceptional point. Further, when noise is included, we show that non-reciprocity is a powerful resource for quantum sensing: it allows one to exceed the fundamental bounds constraining any conventional, reciprocal sensor. Non-reciprocal quantum sensors could be implemented in a variety of systems, including superconducting quantum circuits and quantum optomechanical systems.

8:48AM K28.00003: Saturating the quantum Cramér-Rao bound using LOCC*  SISI ZHOU (Presenter), Yale Quantum Institute, Yale University, CHANG-LING ZOU, Key Laboratory of Quantum Information, University of Science and Technology of China, LIANG JIANG, Yale Quantum Institute, Yale University — The quantum Cramér-Rao bound (QCRB) provides an ultimate precision limit allowed by quantum mechanics in parameter estimation. Given any quantum state dependent on a single parameter, there is always a positive-operator valued measurement (POVM) saturating the QCRB. However, the QCRB-saturating POVM cannot always be implemented efficiently, especially in multipartite systems. In this talk, we show that the POVM based on local operations and classical communication (LOCC) is QCRB-saturating for arbitrary pure states or rank-two mixed states with varying probability distributions over fixed eigenbasis. We also analyze the robustness of our LOCC protocol against noise and show how it can be made noise-resilient. Finally, a four-qubit system is studied as an example of a non-trivial LOCC protocol saturating the QCRB. For details, see ArXiv: 1809.06017.

*We acknowledge support from the ARL-CDQI (W911NF-15-2-0067), ARO (W911NF-14-1-0011, W911NF-14-1-0563), ARO MURI (W911NF-16-1-0349), AFOSR MURI (FA9550-14-1-0052, FA9550-15-1-0015), NSF (EFMA-1640959), Alfred P. Sloan Foundation (BR2013-049), and Packard Foundation (2013-39273).

9:00AM K28.00004: Ramsey interferometry in correlated quantum noise environments*  LEIGH NORRIS (Presenter), FELIX BEAUDOIN, LORENZA VIOLA, Dartmouth College — We quantify the impact of spatiotemporally correlated Gaussian quantum noise on frequency estimation by Ramsey interferometry. While correlations in a classical noise environment can be exploited to reduce uncertainty relative to the uncorrelated case, we show that quantum noise environments with frequency asymmetric spectra generally introduce additional sources of uncertainty due to uncontrolled entanglement of the sensing system mediated by the bath. For the representative case of collective noise from bosonic sources, and experimentally relevant collective spin observables, we find that the uncertainty can increase exponentially with the number of probes. As a concrete application, we show that correlated quantum noise due to a lattice vibrational mode can preclude superclassical precision scaling in current amplitude sensing experiments with trapped ions. This work was recently reported in PRA (Rapid Communications) 98, 020102 (2018).

*This work was supported by the US Army Research Office under Contract No. W911NF-12-R-0012 and by the Fonds de Recherche du Québec—Nature et Technologies.

9:12AM K28.00005: Hamiltonian engineering for quantum sensing  YI-XIANG LIU (Presenter), Massachusetts Institute of Technology, ASHOK AJOY, University of California Berkeley, JORDAN HINES, PAOLA CAPPELLARO, Massachusetts Institute of Technology — Quantum sensing utilizes the interaction between the quantum sensor and the object to be detected. However, limited by the intrinsic system Hamiltonian or experimental capabilities, the implementable Hamiltonian evolution may not be optimal to reveal the information of the target object. Inspired by digital quantum simulation, here we present a general framework in which we use Trotter-like combinations of unitaries to engineer better Hamiltonians for sensing and provide an efficient protocol to reduce the approximation error. We show the application of Hamiltonian engineering to nano-scale magnetic resonance imaging.

9:24AM K28.00006: Provably optimal controls for magnetometry in cluttered environments  VIRGINIA FREY (Presenter), Univ of Sydney, LEIGH NORRIS, LORENZA VIOLA, Dartmouth College, MICHAEL JORDAN BIERCUK, Univ of Sydney — The extreme fragility of quantum systems makes them ideally suited for sensing applications such as magnetometry, biological imaging and noise characterization for quantum computing. However, interpreting a qubit-based sensor’s output is generally complicated by background clutter arising from both out-of-band spectral leakage, and ambiguity in signal origin when the implemented qubit drive is imperfect. Here we present a novel sensing protocol based on the optimal band-limited Slepian functions that overcomes both of these challenges. We construct Slepian-based controls using a finite-difference method that preserves the relevant spectral concentration while removing nonlinearities in the sensor response which arise when targeting ambient noise signatures that couple to the sensor’s signal through an additive dephasing Hamiltonian term, such as magnetic field fluctuations. We experimentally implement a tomographic measurement framework which separates multi-axes contributions using projective measurements on a single trapped ion magnetometer. Experiments validate the spectral concentration of the new finite-difference controls and allow for simultaneous, narrowband spectrum reconstruction of both environmental dephasing and control noise fields.
ROBERT DELANEY (Presenter), ADAM PREED, JILA, REED ANDREWS, HRL Laboratories, LLC, KONRAD LEHNERT, JILA — Quantum mechanics places strict limits on how precisely the two motional quadratures of an object can be simultaneously measured. To noiselessly reconstruct an unknown quantum state of motion, a single quadrature measurement can be repeated over all of phase space, and the density matrix describing the quantum state can be reconstructed via quantum state tomography. Here we demonstrate a pulsed measurement of the motion of a micromechanical oscillator embedded in a superconducting electromechanical circuit. The measurement can be tuned from a nearly quantum-limited simultaneous measurement of both quadratures, to a single quadrature measurement with added noise of -10 dB relative to vacuum fluctuations in one quadrature, resulting in a total measurement efficiency of 92%. The high efficiency measurement is used to accurately reconstruct the density matrix of a dissipatively squeezed mechanical oscillator (-3.3 dB relative to vacuum fluctuations), demonstrating that the measurement is suitable for tomography of arbitrary quantum states of the mechanical oscillator.

DANY LACHANCE-QUIRION (Presenter), SAMUEL PIOTR WOLSKI, YUTAKA TABUCHI, SHINGO KONO, KOJI USAMI, YASUNOBU NAKAMURA, Research Center for Advanced Science and Technology, The University of Tokyo — Opportunities for quantum sensing of quanta of collective spin excitations in a ferromagnet, called magnons, are now possible thanks to the demonstrations of both strong resonant and dispersive couplings between a superconducting qubit and the uniform precession mode, or Kittel mode, of a ferromagnetic sphere [1,2]. Based on operations on the qubit conditional on the state of the Kittel mode, single-shot detection of a single magnon with an efficiency reaching about 50% is demonstrated using the protocol of Ref. [3]. The detection efficiency is mainly limited by the qubit readout fidelity. Furthermore, a magnon detection sensitivity of about $10^{-3}$ magnons/√Hz is demonstrated using a standard Ramsey interferometry technique. These two complementary quantum sensing methods could find applications in quantum technologies based on magnonics and the detection of axions in dark matter searches.


KATHERINE INZANI (Presenter), SINEAD GRIFFIN, Lawrence Berkeley National Laboratory — The direct detection of light dark matter (DM) relies on harnessing low-threshold events in target materials. One such event is the scattering of an electron across a small gap, where our target material’s threshold will determine the range of masses of DM particles we are sensitive to. In this work we investigate spin-orbit semiconductors as DM detection targets. We report the results of a high-throughput search for new small-gapped semiconductors, and estimate their reach as DM targets using first-principles methods. We also discuss how the calculated material properties influence the detector size and geometry.

AKASH DIXIT (Presenter), DAVID SCHUSTER, University of Chicago, AARON CHOU, Fermilab, ANKUR AGRAWAL, SRIVATSAN CHAKRAM, RAVI NAIK, University of Chicago — The axion is a potential solution to the strong CP problem in QCD and could account for the abundance of dark matter observed in the universe. In the presence of an applied magnetic field, the axion field will source a current used to drive a resonant cavity to single photon occupation. A transmon qubit operating as a microwave photon sensor is a viable readout system at frequencies where the added noise of quantum limited amplifiers overwhelsms the signal rate. The use of a direct dispersive quantum non-demolition measurement of the photon number decouples the measurement back action from the experimental uncertainties. In this regime background and dark counts become the dominant sources of detector error. For a transmon qubit operating as a photon counter, the dark rate is typically 1-10% and is orders of magnitude greater than the anticipated signal rate. In order to mitigate the effect of individual bit flip errors of the detector we operate multiple detectors in the same cavity volume. The error rate of the joint N-qubit detector could potentially have exponentially suppressed error rates as compared to the single detector. We will report theoretical performance and progress towards characterizing fidelity and correlations of multqubit detectors.
10:24AM K28.00011: Quantum noise limits for a class of nonlinear amplifiers* JEFFREY EPSTEIN (Presenter), Physics, University of California, Berkeley, JOSHUA COMBES, Rigetti Computing — We introduce a class of nonlinear amplifier input-output relations that allow the measurement of any normal operator using linear measurements with only vacuum fluctuations added at the output. In the limit of large gain, such devices would effectively implement perfect measurements of nonlinear operators in the same way that linear amplifiers permit effectively perfect linear measurements even when paired with realistic, noisy measurement devices. We analyze the application of these amplifiers to photon number measurements and state estimation.

*JE was supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program. JC was supported by the Australian Research Council through a Discovery Early Career Researcher Award (DE160100356) and via the Centre of Excellence in Engineered Quantum Systems (EQuS), project number CE170100009.

10:36AM K28.00012: One from many: Scalar estimation in a multiparameter context* JONATHAN GROSS (Presenter), Institut quantique, Université de Sherbrooke, CARLTON MORRIS CAVES, Center for Quantum Information and Control, University of New Mexico — Achievable sensitivity bounds are difficult to formulate for quantum multiparameter estimation. We consider a specialized case: many parameters of a Hamiltonian are unknown and one seeks an estimate for a scalar function of the Hamiltonian. This problem exhibits genuine multiparameter behavior, though it is superficially similar to single-parameter estimation. By uniting saturable single-parameter quantum bounds with geometric reasoning we prove the conditions, necessary and sufficient, for saturating the fundamental and attainable bound in this context.

*National Science Foundation Grant Nos. PHY-1521016 and PHY-1314763.

10:48AM K28.00013: Optimal measurements in simultaneous multi-parameter estimation of quantum systems* JING YANG (Presenter), Department of Physics and Astronomy, University of Rochester, SHENGSHI PANG, Fermi lab, YIYU ZHOU, Institute of Optics, University of Rochester, ANDREW N JORDAN, Department of Physics and Astronomy, University of Rochester — Simultaneous estimation of multiple parameters is a well-known challenge in quantum metrology. The underlying difficulty is to identify the common optimal measurements for all the parameters, which typically do not coincide or commute. For a general probe state and a projective measurement of arbitrary rank, we find the necessary and sufficient conditions under which the measurement gives rise to the multi-parameter quantum Cramer-Rao matrix bound. We also give an application of these conditions to the specific problem of estimating three-dimensional separation of two point incoherent sources of equal intensities from single photon measurements. By considering the hard-aperture and paraxial approximated pupil function, we find a local optimal measurement for simultaneous estimation of the small three dimensional separation. Furthermore, regardless of the magnitude of longitudinal separation, a local optimal measurement for simultaneously estimating the small transverse separation is also found. The saturation conditions of the multi-parameter quantum Cramer-Rao bound may be further explored in quantum sensing and imaging.

*This work was supported by U.S. Army Research Office, National Science Foundation, and U.S. Office of Naval Research.

Wednesday, March 6, 2019 8:00 AM - 9:30 AM

Session K29 APS: Tutorial for Authors & Referees BCEC 162A

8:00AM K29.00001: Tutorial for Authors & Referees — Publication is an essential part of scholarly research and integral to most scientists’ careers. A good understanding of the authoring and reviewing processes will help authors navigate their way to a published manuscript. In this tutorial, editors from Physical Review Letters and Physical Review will provide advice on topics such as how to write a good paper, how best to respond to reviews, and how to write informative referee reports.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K30 GSOFT DPOLY DBIO: Organization and Dynamics of Functional Liquid Crystals, Polymers, and Biological Assemblies II BCEC 162B - Roy Beck, Tel Aviv University - Tag(s): Focus
**8:00AM K30.00001: DYNAMIC SELF-ASSEMBLY OF VIRUS CAPSIDS** [Invited] URI RAVIV (Presenter), Hebrew University of Jerusalem — The assembly and disassembly of virus capsids, composed of many subunits, are fundamental steps in the viral life cycle. The complete set of possible capsid intermediates is immense, yet the concerted assembly process is done with high fidelity and leads to stable capsids that can efficiently encapsulate and protect genetic material, and when needed, dissociate and release their cargo. Virus capsids are therefore stable and flexible dynamic structures. To better understand and predict the outcomes of these apparently contradictory processes, we precisely analyzed the structure, kinetics, and thermodynamic stability of the experimentally tractable virus assembly reaction, in vitro. High-resolution modern synchrotron solution X-ray scattering measurements of assembly reactions provided statistically reliable and rich structural data. We rigorously analyzed the data by integrating our home-developed state-of-the-art scattering data analysis software D+ (https://scholars.huji.ac.il/uriraviv/software/d-software) with simulations and theory of macromolecular self-assembly. Our accurate and comprehensive analysis provided new insight into the mechanisms of viral self-assembly and the boundaries where thermodynamic products can be realized and function, and when kinetically trapped metastable states may form. This insight could be important for designing antiviral therapeutics as well as noncapsules or nanoreactors.

*(Israel Science Foundation (grant 656/17), NIH (award number 1R01AI118933)*

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**8:36AM K30.00002: Counterion-dependent Dynamics of Nanoconfined Water in Lyotropic Liquid Crystalline Mesophases** MAHESH MAHANTHAPPA (Presenter), University of Minnesota — Understanding how the interfacial chemical functionalities influence nanoconfined water dynamics could potentially inform the design of next-generation permselective and ion-transporting membranes for energy applications. However, lacking access to well-defined systems with tunable interfacial chemistries and nanoconfined geometries has hampered conclusive studies of water dynamics therein. Derived from the water concentration-dependent self-assembly of small molecule surfactants, lyotropic liquid crystals (LLCs) offer a platform for studying confined water dynamics in nanopores (diameters ~0.7-2.5 nm) lined with well-defined chemical functionalities. In this contribution, we describe the synthesis and aqueous phase behavior of ionic gemini dicarboxylate surfactants, which form technologically-useful, normal double gyroid phases in which water is nanoconfined between two carboxylate-lined, convex interfaces. Quasielastic neutron scattering (QENS) measurements indicate that the gyroid water dynamics are significantly slower than in bulk water, and that the observed dynamics are very sensitive to the nature of the charge-compensating counterion (Na+, K+, Me₄N+) associated with the carboxylate surfactant headgroup.

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**8:48AM K30.00003: Phase transformations in lipids confined to colloidally stable nanoscale particles** JACOB RUEBEN (Presenter), Materials Science and Engineering, University of Illinois at Urbana-Champaign, HOKUN KIM, Korea Institute of Science and Technology, CECILIA LEAL, Materials Science and Engineering, University of Illinois at Urbana-Champaign — Lipids – biological, amphiphilic molecules with ability to self-organize into bilayer structures – have found lasting therapeutic application in drug-laden nanoparticles. Of recent interest is the internal structure of these nanoparticles, which influences their endosomal escape in cellular delivery pathways. Lipid nanoparticles with bicontinuous cubic internal structure show improved gene knockdown efficiency over more traditional liposomal particles [1]. Inverse hexagonal-phase lipid materials show further improved fusogenic properties, but are toxic due to pore formation with the plasma membrane [2]. Here we report a lipid-based material with phase-triggering character to avoid such toxicity limitations. In this system, a change from bicontinuous cubic to inverse hexagonal within the nanoparticles can potentially be triggered at any delivery step without requiring endosomal acidification. Instead, local heating is achieved via near-infrared radiation of incorporated gold nanorods, inciting localized surface plasmon resonance. The formulated lipid systems are characterized with cryogenic TEM and small-angle X-ray scattering (SAXS).

References:


*Funded by the NIH under grant no. 1DP2EB024377-01*
9:00AM K30.00004: Modeling the Properties of Liquid Crystal Electrolytes with Replica Exchange Molecular Dynamics*  
MICHAEL QUEVILLON (Presenter), ARSENII PANTELEEV, JONATHAN WHITMER, University of Notre Dame — Ionic liquid crystals exist at the intersection of ionic liquids and liquid crystals; properties from both classes of materials can be utilized in various applications, from nonlinear optical and photonic devices to dye-sensitized solar cells. One intriguing use has been suggested where the ionic liquid crystals act as anisotropic battery electrolytes, where the liquid crystalline order provides global structure and the ionic liquid character provides a medium through which charge transport is facilitated. The ionic liquid crystals in question have bulky ionic groups and mesogenic “tails” with little or no effective charge, qualitatively similar to charged surfactants. This class of materials is relatively unprobed experimentally, as many are nontrivial to synthesize. We leverage atomistic molecular dynamics simulations of these systems as a preliminary way to study their phase behavior, utilizing replica exchange methods to pinpoint and elucidate the observed phase transitions.

*Computational resources provided by the Notre Dame Center for Research Computing (CRC). Additional support from the Midwest Integrated Center for Computational Materials (MICCoM), via the US Department of Energy, Basic Energy Sciences division.

9:12AM K30.00005: Mechanisms to Twist-Bend and Splay-Bend Nematic Phases  
NANDITA CHATURVEDI (Presenter), RANDALL D KAMIEN, University of Pennsylvania — Twist bend phases of liquid crystals have been studied extensively experimentally. However, the mechanism behind their emergence remains debated. Theoretical models have predicted the existence of twist-bend and splay-bend phases as stable states arising from a common mechanism. With the recent experimental observation of splay-bend phases, we look at bond orientational order, such as planar hexatic order, as a way to arrive at splay-bend and twist-bend phases. We find that phase chirality, and the nematic symmetry play a key role in looking at possible interactions of nematic order and bond orientational order.

9:24AM K30.00006: Length segregation in mixtures of spherocylinders induced by imposed topological defects*  
ELSHAD ALLAHYAROV (Presenter), Theoretical Chemistry, University of Duisburg-Essen, HARTMUT LOEWEN, Theoretical Physics II, University of Dusseldorf — We explore length segregation in binary mixtures of spherocylinders of lengths \( L_1 \) and \( L_2 \) which are tangentially confined on a spherical surface of radius \( R \). The orientation of spherocylinders is constrained along an externally imposed direction field which is either along the longitude or the latitude lines of the sphere. We show that the integer orientational defects at the poles induce a complex segregation picture also depending on the length ratio factor \( y=L_2/L_1 \) and the total packing fraction \( \eta \) of the spherocylinders. In longitude preoriented cases shorter rods tend to accumulate at the poles whereas longer rods occupy central equatorial area of the spherical surface. In latitude preoriented cases longer rods are predominantly both in the cap and in the equatorial areas and shorter rods are localized in between. A reference situation with a defect-free flat plane does not show any length segregation at similar \( y \) and \( \eta \). We also develop an Onsager-like density functional theory which is capable to predict length segregation in ordered mixtures. At low density, the results of this theory are in good agreement with the simulation data.

*Deutsche Forschungsgemeinschaft (DFG) through the grants AL 2058/1-1 (for E.A.) and LO 418/20-1 (for H.L.).

9:36AM K30.00007: Temperature-induced coordinated transformation of block copolymer micelles on fcc lattices to hcp structures  
SANGWOO LEE (Presenter), LIWEN CHEN, Rensselaer Polytechnic Institute — We discovered coordinated phase transformation of the strongly-segregated block copolymer micelles in aqueous solution on fcc lattices to hcp structures. The fcc structures formed by direct dissolution of poly(1,2-butadiene-b-ethylene oxide) diblock copolymer in water were gently shear-aligned and contained in sealed thin-wall capillaries. Heating the shear-aligned fcc crystallites to a higher temperature induced highly-coordinated hcp crystallites aligned in the same direction which we believe cannot happen by a nucleation and growth mechanism due to the high symmetry of fcc crystals. Careful analysis of the hcp structures suggests that the phase transformation occurred by sliding specific two-dimensional hexagonal micelle layers of the shear-aligned fcc crystallites likely with the smallest cross-section area.
9:48AM K30.00008: A mean field approach to determine the statistics of bundles of wormlike chains  
GREG MORRISON (Presenter), University of Houston — Crosslinked bundles of macromolecules play an important role in a variety of biologically relevant systems, including the flagella that provide locomotion and the microtubules and actin filaments that compose the cytoskeleton. In this talk, I describe a novel method of studying the statistics of weakly-bending, weakly-shearing bundles of stiff polymers using a mean field approach. I show that the imposition of the constraints of inextensibility and inter-filament separation on average leads to an analytically tractable free energy determined by a single wormlike Hamiltonian coupled to an effective Hamiltonian of a cylindrically confined chain, the latter representing the crosslinking between filaments. This gives rise to a bundle free energy that deviates from a typical wormlike chain, depending on a deflection length that couples the filament stiffness and bundle radius. The free energy of an intrinsically twisted bundle is determined for stiff bundles as well, which produces a significant change in the dependence of the free energy on filament stiffness and cross-sectional width. This mean field approach provides new insight into the statistics of bundled macromolecules with a variety of geometric constraints, useful in a number of biological contexts.

10:00AM K30.00009: Configurable Self-Assembly of Block Copolymers at the Liquid-Liquid Interface*  
FELIPE JIMENEZ (Presenter), HA-KYUNG KWON, MONICA OLVERA DE LA CRUZ, Northwestern University — Self-assembly of charged block copolymers has a range of potential applications such as fabrication of reconfigurable patterns in liquid-liquid systems, thin-film nanopatterning, bottom-up nanofabrication, demulsifying and antifoaming in extraction methods, drug delivery, protein encapsulation, among many others. Here we investigate the configurations of amphiphilic block copolymers at the water-chloroform interface using molecular dynamics simulations. The copolymers are constituted by one hydrophilic block and one hydrophobic block. A fraction of monomers ($f_q$) in the hydrophilic block bear a positive elementary charge which is balanced by free counterions. Our model represents the block copolymer poly(styrene)-poly(2-vinylpyridine) (PS-b-P2VP) with a degree of quaternization ($f_q$). A variety of structures going from circular domains to elongated stripes is observed by varying the polymer charge fraction and the hydrophilic/hydrophobic ratio. The adsorption and the structural changes are driven by a combination of effects such as the dielectric mismatch at the liquid-liquid interface, ionic correlations, hydrophilic-hydrophobic forces, and solvation effects.

*Center for Hierarchical Materials Design (CHiMaD), National Institute of Standards and Technology (NIST), Dept. of Commerce.

10:12AM K30.00010: Block and gradient copoly(2-oxazoline) micelles: striking different on the inside  
SERGEY FILIPPOV (Presenter), Harvard University, BART VERBRAEKEN, Department of Organic and Macromolecular Chemistry, Ghent University, PETER KONAREV, DMITRI SVERGUN, EMBL c/o DESY, NATALYA S. VISHNEVSKAYA, CHRISTINE M. PAPADAKIS, Physik-Department, Technische Universität München, SARAH ROGERS, ISIS Facility, Rutherford Appleton Laboratory, AUREL RADULESCU, Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science JCNS, TIMOTHEE COURTIN, JOSÉ C. MARTINS, Department of Organic and Macromolecular Chemistry, Ghent University, LARISA STAROVOYTOVA, Institute of Macromolecular Chemistry, POTEMKIN POTEMKIN, Physics Department, Lomonosov Moscow State University, RICHARD HOOGENBOOM, Department of Organic and Macromolecular Chemistry, Ghent University — Herein, we provide a direct proof for differences in the micellar structure of amphiphilic diblock and gradient copolymers, thereby unambiguously demonstrating the influence of monomer distribution along the polymer chains on the micellization behavior[1]. The internal structure of amphiphilic block and gradient co poly(2-oxazolines) based on the hydrophilic poly(2-methyl-2-oxazoline) (PMeOx) and the hydrophobic poly(2-phenyl-2-oxazoline) (PPhOx) was studied in water and water-ethanol mixtures by Small-Angle X-ray Scattering (SAXS), Small-Angle Neutron Scattering (SANS), Static and Dynamic Light Scattering (SLS/DLS), and $^1$H NMR spectroscopy. Contrast matching small angle neutron scattering (SANS) experiments revealed that block copolymers form micelles with a uniform density profile of the core. In contrast to popular assumption, the outer part of the core of the gradient copolymer micelles has a distinctly higher density than the middle of the core. We attribute the latter finding to back-folding of chains resulting from hydrophilic-hydrophobic interactions, leading to a new type of micelles that we refer to as micelles with a “bitterball-core” structure.

References
10:24AM K30.00011: Ionic Phase-segregated Liquid Crystal/Polymer Electrolyte for Lithium-ion Transport*
JIACHENG LIU (Presenter), SUNIL UPADHYAY, MATTHEW WINKLER, YUTING XIA, JENNIFER LYN SCHAEFER, University of Notre Dame — Solid polymer electrolytes have been widely studied for applications in lithium-ion batteries due to the potential for improved thermal and electrochemical stability.[1] Poly(ethylene oxide) (PEO) based electrolytes are the most widely studied solid polymer electrolyte. The conductivity of liquid-free PEO-based electrolytes is limited by ethylene oxide chain segmental motion.[2] In the present work, we seek to investigate lithium-ion transport via a different mechanism, lithium-ion transport through ionic domains. Ionic liquid crystal (LC) model small molecules and related single-ion conducting side-chain polymer electrolytes were synthesized. Small-angle X-ray scattering shows that both the LCs and polymers present segregated ionic phases. Impedance spectroscopy measurements indicate that both materials present Vogel-Tammann-Fulcher temperature-dependent conductivity. Current efforts are focused on macroscopic alignment of ionic phase for mitigation of grain boundary effects and studying the effect of anion structure on lithium-ion transport.


*This research is supported by the National Science Foundation through award # DMR-1654162.

10:36AM K30.00012: Rotational Symmetry Breaking of Complex Polymeric Macromolecules*
JUSTIN LITTLE (Presenter), ROBJEN BRUINSMA, Physics and Astronomy, University of California, Los Angeles, ALEXANDER GROSBERG, Department of Physics, New York University — A generalized version of Flory mean-field theory, supported by numerical simulations, indicates that polymeric macromolecules in good solvent with branches and cycles can show a sequence of spontaneous rotational symmetry breaking transitions as a function of increasing strength of the self-repulsion (J. Kelly, A. Grosberg and R. Bruinsma, submitted to PRL). We present here the analysis of the effect of including thermal fluctuations in the mean-field theory on the nature of these transitions for specific polymeric structures.

*We thank the NSF-DMR under Grant 1006128 and the Simons Foundation for funding.

10:48AM K30.00013: Scalable Production of Internally-Structured and Surface-Active Polymer Colloids via Flash NanoPrecipitation
VICTORIA LEE (Presenter), ROBERT K PRUD'HOMME, RODNEY PRIESTLEY, Princeton University — Production of polymer nanocolloids with complex internal structures or anisotropic surface functionality on large scales has been a challenge which has hindered their implementation in applications from drug delivery and biosensing to oil and gas recovery. We have developed Flash NanoPrecipitation (FNP) as a scalable process which can be used to generate kilograms of such polymer colloids per day. This solvent-exchange process relies on the rapid mixing of a polymer solution with an antisolvent stream to produce supersaturated conditions which result in monodisperse polymer colloids. Additional complexity can be achieved using the same low-cost equipment by taking advantage of the phase separation of chemically distinct polymers. Janus, core-shell, patchy, and lamellar morphologies have been produced by incorporating a blend of homopolymers or block copolymers into the system, and hydrophilic coronas can be generated via the use of amphiphilic block copolymers. Amphiphilic Janus colloids have recently been created by combining the phase separation behavior of hydrophobic polymers with the adsorption of amphiphilic block copolymers on one domain. These colloids are surface-active in oil-water mixtures and show promise as Pickering emulsion stabilizers.

Wednesday, March 6, 2019 8:00 AM - 10:48 AM

Session K31 DCP: Biomagnetic Chemical Sensing (QIS3) BCEC 203 - Michael Berman, Air Force Office of Science Research - Tag(s): Focus

8:00AM K31.00001: Quantum Biochemical Compasses [Invited] CHRISTIANE TIMMEL (Presenter), Oxford University — tbd
8:36AM K31.00002: Observations of Coherence in Bacterial Reaction Centers Using Two-Dimensional Electronic Spectroscopy*  
VERONICA POLICHT (Presenter), ANDREW NIEDRINGHAUS, JENNIFER P OGILVIE, Department of Physics, University of Michigan — Bacterial reaction centers (BRC) are photosynthetic proteins which perform electronic energy and charge transfer at ultrafast timescales (fs - ps) with near unity quantum efficiency in wild type proteins. Several recent observations of coherences in BRCs and other photosynthetic proteins have proposed that coherent superposition states are partly responsible for the impressive functionality of these systems. In attempting to answer this question, conflicting origin assignments of the coherences have been proposed. In order to develop our understanding of coherences we have performed Two-dimensional electronic spectroscopy on BRCs from purple bacteria *Rh. capsulatus* and its predominant pigment Bacteriochlorophyll a (BChla). We are able to identify strong intramolecular vibrational contributions in both systems as well as signs of vibronic coherence in the BRC. We additionally resolve the weak upper-excitonic peak of the strongly coupled special pair in the BRC, made visible due to resonance of vibrational modes with excitonic energy gaps. We simulate the signatures of vibronic coherence using a reduced BRC model. These results should inform future efforts to model electronic structure of the BRC.

*We gratefully acknowledge funding from the National Science Foundation (No. 1305450).

8:48AM K31.00003: Optical Tweezers: from Biophysics to Chemical Physics.  
MARIA KAMENETSKA (Presenter), Physics and Chemistry, Boston University, JACOB BLACK, ALEXANDER PAROBEK, ZIAD GANIM, Chemistry, Yale University — Optical Tweezers have resulted in transformative mechanistic understanding of biological processes by allowing unambiguous and reproducible measurements on single molecules. Using this technique, we can trap and isolate a single molecule away from surface heterogeneities and manipulate it with nanometer resolution and piconewton control. The application of this powerful technique to solution-phase chemistry and materials characterization has been hampered by the inability to achieve stable trapping in organic solvents. Here, I present our recent advances in extending optical tweezers to experiments on single molecules in a variety of solvents. Furthermore, I report on our preliminary measurements of optically-induced forces and demonstrate that force-detected absorption spectroscopy allows for nanoscale mapping of absorption profiles.

9:00AM K31.00004: The interplay between magnetism and chemical binding  
SUDIPTO CHAKRABARTI (Presenter), Weizmann Institute of Science — Single molecule spintronics aim to identify new spin transport effects near the limit of electronic component's miniaturization. While the focus in this field is on magneto-transport properties, not much is known about the effect of magnetism on the structure of molecular conductors. Here, we reveal a new phenomenon: the direction of applied magnetic field can affect the properties of a metal-molecule chemical bond. Specifically, we show that magnetic field direction affects the formation of metal-single molecule-metal junctions and the stability of the metal-molecule bond. Our findings reveal the interplay between magnetism and chemical binding at the level of a single chemical bond.

9:12AM K31.00005: Infrared spectroscopic nano-imaging of molecular coupling and dynamics in poly-tetrafluoroethylene  
SVEN A DOENGES (Presenter), BERND METZGER, JUN NISHIDA, ERIC A MULLER, MARKUS B RASCHKE, Department of Physics, Department of Chemistry, and JILA, University of Colorado - Boulder, Boulder, CO, United States — In organic materials, local morphology and environment determine material properties through intra- and intermolecular coupling. Vibrational spectroscopy can be used as a sensitive probe to variations in molecular structure, coupling, and dynamics. However, conventional far-field spectroscopic imaging spatially averages over the molecular ensemble, obscuring the effects of the local chemical environment. Here, we use broadband and ultrafast scattering scanning near-field optical microscopy (s-SNOM) to image nanoscale heterogeneity in the technologically important polymer of polytetrafluoroethylene (PTFE). Probing symmetric and antisymmetric coupled C-F stretch vibrations, from their variations and correlations in vibrational solvatochromism we reveal spatial sub-ensembles and their arrangements from nanometer to micron length scale of ordered and disordered domains in as cast, stretched, and rubbed PTFE films. The work demonstrates the use of vibrational marker resonances as intrinsic labels and molecular rulers as sensitive probes of their local structural environment associated with materials functional properties.
9:24AM K31.00006: Scanned Probe Microscopy Studies of MoS2 Catalysis on Insulating Substrates*  STEVEN ARIAS (Presenter), TAN DAO, SHAWNA HOLLEN, University of New Hampshire — Molybdenum Disulfide (MoS2) is one of the most commonly used commercial hydrodesulfurization (HDS) catalysts, but a microscopic understanding of the active sites and reaction mechanisms has been difficult to develop. Understanding these reactions on an atomic scale provide guidance to catalyst design. Improving HDS catalyst design will also rely on our knowledge of the catalyst on industrially relevant, insulating substrates. We will present data from scanning tunneling microscopy and non-contact atomic force microscopy on exfoliated MoS2 flakes on a silicon dioxide substrate. To determine active sites for HDS, we introduce thiophene molecules that adsorb to the MoS2. This system provides the first opportunities for atomic scale catalysis studies on industrially-relevant substrates.

*Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support (or partial support) of this research.

9:36AM K31.00007: Investigating Tunneling Controlled Reactions with Ring Polymer Molecular Dynamics  XINYANG LI (Presenter), PENGFEI HUO, Chemistry, University of Rochester — Here we present an ab-initio on-the-fly rate constant computation on the decay of methylhydroxycarbene with Ring polymer molecular dynamics (RPMD). Experiments show that hydroxycarbenes can decay rapidly through a high but thin barrier instead of a lower but broader barrier at 11 K. We investigate the tunneling of the transferring proton with RPMD which can accurately describe nuclear quantum effects. Quantum free energy profiles and transmission coefficients are computed in order to construct the full rate constants. We compute RPMD reaction rates at various temperatures which agree with previous experiments and theoretical studies.

9:48AM K31.00008: Self-assembling Ordered Arrays of Virus-like Particles Mediated by Linkers*  NICHOLAS BRUNK (Presenter), Intelligent Systems Engineering, Indiana University Bloomington, MASAKI UCHIDA, TREVOR DOUGLAS, Department of Chemistry, Indiana University Bloomington, VIKRAM JADHAO, Intelligent Systems Engineering, Indiana University Bloomington — Virus-like particles (VLPs), themselves self-assembled from protein subunits, can be exploited to generate hierarchical functional materials for applications in catalysis and photonics. We present an integrated experimental and computational method to understand and control higher-order VLP assembly into three dimensional, ordered arrays that is applicable to a variety of VLP-linker systems. Specifically, we study the assembly of bacteriophage P22 VLPs mediated by oppositely-charged, macromolecular dendrimers. The integrated approach demonstrates VLPs self-assemble into ordered arrays in the presence of dendrimers as the ionic strength is lowered below a threshold value. This threshold may be tuned by genetically engineering the VLP surface charge. At threshold, the common lattice structure exhibits the same long-range order and a similar configuration of bridging dendrimers, regardless of the VLP surface charge. The experimentally-validated model identifies key electrostatic and kinetic mechanisms, predicting dendrimer concentration as a control parameter for modulating assembly. The integrated approach opens new design and control strategies to fabricate active hierarchical materials.

*This work is supported by the National Science Foundation through Awards 1720625 and 1753182.

10:00AM K31.00009: Scaling relations quantify the hierarchical self-assembly of capillary-densified nanofiber arrays into shape-tunable architectures  ASHLEY KAISER (Presenter), ITAI Y STEIN, KEHANG CUI, BRIAN L WARDLE, Massachusetts Institute of Technology — Capillary-mediated densification is a facile and versatile method to create high-density, hierarchical structures from nanofiber (NF) arrays, such as aligned carbon nanotubes, whose exceptional intrinsic properties motivate their use as shape-tunable materials. Here, scaling relations are presented that accurately predict the morphology of capillary-densified NF arrays exhibiting multiple spatial scales, including long-range cellular networks formed from bulk-scale arrays, and solid, micron-scale pins formed via the densification of patterned arrays within the critical pattern size separating cell vs. pin formation. Both experiments and models show that the effective elastic modulus of the densifying NF arrays governs the resulting geometries, including the cell width and area, cell and pin wall thickness, and the NF volume fraction within the densified walls, which increase monotonically with array height. Further structural tunability, including the densification of mm- to cm-tall NF arrays, is possible by altering the NF-substrate adhesion strength. Collectively, these results could enable the broad use of capillary densification to predictably pattern hierarchical NF arrays for applications in optoelectronics, composite reinforcement, and advanced thermomechanical devices.
10:12AM K31.00010: Optical properties of free base tetrasulfonatofenil porphyrin (H2TPPS4), and tetrapyridyl porphyrin (H2TPyP) with ruthenium group

EHSAN ZOLGHADR (Presenter), KESHAV SHARMA, University of Alabama, JEFFERSON MARCIO SANCHES LOPES, Federal University of Pará, RENATO NEIVA SAMPAIO, University of North Carolina at Chapel Hill, ALZIR AZEVEDO BATISTA, Federal University of São Carlos, AMANDO SIUITI ITO, University of São Paulo, NEWTON M BARBOSA NETO, Federal University of Pará, PAULO T ARAUJO, University of Alabama — Recently we proposed new insight to the absorption and fluorescence (FL) of free base tetrapyridyl porphyrin (H2TPyP). In this project, we extend our study to the free base tetrasulfonatofenil porphyrin (H2TPPS4), and to supramolecular structure composed by H2TPyP and four ruthenium groups ([RuCl(terpy)(PPh3)2]PF6). Despite the fact that literature has reported the transitions observed in porphyrins’ absorption and fluorescence spectra, a more accurate interpretation has been evasive and still needed for H2TPPS4 and [RuCl(terpy)(PPh3)2]PF6 systems. We found that these systems follow our recent findings for H2TPyP where each of the absorption Q-bands consist of two quasi-degenerated bands namely Qx1, Qx2 and Qy1, Qy2, respectively. We also explore the FL and its polarization degree (polarization components) via the Stokes spectroscopy method. Using the Stokes method, we found that the FL polarization degree depends on the concentration of the molecules in the solvent. In order to elucidate the polarization mechanisms, further investigations are being conducted via polarization-resolved, temperature-dependent and lifetime spectroscopy experiments.

10:24AM K31.00011: Spin Crossover Predictions in Transition Metal Complexes using the Density Corrected DFT*

LUIS SORIANO (Presenter), ALBERTO VELA, Center for Research and Advanced Studies of the National Polytechnic Institute — The phenomenon of spin-crossover (SCO) in transition metal complexes is of great importance in the development of magnetic materials whose properties are used in visualization, memory, and electrical devices, to mention a few. This phenomenon has been amply studied with Density Functional Theory (DFT) using a broad variety of exchange-correlation (XC) functionals with disappointing outcomes. Such functionals seem incapable of predicting reliably the energy differences between the high- and low-spin configurations. Recently, an approach called HF-DFT, which consists of evaluating the energy of a selected XC functional with the Hartree-Fock (HF) density, has been applied successfully to several problems, including SCO in some iron complexes with small ligands, yielding results that are close to coupled cluster (CC) and Diffusion Monte Carlo calculations, at a much lower computational cost. In this work we show that HF-DFT, using DFT optimized geometries, also offers an excellent alternative to describe SCO in manganocenes with ligands in the cyclopentadienyl rings going from hydrogen to tert-butyl. The results are in excellent agreement with available CCSD calculations.

*LASA and AVA thank Conacyt for grant Fronteras 867.

10:36AM K31.00012: Resonance Energy Transfer on a Metallic Thin Film: Characteristic Distance and the Origin of Plasmon Enhancement*

LIANG-YAN HSU (Presenter), Institute of Atomic and Molecular Sciences, Academia Sinica, JHIH-SHENG WU, physics, Georgia State University — Resonance energy transfer (RET) around metallic structures has received considerable attention during the past few years. In this study, we analyze the mechanisms of RET on a metallic thin film in the framework of macroscopic quantum electrodynamics and investigate the distance dependence of RET enhancements. Our theoretical analysis shows that the mechanisms of RET can be separated into mirror dipoles, surface plasmons, and retardation. Besides, we find the characteristic distance of RET coupled with surface plasmon polaritons and it can be modified by varying the thickness of thin film, indicating that RET can be significantly enhanced at a short range.

*This research was supported by Academia Sinica and the Ministry of Science and Technology of Taiwan (MOST 106-2113-M-001-036-MY3)

Wednesday, March 6, 2019 8:00 AM - 10:48 AM

Session K32 DCP: Accurate Methods for Vibrational Analysis (C) BCEC 204A - Julien Bloino - Tag(s): Focus
8:00AM K32.00001: Collocation Methods for Computing Vibrational Spectra* [Invited] TUCKER CARRINGTON (Presenter), ROBERT WODRASZKA, Queen's University — When the potential energy surface (PES) does not have a special form (e.g. a sum of products), it is common to use quadrature to compute a vibrational spectrum. Direct-product quadrature grids are most popular. The size of a direct-product grid scales exponentially with the number of atoms and it is not possible to store values of the PES for molecules with more than 5 atoms. One option is to use a Smolyak quadrature grid. In this talk, I shall present collocation methods with Smolyak-type grids. Collocation has advantages: 1) point selection is less important; 2) no integrals, no quadratures, no weights; 3) easy to use with complicated kinetic energy operators; 4) it can be used with any (the best possible) coordinates and basis functions; 5) in many cases fewer collocation than quadrature points are required; 6) the length of the vectors one must store is reduced. Collocation can be used with the Multiconfiguration Time-Dependent Hartree (MCTDH) approach. The collocation-based MCTDH method I shall present can be used with general potential energy surfaces. This is imperative if one wishes to compute very accurate spectra. When the basis is good, the accuracy of collocation solutions to the Schrödinger equation is not sensitive to the choice of the collocation points. The original collocation-MCTDH (C-MCTDH) method [J. Chem. Phys. 148, 044115 (2018)] uses, as is also true in standard MCTDH, a direct product basis. Because we do not rely on having a sum-of-products potential energy surface, we also have a direct product grid. By using generalized hierarchical basis functions, that span the same space as the single particle functions we introduced in the first C-MCTDH paper, and a Smolyak grid, we have developed C-MCTDH approach that makes it possible to prune both the basis and the grid.

*The financial support of the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

8:36AM K32.00002: On a New Path to Computing the Vibrational Spectra of PAHs* [Invited] RYAN FORTENBERRY (Presenter), Department of Chemistry & Biochemistry, University of Mississippi, JOSHUA P. LAYFIELD, Department of Chemistry, University of St. Thomas (MN), TIMOTHY J LEE, MS 245-3, NASA Ames Research Center — Polycyclic aromatic hydrocarbons are big, largely amorphous, and ubiquitous. This makes them both incredibly important (notably for environmental science and astrophysics) and incredibly difficult to precisely describe the infrared spectral features of a single unique PAH specimen type in the laboratory. Quantum chemical computations have recently demonstrated the ability to produce vibrational frequencies for a selection of molecules to as good as within 1.0 cm⁻¹ of experiment and can do so conclusively for a single molecule since only one chemical system is input into the computations. However, these computations are incredibly costly making them applicable only to small molecules. Recent work in our group has shown that newer quantum chemical theory such as explicitly correlated methods (F12b) can be utilized effectively to produce experimentally-comparable vibrational frequencies at a reduced cost, but this still only extends the sizes of the molecules to be studied potentially up to benzene. However, reparameterized semi-empirical methods designed solely to treat hydrocarbons are showing promise in predicting the spectra of small molecules with a significant savings in time. Successes include c-C₃H₂, C₃H₅⁺, and HOCO⁺ among others. These methods are currently being extended to PAHs.

*NASA Grant NNX17AH15G

9:12AM K32.00003: Ab initio methods targeting strong electron- and nuclear-correlation in spectroscopy* [Invited] MARKUS REIHER (Presenter), ETH Zurich — The density matrix renormalization group (DMRG) has emerged as an important alternative to multi-configurational self-consistent-field calculations in molecular spectroscopy, replacing standard complete active space approaches for large orbital spaces. We implemented a spin-adapted matrix-product-state (MPS) and -operator formulation of the DMRG, which serves as a flexible and efficient basis for the development of an MPS state-interaction approach for optical spectroscopy and of a short-time resonance Raman spectroscopy model. We extended our approach to vibrational spectroscopy and I will discuss how the DMRG can be exploited to optimize vibrational wave functions expressed as matrix product states.

*Support from ETH Zurich and the Swiss National Science Foundation is gratefully acknowledged.
9:48AM K32.00004: Computational Methods for Excited State Time-Resolved Vibrational Spectroscopies  
ALESSIO PETRONE (Presenter), FEDERICO COPPOLA, FULVIO PERRELLA, NADIA REGA, Chemical Sciences, University of Naples Federico II — Time-resolved Infrared (IR) and Raman\(^1\) spectroscopies, have become increasingly important in modern chemical, biological, and materials research. This modern focus is primarily due to their capability to study non-equilibrium structural dynamics of ultrafast chemical phenomena.\(^2\)

A computational approach based on both \textit{ab-initio} molecular dynamics and transient vibrational analysis is presented to establish a time-dependent density functional theory (TDDFT) based protocol able of describing simultaneously transient IR and Raman active vibrational modes. This work relies on the recent method development for the evaluation of higher-order TDDFT properties and multiresolution time-frequency analysis.\(^3\)

Excited state photo dynamics of prototypical molecules in gas phase will be used as test cases, showing the evolution of the vibrational \textit{signatures} upon the excitation. This protocol is critical to understand how nuclear motions can mediate the photo-dynamics of several photo-active systems.


10:00AM K32.00005: Gadolinium Cation (Gd\(^+\)) Reaction with CO\(_2\): Potential Energy Surface Mapped from Experiment and Theory  
MARIA DEMIREVA (Presenter), PETER B ARMENTROUT, University of Utah — Understanding the activation of CO\(_2\) is of interest because of the role of CO\(_2\) as a greenhouse gas and its potential use as a carbon source in chemical synthesis. In gas phase experiments, the interactions and thermochemistry of CO\(_2\) with metals can be probed without complicating effects from solvent or substrate molecules. Such studies can provide details about the activation processes at a molecular level. This information can potentially be extended to more complicated systems and be valuable in the design of new and improved catalysts. Here, guided ion beam tandem mass spectrometry is used to investigate the energy dependent reaction of gas-phase lanthanide gadolinium cation (Gd\(^+\)) with CO\(_2\) to form GdO\(^+\) and CO. Results show that ground state products are formed in an exothermic and barrierless process, with an electronically excited product ion produced efficiently at high collision energies. Additional experiments on the reverse process as well as Gd\(^+\)(CO\(_2\)) and O\(\text{Gd}^+(\text{CO})\) intermediates allow for an experimental potential energy surface to be determined. Electronic structure calculations help identify the structures and electronic states of these species and help explain the reactivity observed. Periodic trends in reactivity will be briefly discussed.

AMRO DODIN (Presenter), ADAM P. WILLARD, Chemistry, MIT — The statistics of open quantum systems are determined by the interplay of classical uncertainty, describing the lack of knowledge of the initial preparation of the system and bath, and quantum uncertainty, originating from the wave-mechanical nature of quantum states. In this presentation, a classical probability distribution on quantum state space will be defined that separately encodes classical and quantum sources of uncertainty. The dynamics of such distributions will then be explored, revealing similar properties to Hamiltonian classical mechanics. In particular, the dynamics of closed systems is shown to be incompressible and time reversible, proving a quantum analog to the classical Liouville’s theorem and framing quantum microreversibility equivalently to classical systems. This enables the application of tools from classical mechanics, statistical physics and fluid mechanics to quantum systems with applications in quantum information science and quantum thermodynamics.
10:24AM K32.00007: Vibronic Structure and Photoelectron Angular Distribution in the Photoelectron Spectrum of ICN

SOUMITRA MANNA (Presenter), SABYASHACHI MISHRA, Department of Chemistry, Indian Institute of Technology Kharagpur — In some molecular systems, the complex vibronic structure of photoelectron bands demand extensive theoretical and computational efforts to delineate the interactions between vibrational degrees of freedom and electronic motion, further complicated by coupling of orbital and spin momenta of the electrons. The photoelectron spectroscopy of ICN has been a very challenging problem that has received a lot of attention. However, a conclusive interpretation of the spectrum, in particular, the complex spin-vibronic structures of the B 2Π3/2 and B 2Π1/2 states, has remained elusive. In this presentation, we will explain the complex vibronic structure of ICN by analyzing the Dyson orbitals corresponding to the ionized electrons. The simulated spectra have been found to successfully reproduce the position and intensities of the main four photoelectron bands along with the associated vibronic structures. The shape resonances seen in the experimental asymmetry parameters and the trends of ionization cross-section with increasing electron kinetic energies are explained in terms of the partial wave analysis of the departing photoelectron and the contribution of allowed photoelectron angular momentum channels to the ensuing photoelectron wave function.

*University Grants Commission, New Delhi.

10:36AM K32.00008: Quantum Dynamics of Fluorescence Coupled with Surface Plasmon Polaritons and Intramolecular Vibrations

SIWEI WANG (Presenter), Chemistry, Princeton University, LIANG-YAN HSU, Institute of Atomic and Molecular Sciences, Academia Sinica, GREG SCHOLES, Chemistry, Princeton University — We study quantum dynamics of molecular fluorescence on a metal surface based on macroscopic quantum electrodynamics and explore the Purcell factor including non-Markovian effect (beyond Fermi's golden rule). The method we present is general for molecular fluorescence in a variety of plasmonic nanostructures (not limited to metal surfaces). Furthermore, the proposed method allows us to express memory kernels in terms of the parts of surface plasmon polaritons and molecular vibrations and enables us to calculate the kernels via classical electrodynamics, e.g., finite-difference time domain method. We find that, under different strengths of exciton-polariton couplings, the interplay of surface plasmon polaritons and molecular vibrations can lead to distinct characteristics in dynamics. Our study also provides a direction for exploring the effect of vibrational coherence on plasmon-enhanced molecular fluorescence.

*The authors acknowledge financial support by the National Science Foundation, MRI No. DMR-1229217, and by Princeton University through the Innovation Fund for New Ideas in the Natural Sciences.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K33 FIAP: Phase Change Materials, Memristors, and Neuromorphic Computing

BCEC 204B - Ali Gokirmak

8:00AM K33.00001: Evidence of Charge Trapping Giving Rise to Resistance Drift of Metastable Amorphous Ge2Sb2Te5

RAIHAN SAYEED KHAN (Presenter), SADID MUNEER, NAFISA NOOR, HELENA SILVA, ALI GOKIRMAK, University of Connecticut — Phase change memory (PCM) is a high speed, high density, scalable non-volatile memory that utilizes the resistivity contrast between amorphous (high resistivity) and crystalline (low resistivity) phases of chalcogenides like Ge2Sb2Te5 (GST) [1]. The large resistivity window enables programming to intermediate states and hence multi bit storage; however, PCM suffers from spontaneous resistance drift after amorphization [2,3] potentially resulting in overlapping resistance levels. It is difficult to be understand resistance drift from room temperature measurements as multiple processes may be occurring simultaneously, presenting a need for cryogenic measurements. We monitor resistance drift in GST line cells for up to ~10^4 s from 175K to 300K at 25K intervals with varying light exposure. The resistance drift coefficients decrease with decreasing temperature. Light exposure alters cell resistivity at a time scale longer than expected from thermal effects at these temperatures, suggesting a charge-trapping mechanism.

References:

*AFOSR MURI FA9550-14-1-0351
8:12AM K33.00002: Heat transfer as coupling mechanism in VO$_2$-based neurons* JAVIER DEL VALLE GRANDA (Presenter), YOAV KALCHEIM, PAVEL SALEV, IVAN SCHULLER, University of California, San Diego — Neuromorphic computing is a new computation paradigm which imitates the architecture of biological brain. One of the basic tasks is to find materials that mimic the functionality of the two basic components of neural networks: neurons and synapses. Resistive switching offers a unique opportunity to do this. Non-volatile resistive switching has been extensively studied and successfully used to mimic synaptic behavior. On the other hand, finding resistive-switching based neurons has remained an elusive task. Current hardware neurons are based on complex, not-scalable CMOS circuits. In this work, we show how volatile resistive switching in VO$_2$ can be used to do such task. We use heat as a memory mechanism to implement “leaky integrate and fire”, a basic neural functionality. By keeping VO$_2$ nanodevices at the edge of firing and using heat transfer as coupling mechanism, we show signal self-amplification when voltage spikes are transferred form one neuron to the next. This result is key towards the construction of completely scalable, resistive-switching based neuromorphic hardware.

*This research is supported by the Vannevar Bush Faculty Fellowship program, funded by the Office of Naval Research through grant N00014-15-1-2848. J.d.V. thanks Fundación Ramón Areces for their support.

8:24AM K33.00003: Electrical Characterization of Ge$_2$Sb$_2$Te$_5$ Phase Change Memory Cells at Cryogenic Temperatures to Investigate the Physical Phenomena that Give Rise to Resistance Drift of the Amorphous Phase* ABM HASAN TALUKDER (Presenter), RAihan SAYEED KHAN, SADID MUNEER, KIMBERLY NGUYEN, MADISON NADOLNY, ALI GOKIRMAK, HELENA SILVA, University of Connecticut — Electrical measurements of metastable amorphous Ge$_2$Sb$_2$Te$_5$ in the temperature range of 300 - 675 K using a waveform tailored to melt, quench and characterize cells in a single shot [1] have resulted in characterization of temperature dependent carrier activation energies that follow a parabolic behavior with a peak value of ~377 meV at ~465 K [2]. Measurements of cells amorphized at cryogenic temperatures give insights about the physical phenomena that give rise to resistance drift of the amorphous phase as well as the activation energy in a broader temperature range. We have performed electrical measurements in 85 – 300 K temperature range and observed resistance drift over time. As the viscosity of the material is expected to be extremely high at 85 K, we expect charge trapping to be the dominant factor for drift in amorphous Ge$_2$Sb$_2$Te$_5$.

References:

*Supported by NSF ECCS. Award# 1711626.

8:36AM K33.00004: Characteristics and applications of carbon-based ReRAM* PEI-FANG CHUNG (Presenter), MONSHU HO, Physics, National Chung Hsing University — In this work, we anticipate the performance of fullerene molecules could provide a new prototype of the Carbon-based ReRAM model owing to its outstanding electric and magnetic characteristic. Few layers of fullerene molecules ($C_{84}$) ultrathin film were assembled thermally on Si (111)-7×7 substrates under ultra-high vacuum. The top-electrode Pt (50nm) was deposited by RF magnetron sputtering on $C_{84}$ film. The surface electronic states and magnetic characteristics of $C_{84}$ film were studied by UHV-STM and MFM. The STS has revealed the wide band gap of fullerene molecule in which the LDOS can be tuned by different cover density and different combination of fullerene molecules. The ferromagnetic domain has been discovered along the domain boundaries on proposed Si substrate due to the quantum confinement along with localized unpaired electrons in fullerene molecules. The resistance switching behavior of the memory devices were attributed to the formation and rupture of conductive filaments. Thus, we characterized the binding feature and the photoelectric properties with Raman, XPS and VT-PL. We could declare fullerene molecules have potential as a promising candidate for next generation nonvolatile memory and other semiconductor applications.

*Si(111)-7x7, Fullerene molecules, $C_{84}$, ReRam
Finite Element Modeling of Ovonic Switching* JAKE SCOGGIN (Presenter), HELENA SILVA, ALI GOKIRMAK, ECE, UConn — Ovonic switching in amorphous semiconductors was first reported in the 1960s [1] and has since spawned phase change memory, ovonic threshold switches, and a rich debate on the physical phenomena underlying the rapid transition from low to high electrical conductivity in these materials once a sufficient field is applied [2]. We model ovonic switching as a field-assisted thermal phenomenon in 2-D, 2-D rotational, and 3-D finite element simulations. We vary fields, geometries, and transient conditions and obtain I-V characteristics in good agreement with experimental data. We also show 2-D simulations of ovonic switches as current-limiting access devices for reset and set of phase change memory cells in a crossbar array using our finite element phase change model [3], [4].


*AFOSR MURI FA9550-14-1-0351

On attractor states in the dynamics of pulse-driven memristors YURIY PERSHIN (Presenter), Physics and Astronomy, University of South Carolina, VALERIY SLIPKO, Institute of Physics, Opole University — We predict the existence of attractor states in the dynamics of certain pulse-driven memristors (resistors with memory) and memristive networks [1]. A general approach to identify the attractor points in two-terminal memristive circuits driven by alternating polarity voltage or current pulses has been developed and applied to several model cases including the ideal and threshold-type memristors, as well as certain memristive networks. Potential applications of dynamical memristor attractors include the memristor initialization, associative memory, and validation of memristor models, to name a few. In particular, based on specific cases we have demonstrated that the presence or absence of attractor dynamics can be directly related to the window function used in the memristor model. This result paves the way towards a simple experimental test of memristor models, which is just one of several promising applications of dynamical memristor attractors.


Finite Element Simulation of Phase Change Memory Cell* MD TASHFIQ BIN KASHEM (Presenter), JAKE SCOGGIN, SADID MUNEER, HELENA SILVA, ALI GOKIRMAK, University of Connecticut — We perform finite element simulations of read, reset and set operations on Ge2Sb2Te5 phase change memory cells using the model developed in [1], [2]. An electrical circuit model is included to utilize a transistor as an access device. Thermoelastic effects (Thomson and Peltier heat) are incorporated in the current continuity and heat transfer physics which are solved self-consistently to obtain potential and temperature distributions across the device. We use temperature dependent material parameters (Seebeck coefficient, thermal conductivity and electrical resistivity) to precisely model electrothermal phenomena in the cell. We perform successive read, reset and set operations and analyze nucleation, growth and amorphization as well as temperature and resistance profiles during the simulations.

References:

*This work was supported by Air Force Office of Scientific Research (AFOSR) through award FA9550-14-1-0351.
Enhanced Reset Variability in Phase Change Memory for Hardware Security Applications

NAFISA NOOR, SADID MUNEER, RAHAN SAYEED KHAN, ALI GOKIRMAK, HELENA SILVA (Presenter), Electrical and Computer Engineering, University of Connecticut, Storrs, CT 06269, USA — Phase change memory (PCM) relies on the change of resistance of a chalcogenide material, that can be reversibly switched between amorphous and crystalline states by applying appropriate electrical pulses. We have experimentally shown enhanced variability during the amorphization hexagonal close packed (hcp) Ge$_2$Sb$_2$Te$_5$ line cells by using long-narrow cell dimensions and voltage pulses with narrow rise and fall times. Percolation-blocked conduction in long-narrow cells, parasitic capacitive current, and thermal runaway at the onset of melting from the initial hcp state are the possible physical mechanisms behind the significant increase of reset uncertainty, which is useful for implementing hardware security primitives$^{1-4}$.

2N. Noor et al., in International Semiconductor Device Research Symposium (2016).

A simple and highly-scalable artificial neuron using an Ovonic Threshold Switch (OTS)*

SUYOUN LEE (Presenter), MILIM LEE, SEONG WON CHO, JOON YOUNG KWAK, HYUNSU JU, Korea Institute of Science and Technology, YEONJIN YI, Institute of Physics and Applied Physics, Yonsei University, BYUNG-KI CHEONG, Korea Institute of Science and Technology — A scalable and low power-consuming artificial neuron is an essential building block for developing a brain-inspired computing system. Among various features of a biological neuron in the mammalian cortex, the spike-frequency adaptation and chaotic activities are very important ingredients for the realization of the energy-efficient signal processing, learning, and adaptation to environments, which are hard to be achieved up to now. In this work, we have demonstrated those features in a simple artificial neuron device composed of an Ovonic Threshold Switch (OTS) and a few passive electrical components. Furthermore, with our OTS-based neuron device employing the reservoir computing technique combined with delayed feedback dynamics, spoken-digit recognition task has been performed with a considerable degree of recognition accuracy. These results show that our OTS-based artificial neuron device is promising for the application in the development of a large-scale brain-inspired computing system.

*This work was supported by the Korea Institute of Science and Technology (KIST) through 2E27811.

Development of Self-rectifying TaO$_y$/Nanoporous TaO$_x$ Memristor Synapse for Suppressing Non-neural Signal in the Large-scale Neuromorphic Array System

SANGHYEON CHOI (Presenter), SEONGHOON JANG, KU-KIST Graduate School of Converging Science & Technology, Korea University, JUNG-HWAN MOON, Department of Materials Science and Engineering, Korea University, JONG CHAN KIM, HU YOUNG JEONG, UNIST Central Research Facilities and School of Materials Science and Engineering, Ulsan National Institute of Science and Technology (UNIST), PEONGHWAN JANG, KYUNG-JIN LEE, Department of Materials Science and Engineering, Korea University, GUNUK WANG, KU-KIST Graduate School of Converging Science & Technology, Korea University — Memristor that consists of a metal-oxide layer sandwiched between two conductors is being greatly envisioned as a platform to imitate the principal of biological synapses due to its nonlinear and dynamic electrical properties depending on the history of applied electrical programming$^{[1]}$. In this study, we fabricated the nanoporous (NP) TaO$_x$ memristor device by an anodic treatment in the room temperature and utilized the device as the two-terminal artificial synapses$^{[2]}$. The device exhibits a stable self-rectifying I-V switching behavior with $\sim10^4$ nonlinearity, which can effectively prevent the undesired neural signals in the densely-integrated synaptic array. Based on analog shift of the Ohmic-contact site by diverse electrical stimuli, the essential synaptic functions were successfully mimicked. A 16 × 16 crossbar array with only our device was fabricated and statistically evaluated. In addition, we investigated the effect of the nonlinearity of the synaptic device on the accuracy of the pattern recognition using artificial neural network simulation. Taken all together, we believe the designed device can provide a route toward the large-scale neuromorphic computing technology.

References

10:00AM K33.00011: Current-induced resistivity switching in VO₂ micro-electronic oscillators  MILINDA PATTANAYAK (Presenter), Department of Physics & Astronomy, Nano Tech Center, Texas Tech University, MD NADIM F HOQUE, ZHAOYANG FAN, AYRTON A BERNUSSI, Department of Electrical and Computer Engineering, Nano Tech Center, Texas Tech University — Functional metal oxides are a class of emerging materials with novel applications in tunable and reconfigurable microelectronics beyond the CMOS technology. Vanadium dioxide (VO₂) is one such material that is attracting considerable attention for its reversible insulator-to-metal phase transition (IMT). Under electrically controlled IMT process VO₂ devices exhibit electrical switching and negative differential resistance (NDR). Such attributes make VO₂ the ideal candidate for designing tunable micro oscillators for emerging applications such as neuro-morphic computing. We designed, fabricated, and characterized planar VO₂ micro-channel devices with different dimensions. The intrinsic parasitic capacitance of the fabricated devices allowed for stable spontaneous electrical oscillations under current actuation. Our novel approach for controlling the current in the NDR region eliminates the need of an external pulsed power source or external passive components to generate self-sustained electrical oscillations. Such reduction in circuitry complexity is significant for prospective large scale on-chip integration of micro- or nano- oscillators that simplifies the power source design and the connection between oscillators and metal interconnects carrying power to the oscillators.

10:12AM K33.00012: Scalable Free-Space Optical Neural Networks* LIANE BERNSTEIN (Presenter), ALEXANDER SLUDDS, RYAN HAMERLY, DIRK R. ENGLUND, Massachusetts Institute of Technology — The transformative impact of deep neural networks (DNNs) in many fields has motivated the development of hardware accelerators to improve speed and power consumption. We present a novel photonic approach based on homodyne detection where inputs and weights are encoded optically and can be reprogrammed and trained on the fly. This architecture is naturally adapted to free-space optics where both fully-connected and convolutional networks can be implemented and scaled to millions of neurons. By utilizing passive optical fan-out and performing arithmetic coherently with optical interference, this scheme circumvents fundamental limits of irreversible electronic processing. We study the effect of detector shot noise on neural-network accuracy to establish a “standard quantum limit” for this system. This bound, which can be as low as 50 zJ/FLOP, suggests performance below the Landauer (thermodynamic) limit is theoretically possible with photonics.


10:24AM K33.00013: Synaptic Barristor Based on Phase-Engineered Two-Dimensional Heterostructures  WOONG HUH (Presenter), SEONGHOON JANG, JAE YOON LEE, DONGHUN LEE, JUNG MIN LEE, HONG-GYU PARK, Korea University, JONG CHAN KIM, HU YOUNG JEONG, UNIST, GUNUK WANG, CHUL-HO LEE, Korea University — Heterostructures built from various two-dimensional (2D) layered materials are emerging material platforms for low-power and high-performance electronic devices because of their high-quality heterointerfaces. Here, we report a new class of artificial synaptic architecture, a three-terminal device consisting of a monolithically integrated WOₓ memristor and a variable-barrier WSe₂/graphene Schottky diode, termed as a 'synaptic barristor'. The device can implement essential synaptic characteristics, such as short-term plasticity and long-term plasticity. Owing to the electrostatically controlled barrier height in the ultrathin vdW heterostructure, the device exhibits gate-controlled memristive switching characteristics with tunable programming voltages of 0.2–0.5 V. Notably, by electrostatic tuning with a gate terminal, we can additionally regulate the degree and tuning rate of the synaptic weight independent of the programming impulses from source and drain terminals. These capabilities enable the accelerated consolidation and conversion of synaptic plasticity, functionally analogous to the synapse with an additional neuromodulator in biological neural networks. Our demonstration represents an important step toward highly networked and energy-efficient neuromorphic circuits.
10:36 AM K33.00014: Resolving the Metal-Insulator Transition Mechanism of NbO2 for Memristor Applications

MATTHEW WAHILA (Presenter), GALO PAEZ, CHRISTOPHER SINGH, SHAWN SALLIS, Binghamton University, JERZY T. SADOWSKI, Center for Functional Nanomaterials, BROOKS TELLEKAMP, ALAN DOOLITTLE, Georgia Institute of Technology, WEI-CHENG LEE, LOUIS F. J. PIPER, Binghamton University — Electroformed NbOx films show potential for memristor applications, however, their memristive mechanism is not understood. NbO2 filaments with a temperature-dependent MIT have been theorized to be the culprit,[1,2] but this has not been proven due in part to a lack of understanding regarding the MIT nature. Crystalline NbO2 undergoes an MIT with accompanying structural transition at ~810°C, but there are competing claims as to whether it is Mott, Peierls, or cooperative Mott-Peierls like VO2.[3,4] We have investigated crystalline NbO2 using synchrotron-based temperature-dependent and variable energy XPS, µ-LEED, and LEEM/PEEM, and have conclusively found it be a gradual 2nd-order Peierls transition. The gradual nature is then attributed to weakening Nb-Nb dimers causing the formation of a pseudogap as temperature increases. Moreover, calculations fully reproduce experimental spectra without explicit consideration of correlations, indicating minimal Mott character.


*This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0024.

10:48 AM K33.00015: Nb-doped TiO2: Effect of interstitial oxygen atom on charge state of Nb

WEI YAN, XIAOJIE LIU (Presenter), Center for Quantum Sciences and School of Physics, Northeast Normal University — The structural and electronic properties of Nb doped Rutile TiO2 are investigated by first-principles calculations based on density functional theory. Several doping models including 2(NbTi)+Oi, NbTi+Oi, 2(NbTi), and NbTi are investigated. We find that all the doped systems preserve the semiconductor character but have an impurity state inside the band gap. Therefore, the band gaps of the doped systems are reduced by 0.15~1.41 eV, compared to that of the pure rutile TiO2. These results suggest that Nb-doped TiO2 would have higher photocatalytic activity than pure TiO2. The origin of the gap state is different in different doping models. The calculation results show that interstitial oxygen atom play an essential role in manipulating the valence state of Nb impurity. The charge density analysis show that Nb atom in 2(NbTi)+Oi and NbTi+Oi systems can be pentavalent since the Nb atom loses much more electrons due to the interaction with the interstitial oxygen atoms. On the other hand Nb atoms in the NbTi and 2(NbTi) doped systems would be tetravalent.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K34 FIAP FECS: Future of Physics and Evolving Careers of Physicists BCEC 205A - Maria Longobardi, University of Geneva - Tag(s): Careers, Industrial, Invited, Undergraduate
8:00AM K34.00001: Emergence by design in artificial spin ice* [Invited] CRISTIANO NISOLI (Presenter), Theoretical Division, Los Alamos National Laboratory — Intriguing phenomena generally emerge from the collective behavior of numerous simple interacting degrees of freedom. Indeed, physicists typically first discover new systems and then proceed to describe them via higher level models that often deliberately neglect the detail of the building blocks. Instead, they concentrate on the relevant symmetries and interactions of an emergent description [1]. Today, advances in nano and micro fabrication, characterization, and control, can invert that approach. We can realize artificial systems whose interacting, elementary degrees of freedom can be tailor-designed for exotic behaviors in their collective, low-energy kinetics. That is the case of artificial spin ice materials [2], which can now be variously manufactured in arrays of magnetic nano-islands [3], trapped colloids [4], vortices in nano-patterned superconductors [5], or possibly with skyrmions in liquid crystals. They can produce new phenomena often non seen in natural materials, such as complex kinetics of magnetic charges and magnetic monopoles [6], new forms of frustration [7], classical forms of topological order [8], dimensionality reduction [9], or ergodicity breaking in absence of quenched disorder. With the goal of eliciting contributions in this field by early career scientists and students we will briefly summarize the fiend and then report on the more recent results.


*LDRD LANL

8:36AM K34.00002: Imaging Quantum Materials* [Invited] MARIA IAVARONE (Presenter), Physics, Temple University — Future technological breakthroughs require innovations aimed at predicting, designing, developing and manufacturing complex materials with multiple functionalities. Materials research is key to answer these societal needs. In quantum materials, the collective behavior of electrons generates a wide range of novel physical properties. Understanding this behavior together with the ability to control the electronic properties of solids has already led to landmark discoveries in condensed matter physics. These discoveries have opened pathways to novel electronic applications of the new materials and devices. The availability of characterization tools, such as scanning probes, which visualize exotic quantum states with high sensitivity and resolution, allows scientists to improve their ability to design, synthesize and understand materials with exotic functionalities. Examples of applications of some of the scanning probe techniques to the field of superconductivity and two-dimensional materials will be presented.

*The work is supported by the Center for Complex Materials from First Principles (CCM), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #SC0012575 and by U.S. Department of Energy, Office of Science, Basic Energy Science DE-SC0004556.

9:12AM K34.00003: The Role of Communication in the Future of Physics [Invited] JESSICA THOMAS (Presenter), American Physical Society — TBD

9:48AM K34.00004: The Career of a Nuclear Physicist at IBM [Invited] MICHAEL GORDON (Presenter), IBM Thomas J. Watson Research Center — TBD
10:24AM K34.00005: Distinguished Lectureship Award on the Applications of Physics Talk: Career Opportunities from Fundamental Physics to Patient Treatments [Invited] CYNTHIA KEPPEL (Presenter), Thomas Jefferson National Accelerator Facility — Discoveries and technological advances spurred by the demands of fundamental physics research find applications in many disciplines, including providing benefit to society through the treatment and diagnosis of disease. Rather than survey the manifold applications of this topic, a few examples will be presented. With emphasis on the "bench to bedside" implementation of nuclear physics technology, scientific topics ranging from the smaller-scale treatment implementation of fiber-based in-vivo dosimetry to large scale proton radiation therapy treatment to the diagnostic application of breast specific gamma imaging will be presented. In parallel, the variety of physics career options along this path, from fundamental research science on "the bench" to clinically-utilized medical products at "bedside", will be highlighted.

Wednesday, March 6, 2019 8:00 AM - 10:24 AM

Session K35 DQI: Semiconducting Qubits: Interface Characterization BCC5 205B - Patrick Harvey-Collard, Delft University of Technology - Tag(s): Focus

8:00AM K35.00001: A silicon metal-oxide-semiconductor quantum dot patterned with nano-imprint lithography* JOHN ROONEY (Presenter), NICHOLAS PENTHORN, JOSHUA S CHOENFIELD, HONGWEN JIANG, Physics, University of California, Los Angeles — We have transferred the metal gate pattern of a nanoscale depletion mode quantum dot onto a Si/SiO2 substrate with nano-imprint lithography (NIL), eliminating the use of e-beam lithography (EBL) and, consequently, reducing the effects of charge impurities. Critical features with 50 nm scale and separation can be dependably reproduced without making substantial changes to the device design. By studying charge transport through a quantum point contact and quantum dot, the prevalence of impurities was diminished in NIL devices when compared to similar EBL counterparts. Furthermore, 1/f charge noise was measured with an average of 1.4 µeV/√Hz at 1 Hz, equivalent to previous measurements made on EBL devices. This work offers a path toward reliable quantum dot operation in MOS by improving fabrication techniques to reduce charge impurities.

*This work was funded by the U.S. Army Research Office (ARO) through Grant No. # W911NF-17-1-0242

8:12AM K35.00002: Vibrational modes at the Si/SiO2 interface detected by pulse electron spin resonance* MARCO FANCIULLI (Presenter), Department of Materials Science, University of Milano-Bicocca, Milan, Italy, MATTEO BELLI, MDM Laboratory, IMM, CNR, Agrate Brianza, Italy, ROGÉRIO DE SOUSA, Department of Physics and Astronomy, University of Victoria, Victoria, British Columbia, Canada — Electron spin relaxation mechanisms for dangling bonds (Pb centers) at the Si/SiO2 interface in silicon nanowires produced by metal assisted chemical etching have been investigated by pulse electron spin resonance. The increased interface area in the nanowires provides the signal to noise ratio required to detect non-exponential decay of spin magnetization The spin-lattice relaxation rates are reported in the temperature range 4-300 K and the experimentally observed temperature dependence is explained in terms of the excess vibrational modes which manifest as tunneling two level systems (TTLS) giving rise to the so called “boson peak” of the amorphous interface. The experiment together with a theory of the spin relaxation mechanism which involves TTLSs provide a novel method to address the boson peak and other issues related to the role of the TTLSs in determining noise and decoherence in qubits and other sensitive devices.

*R.d.S. acknowledges financial support from NSERC (Canada) through its Discovery (RGPIN-2015- 03938) and Collaborative Research and Development programs (CRDPJ 478366-14).

8:24AM K35.00003: Fidelity of strongly driven electric dipole spin resonance* YASUHIRO TOKURA (Presenter), University of Tsukuba — Coherent control of a single spin confined in a quantum dot (QD) by the microwave electric field (electric dipole spin resonance; EDSR) is an active field of recent research. One of the required mechanisms to couple the orbital motion to the spin degree of freedom is to utilize the slanting magnetic field [1]. J. Yoneda et al.[2] had reported EDSR with a large Rabi frequency up to 100 MHz by optimizing the design of the micro-magnet as well as inducing larger power of microwave. In the largest achievable microwave amplitude, the Rabi frequency is saturated from the expected linear dependence with the microwave amplitude and the fidelity of the Rabi oscillation becomes degraded. Possible origin of this saturation is the non-parabolicity of the confinement potential [3]. In this report, we study the effect of the noise by strongly-driven orbital motion on the fidelity of the spin. In particular, the first (second)-order spin-orbital coupling induces enhanced spin-relaxations (decoherence) with increasing microwave amplitude.


*This work is supported by JSPS Kakenhi (26247051, 18k03479) and CREST JST (JPMJCR15N2).
Low power electric dipole spin resonance in silicon: theory

MONICA BENITO (Presenter), University of Konstanz, JASON R PETTA, Princeton University, GUIDO BURKARD, University of Konstanz, XANTHE CROOT, XIAO MI, Princeton University — Control of individual electron spins is one of the cornerstones of spin-based quantum technology. The application of ac magnetic fields allows to drive coherent spin rotations in electrons placed in gate-defined quantum dots, but there is a strong incentive to avoid magnetic driving since it is technically demanding and limits the Rabi frequency due to sample heating issues. Electric dipole spin resonance techniques, which harness some type of spin-orbit coupling to electrically control the electron spin state, provide a more robust possibility [1,2]. Since the intrinsic spin-orbit coupling for electrons in silicon is very weak, the development of novel efficient tools for spin control applicable to silicon based quantum devices is desirable [2-5]. Here, we present a theoretical investigation of an efficient novel mechanism in silicon quantum dots to induce single electron coherent spin rotations relying on an external magnetic field gradient.


Low power electric dipole spin resonance in silicon: experiment

XANTHE CROOT (Presenter), Department of Physics, Princeton University, Princeton, NJ 08544, USA, MONICA BENITO, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany, XIAO MI, Department of Physics, Princeton University, Princeton, NJ 08544, USA, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany, JASON R PETTA, Department of Physics, Princeton University, Princeton, NJ 08544, USA — Spin-based quantum information processing requires exquisite single spin control. While electron spin resonance is a natural means of controlling spin qubits in gate-defined quantum dots, generating localized ac magnetic fields large enough to drive coherent oscillations is challenging. As an alternative, electric dipole spin resonance (EDSR) can be employed [1]. Spin-orbit coupling often mediates EDSR: however, intrinsic spin-orbit coupling in silicon is small. To overcome this, on-chip micromagnets can be used to generate synthetic spin-orbit interactions [2], with EDSR having now been demonstrated in silicon [3, 4]. Here we present experimental results using a new technique for low-power EDSR in silicon with micromagnets, in a step towards scalable power budgets for large-scale spin-based quantum processors.


Charge offset drift in single electron devices containing aluminum oxide

RYAN MATTHEW STEIN (Presenter), Material Science and Engineering, University of Maryland, College Park, YANXUE HONG, Electrical and Computer Engineering, University of Maryland, College Park, BINHUI HU, ANDREW J MURPHY, NEIL ZIMMERMAN, JOSHUA POMEROY, MICHAEL DAVID STEWART, National Institute of Standards and Technology — Single electron devices (SEDs) suffer from a long-time instability, referred to as charge offset drift (ΔQ0), that hampers integration of SEDs in applications such as quantum metrology and computing. Previous measurements of ΔQ0 show SEDs containing aluminum oxide (AlOx) have been less stable than comparable SEDs containing only silicon dioxide (SiO2). Here, we have fabricated two different types of SEDs: all-metal Al/AlOx/Al tunnel junction-based devices and tunable barrier silicon metal-oxide-semiconductor (MOS) devices. The all-metal SEDs contain plasma-oxidized AlOx as the tunnel barrier. The charge offset stability measured on these devices is better than any other reported metallic SEDs, displaying a very small linear ΔQ0 of 0.1e over 7.5 days and two times lower standard deviation. The MOS SEDs are made on a silicon-on-insulator (SOI) substrate with a thermal SiO2 gate oxide, Al gates, and thermal AlOx as an isolation oxide. Four of the five MOS SEDs measured show a linear charge offset drift of less than 0.07 e over 7 days and standard deviations less than 0.02 e. These results suggest the stability of devices made with AlOx may be significantly better than previously thought and that other factors, such as geometry, are playing as large a role as materials.
9:12AM K35.00007: Probing decoherence at an atom-defect quantum interface† XUE HAN (Presenter), ALEC CAO, ALEC JENKINS, DOLEV BLUVSTEIN, University of California, Santa Barbara, SHUO MA, Physics, Princeton University, KUNAL MUKHERJEE, DAVID MINOT WELD, ANIA CLAIRE JAYICH, University of California, Santa Barbara — The atomic-scale quantum properties of interfaces play a central role in the ubiquitous surface-mediated decoherence that currently limits a wide variety of quantum technologies. We have constructed a novel instrument for quantitatively studying decoherence at active quantum surfaces. This hybrid quantum system combines neutral atoms adsorbed onto a diamond surface in ultrahigh vacuum conditions and subsurface nitrogen vacancy (NV) centers. We present measurements of the decoherence and relaxation rates of shallow NV centers interacting with atomic adsorbates deposited at thicknesses varying from angstroms to nanometers. As adsorbate atoms are added, we observe a significant reduction in spin relaxation time. We present progress towards a detailed understanding of coherence at this model quantum interface, with important consequences for a broad range of quantum interfaces.

*DOE BES Quantum Information Sciences program

9:24AM K35.00008: Ultra-thin body buried oxide 28nm FD-SOI platform for silicon quantum dots† CLAUDE ROHRBACHER (Presenter), SOPHIE ROCHELLE, JULIEN CAMIRAND LEMYRE, ALEXANDRE BÉDARD-VALLÉE, PASCAL LEMIEUX, Institut quantique, Universite de Sherbrooke, PHILIPPE Galy, THOMAS BEDECARRATS, FRANCK ARNAUD, Technology and Design Platforms Research and Development Center, STMicroelectronics, DOMINIQUE DROUIN, Departement de Genie Electrique et Informatique, Universite de Sherbrooke, MICHEL PIORO-LADRIERE, Institut quantique, Universite de Sherbrooke & Canadian Institute for Advanced Research — Silicon spin qubits, with their long coherence time and their compatibility with CMOS industrial technology shows great promise for large scale quantum computing and co-integration. Here we present a UTBB FD-SOI platform that is designed to operate as a transistor and host quantum dots. This platform is composed of NMOS structures with wire gate and split enhancement gate geometries, and is entirely fabricated inside STMicroelectronics’ standard process line. We explore various regimes in gate voltage space and demonstrate reproducible operation of multiples devices at 1.5 K and 10m K. We identify various regime for formation of quantum dots including electrostatic single and double quantum dots. We also present a cryogenic characterization of classical FD-SOI transistors that involves variation of mobility, kink effect and split C-V analysis down to 10 mK. These results set a pathway towards improved FD-SOI devices and quantum dots fully fabricated in standard process line.

*This work was supported by the Fonds de Recherche du Québec Nature et Technologies and the Canada Foundation for Innovation (CFI). This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund.

9:36AM K35.00009: Magnetotransport of metal-oxide-semiconductor devices fabricated on highly enriched 28Si ARUNA RAMANAYAKA (Presenter), KE TANG, HYUN-SOO KIM, Joint Quantum Institute, JOSEPH HAGMANN, National Institute of Standards and Technology, RYAN MATTHEW STEIN, Joint Quantum Institute, MICHAEL DAVID STEWART, CURT A RICHTER, JOSHUA POMEROY, National Institute of Standards and Technology — Isotopically enriched 28Si is regarded as an ideal environment for quantum computation (QC) as elimination of unpaired nuclear spins can result in low error rates for QC. At NIST we have developed a method to grow isotopically enriched 28Si, which provides the unique advantage of targeting a desired enrichment anywhere between natural abundance and the highest possible enrichment > 99.99998 % 28Si isotopic fractions. To explore the electrical properties of 28Si, we fabricate gated Hall bar devices and study the magnetotransport at magnetic fields (B) 12 T and temperatures (T) ranging from 1.2 K to 10 K. The magnetoresistance at |B| ≤ 0.25 T shows maximum mobilities of ≈ 1700 cm²/(V×s) and ≈ 6000 cm²/(V×s) at an electron density of ≈ 2.5×10¹² cm⁻² for devices fabricated on 28Si and natSi, respectively. We use the T dependence of weak-localization and Shubnikov-de Haas oscillations to deduce the dominant scattering mechanisms in these devices. We believe that the lower mobility observed for the devices fabricated on 28Si is due to the dilute adventitious C, N and O detected in 28Si. We will also discuss the preliminary results of fabrication and measurement of gate defined quantum dot devices in 28Si epilayers.
New Linear-Optical Approach to Quantum Information Processing and Quantum Simulation
ALEXANDER SERGIENKO (Presenter), DAVID SIMON, SHUTO OSAWA, Boston University — Linear optical networks formed from beam splitters and phase shifters have been shown capable of carrying out all quantum information processing tasks, but at the cost of rapid growth in resources as the complexity of the task increases. Here, we show that the use of recently introduced directionally unbiased optical multiports (N≥3), where input ports can double as output ports, can achieve results with much more compact setups and with substantial savings in resources. The behavior of such multiports is highly flexible, with a variety of possible behaviors being controlled by a set of parameters that can be changed or tuned in real time. Here we give an overview of the properties and potential applications of these multiports. Applications include their use as high-dimensional coins and lattice sites for quantum walks, new type of logical gates for two-photon entangled states, and elements of optical simulators for solid state systems. We illustrate that the band structures and electronic behavior of a variety of solid state systems, including those with nontrivial topological behavior, can be simulated using relatively compact linear-optical systems based on such directionally unbiased multiports.

Manipulation of entanglement sudden death in an all-optical experimental setup
ASHUTOSH SINGH (Presenter), URBASI SINHA, Raman Research Institute — Entanglement sudden death (ESD) is the phenomenon wherein a multipartite entangled state disentangles in finite time even when individual qubits decohere only asymptotically in time due to noise. Prolonging the entanglement is essential for the practical realization of entanglement-based quantum information and computation protocols. For this purpose, local NOT operation in the computational basis on one or both qubits has been proposed to combat the amplitude damping noise. Here, we aim to discuss an all-optical-experimental implementation of the NOT operations that can hasten, delay, or avert ESD, all depending on when it is applied during the process of decoherence for the polarization entangled photonic qubit system[1]. Further, the preparation and characterization of a polarization entangled photon source instrumental in obtaining the exciting experimental results on the manipulation of ESD along with the attendant theory will be presented.


Implementation and Simulation of Electrostatically Controlled Quantum Dots in CMOS Technology
DIRK LEIPOLD (Presenter), equal1, HANNES LEIPOLD, USC, LUTZ LEIPOLD, equal1, ELENA BLOKHINA, PANAGIOTIS GIOUNANLIS, KRZYSZTOF POMORSKI, ROBERT STASZEWSKI, UCD, IMRAN BASHIR, GEORGE MAXIM, MIKE ASKER, equal1, CAGRI CETINTEPE, ALI ESMAILIYAN, HONGYING WANG, TEERACHOT SIRIBURANON, UCD — A new architecture of a charge qubit suitable for implementation in large scale CMOS circuits is presented. We demonstrate techniques for time-independent / time-dependent simulations of quantum states and transport in such quantum dots. The time-independent technique makes use of a semi-analytical approach in the Schrödinger formalism combining the calculations of the electric field in CMOS structures with a piece-wise potential approximation of eight or more potential wells. The time-dependent technique leverages the semi-analytical approach to obtain the evolution of eigen states in explicit form. The techniques are upgraded to calculations based on the density matrix. This approach allows estimations of transition frequencies, leakage of the wavefunction between quantum states, and decoherence due to finite potentials and asymmetries of CMOS structures. Based on the height of the barrier between the wells, the behavior can be interpreted as semi-classical single electron transport, CNOT quantum gate operation, or quantum annealing. The presented approach allows the design of quantum gates compatible with conventional CMOS technologies and operating at 4K. The structure was standard foundry solution. We describe the implementation including integrated control structure

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K36 DPOLY: Recent Progress in Polymer Crystallization
BCEC 205C - Toshikazu Miyoshi, The University of Akron - Tag(s): Invited
Observation of scrolled single crystals of even-even nylons helped solve the decades long issue of their negative unbalanced surface stresses in the lamellae fold surfaces. These stresses induce twisted and scrolled lamellae, and very recent examples include the impact and identification of helical hand in crystal structures and the origin of branching, scrolled crystals. Their analysis helps reach some very finer details of the crystalline polymers' buildup. Older these constraints lead to unusual features of their diffraction pattern (e.g. specific streaks) or morphology (e.g. lamellar branching, scrolled crystals). Their analysis helps reach some very finer details of the crystalline polymers' buildup. Older and very recent examples include the impact and identification of helical hand in crystal structures and the origin of unbalanced surface stresses in the lamellae fold surfaces. These stresses induce twisted and scrolled lamellae.

Observation of scrolled single crystals of even-even nylons helped solve the decades long issue of their negative spherulites' architecture.

Shape-Symmetry Incommensurate Polymer Crystals

Crystallization is ubiquitous in nature and semicrystalline polymers are of crucial importance in our daily life. Because of their long chain nature, polymers crystallize via a more complex pathway, leading to profound metastable states and morphology. This talk will focus on polymer crystals whose shape is incommensurate with three-dimensional translational symmetry. Examples are helix, tubes and spheres. Not only can this shape-symmetry incommensurateness arise from the intrinsic characteristics of the crystal such as unbalanced chain folding and/or local stress, it also can be imparted by nanoscale confinement. Both cases will be discussed, and emphasis will be given to the formation mechanism, associated properties and possible applications of these unique polymer single crystals.

References


In Situ Real-Time Observation of Polymer Folded-Chain Crystallization by Atomic Force Microscopy at the Molecular Level

The crystallization process of a folded-chain crystal (FCC) was clearly visualized at the molecular level in situ and in real time for the first time [1]. We deposited an amorphous isotactic poly(methyl methacrylate) monolayer on mica, and the crystallization of the monolayer under high humidity was followed by atomic force microscopy. Detailed crystallization behaviors, especially, the stepwise growth of the FCC with blocks shorter than the chain, chain slipping in the FCC, the formation of an anisotropic nucleus and its growth, and the formation of a small nucleus with a short lifetime, were clearly visualized at the molecular level. The stepwise growth of the FCC differed from that expected by the classical Lauritzen-Hoffman theory and was consistent with recent reports that indicated the formation of some ordered states in the amorphous phase. In addition, the crystallization process of a poly(lactide), which formed an extended-chain crystal (ECC) in a monolayer was also visualized, and will be discussed.

The self-assembly, melting behavior and crystallization kinetics of polyethylenes with moieties placed at an exact equal distance along the backbone will be presented with especial focus on recent studies of the crystalline properties of precision polyethylenes with halogens (as pendant), and acetics (in-chain) groups under rapid and isothermal crystallization from the melt. The observed discrete minima in the temperature coefficient of the crystallization kinetics correlates with transitions between polymorphic structures that differ in packing symmetry. The minima or retardation of crystallization kinetics may be due to self-poisoning at the growth front or to differences in nucleation and growth between two polymorphs at the transition temperature. Control over different layered crystalline structures, demonstrate the ability of these novel systems to generate new polyethylene-based materials based on nanostructures at the lamellar and sub-lamellar level not feasible in classical branched polyethylenes.


*Work supported by NSF, DMR-Polymers

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K37 GMAG DCMP DCOMP: Triangular Lattices

8:00AM K37.00001: Hierarchy of Exchange Interactions in the Triangular-Lattice Spin Liquid YbMgGaO₄ [Invited]
FAHAD MAHMOOD (Presenter), XINSHU ZHANG, Johns Hopkins University, MARCUS DAUM, Georgia Institute of Technology, ZHILING DUN, University of Tennessee, JOSEPH PADDISON, Georgia Institute of Technology, NICHOLAS LAURITA, Johns Hopkins University, TAO HONG, Oak Ridge National Laboratory, HAIDONG ZHOU, University of Tennessee, PETER ARMITAGE, Johns Hopkins University, MARTIN MOURIGAL, Georgia Institute of Technology — The spin-1/2 triangular lattice antiferromagnet YbMgGaO₄ has attracted attention recently as a quantum spin-liquid candidate with the possible presence of off-diagonal anisotropic exchange interactions induced by spin-orbit coupling. Whether a quantum spin liquid is stabilized or not depends on the interplay of various exchange interactions with chemical disorder that is inherent to the layered structure of the compound. We combine time-domain terahertz spectroscopy and inelastic neutron scattering measurements in the field-polarized state of YbMgGaO₄ to obtain better insight of its exchange interactions. Terahertz spectroscopy in this fashion functions as a high-field electron spin resonance and probes the spin-wave excitations at the Brillouin zone center, ideally complementing neutron scattering. A global spin-wave fit to all our spectroscopic data at fields over 4 T, informed by the analysis of the terahertz spectroscopy linewidths, yields constraints on the disorder-averaged g factors and exchange interactions. Our results paint YbMgGaO₄ as an easy-plane XXZ antiferromagnet with the combined and necessary presence of subleading next-nearest neighbor and weak anisotropic off-diagonal nearest-neighbor interactions. Moreover, the obtained g factors are substantially different from previous reports. This work establishes the hierarchy of exchange interactions in YbMgGaO₄ from high-field data alone and thus strongly constrains possible mechanisms responsible for the observed spin-liquid phenomenology.
8:36AM K37.00002: Hidden order and its quantum excitations in the triangular-lattice magnet TmMgGaO₄
YAO SHEN (Presenter), CHANGLE LIU, YAYUAN QIN, SHOUDONG SHEN, Fudan University, YAODONG LI, Physics, University of California Santa Barbara, ROBERT BEWLEY, Rutherford Appleton Laboratory, ASTRID SCHNEIDEWIND, Jülich Centre for Neutron Science, GANG CHEN, JUN ZHAO, Fudan University — Certain magnetic materials exhibit exotic hidden-order phases, which are not directly accessible to conventional magnetic measurements due to the lack of internal field. Thus, experimental identification and theoretical understanding of a hidden order are difficult. Here we combine neutron scattering and thermodynamic probes to study the newly discovered rare-earth triangular-lattice magnet TmMgGaO₄. Magnetic Bragg peaks at K points are observed in the elastic neutron diffraction measurements. More interesting, however, is the observation of sharp and highly dispersive spin excitations that cannot be explained by a magnetic dipolar order, but instead is the direct consequence of the preformed multipolar order that arises from a rather weak crystal field splitting and is “hidden” in the conventional magnetic measurements. We demonstrate that the observed unusual spin correlations and thermodynamics can be accurately described by a transverse field Ising model on the triangular lattice with an intertwined dipolar and ferro-multipolar order.

8:48AM K37.00003: Investigating the Dynamic Magnetic Properties of Triangular Antiferromagnet YbZnGaO₄
WILLIAM STEINHARDT (Presenter), SACHITH DISSANAYAKE, ZHENZHONG SHI, Duke University, NICHOLAS BUTCH, Center for Neutron Research, National Institute of Standards and Technology, DAVID E GRAF, National High Magnetic Field Laboratory, YAOHUA LIU, Neutron Scattering Division, Oak Ridge National Laboratory, HONGCHENG LU, CASEY MARJERRISON, SARA HARAVIFARD, Duke University — Recently the antiferromagnetic triangular-lattice family of materials RMM'O₄ (where R = rare earth, M and M' = transition or main group) has attracted much attention, due to their disordered ground state and possible link to quantum spin liquid state. In this talk we present results from our recent field-dependent single-crystal diffuse and inelastic neutron scattering experiments, as well as thermal- and magneto-transport measurements performed on YbZnGaO₄.

9:00AM K37.00004: Elastic and Inelastic Neutron Scattering Study of the Triangular Lattice Ising Antiferromagnet TmMgGaO₄
MARCUS DAUM (Presenter), ZHILING DUN, Georgia Institute of Technology, HAIDONG ZHOU, University of Tennessee, Knoxville, MARTIN MOURIGAL, Georgia Institute of Technology — The LnMgGaO₄ family of materials (with Ln= Yb³⁺, Er³⁺, and Tm³⁺) has been the focus of recent studies in frustrated magnetism due to the combination of anisotropic exchange interactions from strong spin obit coupling, geometrical frustration, and inherent site disorder of Mg²⁺ and Ga³⁺. In order to further understand the original compound, YbMgGaO₄, we have begun to investigate how the non-Kramers ion Tm³⁺ differs from Yb³⁺ when placed in a similar crystal structure. TmMgGaO₄ displays a strong Ising behavior and magnetic scattering at the K-point of the triangular Brillouin zone at T= 0.05K. In this talk, I will present recent neutron scattering results on single-crystals of TmMgGaO₄ that elucidate the temperature and magnetic field dependence of spin correlations in that material.

*This work was supported by NSF Grant DMR 1750186.

9:12AM K37.00005: Gapless chiral spin liquid in spin-1/2 triangular Heisenberg model
SHOUSHU GONG (Presenter), Department of Physics, Beihang University, MAC LEE, DONNA SHENG, California State University, Northridge — We study the ground state of spin-1/2 triangular-lattice antiferromagnet with first- (J₁), second- (J₂), and third-neighbor (J₃) interactions, using large-scale density matrix renormalization group on cylinder geometry. By increasing the couplings, we establish a quantum phase diagram of the system. Besides the previously identified magnetic phases and J₁-J₂ spin liquid, we find a new gapless chiral spin liquid (CSL) phase with growing J₃, which emerges at the neighbor of the J₁-J₂ spin liquid. This CSL spontaneously breaks time-reversal symmetry by showing a robust three-spin scalar chiral order and the chiral edge mode in the entanglement spectrum. The finite-size scaling of spin triplet gap strongly suggests gapless spin excitations, which is further supported by the logarithmic behavior of the subsystem length dependence of entanglement entropy that leads to a finite central charge. The fitted central charge grows rapidly with increasing system width, which does not support a U(1) Dirac spin liquid but indicates an emergent spinon Fermi surface. This CSL realizes an example of interacting topological phase with chiral edge mode and gapless bulk excitations.
9:24AM K37.00006: Anisotropic-exchange magnets on a triangular lattice: dual spin liquids* ALEXANDER
CHERNYSHEV (Presenter), PAVEL MAKSIMOV, ZHENYUE ZHU, STEVEN ROBERT WHITE, University of California, Irvine — We establish a correspondence of the anisotropic-exchange model to an extended Kitaev-Heisenberg model. With the help of Klein dualities, deeper connections between different parts of the parameter space are established. Using these insights, we have performed DMRG studies of the quantum $S=1/2$ anisotropic-exchange model in previously unexplored parts of the phase diagram. The most important implication of the correspondence is that it necessitates an existence of a spin liquid that is Klein dual to the spin liquid found by us earlier. In our present DMRG study, we do confirm existence of this dual spin-liquid phase. With the structure factor $S(q)$, we also confirm that the dual spin liquid can be seen as a result of a melting of the dual 120° phase, same way as the earlier spin liquid is a molten 120° phase. The confirmation of the dual spin liquid strengthens our case for both of them.

*Supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences, Award No. DE-FG02-04ER46174

9:36AM K37.00007: Anisotropic-exchange magnets on a triangular lattice: spin waves and accidental degeneracies* PAVEL MAKSIMOV (Presenter), ZHENYUE ZHU, STEVEN ROBERT WHITE, ALEXANDER CHERNYSHEV, University of California, Irvine — We present an overview of the phase diagram, spin-wave excitations, and finite-temperature transitions of the anisotropic-exchange magnets on a nearest-neighbor triangular lattice. We investigate transitions between five principal classical phases: ferromagnetic, Néel, its dual, and the two stripe phases. Transitions are identified by the spin-wave instabilities and by the Luttinger-Tisza approach. In the stripe phases, quantum fluctuations are mostly negligible, leaving the ordered moment nearly saturated even for $S = 1/2$. However, for a 2D surface of the full 3D parameter space, the spin-wave spectrum in one of the stripe phases exhibits an accidental degeneracy. As a result, the ordering transition temperature in a wide region of the phase diagram is suppressed. This accidental degeneracy is due to a correspondence to an extended Kitaev-Heisenberg model with emergent symmetries.

*Funded by DOE No. DE-FG02-04ER46174

9:48AM K37.00008: Pressure-tuning of the quantum spin Hamiltonian of a triangular lattice antiferromagnet SERGEI ZVYAGIN (Presenter), Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, DAVID E GRAF, National High Magnetic Field Laboratory, Florida State University, TAKAHIRO SAKURAI, Research Facility Center for Science and Technology, Kobe University, SHOJIRO KIMURA, HIROYUKI NOJIRI, Institute for Materials Research, Tohoku University, JOACHIM WOSNITZA, Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, HITOSHI OHTA, Molecular Photoscience Research Center, Kobe University, TOSHIO ONO, Department of Physical Science, Osaka Prefecture University, HIDEKAZU TANAKA, Department of Physics, Tokyo Institute of Technology — Quantum antiferromagnets on a triangular lattice are prototype materials to investigate the phenomena of geometrical frustration in quantum matter. Apart from highly unusual magnetic properties, they possess a very rich phase diagram ranging from a simple unfrustrated square lattice to a quantum spin liquid, yet to be confirmed experimentally. One major obstacle in this area of research is the lack of materials with appropriate (ideally tuned) exchange coupling parameters. Here, we demonstrate an alternative approach where, instead of the chemical composition, the spin Hamiltonian of a triangular lattice antiferromagnet is tuned by hydrostatic pressure. The combination of tunnel-diode-oscillator and electron spin resonance techniques allows us to accurately monitor the spin-Hamiltonian parameters in Cs$_2$CuCl$_4$, revealing a significant increase of its exchange coupling ratio from 0.3 to 0.42 at a pressure of 1.8 GPa. A number of emerging field-induced transitions were observed in the high-pressure phase.
10:00AM K37.00009: Partial Magnetic Order in the Anisotropic Triangular Lattice System CeCd₃As₃  SARAH DUNSIGER (Presenter), TRIUMF, KOLAWOLE AKINTOLA, Department of Physics, Simon Fraser University, ANDRE COTE, Kwantlen Polytechnic University, ALEX FANG, SHAYAN GHEIDI, JEONGHUN LEE, SHYAM SUNDAR, EUNDEOK MUN, JEFF SONIER, Department of Physics, Simon Fraser University — CeCd₃As₃ is one member of a family of rare earth ternary compounds which crystallize into a hexagonal ScAl₃C₃-type structure, where the magnetic Ce-ions form a quasi two dimensional anisotropic triangular lattice. Such model geometrically frustrated systems have been proposed as candidates for quantum spin liquid behavior [1].

We report a muon spin relaxation investigation of the low temperature partially ordered phase and associated spin fluctuations of this material. The growth of an anomalous and sizable magnetic contribution to the specific heat below 10 K in CeCd₃As₃ has been found to correspond to enhancement in the spin lattice relaxation rate, which onsets on a temperature scale 20x the ordering transition. Tuning the conductivity through chemical substitution, we discuss the roles of geometric magnetic frustration, Kondo and Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions in interpreting the response of this Ce based intermetallic compound.


10:12AM K37.00010: Frustrated antiferromagnetic(AFM) order in CeCd₃As₃* KEENAN AVERS (Presenter), Physics, Northwestern University, ROMAN MOVSHOVICH, Condensed Matter and Magnet Sciences, Los Alamos National Laboratory, WILLIAM HALPERIN, Physics, Northwestern University, JOE D THOMPSON, PRISCILA ROSA, Condensed Matter and Magnet Sciences, Los Alamos National Laboratory — The relatively unexplored compound CeCd₃As₃ crystallizes in the P6₃/mmc space group, and has geometrically frustrated triangular arrangements of magnetic cerium atoms in the a/b plane. Magnetization measurements indicate strong out of plane AFM interactions. Our heat capacity, C(T), measurements on a single crystal reveal a sharp peak at Tₙ = 420 mK in zero field, consistent with an out of plane AFM phase transition. Applying a magnetic field within the easy-plane raises Tₙ to 490 mK at 2 T demonstrating lifting of frustration. At high fields Tₙ is suppressed to zero, and C(T) no longer resembles that of an AFM. Instead we observed an excess of entropy at the lowest temperatures measured. These results indicate competition between AFM order and frustration at low fields, and a field induced highly degenerate ground state at stronger fields.

*Work was conducted at Los Alamos National Laboratory under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. KEA and WPH acknowledge the U.S. Dept. of Energy DE-FG02-05ER46248, and the Northwestern Center for Applied Physics and Superconducting Technology. A portion of this work was supported by the Los Alamos Laboratory Directed Research and Development program

10:24AM K37.00011: Magnon topology and thermal Hall effect in trimerized triangular lattice antiferromagnet* KYUNGSU KIM, KI LEE (Presenter), Seoul National University, SUK BUM CHUNG, Department of Physics, University of Seoul, JE-GUIEN PARK, Seoul National University — Magnon band topology and magnon transverse responses have been studied in two-dimensional magnetisms for the last few years. The magnon band topology of the most well-known frustrated two-dimensional spin model antiferromagnetic triangular lattice has got less attention than its cousin Kagome systems because of the spin-chirality cancellation which prohibits thermal Hall effect.

In this work, we study the band topology and thermal Hall effect of triangular lattice antiferromagnet with the nearest-neighbor exchange and external field using linear spinwave theory. We clarify that the effect PT symmetry forces thermal Hall effect in distortion-free triangular lattice antiferromagnets to zero even when a perpendicular external magnetic field is applied. We show, however, that (anti-)trimerization distortion in antiferromagnetic triangular lattice removes the symmetry and gives nontrivial magnon band topology and the finite thermal Hall effect. Finally, we estimate the thermal Hall effect of triangular antiferromagnets with such distortions YMnO₃ and LuMnO₃.

*This work was supported by IBS-R009-G1 (K. K., K.H.L., and J-G. P.) and Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2018R1D1A1B07045899) (S. B. C.).
Selective measurements of intertwined multipolar orders: Non-Kramers doublets on a triangular lattice

CHANGLE LIU (Presenter), Department of Physics, Fudan University, YAODONG LI, Department of Physics, University of California, Santa Babara, GANG CHEN, Department of Physics, Fudan University — Motivated by the rapid experimental progress on the spin-orbit-coupled Mott insulators, we propose and study a generic spin model that describes the interaction between the non-Kramers doublets on a triangular lattice and is relevant for triangular lattice rare-earth magnets. We predict that the system supports both pure quadrupolar orders and intertwined multipolar orders in the phase diagram. We explore the magnetic excitations to reveal the dynamic properties of the systems. Due to the peculiar properties of the non-Kramers doublets and the selective coupling to the magnetic field, we further study the magnetization process of the system in the magnetic field. We point out the selective measurements of the static and dynamic properties of the intertwined multipolarities in the neutron scattering, NMR, and μSR probes and predict the experimental consequences. The relevance to the existing materials such as TmMgGaO₄, Pr-based, and Tb-based magnets, and many ternary chalcogenides is discussed. Our results not only illustrate the rich physics and the promising direction in the interplay between strong spin-orbit-entangled multipole moments and the geometrical frustration, but also provide a general idea to use noncommutative observables to reveal the dynamics of the hidden orders.

Physical properties of the trigonal binary compound Nd₂O₃

GABRIELE SALA (Presenter), MATTHEW BRANDON STONE, BINOD RAI, ANDREW MAY, CLARINA DELA CRUZ, GEORGE EHLERS, VASILE O GARLEA, MARK D LUMSDEN, Oak Ridge National Laboratory, HASITHA SURIYA ARACHCHIGE, Department of Physics and Astronomy, University of Tennessee, VICTOR R. FANELLI, Oak Ridge National Laboratory, DAVID GEORGE MANDRUS, Department of Material Science & Engineering, University of Tennessee, ANDY CHRISTIANSON, Oak Ridge National Laboratory — Nd₂O₃ is a structurally and chemically simple material which crystalizes in a trigonal structure, with Nd³⁺ ions surrounded by cages of 7 oxygen anions. Here we study the physical properties of Nd₂O₃ with neutron diffraction, inelastic neutron scattering, heat capacity, and magnetic susceptibility measurements. The inelastic neutron scattering measurements reveal that the crystal field spectrum consists of four excitations spanning the energy range 3-60 meV. The ground state eigenfunction consists of XY-spins in the ab plane. Fits to the magnetic susceptibility data indicate a Curie-Weiss temperature of θCW=-23.7(1) K. Neutron diffraction measurements show that long range antiferromagnetic order occurs below Tₐ=550 mK implying a frustration index of θCW / Tₐ ~43. These results suggest that Nd₂O₃ may be a model system for competing interactions between magnetic moments subject to strong spin-orbit coupling.

This work was supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K38 GMAG DMP: 2D Magnetism II

Spin Transfer Torques in Monolayer WSe₂/PMA Heterostructures

STEVE NOVAKOV (Presenter), Physics, University of Michigan, NGUYEN VU, Materials Science and Engineering, University of Michigan, BHAKTI JARIWALA, AZIM KOZHAKHMETOV, Department of Materials Science and Engineering, Pennsylvania State University, GUANYU ZHOU, CHRISTOPHER HINKLE, Materials Science & Engineering, University of Texas - Dallas, JOSHUA ROBINSON, Department of Materials Science and Engineering, Pennsylvania State University, JOHN HERON, Materials Science and Engineering, University of Michigan — Transition metal dichalcogenides (TMD), with composition MX₂ (M={Mo, W}, X={S, Se, Te}), are promising candidates for a variety of spintronics applications due to their intrinsic band properties [1]. In comparison to 3D spin Hall effect (SHE) materials, (typically conductive 5d/4f transition metal compounds such as Pt and W) semiconducting TMDs promise spin/charge conversion with a higher efficiency and tunability, which has been shown in heterostructures with insulating magnets [2]. Additionally, TMDs may allow for more efficient switching of magnets with perpendicular magnetic anisotropy (PMA) than 3D SHE systems due to stronger out of plane spin torques [3]. We report on the growth and spin torque measurements of PMA and monolayer WSe₂ heterostructures. The PMA film stacks were grown by pulsed laser deposition and the WSe₂ was deposited with molecular beam epitaxy and chemical vapor deposition. The heterostructures were patterned into Hall bar devices and subject to angle and field resolved spin torque measurements to characterize the torque geometry and switching efficiency.

*SRC nCore New Limits
**Imaging the Electronic Structure of Magnetic and Non-Magnetic Atomic Impurities in Monolayer Semiconductors**

CALEB ZERGER (Presenter), ALEX CONTRYMAN, HONG LI, XIAOLIN ZHENG, HARI MANOHARAN, Stanford University — It has been predicted that a two dimensional dilute magnetic semiconductor (2D DMS) can be formed by suitably doping monolayer transition metal dichalcogenides with magnetic materials. Here we present scanning tunneling microscopy (STM) and spectroscopy (STS) data on these doped monolayers. We identify and characterize multiple impurity types resulting from the doping procedure, observing both magnetic and non-magnetic impurities. Using a full spectral mapping in position and energy space, and through comparison to density functional theory calculations, we can associate these impurity states with different impurity types and incorporation sites. For example, we have found transition metal substitutional dopants and a dichalcogenide substitutional dopant. Specific dopant arrangements demonstrate strong spin splitting, a necessary ingredient towards achieving a 2D DMS state in monolayer semiconductors.

*Supported by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4537 and the U.S. DoE under contract DE-AC02-05CH11231

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**Magneto-Optical Kerr Effect microscopy on the intercalated transition metal dichalcogenides Fe₉TaS₂* ARIELLE LITTLE (Presenter), DYLAN REES, SPENCER DOYLE, CAOLAN JOHN, ERAN MANIV, JAMES G. ANALYTIS, JOSEPH ORENSTEIN, University of California, Berkeley — The layered transition metal dichalcogenide TaS₂ exhibits a broad range of phases including CDW states and superconductivity [1]; the polymorph 1T-TaS₂ has even been predicted to host a spin liquid [2]. Also of interest is the doping of such materials with metallic ions. In TaS₂ the intercalation of Iron between layers stabilizes ferromagnetic order. The magnetic properties vary drastically with the amount of intercalant, x [3]. For example, for x=0.33 chiral superlattice structures form [4]. Here we employ scanning Magneto-Optical Kerr Effect (MOKE) microscopy to image the onset of magnetic order and in some instances optical birefringence in compounds with intercalation from x=0.26 to 0.33. In the x=0.33 compound we report a sharp structural phase transition coincident with the magnetic transition and image the resulting domains on a 10-μm scale.


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**Thermodynamic "valley noise" in monolayer semiconductors: access to intrinsic valley relaxation timescales** MATEUSZ GORYCA (Presenter), Los Alamos National Laboratory, NATHAN WILSON, Department of Physics, University of Washington, PRASENJIT DEY, Los Alamos National Laboratory, XIAODONG XU, Department of Physics, University of Washington, SCOTT CROOKER, Los Alamos National Laboratory — The new class of atomically-thin transition-metal dichalcogenide (TMD) semiconductors such as monolayer MoS₂ and WSe₂ has focused broad attention on the concept of “valleytronics”, founded on the idea of encoding information in an electron’s valley degree of freedom. A key parameter is therefore the intrinsic timescale of an electron’s inter-valley relaxation, and recent optical pump-probe studies have shown long (microsecond) valley relaxation of resident carriers in monolayer TMDs [1,2]. However, a significant drawback of all such pump-probe experiments is that they are by design perturbative: the optical pumping that drives the carrier polarization away from equilibrium also inevitably introduces “dark” excitons, whose presence may mask the intrinsic valley relaxation of resident carriers.

Here we present a completely alternative approach for measuring valley dynamics, based on the idea of passively “listening” to the random spontaneous scattering of carriers between K and K’ valleys that occurs even in strict thermal equilibrium. We demonstrate that the stochastic valley noise is measurable by optical means and, in accord with the fluctuation-dissipation theorem, encodes the true intrinsic timescales of valley relaxation, free from any pumping, excitation, or other perturbative effects [3]. Using this new fluctuation-based methodology we measure very long valley relaxation dynamics of both electrons and holes in a single electrostatically-gated WSe₂ monolayers. Noise spectra reveal long intrinsic valley relaxation with a single sub-microsecond time scale. Moreover, they validate both the relaxation times and the wavelength dependence observed in conventional pump-probe measurements, thereby resolving concerns about the role of dark excitons and trions in studies of long-lived valley relaxation.

9:12AM K38.00005: Gap opening at the Rashba-split states of Janus transition metal dichalcogenides induced by two-dimensional ferromagnetic semiconductor CrI₃* TAO HU (Presenter), WEI REN, Shanghai University — The Janus transition metal dichalcogenides intrinsically have Rashba spin splitting due to the presence of the out-of-plane mirror-symmetry breaking and strong spin-orbit coupling (SOC). Using first-principles calculations, we show that a van der Waals (vdW) heterostructure consisting of WSeTe and CrI₃ has inherently coexistence of Rashba and Zeeman spin splitting near the Brillouin zone center (Γ). The Rashba spin splitting states of WSeTe open an exchange gap of 29 meV when it is placed on the top of two-dimensional (2D) ferromagnetic semiconductor CrI₃. The spin-polarized subbands of Rashba-split states are separated at the Γ point because of the existence of effective perpendicular magnetic field stemmed from CrI₃. In the crossover region of Rashba and Zeeman spin splitting, the spin orientations of the two subbands are locked to the momenta. A single-circle Fermi contour could emerge if the Fermi level is tuned to locate exactly within the gap between the two subbands. Our results provide important insight into the manipulation of spin states for future spintronics applications of 2D vdW heterostructures.

*This research was supported by the National Key Basic Research Program of China (Grant No. 2015CB921600), the Natural Science Foundation of China (Grants No. 51672171).

9:24AM K38.00006: Influence of the spatial fluctuations of the Rashba field and magnetization on the electron and spin transport in 2D systems* ANNA DYRDAL (Presenter), Institut für Physik, Martin-Luther Universität Halle-Wittenberg, D-06099 Halle, Germany, SYLWIA KUDLA, VITALII DUGAEV, Department of Physics and Medical Engineering, Rzeszow University of Technology, Al. Powstancow Warszawy 6, 35-959 Rzeszow, Poland, EVGENY SHERMAN, Department of Physical Chemistry, Universidad del País Vasco UPV-EHU, 48080, Bilbao, Spain, JOZEF BARNAS, Faculty of Physics, Adam Mickiewicz University in Poznan, ul. Umultowska 85, 61-614 Poznan, Poland, JAMAL BERAKDAR, Institut für Physik, Martin-Luther Universität Halle-Wittenberg, D-06099 Halle, Germany — In a general case, spin-orbit coupling contains regular (spatially uniform, periodic) and a random component. Local imperfections, such as a random distribution of donors or impurities, may lead to local modifications of the spin-orbit coupling. Similarly, magnetization in the system may reveal spatial fluctuations as well. Such fluctuations modify transport properties of the system and induce a variety of observable effects [Physica E 42, 2157 (2010); Nat. Phys.12, 920(2016)]. We will present the theoretical description of the selected transport characteristics (electric and spin conductivity and anomalous Hall effect) induced or modified due to the presence of random Rashba field or magnetization fluctuations in 2D systems such as semiconductor heterostructures or topological insulators. We will show an important role of the transport relaxation time for charge and spin currents, that leads to a nontrivial temperature dependence of the conductivity [S.Kudla et al., PRB 97, 245307(2018)]. We will also consider the influence of magnetization fluctuations on the anomalous Hall effect in topological insulators.

*This work has been supported by the National Science Center in Poland (project No. DEC-2017/27/B/ST3/02881) and by German Research Foundation through SFB 726 and SFB TRR 227.

9:36AM K38.00007: Electrically switching the valley polarization of 2D semiconductor LIZHONG LI (Presenter), SHENGWEI JIANG, Applied and Engineering Physics, Cornell University, ZEFANG WANG, Department of Physics, Penn State University, JIE SHAN, KIN FAI MAK, Applied and Engineering Physics, Cornell University — Controlling the valley degree of freedom in transition metal dichalcogenide(TMD) semiconductors is essential to the application of valleytronic devices. The strong magnetic coupling between monolayer TMD semiconductor WSe2 and few layer CrI₃, a recently discovered 2D magnet, provides a novel approach for lifting the valley degeneracy and switching the valley polarization. In this talk we present our result on gate controlled valley polarization in CrI₃/WSe₂ heterostructures. Due to the short-range magnetic proximity interaction, WSe₂ shows clear valley polarization controlled by the spin orientation of CrI₃. We demonstrate that the magnetic coupling between WSe₂ and CrI₃ could be effectively tuned by gate voltage, allowing reversible and efficient electrical switching of the valley polarization in WSe₂.
9:48AM K38.00008: Electrical gate control of photon-spin and photon-charge conversions in van der Waals heterostructures* [Invited] YUNQIU (KELLY) LUO (Presenter), ROLAND KAWAKAMI, Ohio State University — Semiconductor heterostructures of dissimilar materials are inherently limited by their interface quality, lattice mismatch, and intrinsic defects. These obstacles are overcome in van der Waals (vdW) heterostructures forming atomically sharp interfaces even between very different 2D materials. Our recent work demonstrates the efficient optically-created spin-polarized charge transfer across monolayer MoS2/graphene vdW interface, including complete control of spin polarization with photon helicity and photon energy up to room temperature. However, the underlying mechanisms and the qualitative trends in both photon-spin and photon-charge conversions remain elusive. To investigate origins of photon-charge conversion, we build a dual-gated MoS2/graphene field-effect device which allows multi-variable control of photon energy, bias voltage, and top and bottom gates. We observe an intriguing bias enhancement of photoconductivity, which behaves oppositely across graphene Dirac point. We further investigate the origins of photoconductivity using both above and below MoS2 band gap photon excitation. Gate dependence and photon intensity dependence indicate strongly towards the dominance of graphene photothermoelectric effect for below gap excitation, while an interplay of MoS2 photovoltaic effect and graphene photothermoelectric effect mediates above gap excitation. DFT and analytical models connect the role of bias voltage as an independent density of states modulation, which enhances the charge tunneling efficiency across the vdW barrier. In the end, we will briefly discuss the ultrafast photon-spin transfer across monolayer WSe2/graphene interface, as well as an outlook to the challenges and future of photon-spin and photon-charge conversions based on vdW hybrid systems.

*We acknowledge support from Ohio State Presidential Fellowship, collaborations with Dr. M. Neupane at U.S. Army Research Lab and Dr. T. Zhou, Prof. I. Zutic at Univ. at Buffalo, State Univ. of New York.

10:24AM K38.00009: Unconventional transport in low-density two-dimensional Rashba systems* JOEL HUTCHINSON (Presenter), JOSEPH MACJEJKO, University of Alberta — Rashba spin-orbit coupling appears in 2D systems lacking inversion symmetry, and causes the spin-splitting of otherwise degenerate energy bands into an upper and lower helicity band. In this talk, we explore how impurity scattering affects transport in the ultra-low density regime where electrons are confined to the lower helicity band. A previous study has investigated the conductivity in this regime using a treatment in the first Born approximation. In this work, we use the full T-matrix to uncover new features of the conductivity. We first present results for the conductivity within a semiclassical Boltzmann framework and show that it exhibits an unconventional density dependence due to the unusual features of the group velocity in the single particle dispersion, as well as quantized plateaus as a function of the logarithm of the electron density. We support this with results from the Kubo formula and find that these plateaus persist in the full quantum theory. We suggest that this quantization may be seen in a pump-probe experiment.

*This work was supported by NSERC, Alberta Innovates - Technology Futures (AITF), the Canada Research Chair Program (CRC), the Canadian Institute for Advanced Research (CIFAR), and the University of Alberta.

10:36AM K38.00010: Magnetism of a Magnetic-ion-intercalated Transition Metal Dichalcogenide with a Chiral Structure KAI DU (Presenter), JAE WOOK KIM, FEI-TING HUANG, SEONG JOON LIM, Rutgers University, New Brunswick, KASUN GAMAGE, JUNJIE YANG, Central Michigan University, MYUNG-GEUN HAN, Brookhaven National Laboratory, SANG-WOOK CHEONG, Rutgers University, New Brunswick — Chiral magnets are materials where various intriguing spin orders including skyrmions, chiral soliton lattice, and topological domain walls can be found in the presence of the structural chirality. On the other hand, the hunting for exotic magnetic systems that are possible to fabricate functional two-dimensional devices for applications is also in high demand. In this work, we demonstrate that a magnetic-ion-intercalated transition metal dichalcogenide (TMD) is a layered chiral magnet according to our magnetic measurements and Lorenz transmission electron microscopy studies. Using transmission electron microscopy and magnetic force microscopy, we investigated its chiral structural domains and magnetic domains, respectively. Their domain topologies and relations will also be discussed.
Spin-Phonon Coupling, Spin Waves, and Other Magnetic Phenomena in Layered XPS₃ Materials via Raman Spectroscopy

AMBER MCCREARY (Presenter), Nanoscale Device Characterization Division, Physical Measurement Laboratory, National Institute of Standards and Technology, JUN CAO, Department of Chemistry, Boston University, XI LING, Department of Chemistry, Division of Materials Science and Engineering, and The Photonics Center, Boston University, ROBERT D MCMICHAEL, ANGELA HIGHT WALKER, Nanoscale Device Characterization Division, Physical Measurement Laboratory, National Institute of Standards and Technology — Raman spectroscopy is a powerful, non-destructive optical method to probe the fundamental physics of two-dimensional (2D) layered materials through inelastic scattering. An amazing amount of information is quantified from the spectra such as layer thickness, disorder, edge and grain boundaries, strain, etc. More interestingly for 2D materials is that Raman efficiently probes the evolution of the electron-phonon and spin-phonon interactions as a function of temperature, laser energy, polarization, and magnetic field. Using our unique magneto-Raman capabilities, we study the magnetic properties of the metal phosphorus trisulfide family (XPS₃, where X = Fe, Mn, and Ni) which are layered antiferromagnetic semiconductors. While the three materials have the same crystal structure, their varying spin structures result in distinct behavior as a function of temperature and magnetic field, which will be presented herein. In FePS₃, we investigate the splitting and shifting of a non Γ-point phonon mode below the Neel temperature that is not present in MnPS₃, as well as the emergence of a spin wave with anomalous symmetry behavior. In addition, we have studied the apparent two-magnon mode in NiPS₃ under various conditions.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K39 GMAG DMP: Spin Pumping

8:00AM K39.00001: Enhanced spin pumping into superconductors provides evidence for superconducting pure spin currents [Invited] CHIARA CICCARELLI (Presenter), University of Cambridge — Unlike conventional spin-singlet Cooper pairs, spin-triplet pairs can carry spin. Triplet supercurrents were discovered in Josephson junctions with metallic ferromagnet spacers, where spin transport can occur only within the ferromagnet and in conjunction with a charge current. Ferromagnetic resonance injects a pure spin current from a precessing ferromagnet into adjacent non-magnetic materials. For spin-singlet pairing, the ferromagnetic resonance spin pumping efficiency decreases below the critical temperature (Tc) of a coupled superconductor. Ciccarelli and collaborators present ferromagnetic resonance experiments in which spin sink layers with strong spin–orbit coupling are added to the superconductor. Their results show that the induced spin currents, rather than being suppressed, are substantially larger in the superconducting state compared with the normal state; although further work is required to establish the details of the spin transport process, they show that this cannot be mediated by quasiparticles and is most likely a triplet pure spin supercurrent.

8:36AM K39.00002: Probe of spin dynamics in superconducting NbN thin films via spin pumping* YUNYAN YAO (Presenter), QI SONG, International Center for Quantum Materials, School of Physics, Peking University, YOTA TAKAMURA, JUAN PEDRO CASCALES, Plasma Science and Fusion Center and Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, WEI YUAN, YANG MA, YU YUN, XINCHENG XIE, International Center for Quantum Materials, School of Physics, Peking University, BEIJING, JAGADEESH MOODERA, Plasma Science and Fusion Center and Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, WEI HAN, International Center for Quantum Materials, School of Physics, Peking University, BEIJING — The emerging field of superconductor (SC) spintronics has attracted intensive attentions recently. Many fantastic spin-dependent properties in SCs have been discovered, including large magnetoresistance, long spin lifetimes, and the giant spin Hall effect, etc. Regarding the spin dynamics in superconducting thin films, few studies have been reported yet. Here, we report the investigation of the spin dynamics in an s-wave superconducting NbN film via spin pumping from an adjacent insulating ferromagnet GdN film. A profound coherence peak of the Gilbert damping of GdN is observed slightly below the superconducting critical temperature of the NbN, which agrees well with recent theoretical prediction for s-wave SCs in the presence of impurity spin-orbit scattering. This observation is also a manifestation of the dynamic spin injection into superconducting NbN thin film. Our results demonstrate that spin pumping could be used to probe the dynamic spin susceptibility of superconducting thin films, thus pave the way for future investigation of spin dynamics of interfacial and two-dimensional crystalline SCs.

*National Basic Research Programs of China (973 program Grant Nos. 2015CB921104 and 2014CB920902) and National Natural Science Foundation of China (NSFC Grant No. 11574006).
8:48AM K39.00003: Efficient spin current generation from new, low-loss Mg(Al,Fe)2O4 films into heavy metals
LAUREN RIDDIFORD (Presenter), JACOB WISSER, Geballe Laboratory for Advanced Materials, Stanford University, SATORU EMORI, Physics, Virginia Tech, PENG LI, Geballe Laboratory for Advanced Materials, Stanford University, DEBANGSU ROY, EGECAN COGULU, Physics, New York University, OLAF M VAN T ERVE, Naval Research Laboratory, YONG DENG, SHAN X WANG, Materials Science, Stanford University, BEREND JONKER, Naval Research Laboratory, ANDREW D KENT, Physics, New York University, YURI SUZUKI, Geballe Laboratory for Advanced Materials, Stanford University — Low-damping magnetic insulators are essential to the growing field of spintronics since they can generate and transfer spin currents without associated charge currents. We have recently developed a new ferrimagnetic insulator, MgAl0.5Fe1.5O4 (MAFO), which has Gilbert damping as low as 1x10^-3. Through resonant excitation of the MAFO layer, we observed significant spin pumping from MAFO films into adjacent Pt and β-W layers by enhanced Gilbert damping and electrical voltage peaks that appear at ferromagnetic resonance (FMR). There is a reversal of the transverse voltage signal in MAFO/Pt and MAFO/β-W, which is consistent with the opposite signs of the spin Hall angle in these two materials and indicates the signal is due to the inverse spin Hall effect and not to proximity-induced anisotropic magnetoresistance (AMR). Further, angular dependent magnetoresistance (ADMR) measurements reveal that the spin Hall magnetoresistance (SHMR) is 7-10 times larger than the AMR contribution, so spin pumping effects dominate the magnetic dynamics of the bilayers. From FMR and ADMR measurements, we deduced a spin-mixing conductance of ~3x10^14 Ω^-1 m^-2 in MAFO/Pt. Together, these measurements indicate that MAFO is an excellent candidate for efficient spin current-based heterostructures and devices.

9:00AM K39.00004: Ferromagnetic Resonance and Spin Transport in Epitaxial Manganite/Ruthenate Bilayers
PURNIMA BALAKRISHNAN (Presenter), Stanford University, SATORU EMORI, Virginia Tech, YURI SUZUKI, Stanford University — Spin current generation by spin-pumping from a ferromagnet into a non-magnetic metal has been of great interest recently. However the role of the interface in the efficient pumping of spin current into the non-magnetic metal has not been addressed extensively. We address this issue by studying coherent interfaces in epitaxial oxide bilayers. Here we report recent results on spin pumping in pulsed-laser deposited bilayers of the ferromagnetic metal La2/3Sr1/3MnO3 (LSMO) and the paramagnetic metals SrRuO3 (SRO) and CaRuO3 (CRO). X-ray diffraction indicates excellent crystallinity of the bilayers. CRO layers are under tensile strain on LSMO films grown on LSAT substrates, in contrast to SRO layers which are under compressive strain. Ferromagnetic resonance measurements of LSMO films indicate that the Gilbert damping parameter can be as low as 1x10^-3. This damping increases with the addition of an epitaxial ruthenate overlayer of SRO or CRO consistent with spin pumping. From the ruthenate thickness dependence of the Gilbert damping, we estimate that the spin diffusion length is larger in CRO than in SRO. We will also discuss the role of proximity-induced magnetism on spin transport in bilayers with SRO versus CRO, which has no ferromagnetic transition.

MIJIN LIM (Presenter), HYUN-WOO LEE, Physics, Pohang University of Science and Technology(POSTECH), Pohang 37673, Korea — Spin conservation at an interface influences several spin transport phenomena such as spin-to-charge conversion and spin-orbit torque. If spin flips at the interface, the spin information may be lost, which is called a spin-memory loss. [1] We claim that large atomic spin-orbit coupling(SOC) and interfacial inversion symmetry breaking(ISB) are important elements of spin-flip scattering in the heterostructure that consists of a nonmagnetic metal with strong SOC and a ferromagnet. To study those effects, we calculate the change of spin information during the reflection/transmission using the tight-binding method. Here, we report two main findings. The first is about the spin-flip resulting from the SOC-induced entanglement of spin and orbital degree of freedom. The other is that the inversion symmetry breaking at an interface, which allows specific inter-orbital hopping [2], generates an additional spin-flip. We argue that these processes contribute to the interfacial spin-memory loss and spin transparency in spintronics devices. [1, 3]


*Samsung Science & Technology Foundation (Grant No. BA-1501-07)
9:24AM K39.00006: Enhancement of spin-motive force in systems with broken inversion symmetry* YUTA YAMANE (Presenter), RIKEN — The exchange interaction between the conduction electron spin and the local magnetization is responsible for spin-transfer torque, which provides an promising way of manipulating the magnetization by charge current. The same interaction can also mediate an electric-voltage generation by dynamical magnetic textures, i.e., spin-motive force (SMF). A SMF reflects spatiotemporal variation of the magnetization, and thus offers a powerful method to probe and explore various dynamical magnetic textures.

The experimentally observed SMFs thus far are typically 100nV-1μV. To achieve larger SMF is deemed indispensable towards realization of spintronic devices actively exploiting SMF. In this work we address this problem demonstrating that, in the presence of Dzyaloshinskii-Moriya Interaction (DMI), the SMF due to field-induced domain-wall motion can be dramatically enhanced[1]. The presence of DMI leads to extra spatial rotation of the magnetization, which turns out to play a crucial role in the enhancement of SMF. Our results suggest a new perspective on inversion-symmetry-broken systems as a suitable stage for pursuit of larger SMF.


*This research was supported by Research Fellowship for Young Scientists from Japan Society for the Promotion of Science.

9:36AM K39.00007: Optically generated spin currents in platinum/magnetic insulator bilayer structures* JOSEPH MURPHY (Presenter), SUBASH KATTEL, University of Wyoming, JINJUN DING, TAO LIU, MINGZHONG WU, Colorado State University, WILLIAM RICE, University of Wyoming — The generation and detection of pure spin current provides a pathway for solid-state devices to avoid Joule heating losses arising in electrical architectures.

Despite the promise of loss-free, spin-based devices, integrated spin current technology into real-world applications has proven difficult.

Here, we use a Pt/Y₃Fe₅O₁₂ (YIG) bilayer device to detect light from 390 nm to 2200 nm using the spin Seebeck effect (SSE).

We find that the nanometer-thick platinum layer is crucial for both spin current generation and detection.

We use a phase-sensitive, field-modulation technique to determine the temperature gradient across the YIG, \(\nabla T\), created by optical illumination, \(I\), to be \(\nabla T/I = 0.0975^\circ\text{C} \cdot \text{m}/\text{W}\).

From our measured values of \(\nabla T\) and \(\nabla V\), we obtain the SSE coefficient of YIG to be \(S_{\text{spin}} = -\nabla V/\nabla T = -1.1 \text{nV/K}\); this value is consistent with reported literature values for other SSE materials.

This work reveals the possibility of using spin current generation and detection for broadband light optoelectronics.

*JRM, SK and WDR acknowledge support from NASA through Grant No. WY-80NSS17M0049 and through the University of Wyoming School of Energy Resources.

9:48AM K39.00008: Nonlinear magnon study by microwave perpendicular pumping ferromagnetic resonance in thin films* TAO QU (Presenter), ANEESH VENUGOPAL, JAMES ETHERIDGE, KARTHIK SRINIVASA, WILLIAM PERIA, BETHANIE STADLER, PAUL CROWELL, RANDALL VICTORA, University of Minnesota — To investigate the nonlinear effects arising from magnon coupling to microwaves and their application to the new functionality of monolithically integrated magnetic components on semiconductor substrates, it is important to exploit non-linear ferromagnetic resonance in magnetic insulator materials. We have studied the nonlinearity caused by the three magnon scattering mechanism in GHz ferromagnetic resonance in simulation and analytically. The thicknesses of the studied YIG films are varied in the range of nanometers to several micrometers. A realistic micromagnetic simulation is implemented to capture the physical mechanisms coupling magnons of sub-micrometer wavelengths and microwaves of centimeter wavelength using CUDA parallel high-performance computing. Using the Holstein-Primakoff transformation and equation of motion in the theoretical model, we obtain the analytical magnon dispersion and the power threshold function. The power threshold for the three-magnon process is sensitive to the material properties. We find that the non-linearity is due primarily to incoherent magnon modes propagating in the thin film plane, while the modes propagating out of the film plane exist, but with much smaller occupation numbers.

*We thank DARPA and XSEDE for funding this project.
10:00AM K39.00009: Spin pumping in a material with metal-insulator transition  TAQIYYAH SAFI (Presenter), LUQIAO LIU, Massachusetts Institute of Technology — Ferromagnetic resonance driven spin pumping is a powerful tool to study the generation and detection of pure spin currents. Using spin pumping, people have characterized the spin orbit interaction induced charge—spin conversion in various materials, including paramagnetic, ferromagnetic and antiferromagnetic metals, semiconductors, as well as superconductors. It is interesting to ask whether the charge to spin conversion efficiency undergoes any significant change in a material with spontaneous phase transitions. In this talk we will present our work on spin pumping in VO₂, a prototype metal-insulator transition (MIT) material. By exciting ferromagnetic resonance in an adjacent magnetic insulator, we are able to inject spin current into VO₂ and quantify the variation in spin pumping voltage during the phase transition. We find that large spin pumping voltages exist in both metallic and insulating phase of VO₂, despite of the huge resistance change across this transition. To this end, we will present our work on the variation of spin mixing conductance and the spin Hall angle across the phase transition region.

10:12AM K39.00010: Topological Transport of Vorticity in Heisenberg Magnets  JI ZOU (Presenter), Physics, Univ of California - Los Angeles, SE KWON KIM, Physics, University of Missouri, YAROSLAV TSERKOVNYAK, Physics, Univ of California - Los Angeles — We study a robust topological transport carried by vortices in a thin film of an easy-plane ferromagnetic insulator between two metal contacts. A vortex, which is a nonlocal topological spin texture in two-dimensional magnets, exhibits some beneficial features as compared to skyrmions, which are local topological defects. In particular, the total topological charge carried by vorticity is robust against local fluctuations of the spin order-parameter magnitude. We show that an electric current in one of the magnetized metal contacts can pump vortices into the insulating bulk. Diffusion and nonlocal Coulomb-like interaction between these vortices will establish a steady-state vortex flow. Vortices leaving the bulk produce an electromotive force at another contact, which is related to the current-induced vorticity pumping by the Onsager reciprocity. The voltage signal decays algebraically with the separation between two contacts, similarly to a superfluid spin transport. Finally, the vorticity and closely related skyrmion type topological hydrodynamics are generalized to arbitrary dimensions, in terms of nonsingular order-parameter vector fields.

10:24AM K39.00011: Observation of NMR spin pumping*  YUKI SHIOMI (Presenter), University of Tokyo, JANA LUSTIKOVA, SHINGO WATANABE, Tohoku University, DAICHI HIROBE, Institute for Molecular Science, SABURO TAKAHASHI, Tohoku University, EIJI SAITO, University of Tokyo — We report spin pumping from nuclear magnetic resonance (NMR), in which nuclear spin dynamics emits a spin current, a flow of spin angular momentum of electrons. By using the canted antiferromagnet MnCO₃, in which typical nuclear spin-wave formation is established due to the reinforced hyperfine coupling, we find that a spin current is generated from an NMR.

*This research was supported by JST ERATO ‘Spin Quantum Rectification Project’ (JPMJER1402), JSPS KAKENHI (no. 17H04806, no. JP18H04215, no. 18H04311, no. JP16j03699 and no. 17H02927) and MEXT (Innovative Area ‘Nano Spin Conversion Science’ (no. 26103005)).

10:36AM K39.00012: Tunable Quantum Dynamics in a Disordered Magnet  CHRISTOPHER TANG (Presenter), DANIEL SILEVITCH, Caltech, GABRIEL AEPPLI, Paul Scherrer Institutue, THOMAS F ROSENBAUM, Caltech — Quantum memories depend on maintaining coherence in minimally-interacting qubits. In an attempt to engineer such memories, we decouple coherent many-body excitations from their environment in the dilute Ising magnet LiHo₀.₀₄₅Y₀.₉₅₅F₄ by driving the system into a non-linear regime with a Floquet drive. In this material, clusters of dozens to hundreds of spins bind together and can be excited resonantly by a strong ac magnetic field. The structure of these clusters can be studied via a Fano resonance technique using pump-probe magnetic susceptibility measurements, revealing lifetimes and coherent quantum interference between different excitation channels. In addition, we can tune the dynamics of the quantum degrees of freedom by tuning the strength of the pump ac magnetic field, or by introducing a static transverse field that serves to quantum-mechanically mix spin states. At special values of these two fields, zero-crossings of the Fano asymmetry parameter are observed, which are associated with a dissipationless response at the drive frequency. At these points, certain spin-clusters are minimally coupled with their environment, due to quantum interference between different excitation channels. The lifetimes of these excitations can be measured directly in the time-domain.
The behavior of spin propagation in metals in various measurement schemes is shown to be qualitatively different than a simple exponential decay - due to the backflow effect on spin diffusion in the presence of interfaces. We utilize the spin sensitivity of Nb superconducting point contacts to evaluate the spin current depolarization in a normal metal. The spin current was injected from bulk Co$_2$Mn$_{0.5}$Fe$_{0.5}$Si Heusler alloys into gold films of variable thickness. While our phenomenological theoretical results are consistent with gradually decaying spin polarization as the film thickness increases, the spin diffusion length in Au is found to be 285 nm, more than two times larger than without taking the backflow effect into account.

Wednesday, March 6, 2019 8:00 AM - 10:48 AM

Session K40 GMAG DMP: Control of Magnetic Oxides

**8:00AM K40.00001: Control of Quantum States in 4d/5d Transition Metal Oxides** [Invited] GANG CAO (Presenter), Department of Physics, University of Colorado at Boulder — A delicate balance between spin-orbit and other competing interactions inherent in 4d/5d materials offers a unique range of opportunities to uncover exotic states and physical properties that are intimately coupled to the crystal structure [1]. This unique feature provides us fertile ground to control quantum states by tuning the lattice of single crystals. Here we present and discuss two recent examples and their fundamental significance: (i) Pressure-induced transition from interlayer ferromagnetism to intralayer antiferromagnetism in Sr$_4$Ru$_2$O$_{10}$ [2], and (ii) Electrical-current control of structural and physical properties in canted antiferromagnetic iridates [3].


**This work was supported by NSF grant DMR-1712101**

**8:36AM K40.00002: Electric field control of magnetic domains in Y-type hexaferrite single crystals at room temperature** VILMOS KOCSIS (Presenter), TARO NAKAJIMA, Center for Emergent Matter Science (CEMS), RIKEN, MASAAKI MATSUDA, Oak Ridge National Laboratory, AKIKO KIKKAWA, YOSHIO KANEKO, JUNYA TAKASHIMA, Center for Emergent Matter Science (CEMS), RIKEN, KAZUHISA KAKURAI, Comprehensive Research Organization for Science and Society (CROSS), TAKA-HISA ARIMA, University of Tokyo, FUMITAKA KAGAWA, Center for Emergent Matter Science (CEMS), RIKEN, YUSUKE TOKUNAGA, University of Tokyo, YOSHINORI TOKURA, YASUJIRO TAGUCHI, Center for Emergent Matter Science (CEMS), RIKEN — In the trigonal Y-type hexaferrites the magnetoelectric properties are attributed to the emergence of the so-called FE3 phase with co-existing ferrimagnetic and ferroelectric orders [1]. Recently, in the Al-doped Y-type hexaferrite, (Ba,Sr)$_2$Co$_2$Fe$_{11}$Al$_x$O$_{22}$, this multiferroic phase has been observed as a metastable phase close to room temperatures even in the absence of magnetic field [2,3].

In this presentation we report that in bulk Ba$_{0.8}$Sr$_{1.2}$Co$_2$Fe$_{12-x}$Al$_x$O$_{22}$ with x=0.9, the ferrimagnetic and ferroelectric domains have considerable coupling even at room temperature. Cross-control of the magnetic and electric degrees of freedoms, i.e. the direct (P-H) and inverse (M-E) magnetoelectric effect have been observed up to room temperature. Using magnetic force microscopy, control of the magnetic domain pattern by the application of electric field is directly visualized. We demonstrate that magnetization switching is realized via the propagation of two kinds of domain walls; parallel and perpendicular to the applied electric field.

8:48AM K40.00003: Magnetically Controlled Surface Acoustic Waves on Multiferroic BiFeO$_3$* RYO SASAKI (Presenter), YUTA ISHII, Department of Basic Science, University of Tokyo, YOICHI NII, Institute for Materials Research, Tohoku University, TOSHIMITSU ITO, National Institute of Advanced Industrial Science and Technology (AIST), YOSHINORI ONOSE, Institute for Materials Research, Tohoku University — We fabricate a surface acoustic wave (SAW) device on a multiferroic BiFeO$_3$ crystal while SAW devices are usually fabricated on nonmagnetic piezoelectrics and commercially available as bandpass filters. By using the time-domain technique, we demonstrate the SAW excitation on BiFeO$_3$. The amplitude and phase of the SAW signal are modulated by the external magnetic field reflecting the multiferroicity of BiFeO$_3$. The magnetic controllability of the multiferroic SAW device seems useful for the further functionalization of the SAW device.

*This work was in part supported by the Grants-in-Aid for Scientific Research (Grants No. 25247058, No. 16H04008, No. 15K21622, and No. 17H05176) and The Murata Science Foundation.

9:00AM K40.00004: Pressure-induced magnetic behavior in Ca$_2$Mn$_2$O$_5$-type A$_2$B$_2$O$_5$ oxides YONGJIN SHIN (Presenter), JAMES M RONDINELLI, Northwestern University — Brownmillerite oxides with the chemical formula A$_2$B$_2$O$_5$ are derived from stoichiometric ABO$_3$ perovskites and exhibit ordered oxygen vacancies (OOVs). The OOVs transform the octahedral BO$_6$ units into different BO$_6$-x polyhedra, which allows for large changes in the crystal field split orbital structure and subsequent changes in functional properties. The magnetic order of transition metal oxides is governed by the correlation between these orbitals and corresponding electronic configurations. For example, Sr$_2$Mn$_2$O$_5$ (SMO; $d^4$) in the Ca$_2$Mn$_2$O$_5$-type square pyramidal network yields E-type antiferromagnetic (AFM-E) order, consistent with the Goodenough-Kanamori rules, whereas Sr$_2$Fe$_2$O$_5$ (SFO; $d^5$) exhibits AFM-G order within the same structure. Here, we investigate with first principles calculations the effect of hydrostatic pressure on the Ca$_2$Mn$_2$O$_5$-type structure, which drives contrasting behavior in SMO and SFO. We show the AFM-E order in SMO is further stabilized under pressure while SFO exhibits a magnetic transition to a FM state at ~24 GPa arising from a spin crossover. Lastly, we evaluate the pressure effect induced by biaxial strain in OOV structures and discuss the feasibility of such phase transition in thin film geometries.

9:12AM K40.00005: Pressure-induced transition from an antiferromagnetic insulator to a ferromagnetic metal in Ca$_2$Ru$_{1-x}$M$_x$O$_4$ (M=Cr, Mn and Fe)* HAO ZHENG (Presenter), Department of Physics, University of Colorado, Boulder, CO 80309, FENG YE, SONGXUE CHI, Quantum Condensed Matter Division, Oak Ridge National Laboratory, TN 37831, HENGDI ZHAO, YIFEI NI, YU ZHANG, GANG CAO, Department of Physics, University of Colorado, Boulder, CO 80309 — The comparable magnitudes of the Coulomb interaction and 4$d$-bandwidth can leave ruthenates precariously balanced on the border between metallic and insulating behavior, and/or on the verge of long-range magnetic order. Ca$_2$RuO$_4$ is an antiferromagnetic (AFM) Mott insulator with Neel temperature at $T_N = 110$ K and a first-order metal-insulator transition at $T_{MI} = 357$ K. It is recognized that Ca$_2$RuO$_4$ and its derivatives are highly sensitive to the lattice degrees of freedom. Here we report that application of modest pressure (< 2.5 GPa) readily destabilizes the AFM Mott state and precipitates a ferromagnetic metallic state at low temperatures in Ca$_2$Ru$_{1-x}$M$_x$O$_4$ (M=Cr, Mn and Fe). Transport and magnetic properties including neutron diffraction at pressure will be presented and discussed along with other related systems.

*This work was supported by the National Science Foundation via grant DMR-1712101.

9:24AM K40.00006: Strain-induced heteronuclear charge disproportionation in EuMnO$_3$* ULRICH ASCHAUER (Presenter), NATHALIE VONRÜTI, Departement of Chemistry and Biochemistry, University of Bern, NICOLA SPALDIN, Materials Theory, ETH Zürich — Charge disproportionation transitions commonly link high-temperature phases, in which cations of a given element have the same oxidation state, to low-temperature phases, where charge transfers between ions of this element results unequal oxidation states. Based on density functional theory calculations we here propose the concept of heteronuclear charge disproportionation, for which charge transfers occurs between different elements located on different crystallographic sites. Using EuMnO$_3$ as a test case, we show that the transition from Eu$^{3+}$Mn$^{3+}$O$_3$ to Eu$^{2+1}$Mn$^{4+}$O$_3$ can be triggered by pressure or epitaxial strain. We will highlight experimentally accessible signatures of this transition and discuss other crystal chemistries that could show similar phase transitions and resulting novel physics.

*This work was financially supported by the ETH Zürich and by the ERC Advanced Grant program, No. 291151 as well as the SNF Professorship Grant PP00P2_157615.
9:36AM K40.00007: Evidence of the Multiferroic Character of the EuO$_{1-x}$-BaTiO$_3$ Heterojunction* SYED QAMAR

ABBAS SHAH (Presenter), Physics and Astronomy, The University of Nebraska-Lincoln, GAURAB RIMAL, Physics and Astronomy, Rutgers University, Piscataway, GUANHUA HAO, ANDREW J YOST, Physics and Astronomy, The University of Nebraska-Lincoln, JINKE TANG, Physics and Astronomy, The University of Wyoming-Laramie, PETER A DOWBEN, Physics and Astronomy, The University of Nebraska-Lincoln — EuO$_{1-x}$ combines several interesting properties: large magneto-optical effects, colossal magnetoresistance, and enhanced Curie temperature due to bound magnetic polarons. EuO$_{1-x}$ is also one of a very few ferromagnetic insulators and, as an ultra thin film, very sensitive to interface effects. Investigation into the affect of ferroelectric substrates on the ferromagnetic properties of EuO$_{1-x}$ can provide deep insights into how one can manipulate magnetism by changing interface charge populations. Utilizing pulsed laser deposition, a thin film (20nm) of ferroelectric BaTiO$_3$ was grown on top of a thin film (15nm) of ferromagnetic EuO$_{1-x}$. X-ray diffraction indicates the presence of high quality crystalline thin films of EuO$_{1-x}$ and BaTiO$_3$. Magneto optical Kerr effect (MOKE) spectroscopy and magnetoresistance measurements indicate a temperature dependent signature of anti-ferromagnetic magnetoelectric coupling of the ferroelectric/ferromagnetic heterostructure. This study sheds new light on the modulation of magnetoelectric coupling at a device interface.

*This research was supported by the National Science Foundation, through Grant Nos. NSF-ECCS 1740136 and 1508541, as well as by the NCORE, a wholly owned subsidiary of the Semiconductor Research Corporation (SRC).

9:48AM K40.00008: Magnetic structure of hexagonally stabilized (Lu,In)FeO$_3$ KWANGHEE CHO (Presenter), HAKBEOM KIM, SOONYONG PARK, Chung-Ang University — Hexagonal LuFeO$_3$ has recently attracted considerable attention as promising candidates for room-temperature multiferroics, in which ferroelectricity and magnetism coexist in a single phase. However, most studies have been performed in a thin film form due to the instability of the bulk hexagonal LuFeO$_3$. Herein, we report that in LuFeO$_3$ a single hexagonal phase can be stabilized in both polycrystalline and single-crystalline bulk form with a wide range of Indium substitution in Lutetium site. Neutron diffraction results on magnetic spin structures and crystal structures of the Indium substituted LuFeO$_3$ will be discussed.

10:00AM K40.00009: Meta—stability and Transient Phases Triggered by Optically Excited Quasi—particles in Strongly Correlated Systems.* MYRON KAPETANAKIS (Presenter), Physics, University of Alabama at Birmingham, PANAGIOTIS LINGOS, Physics, University of Crete, JIGANG WANG, Physics & Astronomy, Ames Lab & Iowa State University, ILLIAS PERAKIS, Physics, University of Alabama at Birmingham — The interplay between electronic, magnetic and lattice degrees of freedom in colossal magnetoresistant manganites results in a rich phase diagram that provides an ideal model system for phase transition studies. Here we investigate the possibility of phase transitions induced by ultrafast optical laser pulses. We use a generalized tight—binding model, based on Hubbard operators, to describe the interaction between itinerant carrier and localized magnetic moment in multi—electron configurations. Optically—induced quasi—particle excitations introduce inhomogeneities, charge redistributions and spin fluctuations resulting in the formation of meta—stable states that trigger a non-equilibrium ultrafast dynamics. We discuss a theoretical description of optical switching mechanism between coexisting phases and highlight the role of photo—induced non—linearities on quantum femtosecond magnetism.

*This work was supported by the Army Research Office under award W911NF-15-1-0135.

10:12AM K40.00010: Photo-excitation of Mott and charge transfer insulators DENIS GOLEZ (Presenter), PHILIPP WERNER, Department of physics, University of Fribourg, MARTIN ECKSTEIN, Department of physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — I will compare the dynamics after the photo-excitation in Mott and charge-transfer insulators (CTIs). The later is described within the three-band Emery model and a non-equilibrium extension of GW+EDMFT. In contrast to Mott insulators a strong renormalization of the charge-transfer gap and a substantial broadening of bands is present in CTIs. The comparison with different experimental pump-probe techniques, like time resolved ARPES and optical conductivity, shows qualitative agreement and exemplify that dynamical correlations are essential for a proper description of the photo-doped state. I will provide an outlook how to extend these tools to an ab-initio description of strongly correlated materials out of equilibrium.

10:24AM K40.00011: Modulating Charge-Orbital Ordering in SmBaMn$_2$O$_6$ Single Crystals with Tuneable Strain. HAN ZHANG (Presenter), LIN HAO, JUNYI YANG, Physics, University of Tennessee, SHUA SANCHEZ, JIUN-HAW CHU, University of Washington, HAIDONG ZHOU, JIAN LIU, Physics, University of Tennessee — SmBaMn$_2$O$_6$ is a perovskite manganese oxide with A-site ordering where competing interactions lead to a series of phase transitions. The observed orderings include charge-orbital-ordering, antiferromagnetic ordering, ferromagnetic canting and spin re-orientation. The Structural phase transition associated charge-orbital-ordering clearly indicate a strong relation between the lattice, charge and orbital. A systematic study with tunable strain along lattice directions is done to study how the latter two interact with lattice, as well as how the interplay contributes to the macroscopic properties.
10:36AM K40.00012: Field-induced antiferromagnetic cone structure in multiferroic BiFeO3  MASAKI MATSUDA
(Presenter), SACHITH DISSANAYAKE, Oak Ridge National Laboratory, YASUKO OZAKI, TOSHIMITSU ITO, AIST, XINZHI LIU, MACIEJ
BARTKOWIAK, OLEKSANDR PROKHENKO, Helmholtz-Zentrum Berlin — BiFeO3, a rare multiferroic compound that shows
antiferromagnetism and ferroelectricity simultaneously above room temperature ($T_N$~640 K), has been studied intensively.
Recently, a new magnetic phase has been found between the cycloidal and canted antiferromagnetic phase in magnetic
field [1]. We performed neutron diffraction measurements in high static magnetic fields up to 19 T on HFM/EXED facility at
BER II research reactor in Helmholtz Zentrum Berlin. We successfully observed weak incommensurate peaks around 13 T
which split along the magnetic field direction [1,1,-2] at the (1/2, 1/2, 1/2) main peak. The magnetic field and temperature
region, where the incommensurate peaks appear, is consistent with that in the phase diagram obtained by the
magnetization measurements [1]. We confirmed that the magnetic structure in the intermediate phase is the
antiferromagnetic cone structure which is predicted theoretically. We will show the detailed magnetic structure (magnetic
wave vector and cone angle) and discuss the relation between the magnetic structure and the magnetoelectric effect. [1] S.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K41 GMAG DMP: Chiral Magnetism and Structures I  B Cec 209 - Daniele Pinna, Johannes Gutenberg
Universität Mainz - Tag(s): Focus

8:00AM K41.00001: Rise of Chiral Spintronics [Invited]  SEE-HUN YANG (Presenter), IBM Research - Almaden — Chirality is one
of the fundamental asymmetries in nature. Recently chiral nature of magnetic and nonmagnetic structures have been
enormously highlighted and arisen to be very useful for potential application to not only spintronics but biology and
pharmaceutical industries For example, it has been reported that the combination with spin-orbit interaction such as spin
Hall effect can be very efficient in manipulation of magnetic elements [1], and spin currents in chiral molecules induced by
chirality interacts with magnetic structures [2]. I will present recent remarkable progress in emergent novel phenomena
associated with chiral properties from not only emergent magnetic nanostructures but chiral molecules: spin-orbit torques
from perpendicularly magnetized ultrathin films [2], exchange coupling torque [3] and entirely new phase of chiral
exchange drag [4] from synthetic antiferromagnets, and separation of chiral molecules by magnetic structure: enantiomer
[5]. In the end I will discuss potential applications and promising outlooks from these new findings.


8:36AM K41.00002: Unit cell thick ferrimagnetic Mn$_3$Z Heusler Domain Wall motion  PANAGIOTIS CH. FILIPPOU
(Presenter), IBM Almaden Research Center, JAEWOO JEONG, New Memory Technology Lab, Samsung Electronics, YARI FERRANTE,
SEE-HUN YANG, TEYA TOPURIA, MAHESH G. SAMANT, IBM Almaden Research Center, STUART S PARKIN, Max Planck Institute for
Microstructure Physics Halle — Antiferromagnets and ferrimagnets are of particular interest for spintronic devices. In this
talk, we present the Domain Wall (DW) motion of Mn$_3$Z (Z=Ge, Sn, Sb) Heuslers, using the chemical templating layer (CTL)
concept. Unit cell thick, ferrimagnetic, binary Heusler compounds, have low magnetization and high perpendicular
magnetic anisotropy in their tetragonally distorted forms, can sustain current driven DW motion in nanowire racetracks of
-129 ms$^{-1}$ with the lowest current density to initiate motion of 2.8 $10^6$ A cm$^{-2}$. The direction of the DW motion is
determined by the bulk spin polarization of the Heusler. Moreover, the DW motion shows contribution by chiral spin orbit
torques when studied under in-plane fields. We discuss the complex mechanism of the DW motion in Heusler films and
identify a bulk Dzyaloshinskii-Moriya interaction and a spin Hall effect deriving from the CTLs.
One example of the extraordinary abilities of the Mn$_3$Z Heusler family, is shown by systematically tuning by an order of
magnitude the bulk DMI field strength, by varying the composition of the Heusler alloy. These results are the first
demonstration of DW motion in ultra-thin Heusler alloys with complex and tunable magnetic properties and is an
important step to enable Heusler spintronics applications.

The preimages of the spin texture and numerical calculations of $Q_H$ show that the hopfion has $Q_H = 1$. Furthermore, another non-trivial state that includes a monopole–antimonopole pair (MAP) is also stabilized in this system. By applying an external magnetic field, hopfion and MAP states with the same polarization can be switched between each other. The topological transition between the hopfion and the MAP state involves a creation (annihilation) of the MAP and twist of the preimages. Our work paves the way to study non-trivial 3D topological spin textures and stimulates more investigations in the field of 3D spintronics.


*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0016424 and as part of the Spins and Heat in Nanoscale Electronic Systems (SHINES) an Energy Frontier Research Center funded by U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0012670.

Here, we show, on the example of chiral ferrimagnetism in amorphous GdCo, that the concept of chirality driven by interfacial DMI can be generalized to complex multicomponent systems. Utilizing Lorentz microscopy and X-ray magnetic circular dichroism spectroscopy, and tailoring thickness, capping and rare-earth composition, we find that a 2nm-thick interfacial DMI can be generalized to complex multicomponent systems. Utilizing Lorentz microscopy and X-ray magnetic circular dichroism spectroscopy, and tailoring thickness, capping and rare-earth composition, we find that a 2nm-thick GdCo film preserves ferrimagnetism and stabilizes chiral domain walls. The type of chiral domain walls depends on the circular dichroism spectroscopy, and tailoring thickness, capping and rare-earth composition, we find that a 2nm-thick GdCo film preserves ferrimagnetism and stabilizes chiral domain walls. The type of chiral domain walls depends on the type of chiral domain walls depends on the rare-earth composition/saturation magnetization, enabling a possible temperature control of the intrinsic properties of ferrimagnetic domain walls.

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Transport signatures of interfacial exchange coupling and chiral spin textures in magnetic insulator thin films*  QIMING SHAO (Presenter), ECE, UCLA, YAWEN LIU, Physics, UCR, ALEXANDER GRUTTER, Neutron-Condensed Matter Science Group, NIST, GUOQIANG YU, ECE, UCLA, SE KWON KIM, Physics, UCLA, XIAOYU CHE, ECE, UCLA, CHI TANG, Physics, UCR, YAROSLAV TSERKOVNYAK, Physics, UCLA, JING SHI, Physics, UCR, KANG L. WANG, ECE, UCLA — Ferrimagnetic insulators (FMIs) attract tremendous interest for spintronic applications due to high characteristic frequency, low Gilbert damping, and absence of Ohmic loss. First, we demonstrate the critical role of dimensionality on the SOT efficiency by systematically studying the FMI layer thickness dependent SOT efficiency in tungsten/thulium iron garnet (W/TmIG) bilayers. Current-induced switching in FMI thin films is demonstrated with a thickness up to 15 nm [1]. Second, we use temperature dependent Hall measurements to identify contributions of spin Hall, magnetic proximity, and sublattice effects to the anomalous Hall signal in various heavy metal/ferrimagnetic insulator heterostructures. This approach enables detection of both the magnetic proximity effect onset temperature and magnetization compensation temperature and provides essential information regarding the interfacial exchange coupling. At last, we show the transport signatures of chiral spin textures, topological Hall effect, in the platinum/ferrimagnetic insulator bilayer. [1] Q. Shao, et al., Nat. Commun., 9, 3612 (2018)

*We acknowledge funding support from SHINES (DE-SC0012670), MURI (W911NF-16-1-0472 and W911NF-15-1-10561), and TANMS (EEC-1160504).

Z2 topological invariant for magnon spin Hall systems  HIROKI KONDO (Presenter), YUTAKA AKAGI, HOSHO KATSURA, Department of Physics, University of Tokyo — The classification and characterization of different phases of matter based on the topology of band structures has recently attracted much attention. It is known that some of the topological phenomena in electron systems are carried over to bosonic systems [1]. However, the topological invariant of bosonic systems with time-reversal symmetry has not yet been identified, as Kramers' theorem cannot be applied to them. To address this issue, we first introduce the pseudo-time-reversal operator which ensures the existence of “Kramers pairs” of bosons. Then, we define the Z2 topological invariant for magnon spin Hall systems [2] using the Berry connection and curvature for bosons, which are different from those of electrons [3]. Furthermore, we propose two magnetic models with magnon bands carrying the nontrivial Z2 topological invariant. We also demonstrate that the presence (absence) of helical edge states corresponds to the nontrivial (trivial) value of the Z2 topological invariant.


Observation of long-wavelength modulation in chiral Mn1/3NbS2*  SUNIL KARNA (Presenter), DAVID P YOUNG, FRANK N. WOMACK, Physics and Astronomy Department, Louisiana State University, YAN WU, HUIBO CAO, LISA DEBEER-SCHMITT, Oak Ridge National Laboratory, PHILIP W ADAMS, JOHN DITUSA, Physics and Astronomy Department, Louisiana State University — We have investigated the magnetic properties of Mn1/3NbS2, through neutron diffraction and magnetic susceptibility measurements. Mn1/3NbS2 crystallizes in the non-centrosymmetric hexagonal space group P6322 and is built from NbS2 layers intercalated by Mn ions. The Mn atoms are situated in the octahedral holes between trigonal prismatic layers of 2H-NbS2. The magnetic susceptibility and magnetization indicate a magnetic transition at $T_N \sim 45$ K with an anisotropy that is similar to that observed in Cr1/3NbS2. Neutron diffraction reveals increased scattering near the structural Bragg peaks. However, our data indicate that the magnetic scattering had a wider q-dependence than the nuclear Bragg peaks suggesting a long wavelength modulation of the magnetic ordering along the c-axis.

*This material is based upon the work supported by the U.S. Department of Energy under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents.
10:12AM K41.00010: Investigating the stability of incommensurate spin textures in GaV4S8  ELEANOR CLEMENTS (Presenter), University of South Florida, GANESH POKHAREL, DAVID GEORGE MANDRUS, Department of Materials Science and Engineering, University of Tennessee Knoxville, HARIHARAN SRIKANTH, MANH-HUONG PHAN, University of South Florida — The polar noncentrosymmetric GaV4S8 hosts a Néel skyrmion lattice (SkL) below Tc ~ 13 K. The Néel SkL extends over a broad range of temperature and magnetic field relative to the SkL in the chiral B20 helimagnets. It has been proposed that the modulated phases evolve into a ferromagnetic ground state at temperatures below ~ 5 K. By exploiting the magnetocaloric effect, we analyze the temperature and field evolution of the magnetic entropy change to gain insight into the stabilization mechanism of the magnetic phases close to Tc, which are thought to be governed by thermal fluctuations. We also investigate the behavior of the magnetic entropy change at low temperatures approaching the magnetic ground state.

10:24AM K41.00011: Non-trivial topology in 2D magnetic systems without skyrmions*  JIE-XIANG YU (Presenter), University of New Hampshire, WENTAO HOU, Boston College, MORGAN A DALY, JIADONG ZANG, University of New Hampshire — The magnetic skyrmion is a kind of two-dimensional(2D) topological non-trivial spin textures which can be identified by an integer number, called topological charge. However, our study on 2D chiral magnets, however, showed that one topological charge does not necessarily correspond to one skyrmion and the non-trivial topology can be found in a disordered phase. Here, we further investigate non-trivial topology in various systems where no-skyrmion is expected in low magnetic field region. In 2D spin-frustrated systems, such thermally driven topology is dominated in a wide range of magnetic fields; In the antiferromagnetic system with staggered Dzyaloshinskii-Moriya interactions, giant response of topological charge is found in a canted spin-ordering phase. Both two systems are related to real systems so that we expect the topological properties can be observed by thermal magnon and/or anomalous Hall effect.

*Our studies are supported by U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award No. DE-SC0016424 and Extreme Science and Engineering Discovery Environment (XSEDE) under Grant No. TG-PHY170023.

10:36AM K41.00012: Direct imaging of topological phase discontinuities in chiral spin textures via electron ptychography beyond diffraction-limited resolution*  ZHEN CHEN (Presenter), Applied and Engineering Physics, Cornell University, EMRAH TURGUT, Department of Physics, Oklahoma State University, KRISHNAN CHANDER, KAYLA NGUYEN, Applied and Engineering Physics, Cornell University, MATTHEW STOLT, SONG JIN, University of Wisconsin–Madison, DAN RALPH, Department of Physics, Cornell University, GREGORY FUCHS, DAVID ANTHONY MULLER, Applied and Engineering Physics, Cornell University — Real-space imaging of magnetic structures can provide crucial information for understanding many magnetic phenomena. Here, utilizing a new electron microscope detector, EMPAD, we resolve the internal fine structure of skyrmions in single crystal FeGe using Lorentz STEM and electron ptychography. We have unambiguously uncovered the topological phase discontinuities near the skyrmion lattice dislocation and boundaries. We also demonstrate a significant resolution improvement using electron ptychography, allowing magnetic imaging beyond the diffraction limit imposed by the electron optics. Magnetic domain images from ultrathin metallic multilayer films show the outstanding detection limit of our new imaging method. This new direct imaging technique can be applied to determine complex chiral spin structures in a wide variety of materials.

*Supported by NSF DMR-1539918 and MRSEC DMR-1719875 and DARPA D18AC00009

10:48AM K41.00013: Multiple magnetic phases in chiral Mn1/3NbS2  BING SHEN (Presenter), School of Physics, Sun Yat-Sen University, China — The chirality in materials always leads to the intriguing functionalities. In a magnetic system, the spin texture can be chiral due to the competition of Dzyaloshinskii-Moriya (DM) interaction and ferromagnetic coupling. The unique magnetic structure could be modulated into a particlelike order by applying field such as a magnetic soliton. In this talk, we present the systematic magneto-transport study on the chiral magnetic Mn1/3NbS2 single crystal, a proposed candidate of chiral magnetic solation semimetal. With tuning temperature and applied field, the system undergoes several magnetic states. An anisotropic magnetic phase diagram is revealed in this the layered materials.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K42 DQI: Applications of Noisy Intermediate Scale Quantum Computers IV  BCEC

210A - Peter Johnson - Tag(s): Focus
8:00AM K42.00001: Tensorial tools for quantum computing* YANNICK MEURICE (Presenter), University of Iowa — Tensorial methods have been playing an increasingly important role in the context of spin models and lattice gauge theory. In most examples, the variables of integration are compact and character expansion (for instance Fourier analysis for U(1) models) can be used to rewrite the partition function and average observables as discrete sums of contracted tensors. This reformulations have been used for RG coarse-graining but they are also very useful for quantum computing. Their build-in Trotter procedure allows us to write quantum circuit or propose analog simulations. We discuss recent applications and FAQs about the tensor reformulations such as boundary conditions, Grassmann variables, Ward identities, effects of truncations and gauge invariance.

*Department of Energy Office of Science Award Numbers: DE-SC0019139 and DE-SC0010113.

8:12AM K42.00002: How many qubits are needed for quantum computational supremacy?* ALEXANDER DALZELL (Presenter), Caltech, ARAM HARROW, DAX ENSHAN KOH, ROLANDO LA PLACA, Massachusetts Institute of Technology — Quantum computational supremacy arguments, which describe a way for a quantum computer to perform a task that cannot also be done by a classical computer, typically require a computational assumption related to the limitations of classical computation. One common assumption is that the polynomial hierarchy (PH) does not collapse, a stronger version of the statement that P =/= NP, which leads to the conclusion that any classical simulation of certain families of quantum circuits requires time scaling worse than any polynomial in the size of the circuits. However, the asymptotic nature of this conclusion prevents us from calculating exactly how many qubits these quantum circuits must have for their classical simulation to be intractable on modern supercomputers. We refine these quantum computational supremacy arguments and perform such a calculation by imposing fine-grained versions of the non-collapse assumption. Based on these conjectures we conclude that IQP circuits with 180 qubits, QAOA circuits with 360 qubits and boson sampling circuits (i.e. linear optical networks) with 90 photons are large enough for producing samples from their output distributions to be intractable on current technology.

*Supported by the Orr Fellowship, NSF, ARO, MIT-IBM Watson AI lab, and A*STAR.

8:24AM K42.00003: Verifying quantum supremacy by doubling the circuit depth* ANIMESH DATTA (Presenter), SAMUELE FERRACIN, THEODOROS KAPOURNIOTIS, University of Warwick — Any fruitful use of the noisy intermediate-scale quantum computing devices being developed relies crucially on our ability to verify the correctness of their outputs. This verification must be achievable within these noisy intermediate-scale devices. We present a verification protocol in the circuit model where the “desired” computation is verified running several independent “trap” computations, each of which requires (i) no more qubits than the desired computation and (ii) a circuit-depth twice that of the desired computation. Our protocol exploits the fact that single qubit gates are often the best components in noisy intermediate-scale quantum devices. We begin with the assumption that only the single-qubit gates are prefect, and then extend our protocol to account for all operations in intermediate-scale quantum computing devices being noisy. Our protocol applies to sampling problems that underlie quantum supremacy. In particular we provide a verification scheme, with a doubling of the circuit depth, to bound the variation distance between ideal and noisy probability distributions resulting from random circuit sampling - a candidate for quantum supremacy.

*UK EPSRC (EP/K04057X/2), UK Networked Quantum Information Technologies (NQIT) Hub (EP/M013243/1)

8:36AM K42.00004: Variational Quantum Factoring ERIC ANSCHUETZ, JONATHAN OLSON, ALAN ASPURU-GUZIK, YUDONG CAO (Presenter), Zapata Computing — Integer factorization has been one of the cornerstone applications of the field of quantum computing since the discovery of an efficient algorithm for factoring by Peter Shor. Unfortunately, factoring via Shor's algorithm is well beyond the capabilities of today's noisy intermediate-scale quantum (NISQ) devices. In this work, we revisit the problem of factoring, developing an alternative to Shor's algorithm, which employs established techniques to map the factoring problem to the ground state of an Ising Hamiltonian. The proposed variational quantum factoring (VQF) algorithm starts by simplifying equations over Boolean variables in a preprocessing step to reduce the number of qubits needed for the Hamiltonian. Then, it seeks an approximate ground state of the resulting Ising Hamiltonian by training variational circuits using the quantum approximate optimization algorithm (QAOA). We benchmark the VQF algorithm on various instances of factoring and present numerical results on its performance.
8:48AM K42.00005: Variational quantum eigensolver of interacting bosons with NISQ devices  ANDY C. Y. LI (Presenter), ALEXANDRU MACRIDIN, PANAGIOTIS SPENTZOURIS, Fermilab — Interacting boson systems are of broad interest in different fields of physics. Their simulation on classical computers is in general very challenging. The recent advances in variational-quantum-eigensolver (VQE) algorithms offer new scalable ways to investigate these systems with noisy intermediate scale quantum (NISQ) devices. In this work, we present a proof-of-principle experiment of a boson VQE algorithm implemented on Rigetti’s 8Q-device. Our experiment determines the low-energy eigenspectrum of the Rabi model -- a simple boson model with interactions mediated by an atom. Our results illustrate that scalable quantum simulations of interacting boson systems using NISQ devices have a promising future.

9:00AM K42.00006: A Quantum Algorithm for Symmetry-Exploitation in Exact Diagonalization of Quantum Many-Body Systems  ALBERT SCHMITZ, University of Colorado, Boulder, SONIKA JOHRI (Presenter), Intel — Grover's search algorithm can be extended to a minimization procedure on a quantum computer. Here, we find a new application for this procedure – the symmetry-based size reduction of matrices corresponding to quantum many-body Hamiltonians before they are diagonalized. This is currently a memory/computational bottleneck on classical computers. In this case, the minimization problem cannot tolerate an approximate minimum ruling out variational quantum algorithms, and adiabatic minimization is unsuitable since there is no notion of a finite energy gap protecting the ground state during the evolution from the starting to the final state. Instead, Grover's minimization procedure provides a reliable means to obtain a quadratic speedup over classical algorithms. We discuss both the theory and full circuit implementation of Grover minimization as applied to this problem. We find that the oracle for this problem only scales as poly-log in the size of the search space, in contrast to many oracles in proposed applications for Grover's algorithm which scale polynomially. Further, we design an error mitigation scheme that significantly reduces the effects of noise on the computation, making it a plausible candidate for the Noisy Intermediate Scale Quantum era.

9:12AM K42.00007: Variational Quantum Optics  AGUST&iacute;N DI PAOLO (Presenter), Université de Sherbrooke, Institut quantique and Département de Physique, PANAGIOTIS BARKOUTSOS, IVANO TAVERNELLI, IBM Research - Zurich, ALEXANDRE BLAIS, Université de Sherbrooke, Institut quantique and Département de Physique — Quantum processors of intermediate scale have been used to simulate quantum chemistry by means of the variational quantum algorithm (VQA). VQAs have been shown to be robust against noise and can handle limited connectivity by using hardware-efficient state-preparation protocols. This makes VQAs a promising tool for near-term application of quantum co-processors in the hybrid quantum-classical computation paradigm. In this talk, we extend the applicability of variational quantum algorithms to bosonic Hamiltonians with applications to quantum optics.

9:24AM K42.00008: Study network-related optimization problems using quantum alternating optimization ansatz  ZHIHUI WANG (Presenter), Quantum Artificial Intelligence Laboratory, NASA Ames Research Center, MUSTAFA ADNANE, Quantum Artificial Intelligence Laboratory, Universities Space Research Association, NASA Ames Research Center, ELEANOR RIEFFEL, BRYAN O’GORMAN, Quantum Artificial Intelligence Laboratory, NASA Ames Research Center, STUART HADFIELD, RICCARDO MENGONI, DAVIDE VENTURELLI, Quantum Artificial Intelligence Laboratory, Universities Space Research Association, NASA Ames Research Center — Network-related connectivity optimization problems are underlying a wide range of applications and are of high computational complexity. We consider studying network optimization problems using quantum heuristics. In particular, we consider Quantum Alternating Operator Ansatz, an extension of the Quantum Approximate Optimization Algorithms, in which a cost-function based unitary and a non-commuting mixing unitary are applied alternately. We present mappings for a few network optimization problems, including variants of finding the optimal spanning-tree or spanning-graph of a graph. We give special focus on the design of mixers based on the constraints in the problem such that the system evolution remains in a subspace of the full Hilbert space where all constraints are satisfied. In the spanning-tree problem, one such constraint is that a mixer applied to a spanning tree needs also be a spanning tree. This involves checking the connectivity of a subgraph, which is a global condition common for most network-related problems. We show how this feature can be efficiently represented in the mixer in a quantum coherent way, based on manipulation of a descendant-matrix and an adjacent matrix. We further develop a mixer for the spanning-graphs based on the spanning-tree mixer.

9:36AM K42.00009: Adiabatic Quantum Chemistry Simulations with Superconducting Qubits  NIKOLAJ MOLL (Presenter), GIAN SALIS, MARC GANZHORN, DANIEL EGGER, STEFAN FILIPP, IBM Research - Zurich, MARCO ROTH, RWTH Aachen University, SEBASTIAN SCHMIDT, ETH Zurich — The simulation of a quantum system with a classical computer without any approximations is intractable even for moderate system sizes. It has been recognized early that using a controllable quantum system as a simulator could solve this for increasing system sizes. We propose a scalable quantum simulator based on driven superconducting qubits where the interactions are generated parametrically by polychromatic magnetic flux modulation of a tunable bus element. In this system, the XX- and YY-type interactions as well as transverse fields are independently tunable over a large parameter range. We experimentally demonstrate an adiabatic simulation using two superconducting qubits and one tunable bus element. The time required to reach the ground state of the Hamiltonian lies in the few microseconds range and therefore is well within the capability of currently available superconducting circuits.
**9:48AM K42.00010: Faster classical sampling from distributions defined by quantum circuits** [invited] IGOR MARKOV (Presenter), ANEEQA FATIMA, University of Michigan, SERGEI ISAKOV, SERGIO BOIXO, Google — As quantum computers become more capable, the question of when they surpass state-of-the-art classical computation for a well-defined computational task is attracting much attention. The leading candidate task for this milestone entails sampling from the output distribution defined by a random quantum circuit. We develop algorithms and software for massively-parallel simulation. In particular, we propose two new ways to trade circuit fidelity for computational speedups, so as to match the fidelity of a given quantum computer --- a task previously thought impossible. We report massive speedups for the sampling task over prior software from Microsoft, IBM, Alibaba and Google, as well as supercomputer and GPU-based simulations. By using publicly available Google Cloud Computing, we price such simulations and enable comparisons by total cost across hardware platforms. We simulate approximate sampling from the output of a circuit with 7x8 qubits and depth 1+40+1 by producing one million bitstring probabilities with fidelity 0.5%, at an estimated cost of $35184. Simulating circuits of depth to 1+48+1 would cost one million dollars.

**10:24AM K42.00011: Subspace-search variational quantum eigensolver for excited states** KEN M NAKANISHI (Presenter), Physics, The University of Tokyo, KOSUKE MITARAI, Engineering Science, Osaka University, KEISUKE FUJII, Physics, Kyoto University — The variational quantum eigensolver (VQE), a variational algorithm to obtain an approximated ground state of a given Hamiltonian, is an appealing application of near-term quantum computers. To extend the framework to excited states, we here propose an algorithm, the subspace-search variational quantum eigensolver (SSVQE). This algorithm searches a low energy subspace by supplying orthogonal input states to the variational ansatz and relies on the unitarity of transformations to ensure the orthogonality of output states. The k-th excited state is obtained as the highest energy state in the low energy subspace. The proposed algorithm does not employ any ancilla qubits. The disuse of the ancilla qubits in our algorithm is a great improvement from the existing proposals for excited states, which have utilized the swap test, making our proposal a truly near-term quantum algorithm. We further generalize the SSVQE to obtain all excited states up to the k-th by only single optimization procedure. From numerical simulations, we verify the proposed algorithms. This work greatly extends the applicable domain of the VQE to excited states and their related properties like a transition amplitude without sacrificing any feasibility of it.

*This work was supported by QunaSys Inc.

**10:36AM K42.00012: Holistic Error Mitigation Frameworks For Near-Term Computations** EUGEN DUMITRESCU (Presenter), RAPHAEL POOSER, ALEXANDER MCCASKEY, TITUS MORRIS, PAVEL LOUGOVSKI, Oak Ridge National Laboratory — It is necessary to mitigate physical errors in order for NISQ computations to compute quantities with reasonable accuracy. Therefore NISQ programming stacks must include a robust error mitigation infrastructure supplementing principal quantum programs at compile time and operating at a high level of abstraction. We introduce an error mitigation framework consisting of routines built into a software stack aiming to return corrected data from programs run on NISQ devices. As a demonstration, we implement a variety of protocols which increase the accuracy of variational quantum eigensolver-style hybrid algorithms running on multiple NISQ devices.

*This work was supported as part of the ASCR-Testbed Pathfinder Program at Oak Ridge National Laboratory under FWP #ERKJ332

**10:48AM K42.00013: Quantum Kitchen Sinks: An algorithm for machine learning on near-term quantum computers** CHRISTOPHER WILSON (Presenter), Institute for Quantum Computing, University of Waterloo, JOHANNES OTTERBACH, OpenAI, NIKOLAS TEZAK, ROBERT S SMITH, PETER KARALEKAS, ANTHONY POLLORENO, SOHAIB ALAM, GAVIN CROOKS, MARCUS DA SILVA, Rigetti Computing — Noisy intermediate-scale quantum (NISQ) computing devices are an exciting platform for the exploration of the power of near-term quantum applications. We describe a near-term quantum application for machine learning tasks by building upon the classical algorithm known as random kitchen sinks. Our technique, called quantum kitchen sinks, uses quantum circuits to nonlinearly transform classical inputs into features that can then be used in a number of machine learning algorithms. We demonstrate the power and flexibility of this proposal by using it to solve binary classification problems for synthetic datasets as well as handwritten digits from the MNIST database. Simulations show, in particular, that small quantum circuits provide significant performance lift over standard linear classical algorithms, reducing classification error rates from 50% to <0.1%, and from 4.1% to 1.4% in these two examples, respectively. We show comparable performance for these examples in experiments with superconducting qubits.

**Wednesday, March 6, 2019 8:00 AM - 11:00 AM**

Session K43 DCMP: Breakthroughs in Quantum Dynamics BCEC 210B - Anatoli Polkovnikov - Tag(s): Invited
8:00AM K43.00001: Spatio-temporal quenches for fast preparation of ground states of critical models* [Invited]
KARTIEK AGARWAL (Presenter), McGill University, SHIVAJI SONDHI, RAVINDRA BHATT, MATTEO IPPOLITI, Princeton University, PRAHAR MITRA, Institute for Advanced Study — The difficulty of preparing highly entangled quantum states poses an important challenge in engineering artificial quantum systems for the purposes of computation and simulation. Adiabatic methods which slowly evolve unentangled states to entangled states are typically slow and particularly fail at criticality where the gap between eigenstates vanishes. The search for novel non-adiabatic methods for quantum state preparation is a topic of current research interest, and immense experimental relevance. I will describe the state of the art in the field and discuss our proposal(s) using spatio-temporal quenches to efficiently prepare the ground states of arbitrary interacting critical theories in one dimension and beyond.

*UK Foundation
DOE-BES Grant No. DE-SC0002140

8:36AM K43.00002: Localization and Thermalization in Nuclear Spin Chains [Invited] PAOLA CAPPELLARO (Presenter), Massachusetts Institute of Technology — TBD

9:12AM K43.00003: Many body localization with long range interactions* [Invited] RAHUL NANDKISHORE (Presenter), University of Colorado, Boulder — Many-body localization (MBL) has emerged as a powerful paradigm for understanding nonequilibrium quantum dynamics. Folklore based on perturbative arguments holds that MBL arises only in systems with short-range interactions. I will present nonperturbative arguments indicating that MBL can arise in systems with long-range (Coulomb) interactions, through a mechanism dubbed “order enabled localization.” In particular, one can show using bosonization that MBL can arise in one-dimensional systems with \( -r \) interactions, a problem that exhibits charge confinement. One can also show that (through the Anderson-Higgs mechanism) MBL can arise in two-dimensional systems with \( \log(r) \) interactions, and perhaps even in three-dimensional systems with \( 1/r \) interactions. The extension to three dimensions requires developing a theory of localization of extended quantum objects. The arguments are asymptotic (i.e., valid up to rare region corrections), yet they open the door to investigation of MBL physics in a wide array of long-range interacting systems where such physics was previously believed not to arise. They also open the door to using MBL to stabilize driven superconductivity.


*This work is supported in part by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0183 and in part by the Sloan Foundation through a Sloan Research Fellowship.

9:48AM K43.00004: Exploring Quantum Thermalization Near Integrability in a Dipolar Quantum Newton's Cradle* [Invited] BENJAMIN LEV (Presenter), YIJUN TANG, Stanford University, SARANG GOPALAKRISHNAN, Physics, CUNY, MARCOS RIGOL, Physics, Pennsylvania State University, WIL KAO, KUAN-YU LI, Stanford University, KRISHNANAND MALLAYYA, Physics, Pennsylvania State University — Isolated quantum many-body systems with integrable dynamics generically do not thermalize starting from generic initial states when taken far from equilibrium. As one perturbs such systems away from the integrable point, thermalization sets in, but the nature of the crossover from integrable to thermalizing behavior is an unresolved and actively discussed question. We explore this question by studying the dynamics of the momentum distribution function in a dipolar quantum Newton’s cradle consisting of highly magnetic dysprosium atoms. This is accomplished by creating an ultracold one-dimensional Bose gas with strong magnetic dipole-dipole interactions. These interactions provide tunability of both the strength of the integrability-breaking perturbation and the nature of the near-integrable dynamics. We provide the first experimental evidence that thermalization close to a strongly interacting integrable point occurs in two steps: prethermalization followed by near-exponential thermalization. Moreover, the measured thermalization rate is consistent with a parameter-free theoretical estimate, based on identifying the types of collisions that dominate thermalization. By providing tunability between regimes of integrable and nonintegrable, chaotic dynamics, our work sheds light both on the mechanisms by which isolated quantum many-body systems thermalize, and on the temporal structure of the onset of thermalization. Reference: Y. Tang, W. Kao, K.-Y. Li, S. Seo, K. Mallayya, M. Rigol, S. Gopalakrishnan, and B. L. Lev, Phys. Rev. X 8, 021030 (2018).

*AFOSR (FA9550-12-1-0056) and NSF (PHY-1707482)

10:24AM K43.00005: Many body quantum chaos [Invited] TOMASZ PROSEN (Presenter), University of Ljubljana — TBD

Wednesday, March 6, 2019 8:00 AM - 11:00 AM
8:00AM K44.00001: Quantum Oscillations in Kondo Insulators* [Invited]  LU LI (Presenter), University of Michigan — In metals, orbital motions of conduction electrons on the Fermi surface are quantized in magnetic fields, which is manifested by quantum oscillations in electrical resistivity. This Landau quantization is generally absent in insulators. Here, we report a notable exception in an insulator — ytterbium dodecaboride (YbB₁₂). The resistivity of YbB₁₂, which is of a much larger magnitude than the resistivity in metals, exhibits distinct quantum oscillations. These unconventional oscillations arise from the insulating bulk, even though the temperature dependence of the oscillation amplitude follows the conventional Fermi liquid theory of metals with a large effective mass. Quantum oscillations in the magnetic torque are also observed, albeit with a lighter effective mass.

*This work is mainly supported by the National Science Foundation under award DMR-1707620 (high field magnetization and resistivity measurements), by the Office of Naval Research through the Young Investigator Prize under award N00014-15-1-2382 (sample structure and low field electrical transport characterizations). The development of the torque magnetometry technique in intense magnetic fields was supported by the U.S. Department of Energy (DOE) under award DE-SC0008110. Some results are obtained with equipment supported by the National Science Foundation Major Research Instrumentation award under DMR-1428226 (the equipment of the thermodynamic and electrical transport characterizations).

8:36AM K44.00002: Fermi surfaces in Kondo insulators [Invited] SUCHITRA SEBASTIAN (Presenter), University of Cambridge — TBD

9:12AM K44.00003: A Physical-Chemical Understanding of Samarium Hexaboride [Invited] TYREL MCQUEEN (Presenter), Johns Hopkins University — TBD

9:48AM K44.00004: Mixed valence insulators with neutral Fermi surfaces* [Invited] SENTHIL TODADRI (Presenter), Massachusetts Institute of Technology — A number of recent experiments have suggested the possibility that the low-temperature insulating bulk of mixed valence systems like SmB₆ and YbB₁₂ hosts electrically neutral gapless excitations. I will describe a new phase of matter—composite exciton Fermi liquid—a mixed valence insulator with a three dimensional fermi-surface of a neutral fermion, that we name the "composite exciton". I will describe the mechanism responsible for the formation of such excitons, discuss the phenomenology of the composite exciton Fermi-liquid and discuss existing and possible future experiments.

*Research supported US Department of Energy grant DE-SC0008739, and partly by the Simons Foundation.

10:24AM K44.00005: Quantum Oscillation from in-gap states in Kondo insulators [Invited] HUITAO SHEN (Presenter), Massachusetts Institute of Technology — Recent experiments on quantum oscillation in heavy fermion materials, such as SmB₆ and YbB₁₂, has gained great many interests in the community of strongly correlated electrons. Its physical origin has been hotly debated.

In this talk, we present the most direct explanation to this novel phenomenon—quantum oscillation comes from in-gap quasiparticles. The quantum oscillation found in these narrow gap insulators, where the scattering rate controls Lifshitz-Kosevich (LK) factor instead of Dingle factor, is quite the opposite to the case of normal metals, where the scattering rate controls Dingle factor instead of LK factor. This novel result is an important prediction of our theory and differs clearly with other theories. We provide an analytical formula that can be used by experimentalists to fit and interpret their data. Our calculation based on the ARPES data agrees very well with the quantum oscillation experiments.

Wednesday, March 6, 2019 8:00 AM - 10:48 AM
Viscoelastic Thin Films SHEETAL RANGA (Presenter), RABIBRATA MUKHERJEE, Department of Chemical Engineering, Indian Institute of Technology Kharagpur —

Self-organized instability patterns in thin films are of great interest in diverse scientific and technological applications. We investigated the surface instability in a viscoelastic film engendered by externally applied electric field perpendicular to the film surface in a capacitor geometry. Here the main destabilizing force is electrostatic pressure and the restoring effects arising out of stretching of the crosslinked elastomeric film. The external field polarizes the air-polymer interface and the film surface destabilizes itself to align in the direction of the applied field to minimize the energy forming different morphologies. We report here complete bonding-debonding sequence and morphological transformation. During bonding, the patterns appear only when the field strength \( U \) exceeds critical voltage \( U_c \), which depends on the shear modulus, gap spacing, and film thickness etc. With an increase in \( U \), initially columns appear which further evolves into labyrinths and holes before the film surface comes in complete conformal contact with the top electrode. During debonding, the patterns appear following exactly opposite morphological sequence. Though the patterns are completely switchable by electric field we have observed hysteresis during de-bonding.

Transition from spin dewetted droplets to continuous film in a semi-crystalline Polyethylene Oxide thin film SOUMYAMOULI PAL (Presenter), RABIBRATA MUKHERJEE, Department of Chemical Engineering, Indian Institute of Technology Kharagpur — Polymeric thin films are increasingly being utilized for technological applications, such as coatings, functional surfaces, etc. Dewetting and crystallization both play a significant role in determining the film morphology and ultimate film properties. When polyethylene oxide (PEO) is spin coated from a nonpolar solvent (chloroform), crystallization proceeds via formation of spherulites, which correlate well with Avrami kinetics. Spontaneous rupture of the dispersed solution layer during spin coating results in isolated periodic morphologies of the solute at low concentrations (\( C_n \)). Here, the morphology of PEO thin films coated on pre-patterned PDMS substrate transforms from spin-dewetted droplets to elongated threads to continuous films with an increase in \( C_n \). We investigated the effects of RPM variation during spin coating on the transition of spin-dewetted morphologies from droplets at lower RPM to continuous film at higher RPM. We further show that within the spin-dewetted regime, with a decrease in solute concentration and increase in RPM, droplet periodicity (\( \lambda_D \)) reduces and number density of droplets increases. Spherulite structures were observed in both spin-dewetted aligned droplets and continuous films; however, lamellar structures were observed in elongated threads.

Influence of residual stress on dewetted morphology of spin coated polymer thin films ALOK PATRA (Presenter), ANUJA DAS, RABIBRATA MUKHERJEE, Department of Chemical Engineering, Indian Institute of Technology Kharagpur — Spontaneous instability in polymer thin film leading to its rupture and subsequent formation of polymer droplets is called Dewetting. In this regard, it is essential to investigate the fundamental properties of polymer leading to dewetting and its effect on the dewetted morphology. We report the dependence of dewetted morphology of polymer thin film on residual stress generated during spin coating. Unlike applied stress, residual stress arises due to polymer chain entanglement while the polymer is in solution state and endures high centripetal force. The spin-coated polymer film is at a metastable equilibrium state generating a residual stress among the polymer chains. We produce different residual stress in polymer thin film of same thickness by spin coating at different rotation speeds. Based on the degree of stress present, the dynamics of dewetting as well as morphology varies. From this we exhibit the contrast by dewetting the thin film by different techniques: Thermal annealing, solvent vapor and good solvent mediated dissolution. The contrast in the morphology is shown as a measure of droplet periodicity (\( \lambda_D \)) and diameter (\( D_D \)). Consequently, we can qualitatively predict the degree of residual stress in thin film by its dewetted morphology without further characterization.

Structure and dynamics of pseudo-partial wetting precursor films EMILIE VERNEUIL, FRANCOIS LEQUEUX, HELENE MONTES, CLAIRE SCHUNE (Presenter), MARC YONGER, SIMM, ESPCI Paris — Wetting of liquids on high energy solids where the spreading parameter is positive is expected to lead to nanometer-thick precursor films spreading out of the macroscopic liquid body. In this film, Van der Waals interactions induce either disjoining or conjoining Derjaguin pressure that respectively tend to separate the film interfaces or to bring them together.

We report for the first time systematic observations of droplets and their precursor films of high polarisability polymer melts on silica, which lead to a pseudo-partial wetting situation: at equilibrium, the droplet coexists with its film, in which the Derjaguin pressure is conjoining. By ellipsometry, we clearly evidence the unique structure and dynamics of these precursor films compared to total wetting films. Whereas in total wetting, the precursor film ends with a sharp step and consists of dense macromolecules, the profile of pseudo-partial wetting films is diffusive and the molecules form a quasi-two-dimensional gas with a diffusion coefficient specific to each polymer. These results were extended to a series of common organic polymers and rationalized within the framework of Van der Waals interactions, and short range surface interactions.
Theoretical insights into the hydrophobicity of low index CeO$_2$ surfaces

MARCO FRONZI (Presenter), International Research Centre for Renewable Energy, Xi’an Jiaotong University, HUSSEIN ASSADI, Center for Green Research on Energy and Environmental Materials, National Institute for Materials Science, DORIAN HANAOR, Chair of Advanced Ceramic Materials, Institute for Materials Science and Technology, Technische Universität Berlin — The hydrophobicity of CeO$_2$ surfaces is examined here. Since wettability measurements are extremely sensitive to experimental conditions, we propose a general approach to obtain contact angles between water and ceria surfaces of specified orientations based on density functional calculations. In particular, we analysed the low index surfaces of this oxide to establish their interactions with water. and we found the CeO$_2$ (111) surface to be the most hydrophobic, whereas the CeO$_2$ (110) surface is mildly hydrophilic. Also, we found that the O terminated (100) surface was unstable unless fully covered by molecularly adsorbed water. We identified a strong attractive interaction between the hydrogen atoms in water molecules and surface oxygen, which gives rise to the hydrophilic behaviour of (110) surfaces. The findings here shed light on the origin of the intrinsic wettability of rare earth oxides in general and CeO$_2$ surfaces in particular and also explain why CeO$_2$ (100) surface properties are so critically dependant on applied synthesis methods.

*The financial support was provided by the National Natural Science Foundation of China (Grant No. 51323011). Computational resources were provided by the Center for Computational Sciences at the University of Tsukuba.

Inferring Boundary Viscosity Values from Shear Deformation of Molecularly Thin Films

KISHAN MAKWANA (Presenter), Physics, University of Oxford, Oxford OX1 3PN, UK, SANDRA TROIAN, MC128-95, CALTECH, Pasadena, CA 91125 — Derjaguin and co-workers in 1946 introduced a shear technique for inferring the boundary viscosity of ultrathin liquid films. Air blown through a slender horizontal slit is used to apply a constant shear stress to the free surface of an initially flat and uniform film. Newtonian films tend to distort streamwise into a wedge shape whose slope decreases in time. The viscosity of the film can then be extracted from the wedge slope. High resolution measurements of the deformed film shape are normally obtained by interferometry for microscale films or ellipsometry for molecular scale films. Over the years, it has become evident that liquid nanofilms can exhibit a shear response that deviates significantly from this ideal linear behavior. Various physical mechanisms have been proposed to help resolve discrepancies between theory and experiment. Here we present finite element simulations of the liquid deformation process to evaluate help assess the influences of different mechanisms. Based on quantitative comparison to experimental data, we describe which candidate mechanisms best fit the trends observed.

*KM gratefully acknowledges support from the Oxford University Laidlaw Undergraduate Research and Leadership Scholarship.

Dependency of ice adhesion strength on surface wettability and roughness

MARINA MACHADO DE OLIVEIRA (Presenter), SUBASH KATTEL, JOSEPH MURPHY, JOHN ACKERMAN, WILLIAM RICE, VLADIMIR ALVARADO, University of Wyoming — Ice adhesion mechanisms are poorly understood contributing to the limited effectiveness of current ice mitigation techniques. The ideal solution is to prevent ice accretion via suppression of ice adhesion on ice-phobic surfaces, which requires understanding ice-phobicity at a more fundamental level. Given the breadth of published results, we designed an experimental matrix to isolate the effects of roughness and dynamic water spreading on ice adhesion. To this end, we conducted detailed surface roughness maps and novel dynamic contact angle measurements on stainless steel, aluminum, and non-metallic materials. We varied temperature to evaluate a variety of conditions encountered in practice such as clear ice, mixed ice and rime ice. Dynamic hysteresis of the contact angle and adhesion are clear functions of the forcing frequency and amplitude as well as surface roughness in pendant drop experiments. These results are a step towards finding physics-based solutions to ice accretion challenges.

*We acknowledge support through NASA under Grant No. WY-80NSS17M0049
9:24AM K45.00008: Rapid Detection of Thalassaemia Carriers by Image Analysis of Dried Patterns of Blood and Plasma Droplets  
MANISH AYUSHMAN (Presenter), MANIKUNTALA MUKHOPADHYAY, SUNANDO DASGUPTA, Chemical Engineering, Indian Institute of Technology Kharagpur — The drying of drops of biological fluids such as blood/plasma leads to the formation of several interesting and complex patterns. Specific diseases can give rise to distinct drying patterns where the final pattern will depend on a number of factors such as plasma content and the morphology of the red blood cells. Thalassaemia is the most common single gene disorder in which the production of haemoglobin is impaired. At present, the gold standard method, used for carrier detection in hospitals, requires expensive instruments, skilled manpower and significant time, making it difficult to be used as an on-site method. A rapid, portable and automated technology for thalassaemia carrier screening is hence of significant importance. The carrier samples were separated from the healthy ones based on their blood and plasma droplet drying patterns. Image analysis based tools were used to identify the distinct signatory features in the patterns of the respective samples and correlated to the results obtained from the gold standard method. The proposed technique can be instrumental in developing a rapid, less laborious and cost effective ‘on-field’ screening method thus enabling the initial screening of the carriers from the large population.

9:36AM K45.00009: Creeping of Salt Solutions: Influence of Surfactants  
MOHSIN QAZI (Presenter), HERISH SALIM, ETIENNE JAMBON-PUILLET, DANIEL BONN, NOUSHINE SHAHIDZADEH, Institute of Physics, University of Amsterdam — Salt creeping, the growth of crystals from evaporating salt solutions beyond the solution boundary, is a very common and fascinating phenomenon. It has a significant impact in industrial processes involving high salt concentrations, for the sodification of agricultural soils and for the preservation of salt-contaminated buildings and artworks1. In spite of its importance, salt creeping remains poorly understood and there are consequently hardly or no measures to control the phenomenon2. We present new experiments using a custom-made setup, that allows to reproduce the creeping phenomenon in the laboratory and study the influence of environmental conditions and additives. We show that during evaporation of salt solutions, the creeping starts only when the contact angle reaches a well-defined critical value, allowing us to propose a mechanism for the creeping dynamics. In addition, a nucleation promoting surfactant promotes creeping whereas a nucleation inhibitor prevents it.


9:48AM K45.00010: Transient dynamics of viscous drop impact on immiscible liquid bath: A holistic analysis*  
KUMARI TRINAVEE (Presenter), SIRSHENDU MISRA, NAGA SIVA KUMAR GUNDA, SUSHANTA MITRA, Mechanical and Mechatronics Engineering, University of Waterloo — Droplet entry problems offer extensive opportunities to understand the non-trivial multifluid interaction and the resulting complex evolution of phase boundary. Although droplet entry problems on identical or miscible liquid pool has been prolifically studied, its immiscible counterpart is rather unexplored. In this work, we present our holistic approach coupling experimental observation with theoretical and numerical validation to better understand the dynamics of droplet impact for an oil droplet impinged on a water pool. Our focus is laid on understanding the topologically complex temporal evolution of the oil/water liquid interface. Images acquired from a high-speed camera has been processed to obtain the interface acceleration which in turn is used to calculate an assistive force field responsible for the pinch-off. An analysis involving the change in total energy in the penetration process for a flow field with negligible viscous dissipation has been presented. The experimental results are validated with a volume of fluid based numerical model developed in-house. Additionally, we investigated the equilibrium droplet shape beyond penetration and its dependence on the properties of surrounding fluid, which still is an unexplored area in literature.

*NSERC DG.
Investigation of the interaction between graphene membranes suspended and liquid by nano-infrared spectroscopy*

LEONEL MEIRELES (Presenter), Universidade Federal de Minas Gerais, INGRID DAVID BARCELOS, CNPEM, Laboratório Nacional de Luz Síncrotron, GUSTAVO ARRIGHI FERRARI, PAULO ALEXANDRE DE ALMEIDA NEVES, Universidade Federal de Minas Gerais, RAUL OLIVEIRA FREITAS, CNPEM, Laboratório Nacional de Luz Síncrotron, RODRIGO GRIBEL LACERDA, Universidade Federal de Minas Gerais — The chemical properties of biological systems in their native living environment has been a constant ambition in life sciences. Infrared spectroscopy is a unique analytical tool that enables identification of chemical compounds by their natural molecular-vibrational signatures in a label-free mode. Here we report the development of a robust fluidic platform specifically designed for nanoscale resolved infrared spectroscopy of biomaterials in liquid environments. An advantage of our proposed fluidic chip is the use of an atomic-thin graphene layer as an optical window for accessing the liquid stream inside the micro-channels written in the silicon wafer. We demonstrate the feasibility of the platform for scattering scanning near-field optical microscopy for measuring the infrared fingerprint of typical biological fluids based on Dimethyl Sulfoxide, Phosphate, Citric Acid, and Human Serum Albumin. We foresee our development to serve as a template for future studies involving fundamental questions on the chemistry of in-solution nanoscale bio-systems.

*We thank the financial support given by CAPES, Fapemig, (Rede 2D), CNP, INCT/Nanomaterials de Carbono and for Brazilian Synchrotron Light Laboratory (LNLS) for the beamline time.

Underliquid wetting behavior of graphene: Is the hypothesis of wetting transparency valid?*

SIRSHENDU MISRA (Presenter), NAGA SIVA KUMAR GUNDA, SUSHANTA MITRA, Department of Mechanical and Mechatronics Engineering, University of Waterloo — Since the inception of wetting transparency hypothesis, understanding the wetting behavior of graphene and its dependence on the choice of underlying support layer fostered significant attention from scientific community. However, wetting studies on submerged graphene coated substrates are relatively scarce despite promising practical applications (e.g. water harvesting, oil-water separation etc.). Here we attempt to understand the wetting characteristics of a monolayer of graphene coated on a glass substrate when submerged in a liquid bath. A wide range of droplet and surrounding liquid combinations have been investigated to assess the dependency on the interaction potentials. In general, partial transparency towards wetting is observed and the degree of the same is seen to demonstrate a non-trivial dependence on the polar and dispersive interaction potentials between the participating entities with the competition between wetting affinities of the droplet and the surrounding liquid with respect to the coated substrate displaying the most prominent effect. Taking cue from Trinavee et al. (Langmuir 2018, 34, 11695−11705), a modified theoretical model involving formation of an intermediate thin film is proposed to explicate this underliquid wetting phenomenon.

*WIN Nanofellowship

Isotherm kinetics and rapid sorption activity of mesoporous vdW 2D sheets decorated with magnetic nanobeads*

MEENAKSHI TALUKDAR (Presenter), PRITAM DEB, Tezpur University — Two-dimensional (2D) van der Waals (vdW) adsorbent sheets represent as an emerging class of materials overcoming the limitations for oil adsorption. Here, the interaction between adsorbent and adsorbate can be realised by the adsorption isotherm of the adsorption process [Phys. Rev. Lett. 120, 264502, 2018]. Besides, the kinetics of the adsorption process is an important characteristics in understanding the rate of adsorption mechanism in vdW sheets [Rev. Mod. Phys. 89, 035005, 2017]. In addition to the standard isotherm and kinetics retention of the physical phenomena of the host magnetic nanocomposite system, our study has reported a promising adsorbent material for efficient and rapid oil recovery providing feasible solution towards the upcoming oil consumption [arXiv 2018.03037, 2018]-[Indian Patent Application 201831009592, 2018].

*Tezpur University
Effect of Catalysis-clustering on Gas-sensing Performance*

NACIR TIT (Presenter), MUHAMMAD ALI, ALAA SHAHEEN, Physics, UAE University — We present a theoretical investigation, based on a combined of density-functional theory (DFT) and non-equilibrium Green’s-functional (NEGF) formalism, to study the effect of catalysis-clustering on the sensor response. Specifically, the scope is to compare the adsorption and transport properties after chemisorption of CO2 molecules on iron (Fe) ad-atoms deposited on graphene nano-ribbons (GNR) in two different ways: (i) Five Fe ad-atoms deposited on GNR in scattered fashion; and (ii) A cluster of five Fe atoms deposited on GNR. The results of IV-curves calculations confirm stronger deviations in the case of scattered Fe ad-atoms and, consequently, stronger sensor response. This work suggests stronger sensitivity and selectivity to be reached by scattering ad-atoms of the transition-metal catalysis and with an optimization of their density. As the sensor response is based on the deviation of conductance from before to after the exposure to the gas, our results have indeed a direct application to fabricate solid-state based gas sensors working with high sensitivity at room temperature, to detect toxic and hazardous gases such as CO2.

*31R145-Research Center in UAEU - ECEER -2-2017

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K46 DMP: Complex Oxide Interfaces & Heterostructures -- Interfacial two dimensional electron gas

8:00AM K46.00001: Two dimensional t2g electron gas at the oxide interface* [Invited] ALEXANDER DEMKOV (Presenter), University of Texas at Austin — The discovered revolutionary class of polar oxide heterostructures holds tremendous promise for exploiting the physical properties of the novel 2DEG formed at the oxide/oxide interface. SrTiO3 is a widely used substrate for the growth of other functional oxide thin films. The reactivity of the substrate with respect to the film during deposition, particularly with regard to redox reactions, has typically been glossed over. We have recently demonstrated by depositing a variety of metals and measuring the in situ core level spectra of both the metal and SrTiO3 that, depending on the oxide formation energy and work function of the metal, there will be an interfacial layer of oxygen-deficient SrTiO3 at the interface with the top oxide film. I will focus on the integrated highly spin-split ferromagnetic semiconductor EuO onto perovskite SrTiO3 (001). A careful deposition of Eu metal by molecular beam epitaxy resulted in EuO growth via oxygen out-diffusion from SrTiO3. This in turn leaves behind a highly conductive interfacial layer through generation of oxygen vacancies. Below the Curie temperature of 70 K of EuO, this spin-polarized two-dimensional t2g electron gas at the EuO/SrTiO3 interface displays very large positive linear magnetoresistance.

*Air Force Office of Scientific Research (FA9550-12-10494)

8:36AM K46.00002: Engineering BaTiO3 Based Ferroelectric Materials with Reactive Molecular Dynamics Simulations* DUNDAR YILMAZ (Presenter), DOOMAN AKBARIAN, Pennsylvania State University, PANCHAPAKESAN GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, ADRI C VAN DUIN, Pennsylvania State University — Ferroelectric materials such as barium titanate (BaTiO3) have wide applications in nano scale electronic devices due to their outstanding properties. In this study, we developed a ReaxFF reactive force field for BaTiO3 which can reproduce the ferroelectric/non-ferroelectric phases, ferroelectric and thermal hysteresis loops of the BaTiO3 crystal structure and O-vacancy, Ba-O and Ti-O divacancy formation energies and their migration. This ReaxFF description can be straightforwardly extended to a wide range of material interfaces. The force field predicted that a 4.8 nm sample thickness is required to observe the ferroelectric hysteresis effect. Also, we found that oxygen vacancies (OVs) in the BaTiO3 cluster reduce the polarization and the phase transition temperature. Our BaTiO3 ReaxFF reactive force field showed an outstanding ability of predicting the domain walls in BaTiO3. We investigated effect of the defect (O-vacancy, divacancy) densities as well as the thickness on the ferroelectric hysteresis loops of the BaTiO3 thin film structures to lead design efforts of novel BaTiO3 based ferroelectric materials.

*We acknowledge funding from AFRL grant FA9451-16-1-0041. Part of this work was supported by DOE-BES.
Engineered Helicity of One-Dimensional LaAlO$_3$/SrTiO$_3$ Nanowires

MEGAN BRIGGEMAN (Presenter), JIANAN LI, Physics and Astronomy, University of Pittsburgh, MENGCHEN HUANG, Physics, University of California-Santa Barbara, ANTHONY TYLAN-TYLER, Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNGWOO LEE, CHANG-BEOM EOM, Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Physics and Astronomy, University of Pittsburgh — Quantum transport in 1D geometries is fascinating in its own right, but it can also be regarded as a building-block for a variety of quantum devices. We have developed a flexible platform for creating 1D nanostructures at the LaAlO$_3$/SrTiO$_3$ interface using a conductive-AFM lithography technique [1]. Straight nanowire segments behave as electron waveguides with subband occupation that can be tuned with a gate and an external magnetic field [2]. We can periodically perturb this waveguide, with 10 nm periodicity, in two ways. “Kronig-Penney” type modulation results in periodic vertical displacement of the electron waveguide, and sinusoidal lateral displacement of the nanowire can also be achieved. Combining the two perturbations in quadrature yields a helical nanowire which exhibits striking oscillatory transmission as a function of both magnetic field and chemical potential. We discuss these results in terms of an engineered axial in-plane spin-orbit interaction within the spiral electron waveguide.


Determination of Spin-Orbit Scattering Lifetime at the Interface of LaAlO$_3$/SrTiO$_3$ from the Superconducting Upper Critical Fields

WEI-LI LEE (Presenter), AKHILESH SINGH, TSUNG-CHI WU, MING-YUAN SONG, MING-CHIN CHEN, CHI-SHEN LI, Institute of Physics, Academia Sinica — The intrinsic mechanism of the spin-orbit coupling at the LaAlO$_3$/SrTiO$_3$ interface remains a debatable issue. Rashba-type spin-orbit coupling is an appealing candidate that has been demonstrated by several magnetotransport results. On the other hand, the atomic spin-orbit coupling was also shown to play an important role, particularly when the Fermi level is close to the Lifshitz point. Unlike previous works, we focus on the measurements of the anisotropic and superconducting upper critical fields in gated LaAlO$_3$/SrTiO$_3$ devices. By rigorous fittings of the $H_{c2}$-$T$ curves using both the Werthamer-Helfand-Hohenberg theory and Klemm-Luther-Beasley model, the spin-orbit scattering lifetime can be determined with high precision in superconducting state. We found that the extracted spin-orbit lifetime monotonically increase with the transport lifetime that spanned over two orders of magnitude in the regime with sheet density higher than that at Lifshitz point. Those results suggest the dominant role of Elliott-Yafet type spin-relaxation. Comparison to the weak localization fittings will be presented and discussed.

*We acknowledge the funding support from MoST Taiwan (MOST 105-2112-M-001 -012 -MY3).

Nanoscale Inhomogeneous Energy Landscape in LaAlO$_3$/SrTiO$_3$ Heterostructures

ADITI NETHWEWALA (Presenter), MEGAN BRIGGEMAN, JIANAN LI, YUHE TANG, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNGWOO LEE, CHANG-BEOM EOM, Department of Material Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — The energy landscape of LaAlO$_3$/SrTiO$_3$ (LAO/STO) heterostructures plays an important role in determining the transport phenomena. An inhomogeneous energy landscape can lead to the breakdown of 2D transport and the emergence of 1D transport. Thus, knowledge of the energy landscape of the system can play a significant role in understanding correlated electron systems. Here we report a minimally invasive probing technique to map the energy landscape of LAO/STO heterostructures. Using conductive atomic force microscope (c-AFM) lithography [1], we write nanoscale cross-shaped electron waveguides, or “nanocrosses”. Low temperature magnetotransport measurements reveal signs of spatial inhomogeneity. Anisotropic magnetoconductance and anomalous Hall resistance also indicate inhomogeneity. The nanocross geometry provides a powerful tool for exploring the energy landscape of the system and its implications under one frame.


*JL acknowledges support from the Vannevar Bush Faculty Fellowship program, funded by ONR (N00014-15-1-2847). C-BE acknowledges support from NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-4046).
9:24 AM K46.00006: Two-dimensional type-II Dirac fermions in a LaAlO3/LaNiO3/LaAlO3 quantum well

LINGLING TAO (Presenter), EVGENY Y TSYMBAL, Institute of Physics — The type-II Dirac fermions that are characterized by a tilted Dirac cone and anisotropic magnetotransport properties have been recently proposed theoretically and confirmed experimentally. Here, we predict the emergence of two-dimensional (2D) type-II Dirac fermions in LaAlO3/LaNiO3/LaAlO3 quantum-well structures. Using first-principles calculations and model analyses, we show that the Dirac points are formed at the crossing between the dx2−y2 and dz2 bands protected by the mirror symmetry. The energy position of the Dirac points can be tuned to appear at the Fermi energy by changing the quantum-well width. For the quantum-well structure with a two-unit-cell-thick LaNiO3 layer, we predict the coexistence of the type-II Dirac point and the closed nodal line. The results are analyzed and interpreted using a tight-binding model and symmetry arguments. Our findings offer a practical way to realize 2D type-II Dirac fermions in oxide heterostructures.

9:36 AM K46.00007: Density-functional prediction of a spin-orbital entangled two-dimensional electron gas at LaAlO3/SrIrO3 (001) interface

CHURNA BHANDARI (Presenter), SASHI SEKHAR SATPATHY, University of Missouri — With the recent advances on the epitaxial growth techniques, epitaxy grown ultrathin films of SrIrO3 have brought in a considerable research interest as they exhibit thickness dependent metal-insulator transition and other interesting transport properties. SrIrO3 is a Mott insulator below three or four layers of SrIrO3 grown on the SrTiO3 substrate. Using density-functional methods, we study the (001) interface between the non-polar SrIrO3 and the polar LaAlO3 material, where the LaO layer is in contact with the IrO2 layer. We predict the formation of a spin-orbital entangled 2DEG at the interface due to the polar catastrophe, analogous to the n-type LaAlO3/Sr2IrO4 interface. The predicted 2DEG is very well localized at a single layer of Ir near the interface occupying the J\text{eff} = 1/2 conduction bands (upper Hubbard band). The 2DEG leads to a ferromagnetic interface, which is different from the antiferromagnetic bulk.


*This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Grant No. DE-FG02-00ER45818.

9:48 AM K46.00008: Silicon-Integrated Transition Metal Oxide Thin Film Quantum Structures

J. ELLIOTT ORTMANN (Presenter), University of Texas at Austin, SUNAH KWON, University of Texas at Dallas, AGHAM POSADAS, University of Texas at Austin, MOON KIM, University of Texas at Dallas, ALEXANDER DEMKOV, University of Texas at Austin — While the SrTiO3/LaAlO3 (STO/LAO) system has garnered widespread attention since the discovery of a two-dimensional electron gas at the interface of these two band insulators, recent efforts have instead focused on its optical properties. The huge 2.4 eV conduction band offset between STO and LAO allows for charge confinement in STO quantum wells and the optical and electrical modulation of carriers between confined states. Such heterostructures could find use in a multitude of next-generation electrical, optical, and electro-optical devices. However, the technological relevance of such devices hinges on the ability to successfully integrate high-quality STO/LAO quantum structures with silicon. Here, we demonstrate the monolithic integration of high-quality STO/LAO multiple quantum wells on silicon (001) with molecular beam epitaxy. We present electron diffraction, X-ray diffraction and electron microscopy studies establishing the excellent uniformity and crystalline quality with which such heterostructures can be fabricated. Finally, we present examples of how silicon-integrated STO/LAO quantum structures could be used in device fabrication.

10:00 AM K46.00009: Transport regimes of a split gate superconducting quantum point contact in the two-dimensional LaAlO3/SrTiO3 superfluid

HOLGER THIERSCHMANN (Presenter), EMRE MULAZIMOGLU, MANCA NICOLA, Quantum Nanoscience, Delft University of Technology, SRJJIT GOSWAMI, QuTech, Delft University of Technology, TEUN M Klapwijk, ANDREA CAVIGLIA, Quantum Nanoscience, Delft University of Technology — Ever since the observation of the quantized resistance in a point contact in GaAs/AlGaAs heterostructures it has been a long standing goal to achieve similar experimental conditions also in superconductors. Being formed with split gate technology, these structures represent in an ideal manner equilibrium reservoirs which are connected only through a few electron mode channel. Here we demonstrate the formation of a superconducting quantum point contact (SQPC) with split gate technology in a two-dimensional superconductor, utilizing the unique gate tunability of the superfluid at the LaAlO3/SrTiO3 interface. When the constring is tuned through metallic split gates we identify three regimes of transport: First, SQPC for which the supercurrent is carried only by a few quantum transport channels. Second, superconducting island strongly coupled to the equilibrium reservoirs. Third, charge island with a discrete spectrum weakly coupled to the reservoirs.

*We acknowledge funding by the Netherlands Organisation for Scientific Research, Dutch Foundation for Fundamental Research on Matter, the ERC (METIQUM, grant no. 339306, EU H2020 programme/ERC Grant 677458), Quantox of QuantERA ERA-NET cofund in Quantum Technologies and the Russian Science Foundation (RSF) Project No.17-72-30036.

MICHAEL VEIT (Presenter), DI YI, Stanford University, REMI ARRAS, University of Toulouse, ROSSITZA PENTCHEVA, University of Duisburg-Essen, YURI SUZUKI, Stanford University — Emergent metallic behavior at the interface of the Mott insulator LaTiO3 and the band insulator SrTiO3 has been explained in terms of charge redistribution at the interface combined with strain-induced electronic structure modification. We have previously studied ultra-thin (3 unit cell thick) films of LaTiO3 on SrTiO3 substrates and found evidence for unexpectedly large spin-orbit coupling from quantum oscillations with an associated Berry phase, weak anti-localization in the magnetoresistance, and anisotropic in-plane magnetoresistance. In order to tune this material, we have electrically gated these films both on the back side of the SrTiO3 substrate and on top of the LaTiO3 film with an electrolytic gate. Most interestingly, we found a maximum in the resistance that is quantized to the quantum of conductance (2e^2/h). This is independent of the dimensions of the sample. Additionally, by studying samples with four and six contact geometries, we measure nonlocal transport similar. These features are present up to a surprisingly high temperature of 230K. We attribute these observations to helical edge states at the LaTiO3/SrTiO3 interface.

*This work was funded by the Vannevar Bush Faculty Fellowship of the Department of Defense under Contract No. N00014-15-1-0045.*

**10:24AM K46.00011: Anisotropic magnetoresistance for (111) SrTiO3 surfaces within Boltzmann transport theory**

NAZIM BOUDJADA (Presenter), ILIA KHAIT, ARUN PARAMEKANTI, University of Toronto — 2D electron gases formed at (111) surfaces and interfaces of SrTiO3 are highly sensitive to application of in-plane magnetic fields. Motivated by recent magnetoresistance experiments which report different crystalline symmetry components appearing at different gate voltages, we derive a multi-orbital single-layer Hamiltonian which includes spin-orbit coupling, orbital Rashba and broken inversion symmetry at the surface. The anisotropic magnetoresistance is calculated by solving the Boltzmann equation. An explanation for the experimental results observed for SrTiO3 is devised.

*This work was supported by the Natural Sciences and Engineering Research Council of Canada and the Canadian Institute for Advanced Research. NB acknowledges support from the Fonds de Recherche du Québec - Nature et Technologies.*

**10:36AM K46.00012: Adding depth resolution to resonant inelastic X-ray scattering by means of standing-wave excitation**

CHENG-TAI KUO (Presenter), SHIH-CHIEH LIN, Department of Physics, University of California, Davis, YINGYING PENG, Department of Physics and Seitz Materials Research Laboratory, University of Illinois, Urbana, YU-CHENG SHAO, Advanced Light Source, Lawrence Berkeley National Laboratory, GABRIELLA MARIA DE LUCA, DANIELE DI CASTRO, CRN-SPIN, ISMAEL GRAFF, Departamento de Fisica, Universidade Federal do Parana, NICHOLAS B BROOKES, European Synchrotron Radiation Facility, YI-DE CHUANG, Advanced Light Source, Lawrence Berkeley National Laboratory, MARK HUIJBEN, University of Twente, LUCIO BRAICOVICH, GIACOMO GHIRINGHELLI, Politecnico di Milano, CHARLES FADLEY, Department of Physics, University of California, Davis — Resonant inelastic X-ray scattering (RIXS) is a photon-in/photon-out synchrotron-based spectroscopy that uniquely probes the charge transfer, dd, magnetic, phonon and other excitations in correlated oxides and other systems. RIXS is considered to be a probe of bulk properties, reaching depths of the order of 1000 Å. It is thus desirable to give RIXS more quantitative depth resolution, for example to investigate interfaces in oxide heterostructures, which are known to show emergent properties (e.g. interface-induced ferromagnetism at the La_{1.85}Sr_{0.15}CuO_4/La_{0.67}Sr_{0.33}MnO_3 (LSCO/LSMO) heterostructures, 2D electron gases at LaAlO_3/SrTiO_3 (LAO/STO) heterostructure) not present in the single constituents. Here, we demonstrate that, by using standing-wave (SW) excitation from multilayer heterostructures, interface-specific RIXS information can be obtained. We present the results of SW-RIXS measurements on LSCO/LSMO and LAO/STO superlattices. SW effects are clearly observed on the RIXS excitations for these systems and we found to have different depth distribution. SW-RIXS will open up a new spatial dimension to this already powerful technique.

*This work was supported by the US Department of Energy under Contract No. DE-SC0014697 through the University of California Davis.*
Chemically specific termination control of oxide interfaces via layer-by-layer mean inner potential engineering

HAOYING SUN (Presenter), ZHANGWEN MAO, TIANWEI ZHANG, LU HAN, TINGTING ZHANG, Nanjing University, XIANGBIN CAI, Department of Physics, Hong Kong University of Science and Technology, XINGFEI LI, YIPENG ZANG, WEI GUO, JIANHUI SONG, DIANXIANG JI, CHENYI GU, CHAO TANG, ZHENGXIN GU, Nanjing University, NING WANG, Department of Physics, Hong Kong University of Science and Technology, YE ZHU, Department of Applied Physics, The Hong Kong Polytechnic University, DARRELL G. SCHLOM, Department of Materials Science and Engineering, Cornell University, YUEFENG NIE, Nanjing University, XIAOQING PAN, Department of Chemical Engineering and Materials Science and Department of Physics and Astronomy, University of California, Irvine

Creating oxide interfaces with precise chemical specificity at the atomic layer level is desired for the engineering of quantum phases and electronic applications, but highly challenging, owing partially to the lack of in situ tools to monitor the chemical composition and completeness of the surface layer during growth. Here we report the in situ observation of atomic layer-by-layer inner potential variations by analysing the Kikuchi lines during epitaxial growth of strontium titanate, providing a powerful real-time technique to monitor and control the chemical composition during growth. A model combining the effects of mean inner potential and step edge density (roughness) reveals the underlying mechanism of the complex and previously not well-understood reflection high-energy electron diffraction oscillations observed in the shuttered growth of oxide films. General rules are proposed to guide the synthesis of atomically and chemically sharp oxide interfaces, opening up vast opportunities for the exploration of intriguing quantum phenomena at oxide interfaces.

*This work was supported by the National Basic Research Program of China (Grant no. 2015CB654901), the National Natural Science Foundation of China (Nos. 11574135, 11774153, 51772143, 51672125).

Wednesday, March 6, 2019 8:00 AM - 11:00 AM
Session K47: Photovoltaics -- Solar Energy Conversion I

Photovoltaics for High Specific Power: Increasing Markets and Decreasing Package Weight

NANCY HAEGEL (Presenter), National Renewable Energy Laboratory — Emerging markets for lightweight, flexible, and portable power, including unmanned aerial vehicles, portable charging, remote-site power generation, vehicle-integrated and building facades, could benefit from photovoltaic technologies with high specific power (W/kg). Thin-film and emerging technologies offer advantages for lightweight, flexible power, including decreased cost and package weight and the opportunity to utilize new materials and lift-off techniques. We have assessed the role of the substrate, packaging, and interconnects to provide a quantitative assessment of designs to maximize specific power. Including all required components and weight limitations associated with safety and reliability, we estimate a lower bound for a durable lightweight module of ~ 300-500 g/m². For a thin film device with 15% efficiency, this would yield up to 500 W/kg and up to 1200 W/kg for a 35% for a high efficiency III-V multijunction device [1].


*Work supported by the U.S. Department of Energy under Contract No. DE-AC36-08-GO28308 with the National Renewable Energy Laboratory (NREL). Funding provided by the U.S. Office of Naval Research and through NREL's Lab Directed Research and Development initiative.

Stability and the Electronic Properties of Silicon-rich Silicon Carbide Structures by First Principle Calculations

NOURA ALKHALDI (Presenter), SAJIB BARMA, MUHAMMAD NURUL HUDA, University of Texas at Arlington — Silicon carbide has been used in a variety of applications such as solar cells material due to its high stability. Obtaining silicon-rich silicon carbide materials are necessary to tune the band gap for efficient solar light absorptions. In addition, thermodynamically stable Si-rich SiC materials can be used in solar cell applications without requiring the expensive pure grade silicon or pure grade silicon carbide materials. We have used density functional theory (DFT) calculations to examine different phases of silicon-rich silicon carbide to predict stable structures. Different configurations of silicon and carbon atoms in silicon-rich silicon carbide structures have been considered because the configurations play a significant role in getting stable results. The electronic structures have been studied, and the total energies have been calculated as well as the formation energies. These results will be presented. The results show that higher-order hexagonal-phases are more favorable structures than other silicon-rich silicon carbide structures due to their more covalent nature of bonding compared to the cubic counterpart.

*1- University of Hafar Al-Batin
2- Saudi Arabian Cultural Mission (SACM).
3-Texas Advanced Computing Center.
8:24AM K47.00003: Toward the rational design of organic solar photovoltaics: A DFT study of substituent effects on P3MT

DAVID PERRY (Presenter), The University of Akron, SANDILE MAMBA, GUISEPPE PELLICANE, School of Chemistry and Physics, University of KwaZulu-Natal, MESFIN TSIGE, The University of Akron — Organic polymers containing conjugated thiophene rings are among the candidates for the electron-donor materials in organic solar cells. Since material synthesis, device fabrication, and definitive characterization of those devices is tedious and expensive, it is desirable to apply computational methods to a systematic variation of the material chemistry to predict which materials will have the best properties and, potentially, which will yield the highest photon conversion efficiency. Reported here is a model study in which DFT calculations of poly-3-methyl thiophene (P3MT) with a range of 12 different substituents. For each candidate polymer, DFT calculations at the B3LYP-D2/6-31G(d,p) level were extrapolated to the long-chain limit. The following properties relevant to application in a photovoltaic device were estimated from the calculations: (i) the bandgap, (ii) the LUMO energy, and (iii) the steric hindrance to coplanarity of adjacent rings. While (ii) was found to be well correlated with the electron-donating property of the various substituents, (i) and (iii) were much less so indicating a design space in which these three critical properties could, to some extent, be varied independently.

*NRF South Africa (Grants 106020 and 114907) and CHPC at CSIR South Africa

8:36AM K47.00004: Quantitative Nanoscale Mapping of Photovoltaic Properties in Hybrid Organic/Inorganic Solar Cells

HAIAN QIU (Presenter), Department of Physics, Applied Physics, and Astronomy, Binghamton University, JONG HYUN SHIM, JUNGHYUN CHO, Materials Science and Engineering Program, Binghamton University, JEFFREY M. MATIVETSKY, Department of Physics, Applied Physics, and Astronomy, Binghamton University — Conductive atomic force microscopy (C-AFM) has been widely used to map local charge transport in functional materials and photovoltaic active layers. Recently, we have developed and employed C-AFM-based point-by-point current-voltage (PPIV) mapping to quantitatively investigate electrical properties such as local charge carrier mobility and to visualize local spatial variations in photovoltaic parameters such as open-circuit voltage, power conversion efficiency, and charge photogeneration rate. In this talk, we will present two examples in which PPIV mapping is employed to elucidate the influence of local morphology on photovoltaic properties in hybrid organic-inorganic systems. In the case of P3HT: ZnO nanorod active layers, photovoltaic properties are strongly dependent on the local P3HT hole transport layer thickness. Charge generation rate and charge collection probability maps reveal that photocurrent is mainly limited by charge collection. For inverted perovskite solar cells, PPIV photovoltaic characteristic maps exhibit an increased open-circuit voltage at crystal grain boundaries, indicating an important role played by these features.

*This work was supported by NSF CAREER award DMR-1555028 and Binghampton University's Smart Energy TAE.

8:48AM K47.00005: Degradation Mechanisms in Perovskite Solar Cells Probed by Low-Frequency Carrier Kinetics

VINOD SANGWAN (Presenter), MENGHUA ZHU, SARAH CLARK, KYLE LUCK, Materials Science and Engineering, Northwestern University, Evanston, IL 60208, TOBIN MARKS, MERCOURI KANATZIDIS, Chemistry, Northwestern University, Evanston, IL 60208, MARK HERSAM, Materials Science and Engineering, Northwestern University, Evanston, IL 60208 — Hybrid organic-inorganic perovskite solar cells have emerged as leading candidates for third-generation solar cell technology. Despite their superlative power conversion efficiencies (PCEs), hysteresis and degradation limit their applications, thus motivating detailed studies of the underlying physical mechanisms. We introduce correlated low-frequency noise and impedance spectroscopy characterization that reveals carrier kinetics in perovskite solar cells. We employ cells with different hole transport layers that also elucidate tradeoffs between solar cell performance metrics and stability. We focus on the technologically relevant planar cell structure using an emerging SnO2 electron transport layer and two widely used hole transport layers: poly(triarylamine) (PTAA) and Spiro-OMe TAD. PTAA and Spiro-OMe TAD cells with moderate PCEs of 5–12% show a Lorentzian feature at ~200 Hz corresponding to a single fluctuator. Spiro-OMe TAD cells with high PCE (>15%) show four orders of magnitude larger 1/f noise amplitude with a distinctive peak, which is indicative of a cyclostationary process that is correlated with an inductive loop in impedance spectra. The observed current fluctuations are consistent with trapping and de-trapping of methylammonium ions near the SnO2 interface.
9:00AM K47.00006: Domain boundaries in the dipolar order in the perovskite material CH$_3$NH$_3$PbI$_3^*$  
SAHEL ASHHAB (Presenter), MARCELO CARIGNANO, MOHAMED E. MADJET, Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Qatar Foundation, Qatar — We investigate the ordering of the CH$_3$NH$_3$ dipoles in the material CH$_3$NH$_3$PbI$_3$. The dipoles are arranged in a simple cubic lattice. We perform numerical simulations in which we set the boundary conditions such that opposite sides of the simulated sample are ordered in different directions, hence simulating a domain boundary. We calculate the lowest energy state under this constraint. We find that at the level of dipole-dipole interactions, the dipole orientations tend to gradually transform between the two orientations at the two ends of the sample. When we take into consideration the finite spatial size of the CH$_3$NH$_3$ molecules and go beyond the point dipole approximation, we find that the domain boundary becomes sharper. For the parameters of CH$_3$NH$_3$PbI$_3$, our results indicate that the optimal energy structure has a boundary region of a width on the order of a single unit cell.

*This work was made possible by NPRP grant # 8-086-1-017 from the Qatar National Research Fund (a member of Qatar Foundation).

9:12AM K47.00007: Efficient first-principles calculation of phonon assisted photocurrent in large-scale solar cell devices  
MATTIAS PALSGAARD, KURT STOKBRO (Presenter), TROELS MARKUSSEN, Denmark, Synopsys, TUE GUNST, MADS BRANDBYGE, Physics, Technical University of Denmark — We present a straightforward and computationally cheap method to obtain the phonon-assisted photocurrent in large-scale devices from first-principles transport calculations[1]. The photocurrent is calculated using nonequilibrium Green's functions with light-matter interaction from the first-order Born approximation while electron-phonon coupling (EPC) is included through special thermal displacements (STD). We apply the method to a silicon solar cell device and demonstrate the impact of including EPC in order to properly describe the current due to the indirect band-to-band transitions. The first-principles results are successfully compared to experimental measurements of the temperature and light intensity dependence of the open-circuit voltage of a silicon Photovoltaic (PV) module[1]. We use the method to predict the solar cell efficiency of new Janus type 2D devices[2] and show that they outperform the silicon PV module. This work represents a recipe for computational characterization of future PV devices including the combined effects of light-matter interaction, phonon-assisted tunneling and the device potential at finite bias from the level of first-principles simulations.


9:24AM K47.00008: Highly efficient Non-Fullerene Organic Solar Cell with Fine Tuned Hole Transporting Layer  
QIN HU (Presenter), University of Massachusetts Amherst, ZHONG ZHENG, Chinese Academy of Sciences, WENKAI ZHONG, Lawrence Berkeley National Laboratory, JIANHUI HOU, HUIQIONG ZHOU, Chinese Academy of Sciences, FENG LIU, Shanghai jiaotong University, THOMAS RUSSELL, University of Massachusetts Amherst — Non-fullerene organic solar cells have experienced rapid development in the past few years with their impressive optoelectronic properties and great potential in practical applications. Here, we present a facile and effective strategy to improve the device performance through hole-transporting layer (HTL) modification. By optimizing Wox (nanoparticles): PEDOT:PSS composition, the surface free energy of the HTL is improved, hence influences the crystallization mechanism of PBDB-T:IT4F bulk-heterojunction (BHJ) active layer. In-situ grazing incident X-ray diffraction (GIXD) is applied to monitor the crystallization kinetics and morphology formation of the active layer based on different HTLs. The crystal coherence lengths and lamellar stacking distance as well as the phase separation are adjusted by various HTLs. In addition, the optimized HTL can promote more balanced carrier transport ability, leading to reduced non-radiative recombination and higher fill factor. The crystallization to structure, and film property to device performance relationship are established. A power conversion efficiency of 14.2% is achieved based on laboratorial spin-coating process, while an efficiency of 11.9% is obtained via industrial comparable slot-die printing fabrication.

9:36AM K47.00009: Conduction Band Matching in CdSe - Metal Oxide Quantum Dot Solar Cells: The Competition Between Energetics and Electron Transfer Kinetics*  
MATTHEW BECKER (Presenter), SAM AYALA, Saint Mary's College — Quantum dot solar cells were constructed by pairing CdSe quantum dots with metal oxides whose conduction band is very close to that of the CdSe. We hypothesized that the reduced loss of energy due to the closely matched conduction bands would result in a higher open circuit voltage. It was found that the band-matched solar cells perform more poorly and that the improved electron kinetics resulting from a large difference between CdSe and metal oxide conduction band energies seems to have a larger influence on the efficiency of these quantum dot solar cells.

*We wish to acknowledge and thank the Neuhoff Summer Science Communities Grant for providing seed funding for this project.
9:48AM K47.00010: How did solar energy get so cheap, and how much cheaper can it get?  HARRY APOSTOLERIS (Presenter), Khalifa University, MARCO STEFANCICH, Dubai Electricity and Water Authority, MATTEO CHIESA, Khalifa University — In the last several years, the cost of electricity from photovoltaics has fallen to the point where it is now the cheapest source of electricity across large parts of the world. Understanding how this happened is essential to guiding future research in solar energy technology. We have conducted a detailed analysis of the technological and economic factors that led to the realization of ultra low solar electricity prices in the United Arab Emirates, Saudi Arabia, Chile, Mexico and the southwestern US. We show that the primary influences are the declining cost of hardware (PV modules, inverters, trackers) and the low cost of capital available to these projects, combined with local factors such as labor costs and reductions in soft costs. In this presentation we will demonstrate the relative impact of these factors in different locations using a bottom-up LCOE model, and discuss their likely future trends (i.e. future evolution of hardware prices, or the expected impact of interest rate variations on the cost of financing). In this way we aim to provide a "big picture" context for today’s solar energy research.

10:00AM K47.00011: Electrostatic Potential Fluctuations in Thin-Film Photovoltaics†  HARVEY GUTHREY (Presenter), JOHN MOSELEY, MOWAFAK AL-JASSIM, National Renewable Energy Laboratory (NREL) — Increasing the conversion efficiency of photovoltaics based on thin-film absorbers materials requires minimizing the open circuit voltage (Voc) deficit (difference between the band gap and Voc) and producing films with sufficient charge carrier concentrations. However, inherent to these materials are high concentrations of intrinsic point defects and intentional extrinsic defects that can result in 1) significant charge carrier compensation thus reducing the carrier concentration and 2) fluctuations in the local electrostatic potential that define the band structure resulting in increased charge carrier recombination and low Voc values. Understanding both the magnitude and spatial distribution of such potential fluctuations is necessary in order to refine material and device fabrication processes to achieve the highest photovoltaic conversion efficiency. In this contribution, we demonstrate how cathodoluminescence microscopy can be used to monitor such changes in CdSeTe and CuInGaSe2 thin-films with sub-100nm spatial resolution. In addition we discuss the physical mechanisms behind how atomic-scale compositional variations relate to the magnitude and spatial distribution of electrostatic potential fluctuations in these materials.

*U.S. D.O.E. Contract No. DE-AC36-08GO28308

10:12AM K47.00012: Detection of shot noise in perovskite solar cells and related devices†  KEVIN DAVENPORT (Presenter), MARK HAYWARD, LOGAN DRAPER, ANDREY ROGACHEV, University of Utah — Hybrid organic-inorganic perovskite solar cells are one of the most promising emerging technologies with the capability to compete with established silicon devices. The effective commercial rollout of perovskite-based devices, however, requires a fundamental understanding of the material’s electrical transport properties. We have performed current noise spectroscopy on a series of methylammonium lead triiodide perovskite solar cells. Under illumination, the noise power spectrum exhibits two main components: a 1/f6 flicker noise and a frequency-independent white noise. Our main finding is that this white noise is associated with photo-generated shot noise. The extracted Fano factor (0.6 < F < 1) indicates that the observed shot noise is full scale and that the photo-generated carriers have no significant barriers to escape the device. We have performed a similar series of measurements on amorphous silicon solar cells as well as super yellow PPV polymer-based LEDs, the results of which will also be presented.

*This work was supported by NSF CAREER Grant No. 0955484 and NSF Grant No. DMR 1611421.

10:24AM K47.00013: Spectral mapping of open circuit voltage of Cu(In,Ga)Se2 thin-film solar cells via surface photovoltage and its implications for hole carrier transport  JURAN KIM (Presenter), Department of Physics, Ewha Womans University, KIHWAN KIM, JIHYE GWAK, JAE HO YUN, Photovoltaic Laboratory, Korean Institute of Energy Research (KIER), WILLIAM JO, Department of Physics, Ewha Womans University — Due to its suitable physical properties, Cu(In,Ga)Se2 (CIGS) thin-film solar cells are commercialized and expanding its application fields. Thus, the needs for bendable CIGS solar cells are also rising. Up to date, flexible CIGS solar cells have reached power conversion efficiency (PCE) over 20%, but their performance is still limited for low open-circuit voltage. It is related to electron-hole (e-h) carrier transport. Therefore, we need to comprehend carrier behavior in the solar cells and their band structure by analyzing surface photovoltage (SPV) of CIGS thin-films on flexible substrates. By 3-step process and NaF post-deposition treatment we obtained 4 different PCE of 0, 6, 12, and 17%, altering substrate temperatures. Confocal micro-Raman spectroscopy provides phase distribution inside of the materials and the surface. Kelvin probe force microscopy (KPFM) displayed upward surface potential barrier near grain boundaries, helping e-h separation. SPV results was obtained by photo-assisted KPFM under three different wavelength lasers (640, 532, and 405 nm) with different skin depths. These optoelectrical properties from confocal micro-Raman and SPV variation induced by the phase difference can elucidate how non-uniformity affects carrier transport in the solar cell materials.
10:36AM K47.00014: Modeling realistic grain boundaries in CdTe  ERIC SCHWENKER (Presenter), ARUN KUMAR MANNODI KANAKKITHODI, FAITH SEN, LI AN CHEN, SPENCER HILLS, Argonne National Laboratory, JINGLONG GUO, Physics, University of Illinois at Chicago, MOON KIM, Materials Science and Engineering, University of Texas at Dallas, ROBERT KLIE, Physics, University of Illinois at Chicago, MARIA CHAN, Argonne National Laboratory — Grain boundaries (GBs) are performance-limiting in CdTe photovoltaics. Towards understanding and improving GBs, especially in the presence of impurities or alloying elements such as Se and Cl, it is important to perform first principles density functional theory (DFT) modeling on realistic structural models. We develop and use a code FANTASTX (Fully Automated Nanoscale To Atomistic Structure from Theory and eXperiment) which aims at creating atomistic structures which are consistent with scanning transmission electron microscopy (STEM) images as well as are energetically reasonable. We will discuss the electronic structures of realistic CdTe GBs, the effects of impurities on the electronic structure, and the implications for photovoltaic performance.

10:48AM K47.00015: Quasiparticle Band Structure of Iron Pyrite*  GABE LOPEZ-CANDALES (Presenter), WEIYI XIA, Physics, University at Buffalo, YIYANG SUN, Aerospace Engineering and Mechanics, University of Minnesota, PEIHONG ZHANG, Physics, University at Buffalo — Being a non-toxic and abundant material, iron pyrite (FeS2) is an attractive material for photovoltaic applications with a very high quantum efficiency and absorption coefficient. Despite much research effort, the fundamental band gap of FeS2 is still not accurately determined. The measured fundamental band gap of FeS2 ranges from 0.84 to 1.2 eV. Surprisingly, straightforward density functional theory calculations within the generalized gradient approximation (GGA) predict a band gap of 0.46 eV, whereas the supposedly more accurate Heyd-Scuseria-Ernzerhof (HSE) hybrid functional predicts a band gap of 2.6 eV. Perhaps more intriguing is that it was reported [1] that quasiparticle calculations within the GW approximation predicts a band gap of 0.3 eV for FeS2. In this work, we report fully converged G0W0 quasiparticle band structure of FeS2 using a recently developed accelerated method [2]. Contrary to the previous claim, our results predict a 0.81 eV (dipole forbidden) band gap at the Gamma point and a dipole allowed transition energy of about 1.07 eV. Our work illustrates the importance of the convergence issue in GW calculations.

*This work is supported by the NSF under Grants Nos DMR-1506669 and DMREF-1626967.

Wednesday, March 6, 2019 8:00 AM - 10:36 AM

Session K48 DFD GSOFT GSNP: Thin Films, Surface Flows, Interfaces and Microfluidics I

BCEC 251 - Baiou Shi, Penn State Erie - Tag(s): Focus

8:00AM K48.00001: When Salty Water Meets a Hydrophobic Surface  ADELE POYNOR (Presenter), ANTHONY FLORIMBIO, CAYTON HORNBERGER, ZACHARY ZOLL, Allegheny College — The investigation of how water meets a hydrophobic surface suggests that a very low-density layer, called the depletion layer, forms to mitigate the loss of hydrogen bonds at the surface. Salt disrupts the hydrogen-bonding network of water and therefore is expected to affect the formation of the depletion layer. We study this interface using the quantum optical technique of Surface Plasmon Resonance (SPR) for self-assembled monolayers (SAMs) in different aqueous salt solutions.

8:12AM K48.00002: Constant-rate capillary rise in wettability-controlled tubes  BAUYRZHAN PRIMKULOV (Presenter), AMIR PAHLAVAN, RUBEN JUANES, Massachusetts Institute of Technology — Displacement of a viscous liquid by a less-viscous liquid from the solid surfaces is relevant to many practical applications, including flow through porous chemical reactors, immiscible pollutant transport in soils, and hydrocarbon recovery. We study the spontaneous imbibition of water in capillary tubes partially filled with oil slugs of fixed length. High viscosity contrast of viscous-oil with water results in a tunable constant-rate capillary rise. The capability to control both the displacement rates and wettability makes this an attractive system to explore, and the results of the study bear a direct connection to the multiphase flow in porous media, where wettability plays a critical role.
Capillary Flow Dynamics in Open Triangular Grooves: From Flatland to Curvy 3D Trajectories

NICHOLAS WHITE (Presenter), SANDRA TROIAN, MC 128-95, CALTECH, Pasadena, CA 91125 — Capillary flow in straight open triangular grooves finds widespread use in applications such as point-of-care biomedical devices, heat pipes for cooling microelectronics and spacecraft propellant management. Advances in 3D printing and other patterning techniques can now be used to fabricate compact open curved channels in 3D. This capability introduces the potential for multi-layer and multi-functional operation of many types of microfluidic and optofluidic chips. Romero and Yost (1996) and Weislogel (1996) first elucidated how the streamwise gradient in capillary pressure due to the change in curvature of the fluid interface due to local variations in film thickness induces rapid wicking of slender films into straight and open triangular grooves. Here we present an analytic model which extends that original work to arbitrarily curved open triangular grooves in 3D. Despite the complex flow trajectories which can ensue, a first order perturbation analysis yields a compact equation for the moving interface. This finding should be of use to the design and implementation of next generation 3D fluidic devices.

*NCW gratefully acknowledges support from a 2017 NASA Space Technology Research Fellowship.

Capillary Forces Computation for Nano-suspension Droplet Spreading: Molecular Dynamics Simulations

BAIOU SHI (Presenter), Penn State Univ, Behrend, WEIZHOU ZHOU, EDMUND B WEBB III, Lehigh University — With the development of nano-technology, nano-suspension provides us a path to synthesize and disperse nano-particles in fluids, and it has been widely utilized in pharmaceutical and semiconductor industries. Recently, many studies via both experiments and simulations have focused on nano-suspension droplets dynamic spreading and further evaporation on solid surfaces. However, the underlying physics and especially the fundamental driving forces controlling the kinetics of nano-suspension wetting and spreading is still unknown. In this talk, results from molecular dynamics simulations are presented with emphasis on computing capillary forces between advancing liquid fronts and suspended particles. Meanwhile, the effect of nano-particle size, particle loading, and interaction strength examined from atomic scale simulations will be presented. For increasing particle size, a dramatic change of wetting behavior from de-pinning to pinning is observed and also interpreted as the increasing capillary force between suspended nano-particles and the three-phase interface. By tuning down the interaction between the particle and the underlying substrate, de-pinning is observed instead of the exhibiting pinning behavior.

*National Science Foundation, Directorate for Engineering, CBET Division

Water Filtration in Carbon Nanotubes Resulting From Electronic Friction at the Walls

JEFFREY SOKOLOFF (Presenter), Northeastern University — In this talk, a mechanism for removal of salt from salt water is discussed, which results from friction due to Ohm's law heating, resulting from motion of an electron charge induced in the tube walls by the water molecules' dipoles and the ions' charges. The filtration occurs because this friction is larger for salt ions than for water molecules. Friction due to Ohm's law heating might also provide an explanation for the observation by Secchi, et. al., that the flow velocity of water in carbon nanotubes increases rapidly as the tube radius decreases from 50 to 15nm, which does not occur for boron nitride nanotubes which are insulators. This friction is large enough to produce the observed slip-lengths. One possibility is that the nanotubes in this experiment were metallic, whose conductivity becomes large as their radius decreases, due to ballistic conduction. Another possibility is that when the tube circumference drops below the electron mean free path, the wall switches from behaving as a two dimensional conductor to behaving as a one dimensional conductor for which the electrons are more strongly localized. For sufficiently small conductivity, small distortions of the localized states can provide the dominant contribution to the induced charge, rather than current flow.
9:00AM K48.00006: Laser streaming: A novel photoacoustic streaming principle and its application in microfluidic driving  SHUAI YUE (Presenter), Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, China, YANAN WANG, Department of Electrical and Computer Engineering, University of Houston, US, QIUHUI ZHANG, Department of Electrical Information Engineering, Henan University of Engineering, China, FENG LIN, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, China, NZUMBE EPIE, Physics Department and Texas Center for Superconductivity, University of Houston, US, SUCHUAN DONG, Department of Mathematics, Purdue University, US, XIAONAN SHAN, Department of Electrical and Computer Engineering, University of Houston, US, DONG LIU, Department of Mechanical Engineering, University of Houston, US, WEI-KAN CHU, Physics Department and Texas Center for Superconductivity, University of Houston, US, ZHIMING WANG, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, China, JIMING BAO, Department of Electrical and Computer Engineering, University of Houston, US — We report the discovery of a new optofluidic principle and demonstrate the generation of a flow by a pulsed laser beam through a glass window. A plasmonic nanoparticle-decorated cavity had been fabricated by focusing a laser on the interface of a glass and aqueous solution of Au nanoparticles. A flow emerges and remains after the colloidal solution is completely replaced by pure water. Hydrophone signals indicate that the flow is driven via acoustic streaming by a long-lasting ultrasound wave which is resonantly generated by the laser and the cavity through the photoacoustic effect. The principle of this light-driven flow via ultrasound, i.e., photoacoustic streaming by coupling photoacoustics to acoustic streaming had been applied by focusing beams on ion-implanted quartz plate. Manipulating and programming laser beams can easily create a micro single pump, a moving pump, and multiple pumps on any point of the quartz plate without any moving structures. The underlying pumping mechanism of photoacoustic streaming is verified by high-speed imaging of the fluid motion after a single laser pulse. These programmable, fabrication-free micropumps open up a new generation of micropump technology and new opportunities for easy integration and versatile applications.

9:12AM K48.00007: Alignment-dependent growth of unstable patterns in liquid crystals  QING ZHANG (Presenter), Mechanical Engineering, Massachusetts Institute of Technology, SHUANG ZHOU, Department of Physics, UMass Amherst, IRMGARD BISCHOFFBERGER, Mechanical Engineering, Massachusetts Institute of Technology — The displacement of a more viscous fluid by a less viscous one in a quasi-two dimensional geometry leads to the formation of complex fingering patterns. In isotropic systems, disordered dense-branching morphologies arise from repeated tip-splitting of the evolving finger. In anisotropic systems, by contrast, the growth morphology changes to a highly ordered dendritic growth characterized by stable needle-like protrusions decorated with regular side-branches. We investigate such morphology transitions between dendritic growth and dense-branching growth in an intrinsically anisotropic liquid, a lyotropic chromonic liquid crystal in the nematic phase. We show that the transition depends on three parameters; the interface velocity, the concentration of liquid crystal and the viscosity ratio between the less-viscous inner fluid and the more-viscous outer liquid crystal. Remarkably, we find that different aspects of the patterns are experiencing environments of different viscosities; the characteristics of the locally-determined most unstable wavelength are governed by a viscosity that is 20 times lower than that governing the relative length of the fingers. We discuss how these two different viscosities are related to the local alignment of the liquid crystal.

9:24AM K48.00008: Electrokinetics in pH-responsive polyelectrolyte-brush-grafted nanochannels: Effect of the appropriate Strong Stretching Theory representation of the polyelectrolytes*  SIDDHARTHA DAS (Presenter), HANNOOR SINGH SACHAR, VISHAL SANKAR SIVASANKAR, University of Maryland, College Park — Functionalization nanochannels with polyelectrolyte (PE) brushes, contrary to the classical notion, has recently been established to augment electroosmotic (EOS) transport in nanochannels under special conditions where charges of the brushes are localized at the non-grafted ends of the PEs. Here we shall re-visit these calculations as well consider the more readily encountered situations where the entire PE molecule is charged in presence of the most rigorous framework where the PE brushes are modeled using the Strong Stretching Theory (SST) that accounts for the excluded volume (EV) effects and the effect of considering a generalized mass action law. These considerations would significantly affect the monomer distribution (which in turn would affect the drag force imparted by PE brushes) and the resulting EDL (electric double layer) electrostatics (which in turn would affect the EOS body force). This model would be the first rigorous theory for the electrohydrodynamics in the PE-brush-functionalized nanochannels accounting for the appropriate coupled thermodynamic representation of the PE brush configurations and the EDL electrostatics.

*This work has been supported by the Department of Energy Office of Science grant DE-SC0017741.

9:36AM K48.00009: Direct measurement of capillary attraction between floating disks  IAN HO (Presenter), GIUSEPPE PUCCI, DANIEL M HARRIS, School of Engineering, Brown University — It is well known that two particles trapped at a fluid interface may interact due to the deformation they induce on the free surface. In the present work, we present direct measurements of the force between centimetric superhydrophobic disks resting on an air-water interface. Using a novel experimental setup, we characterize how the attraction force depends on the disk mass, diameter, and relative spacing. Our measurements are compared with theoretical predictions. Future directions will be discussed.
observe that the thermal force spectrum is a monotonically increasing function of frequency. A theoretical description involves extracting the spectrum of the thermal force. We compare our experimental measurements with a theoretical description that assumes a long and thin beam fluctuating in a viscous fluid with a frequency dependent thermal driving force. Since the Langevin force excites fluctuations of the resonator in proportion to the square of the linear response function, it is then possible to extract the spectrum of the thermal force. We compare our experimental measurements with a theoretical description that assumes a long and thin beam fluctuating in a viscous fluid with a frequency dependent thermal driving force. We observe that the thermal force spectrum is a monotonically increasing function of frequency.

*We acknowledge support from US NSF through Grant No. CBET-1604075

10:00AM K48.00011: Thickness Dependent Nanofluidic Transport in Nanopores and Nanochannels MOHAMMAD HEIRANIAN (Presenter), N. R. ALURU, University of Illinois at Urbana-Champaign — Due to the high performance water transport through ultrathin membranes, nanopores and nanochannels have drawn a great deal of attention in a variety of applications, such as water desalination, power generation and biosensing. Classically, the transport rate scales inversely with the thickness. However, transport in carbon-based nanopores and nanochannels far exceeds the classical transport governed by the Hagen-Poiseuille (HP) equation, suggesting large transport enhancement factors with respect to the permeation predicted by HP. Here, using molecular dynamics simulations we characterize the thickness dependence by studying the hydrodynamical properties of pores and channels in graphene and finite-length CNTs. Transport in graphene and short CNTs is shown to be dominated by a high interfacial friction and viscosity at the pore/channel entrance. A corrected Hagen-Poiseuille (CHP) model, based on viscosity and friction from Green-Kubo relations, successfully predicts the non-equilibrium pressure driven flows for different sizes of channels. The previously reported enhancement factors (of the order of 1000) approach unity when the permeations are normalized by that of the CHP. The results of our study will help better understand nanoscale flows in nanopores and nanochannels.

10:12AM K48.00012: An electro-coflow based microfluidic route to generation of alginate microcapsules* VENKAT GUNDABALA (Presenter), MD DANISH EQBAL, Chemical engineering, Indian Institute of Technology Bombay — Among various platforms for generation of microgels and microcapsules, microfluidics offers controlled routes for their generation. In this work, a novel interface-based microfluidic device is designed with capability for application of electric fields, and is used to generate alginate microparticles and capsules. Sodium alginate droplets generated through electro-coflow mechanism, cross a liquid-liquid interface and subsequently polymerize into polymeric particles. For microcapsules, double emulsions with an oil core and sodium alginate shell are used. The application of electric fields results in a significant reduction in the drop size and in turn in the particle/capsule size. The study shows a complete on-chip generation of microcapsules with size control achieved through application of external electric fields.

* Venkat Gundabala would like to thank DST (Department of Science and Technology) for research financial support through grant SB/S3/CE/081/2013 and IIT Bombay for travel support

10:24AM K48.00013: Dynamical measurements of receding contact angle for evaporating drops* CHLOE LINDEMAN (Presenter), NICHOLAS SCHADE, SIDNEY ROBERT NAGEL, University of Chicago — We study the receding contact angle of drops during evaporation. Drops of a dyed solution are allowed to evaporate for some time $\tau$ before they are removed via a small hole in the substrate. We record the contact angle as the fluid is removed and extract the receding contact angle — that is, the angle at which the drop first depins — as a function of $\tau$ and dye concentration. For low $\tau$ (i.e., immediate drop removal), the receding contact angle depends only weakly on concentration. For $\tau$ on the order of a few minutes, the receding contact angle decreases with a growing dependence on concentration. This suggests that the concentration of solute near the drop edge grows due to the flows induced by evaporation as in the coffee-ring effect. Surprisingly, even pure water exhibits a significant $\tau$-dependent receding contact angle.

*This material made use of the shared facilities at the University of Chicago Materials Research Science and Engineering Center, supported by National Science Foundation under award number DMR-1420709, and is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1746045.
8:00AM K49.00001: Impact of Antifoam on Rheological Properties of Polynorbornene Membranes for Biobutanol Separation*

SIYUAN LI (Presenter), BRYAN VOGT, Polymer Engineering, The University of Akron — Butanol is a promising alternative to ethanol for bio-based fuel, but its efficient separation from the fermentation broth can be challenging. Poly(butylnorbornene-ran-hydroxyhexafluoroisopropyl norbornene) (BuNB-r-HFANB) is promising for butanol separation from water. Here, we seek to understand how additives in typical fermentation broths interact with this polymer. The sorption of Antifoam 204 in butanol-water solutions in BuNB-r-HFANB films was characterized by quartz crystal microbalance with dissipation (QCM-D). From the QCM-D data, the dependence of concentration on swelling ratio and rheological properties (complex shear modulus and phase angle) of the films was elucidated. By examination of different film thicknesses, it was determined that the antifoam is incorporated within the film. At 100 ppm of antifoam, the swelling ratio increases by a factor of 170, while the phase angle increases to ~90° (liquid-like). The swelling is nearly unchanged at 10 ppm, but decreases markedly at 1 ppm. This suggests that the polymer is saturated by the antifoam even when only present at 10 ppm. These results illustrate the potential impact of dilute additives on new polymers for pervaporation membranes.

*This work was financially supported by the NSF under grant no. CMMI-1462284.

8:12AM K49.00002: The effect of filler distribution in the enhancement of the energy storage in nanocomposites*

ELSHAD ALLAHYAROV, Theoretical Chemistry, University of Duisburg-Essen, LEI ZHU, GUOQIANG ZHANG (Presenter), Macromolecular Science, Case Western Reserve University — Mixing dielectric polymers with high permittivity nano-sized inclusions affects their electrical properties. These nanocomposites are extensively used in actuation applications via employing electrostriction properties of the matrix, and in electrostatic energy storage applications employing high polarization fields of the fillers. In both cases existing theoretical studies mostly utilize mixing rule approaches that consider a homogeneous filler distribution in the matrix. Consequently, the effective permittivity of the composite never exceeds the the permittivity of the filler. We show that much higher effective permittivities can be achieved by manipulating the morphology of the inclusion distribution in the matrix. Simulation results for the field distribution reveal an enhancement of the field localization and dipole-dipole correlation effects in some proposed morphologies. By considering several possible clustering scenarios we found that a cylindrical clustering along the applied field has a potential to achieve an order of magnitude increase in the effective permittivity. The issue of chained filler configurations which lower the breakdown field threshold for the material is also addressed.

*DFG grant AL 2058/1-1 (for E.A.) and ACS PRF grant 57812-ND7 (for E.A. and L.Z.)

8:24AM K49.00003: Analyses of hierarchical structures in vulcanized SBR rubber by using contrast variation USANS and SANS

YUKI WATANABE (Presenter), Graduate School of Engineering, Kyoto University, MIKIITO TAKENAKA, Institute for Chemical Research, Kyoto University, SHOTARO NISHITSUJI, Graduate School of Organic Materials Science, Yamagata University, SATOSHI KOIZUMI, Graduate School of Science and Engineering, Ibaraki University, DAISUKE YAMAGUCHI, Institute for Integrated Cell-Materials Sciences, Kyoto University — The hierarchical structures of poly(styrene-ran-butadiene) (SBR) rubbers vulcanized with sulfur in swollen state were investigated by using ultra small angle neutron scattering (USANS) and small angle neutron scattering (SANS) technique. The scattering intensity can be described by the equation consisting of two Debye-Bueche equations and Ornstein-Zernike-Debye equation indicating that the inhomogeneous structure with the size of 500 to 900 Å exits, in addition to the inhomogeneous structures with the size of 70 to 100 Å with the networks. As the results of the analyses of contrast variation USANS and SANS, The origin of the inhomogeneous structures with the size of 500 to 900 Å was found to consist of ZnO added as activator of sulfur vulcanization, and we was able to yield the size of ZnO being in the order of 1000 Å quantitatively from the partial structure factor of ZnO.
Assignment of the Polymerization Peak in Polystyrene Melt

HE CHENG (Presenter), TAISEN ZUO, GUISHENG JIAO, ZEHUA HAN, China Spallation Neutron Source, Chinese Academy of Sciences, JUNPENG ZHAO, the department of polymer science and engineering, south china university of technology — Polymerization peak at around 0.75 Å⁻¹ in polystyrene (PS) melt was first reported by Katz in 1927, it is origin is still not clear. Here, by combined neutron total scattering, high concentration labelling and molecular dynamic simulation, we visualize the most-probable all-atom positions in polystyrene melt, and assign it to be the inter-chain backbone distance. In our experiments, both the neutron and x-ray total scattering profiles from 0.02 to 30 Å⁻¹ of PS-h8, PS-d8, PS-d5 and their mixtures (1:1 by molar) at different temperatures above their glass transition temperatures were measured. The low q scattering profiles in high concentration labelling mixtures are from the thermo fluctuations, while the intermediate and high q scattering profiles are assigned to the inter- and intra- chain atom-atom correlations.

*This work was funded by National Key Research and Development Program of China (2017 YFA0403703), National Nature Science Foundation of China (21474119 & 21674020), and UK-China Newton Project.

Dynamics of Belousov Zhabotinsky Reaction Based Systems Via Nonlinear Stability Analyses

VANDANA RAJPUT (Presenter), PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Controlling the dynamics of self-oscillating dynamical systems that are far from equilibrium has been a grand challenge for science and engineering. Belousov Zhabotinsky (BZ) reactions, a nonlinear chemical oscillator, has been used to design intrinsically powered self-oscillating dynamical systems. It has been known that the chemical oscillations in BZ reactions are due to the occurrence of Hopf bifurcation (HB). Here, reagent concentrations in the BZ system have been treated as the bifurcation parameter and we perform stability analyses to characterize the dynamics of the BZ system. Specifically, we calculate the first Lyapanov exponent to distinguish quantitatively between the subcritical and supercritical HB. In addition, we also calculate the second Lyapanov exponent to show that for a narrow range of bifurcation parameter, the sustained oscillations in the BZ system transforms in decayed oscillations with sensitive dependence on the initial condition. The transformation of this behavior occurs below a curve called Limit Point of Cycles which is a characteristic of Bautin bifurcation. The outcomes of our study can be utilized to characterize the behavior of dynamical systems and establish design rules for controlling their behavior.

*DST-SERB (EMR/2016/007778)

Directional Motion of Sodium Polyacrylate Gels Initiated by Ca²⁺-Induced Contraction is coupled to an NaCl Gradient

SUSAN KOZAWA (Presenter), Case Western Reserve University, LOREN KREIDER, Indiana Institute of Technology, ANITA VENKATASWAMY, ANNE WALKER, GARY WNEK, Case Western Reserve University — It is known that Na-polyacrylate gel threads contract in the presence of CaCl₂ but we have rather unexpectedly, initiate contraction at or very near the gap, rather than from the side immersed in CaCl₂ while the other side is immersed in NaCl. The main mechanism for ion transport initiates through diffusion; the lowest crosslinked gel allows for bulk diffusion while the higher crosslinked gels primarily propagate surface diffusion. Through surface diffusion, the binding mechanism propagates in a linear fashion, from the CaCl₂ towards the NaCl. The more interesting phenomena, the bulk diffusion, allows the ion gradients to meet within the middle of the gel. We propose this allows time for the chains to condense in the presence of NaCl, which allows for the entropically favored binding to Ca²⁺, immediately collapsing chains and allowing the facilitated binding down either end of the gel. Due to this, we are able to induce overall movement of the gel thread. While the phenomena is correlated to diffusion, the rates are mainly determined by polyelectrolyte dynamics. In all cases, original gel dimensions can be recovered upon treatment with chelators such as sodium triphosphate, an analog to ATP.

*This work is supported by the National Science Foundation under Grant No. NSF #1743475.
Multiscale investigation of polyelectrolyte gel-based electronic devices

Vasilii Triandafilidi

Presenter), Joerg Rottler, Savvas Hatzikiriakos, University of British Columbia — Gel-based electronic devices (sensors and diodes) are attracting attention due to their low cost, favorable mechanical properties, and biocompatibility. We have performed coarse-grained molecular dynamics and continuum simulations of model polyelectrolyte gels used in such devices to study the relationship between voltage and ion distribution on the nanoscale. For sensors, we consider a system consisting of a negatively charged backbone and positive floating counterions. By interfacing two regions with different degree of ionizations, we compute the electrostatic potential difference and show that it obeys a modified Nernst-Donnan equation when accounted for counterion condensation. The pressure is found to be proportional to the Donnan-Potential, which provides a molecular basis for the piezoionic effect observed in experiments. For gel-based diodes, we interface two gels with oppositely charged ions, study its rectifying behavior with molecular simulations and challenge the results obtained through a description based on the Poisson-Boltzmann approximation.


Change in Hierarchical Structure of Segmented Polyurethane Elastomers under Mechanical Deformation

Ken Kojio (Presenter), Institute for Materials Chemistry and Engineering, Kyushu University, Chigusa Nagano, Shiori Masuda, Chao-Hung Cheng, Shuhei Nozaki, Graduate School of Engineering, Kyushu University, Kazutaka Kamitani, Atsushi Takahara, Institute for Materials Chemistry and Engineering, Kyushu University — Polymer materials possess a hierarchical structure such as orientation, conformation, crystal structure, microdomain structure, and so on. When external stimulus is applied to polymers, these various structures would respond depending on the size. In this study, lattice strains obtained from the crystal structure of hard segment domain and microphase-separated structure of segmented polyurethane (SPU) elastomers were evaluated under mechanical deformation by wide-angle X-ray diffraction (WAXD) and small-angle X-ray scattering (SAXS) measurements. SPU elastomers were synthesized with poly(oxytetramethylene) glycol, trans-1,4-bis(isocyanatomethyl) cyclohexane (1,4-H6XDI), and 1,4-butanediol. Change in molecular aggregation structure of the SPU with 20 and 30 wt% hard segment contents were investigated. Both strains (eSAXS and eWAXD) obtained from SAXS and WAXD linearly increased with increasing strain. Compared to HX-20, HX-30 exhibited larger eSAXS and eWAXD in both deformation modes. This is because strain can be easily propagated to whole samples due to well-developed hard segment domains formed in HX-30. eSAXS and eWAXD values obtained by biaxial deformation were larger than for uniaxial one, indicating that the biaxial deformation produces severer condition to the samples.

Thermal analysis of fully zwitterionic copolymers for safer electrochemical energy storage

Andrew Clark (Presenter), Department of Physics and Astronomy, Tufts University, Morgan E Taylor, Matthew J Panzer, Department of Chemical and Biological Engineering, Tufts University, Peggy Cebé, Department of Physics and Astronomy, Tufts University — Current ionic liquid electrolytes used in lithium ion batteries are both volatile and flammable. A safer alternative to liquid electrolytes is to use solid conductive polymer gel electrolytes. In this study, the thermal properties of a group of zwitterionic copolymers designed for electrochemical energy storage are investigated using temperature modulated differential scanning calorimetry (TMDSC) and thermogravimetry (TG). Investigating the thermal properties will reveal how the zwitterionic moieties can affect transition phenomena. Sulfobetaine vinylimidazole (SBVI) and 2-methacryloyloxyethyl phosphorylcholine (MPC) were dissolved in an ionic liquid solution in varying molar ratios and subsequently polymerized to produce fully zwitterionic random copolymers. TG reveals two degradation steps at 290 °C and 390 °C due to MPC degradation and one step at 350 °C due to SBVI degradation. TMDSC at 5 °C/min was used to identify the glass transition of these materials, showing a decrease in Tg from 60 °C to -35 °C with increasing addition of SBVI. A melting endotherm at -18 °C was observed on heating, attributed to the presence of residual ionic liquid.

*This material is based upon work supported by a Tufts Collaborates Seed Grant and NSF DMR-1608125
9:48AM K49.00010: DFT studies of the structural, electronic, and electrochemical properties of copolymers containing ferrocene and imidazole  BENJAMIN TAYO (Presenter), Physics, Pittsburg State University, ERIC MULLINS, Physics, Kansas State University — Ferrocene-based polymers have been used in various applications such as sensors, solar cells, batteries, and photo-oxidation of thin films. Copolymers containing ferrocene and imidazole are unique because of electronic interactions between the ferrocene and neighboring imidazole moiety, leading to the formation of charge transfer complexes in the polymer. Recent electrochemical and UV-Vis studies in the presence of various electrolytes containing metal ions have revealed significant modifications in their properties, e.g., red shifts, and the appearance of multiple oxidation waves in cyclic voltammetry studies. Even though these modifications have been attributed to the ability of the imidazole to coordinate with metal ions, increasing its electron deficiency, thereby enhancing oxidation of the nearby ferrocene moiety if it is in close proximity to it, the equilibrium geometry of the polymer complex is unknown. This talk will discuss the results of DFT studies that was used to address these concerns, for instance determination of equilibrium geometry, and frontier energy levels. We will also discuss the correlation of molecular orbital density plots to the electrochemical properties, specifically the formation of donor-acceptor complexes within the polymer.

10:00AM K49.00011: Viscoelastic Phase Separation as a Route towards Continuously Processed Organic Solar Cells*  JING HE (Presenter), DILHAN M KALYON, STEPHANIE S LEE, Stevens Institute of Technology — Controlling the solution structure of polymer nanocomposite systems prior to thin film deposition is a promising strategy to enhance the efficiency of organic solar cells in a manner compatible with continuous processing methods. Using a model system comprising P3HT and PCBM dissolved in o-DCB, rheological characterization was employed to characterize the thermoreversible gelation of these solutions upon rapid cooling to sub-ambient temperatures. Temperature-variable confocal microscopy imaging of P3HT fluorescence revealed the formation of micron-sized solvent “holes” during cooling, a signature of viscoelastic phase separation. This phenomenon originates from the dynamic asymmetry between the polymer chains and solvent molecules and was found to arrest during the early stages of phase separation due to P3HT interchain crystallization. Cryogen-based scanning electron microscopy images of the gels further uncovered an interfibrillar network with characteristic pore sizes tens of nanometers in diameter. These interconnected polymer structures with hierarchical porosity were deposited as thin films via doctor blading, resulting in a 45% enhancement of light conversion efficiency compared to organic solar cells comprising active layers deposited from uncooled solutions.

*NSF 1635284

10:12AM K49.00012: (Near-) Ambient Pressure XPS for Studying Surface Reconstruction of Hydrated Polymers*  MIKAYLA BARRY (Presenter), EMILY C DAVIDSON, University of California, Santa Barbara, ETHAN J CRUMLIN, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Santa Barbara — Polymer restructuring in response to environmental conditions has made surface characterization of polymers designed for use in hydrated applications difficult. Analysis techniques that provide nanoscale surface composition (e.g. X-ray Photoelectron Spectroscopy (XPS)) have been largely limited to use in vacuum, where the surface presentation no longer matches that of hydrated polymers. Consequently, characterization of the hydrated surface has been relegated to contact angle goniometry and vibrational spectroscopy techniques such as Raman and Sum Frequency Generation (SFG). We present the first synchrotron (Near-) Ambient Pressure XPS (AP-XPS) studies performed on polymer surfaces in contact with water vapor. Water adsorption on polydimethylsiloxane-based polymers was found to increase substantially for those containing even minimal amounts of amphiphilic side chains. The presence of hydrogen-bonding side chains also correlated with greater increases in water adsorption and decreases in silicon-character oxygen (associated with the polymer backbone) at 6 Torr relative to non-hydrogen-bonding side chains.

*This work was supported as part of an Energy Frontier Research Center funded by the U.S. DOE (#DE-SC0019272), with materials provided by a grant from the ONR (N00014-17-1-2047).
10:24AM K49.00013: Self-assembly of Functionalized Nanoparticles in Ordered Phases of Block Copolymers
SUPRIYA GUPTA (Presenter), PARESH CHOKSHI, Chemical Engineering, Indian Institute of Technology Delhi — An emerging application of polymer nanocomposites is to generate self-assembly of nanoparticles leading to novel nanoscale materials with enhanced properties. As particle-based techniques, e.g. molecular simulation, are computationally intensive, we employ the self-consistent field theory (SCFT) combined with density functional theory (DFT) to examine the localization of nanoparticles in ordered domains of block copolymers. The nanoparticles are grafted with polymer chemically identical to either block of the copolymer. To ensure finite size of the particles and excluded volume interactions between species, the free energy is described using DFT. We study the localization of nanoparticles in lamellar and cylindrical morphologies. For lamellar phase, nanoparticles assemble either at the interface between two blocks or at the center of a block domain depending upon particle concentration and grafting density. In cylindrical phase, nanoparticles self-assemble at the center of the cylinders. The role of grafting density, particle size and composition on self-assembly behavior of particles in block copolymer is examined. The comprehensive understanding of factors affecting localization of nanoparticles enable us to control the particulate assembly for desirable material properties.

10:36AM K49.00014: Effect of Synthetic Parameters on Molecular Architecture and Adhesive Performance for Acrylic Emulsion Copolymers
SIPEI ZHANG (Presenter), OWEN (WEN-SHUE) YOUNG, MELINDA EINSLA, JOSEPHINE ELDREDGE, VINITA YADAV, CYNTHIA R. LESLIE, KEBEDE BESHAH, ALAN NAKATANI, ASGHAR PEERA, WILLIAM GRIFFITH, SARAH R. ZOLYNKI, HIMAL RAY, CACHAE PEARSON, SASWATI PUJARI, SEHBAN OZAIR, Dow Chemical Company — It is well known that both the composition and architecture of a polymer affect its performance as a pressure sensitive adhesive (PSA). However, the specific relationships of glass transition temperature (T_g), degree of branching, crosslinking density, and molecular weight with PSA properties are often complicated, and the variables can be difficult to isolate. Here we present a study examining the effects of acrylic monomer, feed time, and styrene content on the molecular architecture of emulsion-based copolymers with systematically varied composition, and their relationships with adhesive performance. The polymer architecture is elucidated using dynamic mechanical analysis (DMA), gel permeation chromatography (GPC), gel fraction/swell ratio (GF/SR), and 13C nuclear magnetic resonance (NMR) spectroscopy. It was found that the primary acrylic monomer had the most significant effect on polymer architecture, followed by styrene content, and then feed time. The resulting impact on adhesive and cohesive strength will also be discussed.

10:48AM K49.00015: Dramatic Mechanical Response of Polymer-metal Inclusions Based Metamaterials
RITUPARNA GHOSH (Presenter), Department of Instrumentation & Applied Physics, Indian Institute of Science, SOURAV DAS, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur, ABHA MISRA, Department of Instrumentation & Applied Physics, Indian Institute of Science — A periodic lattice of metal sphere (steel ball) is arranged in polydimethylsiloxane (PDMS) polymer matrix in multidimensional architecture. At multiple strains there is gradual increases in both the stress and energy absorption capability. Three-dimensional architecture demonstrated maximum loading capacity retaining its elastic behaviour. An enhancement of ~ 50% in absorption capability and stress at 40% strain is recorded as compared to one and two-dimensional architectures. The three-dimensional architecture also showed strain rate independent highly reversible behaviour for 1000 compression cycles at 30% strains and exhibit excellent mechanical stability. However, a dramatic drop in stress by ~ 100% was observed at higher strain (> 50%) in three-dimensional architecture as compared to other metamaterials. Point contacts between multiple disjoint steel balls, which form a periodic chain like structure play the key role in achieving enhanced strength and energy absorption and have importance in numerous mechanical applications where high strength and energy absorption are the prime requirement.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K50 DPOLY DMP: Organic Electronics I: Organic Photovoltaics and Photophysics
BCEC 252B - Elizabeth Von Hauff - Tag(s): Focus
8:00AM K50.00001: Trapped Photons Induced Ultra-high External Quantum Efficiency and Photoresponsivity with Millisecond Response in Hybrid Graphene/Metal-Organic Framework Broadband Wearable Photodetectors

KRISHNA PRASAD BERA (Presenter), Institute of Physics, Academia Sinica —

Metal-Organic frameworks (MOFs) are the promising new class of hybrid materials that has the tremendous attraction in sensing, gas storage, and drug delivery during past two decade due to its unique tunable properties and fascinating architectures. Optoelectronic application of MOF is challenging due to its high porosity and poor electrical conductivity. Combining the superior properties of the MOF along with ultra-high carrier mobility of graphene, we have fabricated and characterize the highly sensitive, broadband, and wearable photodetector on a polydimethylsiloxane substrate. The external quantum efficiency of the hybrid photodetector is found to be > 5×10^8%, under the excitation of 325 nm laser of intensity ~ 0.5 µWcm⁻², which exceeds all the reported values of similar devices. The porosity of the MOF and ripple structure graphene assist the trapping of photons at the light-harvesting layer. The device photoresponsivity is found to be > 10^6 AW⁻¹ with a response time of < 70 ms, which is ~100 times faster than the current standards of the graphene-organic hybrid photodetectors. In addition, utilizing the excellent flexibility of the graphene layer the wearability of the devices is demonstrated, which can be stretched up to 100% of its original dimension.

8:12AM K50.00002: ULTRAFAST ENERGY DISSIPATIONS AND QUANTUM EFFICIENCIES OF CONJUGATED POLYMERS BY SEGMENTAL STRESSES

HSUAN LU (Presenter), CHANG MOU YANG, TZUNG MIN WENG, Material Science, National Tsing Hua University — Quantum efficiencies of conjugated polymers (CPs) were found to increase dramatically by elevation of segmental stresses, therefore, we explore the emission behavior in the time scales comparable to segmental motions to unveil the relationship. We stretched CP (MEH-PPV) to ~300%, resulting photoluminescence (PL) enhancements of 20-60 folds depending on the stress level. By using up-conversion time-resolved confocal PL spectroscopy, we found the absorbed energy quickly dissipates via segmental rotations and vibrations, leading to PL red shifts. The damping via rotations was ~10 times faster than vibrations but stopped after ca. 2 ps, while the latter continued functioning, but abated slowly to diminishment. The segmental stresses can reduce or even switch off the rotation damping but yielded no influences on vibrations. The latter was found in fact heat dissipation, while the rotations, driven by local electrostatics from excitation, can trigger self-trapping and the 2 ps represents the time limit before escape from self-trapping for recombination. This model explains satisfactorily how segmental stresses interacting with CP backbones to result dramatic efficiency enhancements.

8:24AM K50.00003: Quantum-Entangled Triplet-Triplet Excitons in Acene Dimers and their role in Singlet Fission*

SOURATOSH KHAN (Presenter), SUMITENDRA MAZUMDAR, University of Arizona — Singlet fission (SF) in which a photoexcited spin singlet dissociates into a pair of low energy triplet excitons has been claimed in covalently linked acene dimers. Internal covnversion to a quantum entangled triplet-triplet state prior to dissociation makes the process spin-allowed. However, recent experiments based on electron spin resonance as well as transient absorption spectroscopy have both shown this intermediate biexciton to be stable against further decoherence thereby raising questions on SF itself. A disconnect between theory and experimental results have led us to calculate the excited state energies and their optical properties using a correlated electron model (Pariser-Parr-Pople Hamiltonian). We formulate a broad theory of quantum entanglement of triplet-triplet state in symmetric and asymmetric dimers. Based on our calculations, we conclude that i) spectroscopic differences in the ESA signals between free and bound triplets exist beyond the visible, ii) entanglement between the triplets is reduced as proximity between acene units is reduced or in the presence of significant steric hindrance, and iii) ESA from singlet exciton shows absorption in the short-wave infrared due to a transition to an optically forbidden even parity state.

*Supported by NSF-CHE-1764152.
Comparative studies on fluorescent emission of organic semiconductors between optical and electrical pumping* TAIKI MIURA (Presenter), Department of Physics, Graduate School of Science, Tohoku University, THANGAVEL KANAGASEKARAN, WPI-AIMR, Tohoku University, HIDEKAZU SHIMOTANI, SYUN ONUKI, Department of Physics, Graduate School of Science, Tohoku University, KATSUMI TANIGAKI, WPI-AIMR, Tohoku University — Light-emitting devices of organic semiconductors (OSCs), such as organic light-emitting diodes, have widely been used in daily life. Especially, light-emitting organic field effect transistors (LE-OFETs) are considered as candidates for efficient light-emitting devices, such as OSC lasers, in the future. However, the detailed understanding of electroluminescence (EL) by electrical pumping has not fully been understood when it is compared to photoluminescence (PL) by optical excitations. For realizing such a highly performed light-emitting device, the fundamental understanding on the difference between EL and PL is necessary. Here, we report accurate comparative studies on the difference between PL- and EL-mode in the case of single-crystal thin films of BP3T. The result shows that the spectrum shapes are different between PL- and EL-mode and quenching of fluorescent emissions occurs in high current region in the EL-mode. In order to realize highly efficient light-emitting OFETs towards OSC lasers in the future, such annihilation would become a significant obstacle.

*This work is supported by Grant-in-Aid for Scientific Research of JSPS (18H03883, 17H05326, 18H04304) and JST-CREST, and the bilateral country research program.

Theoretical Study on Charge-Transfer Excitations of Buckycatcher-Fullerene Complexes MIHARU HAYASHI, TOMOMI YASOSHIMA, AZUSA MURAOKA (Presenter), Japan Women's University — In particular, p/p stacking compounds have become of interest in new materials for photocatalysis, solar energy and phosphorescent organic light-emitting diodes. We investigate theoretically the photo-induced charge transfer in supramolecular chemistry. Buckycatcher (BC) molecules, bowl-shaped polycyclic hydrocarbons, have attracted attention as a new type of π-conjugated compound. BC molecules with two corannulene or two sumanane subunits can form a complex (BC/C60) with C60 because of the π-π interaction between the convex surface of the C60 and the concave faces of corannulene subunits of the BC. We have performed DFT and TD-DFT calculations on the structures and excitation spectrum of BC molecules and BC/C60 complexes. The most stable structures are BC/C60 in which the p–p stacking of the two corannulene subunits of BC and C60 takes a concave–convex arrangement; therefore, the van der Waals contact is maximized. It is found that the charge-transfer-type excitations from BC to C60 start at the ultraviolet light region. The BC/C60 complexes and their derivatives are potential candidates as key elements for photovoltaic devices and other molecular electronic devices.

The impact of atomic substitution on the photophysics of contorted hexabenzocoronene derivatives GUY OLIVIER NGONGANG NDJAWA (Presenter), TIA S. LEE, NICHOLAS DAVY, JENI SORLI, GREG SCHOLES, LYNN LOO, Princeton University — The photophysical properties of organic semiconductors are strongly influenced by the spin states, lifetimes, populations, and energies of the lowest photoexcited species (S1 or T1). By favoring or limiting the rate of intersystem crossing (ISC), the relative population and lifetime of singlet and triplet excitons can be controlled through molecular design. The incorporation of heavy atoms, such as transition metals, have been reported to enhance spin-orbit coupling in organic systems. Here, we explore the role of peripheral moieties with heteroatoms on the photophysical properties of contorted hexabenzocoronene (cHBCs) derivatives. These chemical alterations may impose steric or enhance spin-orbit coupling, significantly increasing the rate of ISC. With benzofuran moieties, cTBFDBC exhibits the highest degree of molecular contortedness in the series, which is correlated with a high rate of ISC. With much heavier benzothiophene moieties, cTBTDBC uniquely exhibits room temperature and higher phosphorescence yield compared to cTBFDBC, which we correlate to a high degree of spin-orbit coupling induced by the heavy sulfur atom. These findings offer valuable guidelines for enhancing the optoelectronic properties of cHBCs using simple molecular substitution approaches.
9:12AM K50.00007: Coherence and Electron Transport in Pi-Stacked Acceptor-Donor-Acceptor Molecular Triads*
KEVIN KOHLSTEDT (Presenter), MICAELA MATTA, THOMAS ALDRICH, TOBIN MARKS, GEORGE C SCHATZ, Northwestern University — There has been a concerted effort to design non-fullerene acceptors (NFAs) for organic photovoltaic devices, in a large part, due to the processability and stability problems of fullerenes, but concomitantly there is a desire to further understand ultrafast charge generation in donor-acceptor organic molecules. Recently, covalently bonded molecular triads have shown substantial increases in device efficiency when blended with mid-gap polymers. There has been some advances in understanding the details of electron transport with NFA molecules, but there has yet to be quantitative investigation into the relationship of molecular organization in NFA device with its transport capabilities. Here, we present a detailed study of NFA aggregates that show slipped-stacked geometries and strong binding energies between the intermolecular layers. A consequence of strongly coupled LUMO orbitals is intermolecular delocalization leading to transport coherence. We find that for some slip-stacked arrangements favor coherent transport, while others do not, and we propose design strategies to get NFA packings with strong electronic couplings.

*This research is supported by the Air Force Office of Scientific Research (AFOSR) under award number FA9550-14-1-0003

9:24AM K50.00008: Alloy or Blend: Analysis of a Ternary Organic Photovoltaic
XINJING HUANG (Presenter), Applied Physics, University of Michigan, XIAO LIU, EECS, University of Michigan, KAN DING, Physics, University of Michigan, STEPHEN ROSS FORREST, EECS, University of Michigan — The power conversion efficiency of organic solar cells can be enhanced by employing ternary blend bulk heterojunctions, which have been found to have an open-circuit voltage ($V_{OC}$) that depends on the blend ratio of acceptors/donors. It has been proposed that the variation in $V_{OC}$ is due to the formation of molecular alloy between blended acceptors/donors. However, we assert that the formation of a “molecular alloy” should exhibit new electronic states distinguished from those of its constituents. Here, we study the electronic states and energy levels in the P3HT:(ICBA:PC$_{61}$BM) ternary blend system. We find that the ICBA:PC$_{61}$BM acceptors shows the same highest occupied molecular orbital levels and exciton energies as that of ICBA, indicating no new exciton state emerges from the blend. In the ternary blend, the charge transfer states are composed of a linear superposition of those in the corresponding binaries. From these results, no evidence of new emergent electronics state is found which would support the existence of a molecular alloy. Indeed, our results point to the conclusion that blends of these non-interacting molecules differ substantially from our understanding of a conventional alloy. In this talk, we will consider the general criteria in identifying a molecular alloy.

9:36AM K50.00009: Design of Ethanol/Water Soluble Polymers/Fullerenes for Aqueous Processed Organic Solar Cells and Importance of Water Contents for Enhancement of Processability and Device Performance
SEUNGJIN LEE (Presenter), CHANGYEON LEE, YOUNGKWON KIM, JONNHYEONG CHOI, Department of Chemical and Biomolecular Engineering, KAIST, HAN YOUNG WOO, Department of Chemistry, Korea University, BUMJOON KIM, Department of Chemical and Biomolecular Engineering, KAIST — Most of the efficient organic electronic devices have been fabricated using toxic halogenated and/or aromatic organic solvents, which are not desirable in the industrial-scale solution process. Herein, we present a new series of ethanol/water soluble fullerene derivatives with different forms of oligoethylene glycol (OEG) side chains to be utilized in fabricating eco-friendly polymer solar cells (eco-PSCs). Intriguingly, the addition of a typical anti-solvent, water, to ethanol is found to markedly enhance the solubility of the non-ionic OEG side chain-based conjugated polymer (PPDT2FBT-A) and the newly designed fullerene mono-adducts (PC$_{61}$BO12, PC$_{61}$BO15, and PC$_{61}$BO27). A water-ethanol co-solvent with a 1:1 molar ratio provided an increased solubility of PPDT2FBT-A from 2.3 to 42.9 mg mL$^{-1}$ and that of PC$_{61}$BO12 from 0.3 to 40.5 mg mL$^{-1}$. Owing to the improved processability, efficient eco-PSCs with a power conversion efficiency of 2.05% were successfully fabricated. To date, this value is the highest among the devices based on the active layer of water/ethanol-soluble conjugated materials. Our results not only provide important guidelines for the design of electroactive materials, but also signifies the importance of water addition in fabricating environmentally benign eco-PSCs.
Defective conjugated polymers for organic electronics*

MICHAEL SOMMER (Presenter), Institute of Chemistry, Chemnitz University of Technology — This contribution discusses recent progress in the area of the synthesis of conjugated polymers for organic electronics. A first focus is on the role of chemical defects that form during synthesis. Depending on monomer structure, synthetic method and reaction conditions, homocouplings form at varying extent in donor-acceptor copolymers. This deviation from the usually suggested, strictly alternating structure lowers performance and causes a low level of reproducibility. In PCDTBT, homocouplings lower the short circuit current of photovoltaic devices and may be considered as one source for the broad range of reported power conversion efficiencies. The second part includes n-type copolymers from the naphthalene diimide and diketopyrrolopyrrole families. Defect formation, molecular weight control and energy level tuning is elucidated and correlated with charge carrier mobility and photovoltaic performance. A central conclusion is that the general understanding of the occurrence and importance of chemical defects in conjugated polymers has improved, but their entire elimination remains to be solved rendering batch to batch reproducibility a challenge.

*Funding from the German Science Foundation (project SO 1213/8-1) is acknowledged.

Reduced mixed phase interface causes increased charge transfer state separation in polymer solar cells*

THOMAS FERRON (Presenter), MATTHEW C WALDRIP, MICHAEL POPE, BRIAN COLLINS, Washington State University — Investigations into organic solar cells have shown that molecular mixing within domains and interfaces significantly impacts device performance. However, studies often use performance metrics that blur fundamental structure-function mechanisms – in particular, the role of the mixed phase in charge generation versus charge extraction. Here, we present a study based on time-delayed collection field to separately quantify each fundamental step in the charge generation process. Additionally, we utilize a novel resonant X-ray scattering analysis to quantify the state of the nanostructure as it exists within real devices. We find that in a model semicrystalline system, decreasing the mixed interface between donor and acceptor domains has minimal impact on charge transfer (CT) state generation while greatly enhances CT state separation. With both a high correlation (>99%) and a granular quantification of all dynamics, we eliminate competing processes in working devices to determine a causal relationship between the mixed phase volume and the efficiency of charge separation. Our results here support that a reduction in the interfacial mixed phase establishes a steep energy gradient between pure phases to aid charge generation in organic solar cells.

Title: Understanding Quasi-random Nanostructures of the Bulkheterojunctions(BHJ) in Organic Solar Cell Active Layers with Spectral Density Function (SDF)

RABINDRA DULAL (Presenter), University of Wyoming, UMAR FAROOQ GHUMMAN, AKSHAY IYER, Mechanical Engineering, University of Northwestern, JOYDEEP MUNSHI, GANESH BALASUBRAMANIAN, Mechanical Engineering and Mechanics, Lehigh University, WEI CHEN, Mechanical Engineering, University of Northwestern, TEYU CHIEN, University of Wyoming — Bulkheterojunctions in organic photovoltaic solar cell (OPVC) active layers are believed to be determining the performance of the OPVCs. The domain features measured in the active layer exhibits quasi-random nanostructures. Though it is believed that the quasi-random nanostructures in the BHJ play a decisive role on determining the performance, it is unclear how to quantify this quasi-random nanostructures into a quantity that could be used to guide the synthesis. In this work, we will present mathematical description of SDF for two dimensional images followed by a simplified fitting equation for general SDF analysis. The simplified fitting equation will extract the information of domain sizes (average and deviation), and domain distances (average and deviation). Validation of this equation is tested by simulated model data. After testing with the simulated data, this equation is applied to two dimensional cross-sectional scanning tunneling microscopy and spectroscopy (XSTM/S) data and small angle X-ray diffraction data measured on the active layer made of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61 butyric acid methyl ester (PCBM). It will be argued that this method could be applied to various types of data exhibit similar two-domain quasi-random features.
Multiscale Modeling of Organic Photovoltaics*  THOMAS ALLEN (Presenter), PETER JACOB ROSSKY, Rice University — Obtaining a detailed understanding of how molecular configurations impact device performance in polymer-based solar cells is a key problem on the road to enabling improved rational design of these devices. Since direct observation of the relevant morphology is experimentally challenging, computer simulation has become an important tool in gaining insight into correlations between structure and performance in organic photovoltaics. Here, we report on the development and usage of a recent coarse-grained model of poly-3-hexylthiophene (P3HT), parameterized based on an information-theoretic Bayesian approach. On this basis, we discuss insights into not only how to build polymer models, but also which types of observables must be captured in the model in order to faithfully represent device morphology. Additionally, we consider spatial and temporal challenges present even in coarse-grained simulation and sampling and some approaches to alleviate them.

*Welch Award #C-1937

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K51 DBIO: Information Processing in Sensory Systems

8:00AM K51.00001: Making an effort to listen: mechanical amplification by ion channels and myosin molecules in hair cells of the inner ear [Invited]  JIM HUDSPETH (Presenter), Howard Hughes Medical Institute, Rockefeller University — As the gateway to human communication, the sense of hearing is of enormous importance. Hearing commences with the capture of sound energy by hair cells, the ear's sensory receptors, which convert that energy into electrical signals that the brain can then interpret. Each hair cell is a cylindrical epithelial cell surmounted by a hair bundle, an erect cluster of 20-300 rigid, actin-filled rods termed stereocilia. Mechanical force deflects the hair bundle and thereby excites the hair cell and its associated nerve fibers.

Uniquely among our sensory receptors, the hair cell is not a passive recipient of stimuli, but instead uses an active process to enhance its inputs. This active process amplifies mechanical stimuli by as much as a thousandfold, greatly increasing our sensitivity to weak sounds. Amplification is accompanied by frequency tuning, which yields a frequency resolution of less than 0.2 %, one thirtyieth of the interval between piano keys. The active process produces a compressive nonlinearity that renders the ear sensitive to sounds over a millionfold range of amplitude or a trillionfold range of power. Finally, the active process can be so exuberant as to become unstable; as a result, in a very quiet environment most normal ears spontaneously emit sound!

As a result of the cooperative gating of mechanically sensitive ion channels, a hair bundle is dynamically unstable: the relation between the bundle's displacement and the force required to accomplish it possesses two stable fixed points separated by a region of negative stiffness. This situation fosters amplification or oscillation when the hair bundle is pushed into its region of instability by molecular motors, specifically the myosin molecules associated with adaptation of the transduction apparatus to sustained stimuli. Experiments on individual hair bundles indicate that the bundle's operation near this instability—a Hopf bifurcation—accounts for the four characteristics of the active process.

8:36AM K51.00002: Differential Resilience to Perturbation of Circuits with Similar Performance* [Invited]  EVE MARDER (Presenter), Volen Center and Biology Department, Brandeis University — Experimental work on the crustacean stomatogastric ganglion (STG) shows a 2-6 fold variability in the expression of ion channel and receptor genes and in the conductance densities for many of the processes that are important for circuit dynamics. Old and new computational work with conductance-based single neurons and small network models shows that similar network performance can arise from diverse underlying parameter sets. Together, these lines of evidence suggest that each individual animal, at any moment in its life-time, has found a different solution to producing “good enough” motor patterns for normal behavior. This poses the question of the extent to which animals with different sets of underlying circuit parameters can respond reliably and robustly to environmental perturbations and neuromodulation. Consequently, we study the effects of temperature, pH and neuromodulation on the pyloric rhythm of crabs. While all animals respond remarkably well to large environmental perturbations, extreme perturbations that produce system “crashes” reveal the underlying parameter differences in the population. Studies of multiple computational models with similar behaviors under control conditions reveal interesting dynamics when perturbed.

*National Institutes of Health R35 NS 097343.
9:12AM K51.00003: Algorithms and neural circuits in olfaction* [Invited] VENKATESH MURTHY (Presenter), Molecular & Cellular Biology, Harvard University — Animals sense the chemical world to guide their behaviors. Fluctuating mixtures of odorants, often transported in fluid environments, are detected by an array of chemical sensors and parsed by neural circuits to recognize odor objects that can inform behavioral decisions. Unlike other sensory systems, the olfactory system lacks an obvious topographic organization, and neural connectivity across brain regions is seemingly unstructured. These anomalies offer an opportunity to uncover common principles across different sensory systems. We exploit a variety of biophysical, neurophysiological and behavioral methods to understand how odorant features are encoded in the activity of neurons and transformed in different stages of processing. We then use conceptual and computational models to seek algorithmic explanations for how animals solve specific olfactory tasks. In an illustrative set of studies, we have found that mice can be trained to recognize individual odorants embedded in unpredictable and variable background mixtures with high degree of success [doi: 10.1038/nn.3775]. Despite nonlinear interactions and variability in the representations of odor mixtures by odorant receptors, a simple linear feedforward decoding is sufficient to explain the performance of mice in this task [doi: 10.1016/j.neuron.2016.08.007]. Current experiments are aimed at understanding how the mouse brain represents information about odor mixtures to aid odor object identification and categorization.

*Work in the Murthy lab is supported by grants from the NIH, NSF and Harvard University.

9:48AM K51.00004: Information Processing in the Somatosensory System* [Invited] DANIEL O’CONNOR (Presenter), Department of Neuroscience, Johns Hopkins University School of Medicine — Touch perception arises from a closed-loop process in which animals move their sensors in order to actively seek out informative mechanical input, which is then processed to direct further movements. My laboratory uses the mouse whisker system to explore the neural basis of active touch perception, at essentially all levels of the nervous system. Information processing during active touch is constrained by the coding properties of neurons in the skin that transduce mechanical stimuli into action potentials. I will discuss recent work from my laboratory that addresses how specific types of mechanosensory neurons encode (a) mechanical features of the environment during active touch, and (b) self-motion kinematics. These two streams of information allow tactile input to be interpreted with respect to sensor position. After mechanical features of the environment are encoded into action potentials and sent to the central nervous system, multiple factors determine how these neural signals are routed within circuits of the brain to impact perception. I will discuss a second line of work in my lab that addresses how identically encoded sensory inputs can produce quite different perceptual outcomes. By monitoring and manipulating neural activity at multiple levels of the nervous system during behavior, we have gained insight into the mapping between mechanosensation and perception.

*NIH grants R01NS089652 and 1R01NS104834-01.

10:24AM K51.00005: Neural processing and computation in the visual system* [Invited] DAMON CLARK (Presenter), Molecular, Cellular, Developmental Biology, Yale University — Visual systems detect many features of natural scenes, but one of the best studied is how they detect motion, which is a widespread computation across animals. To estimate visual motion speed and direction, the visual system must integrate information nonlinearly over space and over time. Models to estimate visual motion have two essential features: a delay step that delays certain signals with respect to others; and a nonlinear step that integrates signals over space and time to create the motion estimate. The computation itself can be framed as an inference problem, in which spatiotemporal light intensity measurements are combined to estimate a latent variable of image velocity. I will present recent work on understanding how motion is computed in the small brain of the fruit fly Drosophila, where genetic tools allow us to dissect the roles of individual neurons in circuit computations. I will focus on the mathematical operations that describe the transformation from light intensity to motion signals, and how that algorithm performs with different visual inputs. I will also focus on processing steps that appear similar across visual systems. These parallels suggest that there may be a narrow range of motion estimation algorithms that perform well given the constraints of biological systems and the regularities of natural scenes.

*Research in lab is supported by the NIH, NSF, Sloan Foundation, Smith Family Foundation, Searle Scholar Award, and Ziegler Foundation.

Wednesday, March 6, 2019 8:00 AM - 10:48 AM

Session K52 DPOLY: Polymer Nanocomposites II: Block Copolymers and More BCEC 253B - Pinar Akcora, Stevens Institute of Technology - Tag(s): Focus
In recent decades, block copolymer (BCP)-inorganic nanocomposite co-assembly has emerged as a highly tunable route to the synthesis of crystallographically ordered, mesoporous inorganic materials. These materials have found numerous applications in catalysis, energy conversion and storage, and other areas. One notable area in which BCP-directed assembly has made few inroads, however, is the production of electronic-grade materials suitable for studies of emergent phenomena, i.e. quantum metamaterials. For example, superconductors with mesoscale ordering are expected to have properties different from their bulk counterparts. The exploration of these properties has been limited by the lack of tunable, robust synthesis methodologies. We have developed a route to gyroidal NbN superconductors from poly(isoprene-b-styrene-b-ethylene oxide)-Nb$_2$O$_5$ nanocomposites using high-temperature annealing in ammonia gas. In recent work, we have developed synthesis routes using methane gas that enable the synthesis of carbonitrides with superconductor quality comparable to bulk samples and tunable morphology across the BCP phase diagram. These morphologies exhibit differences in the transition onset and magnetization behavior, potentially the first hallmarks of quantum metamaterial behavior.

**8:24AM K52.00003: Nanoparticle Templating via Block Copolymer Self-Assembly**

DEBORAH LIU (Presenter), DANIEL KROGSTAD, University of Illinois at Urbana-Champaign — Many applications of polymer nanocomposites require an ordered configuration. To address this challenge, our group is studying the templating of nanoparticles by block copolymers within a thermoset resin. However, much remains to be understood about the fundamental phase behavior of block copolymers when blended with a thermoset. In this presentation, we will discuss our recent work characterizing the self-assembly behavior of an asymmetric block copolymer blended in an epoxy resin. The nanostructures formed as a function of block copolymer weight fraction within the thermoset resin are characterized by SAXS and TEM, and the evolution of these structures during epoxy curing is evaluated. The effect of increasing weight fraction of block polymer on the thermal characteristics of the cured network are probed using DSC. In addition, we present preliminary work on the abilities of these nanostructures to template gold nanoparticles. The suitability of these materials for high performance applications is also discussed.

**8:36AM K52.00004: Entropy-driven assembly in multicomponent nanocomposite**

LE MA (Presenter), University of California, Berkeley, PETER ERCIUS, Lawrence Berkeley National Laboratory, TING XU, University of California, Berkeley — Hierarchically structured nanocomposites show unique collective properties from nanoparticle (NP) assemblies. Successfully structure control in nanocomposite remains as bottleneck to advance the field. Block copolymer (BCP) and supramolecular systems have been effective in achieving nanoscopic dispersion of fillers. However, NPs with size larger than 30% of the BCP specific domain size tend to aggregation due to the large conformational entropy penalty. This limitation in the particle size restricts the NP incorporation for targeted functionality. Here, we will discuss a new approach to modulate thermodynamic contribution from various components with a special focus of maximizing translational entropy. The present studies suggested that manipulating entropic contribution in multiple components system will lead to new path and opportunity toward structure control and access functionality.

*This work was supported by the Department of Energy, Office of Basic Energy Science, under Contract DE-AC02-05CH11231 through the “Organic–inorganic Nanocomposites” program at Lawrence Berkeley National Laboratory. The tomography was performed at the National Center for Electron Microscopy.*
Electrically Conductive Block Copolymer Nanocomposites for Large-Scale Coating Applications*

JUNPYO KWON (Presenter), KATHERINE EVANS, ROBERT OLIVER RITCHIE, TING XU, University of California, Berkeley — Electrically conductive coatings have been widely applied to convert insulators to electronics for sensing, energy harvesting, or actuator applications. However, commercially available conductive paints have issues regarding low mechanical properties and fatigue resistance. Furthermore, mass production is limited due to the extremely high price of conductive fillers and complicated manufacturing processes. Here, we introduce a low price block copolymer and carbon black nanocomposite possessing superb mechanical flexibility and electrical conductivity. Attractively, its mechanical and electrical properties can be recovered with a thermal annealing process after applying cyclic loadings with high frequencies. The nanocomposite can be coated on a variety of substrates, such as fabric, wood, glass, and plastic. This self-healing composite could be used to design wearable electronics, soft robotics, and strain sensors, which require high flexibility.

*This work was supported by the Jane Lewis Fellowship and the Department of Energy, under Contract DE-AC02-05CH11231 through the “Organic–Inorganic Nanocomposites” program at Lawrence Berkeley National Laboratory.

The effect of chemical structure on the morphology, ion transport, and modulus of hybrid inorganic-organic diblock copolymer electrolytes*

KEVIN GAO (Presenter), GURMUKH SETHI, SAHELI CHAKRABORTY, IRUNE VILLALUENGA, NITASH BALSARA, University of California, Berkeley — Poly(ethylene oxide)-b-polyhedral oligomeric silsequioxane (PEO-POSS) mixed with lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) salt is a nanostructured hybrid organic-inorganic diblock copolymer electrolyte that may enable lithium metal batteries. The organic poly(ethylene oxide) block solvates lithium ions and facilitates ion transport while the inorganic polyhedral oligomeric silsequioxane (POSS) block provides mechanical rigidity, decoupling typically antagonistic mechanical and ion conducting properties. PEO-POSS with different alkyl chain substituents on the POSS monomer's silica cage were synthesized to study the effect of chemical structure on morphology, ion transport, and modulus. Ionic conductivity, salt diffusion coefficient, and steady-state cation transference number were measured for a range of salt concentrations. In general, increasing the alkyl chain length was found to promote ordering and increase mechanical stiffness, while decreasing ionic conductivity.

*This work was supported by a National Defense Science and Engineering Graduate Fellowship.

Ionomer Nanocomposites: The Interplay Between Structural Dynamics and Water Transport

APOORVA BALWANI (Presenter), ALLISON JANSTO, Chemical & Biomolecular Engineering, Clemson University, ANTONIO FARAONE, NIST Center for Neutron Research, National Institute of Standards and Technology, ERIC DAVIS, Chemical & Biomolecular Engineering, Clemson University — Ionomer nanocomposites are gaining popularity as proton exchange membranes (PEMs) in vanadium redox flow batteries due to reduced vanadium ion crossover as compared to traditional PEMs. Understanding the impact of silica nanoparticles (SiNPs) on the structural dynamics and transport kinetics of these nanocomposites can provide vital insights into the mechanism of crossover reduction. Presently, segmental and swelling dynamics of a series of ionomer nanocomposite membranes were characterized using neutron spin echo and time-resolved Fourier transform infrared attenuated total reflectance (tFTIR-ATR) spectroscopy. We found that both viscoelastic relaxations and segmental dynamics in the ionomer network were impeded by the presence of SiNPs. Further, the dynamics of the membranes were highly dependent on the surface chemistry of the SiNPs, for both cationically or anionically charged surfaces. In addition to swelling dynamics, tFTIR-ATR was used to evaluate water sorption kinetics, which were found to be strongly coupled with the viscoelastic relaxation in these hybrid membranes. Anomalous, multi-stage water sorption kinetics were observed and attributed to different stages of structural rearrangement in the ionomer network during membrane hydration.
9:24AM K52.00008: Metal Organic Framework assisted ionic conductivity in solid polymer electrolyte for application in lithium-ion battery  NAGMA ZERIN (Presenter), JANNA MARANAS, XUEYI ZHANG, Pennsylvania State University — Solid polymer electrolytes are safer alternatives to the current flammable liquid electrolytes used in lithium-ion batteries. We are using crystalline PEO6/LiX (X= anion) as the potential polymer electrolyte. In this structure, pairs of PEO chains wrap around each other to form cylindrical tunnels. Inside the tunnel each Li+ coordinates with six ether oxygens. The anions are located outside the tunnel. Low molecular weight PEO6 has been found to be more conductive than its amorphous counterpart. However, it is not useful for practical applications as at room temperature this structure is like viscous liquid. Although increasing molecular weight improves the structural stability of PEO6, it doesn't improve conductivity. High molecular weight PEO6 chains fold into lamellae, preventing direct pathway for lithium ion conduction. We propose that incorporating high aspect ratio nanofillers, containing Lewis acidic surface sites, with PEO6 can resolve the issue. Using metal organic framework as the nanofiller, we have obtained conductivity greater than 10^{-5} S/cm at 30°C.

Reference:

9:36AM K52.00009: EFFECT OF FILLER CONTENT ON ENHANCEMENT OF THERMAL CONDUCTIVITY OF ALIGNED POLYMER GRAPHENE NANOCOMPOSITES  FATEMA TARANNUM (Presenter), JIVTESH GARG, University of Oklahoma — In this work a systematic study of the effect of increment of filler content on enhancement of thermal conductivity(k) of aligned polymer-graphene nanocomposites has been conducted. Using Angstrom Method, it is found that aligned graphene nanoplatelets (GnPs) significantly increase the heat-conducting properties of pure polyethylene (PE) compared to randomly oriented nanoplatelets. The increment in amount of GnPs from 9 weight% to 13 weight% is studied. A combination of melt extrusion processing and compression molding is used to obtain an even dispersion of the filler in the polymer matrix. Alignment of PE and GnPs is observed through confocal laser scanning microscopy. Comparison with effective medium theory reveals the measured thermal conductivity enhancement to be larger than theoretical predictions. Cause of this discrepancy between measurement and theory will be discussed.

9:48AM K52.00010: Molecular Simulations of the Motion of Polymer-Tethered Nanoparticles in Unentangled Polymer Melts  TING GE (Presenter), MICHAEL RUBINSTEIN, Mechanical Engineering and Materials Science, Duke University, GARY GREST, Sandia National Laboratories — Polymer-tethered nanoparticles are commonly added to a polymer matrix to yield superior material properties. Critical to the fabrication and processing of such a composite is the mobility of polymer-tethered nanoparticles. We study the motion of polymer-tethered nanoparticles in unentangled polymer melts using molecular simulations, which offer a precise control of the grafted chain (tail) length N_{tail} and the number Z of tails per particle. For loosely-grafted particles with small Z, the diffusion coefficient decreases with increasing N_{tail}, exhibiting a crossover from particle-dominated to tail-dominated diffusion. If the diffusion is tail-dominated, there are two sub-diffusive regimes in the mean squared displacement \langle \Delta r^2(t) \rangle of particles before diffusion. The sub-diffusion at small t arises from the dynamical coupling of the particle and the melt chains, while the one at large t results from the participation of the particle in the dynamics of the tails. For densely-grafted particles with large Z, \langle \Delta r^2(t) \rangle can be approximated as that of a larger particle. The friction coefficient of the tails is smaller than the prediction based on Rouse dynamics of tails. These results suggest that the particle and tails move as one object with the tails hydrodynamically coupled to each other.

10:00AM K52.00011: Impact of hydrogen bonding interactions on graft-matrix wetting and structure in polymer nanocomposites*  ARJITA KULSHRESHTHA (Presenter), ARTHI JAYARAMAN, University of Delaware — Properties of polymer nanocomposites (PNCs) are linked to their morphology which is dictated by the dispersion/aggregated state of nanoparticles in a polymer matrix. Grafting polymeric ligands onto the nanoparticle surface offers a greater control over morphology by allowing for tuning of effective interactions between graft and matrix polymers. One way to tailor interactions between graft and matrix chemistries is by the introduction of inter-molecular hydrogen bonds between graft and matrix polymers. In this talk, we present our work on the development of a coarse-grained (CG) model that allows us to capture hydrogen bonding type directional and specific interactions between graft and matrix polymers. Using this CG model, we run molecular dynamics (MD) simulations to elucidate the effect of these directional and specific interactions on the PNC morphology by comparing grafted layer wetting, graft and matrix chain conformations and free volume for each graft monomer between PNCs with isotropic graft-matrix interaction and PNCs with hydrogen bonding type graft-matrix interaction. We explore effects over a large design space comprising of grafting density, polymer flexibility, and strengths of isotropic graft-matrix attraction and hydrogen bonding interaction.

*DOE (#DE-SC0017753)
10:12AM K52.00012: Influence of Nanoparticle Surface Chemistry on Properties of Iron Oxide–Poly(ethylene oxide) Nanocomposites*  DONOVAN WEIBLEN (Presenter), GRACE GIONTA, Materials Science and Engineering, Rensselaer Polytechnic Institute, DENIZ RENDE, Center for Materials, Devices, and Integrated Systems, Rensselaer Polytechnic Institute, PINAR AKCORA, Chemical Engineering and Materials Science, Stevens Institute of Technology, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Heating using magnetically susceptible nanoparticles has shown promise in biomedical applications in areas such as tissue engineering and drug delivery. In the current work, the effect of surface coating on iron oxide nanoparticles heated via an alternating magnetic field (AMF) was explored. Two coatings were investigated in addition to bare nanoparticles: poly(ethylene glycol), PEG, coated and amine coated 50–nm–diameter iron oxide nanoparticles. These nanoparticles were dispersed in concentrations varying from 0.010–0.750% by weight in poly (ethylene oxide), PEO. PEO was chosen due to its known biocompatibility and use in the healthcare industry. A significant increase in temperature was observed considering the low loading of particles in all samples. Analysis of heating curves revealed an unusual result. The amine coated particles had a much more significant and rapid response than either the uncoated or PEG coated nanoparticles. Heating properties of samples were also investigated as a function of AMF parameters and iron oxide surface chemistry.

*This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1825254

10:24AM K52.00013: Functional polymer nanocomposites : structural issues in relation to the piezoelectric response*  SOPHIE BARRAU (Presenter), ADELINE MARIN, JULIETTE DEFEBVIN, JOËL LYSKAWA, PATRICE WOISEL, JEAN-MARC LEFEVBRE, UMET, University of Lille, France, ANTHONY FERRI, ANTONIO DA COSTA, RACHEL DESFEUX, UCCS, University of Artois, France — Poly(Vinylidene Fluoride) (PVDF) is a semi-crystalline polymer with complex polymorphism that has attracted considerable interest, owing to the electroactive properties displayed by its polar β and γ phases. Regarding PVDF-based nanocomposites, two strategies are considered in the following :
- The first one deals with the incorporation of piezoelectric inorganic nanofillers (BaTiO3), with primary issues related to nanoparticle dispersion and monitoring of interfacial cohesion, together with promoting the development of the highly polar β phase in the PVDF matrix. It is shown that the piezoelectric response may be modulated as a function of filler content, going through a zero value at some critical filler fraction.
- Alternatively, the introduction of carbon nanotubes in the PVDF matrix is achieved, with the result that the nanotubes induce the formation of the γ polar phase in their vicinity. The local structural organization of the α and γ phases in the PVDF nanocomposite is probed by atomic force microscopy and specific attention is paid to the local electroactive properties through the use of piezoelectric force microscopy (PFM).

*This work was partly supported through grant ANR-16-CE08-0025, ANR NanoPic from the French National Research Agency.

10:36AM K52.00014: Optical Properties of Plasmonic Nanoparticles Polymer Nanocomposites*  ASSAD ULLAH KHAN (Presenter), YICHEN GUO, XI CHEN, GUOLIANG LIU, Virginia Tech — Plasmonic nanoparticles–polymer nanocomposites are used in functional optical materials and devices where light management is essential. However to modulate the optical properties of these nanocomposites, control over the orientation and spatial distribution of the nanoparticles within polymer matrix is very critical. Here we synthesized two-dimensional (2D) Ag nanoplates (AgNPs) with plasmon resonance across the visible and near infrared (NIR) light range via a multi-step approach. Layer-by-layer (LbL) assembly was utilized to control the orientation and density of the AgNPs in the nanocomposite films. The composite thin-films effectively controlled the light transmittance and reflectance across the visible and NIR range. In contrast to the conventional polymer nanocomposites in which the polymer grafted nanoparticles were randomly mixed within the matrix, the thin-film polymer nanocomposites comprise a single layer (~10 nm), or any desired multiple layers, of planarly oriented plasmonic AgNPs separated by a polymer with tunable interlayer thickness. The plasmonic composites filter light selectively and will have enormous effect on energy-efficient tinted glass.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1752611.
8:00AM K53.00001: The Topology and Mechanics of the Formation of Fracture Surface Patterns* [Invited] JAY FINEBERG (Presenter), Hebrew University of Jerusalem, ITAMAR KOLVIN, Physics, University of California Santa Barbara, MOKHTAR ADDA-BEDIA, Laboratoire de Physique, ENS Lyon — How and why are patterns formed on broken surfaces? Faceted fracture surfaces are commonly formed by slow tensile cracks in amorphous materials; hence their formation cannot reflect microscopic order. While fracture mechanics predict that slow crack fronts should be straight and form mirror-like surfaces, facet-forming fronts propagate simultaneously within different planes separated by steps. Why are steps stable, what determines their path and how do they couple to crack front dynamics? By integrating real-time imaging of propagating crack fronts with surface measurements, we demonstrate that steps are topological defects; crack front separation into disconnected overlapping segments provides the condition for step stability. Crack dynamics are enslaved to steps; steps drift at a constant angle to the local front propagation direction while their increased dissipation couples to long-ranged elasticity to determine front shapes. We see how 3D topology couples to 2D fracture dynamics to provide a fundamental picture of how patterned surfaces are generated. We also show that crack front curvature may feed back to deflect step paths via nonlinear focusing of crack fronts, causing steps to converge to form a micro-branch. Thus, our results supply the basis for a unified picture of pattern formation on fracture surfaces.

*This research was funded by the Israel Science Foundation (grant no.1523/15), as well as the US-Israel Bi-national Science Foundation (grant no. 2016950)

8:36AM K53.00002: Topological adhesion [Invited] ZHIGANG SUO (Presenter), Harvard University — TBD

9:12AM K53.00003: Fracture mechanics of self-healing hydrogels [Invited] CHUNG YUEN HUI (Presenter), Cornell University — TBD

9:48AM K53.00004: Active superelasticity in three-dimensional epithelia of controlled shape* [Invited] XAVIER TREPAT (Presenter), ICREA at the Institute for Bioengineering of Catalonia — Fundamental biological processes are carried out by curved epithelial sheets enclosing a pressurized lumen. How these sheets develop and withstand three-dimensional deformations has remained unclear. By combining measurements of epithelial tension and shape with theoretical modeling, here we show that epithelial sheets are active superelastic materials. We produce arrays of epithelial domes with controlled geometry. Quantification of luminal pressure and epithelial tension reveals a tensional plateau over several-fold areal strains. These extreme tissue strains are accommodated by highly heterogeneous cellular strains, in seeming contradiction with the measured tensional uniformity. This phenomenology is reminiscent of superelasticity, a behavior generally attributed to microscopic material instabilities in metal alloys. We show that this instability is triggered in epithelial cells by a stretch-induced dilution of the actin cortex and rescued by the intermediate filament network. Our study unveils a new type of mechanical behavior -active superelasticity- that enables epithelial sheets to sustain extreme stretching under constant tension.

*This work was supported by the Spanish Ministry of Economy and Competitiveness/FEDER (BFU2015-65074-P), the Generalitat de Catalunya and CERCA program, the European Research Council (CoG-616480), and European Commission (project H2020-FETPROACT-01-2016-731957). IBEC is recipient of a Severo Ochoa Award of Excellence from the MINECO.

10:24AM K53.00005: Towards a Unified Model of Soft Adhesives [Invited] MATTEO CICCOTTI (Presenter), Soft Matter Science and Engineering Laboratory (SIMM), ESPCI Paris — Pressure Sensitive Adhesives (PSA) have been widely used in adhesive tapes, stickers, tags in industry and day-to-day use, for decades. PSAs are rate-dependent materials, extremely soft, hence highly deformable. Their bonding strength depends critically on small scale features such the surface properties of the substrates. Understanding quantitatively their behavior has been a enormous challenge. Quite surprisingly, a same adhesive can be described by different models with little connection within each other depending on the adhesion tests used. In this talk, I will present a new modeling strategy to these soft materials [Creton and Ciccotti, Soft Matter, (2016)] based on the identification of the mesoscale mechanisms (cavitation, fibrillation, ...) along with the evaluation of the contribution of the large strain rheology of the PSA into the total work of debonding. I will discuss some original experimental investigations providing insights into the pertinent links between the peel, tack and shear of model PSAs.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K54 DPOLY GSOFT GSNP: Confined Polymer Glasses II: Dynamics, Surface Effects, and Architecture BCEC 254A - George Floudas, University of Ioannina - Tag(s): Focus
8:00AM K54.00001: β-NMR Studies of the Depth Dependence of Secondary Relaxations in Polystyrene Thin Films

IAIN MCKENZIE (Presenter), Physical Sciences Division, TRIUMF, YU CHAI, Physics and Astronomy, University of Waterloo, DAVID CORTIE, Physics and Astronomy, University of British Columbia, JAMES FORREST, Physics and Astronomy, University of Waterloo, DEREK FUJIMOTO, Physics and Astronomy, University of British Columbia, VICTORIA KARNER, Chemistry, University of British Columbia, ROBERT F KIEFL, Physics and Astronomy, University of British Columbia, CDP LEVY, Accelerator Division, TRIUMF, W ANDREW MACFARLANE, Ryan MCFADDEN, Chemistry, University of British Columbia, GERALD D MORRIS, MATTHEW PEARSON, Physical Sciences Division, TRIUMF, ADAM RAEGEN, SHIPEI ZHU, Physics and Astronomy, University of Waterloo — β-detected nuclear magnetic resonance (β-NMR) of implanted $^8$Li$^+$ has been used to probe the depth dependence of secondary relaxation processes in thin films of atactic polystyrene (PS). β-NMR measurements of the average $^8$Li spin-lattice relaxation rate were used to determine the depth dependence of the fluctuation rate of the fast γ-relaxation process in PS films at 317 K, which is well below its glass transition temperature [I. McKenzie et al. Soft Matter, 14, 7324 (2018)]. A novel hole-burning (selective saturation) β-NMR technique has been used to measure the depth dependence of the fluctuation rate of the much slower β-relaxation process at the same temperature. Both the fluctuation rates of the β- and γ-relaxation processes are larger near the free surface than in the bulk and both return to the bulk value over a length scale of several nm.

8:12AM K54.00002: Reducing the Tg-Confinement Effect in Polystyrene Films by Use of Carbon Substrates and Changing the Direction of the Effect in Polystyrene-Carbon Model Nanocomposites

JOHN TORKELSON (Presenter), LAWRENCE CHEN, Northwestern University — Using ellipsometry and fluorescence, we have shown that single-layer polystyrene (PS) films supported on carbon substrate exhibit suppression of the classic $T_g$-confinement effect due to favorable polymer-substrate interactions. Additionally, a bilayer film/fluorescence study has shown that in a bulk PS film, the 15 nm layer at the carbon interface exhibits a $T_g$ nearly 10 K higher than bulk. The ability of PS to favorably interact at the interface with the graphitic substrate (versus silicon dioxide) was demonstrated qualitatively via a dewetting study. Because PS does not naturally wet the native oxide layer on silica, a thin 30 nm-thick, 30 kg/mol PS film readily dewets when annealed at 433 K. However, dewetting of supported thin PS films is greatly suppressed using substrates with favorable interfacial interaction with PS. Model nanocomposites were also made by sputtering a graphitic layer above PS films supported on carbon, sandwiching the film between two graphitic surfaces and providing a consolidated film with constant interlayer distance between the two hard surfaces after annealing. Single-layer PS films in this model nanocomposite geometry exhibit enhanced $T_g$ with decreasing nanoscale thickness due to pi-pi bonding interactions of PS with the graphitic substrates.

8:24AM K54.00003: Polymer dynamics under 2D nanometer confinement

GEORGE FLOUDAS (Presenter), MPI-P, University of Ioannina, CHRISTOS POLITIDIS, STELIOS ALEXANDRIS, University of Ioannina, MARTIN STEINHART, University of Osnabrueck — The effect of confinement on polymer dynamics and the associated liquid-to-glass temperature, $T_g$, has been an issue of great interest in polymer physics. In this study, we investigate the effect of nanometer confinement on the dynamics of several polymers including cis-1,4-polyisoprene with molecular weights both below and above the entanglement limit. As confining medium we employ self-ordered nanoporous alumina (AAO) with diameters, $d$, ranging from 400 nm to 25 nm resulting in a broad $2R_g/d$ range. We employ Broadband Dielectric Spectroscopy (BDS) and Temperature-Modulated Differential Scanning Calorimetry (TMDSC). BDS revealed consistently faster segmental dynamics under confinement with respect to the bulk, leading to a decrease in $T_g$ with increasing degree of confinement ($2R_g/d$). This is discussed in terms of the role of interfacial energy. In addition, we provide evidence for an intermediate process with an Arrhenius temperature dependence whose dielectric strength increases with increasing degree of confinement. These results are discussed in view of recent theoretical and experimental progress in understanding polymer imbibition in nanopores.
Irreversible adsorption: new insights on molecular mobility, thermodynamics and interfacial interactions* [Invited] SIMONE NAPOLITANO (Presenter), DAVID NIETO SIMAVILLA, Polymer and Soft Matter Dynamics, Universite libre de Bruxelles (ULB) — Irreversibly adsorbed polymer layers represent an intriguing class of novel nanomaterials with unexpected properties, strongly deviating from what observed in unbounded polymer melts. These extremely thin films are obtained via a small number of successive steps, easily reproducible: a polymer melt is placed in contact with an adsorbing substrate and nonadsorbed chains are washed away in a good solvent. Importantly, tuning the thickness of the adsorbed layer, an operational parameter equivalent to the number of chains adsorbed on a unit surface, allows modifying the interfacial free volume content and, hence, the performance of polymer coatings without affecting the interfacial chemistry.

Here, we discuss on the physics behind the formation of irreversibly adsorbed layers onto solid substrate. By analyzing the outcome of experiments and simulations, we show how changes in thermal energy and interaction potential affect the equilibrium and the nonequilibrium components of the kinetics. We verify that the monomer pinning mechanism is independent of surface coverage, while the progressive limitation of free sites significantly limits the adsorption rate. Importantly, in neat disagreement with current ideas on surface science, the equilibrium adsorbed amount – and, hence, interfacial interaction potential – is affected by nanocconfinement (1).

Thinner films show a neat drop in adsorbed amount, implying a reduction in interfacial interactions between polymer and substrate upon confinement at the nanoscale level. We demonstrate that this phenomenon is totally ascribable to the smaller amplitude of the dispersive forces in thinner films, that can be parametrized via the Hamaker constant, and discuss on the impact of our new findings on previous experiments on multilayers systems.


*Financial support from the Fonds de la Recherche Scientifique—FNRS under Grant no. T.0147.16 “TIACIC”.

Confinement Effects on Dye Translational Diffusivity in Polystyrene Thin Films Depend on Polymer Molecular Weight: Connection to Fragility-Confinement Effects TONG WEI (Presenter), Department of Chemical and Biological Engineering, Northwestern University, TIAN LAN, Department of Material Science and Engineering, Northwestern University, JOHN TORKELSON, Department of Chemical and Biological Engineering, Northwestern University — The impact of confinement on the translational diffusivity, \(D_{\text{dye}}\), of small-molecule dye 9,10-bis(phenylethynyl)anthracene is studied in supported, thin films by fluorescence. Relative to bulk films and near \(T_g\), \(D_{\text{dye}}\) is reduced by 80 - 90\% in 100-nm-thick, high molecular weight (MW) PS (400 kg/mol) films. In contrast to \(T_g\), which reflects the slow portion of the cooperative segmental relaxation distribution, \(D_{\text{dye}}\) reflects the fast relaxation regions, which can be many orders of magnitude faster than slow regions. \(D_{\text{dye}}\) results are associated with fragility, which reflects the relaxation distribution breadth, and its confinement effects: with sufficient confinement, the relaxation distribution narrows (and high MW PS fragility decreases) with the fast relaxation tail becoming slower, leading to a decrease in \(D_{\text{dye}}\). In yet thinner films, the slow relaxation regions become faster, decreasing \(T_g\). Because low MW PS (6 kg/mol) exhibits a lower bulk fragility than high MW PS, confinement has a much-reduced effect on low MW PS fragility, and both fragility and \(D_{\text{dye}}\) in 100-nm-thick low MW PS films are unchanged from bulk.

Comparing Refractive Index and Density Changes with Decreasing Film Thickness in Thin Supported Films Across Different Polymers YIXUAN HAN (Presenter), CONNIE ROTH, Physics Dept, Emory University — Density or specific volume changes in thin films have been investigated in relation to glass transition and other property changes with decreasing film thickness. Often such density changes are inferred from values of the refractive index through the Lorentz-Lorenz equation. Our group’s previous work on supported polystyrene (PS) films concluded that recently reported large changes in apparent film density are likely erroneous because assumptions in the derivation of the Lorentz-Lorenz relation become invalid for thin films less than ~20 nm. Unexpected non-monotonic changes in refractive index with decreasing thickness were observed for PS films as measured by spectroscopic ellipsometry. Here we compare these PS results to similar measurements of refractive index on poly(2-vinylpyridine) (P2VP) and poly(methyl methacrylate) (PMMA) supported films, polymers typically associated with attractive substrate interactions. Surprisingly, we find P2VP shows identical thickness-dependent refractive index changes to PS, with a more muted behavior for PMMA. We explore whether such trends arise from alignment of monomers near the substrate interface by measuring substrates with different surface chemistries.
9:36AM K54.00007: Prediction of the Structural Relaxation Time from Vibrational Dynamics in Thin Films  ANDREA GIUNTOLI (Presenter), Wesleyan University, MATTEO BECCHI, SISSA, DINO LEPORINI, University of Pisa — The structural relaxation time of glass forming liquids correlates with the cage vibrational dynamics at the picosecond, making it possible to predict one from the other despite a separation of more than ten orders of magnitude in the time scales. This result, found in computer simulations, has been extended over the years to all kind of glassformers in bulk systems. Thin films, though, present additional complications due to finite size effects and complex surface interactions, causing shifts in the glass transition temperature and strong gradients in mobility across the film for reasons that are not fully understood yet. In spite of that, we show that the particle-sized layers of a thin supported film comply without any adjustment with the same scaling observed in bulks, by varying temperature, film thickness and distance from the substrate in a coarse grained molecular dynamics simulation. This result provides new predicting tools for both simulations and experiments and its implications shed light on the physics of confined liquids approaching the glass transition.

9:48AM K54.00008: How does star polymer architecture affect dynamical heterogeneity? JINPENG FAN (Presenter), HAMED EMAMY, Department of Physics, Wesleyan University, ALEXANDROS CHREMOS, JACK DOUGLAS, Materials Science and Engineering Division, National Institute of Standards and Technology, FRANCIS STARR, Department of Physics, Wesleyan University — The formation of an amorphous solid by polymers is one of the most important features for polymer applications. While glass formation of linear chain polymers has been widely explored, comparatively little is known about glass formation of star polymers. We study the dynamical heterogeneity and cooperative nature of star polymer melts via molecular dynamics simulations. In particular, we quantify how the number of arms and the length of those arms affect the collective string-like motion of monomers. We find that, while the star geometry can significantly affect the size and time scale of collective motions, the relationship between the size scale of the collective motions and the overall relaxation time follows the same Adam-Gibbs like relationship previously found to describe simple linear polymers.

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

10:00AM K54.00009: How does polymer architecture affect the fragility of ultra-thin films? AMBER STOREY (Presenter), WENGANG ZHANG, JACK DOUGLAS, National Institute of Standards and Technology, FRANCIS STARR, Wesleyan University — It is widely understood that the glass transition temperature and fragility of thin polymer films can drastically differ from that of the bulk polymer. In this talk, our focus is to show how polymer architecture affects glass formation in thin films, with an emphasis on changes of fragility. We use molecular dynamics simulations to contrast the behavior of coarse-grained supported polymer films of PEO (which has no sidegroup) and PMMA (which does have a sidegroup). The differences between these polymers are most noticeable in the vicinity of the supporting substrate and free interface, where packing consideration are more affected by the polymer architecture.

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

10:12AM K54.00010: Structure and Dynamics of Bio-Based Polymers in the Bulk and under Confinement KYRIAKH CHRISSOPOULOU (Presenter), KRISTALENIA ANDROULAKI, SPIROS ANASTASIAKIS, FORTH-IESL and Univ. of Crete, MASSIMILIANO LABARDI, Univ. of Pisa — The structure and the dynamics of two bio-based polyester polyols are investigated in the bulk and close to surfaces when the polymers are intercalated within the galleries of a hydrophilic sodium montmorillonite, Na⁺-MMT. The morphology of the neat polymers as well as the structure of the nanohybrids are investigated with X-ray diffraction and their thermal properties are studied by differential scanning calorimetry. One of the investigated polyesters is amorphous whereas the second one is a semi-crystalline polymer with an intriguing thermal behavior. Hybrids have been synthesized in a broad range of compositions and intercalated structures are always obtained. Dielectric relaxation spectroscopy was utilized to study the polymer dynamics. It revealed multiple relaxation processes for the neat polymers both below and above their glass transition temperatures whereas, in the nanocomposites, similarities and differences are observed depending on the specific mode of dynamic process. The results are compared with the ones of hyperbranched polymers of similar chemistry but non-linear architecture. This research has been co-financed by the Greek General Secretariat for Research and Technology (Action: Roadmap of Research Infrastructures, project INNOVATION EL, MIS: 5002772).
Existence of irreversibly adsorbed polymer chains in thin polymer films has a huge impact on the wetting, glass transition, aging and polymer chain mobility. Adsorption of polymer chains on the solid substrates is possible due to a delicate balance between enthalpic gain through segment-substrate interactions and reduction in conformational entropy. In this work we have used 4-arm star, 8-arm star, centipede and comb polystyrene (PS) architectures to understand the role of entropy on the structure of irreversibly adsorbed polymer layers using ellipsometry, X-ray reflectivity and atomic force microscopy. Normalized equilibrium adsorbed layer thickness for all architectures is larger than that of the linear PS and for 8-arm star PS it is above 1Rg. Substrate surface energy affects both the adsorbed layer thickness and the density of the layers. Adsorbed star polymers formed thicker and denser layers on HF etched substrates compared to hydrophilic substrates. It is also interesting to note that the adsorbed layer thickness increases with as-cast film thickness initially and reaches a plateau for thicknesses above 200 nm.

*BA acknowledges the support provided by TUBITAK 215Z334, TUBITAK 115C009, TUBA- GEBIP and BAGEP Young Investigator Award.
**8:00AM K55.00001: Monte Carlo Modelling of Phase Separation in Polymer Blends That Contain Branched Molecules**

EMMA WOOD (Presenter), NIGEL CLARKE, Physics and Astronomy, University of Sheffield — Thermoplastic-toughening of thermosetting epoxy resins is becoming increasingly prevalent, particularly for aerospace composites. As the mechanical properties of these materials are highly dependent on morphology, it is extremely important to understand phase separation within blends of branched and linear polymers. Unfortunately, the Flory-Huggins model has significant limitations for systems containing branched polymers. Entropies of branched polymers are often much lower than for linear polymers of the same molecular weight, but the mean field approach of the Flory-Huggins model does not account for this. The impact of polymer conformation on energetic interactions is also ignored. Here, we have developed a simulation approach capable of overcoming these difficulties and calculating free energy for polymers with branched architectures. We have also used Monte Carlo methods to directly simulate concentration fluctuations within industrially relevant blends, and have therefore gained insight into their phase separation characteristics.

*This work was funded by EPSRC and Solvay through the Polymers, Soft Matter and Colloids CDT.

**8:12AM K55.00002: Interface repulsion and arrest of coarsening in thin films of homopolymer blends due to thermal oscillations**

MARCUS MUELLER (Presenter), LOUIS PIGARD, Institute for Theoretical Physics, University of Gottingen, Germany — In equilibrium the interface potential that describes the interaction between two AB interfaces in a binary blend of A and B homopolymers is attractive, and this interface attraction gives rise to a coarsening of the blend morphology even in the absence of interface curvature. Using continuum models we demonstrate that the time-periodic variation of the Flory-Huggins parameter (or temperature or solvent concentration) qualitatively alters this behavior, i.e., for suitable parameter we find that AB interfaces repel each other and adopt a well-defined distance. We explore for which oscillation periods and amplitudes this interface repulsion occurs and how the preferred interface distance depends on these parameters. Using particle-based simulations we explicitly demonstrate that this dissipative self-assembly of a homopolymer blend results in a lamellar structure with multiple planar interfaces in a thin film geometry.

*CRC 1073 / TP A03 and DFG Mu1674/16

**8:24AM K55.00003: The application of Renormalization Group Theory to polymers**

ANNA SINELNIKOVA (Presenter), Department of Physics and Astronomy, Uppsala University, MAXIM ULYBYSHEV, Institut für Theoretische Physik, Julius-Maximilians-Universität, ANTTI J NIEMI, Nordita, Stockholm University — The definition of phases in polymer physics traditionally relies on scaling laws: different critical exponents correspond to different phases. This method requires the length to be varied for a certain polymer chain. This is impossible to do for proteins or other heteropolymer structures where the number of atoms is one of the characteristics of the system. To solve this problem we employ the ideas of Renormalization Group (RG) theory. We propose a scaling procedure and a novel observable through which RG flow determines the phases of polymers. In addition, this method gives rise to the idea of multiphases in heteropolymers: the chain exists in different phases on different length scales. For example, a helical protein can be seen as a collapsed coil at large scales but as a straight rod at scales corresponding to its secondary structure.

*Swedish research council and the Knut and Alice Wallenberg foundation through the Wallenberg Academy Fellow grant of J. Nilsson

**8:36AM K55.00004: Coarse-grained Modeling for Polymer Solutions via the Mori-Zwanzig formalism**

SHU WANG, WENXIAO PAN (Presenter), University of Wisconsin - Madison — In this talk, we present a new method to establish implicit-solvent coarse-grained (CG) modeling for polymer solutions to conserve the dynamical properties of polymers. In the CG modeling, tens to hundreds of atoms were grouped as one CG particle; and the CG dynamic equations were rigorously derived from the atomistic data. The solvent-mediated dynamics of polymers was accurately captured via the generalized Langevin equation (GLE) with a non-Markovian memory kernel based on the Mori-Zwanzig formalism. The computational cost for direct evaluation of the non-Markovian memory kernel and generation of colored noise was significantly reduced by exploiting the equivalence between the non-Markovian dynamics and Markovian dynamics in an extended space. A higher-order time-integration scheme was developed to further accelerate the CG simulations. To assess, validate, and demonstrate the established CG modeling, we have applied it to simulate four different types of polymer solution systems. We find that the proposed CG modeling effectively conserves the velocity autocorrelation function and diffusivity of polymers and enables two orders of speedup in computer time, compared with the reference molecular dynamics simulations.

*National Science Foundation Grant No. CDS&E-1761068
Simulating Diblock Copolymer Micelles in Binary Explicit Solvents  
DONG MENG (Presenter), JING ZONG, Mississippi State University — Amphiphilic block copolymers form nanoscale assemblies when dissolved in a selective solvent. Such self-assembled structures have wide-ranging applications as drug delivery vehicles and nanoreactors, etc. A powerful method to manipulate the assemblies is to vary the composition of solvent mixtures. Unlike single solvent solution, computational studies of amphiphilic block copolymers in solvent mixtures are rarely reported due to high computational cost associated with the necessity of treating solvents explicitly. Here, the Field-Accelerated Monte Carlo [1] simulation is employed in the expanded grand canonical ensemble to study the micelle formation of diblock copolymers in binary solvents: one selective solvent and one good solvent for both blocks. We investigate effects of molecular weight and solvent composition on micelle morphology, critical micelle concentration, and micelle size and aggregation number. It is found that distribution of the good solvent is highly inhomogeneous, concentrating at micelle interface and partitioning unevenly outside/inside micelle cores. Solvent intake by micelle cores increases with polymer molecular weight, affecting the way micelle size and aggregation number change with solvent composition.


Assessment of an Anisotropic Coarse-Grained Model for Cis-Polybutadiene Obtained by a Bottom-up Approach  
IOANNIS TANIS (Presenter), CLAIRE LEMARCHAND, CEA,DAM,DIF, 91297 Arpajon, France, ROUSSEAU BERNARD, Laboratoire de Chimie Physique, UMR 8000 CNRS, Université Paris-Sud, Orsay, France, LAURENT SOULARD, CEA,DAM,DIF, 91297 Arpajon, France — As it has been shown in previous coarse-grained simulations of polymer systems, the spherical representation utilized for the coarse-grained beads cannot capture anisotropic effects that play a crucial role on the structural features as well as on the dynamic response of such systems [1-2]. On these grounds, the aim of this study is to extract a coarse-grained potential for cis-polybutadiene in the melt state by taking into account the shape of the polymer beads. A conservative potential depending on the distance and the relative orientation of the polymer beads is deduced from atomistic molecular dynamics (MD) simulations. The translational dynamics of the beads is tracked using the position and momentum of their center-of-mass, whereas their rotational dynamics is modeled by representing their orientation through the use of quaternions. The efficacy of this approach to reproduce static features of the polymer melt is assessed in coarse-grained simulations and is also compared with respective isotropic models.

References


New Insights into the Glass Transition from Computational Prediction and Evolutionary Design*  
[Invited] DAVID SIMMONS (Presenter), Chemical and Biomedical Engineering, University of South Florida — In most polymers, the glass transition is one of the most important phenomena determining performance properties including mechanical response, processability, and transport behavior. For this reason, understanding and controlling the glass transition is a longstanding goal of polymer science and soft condensed matter physics. However, the vast range of timescales associated with glass formation, coupled with a lack of an agreed-upon theoretical description of the problem, have posed major challenges to achieving this goal. Here I describe a new approach to this problem, combining efficient molecular dynamics simulations, physics-based heuristics, machine learning, and evolutionary algorithms to predict, understand, and design the glass transition.

*The authors acknowledge the W. M. Keck Foundation for generous financial support of this research. This material is based in part on work supported by the National Science Foundation NSF Career Award grant number DMR1554920.
9:48AM K55.00008: Thermodynamics and kinetics of diblock copolymer micelles: chain architecture effect*
PRHASHANNA AMMU, ELENA DORMIDONTTOVA (Presenter), Polymer Program, Institute of Materials Science and Physics
Department, University of Connecticut, Storrs CT, 06269 — Diblock copolymers are actively used in various application, thus
understanding the factors affecting thermodynamics and kinetics of self-assembly is of obvious importance. Computer
modelling is a useful tool to analyze and compare behavior of various complex systems including diblock copolymers. Using
dissipative particle dynamics simulations we investigate the effect of chain architecture on diblock copolymer self-
assembly and the chain exchange kinetics using the example of diblock copolymers with a ring-shaped core or corona
block in comparison with their linear diblock copolymer counterpart. We found a striking difference in both the
equilibrium micelle size and kinetics of chain exchange in these systems. Furthermore, mixed micelles containing block
copolymers of both types exhibit an unexpected synergism of chain exchange, which is not present in mixed micelles
composed solely of linear chains. The origin of this effect and its implication for micelle self-assembly and practical
applications of self-assembled nanostructures will be discussed.

*This work was supported by the National Science Foundation under Grant No.DMR-1410928

10:00AM K55.00009: Simulation of Free Surface of Block Copolymers*
DANIIL BOCHKOV (Presenter), Mechanical Engineering, University of California, Santa Barbara, GADDIEL OUAKNIN, Chemical Engineering, Stanford University, FREDERIC GIBOU, Mechanical Engineering, University of California, Santa Barbara — Due to their self-assembling properties, block
copolymers are used in a variety of engineering applications, from patterning of microchips to targeted drug delivery. The
study of these materials has been significantly accelerated by the powerful self-consistent field theory (SCFT), which has
been particularly effective at studying polymer self-assembly in bulk or in confinements with a-priori known geometry. However,
in many situations the surface of polymer material is free to deform (e.g., polymer/air interface) and its shape must be
determined simultaneously while solving the SCFT equations. In this talk, we present a computational framework for simulating free surfaces block copolymers based on an analytical shape sensitivity analysis. Specifically, we consider an
incompressible polymer melt described by the SCFT equations and derive an analogue of the Young-Laplace equation for
block copolymers. Selective interactions of surrounding materials with distinct polymer chain blocks are taken into
account by a new approach for imposing boundary conditions, consistent with the incompressibility property. To
demonstrate the capabilities of this methodology, we present examples of suspended and substrate-supported diblock
copolymer droplets.

*ARO W911NF-16-1-0136 and NSF DMS 1620471

10:12AM K55.00010: Systematic and Many-Chain-Simulation-Free Coarse Graining of Polymer Melts: Structure-
Based Coarse Graining of the Kremer-Grest Model
YAN WANG (Presenter), QIANG WANG, Colorado State Univ — Our
group recently proposed the systematic and simulation-free strategy for coarse graining of polymeric systems, where the
well-developed polymer reference interaction site model (PRISM) theory, instead of the many-chain molecular simulation
(MCMS), is used to obtain the structural and thermodynamic properties of both the original and coarse-grained (CG)
systems. Our strategy is much faster than those using MCMS, thus effectively solving the transferability problem of coarse
graining. It also avoids the problems caused by the finite-size effects and statistical uncertainties of MCMS, particularly for
the original system, which are the reasons why its coarse graining is needed. Here we apply our strategy to the structure-
based coarse graining of the well-known Kremer-Grest model for homopolymer melts, where the self-consistent PRISM
theory is used to avoid the assumption of ideal-chain conformations in the original system. This paves the way to
quantitatively applying our strategy to more realistic polymers and their multiscale modeling.

10:24AM K55.00011: Extensional Rheology of Neat and Contaminated Ring Polymer Melts*
THOMAS O’CONNOR (Presenter), Sandia National Laboratories, TING GE, MICHAEL RUBINSTEIN, Duke University, GARY GREST, Sandia National
Laboratories — Molecular simulations are applied to study unconcatenated ring polymer melts in uniaxial extensional flow.
Melts of neat rings and neat linear chains with the same length, and rings contaminated with a small fraction of linear
chains are elongated to steady-state for a wide range of Rouse Weissenberg numbers. The rate dependence of the steady-
state stress and viscosity are compared for the three systems and correlated with changes in microscopic chain
conformations. Extensional flows stretch and orient both ring and linear chain conformations along the extension axis.
However, linear chains can stretch to twice the length of a ring with the same molecular weight. The significantly stronger
response of linear chains to extensional flow suggests a small fraction of linear chain contamination might dominate the
extensional viscosity of a nominally neat ring melt. Simulations of ring melts contaminated with varying fractions of linear
chains are used to predict the experimental signature of linear contamination.

*Funding provided by the U.S. Department of Energy through the Harry S. Truman Fellowship at Sandia National
Laboratories.
10:36AM K55.00012: Stress Relaxation in Highly Oriented Melts of Entangled Polymers*  
AUSTIN HOPKINS (Presenter), Physics and Astronomy, Johns Hopkins University, THOMAS O'CONNOR, Sandia National Laboratories, MARK OWEN ROBBINS, Physics and Astronomy, Johns Hopkins University — Molecular dynamics simulations are used to study stress and conformational relaxation in entangled polymer melts deformed far from equilibrium by uniaxial extensional flow. Melts are elongated to a Hencky strain of 6 at Rouse Weissenberg numbers from 0.16-25, producing states with highly aligned chains. Then flow is ceased and the system is allowed to relax until twice the equilibrium disentanglement time. The relaxation of the stress is correlated with changes in the conformation of chains and the geometry of the tube confining them. The primitive path length of chains relaxes towards its equilibrium value on the equilibrium Rouse time and the orientation of the primitive path then relaxes on the equilibrium disentanglement time. Both results are counter to predictions of several recent models that suggest a large reduction in the entanglement density that persists for the disentanglement time, raising fundamental questions about the nature of entanglement in aligned molten polymers.

*Funding through the Harry S. Truman Fellowship at Sandia National Labs, U.S. Army Research Laboratory through Grant No. W911NF-12-2-0022, and NSF DMREF No. 90079795.

10:48AM K55.00013: Plasticizing polymers with small-molecule additives: a not so simple picture revealed by a simple molecular model  
KUSHAL PANCHAL, OLUSEYE ADEYEMI, Department of Chemical Engineering, McMaster University, ROOZBEH MAFI, Canadian General-Tower Ltd., LI XI (Presenter), Department of Chemical Engineering, McMaster University — Processing and manufacturing of many polymer products require the addition of plasticizers for tuning the flow properties of the melt as well as the thermo-mechanical properties of the product (lower Tg and improved material flexibility and ductility). These effects are often collectively described as plasticizers reducing the inter-chain friction and "softening" the material. However, a detailed molecular mechanism has not been fully revealed. We use molecular simulation to show that these effects are often not monotonically correlated. Most notably, additives that are better at reducing Tg may not be as effective at reducing the material stiffness. Indeed, our simulation shows that by simply changing the size of plasticizers, the Tg and Young's modulus vary in opposite directions. In-depth analysis of the free volume distribution and molecular mobility indicates that plasticizers have different effects on the dynamics at different length and time scales. Ongoing research focuses on the plasticizer effects on polymer viscoelasticity. Findings of this study reveal the rich complexity of the plasticization phenomena. In particular, the notion of "plasticization" is indeed a collection of a wide range of physical phenomena that are only loosely correlated at best.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K56 GSNP: Jamming and Glassy Behavior  
BCEC 255 - Andrea Liu, University of Pennsylvania

8:00AM K56.00001: Isostatic jamming of two-dimensional monodisperse system under quenched disorder*  
WEN ZHANG (Presenter), SHIYUN ZHANG, NING XU, Department of Physics, University of Science and Technology of China — The existence of amorphous packings in two-dimensional monodisperse system is a classical unsolved problem. By minimizing the enthalpy of packings of frictionless particles, we obtain isostatic jammed packings under quenched disorder at desired pressures. Quenched disorder is introduced by pinning a fraction of particles $N_f=nfN$. The result shows that there is a unique critical pinning density, $n_{fc}$, at which packings become completely disorder. The static correlation length $\xi_6$ diverges at the same $n_{fc}$ for different pressure $p$, which suggests new ways to investigate the jamming transition in two-dimensional monodisperse system. Finally, we confirm the existence of isostatic jammed packings with packing fraction $\Phi_{jw}=0.845$, and jamming scaling is still satisfied in two-dimensional monodisperse system.

*This work is supported by National Natural Science Foundation of China Grants No.11702289, No.11734014, and No.11574278, and the Anhui Provincial Natural Science Foundation Grant No.1708085QJA07. We thank the Supercomputing Center of University of Science and Technology of China for the computer time.
We numerically study the equilibrium dynamics of a 3D binary hard-sphere (HARD) system and a 3D Kob-Andersen Lennard-Jones (KALJ) system. We provide a quantitative description of dynamical heterogeneity in terms of fluctuations in the local relaxation rates. We extract a recently defined two-point correlator, \( s(q, t) \), that probes those fluctuations. The time decay of \( \chi_{\phi}^2(t) = \lim_{q \to 0} s(q, t) \) is characterized by a certain time scale \( \tau_{ex} \), which we identify as the exchange time of the slow and fast regions, or equivalently the lifetime of the heterogeneities. We calculate the exchange time \( \tau_{ex} \) as a function of either the temperature (for KALJ) or packing fraction (for HARD). We find that, in HARD systems, close to the glass transition, \( \tau_{ex} \) becomes an order of magnitude longer than the \( \alpha \)-relaxation time \( \tau_\alpha \) and \( \tau_{ex}/\tau_\alpha \) increases with packing fractions. However, in KALJ systems, \( \tau_{ex} \) is approximately twice \( \tau_\alpha \) and \( \tau_{ex}/\tau_\alpha \) has no significant dependency on temperature. We also measure the two-point correlation length \( \xi_{\phi}^2(t) \) of the relaxation rates. We find that near the glass transition \( \xi_{\phi}^2(t) \) grows approximately logarithmically with time up to a maximum at time around \( 2\tau_\alpha \), and it decays at long times.
A marginal system is one for which there exists an infinitesimal deformation that will lead to instability. Frictionless sphere packings at jamming, as well as infinite packings above jamming, seem to meet this definition. Further, the scaling of the excess contact number with pressure is consistent with the mean-field expectation of marginal stability. However, the prefactor in three-dimensional systems is slightly larger than predicted. This discrepancy in the prefactor, termed the "marginality gap", is expected to vanish in the mean-field limit. We investigate numerically the Mari-Kurchan model of jammed packings, in which a Gaussian random shift is added to each separation of pairs of particles in the pair potential. By tuning the amplitude of the random shift, we study the range from jammed packings to the mean-field limit to see how the marginality gap evolves.

Jamming as a Multicritical Point*

The discontinuous jump in the bulk modulus B at the jamming transition is a consequence of the formation of a critical contact network of spheres that resists compression. We introduce lattice models with underlying under-coordinated compression-resistant spring lattices to which next-nearest-neighbor springs can be added. In these models, the jamming transition emerges as a kind of multicritical point terminating a line of rigidity-percolation transitions. Tuning the under-coordinated lattice to the jamming critical point yields a faithful description of jamming and its relation to rigidity percolation.

Can a large jammed packing be assembled from smaller ones?

The principle of equivalence of ensembles asserts that, in the thermodynamic limit, a system with periodic boundary conditions behaves identically to a subsystem of the same size, cut out from a larger system. We compare these two ensembles on finite length scales in the case of amorphous jammed packings of soft spheres at zero temperature. Focusing on the statistics of the contact fluctuations, we find that systems with periodic boundary conditions have significantly smaller fluctuations compared to the subsystems. This difference is largest near the jamming transition. Moreover, these two ensembles converge only at a surprisingly large system size. The crossover to the thermodynamic limit defines a length scale for each ensemble. Surprisingly, these diverge, as a function of the distance to the transition, with two different exponents. We argue that this disparity is the result of the system being above the upper critical dimension and that, based on the values of the exponents, the upper critical dimension can be measured.

Response to controlled perturbations in frictional granular jamming

Jamming in frictional granular media results in metastable configurations due to stability imparted by frictional contacts against sliding. We experimentally study the frictional energy difference $\Delta E$ between an unperturbed and a perturbed configuration subject to uni-axial compression under identical conditions in a two-dimensional system comprised of a bidispersed set of disks whose friction we tune through contact roughness $d$. The homogeneous system-wide acoustic perturbations are independently tuned with amplitude $A$ and frequency $f$. We find the frictional stress $\sigma$ released from perturbation follows a stretched exponential form $\sigma = \sigma_0 \exp\left[\frac{\Delta E}{T_{\text{eff}}}\right]^{\beta}$, where $\sigma_0$ is the unperturbed stress, $T_{\text{eff}} = \frac{1}{2}M (A_{\text{RMS}} f_{\text{RMS}})^2$, $M$ is total mass of disks in the configuration, and $A_{\text{RMS}}$ and $f_{\text{RMS}}$ are the respective RMS perturbation amplitude and frequency; the stretched exponent $\beta$ is the only fit parameter. At low $T_{\text{eff}}$, we obtain a best fit around $\beta \sim 1/3$. As $T_{\text{eff}}$ increases and more frictional stress is relieved, the stretched exponent $\beta$ transitions smoothly and approaches an asymptotic value of $\beta \approx 1$ with an Activated or Arrhenius-like relaxation behavior. Eventually when $A_{\text{RMS}} \geq d$, all frictional stresses in the system are relieved and frictionless jamming behavior is recovered.

*This work was supported in part by NSF MRSEC/DMR-1720530 (TCL and OS), NSF DMR-1719490 (DBL), and NSF DMR-1609051 (XM).
9:48AM K56.00010: Aging is a (log-)Poisson Process, not a Renewal Process¹

STEFAN BOETTCHER (Presenter), DOMINIC M ROBE, Physics, Emory University, PAOLO SIBANI, Institut for Fysik Kemi og Farmaci, Syddansk Universitet — Aging is a ubiquitous relaxation dynamic in disordered materials. It ensues after a rapid quench from an equilibrium `fluid" state into a non-equilibrium, history-dependent jammed state. We propose a physically motivated description that contrasts sharply with the trap model² or a continuous-time random walk (CTRW) with broadly distributed trapping times commonly used to fit aging data.³ A renewal process like CTRW proves irreconcilable with the log-Poisson statistic exhibited, for example, by jammed colloids as well as by disordered magnets. A log-Poisson process is characteristic of the intermittent and decelerating dynamics of jammed matter usually activated by record-breaking fluctuations (`quakes'). We show that such a record dynamics (RD) provides a universal model for aging, physically grounded in generic features of free-energy landscapes of disordered systems.⁴


10:00AM K56.00011: Direct Measurement of Force Configuration Entropy in Jamming* JAMES SARTOR (Presenter), ERIC CORWIN, University of Oregon — Thermodynamics connects the microscopic details of a system's entropy to bulk measurements of the system's properties. In granular systems, for which the thermal energy scale is so small as to be irrelevant, this has been proposed using temperature analogues such as compactivity and angoricity. We present a method of linking the measurements of such quantities to the entropy of the force network by measuring the multiplicity directly. For systems at the critical jamming point there is only one mechanically equilibrium force network compatible with the spring network representation of the system, so the force configurational entropy of a jammed system is zero. For each new contact formed, the dimensionality of the space of allowed force configurations increases by one. Within this space lies a subspace of positive-definite forces, which is compatible with a granular packing. We propose that the volume of this subspace is proportional to the multiplicity of the packing's force network configuration. To determine the constant of proportionality, we measure the angoricity over 6 decades of pressure using the method of overlapping histograms.

*This work was supported by the NSF under Career Grant No. DMR-1255370 and a grant from the Simons Foundation No. 454939.

10:12AM K56.00012: Void Percolation Threshold and Critical Properties of the Random Lorentz Gas* PATRICK CHARBONNEAU, Duke University, ERIC CORWIN, Physics, University of Oregon, YI HU (Presenter), Chemistry, Duke University — Percolation and glass formation share interesting dynamical features, in which they both exhibit caging of tracers/particles. Although first noticed long ago, this analogy has grown in physical relevance since a simplified model of structural glasses (Mari-Kurchan) was found to display corrections to caging that are analogous to those observed in percolating systems. Interestingly, our recent study has shown that the glass-like caging transition is absent in lattice percolation for all dimensions. In order to better understand the origin of caging, we consider transport in an off-lattice percolation model. Specifically, we study the caging and critical scaling of transport in the random Lorentz gas, which can be mapped onto the Mari-Kurchan model and to void percolation. We first develop numerical strategies to determine precisely the void percolation threshold in high dimensions, and then study dynamical criticality around that threshold. Our results provide key insights into the dynamics of glass formers and transport in heterogenous media, more generally.

*This research is supported by a grant from the Simons Foundation (#454937, Patrick Charbonneau). This research is also supported in part by the National Science Foundation under Grant No. NSF PHY17-48958.

10:24AM K56.00013: Fluctuation Distributions of Energy Minima in Complex Landscapes* HORST-HOLGER BOLTZ (Presenter), University of Chicago, ANDREA LIU, Physics, University of Pennsylvania, JORGE KURCHAN, LPS, ENS Paris — We discuss the properties of the distributions of energies of minima obtained by gradient descent in complex energy landscapes. Specifically, we study the distribution of energies in minima of the spherical p-spin model and the distribution of jamming threshold packing fractions in jammed particle configurations as archetypal manifestations of disorder-induced complexity. We numerically find universal distributions that resemble the Tracy-Widom distributions often found in problems of random correlated variables, and non-trivial finite-size scaling. Deeper insight into this problem is achieved by realizing the importance of a first-passage process in the eigenvalues of the Hessian to the termination of the steepest descent process, which also manifests the link to problems where the Tracy-Widom distribution is established. This first-passage view of steepest descent dynamics is generic and therefore we expect similar phenomenology in many problems.

*This work is supported within the Simons Collaboration on "Cracking the Glass Problem"
Shear response of jammed disk and sphere packings*  

KYLE VANDERWERF (Presenter), Yale Univ, MARK SHATTUCK, Department of Mechanical Engineering & Materials Science, City College New York, COREY SHANE O’HERN, Yale Univ — The response of purely repulsive disk and sphere packings to athermal, quasistatic simple shear near jamming onset is highly nonlinear. Previous studies have shown that the ensemble-averaged static shear modulus $G$ is nearly constant at small pressure $p$, and at a characteristic pressure $p^*$, $G$ begins to increase as a power-law: $G \sim p^a$, where $a=0.5$. Also, $p^*$ decreases with increasing system size $N$, such that $p^* \sim N^{-\beta}$, where $\beta=1$. Although scaling arguments have rationalized the scaling behavior of $p^*$ and $G$, there is currently no quantitative theoretical framework that can predict the values of $a$ and $\beta$. Here, we carry out numerical simulations of 2D bidisperse disk packings near jamming onset undergoing athermal, quasistatic simple shear at fixed pressure to explain these exponents. We show that $a$ and $\beta$ can be understood by examining the “geometrical families” of jammed packings, which are intervals of shear or pressure where the packings maintain the same network of interparticle contacts without rearrangements. We present a statistical model based on random switching of the packings from one geometrical family to another to predict the values of the exponents $a$ and $\beta$.

*We acknowledge financial support from NSF Grants No. CMMI-1463455 (M.S.) and No. CBET-1605178 (C.O. and K.V.).

Densest vs. jammed packings of 2D bent-core trimers*  

AUSTIN GRIFFITH (Presenter), ROBERT HOY, University of South Florida — We identify the maximally dense lattice packings of tangent-disk trimers with fixed bond angles ($\theta = \theta_0$) and contrast them to both their nonmaximally-dense-but-strictly-jammed lattice packings as well as the disordered jammed states they form for a range of compression protocols. While only $\theta_0 = 0, 60^\circ$, and $120^\circ$ trimers can form the triangular lattice, maximally-dense maximally-symmetric packings for all $\theta_0$ fall into just two categories distinguished by their bond topologies: half-elongated-triangular for $0 < \theta_0 < 60^\circ$ and elongated-snub-square for $60^\circ < \theta_0 < 120^\circ$. The presence of degenerate, lower-symmetry versions of these densest packings combined with several incommensurable families of less-dense-but-strictly-jammed lattice packings act in concert to promote jamming. Systems jam via a two-stage, two-length-scale process. First, randomly-oriented crystalline grains form and grow to a size that increases with decreasing compression rate and depends strongly on $\theta_0$. Since these grains cannot be compressed further, they effectively behave as single nearly-rigid particles as compression continues. Jamming occurs when they can no longer rotate/translate away from one another upon colliding.

*Support from NSF Award No. DMR-1555242 is gratefully acknowledged.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K57 GSNP DPOLY GSOFT: The Extreme Mechanics of Balloons

8:00AM K57.00001: The Extreme Mechanics of Balloons: From Interfacial Films to Inflated Membranes and Back*

[Invited] JOSEPH D PAULSEN (Presenter), Syracuse University — Deformable sheets are ubiquitous in nature and industry across a vast range of scales, from graphene to metal foil to the earth's crust. Thin sheets are also central to advanced applications including flexible electronics and deployable satellites or emergency shelters. Despite their ubiquity, there are still significant fundamental challenges in predicting how a thin elastic sheet will deform under confinement, from the selection of a macroscopic deformed shape all the way down to the fine details of the microstructural features. I will discuss a suite of experiments using interfacial films and inflated membranes to address problems spanning this entire range. First, I will describe how an ultrathin polymer film wrapped around a liquid droplet adopts highly nonsymmetric shapes as the droplet size is decreased, and how this overall shape selection may be understood using a simple model wherein the exposed liquid surface area is minimized [1]. This geometric model reveals a fundamental connection between interfacial films and mylar balloons. Inspired by this connection, we are conducting experiments using inflated membranes to discover how smooth sinusoidal wrinkles transition into sharp “crumples”, a striking behavior that was originally observed on interfacial polymer films in a spherical geometry [2]. We have now isolated these buckled structures on interfacial films in hyperbolic and cylindrical geometries, suggesting that such crumples are a generic building block for confined sheets.


*Support from NSF-DMR-CAREER-1654102 is gratefully acknowledged.
8:36AM K57.00002: Mechanics of interconnected balloon networks  MATJAZ CEBRON (Presenter), MIHA BROJAN, Faculty of Mechanical Engineering, University of Ljubljana, ANDREJ KOSMRLJ, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544 — We investigate the mechanical stability of an array of interconnected thin balloons made from hyperelastic material that are filled with incompressible fluid. Each individual balloon has a nonmonotonic relation between the volume of enclosed fluid and the pressure difference between the inside and the outside of the balloon. While an individual balloon is unstable in the region with the negative slope on the pressure-volume diagram, such state of a balloon can get stabilized when it is interconnected with other balloons. We will present conditions that have to be satisfied for the mechanical stability for the whole network of balloons. Furthermore, we will discuss the dynamics of unstable configurations, which may exhibit an interesting sequence of liquid redistributions between the connected balloons, such that the volumes of balloons change nonmonotonically, before they settle in a new stable state.

8:48AM K57.00003: Beyond the smectic order: splay and amplitude modulations in wrinkle patterns  OLEH TOVKACH, BENJAMIN DAVIDOVITCH (Presenter), University of Massachusetts Amherst — Thin solid sheets and shells tend to suppress compressive stresses by developing wrinkles -- elongated periodic undulations around a smooth enveloping shape, whose characteristic “wavelength”, \( \lambda \), vanishes with the solid's thickness. While an energetically-favored spacing imparts a local smectic order to the pattern, the geometric constraints underlying the mere presence of wrinkles are often incompatible with a global smectic order – implying localized defects and other meso-scale deviations from an "ideal" array of parallel, elongated wrinkles.

We elucidate this generic phenomenon through numerical simulations of a prototypical model of geometrically incompatible confinement – a thin sheet attached to a ball of harmonic springs. In addition to localized defects of various types, we find that a prominent motif is meso-scale modulations of the wrinkle amplitude in domains characterized by smectic order. This finding motivates a coarse-grained theory that describes the variation of wrinkle patterns at scales much larger than their wavelength. In addition to a smectic-like order parameter, whose existence was pointed out previously, we show that such a theory must include other fields, resembling the Ginzburg-Landau theory of superconductors.

9:00AM K57.00004: Self-similar retraction of a shot rubber-band  ALEXANDROS ORATIS (Presenter), JAMES C BIRD, Boston University — Stretching and shooting rubber bands is a familiar experience for both children and adults, yet the initial dynamics are so quick that they are generally missed. When a cut elastic strip is stretched from its end and suddenly released, the dynamics depend on a balance of stretching and inertia. However when a rubber band is stretched, a region of high-curvature is created and it is unclear how this curvature affects the dynamics. Here, we demonstrate that during the retraction of a circular rubber band, a wavelength develops at the rear which increases in size as time progresses. Through a combination of experiments and modeling, we investigate the speed at which the back of the elastic retracts and observe a self-similar shape that depends on stretching, inertia, and bending. These retraction dynamics illuminate how a rubber band can pass by a thumb when discharged without hitting it.

9:12AM K57.00005: All-in-One Design of Soft Machines  TREVOR JONES (Presenter), JOEL MARTHELOT, PT BRUN, Princeton University — In our world filled with human innovation and technology we hardly scratch the surface of what has been formed in nature. While we have increased our control and capabilities of machines in the thrust for biomimicry, the use of soft structures to accomplish complex tasks is still primarily the handiwork of biology. To bridge the gap on nature, we introduce an all-in-one approach to building soft machines. Using the powerful rules of fluid mechanics and silicone elastomers, fluid-mediated networks can be “frozen” to provide unique functional materials. Here a Bretherton-like technique is explored as an elongated bubble deposits a polymer melt film on the inside of tubes. The residual film undergoes drainage as the polymer melts cures into an elastic solid. We characterize these elastic networks, comprised of pneumatic bending actuators, through experiments and predictive models of their constituent parts. By means of this deep integration between the non-linear actuation and the far from equilibrium shape-morphing we reverse engineer targeted soft machines.
Inflatable origami-inspired structures

DAVID MELANCON (Presenter), School of Engineering and Applied Sciences, Harvard University, CHUCK HOBERMAN, Graduate School of Design, Harvard University, BENJAMIN GORISSEN, CARLOS GARCIA MORA, YUNFANG YANG, School of Engineering and Applied Sciences, Harvard University, JASON KU, ERIK DEMAIN, Computer Science and Artificial Intelligence Laboratory, MIT, KATIA BERTOLDI, School of Engineering and Applied Sciences, Harvard University — Origami has long been used as a source of inspiration to design creative and esthetic constructions, from the iconic paper swan to facades of multi-story buildings. More recently, the rules of folding have been applied to fabricate architected materials with functional properties such as compactness, self-foldability, and multi-stability. These properties highlight the potential of origami to become a new design paradigm for rapidly deployable structures. Whereas multiple origami-inspired deployable surfaces have been reported in the literature, there is a lack of research on enclosed deployable geometries. In this work, we introduce a novel type of inflatable origami-inspired structure comprised of a polyhedron with triangular faces and elastic hinges. From simple geometry principles, this star-shaped structure possesses two compatible configurations – flat-folded and deployed – giving rise to a bi-stable behavior. The insights gained from the study of this simple geometry enable the understanding of the folding principles of a novel class of enclosed origami-inspired structures that can be deployed to different stable configurations through inflation.

Buckling of inflatable pouch seams

JAMES HANNA (Presenter), HEE DOO YANG, ALAN ASBECK, Virginia Tech — Inflating a mylar balloon results in a pattern of wrinkles around its seams, and a shape with similarities to those of stuffed paper folders, tea bags, empanadas, and other objects in which the perimeters of thin sheets are attached to form a closed surface around a maximal volume. Our present interest in this problem stems from working with inflatable pouches for soft robotic actuators, made by layering textiles, plastics, and adhesives. We examine circular pouches with annular seams. Inflation of the pouch effectively provides a contractile planar constraint on the interior of the rim, leading to buckling reminiscent of prior results on swelling gel strips attached to rigid bodies. The buckling wavelength coarsens with the width of the seam, until it saturates at four cycles. We examine the effects of seam width, pouch radius, and sheet thickness on the buckling wavelength, through experiments and scaling arguments.

Stress Focusing in Inflated Membranes: Threshold and Morphology

RAJ DE (Presenter), YOUSRA TIMOUNAY, JESSICA L STELZEL, JOSEPH D PAULSEN, Department of Physics, Syracuse University — Thin elastic films may undergo large-amplitude deformations even under small applied force, which makes their behaviors challenging to predict. A symmetry-breaking transition from smooth periodic wrinkles to sharp stress-focusing crumples was recently observed in experiments where an ultrathin polymer film was placed on a spherical water meniscus whose curvature was continuously increased [1]. However, a general set of conditions for crumple formation has remained elusive. We approach this problem on a different scale using ~10-cm-wide square membranes that we construct from polymer sheets, which we then inflate with air. As the internal pressure is gradually increased, sharp crumple form on the surface of the sheet, which then transition to smooth wrinkles at higher pressure. Remarkably, all our data may be described by a single trend for the transition pressure, which depends linearly on the stretching modulus of the film and is inversely proportional to the size of the bag, where we have varied the sheet thickness, Young’s modulus, and bag size over a wide range. Finally, we use a 3D scanner to study the topography of the membrane as we go through the crumpling transition. [1] King et al. PNAS 109 (2012).

From flat sheet to cone without cutting: the wrinkled cone

DOIREANN O’KIELY (Presenter), JOSEPH BLANC, FINN BOX, DOMINIC VELLA, University of Oxford — It is relatively straightforward to roll a sheet of paper into a cone, but in doing so we must “waste” some paper (either by cutting or overlapping the sheet). Here, we show how to create a cone from a very thin polystyrene sheet without cutting or overlapping – instead, the excess length generated by deforming the initially flat sheet is buffered locally by wrinkling. To realise this, we suspend a thin circular sheet on a soap film so that it is held by a small radial tension at the boundary. The sheet is deformed by indenting at the centre. Through wrinkling, the flat sheet deforms to a cone, and subsequent changes in the angle of the cone are accommodated by self-regulated adjustment of the wrinkles. Experimentally, the soap film used to apply the radial tension is deformed by (and hence opposes) wrinkling in the sheet. We discuss the implications of this for the wrinkle pattern selection.

*ERC Grant Agreement no. 637334
Inflating and programming flat inextensible curvilinear paths

EMMANUEL SIEFERT (Presenter), ETIENNE REYSSAT, JOSE BICO, BENOIT ROMAN, PMMH, CNRS/ESPCI/SorbonneU/U. Diderot — Mylar balloons are popular gifts in funfairs or birthday parties. Their conception is very simple: two pieces of flat thin sheets are cut and then sealed together along their edges. Inflation deforms the envelope as it maximises the volume of the balloon. However, while thin sheets are easy to bend or to compress (by forming wrinkles), they barely stretch, which imposes non-trivial geometrical constraints.

Here, we focus on the shape of inflated rings and, more generally, any sealed curvilinear path. We rationalise the shapes obtained for axisymmetric geometries, and in particular describe the location of wrinkles.

We find that inflation modifies the initial curvilinear flat path. How should we choose the initial cut to obtain a mylar balloon of a desired shape? Using our theoretical predictions, we develop a simple numerical tool to solve the inverse problem of programming any 2D curve upon inflation.

*ANR SMART - PSL prematuration BIO-SPASM

Dragonfly-inspired deployable structures: how to inflate and stay flat?

JOEL MARTHELOT, THOMAS DUPUIS, PIERRE-THOMAS BRUN (Presenter), CBE, Princeton University — Programming the final shape of a soft inflatable structure is a nontrivial challenge. Such a task is routinely accomplished in nature, for example when the wing of an emerging dragonfly deploys over just a couple of minutes. This expansion is guided by a network of veins where hemolymph is injected and subsequently solidifies to generate rigidity.

Inspired by dragonflies, we build a model experiment to investigate inflatable deployable structures composed of a tubular network of the veins. We first mimic differential growth to fabricate wrinkled tubular structures. They comprise a soft annular core surmounted by a stiffer and thinner annulus prepared so as to yield a wrinkling instability. We then study the mechanical response of a single wrinkled tubular structure under pressure. We then characterize the in-plane expansion of the structure and study its correlation to the network geometry and the pressure applied to the system. A systematic variation of the geometric and elastic parameters allows us to search for optimal design and operational conditions for a maximal extension while minimizing the input pressure.

Sub-millimeter air-filled toroidal bubbles featuring easily reversible and rapid shape change.

PAUL RUSSO (Presenter), XUJUN ZHANG, ANDREW GORMAN, PETER YUNKER, SAAD BHAMLA, H. QI, Georgia Institute of Technology — Researchers have experimentally observed and generated liquid-filled vesicles in the toroidal topology, but small, air-filled toroids have not been reported. Here we report a facile method to generate air-filled toroidal bubbles coated by a particularly rugged amphipathic protein membrane made from filamentous fungi. The "air donuts" fall into the sub-millimeter size and are believed to be the world's first air-filled toroidal bubbles in this size scale. The major and minor ring radii ratio of the "air donuts" has a value of $\sqrt{2}$, which is in agreement with the liquid-filled vesicle literature. During the formation of "air donuts" under certain easy-to-meet conditions, the bubbles' shapes transform from cylinders to spheres, and ultimately to toroids. The sphere-to-toroid transition is reversible, which is surprising from the topology point of view. The air-filled toroidal vesicles could provide opportunities in the field of aerosol (flavor and fragrance) delivery applications.

*Supported by the Georgia Tech Center for Research on Active Surfaces and Interfaces, a part of the Science and Technology of Advanced Materials and Interfaces initiative.

Control of adhesion through geometrical enhancements

NICOLAS GAILLARD, Nantes University, MICHAL BUDZIK (Presenter), MARCELO AZEVEDO DIAS, Department of Engineering, Aarhus University — We present an experimental and theoretical investigation of interface geometric effects in peel test configuration to study adhesion between a silicone-based rubber (Vinylpolyisiloxane or VPS) film and a 3D printed ABS polymer. Experiments are carried out in which the VPS film is peeled from the 3D printed material. Two loading cases, peel and shear modes (90 and 0 degree respectively), are investigated in detail. Initially, reference specimens, in which VPS is moulded directly on the ABS surface are tested. With reproducible results no significant effects of the loading rate and a significant effect of the loading direction are observed. Subsequently, VPS is moulded to the 3D printed base which included rectangular groves along the crack growth path. Two failure mechanism are introduced which are found to lead to enhancement of apparent fracture energy: (1) local variations in the bending rigidity of the VPS film, (2) deflection of the crack growth path at the corrugation. Effective mechanism of VPS pillars pull-out is observed. Both mechanisms result in the peak (apparent) fracture energies ca. 10 and 1.4 times higher than the reference specimens for the peel and shear modes respectively. Theoretical and analytical arguments are provided to explain the aforementioned scenario.
Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K58 GSOFT: Disordered and Glassy Systems I  BCEC 257A - Matthew Abernathy, United States Naval Research Laboratory

8:00AM K58.00001: Probing the local environment in colloidal glass  WENHAI ZHENG (Presenter), DAVID J PINE, New York University — We developed a method to probe the local environment in colloidal glass by measuring the rotational diffusion of elliptical tracer particles. Using tracers of various aspect ratios as passive micro-probes, we explored the response of the material to different local strains. Special design of the tracers enhances its optical anisotropy, which enables us to follow the 3-dimensional rotation of nearly spherical probes. We found as the volume fraction of the colloidal suspension approaches the glass transition point, the rotational diffusion of the ellipsoids slows down dramatically and differs significantly spatially, which reflects the heterogeneity of the local environment.

8:12AM K58.00002: Tracer Transport Probes Relaxation and Structure of Attractive and Repulsive Glassy Liquids  RYAN ROBERTS (Presenter), RYAN POLING-SKUTVIK, JEREMY C PALMER, JACINTA CONRAD, Chemical Engineering, University of Houston — Dynamic coupling of small penetrants to slow, cooperative relaxations within crowded cells, supercooled liquids, and polymer matrices has broad consequences for applications ranging from drug delivery to nanocomposite processing. Interactions between the constituents of these and other disordered media alter the cooperative relaxations, but their effect on penetrant dynamics remains incompletely understood. We use molecular dynamics simulations to show that the motions of hard-sphere tracer particles probe differences in local structure and cooperative relaxation processes in attractive and repulsive supercooled liquid matrices with equal bulk packing fractions and long-time diffusivities. Coupling of the tracer dynamics to collective matrix relaxations affects the shape of tracer trajectories, which are string-like within the repulsive matrix and compact in the attractive. These results reveal that the structure of relaxations controls penetrant transport and dispersion in cooperatively relaxing systems. We further explore this connection by calculating the tracer and matrix dynamic susceptibilities, characterizing cooperative rearrangements in the matrices, and simulating tracer diffusion in arrested glasses.

8:24AM K58.00003: Controlling fragility via geometry in hard particle glass-formers*  ERIN TEICH (Presenter), University of Pennsylvania, GREG VAN ANDERS, Queen's University, SHARON GLOTZER, University of Michigan — We demonstrate that fragility, a technologically relevant measure of glass-forming ability, may be tuned via slight changes to particle shape in monodisperse, super-compressed systems of hard particles. We simulate systems of tetrahedrally symmetric particles, interacting solely through volume exclusion via Monte Carlo sampling, and show that these glass-formers become stronger as the particle shape becomes increasingly tetrahedral. Moreover, we connect strength and local structure in these systems. Our results parallel similar findings for network glass-formers such as silica, in which short-range tetrahedral bonding yields glasses of exceptional strength, and we show that similar effects can arise from geometry alone.

*E.G.T acknowledges support from the National Science Foundation Graduate Research Fellowship Grant DGE 1256260 and a Blue Waters Graduate Fellowship.

8:36AM K58.00004: Exploring Glassy Physics using Athermal Simulations  FRANCESCO ARCERI (Presenter), ERIC CORWIN, CorwinLab, Department of Physics, University of Oregon — Thermal hard spheres simulations are widely used for probing the low temperature physics of glass formers. However, they suffer from the limitations of Monte-Carlo simulations, which are necessarily slow and not easily parallelizable. Although hard sphere interactions present infinitely strong repulsion upon contact, in the infinite pressure limit when the jamming transition occurs, mean-field theory predicts an effective potential, which is a logarithmic function of the gap between particles. This effective potential can be seen as a proxy for frequent collisions, acting as a measure of the allowed space each particle can travel before interacting with one of its neighbors. Thus, by studying the properties of this effective potential we can learn about the thermal system in a high pressure regime which is otherwise inaccessible. Using deterministic minimization schemes to find local minima of the free energy landscape, we can reach extremely dense configurations. We explore the features of such configurations, comparing their vibrational properties with their thermal counterparts as well as with mean field predictions. Furthermore, their dynamics have been tested using thermal simulations with the aim of using them as valid configurations of low temperature glasses.
Correlations Between Short- and Long-time Relaxation in Colloidal Supercooled Liquids and Glasses

CHANDAN KUMAR (Presenter), XIAOGUANG MA, Department of Physics, University of Pennsylvania, Philadelphia, PA, United States, PIOTR HABDAS, Department of Physics, Saint Joseph's University, Philadelphia, PA, United States, KEVIN B APTOWICZ, Department of Physics and Engineering, West Chester University, West Chester, PA, United States, ARJUN G YODH, Department of Physics, University of Pennsylvania, Philadelphia, PA, United States — The spatiotemporal dynamics of short- (β) and long-time (α) structural relaxation are measured experimentally as a function of packing fraction, φ, in a series of quasi-two-dimensional binary-sphere colloidal supercooled liquids and glasses. The relaxation times associated with both long-time dynamic heterogeneity and short-time intra-cage motion grow by orders of magnitude with increasing φ, and interestingly, the two relaxation times are strongly correlated and suggest power law behavior. Moreover, microscopic analysis of the spatiotemporal dynamics revealed that the fraction of overlapping clusters of most-mobile particles at the long and short timescale increases with φ. Furthermore, the minimum spatial separation between the closest non-overlapping clusters of most-mobile particles across the two distinct timescales shows an exponential distribution. This allows extraction of φ-dependent characteristic length scale that further connects dynamics on short- and long timescales and increases with packing.

*C.K.M, X.M., and A.G.Y. gratefully acknowledge financial support from the National Science Foundation through DMR16-07378, the MRSEC DMR-1720530 including its Optical Microscopy Shared Experimental Facility, and NASA through NNX13AL27G.

How glass responses to laser excitation

BO LI (Presenter), KAI LOU, Center for Soft and Living Matter, Korea Institute of Basic Science, WALTER KOB, University of Montpellier, Laboratoire Charles Coulomb, STEVE GRANICK, Center for Soft and Living Matter, Korea Institute of Basic Science — Glass is a disordered solid that processes distinct dynamical and elastic properties compared with crystal. Elastically, how heterogeneous a glassy materials can be and to what extent such heterogeneity is determined by structure are long standing puzzles in glass science. In this experiment, we probed the responses of binary colloidal glasses towards the local excitations caused by laser pulses. We observed very similar excitation patterns when the laser was repeated in linear region; directly proving that the dynamical heterogeneity is strongly encoded with structure. In non-linear region, we discovered for the first time a non-monotonic dynamical length scale as a function of φ, resulting from the intriguing interplay between cooperative motion and local structure. Our results highlight the crucial role structure plays in the dynamics and elasticity of glasses.

Direct Observation of the Gardner/Marginal Glass Transition within a Colloidal Glass

ANDREW HAMMOND (Presenter), ERIC CORWIN, University of Oregon — It has recently been shown that in the infinite dimensional limit there exists a second phase transition, called the Gardner transition, within the glassy phase, dividing so-called stable glass and marginal glass. We have developed a technique to experimentally probe this phase of matter using a colloidal glass. We avoid the difficulties inherent in measuring the long time behavior of glasses by instead focusing on the very short time dynamics of the ballistic to caged transition. We track a single tracer particle within a sedimenting mixture and measure the resulting mean squared displacement (MSD). By analyzing the MSD we find two distinct transitions at different packing fractions: 1) the transition into the stable glass phase is marked by the appearance of a plateau whose magnitude shrinks with increasing density and 2) the transition into the marginal glass phase is marked by logarithmic growth towards that plateau. This provides the first experimental evidence for the existence of a marginal glass in 3d.

*I would like to acknowledge funding from the Simons Foundation No. 454939, and from the NSF DMR-1255370.
**Frequency-dependent moduli in a supercooled liquid in the close vicinity of the glass transition by molecular dynamics**

**BAOSHUANG SHANG (Presenter),** Laboratoire Interdisciplinaire de Physique, University of British Columbia, **PENGFEI GUAN,** Beijing Computational Science Research Center, **JEAN-LOUIS BARRAT,** Laboratoire Interdisciplinaire de Physique — Amorphous materials have a rich relaxation spectrum which is usually described in terms of alpha, beta, and possibly more complex relaxation mechanisms. In this work, we investigate the local dynamic modulus spectrum in a model glass just above glass transition temperature by performing a mechanical spectroscopy analysis using molecular dynamics. We find that the spectrum, at the local as well as on the global scale, can be well depicted by Cole-Davidson formula in the frequency range explored with simulations. Surprisingly, the Cole-Davidson stretching exponent does not change with the size of the local region that is probed. The local relaxation time displays a broad distribution, as expected based on dynamic heterogeneity concepts, but the stretching is obtained independently of this distribution. Furthermore, we find that the size dependence of local relaxation time and modulus can be well explained by the elastic shoving model.

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**Memory in Solid-Solid Interfaces**

**SAMUEL DILLAVOU (Presenter),** SHMUEL RUBINSTEIN, Harvard University — The interface between two solid, static bodies - your chair and the floor, your cup and the table, two books in a stack - is in fact continuously evolving. Due to small-scale roughness, ostensibly flat surfaces typically have a real area of contact several orders of magnitude smaller than apparent area. As a result, these contact points experience enormous pressures, and slowly deform in time.

By measuring the evolution of the real area of contact, we demonstrate that these multi-contact interfaces (MCIs) store a memory of the pressures they experienced. Unlike simple relaxation, e.g. a spring and dashpot system, which depends only on its current state, MCIs evolve according to their entire loading history.

Understanding of MCIs is not only useful for knowing how much coffee has been in your cup; the real area of contact also determines the friction between two bodies. As a result, the coefficient of static friction also evolves according to this interfacial memory. These effects suggest that MCIs and frictional systems belong in a universality class of glassy systems characterized by disorder and slow relaxation.

*The Harvard Smith Family Fellowship

**Extending the phase space of jamming from a jamming point to a jamming plane**

**YULIANG JIN (Presenter),** Institute of Theoretical Physics, Chinese Academy of Sciences, **HAJIME YOSHINO,** Osaka University — The concept of jamming has attracted great research interest due to its broad relevance in soft matter such as liquids, glasses, colloids, foams, and granular materials, and its deep connection to the sphere packing problem and phase transitions. Here we show numerically that the phase space of frictionless jammed states can be extended from the well-known jamming point, to a jamming line by using deeply super-cooled liquid states as initial configurations, which can be further extended into a jamming plane by adding shear strains. While all jammed states are isostatic and belong to the same universality class, their various anisotropy and amorphous order can be mapped out on the jammed plane. The jamming point is isotropic, with the minimum amorphous order (or maximum randomness), which, in the thermodynamic limit, sets a sharp lower bound for the jamming density of frictionless packings.

*This work was supported by KAKENHI (No. 25103005 “Fluctuation & Structure” and No. 50335337) from MEXT, Japan, and by the Chinese Academy of Sciences Pioneer Hundred-Talent Program.
10:00AM K58.00011: Large, growing length scale controls the melting mechanism of stable glasses*

LUDOVIC BERTHIER, Laboratoire Charles Coulomb, University of Montpellier, CNRS, PATRICK CHARBONNEAU, Chemistry, Physics, Duke University, ELIJAH FLENNER (Presenter), Chemistry, Colorado State University, CHRISTOPHER J. FULLERTON, Physiology, Anatomy and Genetics, University of Oxford — Exceptionally stable vapor-deposited glass films melt via a constant velocity front initiated at the surface, whereas ordinary liquid cooled glass films melt homogeneously. The melting time for stable glass films increase linearly with film thickness until a crossover thickness \( l_c \), which can be as large as a micrometer. For films thicker than \( l_c \) the melting time is constant, suggesting that a bulk transformation mechanism is then prominent. Here we use the swap Monte Carlo algorithm to prepare stable glass films that we subsequently melt films using molecular dynamics simulations, in order to study the microscopic differences between the two melting mechanisms of glass films. Several of our stable films completely melt via a front initiated at the surface for lower melting temperatures, but melt via a bulk mechanism at higher melting temperatures. For intermediate melting temperature we directly determine \( l_c \), and then we use bulk melting simulations to approximate \( l_c \) to lower melting temperatures. We find that \( l_c \) grows with increasing stability and decreasing melting temperature. Using parameters corresponding to toluene, we determine that the crossover length for our most stable glass is comparable to that measured in experiments.

*NSF DMR-1608086
Simons Foundation

10:12AM K58.00012: Quantifying the Structure of Space-Filling Disordered Cellular Patterns with Hyperuniformity Disorder Length Spectroscopy

ANTHONY CHIECO (Presenter), DOUGLAS DURIAN, University of Pennsylvania — A system is hyperuniform if the spectral density decays like \( \chi(q)\sim q^{-\epsilon} \) with \( \epsilon > 0 \) as \( q \) goes to zero. In real space the area fraction variance for randomly placed measuring \( L \times L \) windows can be written \( \sigma^2(L)\sim <a>^2 h(L)/L^3 \) where \( <a> \) is the average particle area and \( h(L) \) is the hyperuniformity disorder length, which is defined by the distance from the window boundary where number density fluctuations occur [1]. The spectrum of \( h(L) \) versus \( L \) quantifies the degree of structural order; smaller \( h(L) \) indicates more order, and at large \( L \) hyperuniform patterns have constant \( h(L)=h_e \). Here, we compare \( \chi(q) \) and \( h(L) \) spectra for cellular patterns given by Voronoi construction around points that are (1) uncorrelated (Poisson), (2) low discrepancy (Halton), and (3) displaced from a lattice by Gaussian noise (Einstein), as well as (4) the centroids of bubbles in a quasi-2d foam. All four types are hyperuniform and have \( \chi(q)\sim q^{-4} \) for small \( q \). The \( h_e \) values indicate that Poisson, Halton, Einstein, and foams are ranked least to most ordered. The foam has \( h_e=0.082<\alpha>^{1/2} \) and the same value of \( h_e \) is found for the other cellular patterns if analyzed in terms of the Voronoi cell centroids; for comparison, \( h_e=0.084<\alpha>^{1/2} \) is found at jamming for bidisperse disks [1].


10:24AM K58.00013: Competition of Crystallization and Vitrification*

MUHAMMAD HASYIM (Presenter), KRANTHI K MANDADAPU, Chemical and Biomolecular Engineering, University of California - Berkeley — The competition between vitrification and crystallization in glass-forming materials manifests as a non-monotonic behavior in the time-temperature transformation (TTT) diagrams. A coarse-grained model, referred to as the Arrow-Potts model, is constructed to explore the physics behind this competition. Using Monte Carlo simulations, the model is shown to produce two regimes of crystal nucleation and coarsening. At high temperatures, crystallization is dominated by the nucleation of compact and fluctuating crystalline clusters. At low temperatures, crystal coarsening proceeds through hierarchical relaxation pathways within the supercooled liquid, producing fractal ramified crystalline clusters. To explain and unify these two regimes, the Kolmogorov-Avrami theory is used as a framework to combine nucleation theory and a random walk theory for crystal coarsening kinetics, both of which govern the high-T and low-T regimes respectively. Finally, we demonstrate how the universal character of low-T crystallization is characterized by scaling exponents which are crucial to accurately account for the timescales observed in the TTT diagram.

*This work was supported by Department of Energy Contract No. DE-AC0205CH11231, FWP No. CH-PHYS02.
TIANXING MA, ADITHYA SRIDHAR, KYLE BUZNITSKY, MATTHEW SIGNORELLI, JONATHAN SINGER (Presenter), Mechanical and Aerospace Engineering, Rutgers University — Focused laser spike (FLaSk) dewetting has been used as a method for the patterning of soft matter thin films for several decades. Through the use of a focused laser beam, a localized heat source is provided along with an extreme thermal gradient. The material melted by the local heating is simultaneously moved down the thermal gradient and forms highly characteristic trench-ridge morphologies. Through micron-scale dot exposures on a universal heating substrate designed in our lab, coupled with optical microscopy, we have studied the characteristic radii of the dewetted ridge feature for various glassy thin films with different molecular weights and glass transition temperatures as a function of time. This was approached through a combination of experiments, simulations, and analytical models. Not only were we able to identify features of the dewetting that revealed differences between the polymer system, but the FLaSk process could give independent information on surface and bulk behavior. In this way, it has been shown that FLaSk dewetting as a metrology method can be employed for high-throughput analysis of thin film materials in high shear, high temperature testing regimes that would otherwise be difficult to reach.

10:48AM K58.00015: How to extract memories from a relaxing granular material
KIERAN MURPHY (Presenter), JONATHON KRUPPE, HEINRICH M JAEGER, University of Chicago — Recent experiments on crumpled sheets have found they can store multiple memories of past loading, and that one can simply watch the system relax over long timescales to read off its memories [1]. The model used to explain the observed nonmonotonic relaxation approximates the system as a population of exponentially relaxing modes with a specific distribution of timescales, though the physical manifestation of the modes in these systems remains ambiguous.

Here we show a granular packing can also exhibit history-dependent and nonmonotonic stress relaxation. We then expand upon the framework to understand glassy dynamics in disordered systems with the following results and insights. First, the history dependence of the relaxation is found to be tied to the shear stresses supported by the granular packing but not isotropic compressive stresses. Second, we extend the above model to incorporate finite duration loading. Third, with frictional contacts in the granular packing as the relaxing elements, each sliding glacially slowly, we move beyond relaxation experiments to explain features in the data of shape-dependent plasticity [2] as well as volumetric compaction and hysteresis during cyclic loading.


Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K59 GSOFT: Rheology of Active Fluids: From Active Polymers to Living Matter
BCEC

8:00AM K59.00001: Symmetric shear bands and collective swarming of bacterial suspensions* [Invited] XIANG CHENG (Presenter), Chemical Engineering and Materials Science, University of Minnesota — Active fluids are a novel class of non-equilibrium complex fluids with examples across a wide range of biological and physical systems such as flocking animals, swimming microorganisms, vibrated granular rods, and suspensions of synthetic colloidal swimmers. Different from familiar non-equilibrium systems where free energy is injected from boundaries, an active fluid is a dispersion of large numbers of self-propelled units, which convert the ambient/internal free energy and maintain non-equilibrium steady states at microscopic scales. Due to this distinct feature, active fluids exhibit fascinating and unusual flow behaviors unseen in conventional complex fluids. Here, by combining high-speed confocal microscopy, rheological measurements and biochemical engineering, we experimentally investigate the flow behaviors of E. coli suspensions, a premier example of active fluids. In particular, we show the microscopic dynamics of bacterial suspensions associated with the abnormal rheology and the emergence of collective swarming. Using theoretical tools of fluid mechanics and statistical mechanics, we develop a quantitative understanding of these interesting behaviors. Our study shows the general organizing principles of active fluids that can be exploited for designing “smart” fluids with controllable fluid properties. Our results also provide new insights into the fundamental transport processes of microbiological systems.

*DARPA YFW D16AP00120, NSF-CBET 1702352
8:36AM K59.00002: Activity effects on the non-linear mechanical properties of fire ant aggregations  
MICHAEL TENENBAUM (Presenter), ALBERTO FERNANDEZ-NIEVES, School of Physics, Georgia Institute of Technology — Individual fire ants are inherently active as they are a living organism that convert stored chemical energy into motion. However, each individual ant is not equally disposed to motion at any given time. In an active aggregation, most of the constituent ants are active, and vice versa for an inactive aggregation. Here we look at the role activity plays on the non-linear mechanical behavior of the aggregation through large amplitude oscillatory shear measurements. We find that the level of viscous non-linearity can be decreased by increasing the activity or by increasing the volume fraction. The level of elastic nonlinearity is not affected by either activity or volume fraction. Applying too large of an applied strain amplitude removes the effect of activity but preserves the effect of the volume fraction. We also compare this to viscosity measurements where we see that the level of nonlinearity decreases with activity as well.

8:48AM K59.00003: Spontaneous migration of cellular aggregates: from giant keratocytes to running spheroids  
FRANCOISE BROCHARD-WYART (Presenter), Curie Institute — We introduce the broad field of entangled active matter. Unlike swarms of fish and flocks of birds, cells are bound by transient links and behave as active viscoelastic pastes. Here, we investigate the collective migration of cell on adhesive gels, using 3D cellular aggregates as a model system. Aggregates spread by expanding outwards a cell monolayer, which may partially dewet, causing the aggregate to move. Varying the substrate rigidity induces different modes of aggregate motion: “Giant Keratocytes”, where the lamellipodium is a cell monolayer that expands at the front and retracts at the back; “Penguins”, characterized by bipedal locomotion; and “Running Spheroids”, for non-spreadin aggregates. We characterize these diverse modes of collective migration by quantifying the flows and force field responsible of the bipedal stick-slip motion. We propose two possible mechanisms to explain the spontaneous migration of cellular aggregates: i)chemical modification of the substrate in analogy to reactive droplets. We show that it is possible to mimic a keratocyte with a droplet of oil containing a surfactant. The reactive droplet adopts a croissant shape also seen for keratocyte fragments and ii) symmetry-breaking arising from cell polarization in analogy to active droplets.

9:00AM K59.00004: Activity Driven Bend Instability under an External Field*  
BIBI NAJMA (Presenter), POOJA CHANDRAKAR, S.ALI AGHVAMI, GUILLAUME DUCLOS, Physics, Brandeis University — Active fluids exhibit complex dynamics such as collective motion, internally generated flows, and spontaneous pattern formation on account of their fundamental nonequilibrium nature. Here, we use a 3D active material composed of extensile microtubule bundles and kinesin motor clusters to investigate how the activity driven bend instability is stabilized by an external flow. With no external flow, the internal stresses generated by kinesin motors drive the system far-from equilibrium causing a proliferation of periodic pattern of bend instabilities with a characteristic spatial period \( \lambda \). We observe that the striated pattern of undulations evolves into a turbulent regime with complex flow patterns. Our study reveals that the growth of unstable modes can be controlled by an externally imposed shear flow. We determine the critical value of the flow above which the bend instability is suppressed with the appearance of a uniform steady state where microtubule are aligned by the external flow. Below the critical flow, the growth of the unstable modes is stabilized and the microtubules form a steady undulated pattern that does not evolve into a turbulent regime.

*Brandeis University and Brandeis Bioinspired Soft Materials MRSEC

9:12AM K59.00005: Impact of Motile Bacteria on Viscous Fingering  
JANE CHUI (Presenter), Massachusetts Institute of Technology, HAROLD AURADOU, Université Paris-Saclay, KAREN FAHRNER, HOWARD C BERG, Harvard University, RUBEN JUANES, Massachusetts Institute of Technology — Viscous fingering is a hydrodynamic instability that occurs when a less viscous fluid displaces a more viscous one. Instead of progressing as a uniform front, the less viscous fluid forms fingers to create complex patterns. Understanding how these patterns and their associated gradients evolve over time is of critical importance in characterizing the mixing of two fluids. Here, we investigate the impact of replacing the less viscous fluid with an active suspension of motile bacteria, relevant to applications such as microbial enhanced oil recovery and bioremediation.

In this series of experiments, a suspension of motile \( E. \) coli capable of collective swimming is injected into a microfluidic Hele-Shaw cell under viscous fingering conditions. Using fluorescent microscopy, we observe changes within the mixing zone compared to inactive fluids, such as “rafting,” where some of the bacteria group together and form a patterned interface between the two fluids. Combined with rheological measurements conducted with a Couette rheometer, we quantify the impact these active suspensions have on the formation of viscous fingering patterns and mixing efficiency between the two fluids, and conversely, report details of the collective swimming behavior in the presence of a viscous-gradient front.
9:24AM K59.00006: Looking into the rheology active microtubule suspensions* [Invited] DANIEL BLAIR (Presenter), DAVID A GAGNON, CLAUDIA DESSI, Physics and Institute for Soft Matter, Georgetown University, ZVONIMIR DOGIC, Physics, University of California Santa Barbara — Active suspensions are inherently out-of-equilibrium and can possess anomalous bulk rheological properties. Previous experimental and numerical studies suggest organisms with extensile swimming behavior (e.g. Escherichia coli) can decrease the apparent viscosity of a fluid, while those with contractile swimming behavior (e.g. Chlamydomonas reinhardtii) can increase the apparent viscosity of a fluid. In this talk we will present combined experimental results on the rheology and dynamics of an active suspension of microtubules and kinesin motors driven by ATP. We use a custom-built confocal rheometer to provide simultaneous macroscale rheological measurements and fluorescent imaging of local microtubule dynamics. We find increasing ATP concentration, and therefore increasing activity, yields a significant decrease in the apparent viscosity of the suspension. Simultaneously, using velocimetry techniques, we find significant increases in local velocity fluctuations and deformation rates, suggesting underlying microscale mechanisms for the observed macroscale rheology. We will present a simple model that captures the connection between the local mechanics and the global viscoelasticity.

*Templeton Foundation Grant #57392

10:00AM K59.00007: Interrogation and manipulation of active nematic films using colloidal probes DAVID RIVAS (Presenter), Johns Hopkins University, ROBERT HENRY, University of Maryland, DANIEL H REICH, Johns Hopkins University, TYLER SHENDRUK, University of Oxford, ROBERT LEHENY, Johns Hopkins University — We report studies of the interactions between active nematic films and disk-shaped colloids. The active nematics are driven by molecular motors that cause the constituent microtubular bundles to slide past each other, generating extensional flows that continuously create pairs of +1/2 and -1/2 defects. Rotating magnetic microdisks in proximity to the films produce hydrodynamic flows that compete with the films' intrinsic flow, leading to significant effects on the director field and defect landscape. Near the disks, the self-propelled +1/2 defects take on a preferred direction that is tangential to the direction of imposed stress, creating orientational ordering of the defect motion. At sufficient rotation rates, a more significant alteration of the director field is observed wherein a vortex-like structure within the director field with topological charge of +1 forms. Additionally, we are able to use the disks as effective microrheological probes to gain insight into the physical properties of the film. For example, by analyzing the velocity profile in the film produced by the spinning disk, we obtain an estimate of the film's viscosity.

10:12AM K59.00008: Shearing Living Liquid Crystals* HEND BAZA (Presenter), Department of Physics and Advanced Materials Liquid Crystal Institute, Kent State University, TARAS TURIV, Advanced Materials Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, O D LAVRENOVICH, ANTAL ISTVAN JAKLI, Department of Physics and Advanced Materials Liquid Crystal Institute, Kent State University — Flagellated bacteria of pusher type, such as B. subtilis and E. coli, change the rheological properties of the surrounding isotropic medium. B. subtilis dispersed in a water-based lyotropic chromonic liquid crystals (LCLCs), form a "living liquid crystal" (LLC). Here, we explore the response of the LLC to shear, in particular, how the effective viscosity of LLC changes with the shear rate and how the flow-aligning effect of shear and liquid crystal-mediated elasticity compete with the activity of bacteria that destabilize the orientational order. Studies with an optical rheometer and polarizing optical microscope demonstrate that upon cessation of shear, the activity of bacteria leads to a progressive development of periodic director undulations (with the wave vector parallel to the shear direction), nucleation and multiplication of disclination pairs that produce the regime of topological turbulence. When the gap height increases, disclinations transform from short segments connecting opposite plates to elongated segments in the plane of the cell. The studies reveal a wealth of intriguing phenomena when the system transforms from 2D to 3D-like confinement.

* The work is supported by NSF DMREF grant DMS-1729509.
On the relationship between velocities, tractions, and intercellular stresses in the migrating epithelial monolayer

YOAV GREEN, JEFFREY FREDBERG (Presenter), JAMES P. BUTLER, Harvard T. H. Chan School of Public Health — Cells migrate collectively in physiological phenomena including cancer metastasis, development, and asthmatic airway remodeling. Within an epithelial monolayer, for example, each constituent cell exerts intercellular stresses on neighboring cells, and exerts traction forces on its substrate. While traction forces exerted by a monolayer have been measured for more than a decade, their relationship to measured cellular velocities remains unknown. Additionally, the relationship between intercellular stresses and tractions also remains unresolved. In passive systems, traction stresses and velocities are linked in principle through a constitutive law. The simplest and commonly assumed form of such a law is a Newtonian fluid, which implies a linear relationship between stress and strain rate. In this talk, I will address the question: To what extent are tractions related to velocities through such a linear constitutive law? Using a newly derived theoretical model, I will show that the tractions predicted from the measured velocity field are uncorrelated with the measured tractions. This implies that current methods for intercellular stress recovery need to be corrected where one such rectification is the inclusion of an active stress term, for which we derive a novel constraint.

Rheological response and direct visualization of collective patterns formation leading to shear-bands formation in a suspension of active E.coli at the super-fluidity transition*

ERIC CLEMENT (Presenter), PMMH, ESPCI, VINCENT M MARTINEZ, JOCHEN ARLT, ICMCS, University of Edinburgh, CARINE DOUARCHE, ADAMA CREPPY, HAROLD AURADOU, FAST, University of Paris-Sud, ANGELA DAWSON, JANA SCHWARZ-LINEK, WILSON POON, ICMCS, University of Edinburgh — Suspensions of motile Escherichia coli were found to display a "negative viscosity increment" at low shear rate viz., adding such bacteria lowers the shear viscosity of the system (H.M.Lopez, J. Gachelin, C. Douarche, H.Auradou, E. Clément, Phys. Rev. Lett. 115, 028301 (2015)). Furthermore at higher concentrations a regime of zero viscosity, akin to a "superfluidity" transition, can be reached. Here, for a strain of very active bacteria, we report a full exploration of the rheological response changing confinement, shear rate and concentration, both in a low-shear Couette rheometer and in a cone-plane rheometer. The last allows a direct visualization of the collective organization under shear and the exploration of the different regimes leading the "superfluidity transition" in relation with the dynamics of shear-band formation.

*This work was supported by the ANR grant "BacFlow" ANR-15-CE30-0013, PRC 1576 (CNRS-Roy.Society) and ESMI project E150200679.

The active force spectrum of a microswimmer - modeling and experiments*

WYLIE AHMED (Presenter), California State University, Fullerton — Chlamydomonas reinhardtii are a widely-studied microswimmer that propel themselves by converting chemical energy to mechanical motion of their flagellum in a breast stroke motion. Fluid dynamics approaches have revealed much about the importance of hydrodynamics at the micron-scale and its role in microswimmer transport. However, the stochastic dynamics which are dominated by active non-thermal fluctuations are not well understood. We use optical tweezers and the photon momentum method to directly measure the stochastic forces generated by a trapped Chlamydomonas microswimmer. We model the microswimmer using the generalized Langevin equation approach with active stochastic forcing. Our combined experimental and theoretical approach, based on microrheological techniques, isolates the active force spectrum generated by Chlamydomonas to quantify their nonequilibrium dynamics. We seek to use this framework to test recent developments in stochastic thermodynamics.

*We acknowledge funds from CSUF RSCA grant.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K60 FECS FIP: Topology Matters: Structure-Property Relationships On Different Length Scales 8CEC 258A - Daniel Dessau, University of Colorado, Boulder - Tag(s): Invited
8:00AM K60.00001: Artificial Ferroic Systems: Magnetic Monopoles, Chirality and Bloch Point Singularities [Invited]
LAURA HEYDERMAN (Presenter), ETH Zurich - Paul Scherrer Institute — In artificial ferroic systems [1], novel functionality is engineered through the combination of designed ferroic structures and the control of the interactions between the different components. We probe their behaviour with large-scale facility methods including synchrotron x-rays and low energy muon spectroscopy, which give unparalleled information on microscopic magnetic phenomena. In hybrid mesoscopic structures incorporating two different ferromagnetic layers, the static and dynamic behaviour result from the mutual imprint of the magnetic domain configurations. Here, vortex core reversal can be induced by displacing the core across a domain boundary with a magnetic field. This reversal occurs via the creation of a pair of Bloch point singularities [2].

In artificial spin ice, consisting of arrays of dipolar-coupled nanomagnets arranged in frustrated geometries, a number of interesting emergent phenomena occur. For example, we have observed the creation and separation of emergent magnetic monopoles in an applied magnetic field [3]. In thermally-active systems with superparamagnetic elements, there is a geometry-dependent evolution of magnetic configurations into the lowest-energy states [4], and this dynamic process can be chiral [5]. We have also demonstrated that these magnetic metamaterials can support thermodynamic phase transitions [6, 7]. Finally, we have developed synchrotron x-ray methods to obtain chemical, structural and magnetic information in 3D, and have directly observed the curling magnetic structure surrounding Bloch points [8].


8:36AM K60.00002: Topological soft matter: from metamaterials to polymers [Invited] JAYSON PAULOSE (Presenter),
Physics, University of Oregon —
The classification of physical systems using topology has ushered in a new paradigm for condensed matter physics. Although topologically nontrivial states, with their accompanied features of exotic edge behaviour and robustness to disorder, were first predicted and observed in electronic systems, they have since been realized in a variety of classical systems. Soft matter provides a particularly rich playground for topological physics across diverse length scales. At the macroscopic scale, topology can be used to control tangible features such as vibrational response and mechanical rigidity, bringing elegant mathematical concepts literally to our fingertips. At microscopic scales, the messiness inherent to thermally fluctuating matter provides challenges as well as opportunities for realizing topologically nontrivial behaviour. Across these varied scales, topology holds promise as a tool to create artificial materials with desirable features that are robust to disorder and imperfections. I will demonstrate the breadth and richness of topological soft matter by describing two examples from either end of the spectrum. At the macroscale, I'll survey a class of mechanical metamaterials in which rigidity can be controlled both locally and globally using topology. At the microscale, I'll how strong interactions and thermal fluctuations can be harnessed to generate robust equilibrium patterns in a system of fluctuating lines, with potential applications in polymer patterning and manipulation of magnetic fields in superconductors.
9:12AM K60.00003: Geometrical Frustration Beyond Magnets* [invited] JOSEPH PADDISON (Presenter), University of Cambridge, ZHILING DUN, MARCUS DAUM, School of Physics, Georgia Tech, ANDREW CAIRNS, PETER THYGESEN, Department of Chemistry, University of Oxford, MATTHEW J CLIFFE, University of Cambridge, MATTHEW G. TUCKER, YAOHUA LIU, Oak Ridge National Laboratory, HELEN PLAYFORD, DAVID KEEN, ISIS Neutron and Muon Source, KARENA CHAPMAN, KEVIN BEYER, Argonne National Laboratory, ARKADIY SIMONOV, MICHAEL HAYWARD, RONGHUAN ZHANG, AMBER THOMPSON, Department of Chemistry, University of Oxford, DOMINIK DAISENBERGER, Diamond Light Source, FX COUDERT, Institut de Recherche de Chimie Paris, CNRS / Chimie ParisTech, HAIDONG ZHOU, University of Tennessee, MARTIN MOURIGAL, School of Physics, Georgia Tech, ANDREW GOODWIN, Department of Chemistry, University of Oxford — Geometrical frustration – the inability of a system to satisfy all of its interactions simultaneously because of geometrical constraints – can suppress conventional ordering and promote the formation of exotic states that are disordered, yet strongly correlated. Materials in which magnetic spins occupy lattices built from corner or edge-sharing triangles have provided many examples of novel magnetic behavior due to frustration. In this talk, I will discuss how frustration of structural (nonmagnetic) degrees of freedom – charge states, orbital orientations, or chain displacements – can determine the structures and properties of materials. I will also discuss how the nonmagnetic frustrated interactions can be mapped to equivalent “toy” spin Hamiltonians, including those that are challenging to realize experimentally in magnets. I illustrate these points using three real examples of nonmagnetic frustration. First, I discuss how the solid phases of silver(I) and/or gold(I) cyanides, in which polymeric chains occupy a triangular lattice, can host structural analogs of the spin vortices of triangular $XY$ magnets [1]. Second, I discuss the pyrochlore oxide $Y_2Mo_2O_7$, and explain how orbital dimerization of Jahn-Teller active $Mo^{4+}$ ions on the frustrated pyrochlore lattice may yield an orbital-ice analog of spin-ice and water-ice states [2]. Finally, I discuss the triangular-lattice-based system $YbMgGaO_4$ [3,4] – of interest because of proposed quantum-spin-liquid-like behaviour of its magnetic $Yb^{3+}$ ions – and show how the charge difference between nonmagnetic $Mg^{2+}$ and $Ga^{3+}$ generates a structurally-frustrated state, with implications for the proposed quantum-spin-liquid behaviour.


*Churchill College, Cambridge (JAMP); EPSRC EP/G004528/2 (JAMP, ALG, MJC, ABC).

9:48AM K60.00004: Experimental realization of higher order topological states in classical systems [invited] ALEXANDER KHANIKAEV (Presenter), City College of CUNY — TBD

10:24AM K60.00005: Self-assembled 1D nanostructures on semiconductor surfaces [invited] MARIA LONGOBARDI (Presenter), University of Geneva — Self-assembled one-dimensional (1D) nanostructures have attracted considerable attention in the last decades since their low dimensional architecture offers the possibility to realize atomically precise patterns on semiconducting surfaces. Moreover, the gapped substrate allows the study of the exotic properties of the 1D physics. Bismuth nanolines and their derived Haiku structure are, in this scenario, a unique 1D structures self-assembled on the $Si(001)$ surface. They can grow several micrometers long, almost defect free, in dense arrays or isolated. Their length and tunable density make them suitable for realizing large area functionalized patterns. Although these systems were deeply investigated over the years, their electronic structures have yet not well understood.

Here, an STM/STS study combined with DFT simulation of the electronic properties of the Bi nanolines and derived Haiku structures is presented. High-resolution STM micrographs reveal a rich variety of periodic electronic features as a function of bias voltage. The atomic structures of Bi nanolines and the interplay between Bi and the Si substrate, essential to understanding the electronic and transport properties, are investigated in great details and reproduced in good agreement by the DFT simulations.

Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K61 GSOFT DBIO GSNP: Active Matter V BCEC 258B - Rui Zhang, University of Chicago - Tag(s): Focus
8:00AM K61.00001: Pushers, pullers, splitters: molecular processes governing the dynamics of active emulsions.*

[Invited] CORINNA MAASS (Presenter), KYLE A BALDWIN, BABAK VAJDI HOKMABAD, Max Planck Institute for Dynamics and Self-Organization — Active emulsions are a versatile microswimmer model system. We study a system of spherical oil droplets gradually dissolving in aqueous surfactant solutions, which move autonomously via self-sustaining Marangoni gradients at the oil-water interface. Owing to this interfacial driving, the droplets are direct experimental analogues to hydrodynamic squirmer models, with the interfacial velocity profile depending on the kinetics of surfactant micelles taking up oil from the swimming droplet. We have observed both hydrodynamic and chemical fields around the droplets and found that the system's geometry, length scales and solubilisation timescales govern various effects: pusher to puller type hydrodynamics; persistent to unsteady swimming; and, for large squeezed droplets, interfacial instabilities leading to deformation and division states.

*We acknowledge funding from the DFG SPP 1726 "Microswimmers" and the Max Planck Society.

8:36AM K61.00002: Light-driven Assembly of Motile Colloidal Clusters from Immotile Building Blocks

FALKO SCHMIDT (Presenter), University of Gothenburg, BENNO LIEBCHEN, HARTMUT LOEWEN, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany, Institut für Theoretische Physik II: Weiche Materie, GIOVANNI VOLPE, University of Gothenburg — Active matter, consisting of self-propelled units locally injecting energy into the system, opens new horizons for the creation of functional soft materials with designable properties. Experiencing a constant energy input, allows active matter to self-assemble into phases with a complex architecture and functionality such as living clusters which dynamically form, reshape and break-up but would be forbidden in equilibrium material by the entropy maximization (or free energy minimization) principle. The challenge to control this active self-assembly has evoked widespread efforts typically hinging on an engineering of the properties of individual motile constituents. Here, we provide a different route, where activity occurs as an emergent phenomenon only when individual building blocks bind together, in a way which we control by laser light. Using experiments and simulations of two species of immotile microspheres, we exemplify this route by creating active molecules featuring a complex array of behaviors, becoming migrators, spinners and rotators. The possibility to control the dynamics of active self-assembly via light-controllable nonreciprocal interactions will inspire new approaches to understand living matter and to design active materials.

8:48AM K61.00003: Failures of defining Effective temperature in an active colloidal system

CHONG SHEN (Presenter), H DANIEL OU-YANG, Lehigh University — Active colloidal systems contain active particles, which convert energy from the environment into directed or persistent motion. Effective temperature, defined from active diffusion, fluctuation, and sedimentation profile, is used sometimes for quantifying the activity of active particles. However, non-thermal fluctuations were found to lead to failures when using effective temperature under some conditions, for examples, at short times and in strong confinement. The reason and conditions under which would the failure appear is not clear even for a single active particle.

We investigate from experimentation and numerical simulation the Effective temperature in a quadratic potential. We found the maximum probability distribution in histograms of position is at a characteristic length away from the center, which can't be described with $T_{\text{eff}}$ and Boltzmann distribution. The average potential energies were not proportional to the effective temperatures. We also found that the fluctuation power spectral density (PSD) plots have two characteristic frequencies, which can't be explained with $T_{\text{eff}}$ and fluctuation-dissipation theorem. Our experiments and numerical simulation provide how the effective temperature fails to describe the system.

9:00AM K61.00004: Fluidic Metamaterials for Controlled Transport of Active Colloids

SHAHRZAD YAZDI (Presenter), JUAN L. ARAGONES, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — In metamaterials, one can design novel properties by tuning the links between constituent elements. Here, we leverage hydrodynamic interactions as designed links to engineer a fluidic metamaterial for non-equilibrium colloidal control. Our system consists of an active particle in a viscous fluid confined in a periodic array of posts. Controlled hydrodynamic and electrostatic interactions of the particle with posts give rise to interesting transport modes, reminiscent of those in Floquet-Bloch systems. We present a wide range of non-equilibrium transport states for various lattice structures and external field parameters. Using Brownian dynamics, we examine the robustness of transport states to thermal fluctuations and design defects. This novel system gives insight into design of new materials for smart transport of colloidal particles.
9:12AM K61.00005: Propulsion of catalytic Janus spheres in viscosified solutions  
MATTEO RICCI (Presenter), EDMUND TANG, PURBA CHATTERJEE, Rensselaer Polytechnic Institute — Many applications of Janus motors involve moving objects through complex environments that are mixtures of components. The flow properties of these mixtures could be Newtonian or non-Newtonian. In other applications, additives may be introduced as a way of controlling the motion of motors. The first step in understanding how the fluid mixtures alter their motion is to examine propulsion in fluids where additives change the shear viscosity while the fluid remains Newtonian. We show how solution viscosity affects Janus motor propulsion keeping all other factors (motor size, fuel concentration, temperature, etc.) constant. The velocity is shown to decay approximately inversely with viscosity. Further, the type of viscosifier used affects the interaction between fuel molecules and motor, which affects propulsion. This is part of the overall goal of understanding how solution properties impact propulsion independent of a particular application. When qualifying the propulsion in crowded environments, it is important to understand how to accurately quantify the response. We have used computer simulations to quantify the errors associated with particle tracking when extracting the propulsion of Janus motors.

9:24AM K61.00006: Interrupted Motility Induced Phase Separation for aligning active colloids.  
MARJOLEIN VAN DER LINDEN, DIRK AARTS, Department of Chemistry, Physical and Theoretical Chemistry Laboratory, University of Oxford, OLIVIER DAUCHOT (Presenter), Gulliver Lab UMR 7083, CNRS — Switching on large activity in a rather dense system of active Janus colloids, we observe fast clustering, followed by clusters aggregation towards full phase separation. The phase separation process is however interrupted when large enough clusters start breaking apart. Following the cluster size distribution as a function of time, we identify four successive dynamical regimes. Tracking both the particle positions and orientations, we characterize the structural and alignment ordering present in the growing clusters, and thereby unveil the mechanisms at play in these regimes. In particular, we identify how alignment between the neighboring particles is responsible for the interruption of the full phase separation. This experimental study, which provides the first large-scale observation of phase separation in active colloids, combined with particle scale analysis of the local mechanisms, points at the new physics observed when both alignment and short-range repulsion are present.

9:36AM K61.00007: The velocity of self-propelled Pt-coated colloids is determined by the substrate.  
STEFANIA KETZETZI (Presenter), RACHEL PAMELA DOHERTY, DANIELA JUTTA KRAFT, Leiden University — Active colloids are typically self-propelling near a substrate. However, the effect of the substrate on the self-propulsion remains unexplored. Here, we investigate whether the substrate influences the self-propulsion by performing systematic experiments on different substrates. Interestingly, we find that the colloid velocities are considerably different on different substrates. We consider various physicochemical properties as the origin for this observation. Our results are useful for future modeling and might be helpful in understanding the details of the still debated self-propulsion mechanism.

9:48AM K61.00008: Light Driven Fuel-Free Thermocapillary Microswimmers*  
MATAN YAH BEN ZION (Presenter), YAEILIN CABA, ALVIN MODIN, PAUL M CHAIKIN, New York University — Surface tension is a powerful agent for driving biological and artificial micron-sized particles. Surface tension gradients however, typically require a chemical reaction, making a capillary based swimmer fuel dependent. By combining a light absorbing bead with a fluid droplet we made a dimer that is propelled by light, and requires no chemical fuel. The 6 μm swimmers’ motility records over 10 μm/s and show good with measured thermocapillary and hydrodynamic parameters. We discuss the swimmers’ manipulation and interactions.

*This work was supported primarily by the Materials Research Science and Engineering Center (MRSEC) program of the National Science Foundation under Award No. DMR-1420073. J.B. acknowledges support by the National Science Foundation under Grant No. DMR-1710163.

10:00AM K61.00009: Tuning the motility of self-propelled droplets: from persistent to stochastic*  
ADRIEN IZZET (Presenter), New York University, PEPIJN MOERMAN, Chemistry, Utrecht University, KATHERINE A NEWHALL, Mathematics, University of North Carolina-Chapel Hill, JASNA BRUJIC, New York University — Active droplets produce isotropic concentration gradients in the solution. These solute-mediated interactions depend on the size of the droplet and on the composition of the solvent, as shown in the case of di-ethyl phthalate (DEP) droplets in an aqueous solution of sodium dodecyl sulphate (SDS) [P. G. Moerman et al. PRE 96, 032607 (2017)]. When the fluctuations of these interactions are sufficient to break the symmetry of this dissolution gradient, a self-sustained motion is initiated. These droplets exhibit different motility profiles, from ballistic to diffusive. We use the rotational diffusion model to describe the motility of these swimmers. For a given droplet size, we tune the concentration of surfactant in the solution in order to control the droplet solubility. We show that contrary to Janus particles, the persistence length of the trajectory decreases when adding more fuel (surfactant) in the system: the sensitivity to fluctuations of local fuel concentration increases.
10:12AM K61.00010: Exploring the origin of self-induced vertical oscillations of dust particles in a plasma  JOSHUA MENDEZ (Presenter), GURAM GOGIA, JUSTIN BURTON, Department of Physics, Emory University — Micron-size charged particles can be easily levitated in a low-density plasma environment. Such “dusty plasmas” are often used to investigate traditional condensed matter and statistical physics at the single-particle level. We have recently observed a novel phenomenon where hundreds of particles can switch between crystalline and gas-like states over minutes-long time scales (Gogia et al., PRL, 2017). The constituent-level source of energy for this “active matter” system is sustained, large-amplitude vertical oscillations of the individual particles. Delayed charging, charge fluctuations, and variations in the plasma number density have been previously invoked to explain such behavior, however, we show that these mechanisms are unlikely to drive the oscillations we observe. Langmuir probe measurements suggest the plasma environment around the grains is time-invariant. Furthermore, grains carry charges on the order of $10^4$ electrons, suggesting that square-root N fluctuations would be too small to drive such large amplitude oscillations. We hypothesize that particle oscillations arise not from electrostatic effects, but from a complicated interaction between the ion wakes streaming out in the lee of the particles and the underlying electrode at low pressures.

10:24AM K61.00011: Diffusive ferromagnetic roller gas: velocity and displacement statistics*  GAŠPER KOKOT (Presenter), ALEXEY SNEZHKO, Materials Science Division, Argonne National Laboratory — Active colloids can display collective motion that is non-directional on average, akin to gas molecules. We experimentally observe and investigate such behavior for ferromagnetic colloidal rollers powered by a vertical alternating magnetic field. We show that the system has a bimodal velocity distribution. Furthermore, the displacement statistics transition from bimodal to quasi-Gaussian distributions (Gaussian core with power-law tails) for all densities. Overpopulated tails are observed at low densities. The system demonstrates the normal diffusive behavior for both active particles and inert glass beads of the same size. The density dependence of the diffusion constant shows a striking difference between active and inert particles. Our work provides insight into statistical properties of active Brownian-like non-equilibrium systems.

*The research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:36AM K61.00012: Collective dynamics and active turbulence in swarms of synchronized self-assembled spinners*  KOOHEE HAN (Presenter), GAŠPER KOKOT, ALEXEY SNEZHKO, Materials Science Division, Argonne National Laboratory — Active magnetic colloids have proven to be an excellent model system to explore emergent out-of-equilibrium dynamics and structures. We demonstrate that ferromagnetic microparticles, suspended at an air/water interface and energized by an external rotating magnetic field, form dynamic ensembles of synchronized self-assembled spinners. The balance between the magnetic and viscous torques determines the size of an individual self-assembled spinner, which can be controlled by the frequency and strength of the applied magnetic field. Each spinner generates local hydrodynamic flows such that the collective interactions of the multiple spinners allow the formation of dynamic crystal lattices. We investigate active diffusion of passive cargo particles in such spinner ensembles and analyze the structure of the underlying self-induced surface flows. We show that induced flows exhibit properties of an active turbulence. The energy spectra of the active turbulence in such synchronized spinner ensembles reveal reverse energy cascade with the exponent significantly different from the classical 2D turbulence.

*The research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

10:48AM K61.00013: Solid-liquid transition in layers of deformable active droplets*  BENJAMIN LOEWE (Presenter), Syracuse University; University of California Santa Barbara, DAVIDE MARENDUZZO, University of Edinburgh, M. CRISTINA MARCHETTI, University of California Santa Barbara — Layers of epithelial tissue have been modeled either as collections of spherical active particles or via the Vertex Model (VM) that describes cells as irregular polygons tiling the plane. The VM is appropriate to describe confluent layers where there are no gaps between cells and does not incorporate variations in the cell packing fraction that is by construction set to one. In contrast, the particle model can account for variation in packing fraction, but does not allow for deformations of individual cells. Both models predict a solid-liquid transition of cellular tissue tuned either by cell shape (VM) or by cell density (particle model). To bridge between these two models, we describe cells as deformable self-propelled droplets each characterized by a scalar field representing the cell's density. We then examine the collective behavior of N droplets modeled as N interacting phase fields. Using this model, we examine the interplay of cell deformability, cell density and cell motility in controlling the solid-liquid transition. We quantify the melting of the hexagonal ground state, as well as the stability of metastable states.

*This work was supported by NSF grant DMR-1609208 and by the Simons Foundation Targeted Grant in the Mathematical Modeling of Living Systems Number 342354.
8:00AM K62.00001: Exoplanets: from Discovery to Characterization and Beyond* [Invited] SARA SEAGER (Presenter), Massachusetts Institute of Technology — Thousands of exoplanets are known to orbit nearby stars with evidence that nearly all stars in our Milky Way Galaxy have planets. Beyond their discovery, a new era of “exoplanet characterization” is underway with an astonishing diversity of exoplanets driving the fields of planet formation and evolution, interior structure, atmospheric science, and orbital dynamics to new depths. Exoplanets with masses and average densities that have no solar system counterparts are mysteries in their formation pathways as well as their interior composition and structure. The push to find smaller and smaller planets down to Earth size is succeeding and motivating the next generation of planetary models and telescopes to have the capability to find and identify planets that may be like Earth.

*Thanks to NASA, the MIT Bose Fellows Program, The Change Happens Foundation, and the Heising-Simons Foundation.

8:36AM K62.00002: Phase transitions in mantle silicates and the internal structure of terrestrial exoplanets [Invited] KOICHIRO UMEMOTO (Presenter), Earth-Life Science Institute, Tokyo Institute of Technology — The highest-pressure form in the Earth of the major mantle silicate MgSiO₃-bridgmanite is post-perovskite (PPv). Knowledge of the fate of PPv at higher pressures relevant for super-Earth-type planets is fundamental for us to start modeling the internal structure and dynamics of these planets. In this talk I will review the sequence of phase transitions we discovered in pure MgSiO₃ up to 4 TPa, as well as in aggregates of MgSiO₃+MgO and MgSiO₃+SiO₂ with variable Mg/Si abundances. New phases in the (MgO)ₙ(SiO₂)ᵦ system have been discovered [1-5]. Such phases involve dissociation and recombination reactions in the MgSiO₃+MgO+SiO₂ system, some of them very surprising, but all ending-up in the dissociated elementary oxides, MgO+SiO₂, above 3.1 TPa [1]. These transitions produce density discontinuities in planetary interiors and the consequences of these transitions for the internal structure of terrestrial planets [6] with up to 20 Earth masses will be discussed.

References
9:12AM K62.00003: Mass-dependent Dynamics of Terrestrial Exoplanets Using ab initio Mineral Properties [Invited]
ARIE VAN DEN BERG (Presenter), Utrecht University, DAVID A. YUEN, Applied Physics and Applied Mathematics, Columbia University, KOICHIRO UMEMOTO, ELSI, Tokyo Institute of Technology, MICHAEL JACOBS, Metallurgy, Technical University Clausthal, RENATA WENTZCOVITCH, Applied Physics and Applied Mathematics and Department of Earth and Environmental Sciences, Lamont Doherty Earth Observatory, Columbia University — We present new modelling results for the internal structure and convective dynamics of large terrestrial (rocky) exoplanets. For up to 20 Earth masses (Me) our results show pressure and temperature (P,T) of several Terapascal (TPa) and 10000 Kelvin in the silicate mantle.
Recent mineral physics predictions show stepwise dissociation into SiO₂ and MgO of the main magnesium-silicate mineral of Earth's mantle under these P,T conditions (Umemoto et al., 2017).
Using material properties from these models we have modelled the internal structure of planets in the range 1-20 Me with an Earth-like core mass fraction of 0.3. We found that full dissociation into oxides occurs in planets with M > 13 Me, where at the core mantle boundary P > 2.4 TPa.
Our Rayleigh-Benard mantle convection results for planet mass 1-20 Me show strong differences in the internal structure and the convection dynamics between different cases.
First, due to increasing pressure the number of phase transitions increases from zero in the smallest case to four, for cases > 13 Me. Furthermore, we observe three regimes of convective dynamics, with: 1) smaller planets (< 4 Me), showing vigorous convection, 2) intermediate cases (< 12 Me), with sluggish penetrative convection, concentrated in a single shallow zone of higher flow velocity, and 3) large planets, (> 12 Me), with vigorous convection in top and bottom zones, separated by a high viscosity mid-mantle with sluggish convection.
These regimes are directly related to the pressure dependence of mantle viscosity, first increasing then decreasing due to pressure weakening. Here the planet mass is the control variable because it sets the mantle pressure range.
For the larger planet cases with a bottom layer of oxides, and reduced viscosity, we observe vigorous convection and small scale structure in the deepest part of the mantle that interacts with the dissociation phase boundary. This impacts the heat-flux from the core and the viability of core dynamo processes.

9:48AM K62.00004: Phase Transitions Beyond Post-Perovskite in Neighborite (NaMgF₃) to 1.6 Mbars* [Invited]
THOMAS DUFFY (Presenter), RAJKRISHNA DUTTA, Princeton University, ERAN GREENBERG, VITALI PRAKAPENKA, University of Chicago — Neighborite, NaMgF₃, is used as a model system for understanding ultra-high pressure phase transitions in ABX₃ systems such as MgSiO₃. In this work, we have studied the high-pressure behavior of NaMgF₃ to 1.6 Mbars using the laser-heated diamond anvil cell technique coupled with synchrotron x-ray diffraction. Our work reveals a complex sequence of high-pressure phases beyond post-perovskite in this ABX₃ system. The phase transition sequence in NaMgF₃ is: NaMgF₃ (perovskite) → NaMgF₃ (post perovskite) → NaMgF₃ (Sb₂S₃-type) → NaF (B2-type) + NaMg₂F₅ (P2₁/c) → NaF (B2) + MgF₂ (cotunnite-type). Our results demonstrate the existence of a post-post-perovskite phase, followed a two-stage dissociation into binary fluorides. This work is the first experimental report of a dissociation of a post-perovskite in any known ABX₃ system. A similar sequence of transition is predicted to occur in MgSiO₃ at ultrahigh pressures where it has implications for the mineralogy and dynamics large, rocky extra-solar planets.

*This research was funded by the National Science Foundation.

10:24AM K62.00005: Laser Focus on Planets* [Invited] GILBERT COLLINS (Presenter), Laboratory for Laser Energetics, Mechanical Engineering, and Physics and Astronomy, University of Rochester — A new laboratory exploration of the deep interior states and processes for solar and extrasolar planets is underway. Kilojoule to Megajoule laser compression data and first principles calculations combined with recent observational planet discoveries provide fresh perspectives for the qualities and implications of these massive objects throughout the universe. Recent experimental results for silicates and water reveal dramatic chemical changes emerge at millions of atmosphere pressure and several thousand Kelvin, giving rise to polymeric silicates and superionic water. New equation of state data for iron to tens of millions of atmospheres provides insight into the deep interior core conditions for extrasolar terrestrial planets. At still higher pressures, approaching atomic pressures (294 Mbar = 29.4 TPa) atoms can be brought together closer than a deBroglie wavelength and even in some cases the Bohr radius where core as well as valence electrons (keV as well as eV energy levels) engage in bonding and where a new quantum behavior emerges.

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Wednesday, March 6, 2019 8:00 AM - 11:00 AM
mechanical outcome of knitted fabrics. Techniques, the innate properties of the yarn and the stitch microstructure has a direct effect on the global geometric and elasticity of the resulting fabric. This puts a new spin on additive manufacturing – not only can stitch pattern control the local and global geometry of a textile, but the topology of knitted stitches has a profound impact on the geometry and elasticity of the resulting fabric. This puts a challenge has been realized in the ancient technology known as knitting. This process for making functional materials 2D and 3D with many functional materials, the key to knitting's extraordinary properties lies in its microstructure.

At the 1D level, knits are composed of an interlocking series of slip knots. At the most basic level there is only one manipulation that creates a knitted stitch – pulling a loop of yarn through another loop. However, there exist hundreds of books with thousands of patterns of stitches with seemingly unbounded complexity.

The topology of knitted stitches has a profound impact on the geometry and elasticity of the resulting fabric. This puts a new spin on additive manufacturing – not only can stitch pattern control the local and global geometry of a textile, but the creation process encodes mechanical properties within the material itself. Unlike standard additive manufacturing techniques, the innate properties of the yarn and the stitch microstructure has a direct effect on the global geometric and mechanical outcome of knitted fabrics.

8:36AM K63.00002: Avalanche dynamic in a knitted fabric*  SAMUEL POINCLoux, Ecole Normale Superieure, Mokhtar Adda-Bedia, Departement de Physique, Ecole Normale Superieure de Lyon, Frederic Lechenault (Presenter), Ecole Normale Superieure — A knitted fabric is a topologically constrained elastic yarn following a periodic path. The mechanical behavior of the fabric appears to be drastically different from the yarn it is made of. To explain this discrepancy, we introduced a network model which features three ingredients, a dominant bending energy, an unaltered topology and yarn length conservation. This model provides a quantitative comparison with experiments done on a model knitted fabric, both in the force-elongation relation and in the deformation field. However, yarn-yarn friction at the crossing points induces fluctuations around the average force and deformation response. The fluctuations are identified as sudden drops of the force correlated with localized slipping lines in the network. Power law distribution of event size and morphological scale invariance suggest an avalanching mechanism producing those fluctuations. A mechanism is indeed identified with local slips propagating and mediated through anisotropic elastic redistribution.

*Funded by the ANR METAMAT.

8:48AM K63.00003: A general geometric framework for knitted fabric elasticity  Michael Dimitriyev (Presenter), Krishma Singal, Elisabeta Matsumoto, Georgia Institute of Technology — Knitting is a process in which yarn, an essentially filament-like material, is shaped in space to form a fabric, an essentially sheet-like material, via stitching together a lattice of slip-knots. Due to fabric-level dependence on the stitch pattern, a single yarn can be used to create a large variety of fabric geometries and material responses. Moreover, the elasticity of knits remains poorly understood, as evidenced by the lackcluster performance of spring-lattice models. We seek a continuum elastic model that predicts the three-dimensional shape of knitted fabric. This model should have the flexibility to be adapted to describe a wide range of stitch patterns and elasticity models. To this end, we have developed a geometric framework for relating the yarn path to the emergent surface geometry of the fabric. The generality of our approach allows for a systematic coarse-graining of yarn degrees of freedom, without a priori specification of a model of yarn elasticity. Thus, we are able to arrive at a stitch pattern-dependent, continuum elastic model of knits by assuming a simple phenomenological model of yarn, whilst allowing for the possibility of including more realistic yarn mechanics and experimental comparison.

9:00AM K63.00004: A topological perspective on knitted fabrics  Shashank Markande (Presenter), Elisabeta Matsumoto, Georgia Institute of Technology — A knitted textile structure can be thought of as a series of slip knots stacked next to each other in multiple rows. In a given row, each loop is held in place by a loop in the preceding row. As a first step towards building a topological theory for knitted textile structures, we take advantage of the doubly periodic structure coming from the ordering of stitches into rows and columns. A two-periodic planar structure has two generators of translational symmetry. We get a minimal unit cell that tiles the original structure by modding out by these elements of symmetry. The resulting embedding of a curve inside the unit cell is equivalent to a knot sitting in the thickened two-torus. To study this class of knots, we aim to construct a knot invariant or link invariant based on the process of knitting -- using two needles to form slip knots in yarn -- to make an arbitrary two-periodic knitted textile structure. Such a knot invariant inherits an algebraic structure that reflects how and which elementary operations are used to make a given knitted textile structure and, as a result, tells us whether a given doubly periodic structure can be realized by knitting.
**9:12AM K63.00005: Top Down Modeling of Complex Knit Structures: Beyond Jersey Knits**

CHELSEA KNITTEL (Presenter), University of Oxford, RANDALL D KAMIEN, Physics and Astronomy, University of Pennsylvania, OANA GHITA, KEN EVANS, College of Engineering, Mathematics and Physical Sciences, University of Exeter, GENEVIEVE DION, Drexel University — Modeling of knit textiles is popular in fields such as mechanical engineering and physics, where researchers are working to understand effects of yarn and loop geometries on fabric properties. Often, this can be computationally expensive, allowing only for modeling of planar fabrics such as jersey, made from all knit stitches. We see potential however, in complex self-folding structures, made with knit and purl stitches, as a means of engineering metamaterial textile properties. To aid in modeling of these structures, we have developed a topological framework for the knit structure using families of bicontinuous surfaces which allow us to geometrically understand the physics of the characteristic boundary condition curling of jersey knits. We then consider complex self-folding as a result of competition between these boundaries, affected by contributing magnitudes of forces from course and wale directions. By characterizing these forces, we are developing a system of predicting this folding, through understanding of generalized behaviors that repeat regardless of material or machine. By studying interactions between segments of knit and purl stitches, rather than loops or yarns, we can more quickly understand this behavior, to engineer novel textile properties.

*NSF-CMMI #1537720

**9:24AM K63.00006: Stable elastic knots with no self-contact**

DEREK MOULTON (Presenter), University of Oxford, SÉBASTIEN NEUKIRCH, Université Pierre et Marie Curie, PAUL GRANDGEORGE, École polytechnique fédérale de Lausanne — Knots are widespread, universal physical structures, from shoelaces to Celtic decoration to the many variants familiar to sailors. They are often simple to construct and aesthetically appealing, yet remain topologically and mechanically quite complex. Knots are also common in biopolymers such as DNA and proteins, with numerous and significant biological implications.

While self-contact is an inevitable feature of tight knots, here we go the other direction and ask whether a knotted filament with zero points of self-contact may be realized physically. Our focus is on the simple hand-held experiment of an elastic rod bent into a trefoil knot, with the ends held clamped. The question we consider is whether there exist stable configurations for which there are no points of self-contact. This idea can be fairly easily replicated with a thin strip of paper, but is more difficult or even impossible with a flexible wire. We search for such configurations within the space of three tuning parameters related to the degrees of freedom in the simple experiment. Mathematically, we show, both within standard Kirchhoff theory as well within an elastic strip theory, that stable and contact-free knotted configurations can be found, and we classify the corresponding parametric regions. Numerical results are complemented with an asymptotic analysis that demonstrates the presence of knots near the doubly-covered ring. In the case of the strip model, quantitative experiments of the region of good knots are also provided to validate the theory.

*U.K. Royal Society through the International Exchanges Scheme (grant IE120203)

**10:00AM K63.00007: Untangling the mechanics of elastic knots**

PAUL JOHANNS (Presenter), PAUL GRANDGEORGE, Institute of Mechanical Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland, CHANGYEOB BAEK, Department of Mechanical Engineering, Massachusetts Institute of Technology (MIT), USA, ALASTAIR FLYNN, Institute of Mathematics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland, TOMOHIKO SANO, Department of Physical Science, Ritsumeikan University, Japan, JOHN MADDOCKS, Institute of Mathematics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland, PEDRO REIS, Institute of Mechanical Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland — In surgery, knots are used as ligatures to bind surgical thread during suturing. Even if breakage or unraveling of knotted configurations can be disastrous, suturing guidelines are mostly empirical. Knot theory, a well-established field of mathematics, tends to focus on idealized, non-elastic knots. Moreover, analytical models based on Kirchhoff's theory for elastic rods are limited to simple knots in loose configurations. However, functioning knots are in general tight and involve elastic deformation of the thread, self-contact and nontrivial frictional interactions. We tackle this problem by performing high precision experiments to acquire unprecedented experimental data on the geometry and deformation of simple open-knots. We make use of X-ray micro computed tomography to acquire volumetric information of knotted configurations on homogeneous elastomeric rods. Emphasis is placed on systematically exploring how the mechanical properties of the rod, friction, and the externally applied loads, all conspire to dictate the mechanical performance of knotted structures. We hope that the physical insight gained from this experimental characterization will form the bases for future predictive models for physical knots.

*Supported by the Fonds National de la Recherche, Luxembourg 12439430
10:12AM K63.00008: Not-knots as the building block of elastic knots* PAUL GRANDGEORGE (Presenter), PAUL JOHANNS, Institute of Mechanical Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland, CHANGYEOB BAEK, Department of Mechanical Engineering, Massachusetts Institute of Technology (MIT), USA, ALASTAIR FLYNN, Institute of Mathematics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland, TOMOHIKO SANO, Department of Physical Science, Ritsumeikan University, Japan, JOHN MADDOCKS, Institute of Mathematics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland, PEDRO REIS, Institute of Mechanical Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland — Knots are key for a wide variety of applications such as mooring ships to docks, ensuring the safety of a falling climber or fastening surgical suture threads. Even if knots have been used in hundreds of configurations for millennia, the understanding of their mechanical behavior remains mainly empirical. Past fundamental studies on knots include ideal knots, purely based on geometry and one-dimensional reduced elasticity models. For tight knots, intricate three-dimensional geometries, large deformations, and friction between rod strands are all present in setting a highly nonlinear and coupled behavior. To gain better insight into this complex class of problems, we study the ‘not-knot’: a simpler model system composed of a clasp of two bent elastic rods brought together in mechanical contact. We use X-ray computed tomography to probe the geometry of not-knots, as well as precise force-displacement measurements to quantify the interplay of bending curvature, elasticity, and friction. We believe that regarding complex tight knots as assemblies of simple not-knots will provide a solid foundation to develop much needed predictive models for knotted structures.

*P. Johanns was supported by the Fonds National de la Recherche, Luxembourg 12439430

10:24AM K63.00009: From knots to weaved baskets: Unravelling the mechanics of a clasp between two contacting filaments through numerical experiments* CHANGYEOB BAEK (Presenter), Department of Mechanical Engineering, Massachusetts Institute of Technology (MIT), PAUL GRANDGEORGE, PAUL JOHANNS, Institute of Mechanical Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), ALASTAIR FLYNN, JOHN MADDOCKS, Institute of Mathematics, Ecole Polytechnique Fédérale de Lausanne (EPFL), PEDRO REIS, Institute of Mechanical Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL) — Tight elastic knots and weaved structures tend to exhibit intricate modes of deformation with nontrivial regions of contact that call for a fully three-dimensional description. Given this complexity, there is a striking lack of predictive models for knotted or weaved structures, the design of which tends to rely mostly on accumulated experience and empirical craftsmanship. Here, we study the elementary, yet rich and informative, canonical case of ‘a clasp’ formed by two elastic rods in crossing contact. We first start with the case of rods that have an originally circular cross-section. We tackle this problem by performing finite element simulations of this clasp configuration and contrast our results with experimental data obtained using X-ray tomography of the corresponding physical structures. We compare our results to a well-established description for ideal claps of geometrically rigid strings (that exclude elasticity), finding that the latter acts as an underlying ‘backbone’ for the full elastic solution. Finally, we extend our framework to a clasp formed by strips of non-circular cross-sections, which is the building block in basket weaving.

*P. Johanns was supported by the Fonds National de la Recherche, Luxembourg 12439430.

10:36AM K63.00010: Detangling hair THOMAS PLUMB-REYES (Presenter), NICHOLAS CHARLES, LAKSHMINARAYANAN MAHADEVAN, Harvard University — Tangled hair is difficult to manage. We investigate the everyday problem of taming a tangle of hair with a comb by focusing on a minimal model of this system: a pair of chiral, elastic helical rods entangled to form a braid. As a single, stiff tine combs through the double-helix, it leaves two untangled filaments in its wake. We use experiments, theory and computation to characterize this problem with both mechanics and topology.

10:48AM K63.00011: Born in the Wrong Geometry: Longitudinal and transverse frustration in non-parallel filament bundles* DARIA ATKINSON (Presenter), CHRISTIAN SANTANGELO, GREGORY GRASON, University of Massachusetts Amherst — Assemblies of one-dimensional, filamentous materials are commonplace in physical systems, from microscopic materials, such as columnar liquid crystals and biopolymer bundles, to familiar, macroscopic materials like wires, cables, and ropes. The geometry of continuous filament bundles with cross sectional ordering in three dimensions is highly constrained, and we show that only two families of such filament bundles permit equidistant configurations of their constituent filaments: those with bend, but no twist, and those with twist, but no bend. The elastic response of bent and twisted bundles with no such ordered ground state, such as those formed by DNA plasmids under confinement, is then doubly geometrically frustrated: the presence of twist frustrates crystalline order in the cross-section, and the presence of bend couples this compromise structure to the filament tangents. In filaments, as in many frustrated systems, the global response to deformations can not be adequately described by a linear energy. We present a fully nonlinear theory for the elasticity of bundles with one-dimensional components which can slide freely along their tangents, and discuss the response of Euclidean filament packings to the imposition of non-equidistant geometries.

*NSF DMR-1608862
NSF DMR-1507377
8:00AM K64.00001: Award for Outstanding Doctoral Thesis Research in Biological Physics Talk: Mechanics and energetics of the bacterial flagellar motor* [Invited] JASMINE NIRODY (Presenter), Center for Studies in Physics and Biology, Rockefeller University — The bacterial flagellar motor (BFM) is an ion-powered nanomachine that drives swimming in many bacteria. This protein complex is comprised of several transmembrane rings connected to a long flagellar filament by a flexible hook. Rotation is known to occur via an interaction between one or more membrane-embedded “stator” units, and protein spokes on the periphery of the spinning “rotor” ring. In this talk, I will touch on three features of the motor: (1) its fundamental mechanochemical cycle, (2) the dynamic remodelling of motor structure in response to its environment, and (3) the efficiency of the motor. First, taking into account all the structural and dynamic biophysical experimental evidence to date, we present a mechanically-specific, testable model of the motor's mechanism of torque generation. We validate this theoretical model of the BFM's mechanochemical cycle against experiments done on motors with a single stator. Second, we extend this base model to consider the behavior of multi-stator motors. Stator units have been shown to dynamically bind and leave the motor. We present several recent experiments that shine light on the nature of this complex process, which is influenced by several factors, including the ion gradient, external load, and motor speed. Finally, we also discuss experiments directly measuring the relationship between ion flux through the membrane and motor speed, towards answering the question of whether the motor is loosely or tightly coupled to ion flux — that is, whether each ion passage constitutes a fully efficient power stroke.

*Moore/Sloan Data Science Fellowship; All Souls College Post-Doctoral Research Fellowship; James S. McDonnell Foundation Postdoctoral Fellowship

8:36AM K64.00002: Invariance properties of bacterial random walks inside domains with variable geometry and structural disorder [Invited] ROBERTO DI LEONARDO (Presenter), Università di Roma — Motile cells often explore natural environments characterized by a high degree of structural complexity. Moreover cell motility is also intrinsically noisy due to spontaneous random reorientation and speed fluctuations. The interplay of different noise sources gives rise to complex dynamical behavior that can be strongly sensitive to details and hard to model quantitatively. In striking contrast to this general picture we show that the mean residence time of swimming bacteria inside artificial complex microstructures can be quantitatively predicted by a generalization to active matter of a recently discovered invariance property of random walks. By systematically varying geometry and structural disorder we produce systems that exhibit strongly different distributions of path length and dwell time but whose mean values is invariant and can be predicted with precision by the sole free volume to surface ratio.

Biological implications include the possibility of predicting and controlling the colonization of complex natural environments using only geometric informations.

9:12AM K64.00003: Spontaneously oscillating synthetic cilia* ISABELLA GUIDO (Presenter), ANDREJ VILFAN, Ramin Golestanian, Eberhard Bodenschatz, Max Planck Institute for Dynamics and Self-Organization, KAZUHIRO OIWA, Advanced ICT Research Institute, National Institute of Information and Communications Technology (NICT) — Cilia and flagella produce rapid and regular bending waves responsible for the propulsion of organisms in fluids or for the promotion of fluid transport. It is known that the main contribution to their beating is due to motor proteins, dynein, which drives sliding of the microtubule doublets. However, the fundamental mechanism of the dynein-microtubule interaction is still a puzzle. Here we investigate their mechanical interaction and emergent behavior by analyzing a minimal synthetic system that we experimentally assemble with two microtubules and few dynein motors. We observe that the microtubule pair undergoes cyclical association/dissociation interaction through rhythmic bending, followed by a complete detachment of the microtubules and subsequent re-attachment. By considering the shearing force produced by the motors when they move along the adjacent microtubule and the finite elasticity of the system, we describe this beating cycle in terms of the curvature and dynein-microtubule binding force.

*This work is supported by the BMBF and MPG through the MaxSynBio initiative
**9:24AM K64.00004: Quantitative in vivo measurements of cerebrospinal fluid flow through perivascular spaces in the brain**

JEFFREY TITHOF (Presenter), University of Rochester, HUMBERTO MESTRE, TING DU, WEI SONG, WEIGUO PENG, AMANDA M SWEENEY, GENARO OLVEDA, University of Rochester Medical Center, JOHN H THOMAS, University of Rochester, MAIKEN NEDERGAARD, University of Rochester Medical Center, DOUGLAS H KELLEY, University of Rochester — Recent discoveries have uncovered a novel route for the flow of cerebrospinal fluid (CSF) through the brain which is important for the removal of protein waste, such as amyloid-β. Characterizing this flow and the mechanisms which reduce it may offer new insight into the development of neurodegenerative diseases, such as Alzheimer's disease, which are correlated with accumulation of protein waste. CSF enters the brain along perivascular spaces (PVSs) — annular tunnels around arteries — and arterial pulsations are hypothesized to drive these flows, but this has never been quantitatively shown. We perform experiments to measure PVS flows by injecting microspheres into the CSF of living mice, imaging PVSs using two-photon microscopy, and performing particle tracking velocimetry. These measurements offer the first quantitative evidence demonstrating that CSF is driven through PVSs by arterial pulsations. Furthermore, by increasing blood pressure, we observe changes in the arterial pulsations and a net reduction in the CSF flow speed. Our results offer one potential causal mechanism which may contribute to reduced protein waste clearance and development of neurodegenerative diseases.

*Funded by NIH grant 1RF1AG057575-01

**9:36AM K64.00005: Flows and Stability of a 3D Active Nematic**

KEVIN SKOWRONSKI (Presenter), GUILLAUME DUCLOS, Brandeis University — Filamentous bacteriophage (fd virus) have an elongated, rod-like shape, and have served as a well-known model for lyotropic passive liquid crystals. At low concentrations, fd virus in suspension maintain an isotropic orientation; however, as the virus concentration is increased, the system undergoes a transition to a liquid crystalline phase where the nematic elasticity induces long range order. We can drive this material out of equilibrium by doping it with active filaments that consume chemical energy to self-propel, and probe for novel far-from-equilibrium behaviors. Here, we use microtubules, clusters of kinesin motors, ATP, and a depletant polymer that induces bundling of the microtubules. We combine this active microtubule system with a dense suspension of fd virus to create a 3D out-of-equilibrium composite liquid crystal. By varying the concentration of fd virus and microtubules in the system, we experimentally determine the extent to which the coupling between activity, nematic elasticity, and confinement influence the emergence of collective flows or control the stability, in both the isotropic and the nematic phases.

*Brandeis University and Bioinspired Soft Materials MRSEC

**9:48AM K64.00006: Live cell and in vitro mitotic spindles as arrested liquid crystal tactoids.**

SUMON SAHU (Presenter), Department of Physics, University of Massachusetts, Amherst, BIANCA EDOZIE, Department of Biochemistry and Molecular Biology, University of Massachusetts Amherst, PATRICIA WADSWORTH, Department of Biology, University of Massachusetts Amherst, JENNIFER ROSS, Department of Physics, University of Massachusetts, Amherst — Microtubule self-organization is a fundamentally important phenomenon from both physics and biological point of view. One interesting and important structure is the mitotic spindle, a football-shaped structure used to align and ultimately separate the chromosomes during cell division. Recent studies have claimed that the meiotic spindle is internally organized like a liquid crystal tactoid with many, short microtubules that are fluid-like and can coalesce like droplets. Using live cell experiments, we find that the regions of mitotic spindle near the chromosomes are more fluidized, but other regions are arrested. Using photoactivation, we can measure the dynamics of different regions of the spindle and the relative concentration of microtubule-associated proteins and motors as a function of the microtubule concentration. In addition, we use in vitro reconstitution experiments of microtubule polymerization in the presence of a microtubule cross linker, MAP65, and depletion agents that can form spindle-like structures. Using FRAP experiments, we found that these spindle-like assemblies are not fluid, but rather arrested, unlike liquid crystals. Using this combination of live cell and in vitro reconstitution, we are uncovering the physical organizations of the mitotic spindle.
10:00AM K64.00007: Actin assembly alone can drive inward and outward membrane deformations  CAMILLE SIMON (Presenter), REMY KUSTERS, VALENTINA CAORSI, Physico Chimie Curie UMR 168, Institut Curie, JOANNEY JEAN-FRANCOIS, ESPCI, CLÉMENT CAMPILLO, LAMBE, Université Evry, JULIE PLASTINO, PIERRE SENS, CÉCILE SYKES, Physico Chimie Curie UMR 168, Institut Curie — The cell membrane is able to deform inward, as during the initiation of endocytosis, or outward, as during the formation of filopodia. Interestingly, both deformations are generated by the same branched, Arp2/3-based, polymerizing actin network. How an inward or an outward deformation can be obtained in the same network structure? What are the physical parameters that will trigger the direction of membrane deformation? To address these questions, we use a reconstituted membrane system of liposomes and purified actin. We investigate the conditions under which the actin cytoskeleton induces inward or outward membrane deformations. We reveal that actin dynamics are the essential player of membrane deformations by photo-damaging the actin structure that relaxes membrane shape. Lowering membrane tension is key to produce filopodia-like structures. Oppositely, endocytic-like structures are robust features that only weakly depend on membrane tension. A pulse-chase two color actin experiment and the labeling of the proteins associated to actin reveal the details of network growth during inward or outward membrane deformation. Our results, supported by theoretical models, explain how such deformations depend on a mechanical balance between the membrane and the actin network.

10:12AM K64.00008: Local, biased polymerization kinetics lead to slow axonal transport of actin  NILAJ CHAKRABARTY (Presenter), Department of Physics and Astronomy, Ohio University, PANKAJ DUBEY, Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, YONG TANG, Department of Molecular and Cellular Physiology, Stanford University, ARCHAN GANGULY, KELSEY LADT, Department of Neurosciences, University of California, San Diego, CHRISTOPHE LETERRIER, CNRS, Aix-Marseille Universite, SUBHOJIT ROY, Department of Neuroscience, University of Wisconsin-Madison, PETER JUNG, Department of Physics and Astronomy, Ohio University — Actin, a key protein constituent of the neuronal cytoskeleton is conveyed along the axon at rates corresponding to slow axonal transport. However, the mechanism of this movement is unknown. Recent advances in live imaging of F-actin and super-resolution imaging has revealed that axonal actin is highly dynamic, undergoing focal assembly, disassembly and elongation bidirectionally along the axon. Actin filaments have an anterograde bias, are locally polymerized and grow with their barbed ends attached to stationary axonal endosomes. We generated the dynamics of axonal actin trail assembly using a model of stochastic filament nucleation and elongation which incorporates imaging data. We then devised a photoactivation simulation to track fluorescently labeled actin in the axon, which closely matches the pulse-chase experiment paradigm. Our simulations predict that local, biased polymerization of actin trails lead to global, anterograde actin transport at rates matching in-vivo pulse-chase experimental rates. Collectively, the simulations and experiments point to local assembly and biased polymerization forming the mechanistic basis of bulk transport. This mechanism is distinct from motor-driven polymer sliding and occurs without any significant contribution from microtubules.

10:24AM K64.00009: Impact of filament dynamics on actomyosin flows  DANIELLE SCHEFF (Presenter), MARGARET GARDEL, Department of Physics, University of Chicago — While myosin driven activity in actin networks has proven to be a good model system for studying active matter, actin filaments have internal dynamics that are less well understood. In cells, filaments continuously depolymerize on one end while repolymerizing on the other, an active process that can both relax stresses by depolymerizing stretched filaments and create forces by driving actin into the cell membrane. Here, we study how this activity affects the ability of actin networks to store energy and propagate forces. Using a minimal system we previously developed, we are able to add actin dynamics to systems composed of both short filaments, which form a liquid crystal, and long ones, which form a contractile-network when in the presence of myosin motors. Preliminary results suggest that filament dynamics cause actomyosin networks to contract uniaxially, implying that dynamic filaments contract through sliding, in contrast to stable filaments which contract through buckling. Simultaneously, dynamics redistribute actin allowing the network to maintain long-lasting contractile flows.
10:36 AM K64.00010: Noise induced escape in delay coupled mixed-reality systems
KLEMENTYNA SZWAYKOWSKA
(Presenter), IRA SCHWARTZ, JASON HINDES, United States Naval Research Laboratory — Networks of coupled subsystems are
common in many fields, from biology to epidemiology and robotics. The emergent behaviors of these systems depend on
the nature of the interaction and the communication network. It is now well-known that delay in communication between
individual agents significantly impacts dynamic pattern formation. In addition, noise propagation through coupling can
lead to complex system-wide behaviors. We consider a mixed-reality (MR) system in which delay-coupled real and
simulated agents fly together in formation, and show how noise acting on the real agents can induce a large transition in
the simulated agents. In order to address this problem, we first analyze a generic model of two weakly delay-coupled
dynamical systems. We show how noise in one system can drive a catastrophic state transition in the other, even as the
noisy system exhibits only small random oscillations; further, we show how the expected transition time scales as a
function of the coupling strength and communication delay. We use an analogous approach to study changes in the flight
formation of MR agents.

*This work was supported by ONR N0001412WX20083 and NRL Base Research Program N0001412WX30002. Ani Hsieh,
Luis Mier, and Brandon Lindley contributed to early versions of this work.

10:48 AM K64.00011: Modeling nonequilibrium self-assembly in the cell through reaction-diffusion simulation
MATTHEW VARGA, Johns Hopkins University, OSMAN YOGURTCU, Food and Drug Administration, MARGARET JOHNSON
(Presenter), Johns Hopkins University — In diverse cellular pathways including clathrin-mediated endocytosis (CME) and viral
bud formation, cytosolic proteins must self-assemble and induce membrane deformation. These essential processes
require localization to the membrane at particular times within the cell, relying in part on the nonequilibrium activity of
energy consuming kinases, phosphatases, and ATPases to produce robust and reversible assemblies. Current
computational tools for studying self-assembly dynamics are not feasible for simulating cellular dynamics due to the slow
time-scales and the dependence on energy-consuming events. We recently developed novel reaction-diffusion algorithms
and software that enable detailed computer simulations of nonequilibrium self-assembly over long time-scales. Our
simulations of clathrin-coat assembly in CME reveal how the formation of structured lattices impacts the kinetics of
assembly, and how localization to the membrane can stabilize large, dynamic assemblies not observed in solution. We also
recently developed a relatively simple theory to quantify how localization of protein binding partners to the membrane
can dramatically enhance binding, via reduction of dimensionality. Membrane localization can thus provide a trigger for
assembly.

*NSF1753174

Wednesday, March 6, 2019 8:00 AM - 10:48 AM

Session K65 DBIO DPOLY GSNP GSOFT: Phase Separation in Biological Systems BCEC 260 - Jean-
Charles Walter, Université de Montpellier - Tag(s): Focus

8:00 AM K65.00001: Permeation of small molecules in phase separated lipid bilayer domains
MARTIN GIRARD
(Presenter), TRISTAN BEREAU, Max Planck Institute for Polymer Research — Membranes of cells are constituted of lipid bilayers,
which can phase separate into ordered domains called rafts. Recent atomic simulations have shown that ionic permeation
is enhanced at the gel-liquid interface of rafts near the melting temperature. Herein, we revisit permeation of small
molecules at raft interfaces using the coarse-grained MARTINI model. Namely, we study how the free energy of insertion
changes with the small molecule, lipid composition and temperature.

*We acknowledge funding from the Emmy Noether program of the Deutsche Forschungsgemeinschaft (DFG).
8:12AM K65.00002: Aggregation of cells dispersed in packed microgels  
CAMERON MORLEY, University of Florida, \( \text{KATHERINE KIWIMAGI, JESSE TORDOFF, RON WEISS, MIT, THOMAS ANGELINI (Presenter), University of Florida} \) — Mixtures of different types of living cells within cultured spheroids segregate in space, sometimes forming core-shell distributions. One long-standing potential mechanism behind this process is described by the differential adhesion hypotheses, which states that cells having differing levels of adhesivity will separate into groups. While this hypothesis has been tested in many ways, alternative driving forces have been proposed. To investigate an extreme limit of cell clustering and segregation, we perform studies using only one cell-type at a time, replacing all other cells with passive, non-adhesive microgel particles. Multiple cell types with tunable cadherin densities are dispersed in polyacrylamide microgels at different volume fractions and monitored over time. In this talk, we will present data on the kinetics of aggregation, the physical characteristics of clusters including fractal dimension, and the role of adhesion energy density on aggregates. By treating microgels as passive, non-adhesive “surrogate” cells, we envision testing theoretical models of active matter designed to study cell-cell phase separation, but in this case setting the appropriate parameters to zero.

8:24AM K65.00003: Evolutionary analysis of pollen patterns as a curious consequence of modulated phases  
ASJA RADJA (Presenter), University of Pennsylvania, \( \text{MAXIM O LAVRENTOVICH, Physics, University of Tennessee, ALISON SWEENEY, University of Pennsylvania} \) — Pollen grain surface morphologies are famously diverse; each species displays a unique, replicable pattern. The function of these microstructures is poorly understood, largely because it is difficult to describe these patterns in a well-defined, mathematical way. It has been shown that the templating of these patterns is created by a phase separation of a polysaccharide mixture on the cell surface. Here we present a characterization of the surface morphologies using a Landau theory of phase transitions to ordered states. We show that 10% of all morphologies can be characterized as equilibrium states with a well-defined wavelength of the pattern. The rest of the patterns have a range of wavelengths on the surface that can be recapitulated by exploring the evolution of a conserved dynamics model. We then perform an evolutionary trait reconstruction where we categorize all extant patterns into one of these two states, further binned by wavelength ranges. Surprisingly, we find that although the equilibrium states have evolved multiple times, evolution has not favored these ordered-polygonal like shapes and perhaps their patterning is simply a natural consequence of a phase separation process without cross-linkers.

8:36AM K65.00004: Spatial control of irreversible protein aggregation  
CHRISTOPH WEBER (Presenter), Biological Physics, Max Planck Institute for the Physics of Complex Systems, \( \text{THOMAS MICHAELS, L MAHADEVAN, Engineering and Applied Sciences, Harvard} \) — Liquid cellular compartments form in the cytoplasm and can regulate aberrant protein aggregation. Yet the mechanisms by which these compartments affect protein aggregation remain unknown. Here, we combine kinetic theory of protein aggregation and liquid-liquid phase separation to study the spatial control of irreversible protein aggregation in the presence of liquid compartments. We find that even for weak interactions aggregates strongly enrich inside the liquid compartment relative to the surrounding cytoplasm. This enrichment is caused by a positive feedback mechanism of aggregate nucleation and growth driven by a flux maintaining the phase equilibrium between the compartment and the cytoplasm. Our model establishes a link between specific aggregating systems and the physical conditions maximizing aggregate enrichment in the compartment. The underlying mechanism of aggregate enrichment could be used to confine cytotoxic protein aggregates inside droplet-like compartments but may also represent a common mechanism to spatially control irreversible chemical reactions in general.

8:48AM K65.00005: Density and viscosity measurements on the liquid condensates of FUS protein low-complexity domain  
CHAO JI (Presenter), \( \text{ERIC GIRARDI, NICHOLAS FAWZI, JAY TANG, Brown University} \) — Recent discoveries have revealed in living cells the formation of liquid droplets consisting of proteins, RNA & DNA. Changes in interactions among these biomolecules may result in devastating diseases, such as amyotrophic lateral sclerosis (ALS). Thus, investigating the physical properties of these liquid droplets in connection with liquid-liquid phase transition is relevant to biomolecular functions and potential therapeutic interventions. We report experiments on the dense liquid droplets formed by FUS (Fused in Sarcoma) low-complexity domain, a section of a protein involved in the development of ALS. By applying a ball drop method under a microscope, we found the density of the protein droplets greater than that of water by 10-15%, indicative of the protein concentration ~200mg/ml. The viscosity of the dilute phase containing FUS droplets is similar to that of water, but viscosity within FUS droplets is very high, ~4000 that of water. Additionally, we found FUS droplets wet solid surface poorly based on the contact angle measurement. These results confirm extremely high protein concentration and strong intermolecular cohesiveness within the condensate state.
Multicomponent Equilibrium Model for the Effects of Charge Regulation on Liquid-liquid Phase Separation of a Globular Eye Lens Protein*  
GEORGE M THURSTON (Presenter), JOHN F HAMILTON, DAVID ROSS, AARON FADDEN, Rochester Institute of Technology, CHRISTOPHER W WAHLE, Video Gaming Technologies, Inc., LEA VACCA MICHEL, JULIA FARAONE, SYMEON BUSHUNOW, Rochester Institute of Technology — We study how charge regulation affects liquid-liquid phase separation of bovine gammaB-crystallin. Our grand-canonical distribution model indicates that hundreds of charging patterns have enough probability to affect protein interactions. We measured times for rotational diffusion via nuclear magnetic resonance, and for translational diffusion to neighbors with quasielastic light scattering. Both times are orders of magnitude faster than time scales for some protonation state changes of titrating residues. Here, we apply chemical equilibrium conditions to a first-order perturbation model for the multicomponent, pattern-dependent free energy. Standard chemical potentials result from our existing dilute solution model. We estimate screened electrostatic, pattern-pair dependent interactions using a linearized Poisson-Boltzmann code that accounts for dielectric heterogeneity and includes all titratable groups. We estimate van der Waals interactions using a simplified protein geometry, and adopt an effective Hamaker coefficient by comparison with the experimental second virial coefficient. This model provides a framework for evaluating how charging pattern probabilities change with increasing concentration, and how they affect liquid-liquid coexistence.

*Supported by NIH R15EY018249

Mediator and RNA polymerase II forms phase-separated bodies and colocalizes with centrosomes during mitosis.*  
CHOONGMAN LEE (Presenter), WON-KI CHO, JAN-HENDRIK SPILLE, IBRAHIM CISSE, Department of Physics, MIT — In interphase, transcriptional proteins such as RNA polymerase II and Mediator are known to form phase-separated bodies to regulate an expression level of SE-controlled genes. However, a behavior of such proteins during mitosis, a cell cycle stage in which most transcriptional activities are silent, is still poorly understood. Here, we show that RNA polymerase II and Mediator form phase-separated bodies during mitosis. Unlike condensates in interphase which are formed based on clustered enhancer elements, condensates in mitosis are formed based on pericentriolar materials, which are phase-separated bodies in mitosis. We suggest that centrosomes play a role of not only microtubule-organizing centers but also protein storages for immediate transcriptional activities after mitosis.

*This work was supported primarily by the NIH director's New Innovator award (DP2CA19569 to I.I.C.) and also by the Pew Charitable Trusts through the Pew Biomedical Scholars Program grant (to I.I.C.)

Liquid-like protein condensates are glassy  
LOUISE JAWERTH (Presenter), Max Planck Institute for the Physics of Complex Systems, ELISABETH FISCHER-FRIEDRICH, ANTHONY HYMAN, Max Planck Institute of Molecular Cell Biology and Genetics, FRANK JULICHER, Max Planck Institute for the Physics of Complex Systems — Liquid-like protein condensates (LLPCs) are intracellular compartments that segregate material without the use of a membrane. The liquid-like behavior of the condensates is a defining characteristic and the viscosity, surface tension and other material properties determine how segregated species diffuse into and within condensates; they, thus, critically impact the biological function of the condensates. It has become increasingly clear that some LLPCs do not have time-independent material properties, but can, instead, transition to more solid, gel-like materials. Here, we present our efforts to quantify these new materials as they age in vitro. We measure the visco-elastic material properties of two proteins, PGL-3 and FUS, by means of a combination of active and passive microrheology. At early times, we find that the droplets behave much like simple liquids but gradually become less elastic. Surprisingly, the changing mechanical properties can all be scaled onto a single master curve using one characteristic time scale which grows as the sample ages. This and other features we observe bear a striking resemblance to the behaviors observed in materials with glass-like aging suggesting that LLPCs are in fact not simple liquids but, rather, a type of soft glass.
Effective long range interactions generated by polymer fluctuations induce bound particle phase separation*  

Gabriel David (Presenter), Jean-Charles Wallter, Laboratoire Charles Coulomb (L2C), CNRS, Univ. Montpellier, Montpellier, France, Chase Broedersz, Arnold Sommerfeld Center for Theoretical Physics and Center for Nanoscience, Ludwig-Maximilian-Universität München, D-80333 München, Germany, Jérôme Dorignac, Frédéric Geniet, Andrea Parmeggiani, Nils-Ole Walliser, John Palmeri, Laboratoire Charles Coulomb (L2C), CNRS, Univ. Montpellier, Montpellier, France — The confinement of chemical species within the cytoplasm is mandatory for the spatio-temporal organization of chemical activities in the cell. Cells indeed compartmentalize the intracellular space using either membrane-bound vesicles or membrane-less organelles. For the latter, cells may employ phase separation of chemical species in order to create localized high density regions in which specific reactions may occur. Such biological phase separation mechanisms often need polymeric scaffolds such as RNA or DNA to bind the chemical species. We propose a general theoretical 3D framework for such polymer-bound particles from which we derive an effective 1D lattice gas model with both nearest neighbor and long range interactions, the latter arising from polymer fluctuations. We argue that 1D phase transitions exist in such system for both Gaussian and self-avoiding polymers and, using a variational method that goes beyond mean field theory, we obtain the mean occupation/temperature phase diagram. To illustrate this model, we apply it to the biologically relevant case of the ParABS system, a prevalent bacterial DNA segregation system, to study the formation of ParBS complexes on DNA.

*This work is funded by the Agence Nationale de la Recherche (Labex Numev) and the CNRS Défi Inphyniti.

Motif Sequences and the Statistical Physics of Intracellular Phase Separation*  

Benjamin Weiner (Presenter), Princeton University, Yigal Meir, Ben Gurion University, Ned Wingreen, Princeton University — Intrinsically Disordered Proteins (IDPs) lack a unique folded structure, and yet perform diverse and important functions inside cells. Recent work suggests that some IDPs promote the formation of membrane-less organelles via phase separation, helping cells spatially organize their biomolecules. Classical theories of phase separation focus on homogeneous polymers, but IDPs have evolved particular sequences of interacting motifs. How does an IDP's motif sequence determine its physical properties? We propose a statistical physics model of IDPs to elucidate the relationship between motif sequence, conformational disorder, and biological function.

We find that motif sequences strongly influence the statistical properties of model IDPs. Intuitively, each sequence has its own set of spatial conformations which determine the relative entropy of inter- and intra-protein bonds. As a result, the concentration of IDPs required for phase separation depends strongly on the motif sequence. Our work demonstrates the emergence of spatial order from conformational disorder, a process which may play a key role in intracellular organization.

*This work was supported in part by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030).

Phase separation and migration in 2D cell co-cultures  

Manuel Gomez-Bera (Presenter), Rochester Institute of Technology, Supravat Dey, University of Delaware, Moumita Das, Rochester Institute of Technology — During morphogenesis, whether in the context of the formation of embryos or of tumors, different types of cells live in close proximity. These cells often have different physical properties. Breast epithelial cells, for example, are generally more adhesive than their cancerous counterparts. This is due to the downregulation of the protein E-cadherin, which facilitates cell-cell adhesion, in cancer cells. Cancer cells are also often more deformable than non-cancerous cells of the same tissue type. We investigate how these differences impact the organization and migration within a binary cell population. To address this, we model and simulate this system as a two-dimensional binary mixture of soft, active particles with different mechanical and adhesive properties. We characterize the phase separation in the system by monitoring the organization and growth of cell clusters with time, and the dynamics in terms of tagged cell trajectories and speeds, mean squared displacements, and non-affine motion. Our results may provide interesting insights into tumor organization, and metastasis.
**10:12AM K65.00012: In vivo dynamics and phase state of natural lipid droplets**  
MARGARITA FOMINA (Presenter), EUGENE MAMONTOV, HUGH O’NEILL, Oak Ridge National Laboratory — All organisms store lipids as energy resource for metabolism. Such lipids are accumulated in the form of intracellular droplets. The lipid droplets (LDs) contain un- and saturated triglycerides. Uncovering biophysics of LDs is crucial for metabolism manipulation or reducing lipid storage. The type and organization of lipids affect their phase state and dynamics in the droplet. We studied LDs in fresh human and porcine subcutaneous fat tissues, as well as yeast cells using quasi-elastic neutron scattering, probing molecular motions in a time scale of 6-400 ps and a length scale of 3-20 Å. The detected two-component dynamics in the droplet is associated with lipid unrestricted diffusion (D~0.006 Å²/ps) and motions of its hydrocarbon chains (D~0.2 Å²/ps) in a restricted volume (5-12 Å). The dynamics of lipids is reduced below 305 K and 266 K in porcine and human tissues, respectively, due to a fluid-gel phase transition of lipids. However, LDs in the yeast cells remain in a fluid-like state within range of 280-310 K. We believe, phase behavior of LDs is different in the tissues and microorganism due to lipid composition. Lipid packing in the droplet is tight in the tissues, having saturated lipids, and loose in the yeast droplet, having equal proportions of un- and saturated lipids.

**10:24AM K65.00013: The role of motility in Myxococcus xanthus droplet formation and droplet geometries**  
CASSIDY YANG (Presenter), KATHERINE COPENHAGEN, JOSHUA SHAEVITZ, Princeton University — Myxococcus xanthus, a rod-shaped soil bacterium lacking long-range interactions, collectively bead from surfaces when starved to form 3D droplet-like aggregates known as fruiting bodies consisting of hundreds of thousands of cells. Active self-propulsive forces of individual bacteria generate local increased pressures that drive the dewetting process. Unlike passive fluids that form axisymmetric spherical cap-shaped droplets, these aggregates are symmetry breaking and are often elongated in an elliptic-like shape. To examine the role of motility in dewetting, we present here the dynamics of both stable and unstable droplet geometries during dewetting and the formation of these fruiting bodies for cells with different Pe numbers. Using sparsely labelled cells, we also track emergent collective flows within these droplets to characterize the internal hydrodynamics and cellular organization.

*This work was supported by the following: NSF-PHY-1401506, NSF PHY-1521553, NSF PHY-1734030, and the NSF GRFP

**10:36AM K65.00014: Mechanical Interplay of Chromatin and Liquid-Liquid Phase Separated Condensates**  
DANIEL LEE (Presenter), Lewis-Sigler Institute for Integrative Genomics, Princeton University, YI-CHE CHANG, Department of Chemistry, Princeton University, YONGDAE SHIN, Department of Mechanical and Aerospace Engineering, Seoul National University, DAVID SANDERS, DAN BRACHA, Department of Chemical and Biological Engineering, Princeton University, PIERRE RONCERAY, Princeton Center for Theoretical Sciences, Princeton University, NED WINGREEN, Lewis-Sigler Institute for Integrative Genomics, Princeton University, CLIFF BRANGWYNNE, Howard Hughes Medical Institute — DNA is organized into chromatin, a complex material which stores information and controls gene expression. One mechanism for biological organization, particularly in the crowded nucleus, is liquid-liquid phase separation (LLPS). Here, we use two optogenetic technologies to show that liquid condensates displace chromatin as they grow. We also demonstrate that these synthetic condensates localize to regions of low-density chromatin. We develop a minimal physical model to explain this stiffness selectivity, wherein droplets prefer low-density chromatin regions due to a lower mechanical energy of deformation. By utilizing these spatiotemporally-controllable optogenetic systems, we construct a phase diagram of an intrinsically disordered transcriptional regulator and estimate the stiffness of the chromatin network. Our work thus not only sheds light on the role of LLPS in chromatin organization but also uses the physical principles of phase separation to elucidate mesoscale features of the nucleus.

*This work was supported in part by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030) and the Graduate Research Fellowship Program (DCE-1656466, D.S.W.L.), and NIH Grants R01 GM082938, U01 DA040601, and the Howard Hughes Medical Institute.

**Wednesday, March 6, 2019 8:00 AM - 11:00 AM**

**Session K66 DBIO: Physics of Cancer**  
BCEC 261 - Rachel Lee, University of Maryland, College Park
8:00AM K66.00001: Mathematical modeling studies on spatial profiles of cytotoxic T cells in solid tumors* XUEFEI LI (Presenter), Rice University, TINA GRUOSSO, MORAG PARK, McGill University, HERBERT LEVINE, Rice University — Infiltration of CD8⁺ T lymphocytes into solid tumors is associated with good prognosis in various types of cancer, including Triple Negative Breast Cancers (TNBC). However, the mechanisms underlying different infiltration-levels are largely unknown. Here, we have characterized the spatial profile of CD8⁺ T cells around tumor-cell clusters in TNBC. Combining mathematical modeling and data analysis, we propose that there exists a possible chemo-repellent inside tumor-cell clusters, which prevents CD8⁺ T cells from infiltrating into tumor-cell clusters. Furthermore, investigation into the properties of collagen fibers suggests that variations in desmoplastic elements does not limit infiltration of CD8⁺ T lymphocytes into tumor-cell clusters, which is consistent with the prediction of our mathematical modeling analysis whereby CD8⁺ T cells are predicted to infiltrate the fibrotic barrier.

*This work was supported by the NSF PHY-1427654, NSF DMS-1361411, The V Foundation, CQDM, the NIH, Merck, Sharpe & Dohme Corp./McGill Faculty of Medicine Grants for Translational Research, the Database and Tissue Bank Axis of the Réseau de Recherche en Cancer of the Fonds de Recherche du Québec-Santé, the Québec Breast Cancer Foundation, and the Charlotte and Leo Karassik Oncology fellowship.

8:12AM K66.00002: Tumor spheroids explode in the presence of interstitial flows revealed by a 3D microfluidic model* YU LING HUANG (Presenter), YUJIE MA, Biological & Environmental Engineering, Cornell University, CINDY WU, Chemical & Biomolecular Engineering, Cornell University, CARINA SHIAU, Biological Sciences, Cornell University, JEFFREY SEGALL, Department of Anatomy & Structural Biology, Albert Einstein College of Medicine, MINGMING WU, Biological & Environmental Engineering, Cornell University — Interstitial flows are ubiquitous in maintaining tissue homeostasis in living systems, and are known to be elevated in malignant tumors. However, most current in vitro assays are carried out in static conditions and do not include fluid flows. In our work, we developed a microfluidic model to study tumor spheroid invasion through 3D collagen architecture under well controlled flows. We discovered that tumor spheroids explode in the presence of flow in contrast to no flow condition. Possible mechanisms underlying this explosion will be discussed in my talk. Our work highlights the importance of biophysical parameters in regulating tumor cell invasion.

*NIH (Award No. R01CA221346, R21CA138366)

8:24AM K66.00003: The Role of Cell Migration Guidance Cues in Emergent Collective Behavior* RACHEL LEE (Presenter), University of Maryland School of Medicine, MATT J. HOURWITZ, PHILLIP ALVAREZ, University of Maryland, College Park, KEYATA N. THOMPSON, MICHELE I. VITOLO, University of Maryland School of Medicine, JOHN T FOURKAS, WOLFGANG LOSERT, University of Maryland, College Park, STUART S. MARTIN, University of Maryland School of Medicine — Studying the dynamics of collective systems can provide insight into how the motion of individual active agents can lead to unexpected emergent collective behavior. As tumors cells migrate to form metastases, a particularly lethal stage of cancer, the cells’ collective behavior is disrupted. Although current research largely focuses on individual cells, recent evidence shows that the most dangerous tumor cells retain the ability to move as collective strands or clusters that metastasize together. In this work, we use quantitative image analysis tools and live-cell imaging to investigate how guidance cues influence cells with different tumorigenicity, leading to distinct migration behavior.

*This research is supported by NIH grant T32-CA154274 and AFOSF grant number FA9550-16-1-0052.

8:36AM K66.00004: Breast cancer cell migration in the bone microenvironment* NATASHA COWLEY (Presenter), RHODA HAWKINS, Physics and Astronomy, University of Sheffield — We are investigating how material confining a cell affects cell motility and behaviour. In particular we look at how rigidity and geometry play a role by investigating the mechanical response of materials with different rigidities to cell generated forces. We model a cell as a viscous droplet with an active contractile boundary analogous to the actin cortex. We use the immersed boundary method to simulate a cell interacting with deformable elastic walls of various geometries. We look at the specific case of breast cancer metastasis to the bone. The majority of patients who die from cancer do so not from the primary tumour, but from the metastasis of cancer to other sites in the body. Breast cancer most commonly metastasises to the bone. We are examining how mechanical forces are involved in this process. Bone tissue is very varied in composition and vastly different from breast tissue. In order to model this varied niche we combine analytical calculations and our simulations, with AFM data from our collaborators. This will further our understanding breast cancer metastasis to the bone and it's motility in the bone microenvironment.

*EPSRC, University of Sheffield
8:48AM K66.00005: Physics of Cancer Metastasis  SEZIN GALIGOLU (Presenter), UNAM, Bilkent University, OZGE AKBULUT, Molecular Biology and Genetics, Bilkent University, ROUJIN GAFFARI, UNAM, Bilkent University, TAYFUN OZCELIK, OZGUR SAHIN, Molecular Biology and Genetics, Bilkent University, SERIM ILDAY, UNAM, Bilkent University — Metastasis is the cause of 90% of deaths related to the cancer. Cancer cells metastasize by entering the bloodstream, where they are dragged to distant parts of the body, and exiting the blood to colonize on another organ. Epithelial-Mesenchymal Transition (EMT) of cancer cells and vice versa (MET), have been proven to be the essential processes underlying metastasis through “static measurements” of biochemical cues. However, it has never been studied under dynamic conditions mimicking the actual physical environment: The blood vessel has an undulated, quasi-2D topology. Blood forms complex flows, e.g., laminar, turbulent, shear flows and their combinations inside this topology. In the bloodstream, the cancer cells are traveling along with many different cells and other entities, where they also face random obstacles. All of these factors are important for the successful completion of the metastasis process. Here, we show how epithelial, mesenchymal, drug-resistant breast cancer cells and healthy breast cells behave in such a dynamic, quasi-2D confined system under complex flows and when faced with random obstacles. We will test their adaptability under extreme physical conditions to conclude the physics of cancer metastasis.

9:00AM K66.00006: Shear stress increases acidic vesicles and proton pumps enhancing prostate cancer progression  ZEINA KHAN (Presenter), FAZLE HUSSAIN, Texas Tech University — Cells in the tumor microenvironment are subjected to increased interstitial fluid pressure due to the angiogenic growth of new leaky blood vessels which triggers lymphangiogenic growth for drainage. This subjects tumor cells to shear stresses of approximately 0.01-0.1 dynes/cm², two to three orders of magnitude smaller than wall shear stresses in blood vessels. While acidic membrane-bound vesicles, such as endosomes and lysosomes, and the V-ATPase proton pumps located on their membranes have been pursued as cancer markers, their role in cancer cell mechanotransduction and enhancing cancer aggressiveness is only recently emerging. We demonstrate that moderately metastatic prostate cancer cells respond to shear stress by increasing endosomes, lysosomes, and proton pumps, thereby activating both complexes of the mechanistic target of rapamycin pathway – mTORC1 and mTORC2 – controllers of autophagy, protein synthesis, glucose and lipid metabolism, and cell cytoskeletal changes. We will also report on shear stress-induced changes in migration and glucose metabolism, where increases accompany enhanced aggressiveness.

9:12AM K66.00007: Spatial heterogeneity of the mechanics of solid tumors  THOMAS FUHS (Presenter), ERIK W. MORAWETZ, FRANK SAUER, STEFFEN GROSSER, JOSEF A KÄS, Peter Debye Institute for Soft Matter Physics, Leipzig University — In solid tumors tissue that is stiffer than healthy tissue is formed by cells that are softer than healthy cells. We try to address this contradiction by spatially resolved investigation of the mechanics of solid tumors tissues. We are able to measure the elasticity of slices of solid tumors on the millimeter scale with micrometer spatial resolution by AFM. This avoids measuring only heavily selected regions or only single cells extracted from dissected tissue. At the same time we are able to precisely align our AFM data with immunohistological stains. We can correlate the spatial heterogeneity of the elasticity maps with the distribution of cytokeratin. We complete these measurements with elasticity data on the whole tissue scale obtained by magnetic resonance elastography and single cell data from optical stretcher measurements. Each set of measurements is performed with tissue and from the same tumor, minimizing the error through biological variance within a dataset. Through the combination of the measurements we are able to bridge the scales from single cells to tissue level, to see how the individual cells contribute to the whole.  

9:24AM K66.00008: Mechanical interactions in 3D tumor/fibroblast co-culture models of pancreatic cancer  ERIC STRUTH (Presenter), JONATHAN P CELLI, Department of Physics, University of Massachusetts Boston — Studies have shown that mechanical interactions between tumor cells and stromal components in the tumor microenvironment impact disease progression and therapeutic response. Tumors of the pancreas are associated with an abundance of stiff fibrous stroma impacting growth and drug delivery. Here we use time lapse imaging to study physical interactions between pancreatic ductal adenocarcinoma (PDAC) cells and stromal fibroblasts grown in 3D culture on laminin rich extracellular matrix (ECM). PDAC cells overlaid on ECM form compact multicellular 3D nodules. When fibroblasts are introduced there is a profound change in growth behavior culminating in the formation of large connected structures. We describe quantitative analysis of this behavior using particle image velocimetry. We contrast stromal interactions of PANC1 PDAC cells and a previously established associated drug-resistant sub-line, showing that drug naïve co-cultures and drug resistant co-cultures are quantifiably different in both distribution of per-frame average magnitude over time, as well as final spatial distribution of spheroids in the co-cultures. Going forward, the methodology for cultivating fibrotic PDAC tumors in vitro may comprise a useful platform for screening drug delivery approaches for this lethal disease.  

*ERC Advanced 741350 - HoldCancerBack
9:36AM K66.00009: Mathematical analysis of the life-span shortening in mice induced by radiation* TAKAHIRO WADA (Presenter), Department of Pure and Applied Physics, Kansai University, TETSUHIRO KINUGAWA, YUICHIRO MANABE, Division of Sustainable Energy and Environmental Engineering, Osaka University, MASAKO BANDO, RCNP, Osaka University — At Institute for Environmental Sciences, Japan, they are conducting experiments to continuously irradiate mice with low dose-rate radiation. In one experiment, they sacrifice a certain number of mice every 100 days and count the number of cancers in the body. They found that, in the irradiated group, the occurrence of cancer happens earlier and the average number of cancer is larger. In the other experiment, they keep the mice until the natural death and they found that the life span is shortened with the increase in the dose rate.

We analyzed the data with a mathematical model. Let $F_C(t)$ be the probability that a mouse has cancers at time $t$ and $P_D(t, s)$ be the probability that a mouse dies by a time $t$ due to a cancer that occurred at time $s$. Then the survival probability at time $t$, $F_S(t)$, is given as $F_S(t) = 1 - \int dF_C(s)/ds P_D(t, s) ds$. In our analysis, $F_C(t)$ is given by the cancer occurrence data. Then by assuming a function form of $P_D(t, s)$, we calculate $F_S(t)$ to compare with the survival data. We found that we can reproduce the survival data by using a simple function for $P_D(t, s)$. We obtained a parameter which expresses the interval between the occurrence of cancer and the death.

*This work was supported by JSPS KAKENHI Grant Numbers JP16H03094, JP16H04637, JP15K12204, JP15K14291.

9:48AM K66.00010: Multiscale simulation of Ras-Raf interaction SUMANTRA SARKAR (Presenter), ANGEL E GARCIA, Center for Nonlinear Studies, Los Alamos National Laboratory — Cells use a limited number of mutually interacting protein-protein interaction networks, called cell-signalling network to communicate with each other. The protein components of these signalling networks have been identified and their individual functions understood. However, how they interact with each other to produce a functional cell-signalling network is relatively poorly understood. An important cell signalling network involved in the growth and proliferation of cells is the MAPK pathway, which is activated through the formation of phosphorylated Ras-Raf protein complex. The formation of this complex at biologically relevant concentrations span multiple timescales, rendering traditional theoretical and experimental tools inadequate to study this problem in its entirety. Using recently developed accelerated simulation techniques, we have been able to overcome this barrier and have studied Ras-Raf interaction in biologically relevant concentrations and timescales. In this talk, I shall present new aspects of Ras-Raf kinetics revealed through these simulations and discuss their potential biological implications.

10:00AM K66.00011: Structure guided development of anti-cancer flexible-heteroarotinoid compounds* DONGHUA ZHOU (Presenter), MARYAM MASHAYEKHI, DIPENDRA BHANDARI, GIL REPA, Oklahoma State University-Stillwater — Flexible-heteroarotinoid compounds have been developed for their anticancer activities. The lead compound SHetA2 is able to inhibit growth of a variety of cancer cell lines and tumors in animal tests, without toxicity to normal tissues. The growth inhibition is about 84% for A2780 ovarian cancer cell cultures; the inhibition efficacy often decreases in real tissues. Therefore, it is desirable to improve efficacy and potency by designing better analogues. We identified the SHetA2 binding site on the receptor protein mortalin using NMR methods. SHetA2 disrupts the interaction of mortalin with other proteins that are upregulated in cancer cells but not in normal cells. Molecular modeling indicated that the binding strength of an analogue could be enhanced by increasing hydrophobicity of the chroman unit and substitution of a certain polar group. Five series of compounds were synthesized to validate the hypotheses. Several redesigned compounds did outperform the parent compound SHetA2, achieving inhibition efficacy of about 94% along with slightly better potency.

*We gratefully acknowledge support by Stephenson Cancer Research Center/Oklahoma Tobacco Settlement Endowment Trust, OSU President’s Fellows Faculty Research Award, and Wentz Research Scholarship (to GR).
10:12AM K66.00012: Anti-cancer drug containing apolioprotein B lipoparticle reconstitution and tracking in living cell

WEI-PING CHANG (Presenter), CHUNG CHING LIN, HSUEH-LIANG CHU, Department of Biological Science and Technology, National Chiao Tung University, Taiwan, PO-YEN LIN, Division of Core Facilities Imaging, Institute of Cellular and Organismic Biology, Academia Sinica, Taiwan, YU-CHUAN LIANG, Agricultural Biotechnology Research Center, Academia Sinica, Taiwan, CALEB G. CHEN, Department of Hematology-Oncology, Mackay Memorial Hospital, Taiwan, CHIA-CHING CHANG, Department of Biological Science and Technology, National Chiao Tung University, Taiwan — Radicicol (Rad), an Hsp 90 inhibitor, is an antitumor drug which loses its antitumor activity during delivery process, in vivo. By adding Rad in the reconstituting apolioprotein B (apoB) process, a Rad containing reconstituted apoB lipoparticle (rABL) complex (Rad@rABL) can be reconstituted and characterized by photonic spectroscopies, differential scanning calorimetry and super resolution imaging. Interestingly, the Rad@rABL single molecule can be tracked within the living cell. The drug delivery route to the mitochondria in the Hep G2 cell line can be monitored. Moreover, the anticancer efficacy of Rad can be enhanced. In summary, rABL is an excellent and native self-assembly drugs carrier and living cell tracking agent.

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

10:24AM K66.00013: Predicting patient outcomes (TNBC) based on positions of cancer islands and CD8+ T cells using machine learning approach

GUANGYUAN YU (Presenter), XUEFEI LI, HERBERT LEVINE, Rice University — The infiltrations of T are different in patients, which could be a tool for the prognosis. High CD8+ T cell counts (both overall and inside cancer-cell islands) is associated with better patient outcome. However, a cut-off of the T-cell count has to be selected manually to separate groups of patients. In this work, we propose a method to classify the small patch of triple-negative breast cancer (TNBC) tumor and use the overall percentage of “good” patches as a marker to predict the prognosis, which is an automatic method of prognosis and could also be used for other cancers. The result shows that the machine learns the importance of cell count and cell infiltration and use the combination as an indicator for prognosis.

*NSF

10:36AM K66.00014: The physics of normal and impaired mitochondrial electron transfer

PAVITHI WEERASINGHE (Presenter), MARTHA VILLAGRAN, Department of Physics and Texas Center for Superconductivity, University of Houston, AIJUN ZHANG, DALE J HAMILTON, Center for Bioenergetics, Houston Methodist Research Institute, BRIAN J MILES, Department of Urology, Houston Methodist, JAREK WOSIK, Department of Electrical and Computer Engineering and Texas Center for Superconductivity, University of Houston, JOHN H MILLER, Department of Physics and Texas Center for Superconductivity, University of Houston — The mitochondrial electron transport chain (ETC) produces most of our bodies’ energy in the form of ATP. Within the ETC, complex II, also known as succinate dehydrogenase (SDH), plays a unique role in that it converts succinate to fumarate as part of the Krebs cycle while simultaneously feeding energetic electrons to the ETC. The electrons travel along a chain of three Fe-S clusters in subunit B (SDHB) before entering the membranous domain containing a heme group and ubiquinone, which ultimately transports them to complex III. Some SDHB mutations in the form of amino acid replacements trigger aggressive growth of certain cancers, such as paraganglioma and pheochromocytoma. We will discuss our collaborative experimental and theoretical program, which includes measurements of human tissue and cell lines, and calculations of normal and mutated electron tunneling rates using Marcus theory. Our preliminary results suggest that some mutations disrupt SDHB electron pathways, causing many electrons to fail to reach their ubiquinone target and instead spill out to generate reactive oxygen species that increase tumorigenicity.

10:48AM K66.00015: Comparison of Subcellular Nanoparticle Size Distributions Across Cell Types with Light Transmission Spectroscopy

ALISON DEATSCH (Presenter), PATRICK SANSONE, NAN SUN, CAROL E TANNER, STEVEN THOMAS RUGGIERO, Physics, University of Notre Dame — The cellular cytoplasm is a complex environment with a wide breadth of both size and concentration of particles, making a comprehensive survey of the subcellular structures interesting and difficult. Using LTS, we measure optical extinction spectra over a wavelength range of ~220-1000 nm, then apply Mie Theory to obtain particle size distributions (PSD). We present improvements to previous spinach cell PSDs, as well as those of new cell types and a comparison of healthy and cancer cells. With a combination of advanced filtration and quantitative LTS (a method of obtaining the concentration directly from the magnitude of the absorption peaks in the extinction spectra), we have improved the measurement of particles <100 nm, allowing the accurate assessment of PSDs over a wide size range: from ~5 nm to 3000nm. These PSDs reveal a power law dependence of particle concentration, \( N(D) \propto D^{-\alpha} \), where \( N(D) \) is the number of particles of diameter, \( D \), per unit volume. This reflects the fractal nature of the cytoplasm as a self-similar system of spheres on many size scales, with the goal to enrich our understanding of the fundamental nature of particle packing in the cytoplasm.
Wednesday, March 6, 2019 8:00 AM - 11:00 AM

Session K69 COM: Committee on Minorities Invited Symposium BCEC 052A - Tag(s): Diversity, Invited, Undergraduate

8:00AM K69.00001: TBD [Invited] IVY JONES (Presenter), Marquette University — TBD

8:36AM K69.00002: TBD [Invited] QUINTON L WILLIAMS (Presenter), Howard University — TBD

9:12AM K69.00003: TBD [Invited] JESUS PANDO (Presenter), DePaul University — TBD

9:48AM K69.00004: TBD [Invited] WILLIE ROCKWARD (Presenter), Morgan State University — TBD

10:24AM K69.00005: TBD [Invited] NADYA MASON (Presenter), University of Illinois at Urbana-Champaign — TBD

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L01 DCMP: Fractional Quantum Hall Effect: Composite Fermions BCEC 106 - Steven Simon, University of Oxford

11:15AM L01.00001: Fractional Quantum Hall Effect at $\nu=2+6/13$: The Parton Paradigm for the Second Landau Level AJIT COIMBATORE BALRAM (Presenter), Niels Bohr International Academy and the Center for Quantum Devices, Niels Bohr Institute, SUTIRTHA MUKHERJEE, Quantum Universe Center, Korea Institute of Advanced Study, KWON PARK, School of Physics and Quantum Universe Center, Korea Institute for Advanced Study, MAISSAM BARKESHLI, Physics, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, MARK RUDNER, Niels Bohr International Academy and the Center for Quantum Devices, Niels Bohr Institute, JAINENDRA JAIN, Physics, Pennsylvania State University — The unexpected appearance of a fractional quantum Hall effect (FQHE) plateau at $\nu=2+6/13$ [Kumar et al., Phys. Rev. Lett. 105, 246808 (2010)] offers a clue into the physical mechanism of the FQHE in the second Landau level (SLL). Here we propose a \texttt{\bar{3}\bar{2}111} parton wave function and demonstrate it to be a good candidate state for this phase. We make several predictions for experimentally measurable properties that can reveal the nature of this state and also distinguish it from the topologically distinct 6/13 state realized in the lowest Landau level. Taking these results together with the recent demonstration that the related \texttt{\bar{2}\bar{2}111} wave function is a good candidate for the ground state at $\nu=2+1/2$ [Balram et al., Phys. Rev. B 98, 035127 (2018)], we propose that the \texttt{\bar{n}\bar{2}111} family of parton wave functions naturally describes the experimentally observed sequence of SLL FQHE plateaus at 2+2/3, 2+1/2 and 2+6/13, and their hole partners.

*DNRF, ERC Grant Agreement No. 678862, Villum Foundation, U. S. DOE Grant no. DE-SC0005042, NSF CAREER (DMR-1753240) and JQI-PFC-UMD. Some of the numerical calculations were performed using the DiagHam package, for which we are grateful to its authors.

11:27AM L01.00002: On the Interpretation of Thermal Conductance of the $\nu=5/2$ Edge STEVEN SIMON (Presenter), University of Oxford — Recent experiments [Banerjee et al, Nature 2018] have measured thermal conductance of the $\nu=5/2$ edge in a GaAs electron gas and found it to be quantized as $K \approx 5/2$ (in appropriate dimensionless units). This result is unexpected, as prior numerical work predicts that the $\nu=5/2$ state should be the Anti-Pfaffian phase of matter, which should have quantized $K = 3/2$. The purpose of this paper is to propose a possible solution to this conflict: if the Majorana edge mode of the Anti-Pfaffian does not thermally equilibrate with the other edge modes, then $K = 5/2$ is expected. I discuss several possible reasons for this nonequilibration, and discuss possible mechanisms in some detail. I further discuss what should be examined further to determine if this is the case.

*EPSRC grants EP/I031014/1 and EP/N01930X/1.
11:39AM L01.00003: Dirac Composite Fermions and Emergent Reflection Symmetry about Even Denominator Filling Fractions*  HART GOLDMAN (Presenter), EDUARDO HECTOR FRADKIN, University of Illinois at Urbana-Champaign — Motivated by the appearance of a “reflection symmetry” in transport experiments and the absence of statistical periodicity in relativistic quantum field theories, we propose a series of relativistic composite fermion theories for the compressible states appearing at filling fractions $\nu = 1/2n$ in quantum Hall systems. These theories consist of electrically neutral Dirac fermions attached to $2n$ flux quanta via an emergent Chern-Simons gauge field. While not possessing an explicit particle-hole symmetry, these theories reproduce the known Jain sequence states proximate to $\nu = 1/2n$, and we show that such states can be related by the observed reflection symmetry, at least at mean field level. We further argue that the lowest Landau level limit requires that the Dirac fermions be tuned to criticality, whether or not this symmetry extends to the compressible states themselves.

*This work was supported by the NSF Graduate Research Fellowship Program Grant No. DGE-1144245 (HG), by NSF Grant No. DMR1725401 (EF), and by the Perimeter Institute for Theoretical Physics. Research at the Perimeter Institute is supported by the Government of Canada through the Department of Innovation, Science and Economic Development and by the Province of Ontario through the Ministry of Research and Innovation.

11:51AM L01.00004: Partial Equilibration of Integer and Fractional Edge Channels in the Thermal Quantum Hall Effect*  KWOK WAI MA (Presenter), DMITRI FELDMAN, Brown University — Since the charged mode is much faster than the neutral modes on quantum Hall edges at large filling factors, the edge may remain out of equilibrium in thermal conductance experiments. This sheds light on the observed imperfect quantization of the thermal Hall conductance at $v=8/3$ and can increase the observed thermal conductance by two quanta at $v=8/5$. Under certain unlikely but not impossible assumptions, this might also reconcile the observed thermal conductance at $v=5/2$ with not only the PH-Pfaffian order but also the anti-Pfaffian order.

*This research was supported in part by the National Science Foundation under Grant No. DMR-1607451

12:03PM L01.00005: Finite-thickness effect of the fractional quantum Hall states in the second Landau level*  PENGJIE WANG (Presenter), JIAN SUN, YIJIA WU, International Center for Quantum Materials, Peking University, HUA CHEN, Department of Physics, Zhejiang Normal University, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, XINCHENG XIE, XI LIN, International Center for Quantum Materials, Peking University — Given the finite thickness of the samples in experiments, the in-plane magnetic field will squeeze the single-particle electron wave function in the direction perpendicular to the plane, effectively decrease the quantum well (QW) width and modify the electron interaction. However, this effect has only been reported in the non-Abelian candidate, 5/2 fractional quantum Hall (FQH) state, while other FQH states in the second Landau level (SLL), including the particle-hole conjugate of 5/2 FQH state, i.e. 7/2 FQH state, remain uninvestigated. We will present our energy gap measurements of the FQH states (7/3, 5/2, 8/3 and 7/2) in the SLL under tilted magnetic fields. A universal critical in-plane magnetic field of around 1.0 T is observed at different fillings, which corresponds to an in-plane magnetic length of around 26 nm. This critical value is comparable with the QW width of 28 nm in our sample, indicating the finite-thickness effect in the SLL. At higher in-plane magnetic fields, we found that the FQH states deviates from its strengthening tendency with in-plane field, further demonstrating the finite-thickness effect.

*The work was funded by NBPRC (2015CB921100), NSFC (11674009), Gordon and Betty Moore Foundation (GBMF4420), NSF MRSEC (DMR-1420541) and Keck Foundation.

12:15PM L01.00006: Strain-induced resistance anisotropy near the FQHE $v=5/2$ in two-dimensional GaAs single quantum wells*  ALEXANDER STERN (Presenter), Physics of Quantum Materials, Max Planck Institute for Chemical Physics of Solids, BRIAN CASAS, Department of Physics and Astronomy, University of California Irvine, JOHANNES POLLANEN, Department of Physics and Astronomy, University of California Irvine, JAMES EISENSTEIN, Department of Physics, California Institute of Technology, KENNETH WEST, LOREN PFEIFFER, Department of Electrical Engineering, Princeton University, JING XIA, Department of Physics and Astronomy, University of California Irvine — We report strain-dependent low temperature magnetotransport measurements of a two-dimensional electrons gas confined in GaAs single quantum wells. The samples are mounted to a piezoelectric-based strain device with which we can apply, and vary, tensile strain in the quantum well in situ. With this apparatus we have achieved strain as large as $-0.5\%$ in GaAs quantum wells at cryogenic temperatures. We find that with increasing strain with a high magnetic field applied causes the magnetoresistance of the two-dimensional electron system confined in the quantum well to develop anisotropic resistance near the FQHE $v = 5/2$. Additionally, we find that this strain and field induced resistance anisotropy is caused by a meta-stable phase that has a temperature dependent decay back to its isotropic state.

*The work at UC Irvine is supported by NSF Grant No. DMR-1350122
12:27PM L01.00007: Principal component analysis of quantum Hall wave functions  NA JIANG (Presenter), SIYAO KE, XIN WAN, Zhejiang University — The fractional quantum Hall effect demonstrates the robustness of topological properties in many-body systems. The effect of mass and interaction anisotropy can be understood in terms of a geometrical description. We present a study of the evolution of quantum Hall wave functions with interaction anisotropy by a statistical learning technique known as the principal component analysis (PCA). We show that the topological and geometrical aspects of a family of wave functions can be readily separated by the PCA. We discuss how to use the PCA to extract wave function metric and to determine the stability of a fractional quantum Hall phase.

12:39PM L01.00008: Hamiltonian theory for Quantum Hall systems in a tilted magnetic field: composite fermion geometry and robustness of activation gaps  KANG YANG (Presenter), University of Paris VI: Pierre-and-Marie-Curie University, MARK OLIVER GOERBIG, University of Paris-Sud, BENOÎT DOUÇOT, University of Paris VI: Pierre-and-Marie-Curie University — In 2011, Haldane showed the existence of an internal geometric degree of freedom in the description of incompressible fractional quantum Hall states. The static value of this metric tells us how the quantum Hall system reacts in the presence of anisotropy, e.g. in the electron-electron interaction. We implement this geometry into Shankar and Murthy's Hamiltonian theory, which provides an analytical framework for Jain's composite fermion (CF) picture according to which the fractional quantum Hall effect arises from an integer number of fully filled CF Landau levels. Here, we study a quantum Hall system in a tilted magnetic field. With a finite width of the system in the z-direction, the parallel component of the magnetic field induces anisotropy into the effective two-dimensional interactions. We find that this anisotropy introduces mixing of CF Landau levels and thus perturbs the Hartree-Fock CF state of the Hamiltonian theory. By changing the internal geometry of the CF, such a perturbation can be minimized by optimizing the underlying metric, and we calculate the corresponding activation gaps for different tilt angles. Our results show that the activation gaps are remarkably robust against the in-plane magnetic field in the lowest and first Landau levels.

12:51PM L01.00009: A Josephson relation for fractionally charged anyons.*  MAELLE KAPFER, PREDEN ROULLEAU, Service de Physique de l'Etat Condense, CEA Saclay, IAN FARRER, Department of Electronic and Electrical Engineering, University of Sheffield, DAVID A RITCHIE, Department of Physics, Cavendish Laboratory, CHRISTIAN GLATTLI (Presenter), Service de Physique de l'Etat Condense, CEA Saclay — Anyons (intermediate between bosons and fermions) occur in two-dimensional electron systems in high magnetic field as fractional excitations with charge \( e^* = e/q \) in the topological ordered states of the Fractional Quantum Hall Effect (FQHE). Owing to their importance for topological quantum phases and possible decoherence free quantum information approaches, understanding anyons is of utmost importance. However, experiments probing their dynamics are lacking. Here we report on a dynamical property of anyons: the long predicted Josephson relation \( f_J = e^* V / h \) for charge \( e^* = e/3 \) and \( e/5 \). It manifests as marked signatures in the Photo Assisted Shot Noise (PASN) versus voltage \( V \) when irradiating contacts at microwaves frequency \( f = f_J \). The validation of FQHE PASN models opens the way to realize time-resolved anyon sources based on levitons to perform time-domain anyon braiding.

*ANR FullyQuantum AAP CE30 grant

1:03PM L01.00010: Non-Magnetic Fractionally Quantized Conductance in Quasi-One Dimensional Semiconductor Structures*  MICHAEL PEPPER (Presenter), SANJEEV KUMAR, YILMAZ GUL, University College London, MAKSYM MYRONOV, Physics, University of Warwick, DAVID A RITCHIE, Physics, University of Cambridge, IAN FARRER, Electrical Engineering, University of Sheffield, HENRY MONTAGU, University College London — We have investigated quasi-one dimensional carrier transport using holes, (electrons), in Ge-SiGe, (GaAs-AlGaAs), heterostructures in the ballistic regime. At values of carrier concentration below about 5.1010 cm-2 the integer ground state disappears to be replaced by fractional values of conductance. This occurs when the confinement of the carriers is relaxed to be on the verge of two-dimensionality. For holes in Ge we find that, in units of \( e^2/h \), the fractional values of conductance are 1/2, spin degenerate, dropping to 1/4 in the presence of a parallel magnetic field and 1/16 which is spin polarized at zero field, (1). The accuracy of the quantization was 0.5%, possibly corresponding to fractional charges of \( e/2 \) and \( e/4 \).

For electrons in GaAs we find a rich structure, the dominant fractional values of conductance, consistently observed, are in the presence of a weak, asymmetric confinement. The values found are 2/5, 1/2 and 1/6. In the presence of a parallel magnetic field a number of other fractions started to appear, (2). These results will be discussed in relation to the formation of a zig-zag electron configuration with strong interactions between the two rows.

2. S. Kumar et al, to be published

*Supported by EPSRC,UK
Melting of interference in the fractional quantum Hall regime: Appearance of neutral modes

MITALI BANERJEE (Presenter), R BHATTACHARYYA, MOTY HEIBLUM, DIANA MAHALU, VLADIMIR UMANSKY, Department of Condensed Matter Physics, Weizmann Institute of Science — The core reason for the absence of interference of fractional charges (in the lowest Landau level) has long been a subject of discussions. Certainly there is dephasing of quasiparticles, but the agent behind this havoc was never singled out experimentally. While interference of electrons has been routinely observed in the integer regime, it gradually reduced as the filling was reduced towards \( \nu = 1 \), where it fully quenched, not to recover in the fractional regime. Here, we have systematically studied the Aharonov-Bohm interference in a Mach-Zehnder interferometer (MZI) and correlated it with the appearance of upstream neutral modes. The latter were determined by an appearance of a conductance plateau of \( \nu = 1/3 \) in a quantum point contact (QPC), which carried shot-noise. As the bulk filling approached \( \nu = 1 \) a substantial drop in the visibility was observed, concomitantly with the appearance \( \nu = 1/3 \) noisy conductance plateau in the QPC (of the MZI) - pointing at the birth of neutral modes at the QPC. Such \( \nu = 1/3 \) conductance plateau persisted throughout the hole-conjugate regime, where interference was absent. We believe that unexpected edge reconstruction, favored in a rather soft edge potential at \( 2 > \nu \geq 1 \) gives birth to upstream neutral modes that dephase the interference.

Landau level subbands as a platform for many-body localization*

AKSHAY KRISHNA (Presenter), Electrical Engineering, Princeton University, MATTEO IPPOLITI, Physics, Princeton University, RAVINDRA BHATT, Electrical Engineering, Princeton University — Previous numerical results [1] have confirmed the theoretical argument [2] that many-body localization is not possible in a Landau level in the presence of interactions and arbitrary disorder. We examine the possibility of many-body localization in subbands (both topological and non-topological) derived from the lowest Landau level. In particular, we use two specific models – a suitably engineered flat band potential, and randomly placed point-like impurities, to create subbands into which we project the problem, including both interactions and disorder. We use exact diagonalization to compute the level spacing ratio as a diagnostic of localization. The results show the absence of localization in topological subbands and the possibility of a finite-disorder many-body localization transition in non-topological subbands. This represents a novel setting for the study of many-body localization in one and two dimensions.


*This work was supported by DOE BES grant DE-SC0002140.

Bulk properties of the 5/2 fractional quantum Hall state with Corbino geometry*

JIAN SUN (Presenter), PENGJIE WANG, ZHEYI ZHU, JIASEN NIU, Peking University, LOREN PFEIFFER, KENNETH WEST, Princeton University, XI LIN, Peking University — The nature of the ground state of the fractional quantum Hall (FQH) effects at half-filling in the second Landau level has been an interesting problem. In high-quality GaAs samples, the exact quantization of the 5/2 FQH state has been observed in van der Pauw geometry, but the fully bulk insulation of the 5/2 FQH state remains unrevealed. Corbino geometry, known for its edge-free nature, has been applied in studying the bulk physics of FQH states and charge density wave states recently. We will show our observation of bulk insulation in the 5/2 FQH state with Corbino geometry at an estimated low electron temperature of 12 mK. With in-plane electrical field, the stability of the 5/2 FQH state was explored. In our measurement, the 5/2 FQH state wasn't enhanced by a weak in-plane electrical field as suggested. Our observation indicates a fully charge insulating nature of the bulk at filling factor 5/2 and could be informative for the proposed thermal conductivity measurements to search the striped Pfaffian and anti-Pfaffian state.

*The work was funded by NSFC (11674009), Gordon and Betty Moore Foundation (GBMF4420), National Science Foundation (DMR-1420541) and Keck Foundation.
1:51PM L01.00014: Half-filled Landau levels: a continuum and sign-free regularization of 3D quantum critical points*  MATTEO IPPOLITI (Presenter), Physics, Princeton University, ROGER MONG, Physics and Astronomy, University of Pittsburgh, FAKHER ASSAAD, Physics, Wuerzburg University, MICHAEL ZALETEL, Physics, University of California, Berkeley — We propose a method to regulate (2+1)-dimensional quantum critical points in which the ultraviolet cutoff is implemented by Landau level quantization, rather than by a lattice [1]. This allows numerical computations on arbitrary manifolds without introducing lattice defects. We focus on $N=4$ flavors (corresponding to the spin and valley degrees of freedom of electrons in graphene) at half filling, and introduce appropriate interaction anisotropies in flavor space to drive different types of magnetic order. We thus obtain a continuum regularization of the O(5) nonlinear sigma model (NLSM) with a topological term, which has been conjectured to flow to a deconfined critical point. We perform infinite-cylinder DMRG [2] simulations of this model and estimate the dimension of the O(5) vector to be $\Delta V \approx 0.55 - 0.70$, depending on the NLSM stiffness. This dependence may be a finite-size effect or further evidence of a weakly discontinuous transition. As the model is sign-problem-free, forthcoming quantum Monte Carlo simulations may be able to discriminate between these cases.


*MI was supported by Department of Energy BES Grant DE-SC0002140.

2:03PM L01.00015: Superconducting correlations in a fractional quantum Hall bilayer interface  JUKKA VAYRYNEN (Presenter), Microsoft Station Q Santa Barbara, MOSHE GOLDSTEIN, Tel Aviv University, YUVAL GEFEN, Weizmann Institute of Science — We consider a fractional quantum Hall bilayer system with an interface between quantum Hall states of filling fractions (0,1) and (1,1/3), motivated by recently fabricated systems by the Heiblum group (Weizmann). We show that disordered tunneling within one of the layers will drive the system to a stable fixed point with two counterpropagating charge modes which have attractive interactions. As a result, superconducting correlations on the edge become slowly-decaying. We discuss the observable effects of the phenomenon and derive general requirements for electron attraction in Abelian quantum Hall states.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L02 DMP: Topological Materials -- Optical and other Spectroscopy  BCEC 107A - Kenneth Burch, Boston College - Tag(s): Focus

11:15AM L02.00001: Magneto-infrared Spectroscopy of Topological Materials [Invited]  ZHIGANG JIANG (Presenter), Georgia Institute of Technology — The topological nature of a material is not only reflected on the surfaces or along the edges but also hidden inside the material in the bulk electronic structure. In this talk, I will describe how the bulk-sensitive magneto-infrared spectroscopy technique can be used to probe the electronic structure topology. I will use transition-metal pentatellurides (ZrTe$_5$ and HfTe$_5$, Dirac semimetals) and monopnictides (NbP, Weyl semimetals) as material examples. For the Dirac semimetals, we find that the observed Landau level transitions are similar to that in graphene but with a finite mass and the Zeeman effect opens the inverted band gap due to the large g-factor in the materials. For the Weyl semimetals, we find that the magnetic field opens a sizable gap at the charge neutrality point (Weyl annihilation) due to the finite coupling between the Weyl points and a new optical transition rule appears when the magnetic field breaks the axial symmetry. For both material systems, a semiquantitative agreement between the experiment and the effective Hamiltonian model calculation is achieved.

11:51AM L02.00002: Quantum oscillation evidence of topological semimetal phase in ZrSnTe  JIN HU (Presenter), University of Arkansas, YANGLIN ZHU, ZHIJIE TANG, Tulane University, ZHIQIANG MAO, Pennsylvania State University, DAVID E GRAF, National High Magnetic Field Laboratory, XIN GUI, WEIWEI XIE, Louisiana State University — The layered WHM - type ($W=Zr$/Hf/La, $H=Si$/Ge/$Sn$/Sb, $M=S$/Se/Te) materials represent a large family of topological semimetals, which provides an excellent platform to study the evolution of topological semimetal state with the fine tuning of spin-orbit coupling and structural dimensionality for various combinations of $W$, $H$ and $M$ elements. In this work, through high field de Haas–van Alphen (dHvA) quantum oscillation studies, we have found evidence for the predicted topological non-trivial bands in ZrSnTe. Furthermore, from the angular dependence of quantum oscillation frequency, we have revealed the three-dimensional Fermi surface topologies of this layered material owing to strong interlayer coupling.
Identification of candidate species for intercalation doping of ZrTe$_5^*$

NORMAND MODINE (Presenter), Sandia National Laboratories — ZrTe$_5$ is an interesting topological quantum material that is predicted to be a Dirac semimetal at the boundary between weak and strong topological insulator phases. In topological materials, it is highly desirable to control the doping of the material in order to adjust the Fermi level to coincide with features in the band structure. Since ZrTe$_5$ is a layered material, one approach to accomplishing this goal is “intercalation doping,” in which a dopant diffuses between the layers of the material. We have used van der Waals-corrected density functional theory to investigate the intercalation of a variety of atoms into ZrTe$_5$ with the goal of identifying promising candidates for intercalation doping. We have calculated bulk absorption energies and diffusion barriers, and where bulk interlayer diffusion rates are reasonably rapid, we have also calculated the corresponding surface properties. We conclude that Li and Pd are promising candidates for intercalation doping of ZrTe$_5$.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA0003525.

Measurements of out-of-plane magnetoresistance in ZrSiS, ZrSiSe, and HfSiS microstructures

KENT SHIRER (Presenter), KIMBERLY MODIC, TINO ZIMMERLING, MARKUS KOENIG, Max Planck Institute for Chemical Physics of Solids, LESLIE SCHOOP, Princeton University, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids — Topological nodal-line semimetals with the general formula XSiY (X = Zr, Hf and Y = S, Se, Te) have recently attracted much experimental and theoretical interest due to their properties, particularly their large magnetoresistances and high carrier mobilities. Due to the platelet-like nature of the XSiY crystals and their extremely low residual resistivities, measurements of the resistivity along the [001] direction are extremely challenging. To accomplish such measurements, microstructures of single crystals were prepared using Focused Ion Beam techniques. Microstructures prepared in this manner have very well-defined geometries and maintain their high crystal quality, verified by the quantum oscillations we observed. We will present magnetoresistance and quantum oscillation data for currents applied along both [001] and [100] in ZrSiS, ZrSiSe, and HfSiS and discuss the role microstructuring can play in the study of these materials.

Revealing Optical Transitions and Carrier Dynamics within the Bulk Band Structure of Bi$_2$Se$_3^*$

GIRIRAJ JNAWALI, SAMUEL M LINSER, IRAJ ABBASIAN SHOJAEI, SEYYEDESADAF POURNIA, HOWARD E JACKSON, LEIGH SMITH (Presenter), Department of Physics, University of Cincinnati, RYAN NEED, STEPHEN WILSON, Materials Department, University of California, Santa Barbara — Bismuth selenide (Bi$_2$Se$_3$) is a prototypical topological insulator which exhibits gapped states within the bulk and topologically protected conducting states on the surface. Here we use mid-infrared pump-probe spectroscopy on Bi$_2$Se$_3$ nanosheets exfoliated from Bridgeman grown single crystals to map the band-edge electronic structure and interrogate carrier relaxation processes over a wide energy range (0.3 to 1.2 eV). We observe direct optical transitions from spin-orbit split valence bands to the Fermi level above the lowest conduction band minimum. The photoexcited carriers thermalize rapidly to the lattice temperature within a couple of picoseconds due to optical phonon emission and scattering with the cold electron gas followed by slow electron-hole recombination within 150 ps at 10 K and 50 ps at 300 K. Knowledge of electronic structure and interaction of electrons and holes within the bulk band structure provides a foundation for understanding coupling of these states with the protected surface states.

*UC acknowledges NSF grants ECCS-1509706, DMR-1531373, and DMR-1507844. S.D.W. acknowledges the support of NSF DMR 1505549.
12:39PM L02.00006: The thickness dependent optical nonlinearity of graphene/Bi$_2$Te$_3$ heterojunction* JIA CHI LAN (Presenter), JUN PENG QIAO, WEI-HENG SUNG, Photonics, National Sun Yat-sen university, CHUN HU CHEN, Chemistry, National Sun Yat-sen university, CHENG MAW CHENG, Condensed Matter Physics Group, National Synchrotron Radiation Research Center, CHAO-KUEI LEE, Photonics, National Sun Yat-sen university — The graphene like surface state of topological insulators (TIs) have been attracted plenty of attentions. However, ultra-low saturation absorption resulting from the intrinsic bulk state of TIs limits its application, such as pulse laser. In this work, thickness dependent optical nonlinearity of graphene/Bi$_2$Te$_3$ heterojunction saturable absorber is investigated. Unlike the low saturation intensity of Bi$_2$Te$_3$ (with order of tens W/cm$^2$), the saturation intensity of graphene/Bi$_2$Te$_3$ heterojunction increases dramatically at least 4 order of magnitude. In addition, the increasing modulation depth of around 60% is characterized and the high quality 1um Q-switched solid state laser based on graphene/Bi$_2$Te$_3$ heterojunction saturable absorber is accordingly performed. Finally, the possible mechanism of carrier dynamics between p-n heterojunction and guideline for material design are proposed and discussed as well.

*The authors would like to thank the financial support by the grant of Ministry of Science and Technology under the project number of MOST 106-2112-M-110-006-MY3 and MOST 107-2218-E-110-016.

12:51PM L02.00007: Measuring the Thermal Conductivity of Semiconductors and Semimetals Using Raman Spectroscopy* IRAJ ABBASIAN SHOJAEI (Presenter), GIRIRAJ JNAWALI, SEYYEDESADAF POURNIA, SAMUEL M LINSER, HOWARD E JACKSON, LEIGH SMITH, Department of Physics, University of Cincinnati, RYAN NEED, STEPHEN WILSON, Materials Department, University of California, Santa Barbara — We present a measurement of the thermal conductivity for Bi$_2$Se$_3$ and Te and semimetals at room temperature by using Raman scattering spectroscopy on a clean prepared sample on a SiO$_2$ substrate. Aluminum is deposited on either side of the flake and is used as a heat sink at room temperature. Using a He/Ne laser (633 nm), we measure the Raman shift of the sample as a function of laser power between 0.1mW and 1mW. The linear red shift of Raman modes due to heating of the sample provides a measure of the temperature of the sample around the incident laser area. We calculate the thermal conductivity of the sample by solving a simplified one dimensional heat diffusion equation, ignoring the heat conduction to the ambient air and substrate. Our results for Bi$_2$Se$_3$ suggest a value of 4 W/mK for the thermal conductivity, comparable to the measurements of others; using the same technique we plan make measurements of several Weyl semimetals (e.g. WTe$_2$ and NbIrTe$_4$).

*UC acknowledges NSF grants ECCS-1509706, DMR-1531373, and DMR-1507844. S.D.W. acknowledges the support of NSF DMR 1505549.

1:03PM L02.00008: Signature of chiral anomaly in TaP through phonon dynamics THANH NGUYEN (Presenter), MINGDA LI, FEI HAN, NINA ANDREJEVIC, Massachusetts Institute of Technology, SONGXUE CHI, JAIME FERNANDEZ-BACA, MASAAKI MATSUDA, Oak Ridge National Laboratory, AHMET ALATAS, ESEN ALP, Argonne National Laboratory — Recent theoretical predictions discussed the possibility of detecting chiral anomaly based on phonon spectra as the exotic electronic degrees of freedom in a Weyl semimetal play an important role to influence the phonon structure. I will discuss measurements made of phonon excitations on a high-quality single crystal sample of type-I Weyl semimetal TaP using inelastic neutron and x-ray scattering spectroscopies. These measurements indicate the presence of phonon softening near the Weyl nodes which is driven by the coupling between the chiral Weyl fermions and phonons. We also observe that this coupling differs between the W1 and W2 Weyl nodes. These results provide a method to extract valuable information about the sought-after electron-phonon coupling strength.

1:15PM L02.00009: Band structure of topological insulators via cyclotron resonance ANDREI PIMENOV (Presenter), Vienna University of Technology — In the quasi-classical approximation the cyclotron mass can be directly connected to the band structure. The analysis based on the cyclotron resonance (CR) is especially useful for thin film materials in which capping layers prevent standard approaches like ARPES. Here, using the CR experiments in the terahertz range, we obtain the band structure of topological insulators (TI) based on mercury telluride (HgTe) quantum wells. In three-dimensional HgTe TI the dispersion of surface carriers is close to parabolic and it dominates the cyclotron signal. In addition, several other features are observed that can be attributed the bulk carriers. In two-dimensional HgTe TI the dispersion of electrons is close to linear showing increasingly complicated character in the region of the hole-like carriers.


This results in the flat bands only having a weak effect on the bulk properties, while the impact of the Dirac cone at the Γ-point is also limited due to it being several hundred meV above EF. We will discuss detailed results of the Fermi surface topology measurements and prospects for tuning the EF to meet either the flat bands or the Dirac cone.


*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE 1256260. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

1:39PM L02.00011: Fermi Surfaces of Flat-Band Intermetallic APd3 (A = Pb, Sn)* KAYA WEI (Presenter), National High Magnetic Field Laboratory, KUAN-WEN CHEN, JENNIFER NEU, YOU LAI, GRETA CHAPPLE, Florida State University, YAN XIN, DAVID E GRAF, LUJIS BALICAS, RYAN BAUMBACH, National High Magnetic Field Laboratory, THEO SIEGRIST, Florida State University — DFT calculations for APd3 (A=Pb, Sn) recently revealed an interesting band structure [1] that includes: a dispersionless branch along the Γ-X line, that could result in a large DOS near EF, and Dirac-like surface states. To test these predictions, we synthesized single crystals of PbPd3 and SnPd3 using the Czochralski growth technique and performed magnetoresistance and torque magnetometry measurements in magnetic fields up to 45 T. Through analysis of quantum oscillations, we uncover Fermi surface topographies that suggest the EF is roughly 50 meV above the flat band for PbPd3. This results in the flat bands only having a weak effect on the bulk properties, while the impact of the Dirac cone at the Γ-point is also limited due to it being several hundred meV above EF. We will discuss detailed results of the Fermi surface topology measurements and prospects for tuning the EF to meet either the flat bands or the Dirac cone.


*The National High Magnetic Field Laboratory is supported by National Science Foundation through NSF/DMR-1644779 and the State of Florida. KW acknowledges support from the Jack E. Crow Fellowship. LB acknowledges support from DOE-BES (No. DE-SC0002613). TS acknowledges support from NSF under grant DMR-1534818 and DMR-1849539.

1:51PM L02.00012: Novel plasmons in quantum anomalous Hall systems* JIANHUI ZHOU (Presenter), High Magnetic Field Laboratory, Hefei Institutes of Physical Science, DI XIAO, Carnegie Mellon Univ, YUGUI YAO, FURU ZHANG, Beijing Institute of Technology — We find that the inverted band structure with the Mexican-hat dispersion could enhance the interband correlation leading to a strong intrinsic plasmon excitation. Its frequency ranges from several meV to tens of meV and can be effectively tuned by the external fields. The electron-hole asymmetric term splits the peak of the plasmon excitation into double peaks. The fate and properties of this plasmon excitation can also act as a probe to characterize the topological phases even in lightly doped systems. We numerically demonstrate the impact of band inversion on plasmon excitations in magnetically doped thin films of three-dimensional strong topological insulators, which support the quantum anomalous Hall states (QAHE). We also study the chiral edge plasmons in QAHE and find many new and remarkable features of chiral edge plasmons. Our work thus sheds some new light on the potential applications of topological materials in plasmonics.


*AFOSR Grant No. FA9550-14-1-0277, the 100 Talents Program of Chinese Academy of Sciences, the MOST Project of China, the National Nature Science Foundation of China.

2:03PM L02.00013: Optical circular dichroism in an antiperovskite Dirac semimetal KATSUHISA TAGUCHI (Presenter), TAKUTO KAWAKAMI, MASATOSHI SATO, YITP, Kyoto University — We theoretically study selective circular dichroism in an antiperovskite type Dirac semimetal, which hosts Dirac fermions with high total angular momentum J. We find that unconventional circular dichroism depends on J : In J =1/2 Dirac fermion, nonzero circular dichroism is generated in Jz · J'z = ±1, where Jz and J'z are the z-component of J of the conduction band minimum and the valance band maximum around Dirac points, respectively. It is noted that this ±1 reflects on the spin angular momentum of the polarization of the applied light. On the other hand, in J =3/2 Dirac fermion, the nonzero circular dichroism is triggered in Jz · J'z = ±3. Its origin is shown in this presentation.
11:15AM L03.00001: Topological Fermi-arcs and Weyl node connectivity in the ferromagnetic Weyl semimetal Co₃Sn₂S₂  NOAM MORALI, RAJIB BATABYAL (Presenter), PRANAB KUMAR NAG, Weizmann Institute of Science, ENKE LIU, QIUNAN XU, YAN SUN, Max Planck Institute for Chemical Physics of Solids, BINGHAI YAN, Weizmann Institute of Science, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, NURIT AVRAHAM, HAIM BEIDENKOPF, Weizmann Institute of Science — Topological “Fermi-arc” surface states are guaranteed to exist on certain surfaces of Weyl semimetals. They connect the surface projection of the bulk Weyl nodes. However, in the presence of multiple pairs of surface projected Weyl nodes the actual connectivity among them is ambiguous. We use scanning tunneling spectroscopy to verify the classification of ferromagnetic Co₃Sn₂S₂ as a Weyl semimetal as well as its time reversal broken origin. By studying three different surface terminations we show that Fermi arc connectivity and Fermi-arc contour in Co₃Sn₂S₂ changes with the specific surface potential. While on the Sn surface we find intra-Brillouin zone connectivity, on the Co surface the Fermi arcs connect Weyl nodes across the Brillouin zone edge. On the S termination the Fermi–arcs hybridise with non-topological bulk and surface states thus obscuring their connectivity.

11:27AM L03.00002: A bi-directional photovoltaic shift on the surface of topological insulators  TOMOKI YOSHIKAWA (Presenter), KAZUKI SUMIDA, Graduate School of Science, Hiroshima University, Japan, YUKIKAISHI, Institute for Solid State Physics, the University of Tokyo, Japan, JAIHAU CHEN, MUNISA NURMAMAT, Graduate School of Science, Hiroshima University, Japan, KONSTANTIN A. KOKH, OLEG E. TERESHCHENKO, Novosibirsk State University, Russia, SHIK SHIN, Institute for Solid State Physics, the University of Tokyo, Japan, AKIO KIMURA, Graduate School of Science, Hiroshima University, Japan — Topological insulators (TIs) possess spin-polarized Dirac states on the surface as a result of the non-trivial topology of the bulk band structure. The surface of TIs is considered as a promising spin-electronic application. Recently, it was suggested that a generation of spin-polarized photocurrent would be possible with bulk-insulating TIs by utilizing surface photovoltage (SPV) effect. To date, SPV effect was observed for the bulk-insulating TI, Bi₂Te₂Se. However, due to the limited controllability of bulk carrier, only a uni-directional shift of the surface potential has been demonstrated. A bi-directional SPV is important for taking control of the ambipolar surface current by light. Here, we have performed time- and angle- resolved photoemission spectroscopy on bulk-insulating TIs of n- and p-type Bi₂Te₃. The experiment was carried out with linearly polarized pump (hv=1.48 eV) and probe (5.92 eV) pulses generated by Ti: sapphire laser system operating at a repetition rate of 250 kHz.

11:39AM L03.00003: Spectromicroscopic Analysis of Surface and Bulk Band Structure at a Disordered Topological Insulator Surface  ERICA KOTTA (Presenter), LIN MIAO, YISHUAI XU, Physics, New York University, AARON BOSTWICK, CHRIS JOZWIAK, ELI ROTENBERG, ALS, Lawrence National Berkeley Laboratory, TAKEHITO SUZUKI, JOSEPH CHECKELSKY, Physics, Massachusetts Institute of Technology, LEWIS A WRAY, Physics, New York University — The technique of angle resolved photoemission spectroscopy (ARPES) is widely applied to measure electronic band structures and has become central to our understanding of quantum material electronic structures over the last few decades. Recent improvements in coherent VUV light sources have driven rapid developments in the focused beam spot for ARPES, down to the d<10um diameter scale with little sacrifice, and the d~100nm scale with reduced flux. For this talk I will present ARPES spectromicroscopy data which was used to map the surface band structure of a beam-sensitive topological insulator sample (disorder-enriched Bi₂Se₃). New data analysis methods are developed to obtain quantitative electronic structure information in spite of the flux sensitivity of the surface, revealing a complex structural environment in which fluctuations in the surface and bulk state energetics are found to be mostly decoupled.
Topological nodal-line semimetals in ferromagnetic rare-earth-metal monohalides

SI-MIN NIE (Presenter), Stanford University, HONGMING WENG, Institute of Physics, Chinese Academy of Sciences, FRITZ PRINZ, Stanford University — Topological semimetals, extending the topological classification from insulators to metals, have greatly enriched our understanding of topological states in condensed matter. Here we identify layered materials as promising candidates for hosting TNLSs. Based on first-principles calculations and effective model analysis, we propose that layered ferromagnetic rare-earth-metal monohalides LnX (Ln=La, Gd; X=Cl, Br) exhibit long pursued topological phases. Specifically, single-layer LaX and single-layer GdX are ideal two-dimensional (2D) Weyl semimetals and large-gap 2D quantum anomalous Hall insulators (QAHIs), with band gaps up to 61 meV, respectively. In addition, 3D LaX and 3D GdX are TNLSs with a pair of mirror-symmetry protected nodal lines and 3D QAHIs, respectively. The nodal lines in 3D LaX extending through the whole Brillouin zone (BZ) are fairly robust against strong spin-orbit coupling (SOC) and located close to the Fermi level, providing a novel platform toward exploring the exotic properties in nodal-line fermions as well as related device designs.

*F. B. P. and S. N. were supported by Stanford Energy 3.0. H. W. was supported by the National Key Research and Development Program of China under grant No. 2016YFA0300600, and NSFC under grant number 11421092.

Weak topological insulator state in quasi-one-dimensional bismuth iodide observed by surface-selective nano-ARPES

RYO NOGUCHI (Presenter), Institute for Solid State Physics, University of Tokyo, TAKANARI TAKAHASHI, Materials and Structures Laboratory, Tokyo Institute of Technology, KENTA KURODA, Institute for Solid State Physics, University of Tokyo, MASAYUKI OCHI, Department of Physics, Osaka University, TETSURO SHIRASAWA, National Metrology Institute of Japan, National Institute of Advanced Industrial Science and Technology, CÉDRIC BAREILLE, MASATO SAKANO, MITSUHIRO NAKAYAMA, Institute for Solid State Physics, University of Tokyo, MATTHEW WATSON, Diamond Light Source, KOICHIRO YAJI, AYUMI HARASAWA, Institute for Solid State Physics, University of Tokyo, HIDEAKI IWASAWA, PAVEL DUDIN, TIMUR KIM, Diamond Light Source, MORITZ HOESCH, DESY, VIKTOR KANDYBA, ALESSIO GIAMPIETRI, ALEXEI VICTOROVICH BARINOV, Elettra-Sincrotrone Trieste, SHIK SHIN, Institute for Solid State Physics, University of Tokyo, RYOTARO ARITA, RIKEN Center for Emergent Matter Science, TAKAO SASAGAWA, Materials and Structures Laboratory, Tokyo Institute of Technology, TAKESHI KONDO, Institute for Solid State Physics, University of Tokyo — Recently, various materials have been confirmed to be topologically non-trivial by angle-resolved photoemission spectroscopy (ARPES) [1]. Despite intensive research on topological materials, a weak topological insulator (WTI) has so far remained hypothetical, since topological surface states (TSS) emerge only on the side surfaces, which are usually undetectable by conventional ARPES. We have overcome this difficulty by employing newly developed nano-ARPES. Its high spatial resolution allows us to perform surface selective measurements, which is necessary for the discovery of a WTI state in real 3D crystals.

In this contribution, we provide first experimental evidence for a WTI state in quasi-one-dimensional $\beta$-Bi$_4$I$_4$. The crystal has naturally cleavable top and side surfaces both stacked via van-der-Waals forces, and TSSs emerge only on the side surface as the WTI phase [2,3]. Our nano-ARPES results reveal quasi-1D Dirac-like surface state emerge only on the side surface while the top surface is topologically dark, which is the hallmark of the WTI state in $\beta$-Bi$_4$I$_4$ [4].

12:15PM L03.00006: Large magnetic gap at the Dirac point in a Mn-induced Bi$_2$Te$_3$ heterostructure* OLIVER RADER (Presenter), EMILE RIENKS, PARTHA M. MANDAL, Helmholtz-Zentrum Berlin, ONDREJ CAHA, JAN RUZICKA, Masaryk University Brno, ANDREAS NEY, HUBERT STEINER, VALENTYN V. VOLOBUYEV, HEIKO H. GROISS, Johannes Kepler Univ. Linz, SALEEM KHAN, JAN MINÁR, University of West Bohemia Pilsen, MIHAELA ALBU, Graz Center for Electron Microscopy, HUBERT EBERT, Ludwig-Maximilians-Universitat Munchen, GÜNTHER BAUER, Johannes Kepler Univ. Linz, ANDREI VARYKHALOV, JAIME SÁNCHEZ-BARRIGA, Helmholtz-Zentrum Berlin, STEFAN WIMMER, GUNTER SPRINGHOLZ, Johannes Kepler Univ. Linz — A magnetic gap at the Dirac point of topological insulators has so far never been observed directly. Here, we use low temperature ARPES to reveal the magnetic gap of Mn-doped Bi$_2$Te$_3$ films which is present only below T$_C$ of 10-12 K. Surprisingly, the gap is 5 times larger than predicted by density functional theory. We show that this enhancement is due to a remarkable structure modification induced by Mn doping. Instead of a disordered impurity system, it forms an alternating sequence of septuple and quintuple layer blocks, with Mn in the center of the septuple layers. Mn-doped Bi$_2$Se$_3$ forms a similar heterostructure, however, only a large, albeit nonmagnetic gap is formed. We explain both differences based on the higher spin-orbit interaction in Bi$_2$Te$_3$. The present findings provide crucial insights for pushing the lossless transport properties of topological insulators towards room temperature.

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12:27PM L03.00007: Directly photoexcited Dirac and Weyl fermions in ZrSiS and NbAs JAEHUN KIM (Presenter), CHRISTOPHER P WEBER, Santa Clara University, LESLIE SCHOOP, Chemistry, Princeton University, STUART S P PARKIN, Max Planck Institute of Microstructure Physics, ROBERT NEWBY, Santa Clara University, ALEXANDR NATEPROV, Applied Physics, Academy of Sciences of Moldova, BETTINA LOTSCH, Max Planck Institute for Solid State Research, M. BALA MURALI KRISHNA, KESHAV M DANI, Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology Graduate University, HANS BECHTEL, Advanced Light Source Division, Lawrence Berkeley National Laboratory, ERNEST ARUSHANOV, Applied Physics, Academy of Sciences of Moldova, MAZHAR ALI, Max Planck Institute of Microstructure Physics — We report ultrafast optical measurements of the Dirac line-node semimetal ZrSiS and the Weyl semimetal NbAs, using mid-infrared pump photons from 86 meV to 500 meV to directly excite Dirac and Weyl fermions within the linearly-dispersing bands. In NbAs the photoexcited Weyl fermions initially form a non-thermal distribution, signified by a brief spike in the differential reflectivity whose sign is controlled by the relative energy of the pump and probe photons. In ZrSiS electron-electron scattering rapidly thermalizes the electrons, and the spike is not observed. Subsequently hot carriers in both materials cool within a few picoseconds. This cooling, as seen in the two materials’ differential reflectivity, differs in sign, shape, and timescale. Nonetheless, we find that it may be described in a simple model of thermal electrons, without free parameters. The electronic cooling in ZrSiS is particularly fast, which may make the material useful for optoelectronic applications.

12:39PM L03.00008: Symmetry protected band crossings of spin-orbit coupled surface states of NbGeSb IGOR MARKOVIĆ (Presenter), OLIVER J CLARK, FEDERICO MAZZOLA, MATTHEW WATSON, University of St Andrews, PHILIP MURGATROYD, MATTHEW DYER, University of Liverpool, CHRISTOPHER ANDREW HOOLEY, University of St Andrews, JONATHAN ALARIA, University of Liverpool, PHILIP KING, University of St Andrews — The electronic structure of materials in the ZrSiS family of nonsymmorphic semimetals hosts, alongside their bulk Dirac line nodes, peculiar surface states created by the breaking of nonsymmorphic symmetry at the surface layer [1-3]. We study the surface electronic structure of NbGeSb (isotransitional to ZrSiS) using spin- and angle-resolved photoemission spectroscopy (ARPES) and density-functional theory (DFT). We observe two pairs of surface states, hosting large Rashba-like spin-splittings, split off from the bulk manifold. We find how these two branches intersect each other, forming a fourfold crossing structure along the Brillouin zone boundary. Surprisingly, we find a counter-intuitive hybridisation structure around these crossings, with three remaining protected and just a single hybridised anti-crossing. We demonstrate how a mirror symmetry line provides protection along the Brillouin zone face, opening new routes to realising complex intertwined spin textures of spin-orbit coupled surface states.

12:51PM L03.00009: Non-Hermitian Hopf-Link Exceptional Line Semimetals* YANG ZHESEN (Presenter), JIANGPING HU, Chinese Academy of Sciences — We study a new class of non-Hermitian topological phases in three dimension, where the topological robust band degeneracies are Hopf-link exceptional lines. As a concrete example, we investigate the non-Hermitian band structure of nodal line semimetals under non-Hermitian perturbations, where the Fermi surfaces can transit from 1d nodal lines to 2d twisting surfaces with Hopf-link boundaries. The topological invariants of these linked exceptional line phases are also proposed. Due to non-Hermitian skin effect, We also find a huge difference between the band structure of periodic and open boundary conditions. After complexification of the momentum in the Bloch Hamiltonian, we find the correct bulk-boundary correspondence in non-Hermitian system. The possible experimental realizations are also discussed.

*Ministry of Science and Technology of China 973 program (No. 2015CB921300, No. 2017YFA0303100), National Science Foundation of China (Grant No. NSFC- 1190020, 11534014, 11334012), and the Strategic Priority Research Program of CAS (Grant No.XDB07000000).

1:03PM L03.00010: Fragility of Fermi arcs in Dirac semimetals* YUN WU (Presenter), NA HYUN JO, LIN-LIN WANG, CONNOR SCHMIDT, KATHRYN NEILSON, BENJAMIN SCHRUNK, PRZEMYSLAW SWATEK, ANDREW EATON, SERGEY L. BUD’KO, PAUL CANFIELD, ADAM KAMINSKI, Iowa State University — We use tunable, vacuum ultraviolet laser-based angle-resolved photoemission spectroscopy and density functional theory calculations to study the electronic properties of Dirac semimetal candidate PtBi2. In addition to bulk electronic states we also find surface states as expected from theory and band calculations. The topological surface states form Fermi pockets rather than double Fermi arcs that were observed in Na3Bi. The surface bands forming the Fermi pockets merge with bulk bands in proximity of the Dirac points, as expected. Our data confirms existence of Dirac states in PtBi2 and reveals the fragility of the Fermi arcs in Dirac semimetals. Because the Fermi arcs are not topologically protected in general, they can be deformed into Fermi pockets, as proposed by Kargarian et al.. Our results demonstrate validity of this theory in PtBi2.

*Research was supported by the US DOE, Office of Basic Energy Sciences under Contract No. DEAC02-07CH11358; Ames Laboratory’s Laboratory-Directed Research and Development (LDRD) funding. Gordon and Betty Moore Foundation EPiQS Initiative (Grant No. GBMF4411); CEM, a NSF MRSEC, under Grant No. DMR-1420451.

1:15PM L03.00011: Intrinsic Fermi Arc Re-wiring in NbIrTe4 SANDY ADHITIA EKAHANA (Presenter), Oxford University-USE 4643, YAN SUN, Max Planck Institute for Iron Research GmbH, HIROMASA NAMIKI, Tokyo Institute Of Technology, HAIFENG YANG, Chinese Academy of Sciences (CAS), JUAN JIANG, Lawrence Berkeley National Laboratory, WUJUN SHI, Max Planck Institute for Iron Research GmbH, CHAOFAN ZHANG, National University of Defense Technology, YIWEI LI, DING PEI, Oxford University-USE 4643, TAKAO SASAGAWA, Tokyo Institute Of Technology, CLAUDIA FELSER, Max planck institute, BINGHAI YAN, Weizmann Institute of Science, ZHONGKAI LIU, ShanghaiTech, YULIN CHEN, Oxford University-USE 4643 — NbIrTe4 which is a semimetal that breaks inversion symmetry predicted to host only four Weyl points. This simplest configuration is confirmed by the measurement from the top and bottom surface of NbIrTe4 showing only a pair of Fermi arcs each. Furthermore, it is found that the Fermi arc connectivity on the bottom surface experiences re-wiring as it evolves from Weyl points energy to the ARPES Fermi energy level. This change is attributed to the hybridisation between the surface and the bulk states as their projection lie within the vicinity of each other. The finding in this work demonstrates that although Fermi arcs are guaranteed in Weyl semimetals, their shape and connectivity are not protected and may be altered accordingly.

1:27PM L03.00012: ARPES study on the electronic structure of VTe2 with double zigzag chains MITSUISHI NATSUKI (Presenter), YUSUKE SUGITA, SAEED BAHRAMY, MANABU KAMITANI, TATSUYA SONOBE, MASATO SAKANO, The University of Tokyo, TAKAHIRO SHIMOJIMA, RIKEN CEMS, KOJI HORIBA, HIROSHI KUMIGASHIRA, KEK-PF, KAZUAKI TAGUCHI, KOJU MIYAMOTO, TAICHI OKUDA, Hiroshima University, SHINTARO ISHIWATA, YUKITOSHI MOTOME, KYOKO ISHIZAKA, The University of Tokyo — Layered transition metal dichalcogenide (TMDC) has been a well-known system to host a variety of charge density waves (CDW) reflecting its quasi-two-dimensionality. More recently, there has been increasing interest in spin-orbit coupling effect and topological aspects of TMDC. VTe2 has a trigonal CdI2-type structure (so-called 17 phase) at high temperature, consisting of trigonal layers formed by edge-sharing VTe6 octahedra. Below ~485 K, it undergoes a peculiar structural phase transition to the monoclinic 17” phase. In this phase, VTe2 exhibits the 3×1×3 superstructure characterized by the formation of double zigzag chains of vanadium [1], which has been discussed in terms of CDW. In this talk, we report on the peculiar modification of the electronic structures via the 17-17” phase transition clarified by utilizing angle-resolved photoemission spectroscopy (ARPES) and first-principles calculations.

1:39PM L03.00013: New class of Chiral topological nodes in transition metal silicide CoSi  
ZHICHENG RAO (Presenter), Institute of Physics — Exotic chiral topological nodes with nonzero chern number and multiple degeneracy, distinct from conventional Dirac and Weyl nodes, could exist in crystalline semimetals with certain space group symmetries. The projections of these chiral topological nodes with opposite chern number are connected by topologically protected surface fermi arcs. Several other types of chiral topological nodes have been predicted by theorists, but the direct experiment evident is still lacked. Here, we will report that two types of new chiral nodes are revealed by using angel-resolved photoemission spectroscopy in transition metal silicide CoSi.

1:51PM L03.00014: Cyclotron antiresonance in the topological insulator Bi$_2$Te$_3$ studied in Voigt geometry  
SASA DORDEVIC (Presenter), The University of Akron, HECHANG LEI, CEDOMIR PETROVIC, Brookhaven National Laboratory, SEONGPHILL MOON, DMITRY SMIRNOV, National High Magnetic Field Laboratory — We have previously observed cyclotron antiresonance in a canonical 3D topological insulator Bi$_2$Te$_3$ in Faraday geometry. We now supplement those results with the recent measurements in Voigt geometry. Antiresonance is also present in this geometry, but an additional absorption feature is also detected, whose origin is currently unknown. Possible explanation of these effects will be discussed within the model which uses an unconventional form of the Lorentz force that external magnetic field exerts on charge carriers.

2:03PM L03.00015: Observation of Quasi-one-dimensional Edge State in ZrTe$_5$ by Angle-resolved Photoemission Spectroscopy  
DONG QIAN (Presenter), FENGFENG ZHU, WENXIANG JIANG, Shanghai Jiao Tong University — Single-layer ZrTe$_5$ was known as a two-dimensional topological insulator, while ZrTe$_5$ bulk crystal consisting of many ZrTe$_5$ layers has been argued as either a three-dimensional strong topological insulator or a weak topological insulator. Using high-resolution photon-energy dependent angle-resolved photoemission spectroscopy, we succeeded in observing a quasi-one-dimensional and linearly dispersive energy band near the Fermi level on the surface that is perpendicular to the two-dimensional ZrTe$_5$ layers. The observed quasi-one-dimensional band comes from the one-dimensional topological edge state of the ZrTe$_5$ layers. The weak dispersion of the quasi-one-dimensional band along the normal direction of ZrTe$_5$ layer indicates that the inter-edge coupling between the ZrTe$_5$ layers are not strong enough to form a three-dimensional strong topological insulator. Our findings provided the comprehensive information about the quasi-one-dimensional edge state and unambiguously indicated that ZrTe$_5$ bulk crystal is a three-dimensional weak topological insulator.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L04 DMP: Dirac/Weyl Semimetals -- Materials Prediction II BCEC 107C - Dmytro Pesin, University of Virginia - Tag(s): Focus

11:15AM L04.00001: Composite Dirac Semimetal  
ZIMING ZHU (Presenter), Hunan Normal University, ZHI-MING YU, WEIKANG WU, Singapore University of Technology and Design, WEI ZHANG, Fujian Normal University, FAN ZHANG, University of Texas at Dallas, SHENGYUAN YANG, Singapore University of Technology and Design — In this work, we investigate the possibility to construct a new topological state, which may be regarded as a combination of a WTI and a Dirac semimetal, hence it may be termed as a composite Dirac semimetal (CDSM). We start with an effective model, which can be derived from a tight-binding model defined on a stacked honeycomb lattice. By analyzing the possible band ordering at the high symmetry points on the rotation axis, we show that a CDSM state can be realized, for which one pair of low-energy bands cross at the Fermi level to form two symmetry-protected Dirac points, whereas another pair of bands have inverted band ordering along the high symmetry path. The hallmark of this state is that on the side surfaces, a pair of Fermi arcs connecting the projected Dirac points coexist with a pair of helical Fermi loops traversing the surface Brillouin zone (BZ). Without breaking any symmetry, the CDSM may undergo a topological phase transition to an insulating state via a band inversion scenario, accompanied by two pairs of helical surface Fermi loops. Finally, by using first-principles calculations, we show that the discussed physics can be realized in a realistic material system.
First-Principles Prediction of New Magnetic Weyl Semimetals: Cobalt-Based Shandites System

YUMA NAKAMURA, WEI LUO (Presenter), JINSEON PARK, Department of Physics and Astronomy, The University of Tennessee (Knoxville), MINA YOON, CNMS, Oak Ridge National Lab — The experimental confirmation of Co3Sn2S2 as the first magnetic Weyl semimetal (MWSM) paved the way to explore new magnetic Weyl semimetals. Cobalt-based shandite consists of T3M2X2 (T = Co; M = Ge, Sn, Pb; X = S, Se) in a rhombohedral arrangement with rotational symmetry, inversion symmetry, and a kagome layer formed by Co. Using a first-principles approach coupled with a global structure search algorithm, we explored energetically stable configurations of Co-based shandites and their alloys (T3M1M2X2, where M1/M2 = Ge, Sn, and Pb). We characterized their electronic properties by establishing a tight-binding Hamiltonian with parameters extracted from maximally localized Wannier functions, and identified new MWSMs. The Weyl points of new MWSMs are formed by p-orbitals of elements M located between the kagome layer and d-orbitals of Co on the kagome layer, where their location and energy level changes as a function of M. A wider class of new MWSMs that can be synthesized experimentally is proposed.

Pairing and charge order in a strongly-interacting Weyl system: Numerically exact results from auxiliary-field quantum Monte Carlo

PETER ROSENBERG (Presenter), NIRAJ ARYAL, EFSTRATIOS MANOUSAKIS, National High Magnetic Field Laboratory, Florida State University — The recent discovery of Weyl semimetals has generated intense interest in their properties. These materials have been predicted to exhibit a number of fascinating behaviors, including topological superconductivity. Here we study a model Weyl system subject to strong interactions using the numerically exact auxiliary-field quantum Monte Carlo technique. We focus on charge and pairing properties, in order to explore the interplay of Weyl physics, charge order, and superconductivity. These high-accuracy results will complement ongoing experimental efforts in Weyl systems, and help guide the search for exotic pairing phenomena in these systems, which can be realized in both real materials and ultra-cold atoms.

Mixed axial-torsional anomaly in Weyl semimetals

YAGO FERREIROS, Royal Institute of Technology, YARON KEDEM, EMIL J BERGHOLTZ, Stockholm University, JENS BARDARSON (Presenter), Royal Institute of Technology — We show that Weyl semimetals exhibit a mixed axial-torsional anomaly in the presence of axial torsion, a concept exclusive of these materials with no known natural fundamental interpretation in terms of the geometry of spacetime. This anomaly implies a nonconservation of the axial current—the difference in current of left- and right-handed chiral fermions—when the torsion of the spacetime in which the Weyl fermions move couples with opposite sign to different chiralities. The anomaly is activated by driving transverse sound waves through a Weyl semimetal with a spatially varying tilted dispersion, which can be engineered by applying strain. This leads to sizable alternating current in presence of a magnetic field that provides a clear-cut experimental signature of our predictions.

Evolution of the surface states of the Luttinger semimetal under compressive strain and broken inversion symmetry

EWELINA HANKIEWICZ (Presenter), JULIAN-BENEDIKT MAYER, MAXIM KHARITONOV, University of Wurzburg — Luttinger semimetal, the quadratic-node semimetal for  electrons under full cubic symmetry, is the parent highest-symmetry minimal model for a variety of topological and/or strongly correlated materials, such as HgTe, α-Sn, and iridate compounds. Recently, Luttinger semimetal has been demonstrated [1] to exhibit surface states of topological origin that can be attributed to approximate chiral symmetry. In the present work, we theoretically study the effect of the symmetry-lowering perturbations on these surface states within an analytical model. Under compressive strain lowering rotational symmetry, Luttinger semimetal becomes a Dirac semimetal with a pair of double-degenerate linear nodes. Breaking further inversion symmetry, the system turns into a Weyl semimetal, with each Dirac node split into four Weyl nodes. We analyze the corresponding evolution of the surface states, and its relation to the surface states of the full Kane model.


We acknowledge financial support from the DFG via SFB 1170 “ToCoTronics” and the ENB Graduate School on Topological Insulators.
12:15PM L04.00006: The effect of interaction and gauge field in topological semimetals

CHAOXING LIU (Presenter), Pennsylvania State University, RUI-XING ZHANG, University of Maryland, PENG YE, Sun Yat-sen University, XIAOLIANG QI, Stanford University, HONGWEI JIA, WENLONG GAO, QINGHUA GUO, BIAO YANG, JING HU, YANGANG BI, Univ of Birmingham, YUANJIANG XIANG, Shenzhen University, SHUANG ZHANG, Univ of Birmingham — Topological semimetals possess topologically protected nodal points or lines with exotic physical properties. Here I focus on the effects of interaction and gauge field on topological Weyl or Dirac semimetals. I will first show that in a nanowire made of Dirac semimetals, interaction enables the emergence of boundary Majorana zero modes that are protected by rotation symmetry under magnetic fields [1]. Therefore, the Dirac semimetal nanowire provides an ideal platform for the realization of 1D interacting topological phase with Majorana physics, which does not require superconductivity and is thus number-conserving. Next I will describe the influence of generalized gauge fields in Weyl semimetals [2,3]. Due to the chirality of Weyl nodes, it was realized that more general form of gauge fields beyond conventional electromagnetic fields can be induced by magnetic fluctuation or strain in Weyl semimetals. As a consequence of gauge fields, zeroth Landau levels can be induced and only propagate in one direction (chiral). The presence of chiral zeroth Landau levels is the origin of chiral anomaly and allows for a robust bulk transport. Such generalization of gauge fields is recently demonstrated in an inhomogeneous Weyl metamaterial experimentally [3].

References:

* I acknowledge the support from ONR under No. N00014-18-1-2793, DOE under award No. DE-SC0019064 and Charles E. Kaufman Foundation.

12:51PM L04.00007: Level statistics of disordered Weyl semimetals

XIANG RONG WANG (Presenter), Hong Kong University of Science and Technology, CHEN WANG, PENG YAN, School of Electronic Science and Engineering, University of Electronic Science and Technology of China — The level statistics and the fractal nature of electron wavefunction around Weyl nodes of disordered Weyl semimetals are numerically investigated. The nearest-neighbor level spacing follows a new universal distribution originally proposed for the level statistics of critical states in the integer quantum Hall systems or normal dirty metals (diffusive metals) at metal-to-insulator transitions, instead of the Wigner-Dyson distribution for diffusive metals. The wavefunction at a Weyl node occupies a fractal space of dimension 2.18, in contrast to the extended states that spread over the whole space (D=3). The finite size scaling of the inverse participation ratio (IPR) suggests that the correlation length of wavefunctions at Weyl nodes (E=0) diverges as ξ \sim |E|^{-\nu} with \nu=0.89. In the ergodic limit, the level number variance around Weyl nodes increases linearly with the average level number N.

* National Natural Science Foundation of China (Grants No.~11374249 and 11704061) and Hong Kong RGC (Grants No.~16301518 and 16300117). CW is supported by UESTC and the China Postdoctoral Science Foundation (Grants No.~2017M610595 and 2017T100684)
1:03PM L04.00008: Emergent Weyl Nodes and Monopole Charge Density Wave State*  
YI LI (Presenter), ERIC BOBROW, CANON SUN, Johns Hopkins University — We study a new class of topological charge density wave states exhibiting monopole harmonic symmetries. When electron and hole Fermi surfaces carry different Chern numbers, the particle-hole pairing exhibits a non-trivial Berry phase inherited from band structure topology independent of concrete density-wave ordering mechanism. The associated density-wave gap functions become nodal, and the net nodal vorticity is determined by the monopole charge of the pairing Berry phase. The gap function nodes become zero-energy Weyl nodes of the bulk spectra of quasi-particle excitations. These states can occur in doped Weyl semimetals with nested electron and hole Fermi surfaces enclosing Weyl nodes of the same chirality in the weak coupling regime. Possible signatures of monopole harmonic charge density waves are proposed for scattering experiments.

*We acknowledge the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, Grant No. DE-FG02-08ER46544 and support from the Alfred P. Sloan Research Fellowships.

1:15PM L04.00009: Non-Abelian Statistics in Momentum Space*  
QUANSHENG WU, EPFL Lausanne, ALEXEY A SOLUYANOV, University of Zurich, TOMAS BZDUSEK (Presenter), Stanford University — We develop a general theory describing the stability and conversions of a wide range of band-structure nodes. The technique readily applies to a plethora of nodes existing in semimetals and superconductor, while it also reveals various previously unknown nodal features. Especially, we find that band-structure nodes in PT-symmetric systems with negligible spin-orbit coupling carry a non-Abelian charge, thus suggesting non-trivial braiding rules in momentum space. The non-Abelian charge also poses constraints on admissible nodal-line composition in 3D systems, and on the topological transitions between various such compositions. We emphasize that the non-Abelian property arises without the need of electron interactions.

In this talk, I motivate our description of band-structure nodes based on homotopy theory, and demonstrate its power on several simple examples. Afterwards, I clarify the meaning of the non-Abelian charge arising in PT-symmetric systems, and show how it constraints nodal compositions in a simple metal, namely elemental scandium (Sc) under strain. Our predictions could be experimentally tested in photoemission experiments.

*T. B. was supported by the Gordon and Betty Moore Foundations EPIQS Initiative, Grant GBMF4302.

1:27PM L04.00010: Classification of composite Weyl fermions  
DANIEL GOSÁLBEZ MARTÍNEZ (Presenter), OLEG YAZYEV, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland — Weyl nodes with chiral charge ±1 are classified as types I and type II according to the tilting of the conical band dispersion at the band degeneracy. Their Fermi surface, described by a quadratic form, is different for these two types. We extend this classification to the case of composite Weyl nodes with chiral charge larger than one. When the C4 and C6 rotation symmetries forbid the linear band dispersion on the plane perpendicular to the symmetry axis, new terms with quadratic and cubic momentum dependence must be included. Consequently, the Fermi surface produced by these band degeneracies are described by a 4 or 6 order algebraic surfaces. In this more complex situation, instead of classifying Fermi surfaces, we study numerically the possible Lifshitz transitions of the Fermi surface produced by a composite Weyl node as the chemical potential is varied. We use this methodology to study quadratic Weyl nodes generated by the C4 rotation symmetry. We find that such band degeneracies present four different types of morphologies, two analogous to the type-I and type-II case of the conical Weyl nodes, and two new distinct morphologies within the type-II class. We illustrate the existence of these new types of band degeneracies in real materials such as bcc iron.

1:39PM L04.00011: Computational search for magnetic Weyl semimetals in rare-earth compounds*  
LIN-LIN WANG (Presenter), Ames Laboratory, NA HYUN JO, YUN WU, BRINDA KUTHANAZHI, ADAM KAMINSKI, PAUL CANFIELD, Iowa State University — Weyl fermions are of interests for both basic science and future technology. Weyl points in electronic band structure can be generated by breaking inversion or/and time-reversal symmetry to realize linear crossings having monopoles of Berry curvature. Here we have used high throughput band structure calculations based on density functional theory to search for magnetic Weyl semimetals in rare-earth compounds. The existence of Weyl points is identified by calculating Berry curvature. We find that the magnetic Weyl points depend on the specific magnetic ordering structure.

*This work is supported by the Center for Advancement of Topological Semimetals, an Energy Frontier Research Center funded by the US DOE Basic Energy Sciences, through the Ames Laboratory under Contract No. DE-AC02-07CH11358. NHJ is funded by the Gordon and Betty Moore Foundation’s EPIQS Initiative through Grant GBMF4411.
1:51PM L04.00012: Optical Properties of Weyl Semimetals from First Principles
CHRISTINA GARCIA (Presenter), JENNIFER COULTER, PRINEHA NARANG, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Recent experiments have shown interesting optical behavior in Weyl semimetals, a topologically nontrivial class of materials. Weyl semimetals (WSMs) are characterized by linearly dispersive band touchings in the bulk states (in three dimensions) where electrons can be treated as massless Weyl fermions. This talk will focus on our evaluation of optical properties, hot carrier generation and dynamics in different Weyl semimetals using first principles calculations incorporating electron-phonon interactions. In particular, we explore TaAs, in which record-breaking second-harmonic generation and bulk photovoltaic effects have been recently reported. We will build upon our ab initio framework to include nonlinear optical properties for direct comparison with these exciting observations.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L05 DMP: Topological Superconductivity: Theory
BCEC 108 - Gregory Fiete, University of Texas at Austin
- Tag(s): Focus

11:15AM L05.00001: Designing topological superconductors [Invited] LIANG FU (Presenter), Massachusetts Institute of Technology — I will discuss routes to creating topological (and other unconventional) superconductors by tuning the Fermi surface of materials with gating, electric/magnetic field and strain. Candidate systems include 2D materials with spin-orbit coupling, with tunable van Hove singularity, or with moire superlattice.

11:51AM L05.00002: Extension of symmetry-based indicators and its application* SEISHIRO ONO (Presenter), Institute for Solid State Physics, HARUKI WATANABE, Applied Physics, University of Tokyo — The goal of the study of topological phases is to achieve the complete classification of phases for all spatial and internal symmetries. The topological periodic table, the classification table of topological insulators for each internal symmetry class, is a milestone in this line of research. Recently, the method of “symmetry-based indicators (SI)” has been developed. It diagnoses the topology of band structures based on their symmetry representations. The prototypical example of SI is the Fu-Kane formula, which distinguishes topological insulators from normal insulators in terms of inversion parities. So far, as an internal symmetry, only the time-reversal symmetry has been taken into account in the calculation of SI. In this talk, we discuss how to incorporate with the chiral symmetry and the particle-hole symmetry.

*H.W. is supported by JSPS KAKENHI Grant No. JP17K17678.

12:03PM L05.00003: Classification of topological crystalline superconducting nodes on high-symmetry line* SHUNTARO SUMITA (Presenter), Department of Physics, Kyoto University, TAKUYA NOMOTO, Department of Applied Physics, The University of Tokyo, KEN SHIOZAKI, Yukawa Institute for Theoretical Physics, Kyoto University, YOUICHI YANASE, Department of Physics, Kyoto University — Recent development in exact classification of a superconducting gap has elucidated various unconventional gap structures [1-8], which have not been predicted by the classification of order parameter based on the point group [9]. One of the important previous results is that all symmetry-protected line nodes are characterized by nontrivial topological numbers [6, 7]. Another intriguing discovery is the gap structures depending on the angular momentum of electrons $j_z$ on threefold and sixfold rotational-symmetric lines [1, 3, 8]. Stimulated by these findings, we classify all crystal symmetry-protected nodes (including such $j_z$-dependent nodes) on high-symmetry $n$-fold ($n = 2, 3, 4, and 6$) axes, by using the combination of group theory and $K$-theory [10]. As a result, it is shown that the classification by group theory completely corresponds with the topological classification. Based on the obtained results, we discuss superconducting gap structures in several candidate superconductors.

*“J-Physics” (15H05884)
“Topological Materials Science” (16H00991 and 18H04225)
"J-Physics: Young Researchers Exchange Program" (JP15K21732)
JSPS KAKENHI Grants No. 15K05164, No. 15H05745, No. 17J09908, No. 18H05227, and No. 18H01178.
12:15PM L05.00004: Weak-Pairing Higher Order Topological Superconductors*  MAO LIN (Presenter), YUXUAN WANG, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — We consider a new class of superconductors, second-order topological superconductors (SOTSC), that have gapped, topological surfaces and gapless Majorana modes on lower-dimensional boundaries: corners of a 2D system or hinges for a 3D system. We propose two general scenarios that SOTSC can be realized spontaneously with weak-pairing instabilities. First, we show that p-wave pairing in a Dirac semimetal in 2D with four mirror symmetric Dirac nodes realizes SOTSC. Second, we show that p+id pairing on an ordinary Fermi surface realizes SOTSC as well. We show that these exotic states can be intrinsically realized in a metallic system with electronic interactions. In the latter case we find that the topological invariants describing the system can be written using simple formulae involving only the low-energy properties of the Fermi surfaces and superconducting pairing, and we also show it can be induced by proximity effect in a heterostructure of cuprate and superconductor.

*YW acknowledges support from the Gordon and Betty Moore Foundations EPiQS Initiative through Grant No. GBMF4305. ML thanks NSF Emerging Frontiers in Research and Innovation NewLAW program Grant EFMA-1641084 and NSF CAREER Grant DMR1351895 for support. TLH was supported by the ONR YIP Award N00014-15-1-2383.

12:27PM L05.00005: Exotic superconductivity with enhanced energy scales in materials with three band crossings*  YU-PING LIN (Presenter), RAHUL NANDKISHORE, Department of Physics, University of Colorado Boulder — Three band crossings can arise in three-dimensional quantum materials with certain space group symmetries. The low energy Hamiltonian supports one fermions and a flat band. We study the pairing problem in this setting. We write down a minimal BCS Hamiltonian and decompose it into spin-orbit coupled irreducible pairing channels. We then solve the resulting gap equations in channels with zero total angular momentum. We find that in the s-wave spin singlet channel (and also in an unusual d-wave 'spin quintet' channel), superconductivity is enormously enhanced, with a possibility for the critical temperature to be linear in interaction strength. Meanwhile, in the p-wave spin triplet channel, the superconductivity exhibits features of conventional BCS theory due to the absence of flat band pairing. Three band crossings thus represent an exciting new platform for realizing exotic superconducting states with enhanced energy scales. We also discuss the effects of doping, nonzero temperature, and of retaining additional terms in the k.p expansion of the Hamiltonian.

*Supported by the Army Research Office and was accomplished under Grant No. W911NF-17-1-0482.

12:39PM L05.00006: Anomalous symmetry protected topological states in interacting fermion systems*  QING-RUI WANG, Physics, The Chinese University of Hong Kong, YANG QI, Physics, Fudan University, ZHENGCHENG GU (Presenter), Physics, The Chinese University of Hong Kong — The classification and construction of symmetry protected topological (SPT) phases have been intensively studied in interacting systems recently. To our surprise, in interacting fermion systems, there even exists a new class of the so-called anomalous SPT (ASPT) states which are only well defined on the boundary of a trivial fermionic bulk. The physical reason is that certain symmetry action might change the fermion parity locally, but is conserved if we introduce a bulk. We demonstrate the essential idea by considering anomalous topological superconductor with time reversal symmetry $T^2 = 1$. Finally, we also discuss the classification scheme of anomalous SPT states for interacting fermions with a total symmetry $G_f = G_b \times \mathbb{Z}_2$ and relevant experimental implications.

*ZCG acknowledges Direct Grant no. 4053300 from The Chinese University of Hong Kong and funding from Hong Kong’s Research Grants Council (ECS 24301516).
12:51PM L05.00007: Superconducting higher-order semimetals: Second-order Dirac superconductors and magnetic field induced higher-order topological superconductivity* SAYED ALI AKBAR GHORASHI (Presenter), XIANG HU, Physics, College of William and Mary, TAYLOR HUGHES, Physics Institute for Condensed Matter Theory, University of Illinois Urbana-Champaign, ENRICO ROSSI, Physics, College of William and Mary — We identify three dimensional superconductors that exhibit various forms of higher order topology. We show how such superconductors can be obtained through superconducting instabilities induced in higher order quadrupole topological semimetals [1]. In our models the normal-state degrees of freedom consist of two orbitals and spin in an electronic structure that forms a quadrupolar topological semimetal. We consider all possible s-wave superconducting pairing terms satisfying Fermi-Dirac statistics and obtain six different superconducting models. We find that four of the models have a non-zero residual quadrupole-like topology, and therefore topologically protected Majorana hinge states on the four hinges of the sample. The other two models have no quadrupolar topology yet, in the presence of an external magnetic field, exhibit helical hinge states localized at only two of the four hinges. For these two models we also find that the pair of corners exhibiting hinge states switches upon a change of sign of the magnetic field.


*Work supported by ONR, NSF, and ARO

1:03PM L05.00008: Higher Order Topological Phases: A General Principle of Construction DUMITRU CALUGARU (Presenter), Max-Planck-Institut fur Physik komplexer Systeme, Dresden, Germany, VLADIMIR JURICIC, NORDITA, the Nordic Institute for Theoretical Physics, Stockholm University and KTH, Stockholm, Sweden, BITAN ROY, Max-Planck-Institut fur Physik komplexer Systeme, Dresden, Germany — In this talk, we discuss a general principle for constructing higher-order topological (HOT) phases [1]. We argue that if a D-dimensional first-order or regular topological phase involves m Hermitian matrices that anti-commute with additional p-1 mutually anti-commuting matrices, it is conceivable to realize an n\textsuperscript{th}-order HOT phase, where n=1,..., p, with appropriate combinations of discrete symmetry-breaking Wilsonian masses. An n\textsuperscript{th}-order HOT phase accommodates zero modes on a surface with co-dimension n. We exemplify these scenarios for prototypical three-dimensional gapless systems, such as a nodal-loop semimetal possessing SU(2) spin rotational symmetry, and Dirac semimetals, transforming under (pseudo-)spin-1/2 or 1 representation. The former system permits an unprecedented realization of a 4\textsuperscript{th}-order phase, without any surface zero modes. Our construction can be generalized to HOT insulators and superconductors in any dimension and symmetry class.


1:15PM L05.00009: Gauge Theory of the Superconductor-Insulator Transition* VALERII VINOKOUR (Presenter), Argonne National Laboratory, CRISTINA DIAMANTINI, LUCA GAMMAITONI, Dipartimento di Fisica e Geologia, University of Perugia, IGOR LUKYANCHUK, Laboratory of Condensed Matter Physics, University of Picardie, CARLO TRUGENBERGER, SwissScientific Technologies SA — The standard model of particle physics is extraordinarily successful at explaining much of the physical realm. Yet, one of its most profound aspects, the mechanism of confinement, that binds quarks into hadrons and is supposedly mediated by chromo-electric strings in a condensate of magnetic monopoles, is not thoroughly understood and lacks direct experimental evidence. We demonstrate that the infinite-resistance superinsulating state, a mirror analog of superconductivity, emerging at the insulating side of the superconductor-insulator transition (SIT) is a condensed matter realization of the quark confinement. We reveal that the mechanism ensuring the infinite resistance of superinsulators is the binding of Cooper pairs into neutral “mesons” by electric strings and establish a mapping of quarks onto Cooper pairs in superinsulators. We reveal a Cooper pair analog of the asymptotic freedom effect implying that systems smaller than the string scale appear in a quantum metallic state.

* M.C.D. thanks CERN. The work at Argonne (V.M.V.) was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. I.L was supported by the H2020-RISE-ENGIMA action.
1:27PM L05.00010: Superconducting vortex from magnetic skyrmions*  SHU-PING LEE (Presenter), YI LI, Johns Hopkins University — We show topological superconductivity can arise at the interface of ferromagnetic skyrmion material in proximity to an s-wave superconductor in the presence of strong spin-orbit coupling. We study the Majorana zero modes localized at the interface of the heterostructure and propose a pathway towards a useful platform for the manipulation of Majorana fermions via controlling skyrmions.

*S.-P. Lee and Y. L. acknowledge the support by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, Grant No. DE-FG02-08ER46544. Y. L. also acknowledges the support from the Alfred P. Sloan Fellowship.

1:39PM L05.00011: Magnon-induced superconductivity in a topological insulator coupled to ferro- and antiferromagnetic insulators*  HENNING HUGDAL (Presenter), Norwegian University of Science and Technology, STEFAN REX, Karlsruhe Institute of Technology, FLAVIO NOGUEIRA, IFW Dresden, ASLE SUDBO, Norwegian University of Science and Technology — We study the effective interactions between Dirac fermions on the surface of a three-dimensional topological insulator due to the proximity coupling to the magnetic fluctuations in a ferromagnetic or antiferromagnetic insulator. Magnetic fluctuations can mediate attractive interactions between Dirac fermions of both Amperean and BCS type. In the ferromagnetic case, we find pairing between fermions with parallel momenta, so-called Amperean pairing, whenever the effective Lagrangian for the magnetic fluctuations does not contain a quadratic term. If a quadratic term is present, the pairing is instead of BCS type above a certain chemical potential. In the antiferromagnetic case, BCS pairing occurs when the ferromagnetic coupling between magnons on the same sublattice exceeds the antiferromagnetic coupling between magnons on different sublattices. Outside this region in parameter space, we again find that Amperean pairing is realized

*H.G.H. and A.S. were supported by the Research Council of Norway through Grant Number 250985, “Fundamentals of Low-dissipative Topological Matter”, and Center of Excellence Grant Number 262633, Center for Quantum Spintronics. S. R. was supported by DFG through SPP 1666, “Topological Insulators: Materials - Fundamental Properties - Devices”.

1:51PM L05.00012: Reproducing topological properties with quasi-Majorana states  ADRIAAN VUIK, BAS NIJHOLT, ANTON AKHMEROV, Kavli institute of nanoscience, Delft University of Technology, MICHAEL WIMMER (Presenter), QuTech and Kavli institute of nanoscience, Delft University of Technology — Andreev bound states in hybrid superconductor-semiconductor devices can have near-zero energy in the topologically trivial regime as long as the confinement potential is sufficiently smooth. We show that in addition to the suppressed coupling between the quasi-Majorana states, also the coupling of these states across a tunnel barrier to the outside is exponentially different. As a consequence, quasi-Majorana states mimic most of the proposed Majorana signatures: quantized zero-bias peaks, the 4π Josephson effect, and the tunneling spectrum in presence of a normal quantum dot. We identify a quantized conductance dip instead of a peak in the open regime as a distinguishing feature of true Majorana states in addition to having a bulk topological transition. Because braiding schemes rely only on the ability to couple to individual Majorana states, the exponential control over coupling strengths allows to also use quasi-Majorana states for braiding.

2:03PM L05.00013: Fulde-Ferrell-Larkin-Ovchinnikov phases in Proximitized Josephson junctions  CHIEN-TE WU (Presenter), Electrophysics, National Chiao Tung University, FNU SETIAWAN, KATHRYN LEVIN, James Franck Institute, University of Chicago — Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phases, which are notoriously difficult to find in more homogeneous systems, have been observed in proximitized superconductors. Of particular interest are those heterostructures which are associated with topological phases[1,2]. In this talk, we establish the effects of spin-orbit coupling and show why these elusive phases are observable in the presence of proximitization. We focus on that FFLO phase which appears inside a substrate (subjected to an in-plane magnetic field) and formed in a Josephson junction configuration. To do so, we solve the Bogoliubov-de Gennes equations for the full multi-component system. The substrates consist of (1) a conical Holmium magnet with an effective 1D spin-orbit coupling, and (2) a two-dimensional electron gas.

Exploring electronic anisotropy with strain in CeRhIn$_5$*  
SEAN THOMAS (Presenter), ADAM P DIOGUARDI, JOE D THOMPSON, PRISCILA ROSA, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory — Strongly correlated material CeRhIn$_5$ hosts a helical antiferromagnetic ground state at zero applied field. When a magnetic field of ~30 T is applied slightly away from the c-axis, a new phase emerges within the antiferromagnetic state with an XY electronic nematic character [1]. Here, we use a combination of uniaxial and biaxial strain devices to investigate the nematic susceptibility of CeRhIn$_5$. A similar approach has been extensively used to investigate the nematic order in iron-based superconductors [2]. We will discuss signatures of the nematic susceptibility in the low-field region of the H-T phase diagram.


*Work at Los Alamos was performed under the auspices of the US DOE, Division of Materials Science and Engineering.

Spin density wave and possible Fulde-Ferrell-Larkin-Ovchinnikov states in CeCoIn$_5$*  
DUK YOUNG KIM, Institue of Basic Science, SKKU, South Korea, SHIZENG LIN, ERIC BAUER, FILIP RONNING, ROMAN MOVSHOVICH (Presenter), Los Alamos National Laboratory — We examine interplay between spin density wave (SDW) and the putative Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state in CeCoIn$_5$. We use thermal conductivity measurement along a-axis in magnetic field applied at various angles away from the c-axis within the bc plane of this tetragonal compound. We compare our results to those of our theoretical model which shows that SDW state in CeCoIn$_5$ is stabilized when the field is directed close to the ab plane. The SDW phase disappears when the field is rotated away from the ab plane. When the field is rotated toward the c axis, the FFLO state emerges while the SDW phase disappears. As a function of field, we observed the reduction of thermal conductivity for field close to the ab plane and the enhancement of thermal conductivity when field is close to the c axis, consistent with the theoretical expectations of additional contribution to the heat transport from the FFLO nodal planes.

*Work was supported by the Los Alamos National Laboratory Directed Research and Development program.

Fermi surface evolution and crystal-field excitations in heavy-fermion compounds probed by time-domain terahertz spectroscopy*  
SHOVON PAL, CHRISTOPH WETLI, Department of Materials, ETH Zürich, FARZANEH ZAMANI, Physikalisches Institut, University of Bonn, OLIVER STOCKERT, MPI-CPFS Dresden, HILBERT V. LÖHNEYSEN, Physikalisches Institut and Inst. für Festkörperphysik, KIT Karlsruhe, MANFRED FIEBIG, Department of Materials, ETH Zürich, JOHANN KROHA (Presenter), Physikalisches Institut, University of Bonn — In heavy-fermion (HF) compounds, the existence of heavy quasiparticles (QPs) is signaled by an enlarged Fermi volume. The energy scale for heavy QP formation is believed to be the Kondo lattice temperature. Hence, the origin of a large Fermi volume observed at temperatures much higher than the Kondo lattice temperature has recently been a controversial issue. We measure the quasiparticle weight in the HF compound CeCu$_6-x$Au$_x$ (x=0, 0.1) by time-resolved THz spectroscopy for temperatures from 2 K up to 300 K. This method distinguishes contributions from the heavy Kondo band and from the crystal-electric-field satellite bands by different THz response delay times [1,2]. We find that the formation of heavy bands is controlled by an exponentially enhanced, high-energy Kondo scale once the crystal-electric-field states become thermally occupied. We corroborate these observations by temperature-dependent, high-resolution dynamical mean-field calculations for the multi-orbital Anderson lattice model and discuss the relevance for quantum critical scenarios.


*Funded in part by SNSF and DFG.
11:51AM L06.00004: Kondo effects in α and γ phases of Ce  JUNWON KIM (Presenter), DONG-CHOON RYU, Department of Physics, Pohang University of Science and Technology, HONGCHUL CHOI, Scuola Internazionale Superiore di Studi Avanzati, KYOO KIM, Max Plank Research Center, Pohang 37671, Korea, BYUNG IL MIN, Department of Physics, Pohang University of Science and Technology — The Kondo effect is one of the fascinating correlation phenomena in condensed matter physics. The monoatomic compound Ce, which is famous for the α - γ phase transition and the extremely rich phase diagram with at least seven allotropes, is a good sample for observing the Kondo effect and its change with respect to the temperature or pressure variations. In this research, we focused on the Kondo physics in α and y phase among the various phases of Ce. To capture the Kondo physics, we used the first principles Dynamical Mean-Field Theory (DMFT) approach combined with Density Functional Theory (DFT)[1,2]. Unlike the cases of using DFT only, we have observed in the DFT+DMFT scheme that Kondo resonances are formed distinctly for α and γ phases of Ce, which yields different band structures between two phases, especially at around EF. We theoretically discuss the temperature-dependent physical properties of both phases, and compare their band structures with photoemission experimental results.

12:03PM L06.00005: Magnetic complexity in RScT (R=Gd, Pr, T=Sb, Ge) based compound*  ARJUN PATHAK (Presenter), FRANCOIS GUILLOU, YAROSLAV MUDRYK, VITALIJ K PECHARSKY, Materials sciences and engineering, Ames Laboratory, US DOE, Ames IA — Ternary RTX intermetallics, where R = rare earth, T = transition metal, X = p-block element, are structurally and magnetically diverse and are among the most interesting intermetallic compounds to explore (Gupta et. al. JALCOM 618 (2015) 562). For example, GdScGe crystallizes in tetragonal CeScSi-type structure and undergoes a ferromagnetic (FM) transition at TC = 350K, while PrScGe (same CeScSi-structure type) has an antiferromagnetic (AFM) transition at TN = 88K and then a FM transition at TC = 80K. When germanium is replaced by antimony, the GdScSb compound crystallizes in a closely related tetragonal CeFeSi-type and orders AFM at TN ~55K. Here we present a systematic study of the interplay between crystal structure and magnetism in Gd1-xPrxScGe and GdSc(Ge1-xSbx). The substitution of heavy lanthanide, Gd, with light lanthanide, Pr, results in a complex magnetic ground state with a large exchange bias of HE ~ 1.06 kOe at T = 2K.

*The Ames Laboratory is operated for the U. S. DOE by Iowa State University of Science and Technology under contract No. DE-AC02-07CH11358. This work was supported by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

12:15PM L06.00006: The Ho₆Mo₄Al₄₃ structure type as a cage for Uranium and Plutonium*  KEVIN HUANG, National High Magnetic Field Laboratory, WILLIAM NELSON (Presenter), Physics, Florida State University, ALEXANDER CHEMEY, THOMAS ALBRECHT-SCHMITT, Chemistry, Florida State University, RYAN BAUMBACH, National High Magnetic Field Laboratory — Single crystals of A₆W₄Al₄₃ (A=U/Pu) were synthesized for the first time using a molten Al flux. This structure features large lattice constants (a=10.97, c=17.71Å) and cage-like W-Al polyhedra that surround the A ions. XRD suggests that, unlike for some other cage-like structures, the A ions do not exhibit soft lattice modes. Magnetic susceptibility measurements for U₆W₄Al₄₃ show Curie-Weiss behavior, where fits to the data yield an effective magnetic moment near 2.0 µB/U. At low-T the magnetic susceptibility deviates from the Curie-Weiss law and saturates to a constant value, as seen for other spin fluctuating materials. There is evidence from the electrical transport and heat capacity for the formation of a heavy Fermi liquid ground state due to Kondo lattice behavior. In contrast, Pu₆W₄Al₄₃ exhibits nearly T-independent Pauli paramagnetism, suggesting delocalization of the 5f electrons. We will discuss these results in the context of the Hill plot, where both compounds are found near the inter-actinide distance that separates delocalized and localized f-electron behavior.

*Work was performed at the NHMFL-FSU, supported by NSF coop. agreements DMR-1157490 and DMR-1644779 and the state of FL. We acknowledge support from US-DOE, BES, under Award No. DE-SC0016568 EFRC-CAST.
Multiple electronic instabilities and the anomalous thermodynamics of plutonium

NEIL HARRISON (Presenter), JONATHAN B BETTS, FEDOR BALAKIREV, MARCELO JAIME, PAUL H TOBASH, Los Alamos National Laboratory — Given plutonium’s importance in energy production, an understanding of its anomalous electronic and thermodynamic properties is essential for its safe handling and long term storage. In common with rare earth and other actinide elements and compounds, plutonium’s physical and chemical properties are determined by $f$-electrons, whose transformation from localized to itinerant behavior are known to drive a significant collapse in volume. However, the occurrence of a volume collapse on both reducing and increasing the temperature and its anomalously large magnitude, reaching as much as 25% at low temperatures, represent extreme departures from the behavior of other known metals. Here we discuss new magnetostriction measurements on $\delta$ Pu, made using an optical fiber Bragg grating technique adapted for use on encapsulated radiological materials, that plutonium’s exceptional thermodynamic behavior with temperature derives from its $f$-electron shell having multiple electronic instabilities.

*This work is supported by the LANL LDRD program.

Fermi Surface Topology and Correlation Effects in the Electronic Structure of Plutonium

ROXANNE TUTCHTON (Presenter), JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory — Due to its position at the boundary between the light and heavy actinides, the electronic structure of Pu has exotic physical properties that are complex and challenging to model. The difficulties in performing accurate theoretical calculations for this element stem from the liminal characteristics of Pu-$5f$ orbital electrons and understanding the role of the fluctuating magnetism in the electronic structure. Two methods for treating the magnetic behavior in Pu are currently debated. One is the “disordered local moment” model described by density functional theory (DFT) and the other is the “valence fluctuation” model as captured by dynamical mean-field theory (DMFT). Focusing on the $\delta$-phase of elemental Pu, we perform a careful comparison of Fermi surface topology calculations using DFT and DFT+$U$. The de Haas-van Alphen (dHvA) frequencies at the Fermi surface and band masses are calculated in both magnetic and nonmagnetic states. We also analyze the effective mass enhancement due to $5f$-electron correlation effects with DMFT. The comparison study will be helpful for future experiments to validate theoretical modeling.

*This work was performed under the auspices of the U.S. DOE National Nuclear Security Agency through the LANL LDRD program.

Isotropic Giant Magnetoresistance in URhIn$_5$

CARSTEN PUTZKE (Presenter), École Polytechnique Fédérale de Lausanne (EPFL), Institute of Materials, Lausanne, Switzerland, ETERI SVANIDZE, MAJA BACHMANN, MARKUS KOENIG, KENT SHIRER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, JONAS DIAZ, École Polytechnique Fédérale de Lausanne (EPFL), Institute of Materials, Lausanne, Switzerland, TOBIAS FOERSTER, Highfield Magnetlaboratory Dresden, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany, ANDREAS LEITHE-JASPER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, YURI GRIN, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, PHILIP MOLL, École Polytechnique Fédérale de Lausanne (EPFL), Institute of Materials, Lausanne, Switzerland — We will show results of the resistivity anisotropy in focused ion beam (FIB)-fabricated microstructures of URhIn$_5$ and compare them to CeRhIn$_5$. Both systems order antiferromagnetically (AFM) at 94 K and 3.8K K, respectively. Marked differences are found in their response to magnetic field, despite their structural and electronical similarities. In CeRhIn$_5$, the AFM order leads to an increase in the ratio of in-plane to out-of-plane resistivity with a modulation of the angle-dependent magnetoresistance. In contrast, the onset of AFM order in URhIn$_5$ has no effect on the anisotropy of the system, but leads to a giant magnetoresistance (GMR), resembling semi-metals like Bi$^1$ and WTe$_2$$^2$, rather than other 115-heavy fermion systems. By performing detailed angle-dependent measurements of the magnetoresistance in the U-based system, we can show that the GMR originates mainly from orbital magnetoresistance, making it unique among $f$-electron containing system.
Large anomalous Hall effect in kagome antiferromagnet $U_3Ru_4Al_{12}$

TOMOYA ASABA (Presenter), ERIC BAUER, JOE D THOMPSON, FILIP RONNING, MPA-CMMS, Los Alamos National Laboratory — The Berry curvature in ferromagnets and antiferromagnets has been attracting huge interests due to the tunability of topological features via the magnetic structure. However, topological features in magnetic heavy fermion systems have been sparsely studied so far. In this study, we measured the anomalous Hall effect (AHE) of kagome heavy fermion antiferromagnet $U_3Ru_4Al_{12}$. A large intrinsic AHE at high fields was observed, suggesting the presence of a large Berry curvature due to Weyl fermion. Moreover, the fields required to obtain the large Berry curvature are significantly different between $B//a$ and $B//a^*$, providing a mechanism to control the topological response in this system. These results may not only help to understand the topological heavy fermion physics, but also shed light on this system as an ideal playground for studying field-tuned topological states.

Magnetic torque of uranium dioxide single crystals

KRZYSZTOF GOFRYK (Presenter), Idaho National Laboratory, YOU LAI, NHMFL-FSU, DANIEL ANTONIO, Idaho National Laboratory, RYAN BAUMBACH, DAVID E GRAF, NHMFL-FSU, MARCELO JAIME, NHMFL-LANL, ANDRES SAUL, Aix-Marseille University, MYRON B SALAMON, NHMFL-LANL, JAMES L SMITH, LANL — Uranium dioxide is one of the most studied actinide compounds due to its fundamental and applied importance. Recently, we have performed a low-temperature magnetostriction study of UO$_2$ in magnetic fields up to 95 T [Nature Comm. 8, 99 (2017)], and uncovered the appearance of linear magnetostriction, leading to a trigonal distortion and piezomagnetism (the first example of piezomagnetism in $f$-electron spin system). The unusually strong correlations between the magnetic moments in U-atoms and lattice distortions are a direct consequence of the non-collinear symmetry of the magnetic state that breaks time reversal symmetry in a non-trivial way that leads to the piezomagnetism. The microscopic nature of these interactions, however, remains unclear. During the talk, we will present magnetic torque measurements (up to 35 T) performed on oriented UO$_2$ single crystals. We will discuss implications of these results in the context of the origin of the piezomagnetic ground state in this material.

Magnetoelectric Quantum Oscillations and the Fermi Surface of UPt$_3$

BELLA VE SHIVARAM, LUDWIG HOLLEIS (Presenter), VERN ULRICH, University of Virginia — We report details of magnetoelectric quantum oscillations measured for several different angles of the magnetic field away from the $a$-axis as well as the $c$-axis in UPt$_3$ for temperatures down to 35 mK. The effective masses of the electrons in the observed orbits obtained from the temperature dependence of the amplitudes of the oscillations will be presented. The field dependence of the frequencies of the orbits will be discussed and the low field values will be compared with the known band structure predictions of UPt$_3$.

Field Angle Tuned Metamagnetism, Lifschitz Transitions and Hidden Order in UPt$_3$

BELLA VE SHIVARAM (Presenter), LUDWIG HOLLEIS, University of Virginia, MARCELO JAIME, JOHN SINGLETON, NHMFL, Los Alamos National Labs, VERN ULRICH, University of Virginia — We report ultrasound velocity measurements carried out on single crystals of UPt$_3$, in magnetic fields, $B$, applied at various angles between $c$-axis and the basal plane. For $B//c-axis, \theta=90^\circ$, we observe magneto-acoustic oscillations that commence at fields as low as 12T. These oscillations suddenly break into a very large amplitude at 24.8 T implying a Lifshitz transition. Continuing to higher fields these large amplitude oscillations disappear at 30 T beyond which much smaller oscillations with altered frequencies are observed. Magnetoelectric measurements performed at fields up to 65 T for $\theta=90^\circ$ reveal small features that are consistent with boundaries at similar magnetic field values. Further, the 30 T transition appears to merge with the angle dependent metamagnetic transition at the intermediate angle $\theta=50^\circ$. For field along this unique angle the magnetoelectric along c-axis vanishes precisely for all magnetic field values. High resolution magnetization measurements vs. field are, surprisingly, featureless and near linear when $\theta=90^\circ$.

The work at the University of Virginia was funded by NSF DMR 0073456. The National Magnet Laboratory in Tallahassee is supported by the National Science Foundation and the State of Florida.
1:51PM L06.00014: Anisotropic Magnetostriction Measurements in UPt₃ to 65 T*  BELLAVE SHIVARAM, University of Virginia, FRANZISKA WEICKERT (Presenter), MARCELO JAIME, NHMFL, Los Alamos National Labs — We present magnetostriction measurements obtained in pulsed magnetic fields up to 65 T at the NHMFL/Los Alamos in single crystals of UPt₃ for fields both parallel and perpendicular to the c-axis. While we reproduce published results at low fields the measurements at the highest fields for field parallel to the basal plane reveal a surprising downward trend in the magnetostriction. All these observations will be examined in the context of the single energy scale model of metamagnetism in heavy electron materials.

*The work at NHMFL/Los Alamos is supported by the National Science Foundation.

Wednesday, March 6, 2019 11:15 AM - 1:51 PM

Session L07 DCMP: Theory of Topological Phases  BCEC 109B - Itamar Kimchi, University of Colorado at Boulder

11:15AM L07.00001: Anomaly manifestations in topological insulator surfaces with strong correlations and disorder  ITAMAR KIMCHI (Presenter), YANG-ZHI CHOU, RAHUL NANDKISHORE, MICHAEL A HERMELE, LEO R RADZIHOVSKY, Physics, University of Colorado, Boulder — Three-dimensional topological insulators exhibit a bulk quantum anomaly that protects certain properties of their surface. For example, theoretical studies of weakly interacting strong and weak topological insulators show that their surface stays conducting, even with arbitrarily strong disorder, as long as the relevant symmetries are preserved on average. However, the combination of strong interactions and disorder offers theoretical questions which have not yet been addressed. Here we address this interplay and show that it can lead to a type of localized surface state, even while the disorder ensemble preserves all symmetries. We discuss how the quantum anomaly is manifested within the localized surface. These minimal manifestations of the quantum anomaly can constrain possible Lieb-Schultz-Mattis-type theorems for disordered systems.

11:27AM L07.00002: Free and Interacting SRE Phases of Fermions: Beyond the Ten-Fold Way*  YU-AN CHEN, ANTON KAPUSTIN, ALEX TURZILLO (Presenter), MINYOUNG YOU, Caltech — It is well-known that sufficiently strong interactions can destabilize some SPT phases of free fermions, while others remain stable even in the presence of interactions. It is also known that certain interacting phases cannot be realized by free fermions. We systematically study both of these phenomena in low dimensions and determine the map from free to interacting SPT phases for an arbitrary unitary symmetry G. In particular, in dimension zero and one we describe precisely which SPT phases can be realized by free fermions. We show that in dimension three there are no non-trivial free fermionic SPT phases with a unitary symmetry. We also describe how to compute invariants characterizing interacting phases for free band Hamiltonians with symmetry G (in any dimension) using only representation theory.

* U.S. Department of Energy, Office of Science, Office of High Energy Physics, Award Number de-sc0011632. The work of A. K. was partly performed at the Aspen Center for Physics, which is supported by National Science Foundation grant PHY-1607611. A. K. was also supported by the Simons Investigator Award.

11:39AM L07.00003: Emergent Dirac fermions in Composite-Fermi-Liquids.*  JIE WANG (Presenter), Princeton University, EDWARD H REZAYI, California State University, Los Angeles, FREDERICK D HALDANE, Princeton University — Composite Fermi Liquids (CFLs) are compressible states that can occur for 2D interacting fermions in the lowest Landau level at 1/2m Landau level fillings when m is an integer. They have been understood as Fermi seas of electromagnetic-flux-attached fermions due to Halperin, Lee and Read. At 1/2 filling, an alternative particle-hole symmetric description based on Dirac fermions was proposed by Son. In this talk, we numerically examined the Berry phase associated with transporting one composite fermion around the Fermi sea at filling 1/2 and 1/4. At one-half, a PI Berry curvature singularity was observed [1,2], supporting Son's effective theory. At one-quarter, we found a uniform Berry curvature and an additional PI strength at Fermi sea center. We explained the 1/4 phenomenon from CFL model wavefunctions. We also proposed a flux-attached Dirac fermion effective action [3], which generalized Son's theory from 1/2 filling to all other filling fractions. The Fermi-sea in this new theory is interpreted as formed by internal-gauge-flux-attached Dirac fermions.


*Department of Energy BES Grant de-sc0002140; Princeton U. compton fund.
11:51AM L07.00004: Fragile topological phases in interacting systems  DOMINIC ELSE (Presenter), HOI CHUN PO, Massachusetts Institute of Technology, HARUKI WATANABE, University of Tokyo — Topological phases of matter are defined by their nontrivial patterns of ground-state quantum entanglement, which is irremovable so long as the excitation gap and the protecting symmetries, if any, are maintained. Recent studies on noninteracting electrons in crystals have unveiled a peculiar variety of topological phases, which harbors nontrivial entanglement that can be dissolved simply by the addition of entanglement-free, but charged, degrees of freedom. Such topological phases have a weaker sense of robustness than their conventional counterparts, and are therefore dubbed "fragile topological phases." In this work, we show that fragile topology is a general concept prevailing beyond systems of noninteracting electrons. We identify the key ingredients for fragile topological phases, and demonstrate their existence not only in interacting systems of fermions, but also bosons.

12:03PM L07.00005: Gapped boundary theory of the twisted gauge theory model of three-dimensional topological orders  HONGYU WANG (Presenter), YINGCHENG LI, Physics Department, Fudan University, YUTING HU, Department of Physics and Institute for Quantum Science and Engineering, Southern University of Science and Technology, YIDUN WAN, Physics Department, Fudan University — We extend the twisted gauge theory model of topological orders in three spatial dimensions to the case where the three spaces have two dimensional boundaries. We achieve this by systematically constructing the boundary Hamiltonians that are compatible with the bulk Hamiltonian. Given the bulk Hamiltonian defined by a gauge group G and a four-cocycle \( \omega \) in the fourth cohomology group of G over U(1), we construct a gapped boundary Hamiltonian using \( \{K, \alpha\} \), with a subgroup \( K \subseteq G \) and a 3-cochain \( \alpha \) of K over U(1), which satisfies the generalized Frobenius condition. The Hamiltonian is invariant under the topological renormalization group flow (via Pachner moves). Each solution \( \{K, \alpha\} \) to the generalized Frobenius condition specifies a gapped boundary condition. We derive a closed-form formula of the ground state degeneracy of the model on a three-cylinder, which can be naturally generalized to three-spaces with more boundaries. We also derive the explicit ground-state wavefunction of the model on a three-ball. The ground state degeneracy and ground-state wavefunction are both presented solely in terms of the input data of the model, namely, \( \{G, \omega, K, \alpha\} \).

12:15PM L07.00006: SU(3) trimer resonating-valence-bond state on the square lattice  XIAOYU DONG (Presenter), California state University, Northridge, USA, JI-YAO CHEN, C. N. R. S. and Université de Toulouse, Toulouse, France, HONG-HAO TU, Technische Universität Dresden, Dresden, Germany — We propose and study an SU(3) trimer resonating-valence-bond (tRVB) state with C4v point-group symmetry on the square lattice. By devising a projected entangled-pair state (PEPS) representation, we show that all (connected) correlation functions between local operators in this SU(3) tRVB state decay exponentially, indicating its gapped nature. We further calculate the modular S and T matrices by constructing all nine topological sectors on a torus and establish the existence of Z3 topological order in this SU(3) tRVB state.

12:27PM L07.00007: Quantum phase transitions between gapped topological phases: a percolation approach  XIN DAI (Presenter), SAAD KHALID, ILYA A GRUZBERG, YUANMING LU, Physics, Ohio State University — We study continuous quantum phase transitions between two gapped topological orders, where a gapped boundary exists at the interface of the two phases. Using a percolation picture, we derive the effective Hamiltonian and the universality class of the quantum phase transition.

12:39PM L07.00008: Anyon exclusions statistics on surfaces with gapped boundaries  YINGCHENG LI (Presenter), YIDUN WAN, HONGYU WANG, YUTING HU, Fudan University — Anyon exclusion statistics, proposed by Haldane, generalizes the Bose-Einstein and Fermi-Dirac statistics. When fusion of anyons is involved, certain 'pseudo-species' anyons appear in the exotic statistical weights of non-Abelian anyon systems, whose meaning and significance remains an open problem. The relevant past studies had considered only anyon systems without any physical boundary. In this paper, we propose an extended anyon exclusion statistics on surfaces with gapped boundaries, introducing mutual exclusion statistics between anyons as well as the boundary components. We present a formula for the statistical weight of many-anyon states obeying the proposed statistics. We develop a systematic basis construction for non-Abelian anyons on any Riemann surfaces with gapped boundaries. The basis construction offers a standard way to read off a canonical set of statistics parameters and hence write down the extended statistical weight of the anyon system being studied. The basis construction reveals that a pseudo-species has different 'excitation' modes corresponding to good quantum numbers of subsystems of a non-Abelian anyon system. This is important because often (e.g., in topological quantum computing) we may be concerned about only the entanglement between such subsystems.
Lattice model constructions for gapless domain walls between topological phases

CHENFENG BAO, Perimeter Institute for Theoretical Physics, Waterloo, Ontario, N2L2Y5, Canada, SHUO YANG (Presenter), State Key Laboratory of Low-Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing 100084, China, CHENJIE WANG, Perimeter Institute for Theoretical Physics, Waterloo, Ontario, N2L2Y5, Canada, ZHENGCHENG GU, Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong — Lattice models of gapless domain walls between twisted and untwisted gauge theories of finite group G are constructed systematically. As simple examples, we numerically studied the gapless domain walls between twisted and untwisted Z_N (with N=6) gauge models in 2+1D using the state-of-art loop optimization of tensor network renormalization algorithm. We also studied the physical mechanism for these gapless domain walls and obtained quantum field theory descriptions that agree perfectly with our numerical results. By taking the advantage of the systematic classification and construction of twisted gauge models using group cohomology theory, we systematically construct general lattice models to realize gapless domain walls for arbitrary finite symmetry group G. Such constructions can be generalized into arbitrary dimensions and might provide us with a systematical way to study gapless domain walls and topological quantum phase transitions.

* *

Effect of Electron-Phonon Interactions on Dirac Fermions

YUXI ZHANG (Presenter), Department of Physics, University of California, Davis, GEORGE BATROUNI, Institut de Physique de Nice, Universite de Nice-Sophia Antipolis, WETING CHIU, Department of Physics, University of California, Davis, NATANAE DE CARVALHO COSTA, Universidade Federal do Rio de Janeiro, HUAIMING GUO, Department of Physics, Beihang University, RICHARD THEODORE SCALETTAR, Department of Physics, University of California, Davis — The effect of electron-electron interactions on Dirac fermions, and the possibility of an intervening spin liquid phase between the semi-metal and antiferromagnetic (AF) regimes, has been a focus of intense quantum simulation effort over the last five years. We use determinant quantum Monte Carlo (DQMC) to study the Holstein model on Honeycomb lattice and pi-flux lattice and explore the role of electron-phonon interactions on Dirac fermions. We show that they give rise to charge density wave (CDW) order, and present evidence that this occurs only above a finite critical interaction strength. We evaluate the temperature for the transition into the CDW which, unlike the AF transition, can occur at finite values owing to the discrete nature of the broken symmetry.

*This work was supported by the Department of Energy, grant DE-SC0014671.

Charge-Density-Wave Transitions of Dirac Fermions Coupled to Phonons

CHUANG CHEN (Presenter), Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, XIAO YAN XU, Department of Physics, Hong Kong University of Science and Technology, ZI YANG MENG, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, MARTIN HOHENADLER, Institut für Theoretische Physik und Astrophysik, Universität Würzburg — The spontaneous generation of charge-density-wave order in a Dirac fermion system via the natural mechanism of electron-phonon coupling is studied in the framework of the Holstein model on the honeycomb lattice. Using two independent and unbiased quantum Monte Carlo methods, the phase diagram as a function of temperature and coupling strength is determined. It features a quantum critical point as well as a line of thermal critical points. Finite-size scaling appears consistent with fermionic Gross-Neveu-Ising universality for the quantum phase transition, and bosonic Ising universality for the thermal phase transition. The critical temperature has a maximum at intermediate couplings. Our findings motivate experimental efforts to identify or engineer Dirac systems with sufficiently strong and tunable electron-phonon coupling.

*MH acknowledges support by the DFG through SFB 1170 ToCoTronics; CC and ZYM by the Ministry of Science and Technology of China through the National Key Research and Development Program (grant 2016YFA0300502), the Strategic Priority Research Program of the Chinese Academy of Sciences (XDB28000000), and the National Science Foundation of China (11574359); XYX by HKRGC (C6026-16W,16324216, 16307117).
1:27PM L07.00012: Diagnosing fractionalization and anyonic statistics in magnetic insulators via noise magnetometry with spin qubits*  
SHUBHAYU CHATTERJEE (Presenter), Physics, University of California Berkeley, JOAQUIN RODRIGUEZ NIEVA, EUGENE DEMLER, Physics, Harvard University — Two-dimensional magnetic insulators exhibit a plethora of competing ground states, such as ordered (anti)ferromagnets, quantum spin liquids with topological order and anyonic excitations, and random singlet phases emerging in the presence of disorder and frustration. We propose that single spin qubits, which interact directly with the low-energy excitations of magnetic insulators, can be used as a diagnostic of magnetic ground states. Experimentally tunable parameters, such as qubit level splitting, sample temperature, and qubit-sample distance, can be used to measure spin correlations with energy and wavevector resolution. Such resolution can be exploited to distinguish between fractionalized excitations in spin liquids and spin waves in magnetically ordered states, or to detect anyonic statistics in systems with a finite energy gap.

*SC acknowledges support from the NSF under Grant No. DMR-1664842. JRN and ED acknowledge support from Harvard-MIT CUA, NSF Grant No. DMR-1308435 and AFOSR-MURI: Photonic Quantum Matter (award FA95501610323).

1:39PM L07.00013: Chiral Tricritical Point: A New Universality Class in Dirac Systems  
SHUAI YIN (Presenter), SHAO-KAI JIAN, HONG YAO, Institute for Advanced Study, Tsinghua University — Tricriticality, as a sister of criticality, is a fundamental and absorbing issue in condensed-matter physics. It has been verified that the bosonic Wilson-Fisher universality class can be changed by gapless fermionic modes at criticality. However, the counterpart phenomena at tricriticality have rarely been explored. In this Letter, we study a model in which a tricritical Ising model is coupled to massless Dirac fermions. We find that the massless Dirac fermions result in the emergence of a new tricritical point, which we refer to as the chiral tricritical point (CTP), at the phase boundary between the Dirac semimetal and the charge-density wave insulator. From functional renormalization group analysis of the effective action, we obtain the critical behaviors of the CTP, which are qualitatively distinct from both the tricritical Ising universality and the chiral Ising universality. We further extend the calculations of the chiral tricritical behaviors of Ising spins to the case of Heisenberg spins. The experimental relevance of the CTP in two-dimensional Dirac semimetals is also discussed.


Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L08 DCMP: Superconductivity: Copper Oxide - Methods and Probes BCEC 150 - Timir Datta, University of South Carolina

11:15AM L08.00001: Circular photogalvanics study of BSCCO high temperature superconductors*  
SE JOON LIM (Presenter), Stanford University, MARTIN GREVEN, University of Minnesota, AHARON KAPITULNIK, Stanford University — Recent studies have reported that bulk inversion symmetry may be broken inside the pseudogap region of the phase diagram in YBa2Cu3Oy single crystals. Here, we report signatures of inversion symmetry breaking in another family of cuprate high temperature superconductors, Bi2Sr2CaCu2O8+δ, using circular photogalvanic measurements.

*This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515 and the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4529.

11:27AM L08.00002: Three Laws of Electronic Thermal Conductivity of High Temperature Superconductors via Dipolon Theory  
RAM SHARMA (Presenter), University of Illinois at Chicago — Recently we predicted [1] a universal peak in electronic thermal conductivity (ETC) of high-Tc superconductors (HTSCs) via the dipolon theory [2-5]. Previously the dipolon theory has predicted the two high energy and one low energy kinks besides a new very low energy kink in HTSCs. Here we present the three laws of ETC which explain not only the origin but also the behavior of ETC in HTSCs: First Law: The ETC is due to the rate of increase of the quasiparticle energy distribution (ROIOTQED) with temperature particularly near the Fermi level. Second Law: The ROIOTQED becomes maximum at temperature \( T^{(p)} \) given by \( \Delta(0)/k_B T^{(p)} = 2.40 \). Third Law: Where there is a superconducting energy gap, there is a peak in the ETC at the temperature \( T^{(p)} \).

11:39 AM L08.00003: High Pressure 3D to 2D Tuning of Magnetism in Cuprates  
MARKUS HUECKER (Presenter), Condensed Matter Physics Department, Weizmann Institute of Science, GENDA GU, JOHN TRANQUADA, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, BERND BÜCHNER, Institute for Solid State Physics, IFW Dresden  
— Broken lattice symmetries often play an integral part in the selection process of the electronic ground state. A prime example is found in the La-214 cuprates, where lattice distortions result in a complex relationship between superconductivity, charge and magnetic orders. In an attempt to dissect this problem into its various parts, here we highlight the impact of lattice distortions on the pristine magnetism of a cuprate parent compound.

11:51 AM L08.00004: Uniaxial strain susceptibilities of superconducting Tc and charge order transition temperature from sound velocity measurements in YBCO*  
DAVID LEBOEUF (Presenter), SIHAM BENHABIB, MEHDI FRACHET, FRANCIS LALIBERTÉ, CYRIL PROUST, LNCMI - CNRS, TOSHINAO LOEW, JUAN PORRAS, MATHIEU LE TACON, BERNHARD KEIMER, max planck institut  
We study the uniaxial strain dependence of superconducting Tc in YBCO as a function of doping using ultrasounds. We focus on the strain dependence along the a-axis dTc/dε1 and along the b-axis dTc/dε2. For dopings 0.08<p<0.12 we find an anisotropic strain dependence with dTc/dε2 >> dTc/dε1. We attribute this anisotropy to a strain-tuned competition between superconductivity and 3D uniaxial CDW. This is supported by sound velocity measurement of the 3D CDW for longitudinal modes along a and b-axis. The elastic behaviour through this CDW transition is anisotropic with |dTCDW/dε2| >> |dTCDW/dε1|. The uniaxial CDW appears as an intrinsic instability even in zero magnetic field and in the zero strain limit probed here.  
For 0.12<p<0.15 where the uniaxial strain dependencies are maximum, we observe dTc/dε2 = dTc/dε1.  
An isotropic dTc/dεi is difficult to explain as being due to a competition to a uniaxial electronic order or as being due to the orthorhombic structure. It indicates that other mechanisms must be at play. This maximum in the strain dependence of Tc with in-plane isotropy could reflect an extrema in the electronic compressibility.  
*CNRS, European Magnetif Field Laboratory, French ANR (ANR-14-CE05-0007), Laboratoire d'Excellence LANEF (ANR-10-LABX-51-01), Université Grenoble-Alpes.

12:03 PM L08.00005: Noisy defects in a doped Mott insulator*  
FREEK MASSEE (Presenter), University of Paris-Sud, YINGKAI HUANG, MARK GOLDEN, University of Amsterdam, MARCO APRILI, University of Paris-Sud  
Detailed studies of the effect of single dopant atoms on the local electronic properties are crucial for a full understanding of the macroscopic characteristics of host materials ranging from semiconductors to high temperature superconductors. Due to limited time resolution of conventional scanning tunnelling microscopes, most atomic scale studies of the latter systems focussed on the time averaged effect of dopants on the electronic structure. I will present how, by using atomic scale shot-noise measurements in the high temperature superconductor Bi2Sr2CaCu2O8+, we visualize sub-nanometre sized objects where remarkable dynamics leads to an enhancement of the tunnelling current noise by at least an order of magnitude. From the position, current and energy dependence we deduce that these defects are oxygen dopant atoms whose local environment leads to charge dynamics that strongly affect the tunnelling mechanism. Possible effects on superconductivity will be discussed.  
*We acknowledge funding from H2020 Marie Sklodowska-Curie Actions (# 659247) and the ANR (ANR-16-ACHN-0018-01)

12:15 PM L08.00006: Steady-state superconductivity in electronic materials with repulsive interactions*  
OLIVER HART (Presenter), University of Cambridge, GARRY GOLDSTEIN, Rutgers University, CLAUDIO CHAMON, Boston University, CLAUDIO CASTELNOVO, University of Cambridge  
We study the effect of laser driving on a minimal model for a hexagonal two-dimensional material with broken inversion symmetry. Through the application of circularly polarised light and coupling to a thermal free electron bath, the system is driven into a nonequilibrium steady state with asymmetric, nonthermal carrier populations in the two valleys. We show that, in this steady state, interband superconducting correlations between electrons can develop independent of the sign of the electron-electron interactions. We discuss how our results apply, for example, to transition metal dichalcogenides. This work opens the door to technological applications of superconductivity in a range of materials that were hitherto precluded from it.  
*This work was supported in part by Engineering and Physical Sciences Research Council (EPSRC) Grants No. EP/P034616/1 and No. EP/M007065/1 (C.Ca. and O.H.), by NSF grant No. DMR-1733071 (G.G.), and by DOE Grant No. DE- FG02-06ER46316 (C.Ch.).
12:27PM L08.00007: Tuning the Josephson vortex lattice structure with pancake vortices in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ single crystals* SIMON BENDING (Presenter), PETER J CURRAN, HUSSEN A MOHAMMED, Department of Physics, University of Bath, ALEXEI E KOSHELEV, Materials Science Division, Argonne National Laboratory, YUJI TSUCHIYA, Department of Electrical Engineering, Nagoya University, TSUYOSHI TAMEGAI, Department of Applied Physics, University of Tokyo — Vortex structures in the highly anisotropic superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ depend on the angle the applied field makes with the CuO$_2$ layers; stacks of pancake vortices form when the field is perpendicular to these and highly elliptical Josephson vortices form when it is parallel to them. For tilted magnetic fields, pancake and Josephson vortices coexist and interact in complex ways to form vortex chains and composite vortex lattices, reflecting the delicate balance between attractive and repulsive interactions. Scanning Hall microscopy has been used to map the rich tilted-field vortex phase diagram in an underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ single crystal. We find that the Josephson vortex lattice spacing has an unexpected non-monotonic dependence on pancake vortex density linked to a field-driven structural transformation with increasing out-of-plane fields. We establish the exact evolution of vortex-chain phases as the out-of-plane field is increased and identify especially stable structures spaced by an integer number of rows of interstitial pancake vortex stacks. Our experimental results are in good semi-quantitative agreement with a theoretical model.


12:39PM L08.00008: Enhancement of critical current density and mechanical properties of BiPb-2223 superconductor phase added with Nano-sized Gd-123 phase ALY ABOU-ALY (Presenter), NAYERA MOHAMMED, MAI BARAKAT, MOHAMMED HASSAN, RAMADAN AWAD, Physics Department, Alexandria University — Ball milled Nano-sized of Gd-123 superconductor phase was added to the high temperature superconductor (HTSC) BiPb-2223 phase with weight percentage 2.0 wt.%. The milling times t was varied up to 180 min. The samples have a general stoichiometry of (Gd$_{1.0}$Ba$_{2.0}$Cu$_{3.0}$O$_{8+\delta}$)$_{2.0}$/Bi$_{1.8}$Pb$_{0.4}$Sr$_{2.0}$Ca$_{2.0}$Cu$_{3.2}$O$_{10+\delta}$. The samples were prepared by the standard solid-state reaction method. The ball milled superconductor Gd-123 phase was characterized by X-ray powder diffraction (XRD) and transmission electron microscope (TEM) confirming the Nano-scale crystallite size. The prepared samples were characterized by XRD and the scanning electron microscope (SEM). Samples were examined by electrical resistivity and IV measurements in addition to Vickers micro hardness. No significant change in the superconducting transition temperature $T_c$ has been noticed for all samples. The highest relative volume fraction for BiPb-2223 phase was recorded for the sample with $t = 120$ min. The critical current density $J_c$ was increased from 326, for free sample, up to 1860 A/cm$^2$, for added sample, with grain size 17.52 nm. The micro hardness data was analyzed using several models. The modified proportional sample resistance (MPSR) model is the model that can describe the behavior of our samples successfully.

12:51PM L08.00009: Structural Phase Transitions: a Limiting Factor for Quantum Criticality and Superconductivity in La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$* QIANLI MA (Presenter), MIRELA DRAGONMIR, JAMES P.I. CLANCY, McMaster University, ASHFIA HUQ, Oak Ridge National Laboratory, BRUCE GAULIN, McMaster University — One branch of the La-214 family of cuprate superconductors, La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$, has been of great interest as it displays the full complexity of the canonical hole-doped high TC phase diagram. The strong dependence of the electronic properties on the crystal symmetry has motivated careful diffraction studies of the La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ structural phase diagram.

We present our recent findings on the structural transitions in the La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ system. Our group has synthesized single-phase polycrystalline samples with $x$ spanning from 0.01 to 0.40, and grew large single crystals of La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ for select $x$. To the best of our knowledge, such high Sr concentrations have not been achieved thus far. Systematic neutron and X-ray diffraction studies were performed at both low and high temperatures. These analyses allowed us to follow the sequence of structural phase transitions and to propose an updated La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ phase diagram that now covers Sr doping concentrations up to $x = 0.40$. Furthermore, our findings suggest that the persistence of the high temperature tetragonal structure, HTT, down to low temperatures when $x = 0.27$ might be a limiting factor for both superconductivity and the putative quantum critical point proposed for La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$.

*NSERC
1:03PM L08.00010: d-wave Andreev reflection study of the ab-plane proximity effect in cuprate/manganite and cuprate/nickelate thin films* RAINNI CHEN (Presenter), CHAO ZHANG, CHRIS GRANSTROM, JOHN Y.T. WEI, Physics, University of Toronto — An anomalously long-range proximity effect was previously reported in c-axis thin-film heterostructures of ferromagnetic La$_{2/3}$Ca$_{1/3}$MnO$_3$ (LCMO) and superconducting YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO), and attributed to spin-triplet d-wave pairing [1]. However, there is debate over the existence of such long-range proximity effect, given the short c-axis coherence length of YBCO, and since scanning tunneling spectroscopy (STS) on c-axis LCMO/YBCO bilayers has failed to observe any direct evidence [2]. For YBCO/LCMO bilayers oriented along the a-axis, similar STS measurements have reportedly observed a proximity length scale of ~ 30 nm [3]. In this work, we extend these prior STS studies to YBCO/LCMO bilayers oriented along the <110> axis, a geometry that is expected produce the most robust d-wave Andreev resonance states. We also measure <110>-oriented LaNiO$_3$/YBCO bilayers, as a non-magnetic control. Our data are analyzed in terms of the overlayer thickness, in an effort to determine the actual length scale of the manganite/cuprate proximity effect in the ab-plane.


*This work was supported by NSERC, CFI, OIT, and CIFAR.

1:15PM L08.00011: Atomically thin high-temperature superconductors YUYING ZHU (Presenter), MENGHAN LIAO, JIN ZHANG, Tsinghua University, RUIDAN ZHONG, JOHN SCHNEELOCH, GENDA GU, Brookhaven National Laboratory, KAILI JIANG, DING ZHANG, XUCUN MA, QIKUN XUE, Tsinghua University — The emergent technique of van der Waals stacking has started to impact on high temperature superconductivity [1][2]. Here we report the realization of superconducting unprotected Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) flakes down to 2.5 unit cells for studying high Tc superconductivity mechanism. We employ a novel solid state gating technique to effectively tune the carrier density of thin flakes, inducing the superconductor-insulator transition (SIT) in BSCCO. The corresponding evolution of the density of states (DOS) is unveiled by using planar tunnel junctions of graphite/BSCCO. The combination of gate tuning and tunneling spectroscopy shall be applicable to other two-dimensional materials.


1:27PM L08.00012: New Mechanism of Umklapp Scattering in Cuprate High-Tc Superconductors RONG LI (Presenter), ZHEN-SU SHE, Peking University — Cuprates display several novel symmetry-broken orders such as spin stripe, charge density wave (CDW). We propose a novel mechanism of dissipative umklapp scattering contributing to anomalous transport by fluctuating order beyond fermi surface reconstruction to electronic spectrum. Spatial-temporal fluctuating order is assumed to introduce umklapp scattering of holes, which yields a relaxation time proportional to square of order's periodicity ($l_o$) and a resistivity $\rho=\hbar/(\pi^2e^2ncl_o^2)$. This achieves a remarkable link between microscopic fluctuating orders and macroscopic transport, which yields a length mapping method (i.e. $l_o\propto \rho^{-1/2}$) to derive orders' periodicity from resistivity data. The theory is validated by data of three classes of samples in LSCO, Bi-2201 and Bi-2212. We show that at underdoped regime at 'knee' temperature (of $\rho$ vs $T$), $l_o$ is indeed close to $2a_0$, which is the periodicity of antiferromagnetism, while at overdoped regime $l_o$ is near $4a_0$, the CDW periodicity. In a vortex liquid, $l_o$ is found to vary as reduced vortex distance (-$B^{1/2}$), and in strange metal as reduced de Broglie wave length (-$T^{-1/2}$). These results demonstrate the universal validity of the new umklapp scattering mechanism and the length mapping method, providing a new tool to study order transitions.
1:39PM L08.00013: Reconfigurable SQUID Arrays  
SICHAO YU (Presenter), New York University Tandon School of Engineering, WILLIAM ANDREW MAYER, MATTHIEU DARTAILH, KAUSHINI WICKRAMASINGHE, JOSEPH YUAN, JAVAD SHABANI, Center for Quantum Phenomena, Department of Physics, New York University — Superconducting quantum interference devices (SQUID) are widely used for sensitive magnetic field detection. Traditional SQUID arrays based on Superconductor/Insulator junctions have limited flexibility as junction properties are not tunable. The realization of Superconductor/Semiconductor junctions allows for gate-tunable junction properties. This allows for complex tunable SQUID arrays that can be continuously adjusted with voltage gates. We numerically study tunable SQUID arrays with various circuit geometries. Potential applications of these arrays include increased sensitivity to spatial inhomogeneity of fields and variable spatial resolution. Another potential advantage that is numerically explored is leveraging time dependent gate voltages to filter noise and increase sensitivity.

1:51PM L08.00014: Scanning SQUID Microscopy on fractional flux quanta with on-chip field control  
PIM REITH (Presenter), MESA+ Institute for Nanotechnology, University of Twente, MICHAEL FALEY, PGi-5, Forschungszentrum Jülich, CHRISTOFORUS DIMAS SATRYA, ALEXANDER GOLUBOV, HANS HILGENKAMP, MESA+ Institute for Nanotechnology, University of Twente — Scanning Superconducting Quantum Interference Device (SQUID) Microscopy (SSM) is a scanning probe technique that utilizes the high magnetic field sensitivity of a SQUID to image local magnetic field of a sample surface. SSM played a vital role in showing the d-wave symmetry in cuprate superconductors by measuring fractional flux quanta, created spontaneously due to the cuprate acting as a π-shift element.

Now we continue on this by incorporating an on-chip bias line that can produce a local magnetic field. This allows us to control the flux state of nearby Nb-YBCO hybrid loops that exhibit fractional flux behavior. We have demonstrated the ability to freely change between the +1/2 Φ₀ and -1/2 Φ₀ states. Additionally, we study transitions into higher flux states (+3/2 Φ₀, ±5/2 Φ₀). These results are a crucial step to using controllable superconducting loops with π-shift elements in quantum annealing computing.

2:03PM L08.00015: Modeling Resonances in the Current-Voltage Characteristics of SQUID Susceptometers*  
SAMANTHA DAVIS (Presenter), Physics, Stanford University, JOHN KIRTLEY, GLAM, Stanford University, KATHRYN ANN MOLER, Physics and Applied Physics, Stanford University — In Scanning SQUID Microscopy, SQUID susceptometers are tools for achieving extremely precise magnetic imaging and local susceptibility measurements with high spatial resolution. Further development of scanning SQUID microscopy demands a thorough understanding of the properties of SQUID susceptometers. One mysterious behavior is the presence of resonances in the current-voltage characteristics of SQUID susceptometers for scanning applications. The origins and the effects of the resonances on the performance of these SQUIDs is unknown. To illuminate the origin and impact of the resonances, we have developed a model that successfully reproduces the experimentally-determined current-voltage characteristics of SQUIDs for one resonance. We explore the limitations of our model by calculating the noise characteristics of SQUIDs of different designs and comparing the results with experimental noise measurements. Looking forward, we aim to extend the model to encompass all the resonances that appear in experimental data. We will then use the model to optimize the signal-to-noise characteristics of scanning SQUID susceptometers.

*Part of this work was performed at the Stanford Nano Shared Facilities (SNSF), supported by the National Science Foundation under award ECCS-1542152.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L09 DCMP: Superconductivity: Proximity Effect and Josephson Junctions I  
Michael Ososfky, United States Naval Research Laboratory
11:15AM L09.00001: Quantum Vortex Melting and Superconductor Insulator Transition in a 2D Josephson Junction Array in a Perpendicular Magnetic Field via Diffusion Monte Carlo* PRAGALV KARKI (Presenter), YEN LEE LOH, University of North Dakota — In this study [1], we simulated a quantum rotor model describing a Josephson junction array (JJA) in the phase representation at zero temperature in a perpendicular magnetic field $B=0.1,0.2,0.3,0.4$ (in units of $h/4\pi ea^2$) on a $L_xL_y$ square lattice with spacing $a$ for $L=6,8,10,12$. The superconductor-insulator transition (SIT) is tuned by the ratio of charging energy to Josephson coupling, $U/J$. Abrupt drops in the magnetization values were observed in the bigger lattices at certain values of $B$ and $U/J$ caused by the formation of vortices. Increasing $U/J$ at a fixed $B$ field causes quantum vortex melting. The magnetization drops to zero around $U/J \sim 5$ indicating SIT. For $B=0.1$ the SIT occurs without an intermediate vortex state and the magnetization scales as $M \sim L^4$, whereas for $B=0.4$ the scaling is $M \sim L^4$ during the vortex melting. For $B$ between 0.1 and 0.4 the scaling is not clear. We used the diffusion Monte Carlo (DMC) method with a guiding wavefunction optimized using the variational Monte Carlo (VMC) method.


*ND EPSCoR through NSF grant #OIA-1355466

11:27AM L09.00002: Protected gap closing in Josephson junctions constructed on Bi$_2$Te$_3$ surface ZHAOZHENG LYU (Presenter), YUAN PANG, JUNHUA WANG, GUANG YANG, GUANGTONG LIU, FANMINING QU, LI LU, JIE FAN, ZHONGQING JI, XIUNIAN JING, institute of physics — On the road of searching for Majorana zero modes (MZMs) in topological insulator-based Josephson junctions, a highly-sought signature is the protected full transparency of electron transport through the junctions due to the existence of the MZMs, associated with complete gap closing between the electronlike and holelike Andreev bound states (ABSs). We fabricated Pb-Bi$_2$Te$_3$-Pb Josephson junctions and developed the method of using nonsuperconducting Pd electrodes to detect the ABS spectra in the junctions area. We generalized the Blonder-Tinkham-Klapwijk theory to describe the measured contact resistance of the Pd-Bi$_2$Te$_3$ interface. Our results provide direct experimental evidence of complete gap-closing and full transparent transport in single Josephson junctions constructed on the surface of Bi$_2$Te$_3$.


11:39AM L09.00003: A Mesoscopic Spectrometer Based on the Josephson Effect* JOEL GRIESMAR (Presenter), VINCENT BENZONI, FABIEN LAFONT, LEO PEYRUCHAT, JEAN-LOUP SMIRR, CAGLAR GIRIT, Flux Quantum Lab, CNRS USR 3573, College de France — A key element of mesoscopic topological systems, such as hybrid semiconductor-superconductor circuits, are Andreev Bound States, single quasiparticles localized at superconducting weak links. The characteristic transition energy of these states is twice the superconducting gap (90 GHz in aluminum). Conventional microwave techniques allow probing these states but only in a limited bandwidth. We propose a new broadband spectrometer operating at frequencies up to 180 GHz based on the Josephson effect which converts a DC voltage to microwave oscillations at a frequency proportional to this voltage. Using a symmetrical SQUID biased at half a flux quantum allows decoupling the spectrometer from environmental modes. In addition, careful design of the biasing circuit reduces the number of remaining modes and damps them. The fabricated mesoscopic spectrometer has a linewidth of 2 MHz, a bandwidth of 180 GHz and a minimal theoretical sensitivity of 5 kHz.

*This research was supported by IDEX grant ANR-10-IDEX-0001-02 PSL, a Paris Programme Emergence(s) Grant and the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement 636744).

11:51AM L09.00004: Quantum Hall Supercurrent in a locally gated Graphene Josephson Junction - Part 1: Induction of Local Filling Factors and Quantum Hall Supercurrent* ANDREW SEREDINSKI (Presenter), ANNE M DRAELOS, ETHAN ARNAULT, MING-TSO WEI, Physics, Duke University, HENGMING LI, TATE FLEMING, Physics and Astronomy, Appalachian State University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, NIMS, FRANCOIS AMET, Physics and Astronomy, Appalachian State University, GLEB FINKELSTEIN, Physics, Duke University — We present a study of a graphene-based Josephson junction with local gates modulating the carrier density along either edge of the junction in a wide range. In magnetic fields in the 1-2 Tesla range, we populate the next Landau level, resulting in Hall plateaus with conductance that differs from the bulk filling factor. We observe robust supercurrent when the gating introduces counter-propagating quantum Hall edge states along either edge of the junction.

*The authors were supported by ARO Award W911NF-16-1-0122 and NSF awards ECCS-1610213 and DMR-1743907.
12:03PM L09.00005: Quantum Hall Supercurrent in a locally gated Graphene Josephson Junction - Part 2: Evolution of Interference patterns with Carrier Density and Field* ETHAN ARNAULT, ANDREW SEREDINSKI, ANNE M DRAELOS, MING-TSO WEI, Department of Physics, Duke University, HENGMING LI, TATE FLEMING (Presenter), Department of Physics, Appalachian State University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Material Lab, NIMS, FRANCOIS AMET, Department of Physics, Appalachian State University, GLEB FINKELSTEIN, Department of Physics, Duke University — We explore supercurrent induced along individual edges in a locally gated graphene-based Josephson junction in the quantum Hall regime. When supercurrents are present along both sides of the junction, they produce interference pattern as a function of magnetic field, bulk and edge carrier densities. This behavior allows us to infer information about the position of the edge states. We present electrostatic models relating the evolution of the interference patterns to the physical location of quantum Hall edge states in the device.

*The authors were supported by ARO Award W911NF-16-1-0122 and NSF awards ECCS-1610213 and DMR-1743907.

12:15PM L09.00006: Realization of Hybrid Superconductor–Semiconductor Systems by Homoepitaxial Growth of Non-equilibrium P-doped Si(111)* KASRA SARDASHTI (Presenter), Department of Science and Math, Fashion Institute of Technology, KAUSHINI WICKRAMASINGHE, Department of Physics, New York University, TRI NGUYEN, Department of Physics, City College of New York, WILLIAM ANDREW MAYER, MEHDI HATEFIPOUR, JOSEPH YUAN, JAVAD SHABANI, Department of Physics, New York University — To fulfill the long-term vision of reliable quantum computation, the ideal hybrid platform allows quantum information to be processed, stored and transmitted in the same materials system. Silicon can be a promising candidate for fault-tolerant hybrid quantum systems due to its multifunctionality, reliability and long coherence times. Superconducting Si could provide a viable pathway for realization of Si qubit circuits, by forming homogeneous Superconductor (SC)–Semiconductor–SC Josephson junctions. In this work, non-equilibrium p-doping of Si thin-films by homoepitaxial growth of Ga-rich Si on Si(111) is studied. Surface structure and morphology of the p-doped films were evaluated by reflection high-energy electron diffraction and atomic force microscopy. Doping levels and carrier concentrations were determined by temperature-dependent resistivity (ρ–T) measurements in van der Pauw configuration and on Hall bars. Upon increase in Ga incorporation, ρ–T characteristics of the p-doped films transitioned from insulating to quasi-reentrant superconductivity with $R_{min}/R_N$ of 0.82–0.89. Based on the known theories, mechanisms and strategies to go beyond the quasi-reentrant regime will be discussed.

*US Air Force Office of Scientific Research Young Investigator Award, FA9550-16-1-0348.

12:27PM L09.00007: Spin-orbit splitting of Andreev states revealed by microwave spectroscopy* LEANDRO TOSI (Presenter), CYRIL METZGER, MARCELO GOFFMAN, CRISTIAN URBINA, HUGUES POTHIER, Quantronics Group, SPEC, CEA-Saclay, SUNGHUN PARK, ALFREDO LEVY YEYATI, Departamento de Materia Condensada, Universidad Autonoma de Madrid, PETER KROGSTRUP, JESPER NYGÅRD, Center for Quantum Devices — The Josephson supercurrent that flows through a weak link between two superconductors is mediated by fermionic quasiparticle states localized at the weak link: the Andreev bound states. To explore the role of the spin of these states, we have performed their microwave absorption spectroscopy in superconducting weak links with strong spin-orbit coupling: an InAs-Al (core-full shell) epitaxially-grown nanowire. The spectra present distinctive features that we interpret as arising from zero-field spin-split Andreev states. A simple empirical model, which takes into account the Rashba spin-orbit interaction in a multichannel nanowire, explains these features and their evolution with magnetic field. Our results show that the spin of quasiparticles can be a relevant degree of freedom in Josephson weak links.

*Marie Sklodowska-Curie individual fellowship grant 705467
Anomalous interference in planar WTe₂ Josephson junctions

ANDREW PIERCE (Presenter), Department of Physics, Harvard University, JOHANNES GOOTH, Max Planck Institute for Chemical Physics of Solids, MICHAEL KOSOWSKY, Department of Physics, Harvard University, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, AMIR YACOBY, Department of Physics, Harvard University — Josephson junctions fabricated on materials with strong spin-orbit coupling (SOC) have driven substantial research efforts due to the possibility of realizing topological superconductivity (TSC) in such devices. Layered materials with strong SOC, especially those which can be isolated via mechanical exfoliation, are particularly attractive due to their natural compatibility with large in-plane magnetic fields. This talk discusses the evolution of the critical current of WTe₂ Josephson junctions as a function of in-plane magnetic field. Thin (<100 nm) samples of WTe₂ are of interest for applications to TSC as they provide strong SOC with the required type of Fermi-surface spin texture. Under certain conditions, the interference patterns observed in these devices diverge from the standard Fraunhofer-like pattern that follows from the simplest set of assumptions, suggesting the presence of important orbital effects.

Numerical modelling of capacitively-shunted Josephson junctions including quasiparticle excitations

WILLIAM COLE (Presenter), University of Maryland, College Park, CHAITANYA MURTHY, University of California, Santa Barbara, BERNARD VAN HECK, Microsoft Quantum, Microsoft Station Q, UCSB — We have developed a numerical framework for calculating the many-body spectrum of Cooper pair box hamiltonians where the Josephson potential is matrix-valued in the space of (non-conserved) quasiparticle occupation numbers. We will describe this general formalism and then demonstrate its applicability to various semi-realistic superconducting junctions of current interest, as specified by real-space Bogoliubov-de Gennes hamiltonians.

Manipulation of Phases and Supercurrents in S-TI-S Lateral Josephson Junction Networks

ERIK HUEMILLER (Presenter), Inprentus Precision Optics, CAN ZHANG, GUANG YUE, University of Illinois at Urbana-Champaign, SEONGSHIK OH, Physics, Rutgers, The State University of New Jersey, DALE J VAN HARLINGEN, University of Illinois at Urbana-Champaign — Quantum computing using topological Q-bits composed of Majorana Fermions (MF) shows promise for its robustness against disorder and its scalability with existing lithography infrastructure. In lateral Josephson junction networks, the MFs are localized to points in the junction where the phase difference of the superconducting order parameter across the junction is equal to an odd multiple of π. Quantum computations are performed by physically moving MFs pinned to odd π crossings around one another, encoding the quantum state of the system in the historical locations of the MFs relative to each other. Understanding the phase distributions around multi-junction nodes in the network is one key hurdle that needs to be overcome before the implementation of this architecture is a reality. Measurements and modeling of Nb-BiSe-Nb lateral Josephson junctions in three and four junction geometries will be presented. The results will be discussed with their implication for the realization of a topological quantum architecture.

Transport Studies in Gate-Tunable Multi-Terminal Josephson Junctions

GINO GRAZIANO (Presenter), School of Physics and Astronomy, University of Minnesota, JOON SUE LEE, California NanoSystems Institute, University of California, Santa Barbara, MIHIR PENDHARKAR, Department of Electrical and Computer Engineering, University of California, Santa Barbara, CHRIS PALMSTROM, Materials Department, University of California, Santa Barbara, VLAD S PRIBIAG, School of Physics and Astronomy, University of Minnesota — Josephson junctions with three or more superconducting leads are predicted to exhibit topological physics in the presence of few conducting modes within the interstitial normal material.[1][2] Such topological behavior manifests itself as signatures in the complex transport properties between the different terminals, with topological phase transitions occurring as a function of phase and voltage bias.[3] Here we study the superconducting and resistive properties of top-gated multi-terminal Josephson devices, based on an InAs 2DEG proximitized with epitaxial aluminum. The top gate is used to deplete the 2DEG, and resistances are analyzed under various bias currents and magnetic fields.


*This work was conducted under NSF DMR grant 16-10114
Spin-triplet supercurrents in Josephson junctions with Co/Py exchange-spring interfaces

EKTA BHATIA (Presenter), Physical Sciences, National Institute of Science Education and Research, HBNI, JAMES DEVINE STONEMAN, SACHIO KOMORI, ANAND SRIVASTAVA, ZOE BARBER, Department of material science and metallurgy, University of Cambridge, KARTIK SENAPATI, Physical Sciences, National Institute of Science Education and Research, HBNI, JASON ROBINSON, Department of material science and metallurgy, University of Cambridge — Conventional (spin-singlet) s-wave superconductivity (S) and ferromagnetism (F) are incompatible. However, it is now established that s-wave S can coexist with F through the conversion of spin-singlet to spin-triplet Cooper pairs at a magnetically inhomogeneous interface [1]. Here we report Josephson coupling in Nb/Co/Py/Nb Josephson junctions in which the total bilayer (Co/Py) thickness exceeds the singlet pair coherence length [1nm in Py [2]]. At a Co/Py interface, the interface exchange coupling is strong compared to the weak magnetic anisotropy of Py and so, depending on the direction and magnitude of an external magnetic field, an in-plane Bloch domain wall can form in Py creating the necessary magnetic non-collinearity for pair conversion [3]. We observe Josephson coupling for Py layer thicknesses up to 11 nm which greatly exceeds the singlet coherence length, strongly suggesting the propagation of spin-polarized triplet supercurrents. Furthermore, through magnetic field history we are able to programme the magnetic state, which offers the potential for active control of triplet supercurrents.


Non-local Josephson effect in Andreev molecules*

CAGLAR GIRIT (Presenter), JEAN-DAMIEN PILLET, VINCENT BENZONI, JOEL GRIESMAR, JEAN-LOUP SMIRR, CNRS USR 3573, Collège de France — We propose the Andreev molecule, an artificial quantum system comprised of two closely spaced Josephson junctions. As in a real molecule, the coupling between Josephson junctions in an Andreev molecule occurs through the overlap and hybridization of the junction's "atomic" orbitals, the Andreev Bound States. One of the striking consequences of molecular hybridization is that the supercurrent flowing through one junction depends on the superconducting phase difference across the other junction. The energy spectrum of Andreev molecules have gaps which open as the inter-junction separation is reduced. The current-phase relations are non-local and demonstrate the possibility of a non-zero supercurrent at zero phase difference, a \( \phi \)-junction. In order to synthesize and detect Andreev molecules, we propose experiments on devices fabricated only with conventional materials and standard nanofabrication techniques. Andreev molecules are a new class of superconducting quantum devices with potential applications in quantum information, metrology, sensing, and molecular simulation.

*IDEX Grant ANR-10-IDEX-0001-02 PSL
Paris “Programme Emergence(s)” Grant
European Research Council (ERC) Horizon 2020 research and innovation programme (grant agreement 636744).

Phase transitions in current biased superconductors*

VADIM OGANESYAN, NEGIN MOHARRAMI ALLAFI (Presenter), Physics and Astronomy, CSI and GC, CUNY — We consider models of Josephson coupled superconducting wires and sheets in the presence of current biasing. We study signatures of a phase transition between fully locked ("locked") and unlocked ("soliton") phases akin to the conventional commensurate-incommensurate transition in mutual inductance and tunnelling spectroscopy.

*NSF DMR1508538 and DMR1420634
Probing the magnetic screening properties of superconductor-ferromagnet hybrids.*

NATHAN SATCHELL (Presenter), Department of Physics and Astronomy, Michigan State University, PATRICK QUARTERMAN, National Institute of Standards and Technology, REZA LOLOEE, Department of Physics and Astronomy, Michigan State University, BRIAN KIRBY, JULIE BORCHERS, National Institute of Standards and Technology, NORMAN OWEN BIRGE, Department of Physics and Astronomy, Michigan State University — Ferromagnetic Josephson junctions are a strong candidate for a dissipationless cryogenic memory alternative to dissipative CMOS technologies. Much attention has been focused on what happens to the supercurrent propagating through the Josephson junction, including the discovery of spin aligned triplet Cooper pairs in these systems [1]. In parallel, the magnetic screening properties of superconductors in electronic proximity to ferromagnetic materials have been studied, as an additional component of the screening is expected to be induced by the proximity effect [2]. These additional screening currents may account for several experimental observations, most notably in Co/Nb/Cu trilayers where an anomalous Meissner effect is reported by the low energy muon spin rotation technique [3]. In this work, we report our progress characterising the magnetic screening properties of isolated Nb (200 nm) and a bilayer of Ni (x nm)/Nb (200 nm) using polarized neutron reflectometry and the Fraunhofer characteristic of Josephson junctions.


*Marie Sklodowska-Curie Action (MSCA-IF-GF Grant No. 743791-SUPERSPIN).

Wednesday, March 6, 2019 11:15 AM - 1:51 PM

Session L10 DMP DCOMP: Fe-based Superconductors -- FeSe Intercalates and Interfaces

11:15AM L10.00001: Spectroscopic evidence of pair-mediated bosonic modes in superconductor FeSe/SrTiO3(100) film

MINJUN LEE (Presenter), MYUNCHUL OH, Seoul National University, JUNGSEOK CHAE, Institute for Basic Science, YOUNG KUK, Seoul National University — Single layer FeSe on SrTiO3(100) is atypical but noticed system in superconductivity. This has unique properties due to the substrate phonon. Unlike other bulk systems, the presence of the interface allows the substrate phonons to affect the superconducting layer. We have investigated substrate phonon effects on superconducting FeSe layer by using scanning tunneling spectroscopy and Eliashberg theory. We were able to measure acoustic, optical and substrate phonons in d²I/dV² spectroscopy. We found these phonon modes attribute to the paring of electrons in this superconducting layer. These results are analyzed by Eliashberg model and we will discuss the coupling strength of these bosonic features. We have found that the substrate phonon has major contribution to increase the transition temperature of this system.
11:27AM L10.00002: Replica bands in FeSe monolayers on STO [Invited]  FENGMIAO LI (Presenter), GEORGE ALBERT SAWATZKY, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z4, Stewart Blusson Quantum Matter Institute — The recent observation of replica bands in FeSe monolayers on STO in angle-resolved photoemission spectroscopy (ARPES) [1] has triggered intense discussions concerning the influence of FeSe electron coupling with STO phonon on the enhanced superconductivity. To obtain narrow replica bands tracing closely the dispersion of main bands rather than broad shake-off features or kinks, one has to require the coupling to be strongly peaked at q=0. However, whether the uniform electric field generated by q=0 STO phonon can strengthen the Cooper pairing in FeSe monolayer is still in discussion. We follow up with a new interpretation of the replica bands demonstrating they are largely due to the energy loss process of the escaping photoelectron, resulted from the well-known strong coupling of external propagating electrons to q=0 Fuchs-Kliewer (FK) surface phonons in STO [2]. Photoelectron energy loss on FeSe monolayer is calculated using the demonstrated successful semiclassical dielectric theory in describing low energy high-resolution electron energy loss spectroscopy (HREELS) [2]. We reduce the loss probability in HREELS by a factor 2 since the electron traveling path in ARPES is 1/2 of the HREELS one. Our calculation turns out to be able to reproduce the replica intensity and other experimental features in detail very well without the need for any fitting parameter [3]. This strongly suggests that the observed replica bands are mostly due to extrinsic photoelectron energy loss and not a result of the electron-phonon interaction of the Fe d electrons with the STO phonons. Therefore, the mechanism of the enhanced superconductivity in these monolayers remains an open question although other phonons than the FK types may still contribute.


12:03PM L10.00003: Quantum phase transition in monolayer FeSe films by tunable thickness of graphene substrate  WAN-TONG HUANG (Presenter), HAICHENG LIN, CHENG ZHENG, YUGUO YIN, SHUAI-HUA JI, XI CHEN, Tsinghua University — Insulator to superconductor transition in Fermi systems is one of the most fascinating issues, which goes beyond the BCS paradigm of superconductivity as the Fermi surface instability. Although exotic physics has been predicted theoretically, the experimental realization of such transition in solid-state systems has been more or less elusive. Here we show that the monolayer FeSe films grown on epitaxial graphene on nitrogen-doped SiC(0001) exhibit phase transition from insulator to superconductor. The Fermi energy of monolayer FeSe is remarkably low and can be tuned by the thickness of graphene through carrier doping. Furthermore, the Fermi energy is comparable to the superconducting gap, providing opportunity to probe exotic physics.

12:15PM L10.00004: Molecular Beam Epitaxy Growth of FeSe/SrTiO3 Heterostructures*  ZHENG REN (Presenter), HE ZHAO, ALEXANDER LAFLEUR, SHANG GAO, BRYAN RACHMILOWITZ, ILIJA ZELJKOVIC, Boston College — Monolayer of FeSe grown on SrTiO3 surface has shown to exhibit a large increase in superconducting transition temperature, from ~8K in bulk FeSe to above 100K (Ge J, et al. Nature Materials 14, 285-289(2015) ). Extensive studies performed on this system to date suggested that both electronic and phononic mechanism might be responsible for this enhancement of superconductivity. Therefore, a route towards increasing the Tc even further might involve using oxide substrates with carefully engineered chemical composition. We use molecular beam epitaxy to grow thin film SrTiO3 on commercial substrates with a precise control of the surface termination (SrO vs. TiO2). Furthermore, we discuss our preliminary results on comparing the structural and electronic properties of FeSe deposited on SrTiO3 thin films and bulk commercial substrates.

*We gratefully acknowledge the funding from DARPA N66001-17-1-4051.
**12:27PM L10.00005: Suppression of superconductivity and the magnetotransport behaviour in ultra-thin flakes of FeSe**

LIAM FARRAR (Presenter), Department of Physics, University of Bath, MATTHEW BRISTOW, Department of Physics, University of Oxford, AMIR HAGHIGHIRAD, Institute for Solid-State Physics, Karlsruhe Institute of Technology, ALIX MCCOLLAM, High Field Magnet Laboratory (HFML-EMFL), Radboud University, SIMON BENDING, Department of Physics, University of Bath, AMALIA COLDEA, Department of Physics, University of Oxford — The discovery of high temperature superconductivity in a monolayer of FeSe on SrTiO3 has ignited significant interest in understanding its two-dimensional superconductivity and the interfacial phenomena that determine its properties. To address these aspects, we examine the superconducting and electronic properties of exfoliated thin flakes of FeSe as a function of decreasing thickness, from bulk down towards 10 nm. We present a magnetotransport study in magnetic fields up to 38 T, which allows us to assess the changes in the multi-band electronic properties as a function of thickness. By reducing the thickness, the superconductivity of FeSe flakes is suppressed and the superconducting phase diagrams show significant changes in anisotropy.

*The research was supported by the Oxford Centre for Applied Superconductivity (CFAS), the John Fell Fund of the Oxford University and by EPSRC, UK (EP/L015544, EP/M020517/1, EP/I004475/1).

**12:39PM L10.00006: Coexistence of Magnetism and Superconductivity in Separate Layers of Iron-Based Superconductor Li_{1-x}Fe_{y}(OH)Fe_{1-y}Se**

CRAIG TOPPING (Presenter), School of Physics and Astronomy, University of St Andrews, FRANZISKA KIRSCHNER, STEPHEN BLUNDELL, Department of Physics, University of Oxford, PETER J. BAKER, ISIS Facility, Rutherford Appleton Laboratory, DANIEL WOODRUFF, FRANCESCA SCHILD, HUALEI SUN, SIMON CLARKE, Department of Chemistry, University of Oxford — The family of compounds of general formula Li_{1-x}Fe_{y}(OH)Fe_{1-y}Se, consisting of alternating Fe_{1-y}Se and Li_{1-x}Fe_{y}(OH) layers, have been found to superconduct with $T_c$'s of $\approx 40$ K. The hydroxide layer, containing roughly 20 % substitution of Li for Fe, has been shown to display magnetism well below the superconducting transition in the region of 10 K. This has been alternately reported as an ordering of the hydroxide layer Fe moments ferromagnetically and antiferromagnetically. Our study elucidates this magnetism by taking advantage of the flexible synthesis of these compounds allowing investigation of superconducting and non-superconducting variants in an effort to disentangle magnetism from superconductivity. Utilizing static and dynamic magnetometry, measurement of heat capacity and muon spin relaxation we propose the magnetism of the hydroxide layer to be glass-like and coexist with superconductivity.

PRB, 95, 134419 (2017)

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**12:51PM L10.00007: Sign reversal of order parameter in single layer FeSe/SrTiO3 film**

HUIMIN ZHANG (Presenter), ZHUOZHI GE, LIAN LI, Department of Physics and Astronomy, West Virginia University — Single layer FeSe film grown on SrTiO3 substrate has drawn much interest for its novel interfacial effects, which have led to the highest superconducting temperature ($T_c$) to date amongst all Fe-based superconductors. While several paring symmetries, such as $s^{++}$-wave, nodeless $d$-wave, as well as $s_{2}$-wave have been suggested, the experimental determination of its superconducting paring symmetry remains elusive. Here we investigate the intrinsic impurity-induced in-gap bound states and quasiparticle interference (QPI) patterns in single layer FeSe/SrTiO3 by scanning tunneling microscopy/spectroscopy. We observed bound states induced by nonmagnetic impurities, which strongly suggests a sign-changing order parameter. Through detailed analysis of the phase-sensitive QPI patterns, we further confirm that the order parameter indeed changes sign within the electron pockets. This identification of a sign change pairing symmetry in single layer FeSe/SrTiO3 presents an important step towards the understanding of the mechanism of its high $T_c$ superconductivity.

*This research is supported by DOE (DE-SC0017632).
of superconducting paths connecting superconducting islands within Fe(Te$_{0.7}$Se$_{0.3}$) thin flakes to describe the behavior of model is supported by the observed thickness dependence of the superconducting transition. We propose a 2D network confirmed using the BKT transition for inhomogeneity model, as well as finite state effects (FSE). This inhomogeneous transition. Due to non-uniform Te/Se spatial distribution, we find that $R(T)$ behavior in flakes $<$10nm can be explained and $>$10nm flakes we find a systematic suppression of the superconductivity and broadening of the superconducting phase modulation caused by the ferromagnetism, which can lead to the decrease of the pairing and critical temperature. 

The presence of Hubbard on-site interaction. Using a single-band model for the superconductor-ferromagnet vacancies. We find that a robust surface ferromagnetism can emerge due to the periodic pattern of oxygen vacancies in FeSe/SrTiO$_3$, and demonstrates that quasiparticle scattering at boundaries can be a viable phase sensitive probe of pairing symmetry in Fe-based superconductors. 

This research is supported by NSF (DMR-1335215).

Evidence of Two-dimensional Superconducting Behavior in Atomically Thin Fe(Te$_{0.7}$Se$_{0.3}$) Flakes

ANDREW STEELY (Presenter), CHUNLEI YUE, YUN LING, ABIN JOSHY, Tulane University, ZHIQIANG MAO, Pennsylvania State University, JIANG WEI, Tulane University — We report detailed thickness-dependent transport studies on strain-free Fe(Te$_{0.7}$Se$_{0.3}$) thin flakes. Notably, we present evidence of two-dimensional superconducting behavior in flakes $<$10nm. For $>$10nm flakes we find a systematic suppression of the superconductivity and broadening of the superconducting phase transition. Due to non-uniform Te/Se spatial distribution, we find that $R(T)$ behavior in flakes $<$10nm can be explained and confirmed using the BKT transition for inhomogeneity model, as well as finite state effects (FSE). This inhomogeneous model is supported by the observed thickness dependence of the superconducting transition. We propose a 2D network of superconducting paths connecting superconducting islands within Fe(Te$_{0.7}$Se$_{0.3}$) thin flakes to describe the behavior of this natural percolating system.

*This work was supported by the DOE under grant DESC0014208 and by the Board of Regents Support Fund (BoRSF) under grant LEQSF(2015-18)-RD-A-23.

Hydrothermal design of magnetic heterolayer iron-based superconductors

BRANDON WILFONG (Presenter), XIUQUAN ZHOU, HUAFEI ZHENG, NAVNEETH BABRA, EFRAIN RODRIGUEZ, JOHNPIERRE PAGLIONE, University of Maryland, College Park — Recently, a new iron-based superconductor, (Li$_{1-x}$Fe$_x$OH)FeSe (critical temperature, $T_c = 43$ K), was reported. Pachmayr et al. and Lu et al. reported observation of ferromagnetism and antiferromagnetism, respectively, in this 43 K superconductor, but no magnetic peak(s) have been observed for this system in several neutron diffraction studies. Thus, our current work aimed at controlling this magnetism through selective doping of other transition metals onto the Li site within the (Li$_{1-x}$Fe$_x$OH)$5^+$ spacer layers. We have synthesized powder and single crystals (Li$_{1-x}$yFe$_x$M$_y$OH)FeSe samples ($M = Cr$, Mn, Co, Ni, Cu, Zn) through a hydrothermal ion-exchange reaction of KFe$_{2-2x}$M$_2$Se$_2$ precursors. These samples have been characterized by x-ray diffraction, electrical resistivity, and magnetic susceptibility to confirm their crystal structure, chemical composition and the influence of transition metal dopants on their superconductivity and magnetism. Neutron diffraction revealed correlation between magnetism and the crystal structure tuned by transition metal dopants in the spacer layers which coexists with superconductivity. Our work demonstrates coexistence of superconductivity and magnetism can be designed through chemical manipulation of heterolayer transition metal chalcogenides.

Engineering nanoscale superconductivity through the competition between ferromagnetism and superconductivity

MATTHEW REDELL (Presenter), WEI-CHENG LEE, Binghamton University — As electronic devices continue to decrease in size, it becomes increasingly more important to understand how to engineer nanoscale systems. Reduced dimensionality in superconductors allows fluctuations to play a greater role in the behavior of the system. For example, bulk iron selenide (FeSe) has a superconducting critical temperature of 8K, but the single layer FeSe grown on SrTiO$_3$ exhibits a significantly higher critical temperature. Motivated by these results, we have performed density functional theory (DFT) calculations for various systems of SrTiO$_3$ with different surface reconstructions for oxygen vacancies. We find that a robust surface ferromagnetism can emerge due to the periodic pattern of oxygen vacancies in the presence of Hubbard on-site interaction. Using a single-band model for the superconductor-ferromagnet heterostructure, we demonstrate that for nanoscale systems the superconducting properties are highly susceptible to modulation caused by the ferromagnetism, which can lead to the decrease of the pairing and critical temperature.
Wednesday, March 6, 2019 11:15 AM - 1:51 PM

Session L11 DMP DCMP FIAP: Materials for Quantum Information Science -- Engineering Quantum States  BCEC 152 - Tag(s): Focus

11:15AM L11.00001: InSb Nanowires for Quantum Devices  GHADA BADAWY (Presenter), SASA GAZIBEGOVIC, Applied Physics, Eindhoven University of Technology, SEBASTIAN HEEDT, FRANCESCO BORSOI, QuTech, Delft University of Technology, SEBASTIAN KOELLING, MARCEL VERHEIJEN, Applied Physics, Eindhoven University of Technology, LEO P KOUWENHOVEN, QuTech, Delft University of Technology, ERIK P. A. M. BAKKERS, Applied Physics, Eindhoven University of Technology — Indium-antimonide (InSb) nanowires (NWs) are considered prime candidates for hosting topological states, known as Majorana zero modes, a key ingredient for future fault-tolerant quantum computing. More specifically, the properties of InSb, such as its high electron mobility and strong spin-orbit coupling, grant it with the ability to deliver stringent requirements needed for bearing topological phases when combined with a superconductor.
Yet, synthesis of this superior material remains a challenge. InSb NWs have been so far synthesized on top of a “stem” of a foreign material, posing two main hurdles; incorporation of the stem material into the grown InSb segment and limiting the length of the InSb NW, restricting it to a maximum of about 3.5 μm. Here, we report growth of pure zinc blende InSb nanowires tens of microns long. These NWs demonstrate significantly higher electron mobility values than obtained for InSb NWs on stems. Thus, this technique meets the strict length and purity prerequisites for realizing Majorana devices and provides flexibility for intricate device designs.

11:27AM L11.00002: In-plane Selective Area InSb Networks for Scalable Majorana Devices  ROY OP HET VELD (Presenter), Applied Physics, Eindhoven University of Technology, DI XIU, QuTech, Delft University of Technology, MARCEL VERHEIJEN, Applied Physics, Eindhoven University of Technology, MIHIR PENDHARKAR, JOON SUE LEE, Dept. of ECE, University of California Santa Barbara, STAN PETERS, SEBASTIAN KOELLING, Applied Physics, Eindhoven University of Technology, LEO P KOUWENHOVEN, Qutech, Delft University of Technology, CHRIS PALMSTROM, Dept. of ECE, University of California Santa Barbara, HAO ZHANG, QuTech, Delft University of Technology, ERIK P. A. M. BAKKERS, Applied Physics, Eindhoven University of Technology — Theoretical proposals predict that networks of Indium Antimonide (InSb) nanowires are suitable for Majorana based quantum computing.
Here we show In-plane Selective Area Networks (InSANe) of InSb nanowires grown catalyst free with a high crystal quality. Although InSb has a large lattice mismatch with Indium Phosphide (InP) (high bandgap substrate material), we manage to synthesize single crystal networks. Transmission electron microscopy (TEM) analysis confirms a zincblende InSb nanowire with a single twin defect at the interface with the underlying substrate. Low temperature transport measurements (e.g. Aharonov-Bohm interference) demonstrate a large electron coherence length of up to 10 μm. An epitaxial superconductor on these networks induces a hard superconducting gap and gives rise to a 2e-periodic Coulomb blockade, making this platform very promising for Majorana topological quantum computing.

11:39AM L11.00003: Fabrication and Characterization of Template-Defined Scalable InAs Nanowire Networks*  KRISTOPHER CERVENY (Presenter), University of Basel, MARTIN FRIEDL, Ecole Polytechnique Federale de Lausanne, TARAS PATLATIUK, CHRISTIAN SCHELLER, LORIN DIRSCHERL, University of Basel, DIDEM DEDE, ANNA FONTCUBERTA I MORRAL, Ecole Polytechnique Federale de Lausanne, DOMINIK ZUMBUHL, University of Basel — Semiconductor nanowires with strong Rashba-type spin-orbit interaction are a great platform to create and study novel quasiparticles, such as Majorana- and para-fermions. These excitations with non-Abelian statistics are of fundamental interest offering promising applications in topological quantum computing. Here, we report recent results on templated InAs nanowire networks grown on GaAs nanomembranes[1]. A fabrication process for contacting, encapsulation in an ALD dielectric, and electrostatic gating of wires grown on [111] and [100] GaAs substrates has been developed and implemented. The low-temperature conductance behavior of the devices has been analyzed as a function of applied magnetic field and gate voltage. The investigation aims at fundamental system properties like mean free path, coherence length, and spin-orbit length. Further, transport behavior over junctions between the nanowires - enabled by the crystal-lattice symmetries - has been explored. The work lays the foundation for the integration of superconductors in the devices, which provides a means for studying the behavior of hybrid structures with strong spin-orbit interaction.


*Supported by Swiss NSF, NCCR QSIT, SNI, and European Microkelvin Platform (EMP)
11:51AM L11.0004: Scalable quantum photonics using quantum dots [Invited]  EDO WAKS (Presenter), University of Maryland, College Park —
In this talk I will describe an experimental realization of strong interactions between single photons mediated by a single electron trapped in a quantum dot. I will first present a quantum transistor where a single photon can control a single electron spin and vice versa 1. This switch realizes a transistor operating at the fundamental quantum limit, where in picoseconds timescales a single photon flips the orientation of a spin and the spin flips the polarization of the photon. I will show how this transistor creates strong interactions between single photons, and enables a single photon to switch a bright field composed of many photons. 2

Subsequently, I will also describe our efforts to incorporate these interactions in quantum photonic circuits to create complex nonlinear devices. I will show a technique to achieve on-chip tuning of quantum dots in order to create indistinguishable emitters coupled to cavities and waveguides 3–5. I will also describe new fabrication methods we are pursuing for hybrid integration of quantum dots with silicon photonics 4, as well as novel topological photonic structures that enable photons to propagate through chiral edge states 6, providing new possibilities for photonic quantum simulation.

References:

12:27PM L11.0005: Improved control of quantum dots in Ge/SiGe quantum wells for spin qubit applications*  WILL HARDY (Presenter), Sandia National Laboratories, YI-HSIN SU, YEN CHUANG, Electrical Engineering, National Taiwan University, LEON MAURER, MITCHELL BRICKSON, ANDREW BACZEWSKI, Sandia National Laboratories, JIUN-YUN LI, Electrical Engineering, National Taiwan University, TZU-MING LU, DWIGHT R LUHMAN, Sandia National Laboratories — Much work on semiconductor spin qubits has focused on extending capabilities and understanding limitations of Si and GaAs. In parallel, alternative materials are being scrutinized for potential advantages in terms of coherence times, control, and extensibility, without sacrificing key features. One such quantum well system, undoped strained Ge/SiGe, appears promising as a candidate spin qubit host due to low disorder, small hole effective mass, and large spin-orbit coupling, and has already been used to demonstrate basic single quantum dots. We take the next steps toward hole spin qubits by preparing a double quantum dot in a one-layer gate structure, then using multilayer gate stacks to demonstrate improved quantum dot control.

*This work was funded in part by the LDRD Program and performed in part at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the USDOE Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the USDOE National Nuclear Security Administration under contract DE-NA0003525. The views expressed in this work do not necessarily represent the views of the USDOE or the US Government.

12:39PM L11.0006: A solvable quantum model of dynamic nuclear polarization in quantum dots*  THOMAS NUTZ (Presenter), Physics, Imperial College London, EDWIN BARNES, SOPHIA ECONOMOU, Physics, Virginia Tech — Dynamic nuclear polarization (DNP) in quantum dots has given rise to a variety of unexpected and potentially useful effects, yet a consistent theoretical description with predictive power is still lacking. We present a quantum mechanical theory of optically induced DNP applicable to quantum dots and other interacting spin systems. The exact steady state of the optically driven coupled electron-nuclear system is calculated under the assumption of constant hyperfine coupling strengths (box model) for an arbitrary number of nuclear spins. Based on this analytical result we investigate the nuclear spin behaviour for different experimental parameter regimes and find that our model reproduces the flat-top and triangular absorption lineshapes (linedragging) seen in various experiments. Furthermore we predict a novel DNP effect. Under particular and achievable experimental conditions the nuclear spin system tends to polarize in such a way as to cancel the effect of the external magnetic field. The predicted sharply peaked nuclear spin polarization probability distributions centered at the value corresponding to degenerate electronic transitions would be of great significance for quantum technological applications.

*EPSRC and Frontiers in Quantum Technologies programme
12:51PM L11.00007: Plasmon mediated quantum communication between quantum dot clouds* RAVINDRA YADAV
(Presenter), Department of Physics, Indian Institute of Science, Bangalore, India, MATTHEW OTTEN, Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439, USA, WEIJIA WANG, Applied Physics Program, Northwestern University, Evanston, Illinois 60208, United States, STEPHEN K GRAY, D. J. GOSZTOLA, GARY P WIEDERRECHT, Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439, USA, TERI W. ODOM, Applied Physics Program, Northwestern University, Evanston, Illinois 60208, United States, JAYDEEP K BASU, Department of Physics, Indian Institute of Science, Bangalore, India — We report experimental and theoretical studies of the interaction of a quantum dot (QD) cloud [1] with a remote QD cloud mediated by surface lattice resonances (SLR) in two dimensional array of plasmonic nanoparticles[2]. By exciting one QD cloud and collecting the photoluminescence from a remote, unexcited QD cloud, we experimentally demonstrate long range, SLR mediated coupling between the two clouds. We explore the coupling between the two QD clouds through the SLR. Our results suggest an exciting new direction where coherent plasmonic systems can mediate interactions between remote QDs, having various applications in quantum information processing and quantum computation, such as realizing two qubit gate interactions between the QD clouds.

References:

*The authors acknowledge Indo-U.S. Science and Technology Forum (IUSSTF) for funding through Virtual center on quantum plasmonics. The authors aknowledge DST Nanomission, India for funding.

1:03PM L11.00008: Simulating topological insulators with donors and quantum dots* NGUYEN LE (Presenter), University of Surrey, ANDREW JAMES FISHER, University College London, ERAN GINOSSAR, University of Surrey — We explore the possibilities of simulating the Su-Schrieffer–Heeger (SSH) model of topological insulators with a one dimensional chain of donors or quantum dots. A measurement of the transverse tunneling current through one end of the chain is proposed for confirming the existence of the edge state in the topologically non-trivial phase. For donors and quantum dots the electron-electron interaction is typically larger than the hopping amplitude, resulting in strong correlation in the ground state. We investigate the effect of interaction on the spin correlation, entanglement, excitation energy spectrum and the Zak phase. We discuss bulk-edge correspondence between the Zak phase and the edge state in the correlated case. An external magnetic field can be used to induce a transition to the well-understood limit of the non interacting SSH model. This transition is accompanied by a strong enhancement of the edge state’s spatial localization, and hence can be identified by observing a sharp increase in the conductance signal.

*We acknowledge financial support from the UK Engineering and Physical Sciences Research Council [COMPASSS/ADDRFSS, Grant No. EP/M009564/1] and EPSRC strategic equipment grant no. EP/L02263X/1.

1:15PM L11.00009: Kitaev chain with a quantum dot* CHUANCHANG ZENG (Presenter), CHRISTOPHER MOORE, APARAO MOHAN RAO, Department of Physics and Astronomy, Clemson University, TUDOR DAN STANESCU, Department of Physics and Astronomy, West Virginia University, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University — We solve analytically the problem of a finite length Kitaev chain coupled to a quantum dot (QD), which extends the standard Kitaev chain problem making it more closely related to the quantum dot-semiconductor-superconductor (QD-SM-SC) nanowire heterostructure that is currently under intense investigation for possible occurrence of Majorana zero modes (MZMs). Our analytical solution reveals the emergence of a robust near-zero-energy Andreev bound state (ABS) localized in the quantum dot region as the generic lowest energy solution in the topologically trivial phase. By contrast, in the bare Kitaev chain problem such a solution does not exist. The robustness of the ABS in the topologically trivial phase is due to a partial decoupling of the component Majorana bound states (MBBs) over the length of the dot potential. As a result, the signatures of the ABS in measurements that couple locally to the quantum dot, e.g., tunneling measurements, are identical to the signatures of topologically-protected MZMs, which arise only in the topological superconducting (TS) phase of the Kitaev chain.

*ARO Grant No. W911NF-16-1-0182.
NSF Grant No. DMR-1414683.
Simple and Re-useable Flip-Chip Method for Hybrid Quantum Systems

CHRISTOPHER CONNER (Presenter), Institute for Molecular Engineering, University of Chicago, KEVIN SATZINGER, Department of Physics, University of California, Santa Barbara, YOUPENG ZHONG, HUNG-SHEN CHANG, Institute for Molecular Engineering, University of Chicago, GREGORY A PEAIRS, Department of Physics, University of California, Santa Barbara, AUDREY BIENFAIT, MING-HAN CHOU, AGNETTA CLELAND, ETIENNE DUMUR, JOEL GREBEL, RHYS G POVEY, SAMUEL WHITELEY, DAVID AWSCHALOM, Institute for Molecular Engineering, University of Chicago, DAVID SCHUSTER, Department of Physics, University of Chicago, ANDREW N CLELAND, Institute for Molecular Engineering, University of Chicago — The flexibility and scalability of solid-state qubit systems can be greatly improved with the use of flip-chip geometries, as these provide a third dimension for interconnects and allow coupling of systems on different substrates [1,2]. Indium bump-bonded flip-chips can be prohibitively costly for a university lab, and do not offer a means to re-use the substrates. Here, we describe a simple, low cost, non-galvanic approach to flip-chip bonding, demonstrated using superconducting qubits coupled to other quantum systems, including acoustic and electromagnetic resonators. We achieve less than two microns of placement error, and provide a cryogenically-compatible bonded structure that can be disassembled using acetone. We have tested the approach using inductively coupled coplanar waveguide resonators, and we have designed a multi-qubit experiment with direct inductive coupling between qubits on separate substrates.


*Supported by AFOSR MURI program, UChicago MRSEC (NSF DMR-1420709), and the ARL. We made use of the Pritzker Nanofabrication Facility, supported by the NSF award NNCI-1542205.

High Temperature Superconducting nano-meanders made by ion irradiation

PAUL AMARI (Presenter), C FEUILLET-PALMA, FRANÇOIS COUËDO, NICOLAS BERGÉAL, J LESUEUR, LPEM, Sorbonne Université, ESPCI, CNRS, PSL — Low temperature Superconducting single photon detectors (SSPD) are suitable for quantum information and space communications applications. They show unrivaled performances from visible wavelength to 10μm that require complex cryogenics at 4K that limit applications. In this respect, high temperature superconductors (HTS) are attractive materials to design SSPDs operating at 40K.

We report the fabrication of YBa2Cu3O7-x nano-meanders showing the highest aspect ratios ever reported so far (30nm thick, 100nm wide, 450μm long) by e-beam lithography and high-energy ion implantation [Amari et al. SUST (2018)]. DC measurements prove that superconducting properties in nanowires are preserved with respect to raw YBCO thin-film. We report large hysteretic IV curves in our nanowires, which is a key requirement for hot-spot creation in SSPD. The inductive part of the nanowires plays an important role in the dynamics of the detector. We study the nanowire's inductance using a resonant method over a wide range of temperature up to Tc. The London penetration depth around 190nm extracted from the microwave measurement confirms that superconducting properties are conserved. Our ion irradiation technique paves the way for a suitable nanofabrication process of robust SSPDs made of HTS materials.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L12 DMP: 2D Materials (Metals, Superconductors, and Correlated Materials) -- TMDC Theory

BCEC 153A - Ting Cao, University of California, Berkeley - Tag(s): Focus
**11:15AM L12.00001: Transport, Interactions, and Flavortronics in 2D Transition Metal Dichalcogenides**

FAN ZHANG (Presenter), Department of Physics, University of Texas at Dallas — Transition metal dichalcogenides (TMDs) provide a unique 2D material platform for discovering novel physics. First, I will briefly discuss our original predictions on the unconventional quantum Hall effect and “topological” valley Hall effect of massive Dirac fermions in monolayer TMDs, which have been confirmed by optical spectroscopy, quantum transport, and local compressibility measurements. Next, I will introduce our recent theories and experiments that have discovered the G-valley holes and Q-valley electrons in the quantum transport of few-layer TMDs. Particularly, the G-valley holes have an extremely large effective mass that produces an odd-integer predominated quantum Hall effect with giant spin susceptibility and extreme density sensitivity, prerequisites for the Wigner crystal phase. Finally, I will elucidate that the TMD Q valleys offer an unprecedented opportunity to realize the solid-state version of SU(3) flavor symmetry that is rare in electron systems. In the quantum-Hall regime, we have predicted that the spontaneous flavor symmetry breaking yields ferroelectric valley nematics tunable by an in-plane electric field. In the quantum-dot geometry, we have predicted flavor enforced irrational Coulomb peaks and fractional Kondo peaks. These effects lead to a new concept—flavortronics.

*(F.Z. is supported by ARO under Grant No. W911NF-18-1-0416.)*

**11:51AM L12.00002: Mott metal-insulator transitions in pressurized layered trichalcogenides**

HEUNG SIK KIM (Presenter), KRISTJAN HAULE, DAVID VANDERBILT, Rutgers University, New Brunswick — Transition metal phosphorous trichalcogenides, $\text{MP}_X_3$ ($M$ and $X$ being transition metal and chalcogen elements respectively), have been the focus of substantial interest recently because of their possible magnetism in the two-dimensional limit. Here we investigate material properties of the compounds with $M = \text{Mn}$ and $\text{Ni}$ employing *ab-initio* density functional and dynamical mean-field calculations, especially their electronic behavior under external pressure in the paramagnetic phase. Mott metal-insulator transitions (MIT) are found to be a common feature for both compounds, but their lattice structures show drastically different behaviors depending on the relevant orbital degrees of freedom, i.e., $t_{2g}$ or $e_g$. MnPS$_3$ undergoes an isosymmetric structural transition by forming Mn-Mn dimers due to the strong direct overlap between the neighboring $t_{2g}$ orbitals, accompanied by a significant volume collapse and a spin-state transition. In contrast, NiPS$_3$ and NiPSe$_3$, with their active $e_g$ orbital degrees of freedom, do not show a structural change at the MIT pressure or deep in the metallic phase. Hence NiPS$_3$ and NiPSe$_3$ become rare examples of materials hosting electronic bandwidth-controlled Mott MITs, thus showing promise for ultrafast resistivity switching.

*Supported by NSF DMR-1629059.

**12:03PM L12.00003: Giant spin Hall effect in two-dimensional monochalcogenides**

JAGODA SLAWINSKA (Presenter), FRANK T CERASOLI, HAIHANG WANG, Department of Physics, University of North Texas, SARA POSTORINO, Dipartimento di Fisica, Università di Roma Tor Vergata, ANDREW SUPKA, Department of Physics and Science of Advanced Materials Program, Central Michigan University, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science, Duke University, MARCO FORNARI, Department of Physics and Science of Advanced Materials Program, Central Michigan University, MARCO BUONGIORNO NARDELLI, Department of Physics, University of North Texas — One of the most exciting properties of two dimensional materials is their sensitivity to external tuning of the electronic properties, for example via electric field or strain. Recently discovered analogues of phosphorene, group-IV monochalcogenides (MX with $M = \text{Ge}$, Sn and $X = \text{S}$, Se, Te), display several interesting phenomena related to the in-plane strain, such as giant piezoelectricity and multiferroicity, which combines ferroelastic and ferroelectric properties. Here, using calculations from first principles, we predict for the first time giant spin Hall effect (SHE) in these materials which suggests their high potential for 2D spintronics. We reveal that the spin Hall conductivity is tunable via combinations of external strain and doping. In some configurations, the strain-induced semiconductor to metal transition enables the logic functionality of switch on/off control of spin currents indicating a new route for the design of multi-tunable spintronics devices.

*The members of the AFLOW Consortium acknowledge support by DOD-ONR (N00014-13-1-0635, N00014-11-1-0136, N00014-15-1-2863). MBN and FTC acknowledge partial support from Clarkson Aerospace Corporation.*
12:15PM L12.00004: Evolution of Weyl fermions along the polarity reversal paths in MoTe$_2$  SOBHIT SINGH (Presenter), JIUNWOONG KIM, KARIN RABE, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ-08854, USA — MoTe$_2$ is a layered material with rich physics arising from structural and electronic phase competition. The three observed crystal phases - 2H, 1T', and T$_d$ - have distinct electronic properties. The non-centrosymmetric T$_d$-MoTe$_2$ is particularly fascinating due to the presence of type-I and type-II Weyl nodes in this system. In this study, we investigate the energetics of the possible structural phase transitions in MoTe$_2$, and explore the possibility of controlling the dynamics of Weyl fermions in MoTe$_2$. Our first-principles calculations reveal that one can systematically tune the location and chirality of Weyl nodes by exploiting the connection between polar distortions and spin-orbit coupling effects in T$_d$-MoTe$_2$. By restoring the broken inversion symmetry, we locate a highly symmetric saddle point structure (T$_d^0$) on the energy landscape of MoTe$_2$, establishing a polarity reversal path connecting up and down variants of T$_d$. The T$_d^0$ phase resembles a paraelectric phase of a ferroelectric compound, and it is dynamically and elastically unstable leading to structural phase transitions into the T$_d$ and 1T' phases. We study the evolution of Weyl nodes as a function of structural distortions in the vicinity of T$_d^0$.

12:27PM L12.00005: Statistical mechanics of anisotropic 2D sheets*  MOHAMED EL HEDI BAHRI (Presenter), ANDREJ KOSMRLJ, Princeton University — Atomically thin 2D sheets are now routinely produced and are used in a variety of electronic applications as well as in self-folding origami structures. The majority of 2D sheets, such as graphene, hexagonal boron nitride and the H phase of Transition Metal Dichalcogenides (TMDs), are isotropic. However, there also exist anisotropic 2D sheets, such as the T' phase of TMDs. Note that in equilibrium most are in the isotropic H phase, however the T' phase is stable for WTe$_2$. This motivated us to investigate the statistical mechanics of freely suspended anisotropic 2D sheets. Similar to isotropic sheets, thermal fluctuations effectively renormalize elastic constants for anisotropic sheets and make them scale dependent. Thermal fluctuations effectively increase flexural rigidities, while the in-plane elastic constants are reduced. We found 3 different universality classes (isotropic, orthorhombic and monoclinic) that are characterized with different power-law exponents of the renormalized elastic constants. The T' phase of TMDs falls in the orthorhombic universality class. Therefore, the elastic constants for WTe$_2$ are expected to scale differently than for other isotropic 2D sheets.

*This work was supported by NSF award DMR-1752100 (CAREER).

12:39PM L12.00006: Dynamical synchronization transition in interacting electron systems*  TANAY NAG (Presenter), condensed matter theory, Max Planck Institute for Physics of Complex Systems (MIPPKS) — Synchronization processes are a ubiquitous phenomenon in nature. We propose a new perspective centered around the topic of a novelly introduced dynamical synchronization transition (DST) in interacting electron systems. In particular, using graphene irradiated by an intense bi-circular pulse laser as a prototypical and experimental viable example, we theoretically investigate how to selectively generate a coherent oscillation of electronic order such as charge density waves (CDW), where the key is to use tailored fields that match the crystalline symmetry broken by the target order. After the pump, a macroscopic number of electrons start oscillating and coherence is built up through a transition. Using an analogy to the celebrated Kuramoto model, describing the classical synchronization of coupled pendulums, we formulate a general framework to encapsulate the induced coherent electronic order. The resulting physics is detectable as a coherent light emission at the synchronized frequency and may be used as a purely electronic way of realizing Floquet states respecting exotic space time crystalline symmetries. In the process, we also explore possible flipping of existing static CDW orders and generation of higher harmonics.

*Max Planck Society, Germany
1:27PM L12.00007: Symmetry, spin-texture, and tunable quantum geometry in WTe2 monolayer* LI-KUN SHI, Institute of High Performance Computing, JUSTIN SONG (Presenter), Nanyang Technological University Singapore and Institute of High Performance Computing Singapore — The spin orientation of electronic wavefunctions in crystals is an internal degree of freedom, typically insensitive to electrical knobs. We argue from a general symmetry analysis and a k.p perspective, that monolayer 1T'-WTe2 possesses an electrically tunable bulk band quantum geometry arising from a gate-activated canted spin texture. In particular, we find that due to its out-of-plane asymmetry, an applied out-of-plane electric field breaks inversion symmetry to induce both in-plane and out-of-plane electric dipoles. These in-turn generate spin-orbit coupling to lift the spin degeneracy and enable a bulk band Berry curvature and magnetic moment distribution to develop. Further, due to its low symmetry, Berry curvature and magnetic moment in 1T'-WTe2 possess a dipolar distribution in momentum space, and can lead to unconventional effects such as a current induced magnetization and quantum non-linear anomalous Hall effect. These render 1T'-WTe2 a rich two-dimensional platform for all-electrical control over quantum geometric effects.

*This work was supported by the Singapore National Research Foundation (NRF) under NRF fellowship award NRF-NRFF2016-05

1:03PM L12.00008: Edge photocurrent response of type-II Weyl semimetal WTe2* QINSHEGNG WANG (Presenter), JIN CAO, JINGCHUAN ZHENG, YUAN HE, Physics, Beijing Institute of Technology, DONG SUN, ICQM, Peking University, YUGUI YAO, Physics, Beijing Institute of Technology — Photodetectors based on new materials or new structures are of great potentials to promote the performance limits of existing photo detection devices. As topological nontrivial materials, Weyl semimetals were reported to have novel optoelectronic properties and potential applications arising from their gapless linear dispersion near Weyl nodes, berry curvature divergence of Weyl nodes, internal broken of inversion or time reversal symmetry, robust fermi-arc type surface states. These unique properties lead to extraordinary optoelectronic response of Weyl semimetals. Here, using scanning photocurrent microscopy, we demonstrate that robust photocurrent will generate on edges with certain crystal direction in type-II Weyl semimetal WTe2, this photocurrent persists under a wide excitation photon energy range from near Weyl point region to high above Weyl point region. We show that the direction of photocurrent did not change with the polarization of excitation photon and a photon energy range from 0.12 eV to 1.96 eV, this edge photocurrent was determined by the symmetry of edges and may come from the nontrivial Fermi-arc type edge state of Weyl semimetal, and may result in a new type of photodetector based on it.

*National Natural Science Foundation of China (Nos. 11704031, 11734003)

1:15PM L12.00009: Quantum Mechanical Calculations of the Dielectric Properties of Metallic 2D Transition Metal Dichalcogenides XIAO SHEN (Presenter), University of Memphis — 2D materials are widely studied for their optical properties due to their reduced dimensionality. The key optical properties are reflectivity and absorption coefficients, which can be determined from the complex dielectric function obtained from first-principles quantum mechanical calculations based on time-dependent current-density functional theory (TDCDFT) [1]. Here we focus on the metallic phases of 2D transition metal dichalcogenides (TMD), including MoS2, MoSe2, and WSe2. We reveal their unique optical properties and discuss how the optical properties change upon the change of the chemical composition.


1:27PM L12.00010: First-Principles Prediction of Stable Transition Metal Dichalcogenide Alloys* JOHN CAVIN (Presenter), Physics Department, Washington University in St. Louis, SUNG BEOM CHO, Virtual Engineering Center, Korea Institute of Ceramic Engineering and Technology, ROHAN MISHRA, Department of Mechanical Engineering and Material Science, Washington University in St. Louis — Quasibinary alloying among pairs of 2-dimensional (2D) transition metal dichalcogenides (TMDs) is an attractive method for tuning properties for applications such as optoelectronics and catalysis. Of the many possible combinations of TMDs, the small subset of semiconducting alloys have garnered widespread attention. Outside this limited subset, the synthesizability of alloys remains largely unknown. In order to the guide synthesis of such alloys, we present ab initio calculations of equilibrium phase diagrams with regions of stability for 27 TMDC alloys: $M_{1-x} M'_{x} X_2$ and $M_{2(1-x)} X_{2x}$ ($M, M' = V, Nb, Ta, Mo, or W; XX' = S or Se$) and two heterostructural alloys, $M_{0.1-x} W_{x}Te_{2}$ and $W_{2(1-x)}Te_{2x}$. We predict four new alloys that are miscible at all temperatures: $Nb_{1-x}Ta_{x}S_{2}$, $Nb_{1-x}Ta_{x}Se_{2}$, $VS_{2(1-x)}Se_{2x}$, and $TaSe_{2(1-x)}$. For the rest of the alloys, we present a qualitative analysis of synthesizability based on miscibility temperatures. We relate TMDC size mismatch with a mixing asymmetry that indicates the synthesizability of low concentration alloys. Our results open new compositional spaces that can be used to design and synthesize TMDC alloys for various applications.

*This work was funded by NSF DMREF-1729787.
minimize electron leakage. 2D oxide nanosheets such as Ca$_2$Nb$_3$O$_{10}$ exhibit both high dielectric constants and good thermal stability, suggesting their potential for use in 2D-material-based FETs. In this work, we perform quantum mechanical calculations using density functional theory in order to model interface and defect properties of Ca$_2$Nb$_3$O$_{10}$. Calculations of interface band alignments of Ca$_2$Nb$_3$O$_{10}$ and various candidate 2D semiconductors allow for the determination of suitable material pairings for p- or n-type transistors. Atomic defects that arise during material fabrication and preparation, like oxygen vacancies, can create defect levels within the oxide band gap. Therefore, we calculated the position of these defect energy levels and how they align relative to the semiconductor band edges to provide insights into potential sources of electron leakage and device degradation in the proposed structures.

S.S. is supported by NSF REU grant PHY-1560035. A.O. and S.T.P. are supported by NSF grant DMR-1508433.
11:27AM L13.00002: Unified Dielectric Nature of Two-Dimensional Materials* ELTON SANTOS (Presenter), School of Mathematics and Physics, BT71NN, United Kingdom, Queen’s University Belfast — Dielectric constant, which defines the polarization of the media, is a key quantity in condensed matter. It describes to a large degree the electron-electron interaction, which has a crucial effect on band gaps, optical excitations, and screening. Here we show that instead of the dielectric constant ε, the 2D polarizability α correctly captures the dielectric nature of a 2D material for both in-plane and out-of-plane polarizations. We reveal that the long-sought universal dielectric-scale relationships in the 2D world: the in-plane polarizability α|| is inversely proportional to the minimal bandgap Eg, while the out-of-plane polarizability α⊥ is directly related to intrinsic thickness of the 2D material. An analytical quantum-mechanical model is developed which give a sound background to the dielectric-scale relationships, which is supported by a broad high-throughput screening over thousands of materials. Moreover, such relations unify the dielectric properties between the 2D materials and their 3D counterparts in a natural manner, which ultimately pushes the boundary of the understanding of electronic screening in both dimensions.

*ARCHER supercomputer, via UKCP (EP/K013564/1); the UK MMM Hub for access to THOMAS (EP/P020194/1). The Queen’s Fellow Award (M8407MPH), DfE (USI 097).

11:39AM L13.00003: Synthesis and structural characterization of the single chain limit of van der Waals materials THANG PHAM (Presenter), SEHOON OH, SCOTT MEYER, BRIAN SHEVITSKI, KYUNGHOON LEE, JEFFREY CAIN, University of California, Berkeley, CHENGYU SONG, PETER ERCIUS, CHRISTIAN F. KISIELOWSKI, Lawrence Berkeley National Laboratory, MARVIN L COHEN, ALEX ZETTL, University of California, Berkeley — The successful isolation of a single layer of van der Waals (vdW) materials, such as graphene and transition metal dichalcogenides (TMDs), and the renewed interests in their emergent properties in the atomically thin limit have motivated the exploration of other vdW materials. Transition metal trichalcogenides (TMTs), such as niobium triselenide (NbSe3), are closely related quasi one-dimensional (1-D) vdW materials consisting of trigonal prismatic chains binding together by weak vdW interaction. The bulk TMTs abound with peculiar properties, such as sliding charge density wave and superconductivity.

In our talk, I will present our recent effort in isolation and study of the single chain of these 1-D vdW materials encapsulated within carbon and boron nitride nanotubes. In the single chain limit of NbSe3, we found an unusual structural helical torsional wave not seen in bulk NbSe3 crystal, by aberration-corrected transmission electron microscopy (TEM). Density functional theory (DFT) calculation shows that the charge transfer from the encapsulating nanotubes to the single chain induces such torsional wave. We term the phenomenon Charge-induced Torsional Wave (CTW). I will also discuss our efforts in synthesis of other TMTs, beyond NbSe3, in the single chain limit.

11:51AM L13.00004: Revealing the Full Spectrum Layered Materials with Super-Human Predictive Abilities [Invited] GOWOON CHEON, EKIN DOGUS CUBUK, EVAN ANTONIUK, Stanford University, JOSHUA E. GOLDBERGER, Ohio State University, EVAN REED (Presenter), Stanford University — We have utilized data mining approaches to elucidate over 1000 2D materials and several hundred 3D materials consisting of van der Waals bonded 1D subcomponents, or molecular wires. We find that hundreds of these 2D materials have the potential to exhibit observable piezoelectric effects, representing a new class of piezoelectrics. A further class of layered materials consists of naturally occurring vertical hetero structures, i.e. bulk crystals that consist of stacks of chemically dissimilar van der Waals bonded layers like a 2-D super lattice. We further combine this data set with physics-based machine learning to discover the chemical composition of an additional 1000 materials that are likely to exhibit layered and two-dimensional phases but have yet to be synthesized. This includes two materials our calculations indicate can exist in distinct structures with different band gaps, expanding the short list of two-dimensional phase change materials. We find our model performs five times better than practitioners in the field at identifying layered materials and is comparable or better than professional solid-state chemists. Finally, we find that semi-supervised learning can offer benefits for materials design where labels for some of the materials are unknown.
12:27PM L13.00005: A Defect-Enabled Reconfigurable Surface* BENJAMIN KATZ (Presenter), VINCENT HENRY CRESPI, Pennsylvania State University — A novel class of surfaces holds the possibility of reversible reconfiguration into dramatically distinct, stable shapes. This property stems in part from their defects—they have equal numbers of pentagon and heptagon disclinations. Exploring these surfaces with an example constructed out of a graphene monolayer with the disclinations arranged in a kagome-like superlattice, we model its mechanical response with semiclassical molecular dynamics. The pentagon disclinations form cones with a two-fold degree of freedom in their up/down orientation, yielding a reconfigurable surface with a large number of stable shapes. Enumerating a complete ‘zoo’ of such shapes for a small patch of this material reveals that not only are the interactions between these degrees of mechanical freedom long-range enough to produce a gaussian-like ‘density of states’ for given cone orientations, but also that the surface possesses other hidden degrees of freedom in certain orientations—further increasing the number of stable shapes it can hold. These shapes cover a broad range of physical forms and a scale comparable to important biomolecules, raising the possibility of biological applications.

*Research performed under a training fellowship for CoMET, an NRT at Penn State funded by NSF.

12:39PM L13.00006: Fabrication of atomically thin nanowire for mesoscopic transport study* ABIN JOSHY (Presenter), YUN LING, Tulane University, XUE LIU, Physics and Applied Physics, Nanyang Technological University, ANDREW STEELY, Tulane University, JINYU LIU, Physics and Astronomy, University of California, Los Angeles, LIUBOV YU. ANTIPINA, PAVEL B. SOROKIN, Structural Research, Technological Institute for Superhard and Novel Carbon Materials, ANA M. SANCHEZ, University of Warwick, ZHIQIANG MAO, Pennsylvania State University, JIANG WEI, Tulane University — Layered transition metal chalcogenides(TMC) have attracted tremendous attention owing to their weak van der Waals(vdW) interactions between chalcogens, allowing easy mechanical exfoliation of single atomic layer from the bulk. We extend this idea of “exfoliating layers” to “exfoliating atomic chains” in Ta2(Pd or Pt)3Se8, which is a vdW bonded stack of molecular strands. In this work, we succeeded to achieve Ta2Pd3Se8 single and few molecular thin (0.7nm, 1.3nm, 2nm) wires through micromechanical exfoliation. High-resolution TEM confirms 1D chain like morphology of these wires. In addition, we also demonstrated that this method can be applied to other isostructures, such as Ta2Pt3Se8. We also discovered that intrinsic semiconducting properties can be largely preserved in the Ta2Pd3Se8 nanowire transistor as evidenced by high on/off ratio (up to 10⁴) and mobility (up to 80 cm²V⁻¹s⁻¹). Finally, our work provides a new strategy for obtaining air-stable and strictly 1D material system, which offers excellent opportunities for the study of 1D physics.

*This work is supported by National Science Foundation under grant #1752997

12:51PM L13.00007: Linking interlayer twist angle to geometrical parameters of self-assembled folded graphene structures* DAWEI ZHAI (Presenter), Ohio University, JOHANNES RODE, CHRISTOPHER BELKE, SUNG J. HONG, HENNRIK SCHMIDT, Leibniz Universität Hannover, NANCY PATRICIA SANDLER, Ohio University, ROLF J. HAUG, Leibniz Universität Hannover — Previous studies have shown the possibility of obtaining folded bilayer graphene ribbons through spontaneous self-tearing and peeling from a substrate [1]. However, the effect of interlayer twist angle has been neglected. Here we investigate the morphology of spontaneously self-grown nanoribbon structures using AFM. Data reveal similar twist angle dependence of the width and interlayer separation, as well as a width-dependent fold radius. As the self-growth involves bilayer formation, bending, tearing and substrate peeling processes, these observations are well described by an energy minimization model that includes the bilayer adhesion energy density as represented by a distance dependent Morse potential. We obtain an explicit expression for the radius-width dependence that predicts a renormalized bending rigidity and stand in good agreement with experimental observations. The newly found relations between these geometrical parameters suggest a mechanism for tailored growth of folded twisted bilayer graphene- a platform for many intriguing physics phenomena.


*We acknowledge support from the DFG within the priority program SPP 1459 and the "Fundamentals of Physics and Metrology" initiative (Germany), NSF-DMR 1508325 (USA).
1:03PM L13.00008: First principles prediction of 2D lattice coherency in van der Waals heterostructures  BENOIT VAN TROEYE (Presenter), JEAN-CHRISTOPHE CHARLIER, XAVIER GONZE, SIMON DUBOIS, AURÉLIEN LHERBIER, Université catholique de Louvain — Beginning with graphene-hBN van der Waals (vdW) heterostructures [1], many Moiré patterns between 2D materials have been observed [2,3]. Still, predicting the coherent, semi-coherent (Moiré) or incoherent matching of 2D lattices at their interface is a challenge for Density Functional Theory (DFT), due to the very large size of the supercells needed in such studies. We introduce a first-principles-based model that bypass the need for large supercells. It generalizes the well-known Frenkel-Kontorova model [4] by including physical effects present in real materials, as derived from a perturbative approach to the problem. In particular, a mean-field modification of the 2D lattice parameters and elastic constants appears, even if the matching of the lattices is incoherent. The results are compared to plain DFT computations and to experimental observations of lattice accommodation in vdW-heterostructures. Then, we predict lattice (in)coherency for a set of 36 vdW-heterostructures based on graphene, phosphorene and different transition metal dichalcogenides.


1:15PM L13.00009: Modeling mechanical relaxation in misaligned 2D heterostructures*  ZIYAN ZHU (Presenter), STEPHEN CARR, SHIANG FANG, STEVEN TORRISI, Harvard University, PAUL CAZEAUX, Department of Mathematics, University of Kansas, MITCHELL LUSKIN, School of Mathematics, University of Minnesota, EFTHIMIOS KAXIRAS, Harvard University — Two-dimensional van der Waals layered materials (e.g., twisted bilayer graphene) provide a platform to study correlated many-body physics and have potential device applications. However, these layered systems are computationally challenging to model by conventional methods due to their large supercells. Here, we present a multi-scale model to efficiently calculate the mechanical relaxation pattern in incommensurate van der Waals heterostructures at arbitrary twist angles and lattice mismatch. We adopt a continuum model to describe lattice relaxation and a generalized stacking fault energy, computed from the density functional theory, to account for interlayer couplings. We obtain the optimized structure by minimizing the total energy. Our model extends the computationally accessible regime to layered systems with relatively small twist angles and large moiré patterns. This model can be applied to a wide range of materials, including those with no empirical interlayer coupling potential available, such as graphene and the transition metal dichalcogenides.

*This work was supported by the STC CIQM, NSF Grant No. DMR-1231319 and the ARO MURI Award No. W911NF-14-0247. S.B.T. was supported by a DOE Computational Science Graduate Fellowship.

1:27PM L13.00010: Evidence of Moiré Excitons in van der Waal(vdW) Heterostructure*  KHA TRAN (Presenter), University of Texas at Austin, GALAN MOODY, NIST, FENGCHENG WU, Argonne National Lab, XIAOBO LU, Physics, Washington University in St. Louis, JUNHO CHOI, JIAMIN QUAN, University of Texas at Austin, AKSHAY SINGH, Massachusetts Institute of Technology, JACOB S EMBLEY, ANDRÉ ZEPEDA, MARSHALL CAMPBELL, KYOUNGHWAN KIM, AMRITESH RAI, University of Texas at Austin, TRAVIS AUTRY, NIST, DANIEL SANCHEZ, University of Texas at Austin, TAKASHI TANIGUCHI, KENJI WATAÑABE, National Institute of Material Science, NANSHU LU, SANJAY BANERJEE, EMANUEL TUTUC, University of Texas at Austin, SUENNE KIM, Hanyang University, LI YANG, Physics, Washington University in St. Louis, KEVIN SILVERMAN, NIST, ALLAN MACDONALD, XIAOQIN (ELAINE) LI, University of Texas at Austin — We report spectroscopy evidence of interlayers excitons confined by a moire superlattice in hBN encapsulated MoSe2/WSe2 heterostructures with small twist angles. Low temperature photoluminescence(PL) measurement shows that interlayer exciton splits into multiple peaks with alternating circular polarization. We assign these peaks to the ground state and excited state excitons localized within a Moiré supercell and explain how the spatial variation of optical selection rule can give rise to multiple peaks with alternative circular polarization. Temperature dependence PL, twist angle dependence, and recombination dynamics all agrees with the localized exciton picture. Our results suggest the feasibility of engineering artificial excitonic crystal using vdW heterostructures for nanophotonics and quantum information applications.

*We gratefully acknowledge funding support from NSF MRSEC under grant DMR-1720595, NSF EFMA-1542747, NSF DMR-1306878, Welch Foundation via grant F-1662, Army Research Office (ARO) #W911NF-17-1-0312 (MURI), Air Force Office of Scientific Research (AFOSR) FA9550-17-1-0304 and NSF DMR-1455346, Japan Elemental Strategy Initiative grant No. JP15K21722.
1:39PM L13.00011: Plate Theory for 2D Crystal Flakes on Curved Surfaces  HENRY YU (Presenter), NITANT GUPTA, KSENIA V. BETS, BORIS YAKOBSON, Rice University — Recent studies demonstrated the use of substrate topography as means to engineer strain patterns in 2D materials. These strain motifs further impart interesting electronic/optical properties in materials. Although there exist theories on the elasticity of layered materials on curved surfaces, these theories rely on 2 restrictive assumptions: 1) gradually varying surfaces and 2) infinite flakes absent of edges. Recent experimental works have shown the capability of creating surfaces with sharp features such as pyramids and tori, crucial for pronounced property modulation, and invalidating the first assumption. Further, in nanoscale growth conditions finite-size and edge effects cannot be ignored due to different strain distribution compared to the infinite case. In this work, we present the exact elastic equations to calculate strain in 2D crystal flakes on curved surfaces. We also show numerical solutions to the strain configurations for graphene and MoS$_2$ flakes on various topographies, with elastic moduli parametrized from atomic simulations; further, we calculate the resulting band-gap modulation or pseudo-magnetic field. Presented formulation allows for the design of the substrate topography to achieve desired strain pattern and associated properties of the 2D materials.

1:51PM L13.00012: First-Principles Study of Chemical doping in WSe$_2$  MAOHUA DU (Presenter), Oak Ridge National Laboratory, DAN HAN, East China Normal University, WENMEI MING, Oak Ridge National Laboratory, HAIXUAN XU, University of Tennessee, SHIYOU CHEN, East China Normal University — 2D transition metal dichalcogenides (TMDs) are promising nano-electronic materials. The ability to dope 2D TMDs both n- and p-type with high carrier concentration and mobility is essential to the development of MOSFET and CMOS technologies. WSe$_2$ has been shown to exhibit both p- and n-type conductivities after chemical doping; however, the n-type doping is much less efficient than the p-type doping. We have carried out density functional theory calculations of a wide range of transition metal dopants in WSe$_2$ with the goal to understand the different dopant behaviors and to design new n-type dopants with improved doping efficiency. We have also studied in details the native defect properties since defects can potentially compensate the dopants. The calculated trend of dopant formation energies is consistent with the available experimental results. We will discuss the underlying mechanisms that are responsible for the different dopant formation energies based on the local symmetries of the dopants in WSe$_2$ and in competing secondary phases, which affect the crystal field splitting and the relative chemical stability of dopants in different crystal environments. We will also suggest new dopants based on our calculations.

2:03PM L13.00013: Ab Initio Calculations of Bonding and Charge Transfer in Borophene Sheets on a Cu(111) Substrate*  STEPHEN ELTINGE (Presenter), Department of Physics, Yale University, New Haven, CT 06520, USA, RONGTING WU, Department of Applied Physics, Yale University, New Haven, CT 06520, USA, ILYA K. DROZDOV, PERCY ZAHL, IVAN BOZOVIC, Brookhaven National Laboratory, Upton, NY 11973, USA, ADRIAN GOZAR, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University, New Haven, CT 06520, USA — Borophene, the two-dimensional hexagonal lattice form of boron, is predicted to have technological uses in flexible electronics and as a precursor to metallic boron nanotubes. Boron's electron deficiency leads to borophene sheets that have both hexagonal and triangular bonding, and different arrangements of these motifs lead to a wide range of nearly isoenergetic phases. Previous work has grown boron on Ag(111) substrates and reported the striped $\beta_{12}$ and $\chi_3$ borophene phases, but more recent growth on a Cu(111) substrate by our team describes a more complex sheet structure with a much larger unit cell. We describe ab initio density functional theory simulations of borophene sheets on the Cu(111) surface to understand and explain this observed lattice structure. We discuss the bonding structure within the borophene sheet, paying special attention to electron doping via charge transfer from the Cu substrate. In addition, we compare our results to calculations of free-standing borophene sheets and discuss implications for practical growth of borophene on substrates.

R. Wu et al., “Large-area single-crystal sheets of borophene on Cu(111) surfaces”, Nature Nanotechnology 14, 44-49 (2019)

*This work is supported by a National Science Foundation (NSF) Graduate Research Fellowship.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L14 DCMP: Electronic Interactions in Twisted Bilayers  BCEC 153C - Cory Dean
11:15AM L14.00001: Chiral SDW and d + id superconductivity in the magic-angle twisted bilayer-graphene  
CHENG-CHENG LIU (Presenter), LI-DA ZHANG, School of Physics, Beijing Institute of Technology, Beijing, China, WEI-QIANG CHEN, Department of Physics, Southern University of Science and Technology, Shenzhen, China, FAN YANG, School of Physics, Beijing Institute of Technology, Beijing, China — We model the newly synthesized magic-angle twisted bilayer-graphene superconductor with two px,y-like Wannier orbitals on the superstructure honeycomb lattice, where the hopping integrals are constructed via the Slater-Koster formulism by symmetry analysis. The characteristics exhibited in this simple model are well consistent with both the rigorous calculations and experimental observations. Van-Hove singularity and Fermi-surface nesting are found in the doping levels relevant to the correlated insulator and unconventional superconductivity revealed experimentally, base on which we identify the two phases as weak-coupling FS instabilities. Then, with repulsive Hubbard interactions turning on, we performed random-phase-approximation (RPA) based calculations to identify the electron instabilities. As a result, we find chiral d + id topological superconductivity bordering the correlated insulating state near half-filling, identified as noncoplanar chiral spin-density wave (SDW) ordered state, featuring quantum anomalous Hall effect. The phase-diagram obtained in our approach is qualitatively consistent with experiments.


11:27AM L14.00002: Multiple topological transitions in magic angle twisted bilayer graphene I  
KASRA HEJAZI (Presenter), CHUNXIAO LIU, University of California, Santa Barbara, HASSAN SHAPOURIAN, University of Chicago, XIAO CHEN, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara — The physics of twisted bilayer graphene (TBG) structures has attracted a lot of interest experimentally and theoretically. Attention was drawn to these systems largely by recent experimental works, which showed strong correlation effects in bilayer graphene systems with a twist angle of roughly 1°, the so-called magic angle. A continuum model for describing such systems is used in our study, and instead of observing flat bands only at the magic angle, we notice that the bands remain almost flat within a small range around the magic angle, where multiple topological transitions occur. The topological transitions are caused by creation and annihilation of Dirac points, which are transported within the moire Brillouin zone as the angle is varied around the magic angle. Furthermore, we propose an effective low energy six-band model near the Γ point, which we argue is the minimal model to explain the motion of the Dirac points around Γ as the angle is varied. These observations can also be exploited for explaining the experimental results regarding the response of the magic angle TBG systems to external magnetic field.

*LB, CL, KH were supported by NSF-DMR1506119, XC by GBMF4304(Moore), HS by NSF-DMR1455296 and KITP(NSF-PHY1748958)  
We acknowledge UCSB Center for Scientific Computing

11:39AM L14.00003: Electron-phonon superconductivity and Landau levels in twisted bilayer graphene  
BIAO LIAN (Presenter), ZHIJUN WANG, FANG XIE, ANDREI B BERNEVIG, Princeton University — In the first half of the presentation, we show the analytical calculation of the electron-phonon coupling in twisted bilayer graphene (TBG), which was recently experimentally observed to exhibit superconductivity around the magic twist angle θ ≈ 1.05°. We show that phonon-mediated electron attraction at the magic angle is strong enough to induce a conventional intervalley pairing between graphene valleys K and K′ with a superconducting critical temperature T_c ~ 1K, in agreement with the experiment. In the second half of the talk, we show the existence of topological Landau levels at large magnetic fields due to nontrivial topology of the flat bands.

*We acknowledge the support of Princeton Center for Theoretical Science at Princeton University, the Department of Energy Grant No. de-sc0016239, the National Science Foundation EAGER Grant No. noaawd1004957, Simons Investigator Grants No. ONRN00014-14-1-0330, No. ARO MURI W911NF-12-1-0461, and No. NSF-MRSEC DMR- 1420541, the Packard Foundation, the Schmidt Fund for Innovative Research.

11:51AM L14.00004: Magic angle twisted bilayer graphene: strong correlations and Landau level  
GAURAV CHAUDHARY (Presenter), ALLAN MACDONALD, University of Texas at Austin — The electronic structure of twisted bilayer graphene (TBLG) features a peculiar Fermi velocity renormalization property which leads to vanishing Fermi-velocities near neutrality at certain “magic” twist angles. At the magic angle the system has strong correlations which have been shown experimentally to lead to Mott insulator and superconducting phases. I will discuss the Landau level structure of TBLG near magic angles, the relationship between electronic structure and experimentally observed Landau levels, and the relationship between magic angle behavior and the system's response to external magnetic fields. We show that the Landau level structure near neutrality is highly sensitive to self-energy modifications of magic angle electronic structure.
**12:03PM** L14.00005: High temperature quantum transport in 2D moiré superlattices  
ROSHAN KRISHNA KUMAR (Presenter), JOHN WALLBANK, XI CHEN, GREGORY AUTON, MATTHEW HOLWILL, ARTEM MISHCHENKO, Konstantin S. Novoselov, Vladimir Falko, Andre Geim, School of Physics & Astronomy, University of Manchester — Van der Waals heterostructures based on moiré superlattices have become increasingly popular due to their large tunability unprecedented by any other solid-state system. In this talk, we review recent experimental results on high-temperature electron transport studies in heterostructures based on 2D moiré superlattices. Our experiments describe two fundamental phenomena of electron transport that manifest profoundly at high temperatures and are extremely sensitive to the twist-angle. First, we show that electron-electron collisions in graphene superlattices are dominated by umklapp processes [1]. They cause a giant increase in resistivity that grows rapidly upon decreasing the twist-angle between 2D layers, degrading the intrinsic mobility of graphene by more than an order of magnitude. Second, we show that moiré superlattices feature a novel class of quantum magnetoresistance oscillations [2] that differ fundamentally from the Shubnikov de Haas effect and all known quantum oscillatory phenomena.


MAREC SERLIN (Presenter), CHARLES TSCHIRHART, HRYHORIY POLSHYN, JIACHERG ZHU, University of California, Santa Barbara, Martin E HUBER, University of Colorado, Denver, Andrea Young, University of California, Santa Barbara — Bilayer graphene, rotationally faulted to ~1.1 degree misalignment, has recently been shown to host superconducting and resistive states associated with the formation of a flat electronic band. While numerous theories exist for the origins of both states, direct validation of these theories remains an outstanding experimental problem. Here, we focus on the resistive states occurring at commensurate filling (1/2, 1/4, and 3/4) of the two lowest superlattice bands. We test theoretical proposals that these states arise due to broken spin—and/or valley—symmetry by performing direct magnetic imaging with nanoscale SQUID-on-tip microscopy. This technique provides single-spin resolved magnetometry on sub-100nm length scales. I will present imaging data from our 4.2K nSOT microscope on graphite-gated twisted bilayers near the flat band condition and discuss the implications for the physics of the commensurate resistive states.

**12:27PM** L14.00007: Multiple topological transitions in magic angle twisted bilayer graphene II  
CHUNXIAO LIU (Presenter), Kasra Hejazi, Leon Bales, Kavli Institute for Theoretical Physics, University of California, Santa Barbara — Recent experiments have observed strongly correlated physics in twisted bilayer graphene (TBG) at very small angles $\theta_0 = 1.05$, along with nearly flat electron bands (FBs) at certain fillings. A good starting point to understand this is a continuum model [PNAS 108, 12233 (2011)] which successfully predicts the formation of FBs at $\theta_0$. Following this work, we investigate the low energy FB structure in the entire moiré Brillouin zone (mBZ) as twisting angle is changed; the effect of transverse lattice distortion is also considered. We notice that the bands remain almost flat within a small range around $\theta_0$, where multiple topological transitions occur. In addition to the previous understanding that the FBs are caused by the highly renormalized dispersion at K, we propose that there are other mBZ regions responsible for the low energy physics and the FBs. We trace the evolution of the Dirac points (DPs), which are very sensitive to the twist angle, and specify several processes of DP transfer within the mBZ. Furthermore, we study the effect of magnetic field to the system; comparison to the experimental results is given.

*LB, CL, KH were supported by NSF Grant DMR1506119. XC was supported by Grant GBMF4304 at KITP. HS was supported by NFS Grant DMR-1455296 and NSF PHY-1748958 (KITP).*

**12:39PM** L14.00008: Role of lattice relaxations in magic angle twisted bilayer graphene  
STEPHEN CARR (Presenter), Shiang Fang, Ziyan Zhu, Efthimiios Kaxiras, Harvard University — Understanding the origin of correlated effects in twisted bilayer graphene (tBLG) first requires a complete single-particle picture of its low-energy electronic states. Previous models of tBLG have had either high accuracy (e.g. DFT, tight-binding supercells), or high twist angle resolution (e.g. continuum or k-dot-p models), but not both. We introduce an ab initio k-dot-p model that includes lattice relaxations which can exactly reproduce DFT tight-binding electronic band-structures, but with the ability to continuously tune the twist angle. Inclusion of relaxation significantly changes the bandstructure near tBLG's first magic angle, and suppresses the appearance of the second magic angle. We find that a geometric interpretation of tBLG's relaxed atomic structure extends to its low-energy electronic states, creating a comprehensive picture of both mechanical and electronic effects at small twist angle.

*This work was supported by ARO MURI Award W911NF-14-0247 and by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319. Computations were run on the Odyssey cluster supported by the FAS Division of Science, Research Computing Group at Harvard University.*
12:51PM L14.00009: Localized eigenstates in dodecagonal twisted bilayer graphene  MOON JIP PARK (Presenter), HEESEUNG KIM, SUNGBIN LEE, Physics, KAIST — Dodecagonal quasicrystalline order has been experimentally demonstrated in twisted bilayer graphene systems. In this talk, we report emergence of localized eigenstates in the dodecagonal quasicrystals without additional random disorder. That is to say, the non-periodic quasicrystalline order causes the localization. These localized states are evidenced by the scaling behaviors of inverse participation ratio and energy level statistics, which have been used to characterize Anderson localization phenomena. Using exact diagonalization method, we show that the localization can be driven by increasing the interlayer coupling strength. In addition, we will compare our result with the conventional two-dimensional Anderson localization transitions.

1:03PM L14.00010: Atmospheric Pressure Chemical Vapor Deposition of Twisted Bilayer Graphene on Copper Foil Substrates*  LUCAS HANSON (Presenter), NIKHIL M TILAK, MICHAEL ALTVATER, BRIAN J ELLSWORTH, EVA ANDREI, Rutgers University, New Brunswick — Atmospheric pressure chemical vapor deposition (APCVD) of graphene bilayers on copper foil substrates represents a promising paradigm for the fabrication of Bernal stacked and twisted bilayer graphene samples. Large scale growth techniques will be essential in developing the potential applications of bilayer graphene, such as ultra high frequency field effect transistors or novel photonic devices. Using a quartz tube and tube furnace, copper foil substrates, argon and hydrogen forming gas, and a methane carbon feedstock, we studied a variety of different APCVD recipes to determine the optimal growth parameters for depositing graphene bilayers. Additionally, various copper substrate pretreatment techniques were tested, including surface etching, electrochemical polishing, wet oxidation, and argon annealing. Preliminary results suggest that increased bilayer grain sizes can be achieved by flowing higher methane concentrations for longer time periods during the growth stage, and optical microscopy of single and bilayer grain alignment suggest that small twist angles can be achieved using our APCVD method.

*Work supported by DOE-FG02-99ER45742, NSF DMR 1708158, NSF EFRI 1433307.

1:15PM L14.00011: Strong Correlations in Magic Angle Twisted Bilayer Graphene Investigated by Scanning Tunneling Microscopy  ALEXANDER KERELSKY (Presenter), LEO MCGILLY, Physics Department, Columbia University, SHAOWEN CHEN, Applied Physics and Math Department, Columbia University, MATTHEW YANKOWITZ, Physics Department, Columbia University, LEDE XIAN, DANTE KENNES, Max Planck Institute for the Structure and Dynamics of Matter, ANGEL RUBIO, Max Planck Inst Structure & Dynamics of Matter, CORY R DEAN, ABHAY PASUPATHY, Physics Department, Columbia University — Recent results on twisted bilayer graphene near the “magic” angle of 1.1 degrees reveal gate-tunable superconducting and correlated insulating states generally attributed to the flat band emerging from the moire superlattice and hybridization between the two layers. To date, the investigation of these states has been limited to bulk probes, inherently hindered by overall sample disorder and inhomogeneity. Using gated scanning tunneling microscopy and spectroscopy (STS), we directly locally investigate twisted bilayer graphene around the magic angle. Many theories have been proposed as to the precise band structure which causes the insulating and superconducting states to emerge, but the question remains for instance as to the size of the gap at charge neutrality and at half filling of the moire superlattices. We show the real experimental L-DOS probed by STS at and near the magic angle with gate tunable doping. Our results show the size of the gap at charge neutrality as well as the half filling state which enables a better understanding of the correlation effects leading to the insulating and superconducting states. Additionally, we study the effects of the local inhomogeneity which likely leads to the variable results observed in transport.

1:27PM L14.00012: Scanning tunneling microscopy of gated twisted bilayer graphene: Suppression of tunneling density of states due to electronic correlations*  YOUNGJOON CHOI (Presenter), JEANNETTE KEMMER, HARPREET SINGH ARORA, ROBERT POLSKI, YIRAN ZHANG, HECHEN REN, Caltech, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, STEVAN NADJ-PERGE, Caltech — ‘Magic’ angle(~1.1°) twisted bilayer graphene(TBG) is predicted to host narrow, non-dispersive electronic bands, where the kinetic energy of electrons becomes much smaller than Coulomb interactions. Recent transport measurements in this system showed insulating behavior and superconductivity around half filling of the bands, key signatures of the strongly correlated electronic systems. But the detailed electronic structure and the many-body properties of this system are still not well-understood. We used scanning tunneling microscopy and spectroscopy to measure gated TBG with angles ranging from 0.9° to 2°. When the twist angle was close to the magic angle, at certain carrier densities, we observed strong suppression of the tunneling density of states at the Fermi level associated with electron-electron interactions. Our results may deepen the understanding of strongly correlated behavior in magic angle TBG.

*This work was supported by NSF (Partly through grants DMR 1744011 and DMR 1753306). Y. C. was supported by Kwanjeong Educational Foundation.
1:39PM L14.00013: Constructing low-energy models for the electronic structure of twisted bilayer graphene
ZACHARY GOODWIN (Presenter), Materials, Imperial College London, ARASH A MOSTOFI, JOHANNES LISCHNER, Materials and Physics, Imperial College London — The recent, unexpected discovery of insulating and superconducting behaviour in magic angle twisted bilayer graphene (tBLG) has generated tremendous interest in theoretical communities to rationalise these observations. To study the angle dependent electronic properties, we have developed a tight binding model for tBLG. Importantly, the developed tight binding model accounts for atomic corrugation, and therefore, different interactions between AA and AB regions. Such asymmetry has been attributed to the isolation of bands near the Fermi energy, which has been experimentally observed. From the tight binding model, the Wannier orbitals and interaction matrix of these orbitals can be obtained. These calculations permit the construction of simplified Hamiltonians with no free parameters. Such downfolded Hamiltonians can be used in state-of-the-art functional renormalisation group methods to calculate the electronic phase diagram. The developed methodology naturally lends itself to systematic improvements and to other bilayer materials.

1:51PM L14.00014: Intralayer and interlayer electron-phonon interactions in twisted bilayer graphene
MARCOS PIMENTA (Presenter), ARIETE RIGHI, ELIEL GOMES DA SILVA NETO, ANDREIJ DE CARVALHO GADELHA, LEONARDO CRISTIANO CAMPOS, Departamento de Física, UFMG, Brazil, MARCUS MOUTINHO, Núcleo Multidisciplinar de Pesquisas em Computação - NUMPEX-COMP, Unifed. do Rio de Janeiro, PEDRO VENEZUELA, Instituto de Física, Universidade Federal Fluminense, PO-WEN CHIU, EE, National Tsing Hua University — In this work we report on the possibility of using resonance Raman spectroscopy to distinguish intralayer and interlayer electron-phonon (el-ph) interactions in twisted bilayer graphene (TBG). This is experimentally attained by tuning the energy of the excitation photon and observing the resonances of the Raman modes in different samples of TBGs. In the intralayer process, the el-ph scattering occurs in a single graphene layer and the other layer imposes a periodic potential that back scatters the excited electron, whereas for the interlayer process the el-ph scattering occurs between states in the Dirac cones of adjacent graphene layers. Our methodology can be extended to study any kind of graphene-based heterostructure. [Eliel et al., Nature Comm. 9, 1221 (2018)]

*This work was supported by the Brazilian Agencies Fapemig, CNPq and CAPES, and by the INCT Nanocarbono.

2:03PM L14.00015: Lattice relaxation and energy band modulation in twisted bilayer graphene
NGUYEN NAM (Presenter), National Institute of Advanced Industrial Science And Technology (AIST), MIKITO KOSHINO, Physics, Osaka University — We theoretically study the lattice relaxation in the twisted bilayer graphene (TBG) and its effect on the electronic band structure. We develop an effective continuum theory to describe the lattice relaxation in general TBGs and obtain the optimized structure to minimize the total energy. At small rotation angles < 2 degrees, in particular, we find that the relaxed lattice drastically reduces the area of the AA stacking region and forms a triangular domain structure with alternating AB and BA stacking regions. We then investigate the effect of the domain formation on the electronic band structure. The most notable change from the nonrelaxed model is that an energy gap of up to 20 meV opens at the superlattice subband edges on the electron and hole sides. We also find that the lattice relaxation significantly enhances the Fermi velocity, which was strongly suppressed in the nonrelaxed model.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L15 DMP: 2D Materials (Semiconductors) -- Quantum Interactions in Transport and Optical Phenomena BCEC 154 - Jifa Tian, U. Wyoming

11:15AM L15.00001: Transport theory of quantum dots based on transition metal dichalcogenides
ZHI-QIANG BAO (Presenter), PATRICK CHEUNG, FAN ZHANG, University of Texas at Dallas — Atomically thin transition metal dichalcogenides (TMDs) represent a conceptually new class of materials that have large bandgaps, strong spin-orbit couplings, and multiple valley degrees of freedom. One particular characteristic of TMDs is their even-odd layer-dependent band structures that have been theoretically predicted and experimentally observed. We study the transport properties of few-layer TMDs in the quantum dot geometry and predict unconventional Coulomb peaks and Kondo resonances when such a dot is tunnel coupled to two normal leads. The irrational peak ratios and fractional resonance conductances found in our study suggest that TMDs provide a unique platform for novel quantum dot physics.

*Research is sponsored by the Army Research Office and was accomplished under Grant Number W911NF-18-1-0416.
11:27 AM  L15.00002: Single photon-phonon entanglement in WSe$_2$ quantum dots*  XIAOTONG CHEN (Presenter), XIN LU, SUDIPTA DUBEY, QIANG YAO, Emory University, SHENG LIU, XINGZHI WANG, QIHUA XIONG, Nanyang Technological University, LIFA ZHANG, Physics, Nanjing Normal University, AJIT SRIVASTAVA, Emory University — We study photoluminescence of optically active quantum dots (QDs) in monolayer WSe$_2$ FET at low temperature (4K) and magnetic fields up to 8T. In addition to the neutral QD emission, a 21.8 meV red-shifted peak is observed. This replica peak shows correlated spectral jitters identical to the parent peak and exhibits similar excitation power dependence and magnetic field induced Zeeman splitting. Raman spectroscopy and phonon dispersion calculations are used to assign this peak to doubly-degenerate chiral phonons. Different to linearly polarized neutral QD, the phonon replica is completely unpolarized. This unusual behavior is not expected in a coherent phonon scattering. We understand it as a result of phonon-phonon entanglement resulting from two indistinguishable paths in the phonon scattering process. As the phonon part of the entanglement is never measured, the photon part gets fully unpolarized. Under magnetic field this indistinguishability is lost and the replica peak recovers its polarization, corroborating our claim. Our results highlight an intriguing feature of 2D honeycomb lattice which can host chiral phonons. This single photon-phonon entanglement can be further explored for non-reciprocal light propagation at the quantum level.

*NSF EFRI NewLAW grant #EFMA-1741691

11:39 AM  L15.00003: Control of spin-valley state in a charged WSe$_2$ quantum dot by optical helicity*  XIN LU (Presenter), XIAOTONG CHEN, SUDIPTA DUBEY, QIANG YAO, Department of Physics, Emory University, XINGZHI WANG, QIHUA XIONG, Division of Physics and Applied Physics, Nanyang Technological University, AJIT SRIVASTAVA, Department of Physics, Emory University — We present low temperature (~4 K) photoluminescence study of positively charged quantum dots (QDs) in an ambipolar WSe$_2$ field effect transistor. At a negative gate voltage when the monolayer sample is lightly hole-doped, a single peak (S-peak) and a doublet (D-peak) appear simultaneously and spectrally wander in an identical manner. We thus assign S- and D-peaks originate from the same QD. D-peaks are the neutral ($X^0$) QD with fine structure splitting of ~600 µeV resulting from the e-h exchange interaction. While the exchange interaction in a singly, positively charged ($X^+$) QD is expected to vanish due to holes forming a singlet and Pauli blocking. We assign S-peaks to be $X^+$ QD which has a binding energy of -10 meV with respect to $X^0$. $X^+$ QD is doubly degenerate at $B = 0$ T. The degeneracy of $X^+$ is lifted in finite $B$ field, allowing us to spectrally distinguish between the spin-valley states (with excess hole spin up in -K valley or spin down in K valley). By controlling the helicity of the excitation laser, we observe selective initialization of spin-valley of excess hole in $X^+$ QD under small $B$ field. Our results show that spin-valley degree is robust in charged WSe$_2$ QDs and enables valleytronics on single localized charge carriers.

*NSF EFRI NewLAW grant #EFMA-1741691

11:51 AM  L15.00004: Potential landscape engineering in two-dimensional transition metal dichalcogenides: towards hybrid optical-electrical quantum dots*  ANDREY SUSHKO (Presenter), KRISTIAAN DE GREVE, LUIS JAUREGUI, Physics, Harvard University, KE WANG, School of Physics and Astronomy, University of Minnesota, KATERNYA PISTUNOVA, ANDREW Y JOE, DOMINIK S WILD, GIANNI SCURI, Physics, Harvard University, ALEXANDER A HIGH, Institute for Molecular Engineering, University of Chicago, YOU ZHOU, Chemistry and Chemical Biology, Harvard University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, PHILIP KIM, Physics, Harvard University, HONGKUN PARK, Chemistry and Chemical Biology, Harvard University, MIKHAIL LUKIN, Physics, Harvard University — Monolayer transition metal dichalcogenides (TMDCs) have attracted recent interest due to their unique excitonic and electronic properties. As gapped, semiconducting counterparts to graphene, they show particularly strong excitonic effects, which can be exploited both in pure monolayer devices, as well as in van der Waals heterostructures where the TMDC is encapsulated between layers of insulating hexagonal boron nitride (hBN). In this work, we discuss progress towards a unique platform that exploits the strong excitonic binding energies of the TMDCs to create a hybrid, electrically controlled yet optically active quantum dot device. Further, we report on recent experiments showing optically induced current from hole-doped molybdenum diselenide to graphite or metal electrodes across over 90nm of hBN, indicating a limitation of hBN encapsulation for hybrid optical-electronic devices in TMDCs along with a method for unipolar charge injection into uncontacted TMDC layers. Finally, we discuss methods for making tunable excitonic potential landscapes in TMDC heterostructures via modulation of the dielectric environment in reconfigurable moiré structures.

*Hertz, PD Soros fellowships
**12:03PM L15.00005: Spontaneous emission enhancement of single-layer WSe$_2$ coupled to a microcavity**

HYUNSEUNG LEE (Presenter), JIEUN LEE, Physics and Energy System Researches, Ajou University — Atomically thin layers of transition metal dichalcogenides such as single-layer WSe$_2$ have recently attracted much attention as promising material candidates for optoelectronic applications. Engineering the spontaneous emission rate in these materials is expected to improve the performance and functionalities of optoelectronic devices. In this talk, we show the photoluminescence (PL) enhancement of mechanically exfoliated single-layer WSe$_2$ integrated to a microcavity. We directly contact silicon dioxide microspheres with diameters ranging from 2 to 7 μm on single-layer WSe$_2$ to control the enhancement rate. We found that the experimentally obtained Purcell factor agrees well with that calculated by the finite-difference time-domain (FDTD) simulation. The Purcell enhancement is further supported by the direct measurement of the radiative decay rate of WSe$_2$ with and without microspheres. Our finding provides a way to manipulate optical properties of single-layer semiconductors for optoelectronic applications and integrated nanophotonics.

**12:15PM L15.00006: Room Temperature Control of Valley Coherence in Microcavity Bilayer WS$_2$ Exciton-Polariton**

MANDEEP KHATONIAR (Presenter), Physics, Graduate Center, City University of New York, New York, NY 10016, NICHOLAS YAMA, Physics, University of Hawaii, Honolulu, HI 96822, SRIRAM GUDDALA, AREG GHAZARYAN, POUYAN GHAEMI MOHAMMADI, VINOD M MENON, Physics, City College of New York, New York, NY 10031 — Transition metal Dichalcogenides (TMD) have emerged as promising candidate for many optoelectronic and photonic applications. Their lack of inversion symmetry, presence of strong spin-orbit coupling and spin-valley locking make them ideal for realizing “Valleytronics”, a valley counterpart of spintronics. An important aspect of using the valley degree of freedom for information technology is manipulating the coherent circularly polarized photoluminescence (PL) from both valleys which is realized in experiment via the retention of linear polarization of the PL. Bare TMD however suffer from many dephasing mechanisms with electron hole exchange being the dominant one. Embedding these TMD’s in microcavities allow us to form polaritons in the strong coupling regime which is a hybrid light-matter system. We thus earn additional control knobs provided by the photon component of the quasiparticle. Also, the lifetime of the polariton species, dictated by the quality factor can be made comparable to that of the dephasing mechanisms to ease their effects. Here we report robust room temperature valley coherence from bilayer WS$_2$ exciton polaritons and show control of the valley coherence without the application of external magnetic field.

*NSF DMR 40G70 , NANO-NY Program NSF award EEC-1659808

**12:27PM L15.00007: Tracking the origin of single photon emitters in WSe$_2$**

LUKAS LINHART (Presenter), Institute for Theoretical Physics, TU Vienna, MATTHIAS PAUR, Institute of Photonics, TU Vienna, VALERIE SMEJKAL, Institute for Theoretical Physics, TU Vienna, THOMAS MUELLER, Institute of Photonics, TU Vienna, JOACHIM E BURGDOERFER, FLORIAN M LIBISCH, Institute for Theoretical Physics, TU Vienna — Single photon emitters (SPE) in WSe$_2$ have been investigated in several recent publications [1, 2], receiving considerable attention in the field of two-dimensional materials. Although the origin of these emitters is generally attributed to defects and/or local strain, an exact microscopic explanation has proven elusive. Using a multiscale approach we established a tight-binding model capturing non-uniform strain, defects and coulomb-interactions we elucidate this mystery. Tight-binding calculations with local strain patterns and open boundary conditions for a large WSe$_2$ flake yield quantum-dot-like localization. Including defects we can reproduce and explain the large g-factor (≈ 9) as well as the zero field splitting, the linear polarization and the electric field dependence. We conclude that local strain shifts excitonic energy levels into an energy of otherwise unoccupied inter-gap defect states, acting as a doorkeeper to fill these states. Together with localized valence bands, this leads to sharp SPE.

SON T. LE (Presenter), Theiss Research & NIST, NICHOLAS GUROS, University of Maryland, College Park, ROBERT C. BRUCE, Virginia Tech University, ANTONIO CARDONE, National Institute of Standards and Technology, NIRANJANA D. AMIN, National Institutes of Health, SIYUAN ZHANG, Theiss Research & NIST, JEFFERY B. KLAUDA, University of Maryland, College Park, HARISH C. PANT, National Institutes of Health, ARVIND BALIJEPALLI, CURT A RICHTER, National Institute of Standards and Technology — We have fabricated and characterized ionic liquid-gated 2D-MoS2 field effect transistors (2D-ILFETs) that operate at the quantum capacitance limit of the 2D channel material. These devices were used to measure pH with high sensitivity (~75 times higher than the Nernst value of 59 mV/pH) and low noise (~2 orders of magnitude higher signal-to-noise ratio over ion-sensitive FETs) at room temperature. This high device performance in pH sensing is attributed to the large asymmetric capacitive coupling between the top ionic liquid gate and bottom silicon gate to the 2D semiconducting channel. This behavior is fundamentally different from dual-gate silicon FET pH sensors that control two coupled channels. To demonstrate the usefulness of ultra-sensitive pH measurements based on 2D-ILFETs, we experimentally quantified the function of enzymes implicated in Alzheimer's disease at physiological concentrations and with sufficient time-resolution to allow the estimation of both steady-state and kinetic parameters in a single experiment.

*S.T.L. acknowledges support by the National Institute of Standards and Technology (NIST) grant 70NANB16H170. J.B.K. and N.B.G. acknowledge support by NIST grant 70NAHB15H023. A.C. acknowledges support by the NIST grant 70NANB17H259.

ELYSE BARRÉ (Presenter), Stanford University, JEAN ANNE INCORVIA, University of Texas at Austin, SUK HYUN KIM, CONNOR MCCLELLAN, ERIC POP, H. S. PHILIP WONG, Stanford University, TONY F. HEINZ, Stanford University and SLAC — Monolayers of semiconducting transition metal dichalcogenides (TMDCs) exhibit a valley Hall effect (VHE) in which the carriers in the K (K') valley acquire a velocity, \( \mathbf{v}(\mathbf{v}) \) perpendicular the applied electric field, \( \mathbf{E} \) [1,2,3]. As the K and K' bands split by spin, the resulting valley current is also a spin current. For a sample of finite width perpendicular to the direction of an applied electric field \( \mathbf{E} \), this leads to a steady-state accumulation of spin and valley polarized carriers at the edges. We have investigated the VHE in ambipolar WSe2 field-effect transistors in both n- and p-type regimes using spatial imaging of the spin and valley polarization by the optical Kerr rotation (KR) at 20 K. Here we quantitatively interpret the magnitude of the measured KR through a model of the optical response for unequal carrier populations in the valleys to obtain an estimate of the experimental spin/valley imbalance. We compare our findings to predictions of a spin diffusion model. This allows us to infer a spin and valley lifetime compatible with previous time-resolved measurements of spin-polarized carriers [4].


MAXIM TRUSHIN (Presenter), Centre for Advanced 2D Materials, NUS — The standard theory of thermionic emission developed for three-dimensional (3D) conductors does not apply to two-dimensional (2D) materials even for making qualitative predictions because of the vanishing out-of-plane quasiparticle velocity [1]. Here, we focus on two mechanisms possibly responsible for out-of-plane quasiparticle transport in 2D-3D and 2D-2D heterojunctions. First, we consider the fundamental origin of the out-of-plane charge carrier motion in a perfect 2D conductor due to the finite quasiparticle lifetime and huge uncertainty of the out-of-plane momentum. The theory is applied to a Schottky junction between graphene and a bulk semiconductor to derive a thermionic constant, which, in contrast to the conventional Richardson constant, depends on the barrier height and Fermi level [2]. Second, we focus on electron transport from a 2D conductor to a 2D semiconductor assuming some short-range interface disorder that results in momentum randomization and interlayer hopping. The model is applied to electron transport in graphene-MoS2 heterostructures [3].


*Supported by the Director's Senior Research Fellowship from CA2DM at NUS.
1:15PM L15.00011: Hall and thermoelectric measurement of Type-II Weyl semimetal TaIrTe₄

(Presenter), YU JIAN, QINSHENG WANG, YUGUI YAO, Beijing Institute of Technology — Weyl semimetal has gapless band structures protected by topology and symmetry which possess many interesting properties, like Fermi arc surface states, chiral anomaly etc. Without the constraint from the Lorentz invariance, type-II Weyl semimetal has a tilted Weyl cone that electron and hole pockets exist at the node energy. TaIrTe₄ is theoretically predicted to be a type-II Weyl semimetal hosting four well-separated Weyl points which is the minimum required by the symmetry. Here, we present our study of TaIrTe₄ with Hall and thermoelectric measurement. In the Hall measurement, two pairs of electron-hole pockets with quite different mobility could be identified by fitting the Hall curves. The temperature dependence of the carrier density shows an obvious movement of the Fermi level which is quite similar to the reported temperature-induced Lifshitz transition in WTe₂. The Hall result suggests that hole-type carrier dominate the transport properties which is in the opposite to the negative Seebeck coefficient. The Nernst coefficient has the same temperature dependence as the mobility of the dominate hole band.

*Work supported by NNSF of China (NO. 11734003, NO. 61804008).

1:27PM L15.00012: Quantum Oscillation in WTe₂ Flakes

XURUI ZHANG (Presenter), XIAOYAN SHI, Department of Physics, University of Texas at Dallas — WTe₂ is theoretically predicted to have two pairs of electron and hole pockets along Γ-X direction, which have been observed in ARPES. However, ARPES also revealed an additional hole pocket which is very closed to Γ point, the center of Brillouin zone. The two predicted pairs of Fermi pockets have already been verified in transport measurements but there’s few evidence of the existence of the hole pocket at Γ point. Here we report the quantum oscillations study in semimetallic WTe₂ flakes with different thickness. An oscillation signal from the hole pocket at Γ point is very likely to be observed.

*UT Dallas research enhancement funds

1:39PM L15.00013: Quantum Transport in N-doped 2D Tellurene

CHANG NIU (Presenter), GANG QIU, YIXIU WANG, WENZHUO WU, PEIDE (PETER) YE, Purdue University — Tellurium (Te) is a p-type narrow-bandgap high-mobility semiconductor with one dimensional van der Waals (vdW) structure. It has a unique chiral-chain crystal lattice in which individual helical chains of Te atoms are stacked together by vdW type bonds and spiral around c-axis. With recently developed solvent-based growth method, we are able to probe the magneto-transport of Te in its 2D limit, coined as tellurene. In this work, we demonstrate an effective dielectric doping technique to realize n-type tellurene. We report on the pronounced weak anti-localization, quantum Hall effect, strong Shubnikov-de Haas oscillations on n-doped tellurene with temperature down to tens of mK and magnetic fields up to 31 Tesla. Angle, electron density and temperature dependence of the oscillations were systematically measured and analyzed.

*A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1644779* and the State of Florida.

1:51PM L15.00014: Substrate Renormalization of Quasiparticle Band Gaps, Exciton Binding Energies and Transport Properties of Quasi-2D Materials

CHIN SHEN ONG (Presenter), FELIPE DA JORNADA, DIANA QIU, STEVEN G. LOUIE, Physics, University of California at Berkeley — Electrons in atomically thin quasi-2D materials, such as monolayer transition-metal dichalcogenides, are spatially confined in the out-of-plane direction and are also more weakly and differently screened than in bulk materials. Consequently, electron-electron and electron-hole interactions in quasi-2D materials are stronger and different compared to the bulk. Similarly, owing to the atomic dimension of layer thickness, quasi-2D materials are sensitive to screening environment produced by substrates, allowing one to dramatically tune their quasiparticle and optical properties. Here, we discuss a method recently developed in our group to incorporate substrate screening into the calculation of quasiparticle and optical properties of quasi-2D materials. We perform ab initio GW and GW-Bethe Salpeter equation (GW-BSE) calculations to quantify this effect on electronic and optical gaps of these systems. We will also discuss a theoretical upper bound of the screening effect. Lastly, we will show how substrate screening can be used to engineer a lateral heterojunction within homogeneous MoS₂ monolayer.

*This work is supported by NSF Grant DMR-1508412, DOE under Contract DE-AC02-05CH11231. Computational resources are provided by DOE at Lawrence Berkeley National Laboratory’s NERSC facility.
Multiscale Modeling of 2D Materials with the Phase-Field Crystal Model

TAPIO ALA-NISSILA

(Presenter), Applied Physics & Mathematical Sciences, Aalto and Loughborough University — Novel 2D materials have unusual properties, many of which are coupled to their large scale mechanical and structural properties. Modeling is a formidable challenge due to a wide span of length and time scales. I will review recent progress in structural multiscale modeling of 2D materials and thin heteroepitaxial overlayers [1], and graphene and h-BN [2,3], based on the Phase Field Crystal (PFC) model combined with Molecular Dynamics and Quantum Density Functional Theory. The PFC model allows one to reach diffusive time scales at the atomic scale, which facilitates quantitative characterisation of domain walls, dislocations, grain boundaries, and strain-driven self-organisation up to micron length scales. This allows one to study e.g. thermal conduction and electrical transport in realistic multi-grain systems [3,4].


*This work has been supported in part by the Academy of Finland QTF Centre of Excellence program (project 312298).

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L16 DCOMP DCP: Aqueous Solutions, Solvated Interfaces, and Ionic Polarization

II BCEC 155 - Jeffrey Greeley, Purdue University - Tag(s): Focus

11:15AM L16.00001: Unraveling correlation effects in water from microscopic response functions* [Invited] DEYU LU

(Invited) DEYU LU

(Presenter), Center for Functional Nanomaterials, Brookhaven National Laboratory — Electronic correlation effects play a crucial role in determining the structural and chemical properties of water. Over past decades, first-principles theory has been widely used to obtain physical insights of water and interpret experimental results. However, direct analysis of the electronic correlation in water from first principle is non-trivial, which motivates the development of new descriptors based on the microscopic response functions and formal methodologies to efficiently evaluate them. Recently, we have developed an ab initio local dielectric response theory [Phys. Rev. B 92, 241107, 2015] that partitions the microscopic electric susceptibility in real space based on the Wannier representation. Several applications of the local dielectric response theory are discussed. We demonstrate how to compute the molecular polarizability of water in the condensed phase and analyze the effects of the hydrogen-bonded network resulting from the crystal field and charge transfer. In another example, we studied the non-local correlation behaviors between water and solvated ions, and identified different screening characteristics of longitudinal and transverse modes.

*This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility at Brookhaven National Laboratory under Contract No. DE-SC0012704, and the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported under Contract No. DE-AC02-05CH11231.

11:51AM L16.00002: Tracking holes and their reactivity in photon-driven reactions using Real-Time Time-Dependent Density Functional Theory (RT-TDDFT)* VIDUSHI SHARMA (Presenter), MARIVI FERNANDEZ SERRA, Department of Physics and Astronomy, and Institute for Advanced Computational Science, Stony Brook University — Photocatalytic reactions on semiconductor surfaces that produce hydrogen have the potential of addressing our growing energy needs. However, the possible reaction intermediates and trajectories associated with such photon-driven reactions are currently not well understood. Our aim is to study the response of molecular systems upon photoexcitation. We are particularly interested in the evolution of a system on the excited-state potential energy surface and the interaction of the molecular intermediates with its surroundings after excitation which leads to the desired reaction. We use ab initio nonadiabatic simulations to study the time evolution of photoexcited states, and we simulate the coupled electron-ion dynamics using RT-TDDFT-based Ehrenfest dynamics. This is a promising nonadiabatic dynamics scheme given the considerable sizes of the molecular systems of interest. We compare the ultrafast dynamics of the "photogenerated-hole" as captured by RT-TDDFT Ehrenfest dynamics with the commonly used Born-Oppenheimer dynamics at similar time scales and identify the key physical characteristics that differentiate one from the other, thereby empirically testing a more computationally intensive nonadiabatic scheme for elucidating the physics of photoexcited systems.

*DE-FG02-09ER16052
Energy fluctuations in water: How are they coupled to protein dynamics and vice versa?*
SAUMYAK MUKHERJEE, SAYANTAN MONDAL, BIMAN BAGCHI (Presenter), Indian Institute of Science — The exotic properties of water have intrigued researchers over a long time. Aqueous solutions of complex biomolecules like proteins trigger further interest. Several theories address the complexity of protein-water interactions. Frauenfelder et al. hypothesized the solvent slaving of protein dynamics. In this work, for the first time, we propose a mechanistic pathway of such protein-water coupling. Using atomistic molecular dynamics simulations on five proteins, we find that water dipoles efficiently interact with polar groups at the protein core. The forces thus experienced are comparable to the forces of interaction with other protein atoms. We also find that the fluctuations in self-energy of protein are significantly anti-correlated to the fluctuations in protein-water interaction energy. This signifies a microscopic channel of energy flow between protein and water. This coupling is also manifested in the total energy spectrum of protein which shows bimodal $1/f$ noise characteristics. The additional slope in the spectrum shows signature of perturbation from water as shown by Ohmine et al.

Ohmine et al. Chem. Rev. 93, 2545 (1993)

Multiscale modeling of systems with confined electrolytes FRANCISCO SOLIS (Presenter), Arizona State University — Macroscopic models of physiological materials describe often tissues as passive homogeneous electric materials. At the mesoscopic level, these materials are typically composed of cells or other structures of similar scale which can be considered as confined electrolytes. Conduction and polarization of these structures can be effectively described by means of density functional theories. In this presentation it will be shown how computations for confined electrolytes can be used to build effective macroscopic models. In particular, we interpret the macroscopic conductivity and polarizability in terms of the properties of the confined electrolytes, analyzed by means of dissipative dynamics.

Salt Ion Transport Through Carbon Nanotubes: Insights from Polarizable Force Field-Based Molecular Dynamics Simulations RAHUL PRASANNA MISRA (Presenter), DANIEL BLANKSCHTEIN, Department of Chemical Engineering, Massachusetts Institute of Technology — Carbon Nanotubes (CNTs) which are cylindrical 1D allotropes of carbon are emerging as promising materials for membrane-based applications, including seawater desalination and osmotic power harvesting. For the rational design of CNTs in membrane-based applications, it is imperative to develop a fundamental understanding of the interactions of salt ions such as Na$^+$ and Cl$^-$ with the carbon atoms of CNTs. Given the large polarizability tensors of CNTs, salt ions inside CNTs can exert strong electric fields which can result in a significant polarization of the CNTs. Although the ion - CNT polarization energy is high (e.g., 27 kcal/mol inside a 0.8 nm diameter CNT) and makes the dominant contribution to the ion - CNT binding energy, previous MD simulation studies have neglected the polarization of CNTs in the presence of water molecules and salt ions. In this talk, we discuss our formulation of polarizable force fields parameterized using quantum chemical simulations which can self-consistently model the anisotropic polarizability tensors of CNTs, as well as reliably model water-CNT and ion-CNT interactions. Finally, by performing classical MD simulations with polarizable force fields, we carry out a comprehensive investigation of salt ion transport through 0.8 – 2 nm diameter CNTs.

Cation-specific effects on the attraction of anions to a hydrophobic surface TRAVIS DOUGLAS (Presenter), Department of Physics and Astronomy, Northwestern University, MIAOQI CHU, X-Ray Science Division, Argonne National Laboratory Advanced Photon Source, SANGJUN YOO, Department of Physics and Astronomy, Northwestern University, CHUNG-JONG YU, Pohang Accelerator Laboratory, Pohang University of Science and Technology, PULAK DUTTA, Department of Physics and Astronomy, Northwestern University — Halides such as bromide and iodide are known to accumulate near the free surface of an electrolyte solution. Solid hydrophobic surfaces in contact with water induce a density-depleted gap near the interface, creating a water density profile similar to the free surface. It is therefore possible that polarizable ions like halides are also attracted to hydrophobic surfaces, a notion that is supported by MD simulations. However, the buried solid-liquid interface is more difficult to access experimentally than the free surface of water and is thus much less studied. We present results of an x-ray reflectivity study of aqueous alkali metal-iodide solutions in contact with a hydrophobic self-assembled monolayer. A layer of enhanced anion density is observed at the SAM-water interface, but with an unexpected strong dependence on the cation present in the solution. This experiment attempts to provide insight into the less understood yet ubiquitous interactions between ions and real hydrophobic/non-polar materials, such as proteins and organic materials present in the atmosphere and soil.
coordinated by two G4 molecules and not in direct contact with TFSA− anions at a low concentration of the Li salt. The case of equimolar Li salt concentration, a positive correlation between the total coordination number of Li+ ions and the simulation to study the lithium bis(trifluoromethylsulfonyl)-amide (LiTFSA) and tetraglyme (G4) electrolyte system. For the oxidative stability, low vapor pressure, and non-flammability. Here we employ the first-principles molecular dynamics significantly increased probability of pairing between the Li-G4 complexes and TFSA− anions at the equimolar ratio could phase stability is clearly established. At the ground state of equimolar LiTFSA-G4 electrolyte, most of Li+ ions are

Materials Science, IKUTARO HAMADA, Department of Precision Science and Technology, Graduate School of Engineering, Osaka University — Glyme based electrolytes for rechargeable Li secondary batteries are of great interest, due to the high oxidative stability, low vapor pressure, and non-flammability. Here we employ the first-principles molecular dynamics simulation to study the lithium bis(trifluoromethylsulfonyl)-amide (LiTFSA) and tetraglyme (G4) electrolyte system. For the case of equimolar Li salt concentration, a positive correlation between the total coordination number of Li+ ions and the phase stability is clearly established. At the ground state of equimolar LiTFSA-G4 electrolyte, most of Li+ ions are coordinated to four O atoms of a curled G4 molecule and one O atom of a TFSA− anion. By contrast, Li+ ions prefer to be coordinated by two G4 molecules and not in direct contact with TFSA− anions at a low concentration of the Li salt. The significantly increased probability of pairing between the Li-G4 complexes and TFSA− anions at the equimolar ratio could be highly relevant to its ionic-liquid-like properties [1].


**1:03PM L16.00008: First-Principles Study of the Solvation Structure of Tetruglyme based Electrolytes** YANG SUN (Presenter), Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute for Materials Science, IKUTARO HAMADA, Department of Precision Science and Technology, Graduate School of Engineering, Osaka University — Glyme based electrolytes for rechargeable Li secondary batteries are of great interest, due to the high oxidative stability, low vapor pressure, and non-flammability. Here we employ the first-principles molecular dynamics simulation to study the lithium bis(trifluoromethylsulfonyl)-amide (LiTFSA) and tetraglyme (G4) electrolyte system. For the case of equimolar Li salt concentration, a positive correlation between the total coordination number of Li+ ions and the phase stability is clearly established. At the ground state of equimolar LiTFSA-G4 electrolyte, most of Li+ ions are coordinated to four O atoms of a curled G4 molecule and one O atom of a TFSA− anion. By contrast, Li+ ions prefer to be coordinated by two G4 molecules and not in direct contact with TFSA− anions at a low concentration of the Li salt. The significantly increased probability of pairing between the Li-G4 complexes and TFSA− anions at the equimolar ratio could be highly relevant to its ionic-liquid-like properties [1].


**1:15PM L16.00009: Ionic Structure in Highly-Concentrated Confined Electrolytes** NASIM ANOUSHEH (Presenter), Intelligent Systems Engineering, Indiana University Bloomington, FRANCISCO SOLIS, School of Mathematical and Natural Sciences, Arizona State University Glendale, VIKRAM JADHAO, Intelligent Systems Engineering, Indiana University Bloomington — Recent surface force measurements have shown that the effective force between mica surfaces does not decay as sharply as predicted by mean-field models such as the Debye-Huckel theory when the concentration of the confined electrolytes is high (around 2 M for NaCl). In other words, the interaction between charged surfaces is “under-screened” at high electrolyte concentrations. Motivated by these experiments, we use molecular dynamics simulations and strong coupling theory to extract the ionic structure in aqueous NaCl electrolytes confined by two interfaces. Ionic density profiles, effective force (pressure) between surfaces, and pair correlation functions are extracted for electrolytes confined between uncharged, charged, and polarizable interfaces at different concentrations (0.1 M to over 2 M). Effects of varying ion sizes, surface separation, and dielectric properties of the solvent are outlined. Simulation results are correlated with strong coupling theory calculations where “underscreening” behavior is associated with the formation of highly correlated groups of ions that act as individual entities.

**This work is supported by the National Science Foundation through Award 1720625.**

**1:27PM L16.00010: Examining Electronic Excitations in Liquid Water under Proton and Photon Irradiation** CHRIS SHEPARD (Presenter), DILLON C. YOST, YI YAO, YOSUKE KANAI, University of North Carolina at Chapel Hill — Proton and Photon irradiation of liquid water is important in many areas of modern technology, including cancer beam therapies. However, understanding the molecular level details of induced electronic excitation has been elusive. Using real-time time-dependent density functional theory, we study the dynamics of electron excitation in liquid water through the propagation of maximally-localized Wannier functions (MLWFs). The MLWF dynamics provide a convenient “molecular orbital” picture of the electronic structure, to understand electronic excitation in terms of localized electrons. We examine the extent to which photo-excitation and electronic stopping excitation differ at the molecular level.

**This work is supported by the National Science Foundation under Grants No. CHE-1565714. An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02- 06CH11357.**
1:39PM L16.00011: TDDFT approach on laser field enhancement by carbon nanotube and photo-decomposition of water
Hong Zhang¹, Yoshiyuki Miyamoto², Xinlu Cheng¹, Angel Rubio³ ¹College of Physical Science and Technology, Sichuan University, Chengdu 610065, China   HONG ZHANG (Presenter), Physics, Sichuan University, China —
In this presentation, we discuss field enhancement of femtosecond laser by carbon nanotubes and application to accelerating water photo-decomposition. The real-time time-dependent density functional theory (TDDFT) was employed for simulating water photo-decomposition near (8,0) semiconducting carbon nanotube. A short pulse with full-width of half-maximum 10fs was considered. When optical field is perpendicular to the tube axis, we found significant laser field enhancement corresponding to laser-power enhancement by factor 2 with laser wavelength 800 nm, and by factor around 8 with wavelength 400 nm. The enhancement is due to polarizability and wall-curvature of carbon nanotube that helps to reduce threshold power for photo-decomposition of water.

1:51PM L16.00012: A Molecular Dynamics Study of Ion Separation and Water Purification Using Graphene/Carbon Nanotube Filter
SAMANEH RIKHTEHGARAN (Presenter), LUC T WILLE, Physics, Florida Atlantic University — Molecular dynamics (MD) simulations have been used to design a graphene carbon nanotube (CNT) filter with an efficiency greater than 90% to separate Na⁺ and Cl⁻ ions from water molecules. The results show that the magnitude of the charge density that covers the surface of the CNT can noticeably influence the performance of ion separation and water purification. Therefore, the ion separation is improved by increasing the magnitude of the surface charge density enormously. In addition, it is observed that the velocity of the piston can have a huge impact on the filter's performance. This work establishes an atomic-level understanding of the effects of graphene and nanostructures on desalination and can be helpful for designing new nanofilter.

2:03PM L16.00013: K-shell Core Electron Excitations in Electronic Stopping of Protons in Water from First Principles*
YI YAO (Presenter), DILLON C. YOST, YOSUKE KANAI, Department of Chemistry, University of North Carolina at Chapel Hill — Understanding the role of core electron excitations in liquid water under proton irradiation has become increasingly important due to the growing use of ion beams in radiation oncology as an alternative to the X/γ-ray photon radiation. Using a first-principles, non-equilibrium simulation approach based on real-time TDDFT, we accurately determine the electronic stopping power over a wide range of proton velocities. The result agrees with available experimental data and also with the SRIM model. Explicit treatment of the K-shell, 1s electrons of oxygen atoms in water was found to be necessary to accurately predict the electronic stopping power for large velocities. The simulations also reveal that excitations of K-shell core electrons influence the valence electron excitation itself, and the separate treatment of valence and core electron excitation is not satisfactory for large velocities.

*This work is supported by the National Science Foundation under Grants No. OAC-1740204. Computer time was provided by the INCITE program with resources of the Argonne Leadership Computing Facility, a DOE Office of Science User Facility supported under Contract DE-AC02– 06CH11357.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L17 DCOMP: Matter in Extreme Environments: Planetary Materials BCEC 156A - Thomas Duffy, Princeton University - Tag(s): Focus

11:15AM L17.00001: Material Properties of Super-Earths and mini-Neptunes* [Invited] DIANA VALENCIA (Presenter), University of Toronto — The most common planets in the galaxy are now known to be low-mass exoplanets that either are rocky, known as super-Earths or may have an incipient envelope, the so-called mini-Neptunes. As the data grows for measured masses and radius for these planets the types of questions that we aim to answer have moved from discovery to characterization. I will talk about synergies between the study of material properties in the PT regime of these planets and the inferences we are able to make now in terms of composition and structure.

*DV thanks the Natural Sciences and Engineering Research Council of Canada
**11:51 AM L17.00002: Ab initio study of water speciation in forsterite**  KOICHIRO UMEMOTO (Presenter), Earth-Life Science Institute, Tokyo Institute of Technology, TIAN QIN, Department of Earth Sciences, University of Minnesota, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics, Columbia University — The Earth's interior contains 0.5 to 100 times of water on the Earth's surface based on different studies. Water or hydrogen (in hydroxyl form) can be stored as hydrous defects in nominally anhydrous minerals (NAMs) in the Earth's mantle. Although in modest concentrations, these defects change the physical properties of their hosts, including electrical conductivity and viscosity, properties that affect mantle processes such as convection. The most likely incorporation mechanism of hydrogen in mantle minerals is the substitution of Mg and Si cations by hydrogens. However, a long-standing debate remains concerning the relative thermodynamic stability of these defects. Using *ab initio* calculations we investigate the energetics of these defects, $(4H)^{\chi}$ Si and $(2H)^{\chi}$ Mg, in forsterite, the Mg end-member of olivine, the most abundant upper mantle phase. We address the role of vibrational free energy and lattice and internal defect configurational entropy in the relative stability of these defects. We conclude that entropic effects are key to the stabilization of the hydrous Mg defect, which should predominate over the hydrous Si defect at typical upper mantle conditions.

*NSF/EAR grant 1161023

**12:03 PM L17.00003: First-principles studies of oxidized carbon in water under extreme conditions**  NORE STOLTE, Department of Physics, Hong Kong University of Science and Technology, DING PAN (Presenter), Department of Physics and Department of Chemistry, Hong Kong University of Science and Technology — The properties of oxidized carbon and water mixtures at high pressure (HP) and high temperature (HT) are of great importance to the deep carbon cycle, which involves more than 90% of Earth's carbon and substantially impacts the carbon budget near Earth's surface. We studied CO$_2$ in supercritical water up to ~13 GPa and 1400 K using *ab initio* molecular dynamics, and found that while the major form of dissolved carbon is CO$_2$(aq) at ambient conditions, carbonic acid (H$_2$CO$_3$(aq)) can be more abundant than CO$_2$(aq) at HP-HT when the total mole fraction of carbon is below 40%. We investigated the aqueous reaction mechanisms of H$_2$CO$_3$(aq) formation and dissociation at HP-HT at the molecular scale. We will discuss the possible P-T range for the stability of H$_2$CO$_3$(aq). Our study suggests that H$_2$CO$_3$(aq) may be an important carbon transport host in the deep carbon cycle.

*The work is supported by the Alfred P. Sloan Foundation through the Deep Carbon Observatory, Hong Kong Research Grants Council (Project No. ECS-26305017), the National Natural Science Foundation of China (Project No. 11774072), and the Croucher Foundation through the Croucher Innovation Grant.

**12:15 PM L17.00004: First-principles prediction of new gas hydrates**  LEWIS CONWAY (Presenter), ANDREAS HERMANN, University of Edinburgh — Gas hydrates can form under low temperature and high pressure (~kbars) conditions and as a result occur naturally on Earth and within the solar system. They have applications in industry in storage and transport of gases. We explore computationally the stability of new gas hydrates, with a focus on the chiral water network S$_X$, the metastable ice structure ice XVII, associated with the C$_0$ hydrogen hydrate and the CO$_2$ HP-hydrate [1]. S$_X$ has been shown experimentally to be readily emptied [2]. Computationally, S$_X$ has been shown to form at least metastable hydrates with He, Ne and Ar [3]. Here we present a density functional theory (DFT) study of molecular N$_2$ and O$_2$ gas hydrates based on filled S$_X$ and analyse the phase evolution in the ground state, which shows a strong dependance on pressure and filling ratio. O$_2$ gas hydrate has the curious potential to form a magnetically ordered structure.


*UK Materials and Molecular Modelling Hub and the UK national HPC service, ARCHER, via the UKCP. EPSRC grants EP/P020194 (partial), EP/P022561/1 and EP/L015110/1 (studentship).
crystals, ammonia (\(\text{NH}_3\)) and ice (\(\text{H}_2\text{O}\)) by density functional theory calculations. We found that \(\text{NH}_3\) and He can form electrostatic energy under high pressure. In this work, we explore and show the reactivity of He with two molecular elements are usually quite inert to chemical reactions due to their closed shell configurations. He is the most stable noble gas since its ionization energy is almost twice as large as that of Xe. It was recently demonstrated that He could react with a large number of ionic compounds with unequal number of cations and anions due to the substantial change of the electrostatic interaction is the driving force for the He insertion under high pressure. In this work, we explore and show the reactivity of He with two molecular crystals, ammonia (\(\text{NH}_3\)) and ice (\(\text{H}_2\text{O}\)) by density functional theory calculations. We found that \(\text{NH}_3\) and He can form stable structure above 50 GPa with a \(\text{NH}_3\):He ratio of 1:1, while \(\text{H}_2\text{O}\) and He can form stable structure above 300 GPa with a \(\text{H}_2\text{O}:\text{He}\) ratio of 2:1. Although change of the electrostatic interaction is the driving force for the He insertion under high pressure, the mechanism is very different between ammonia and ice. This work extends the reactivity of He into a new area of molecular crystals, showing the richness of the chemistry of this most inert element in the periodic table. Since He, \(\text{NH}_3\) and \(\text{H}_2\text{O}\) are the major components of giant gas planets, the new chemistry revealed in our work is important for the understanding of the structure and the evolution of these planets.

**Predicted novel helium compounds under high pressure via CALYPSO**

HANYU LIU (Presenter), JURONG ZHANG, Innovation Center for Computational Physics Method and Software, College of Physics, Jilin university, YINWEI LI, School of Physics and Electronic Engineering, Jiangsu Normal University, JIAN LV, Innovation Center for Computational Physics Method and Software, College of Physics, Jilin university, YANSUN YAO, Department of Physics and Engineering Physics, University of Saskatchewan, XIAOLEI FENG, SIMON REDFERN, Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, CHANGFENG CHEN, Department of Physics, University of Nevada, Las Vegas, YANMING MA, Innovation Center for Computational Physics Method and Software, College of Physics, Jilin university — The knowledge of the structures that can exist in compounds containing helium is of interest for understanding the conditions where and if this inert element can form structures where closed shell electrons of helium can participate in bonding that is not describable exclusively by van der Waals interactions alone. In this work, we examine some mixtures of He and \(\text{H}_2\text{O}\), \(\text{N}_2\) or some minerals at high pressures using a first-principles structure searching method (CALYPSO). We find some thermodynamically stable structures under pressure. These mechanically and dynamically stable structures are found at pressures that are now becoming accessible to high-pressure technique. The present results offer insights for the understanding of the plausible reaction between helium with minerals in the Earth's or other exoplanetary interiors.

**Helium insertion reactions with ammonia and water under pressure**

YIHONG BAI (Presenter), Department of Physics, Beijing Normal University, ZHEN LIU, JORGE BOTANA, Beijing Computational Science Research Centre, DADONG YAN, Department of Physics, Beijing Normal University, HAI-QING LIN, Beijing Computational Science Research Centre, JIAN SUN, School of Physics and Collaborative Innovation Center of Advanced Microstructures, Nanjing University, CHRIS PICKARD, Department of Materials Science and Metallurgy, University of Cambridge, RICHARD NEEDS, Cavendish Laboratory, University of Cambridge, MAOSHENG MIAO, Department of Chemistry and Biochemistry, California State University Northridge — The noble gas elements are usually quite inert to chemical reactions due to their closed shell configurations. He is the most stable noble gas since its ionization energy is almost twice as large as that of Xe. It was recently demonstrated that He could react with a large number of ionic compounds with unequal number of cations and anions due to the substantial change of the electrostatic energy under high pressure. In this work, we explore and show the reactivity of He with two molecular crystals, ammonia (\(\text{NH}_3\)) and ice (\(\text{H}_2\text{O}\)) by density functional theory calculations. We found that \(\text{NH}_3\) and He can form stable structure above 50 GPa with a \(\text{NH}_3\):He ratio of 1:1, while \(\text{H}_2\text{O}\) and He can form stable structure above 300 GPa with a \(\text{H}_2\text{O}:\text{He}\) ratio of 2:1. Although change of the electrostatic interaction is the driving force for the He insertion under high pressure, the mechanism is very different between ammonia and ice. This work extends the reactivity of He into a new area of molecular crystals, showing the richness of the chemistry of this most inert element in the periodic table. Since He, \(\text{NH}_3\) and \(\text{H}_2\text{O}\) are the major components of giant gas planets, the new chemistry revealed in our work is important for the understanding of the structure and the evolution of these planets.

**Helium reaction with sodium halides under pressure**

ZHENG LIU (Presenter), Division of Simulation of Physical Systems, Beijing Computational Research Center, YIHONG BAI, Department of Physics, Beijing Normal University, ORTEGA FERNANDO, Department of Chemistry and Biochemistry, California State University, Northridge, CHRIS PICKARD, Department of Materials Science and Metallurgy, University of Cambridge, DADONG YAN, Department of Physics, Beijing Normal University, HAI-QING LIN, Division of Simulation of Physical Systems, Beijing Computational Research Center, MAOSHENG MIAO, Department of Chemistry and Biochemistry, California State University, Northridge — The noble gas elements are usually quite inert to chemical reactions due to their closed shell configurations. He is the most stable noble gas since its ionization energy is almost twice as large as that of Xe. It was recently demonstrated that He could react with a large number of ionic compounds with unequal number of cations and anions due to the substantial change of the electrostatic energy under high pressure. Unexpectedly, we found in the current work that He can react with NaX (X=Cl, Br, I) under high pressure also with considerable formation energy. The pressure needs to form stable NaXHe compounds decreases with increasing size of the halogen atoms. By analyzing the enthalpy components, the geometry change, and the electronic structures, we find the driving force of the He insertion reaction with AB type compound is the transformation of the structures that disproportionate the interstitial sites, making them ready to accommodate He atoms under high pressure. With the previous work, we greatly extend the reactivity of He with compounds under high pressure.

*We thank the computational resources from Beijing CSRC, National Natural Science Foundation of China (NSFC) for the grants under Nos. 21434001 and 21374011, and China Postdoctoral Science Foundation (No. 2018M630064).
1:03PM L17.00008: Phase relations in δ-AlOOH investigated with ab-initio calculations  
TIANQI WAN, ZIYU CAI, CHENXING LUO (Presenter), Department of Applied Physics and Applied Mathematics, Columbia University in the City of New York, TIAN QIN, Department of Earth Sciences, University of Minnesota, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics, Columbia University in the City of New York — As a high-pressure phase of diaspore and boehmite, δ-AlOOH is a crucial hydrous phase that can transport water in subducted slabs to the Earth's interior. Knowledge of phase relations in AlOOH is vital to understanding the state of water and the mechanisms of water transportation to the deep mantle. Most previous theoretical studies focused on the low-pressure static behavior of δ-AlOOH, leaving not only issues such as hydrogen-bond symmetrization under pressure unresolved but also high-temperature high-pressure phase boundaries not fully discussed. Recent experiments [1] show that the stability field of δ-AlOOH covers the entire pressure range of the Earth's lower mantle and this phase could remain stable in colder slabs down to the core-mantle boundary. We present an ab initio study of the structural and thermodynamic stability of δ-AlOOH and its related polymorphs to multi-Mbar pressures. We address hydrogen-bond symmetrization in AlOOH and the phase boundaries between its well-known phases. Moreover, we are also interested in assessing the dehydration boundary up to pressures exceeding those of the Earth's mantle as well as the possibility of alternative polymorphs at pressures relevant to terrestrial exoplanets.


1:15PM L17.00009: Proton dynamics in high-pressure ice-VII from density functional theory*  
FLORIAN TRYBEL (Presenter), GERD STEINLE-NEUMANN, THOMAS MEIER, Bavarian Research Institute of Experimental Geochemistry and Geophysics (BGI) — Recent Nuclear Magnetic Resonance (NMR) data on high-pressure ice-VII (Meier et al., Nature Comm., 2018) have revealed significant mobility of protons in the pressure range of 20-95 GPa at room temperature. Using a density-functional-theory-based approach, we explore the compression-dependent proton dynamics in ice-VII by directly sampling the proton potential along the diagonal O-O direction in the disordered body centered cubic configuration. We describe a configuration showing a double-well potential with a barrier that permits tunneling at compressions corresponding to 20 GPa. The double-well character disappears near 45 GPa, but a broad minimum indicates significant proton mobility to persist to 95 GPa. Tunneling frequencies are computed using the approximation of Wentzel, Kramers and Brillouin, with frequencies in the THz range.

*This work was supported by the DFG within FOR2440.

1:27PM L17.00010: Role of hydrogen bonding in the phase transformation of bulk liquid water to ice VII under shock loading*  
NILANJAN MITRA (Presenter), DIPAK PRASAD, Indian Institute of Technology Kharagpur — It has been widely reported both through experimental and theoretical investigations that bulk liquid water under shock loading partially transforms into Ice VII – one of the densest forms of ice. It is also known from literature that hydrogen bonding plays the main role in conversion of random arrangement of water molecules in bulk liquid water to that of periodic crystalline arrangement of ice in the event of conventional freezing. Thereby, it can be quite anticipated that the hydrogen bond plays the main role in phase transformation of bulk liquid water to that of ice VII on shock compression. The current manuscript describes the changes in the spectra of water in the 0-1000 cm^{-1} wavenumber regimes as bulk water is shock compressed to form ice VII. The molecular dynamic simulations carried out for this study also compares between different commonly used force potentials that are used to define water.

*Office of Naval Research Global
First-principles modelling of hydrogen-rich planetary materials

ANDREAS HERMANN

Accurate models of the interior structure of planetary bodies, in our or other solar systems, are key to understanding their formation, their evolution to the present day, and many of their properties. The stratification (or lack thereof) of molecular mixtures inside icy planets’ mantles influences their luminosity and cooling rates; and the presence (or not) of water stored inside rocky planets’ mantles influences their convection rates, the magnitude of plate tectonics and presence of surface water. In my talk I will give an overview of our ongoing research aimed at a better understanding of planetary materials using electronic structure calculations, focussing on hydrogen-containing systems on several different pressure scales. For molecular gas hydrates stabilized in the kbar range, crucial in the formation of icy moons and planets, I will show how wave-function based calculations can overcome density functionals’ ambiguities in capturing weak host-guest interactions [1]. For hydrous minerals, which store water inside Earth’s mantle in the GPa range, I will illustrate how crystal structure prediction methodology can help develop a more complete picture on their formation and internal phase transformations [2]. Lastly, I will discuss the properties of mixtures of planetary ices at conditions found in the mantle of Neptune-like bodies, at pressures beyond 1 Mbar and high temperatures [3,4].


Funding from the UK’s EPSRC (EP/L015110/1) and computational resources provided through the UKCP consortium (EP/P022561/1), the UK Materials and Molecular Modelling Hub (EP/P020194) and the Royal Society (RG-150247) are gratefully acknowledged.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L18 DCOMP: Quantum Manybody Systems: Theory and Computation I

Entanglement Entropy from Nonequilibrium Work

JONATHAN D’EMIDIO

The Rényi entanglement entropy of quantum many-body systems can be viewed as the difference in free energy of partition functions with different trace topologies. We introduce an external field that controls the partition function topology, allowing us to define a notion of nonequilibrium work as is varied smoothly. Nonequilibrium fluctuation theorems of the work provide us with statistically exact estimates of the Rényi entanglement entropy. We put these ideas to use in the context of quantum Monte Carlo simulations of SU(N) symmetric spin models in one and two dimensions. In both cases we detect logarithmic violations to the area law with high precision, allowing us to extract the central charge for the critical 1D models and the number of Goldstone modes for the magnetically ordered 2D models.

Entanglement Entropy and Negativity in Inhomogeneous (1+1)D Systems: The Rainbow Chain, the SSD and their Holographic Dual

IAN MACCORMACK

Starting with a system described by a conformal field theory (e.g. a critical spin chain or free fermions), one can find interesting violations to the typical logarithmic behavior of the bipartite entanglement entropy by introducing an inhomogeneous kinetic term in the Hamiltonian. Two examples of recent interest are the rainbow chain and the sine-squared deformed (SSD) model. Such systems can be equivalently described by placing the original CFT on a curved background manifold. Using the AdS/CFT correspondence, we develop a holographic dual description of inhomogeneous (1+1) dimensional systems by foliating the bulk spacetime with curved surfaces. Extending these foliations to the BTZ spacetime allows us to describe inhomogeneous systems at finite temperatures. Using field-theoretic, holographic, and numerical techniques, we are able to compute the entanglement entropy and negativity, for various configurations of intervals, both at zero and finite temperatures, for the rainbow chain and the SSD.

Shinsei Ryu is supported by a Simons Investigator Grant from the Simons Foundation.
11:39AM L18.00003: Crossover Behavior of Entanglement Entropy for Energy Eigenstates of 1d and 2d Fermionic Systems  QIANG MIAO (Presenter), THOMAS BARTHEL, Physics Department, Duke University — The entanglement entropy in ground states of typical condensed matter systems obeys the area law or a log-area law for critical systems. Subsystem entropies in random and thermal states obey a volume law. Here, we discuss the distribution of entanglement entropy in energy eigenstates of quasi-free fermionic systems as a function of energy and subsystem size. Numerical results are obtained with a Monte Carlo approach. We characterize the crossover behavior from the area or log-area law in the vicinity of the ground state and for small subsystem size to the volume law at higher energy and larger subsystem size. The coefficients of the volume law scaling can be matched to entropy densities in equilibrium thermal ensembles. For critical 1d systems at low energies, the universal crossover function matches the prediction from 1+1d conformal field theory for systems at nonzero temperatures. For 2d systems, we find a similar crossover behavior.

11:51AM L18.00004: Relating different localization lengths via non-perturbative construction of local integrals of motion in the many-body localized phase  PAI PENG (Presenter), XUAN WEI, ZEYANG LI, HAOXIONG YAN, PAOLA CAPPELLARO, Massachusetts Institute of Technology — Many-body localization (MBL) is characterized by the absence of thermalization and the violation of conventional thermodynamics. The phenomenological model, which describes the system using a complete set of local integrals of motion (LIOMs), provides a powerful tool to understand MBL. We explicitly compute a complete set of LIOMs non-perturbatively by maximizing the overlap between LIOMs and physical spin operators. This method enables a direct mapping from real space Hamiltonian to the phenomenological model. We demonstrate the exponential decay of weight of LIOMs in real-space and interaction strength of LIOMs in range. We further compare the localization lengths extracted from LIOMs, their interactions and dynamics. Our scheme is immune to accidental resonances and can be applied even at the phase transition point, providing a novel tool to study the microscopic features of the phenomenological model of MBL.

12:03PM L18.00005: A numerical procedure for non-integrable many-body quantum systems*  PAVAN HOSUR (Presenter), University of Houston — Numerical computations of properties of quantum many-body systems generally get drastically simplified by the presence of conserved quantities. Non-integrable quantum systems are those that lack, or have very few, conserved quantities and hence, are invariably intractable numerically. However, the eigenstate thermalization hypothesis postulates certain properties that non-integrable quantum systems must have and so far, computations on small systems have validated these properties. In this talk, a numerical procedure will be described that exploits the eigenstate thermalization hypothesis to discard, at the outset, vast amounts of useless quantum information and extract useful information about a non-integrable system more efficiently. The utility of the algorithm will be demonstrated via comparisons with exact diagonalization studies on prototypical non-integrable models.

*This work was supported by the Department of Physics, College of Natural Sciences and Mathematics and the University of Houston.

12:15PM L18.00006: Product Spectrum Approximation  JOHN MARTYN (Presenter), BRIAN SWINGLE, University of Maryland, College Park — Calculating the physical properties of quantum thermal states is a difficult problem for classical computers, rendering it intractable for most quantum many-body systems. To address this problem, we propose a variational scheme to prepare approximate thermal states on a quantum computer by applying a series of two-qubit gates to a product state. We apply our method to a non-integrable region of the mixed field Ising chain and the Sachdev-Ye-Kitaev model. We demonstrate how our method can be easily extended to large systems governed by local Hamiltonians and the preparation of thermofield double states. By comparing our results with exact solutions, we find that our construction enables the efficient preparation of approximate thermal states on quantum devices. Our results imply that the details of the many-body energy spectrum are not needed to capture simple thermal observables.

12:27PM L18.00007: Non-Markovian Quantum Dynamics via General Quantum Master Equation and Tensor Networks*  ERIKA YE (Presenter), AUSTIN MINNICH, GARNET CHAN, Caltech — Computing real-time dynamics of a quantum many-body system is challenging due to the exponential growth of entanglement. While many different approaches have been investigated, how to compute the real-time dynamics of generic condensed matter systems, or how to best classify for which systems the dynamics cannot feasibly be computed on a classical computer, remain open questions. In this work, we treat the Nakajima-Zwanzig general quantum master equation with tensor network methods to identify the limits of classical time evolution algorithms. Though the memory kernel is difficult to compute even numerically, tensor networks provide a systematic means of obtaining the kernel for diverse complex systems, such as the spin-boson model with anharmonic bath sites. In this work we focus on the spin-boson model and analyze how the types and strengths of interactions affect the lifetime of the memory kernel. Our work provides general insight into the classical simulatability of quantum dynamics.

*2018 Google PhD Fellowship
12:39PM L18.00008: Collective Excitations in a Landau-Majorana Liquid  
JOSHUAH HEATH (Presenter), KEVIN BEDELL, Boston College — Landau-Fermi liquid theory is one of the foundational theories of interacting many-body fermions. Its simplicity has led to its continued application to real materials, and the rare instances where it fails (e.g., the case of a non-Fermi liquid) have become a major concern in the condensed matter community. In this study, we apply the formalism of Landau-Fermi liquid theory to describe a quantum liquid of interacting Majorana fermions. As opposed to Majorana zero modes, which characterize topologically non-trivial materials and obey anyonic statistics, Majorana fermions are spin-1/2 particles that experience mutual pairwise annihilation. Drawing on a previous work (arXiv:1709.04483), we describe the quasiparticles in such a system and construct the Landau-Silin kinetic equation. The presence of a robust Fermi surface in the screened Majorana system leads to a Lifshitz transition in the limit of large driving frequency. In addition, a calculation of the zero sound leads to the presence of an enhanced stability of the Landau-Majorana liquid against Pomeranchuk instabilities. These results lead to important differences in the fundamental physics of interacting Majorana fermion ensembles that has potential applications in various condensed matter systems and astrophysical phenomena.

12:51PM L18.00009: Divergences of the irreducible vertex functions in correlated metallic systems: Insights from the Anderson Impurity Model  
PATRICK CHALUPA (Presenter), PATRIK GUNACKER, TU Wien, THOMAS SCHAEFER, College de France, KARSTEN HELD, ALESSANDRO TOSCHI, TU Wien — We analyze the occurrence of divergences in the irreducible vertex functions of the Anderson impurity model (AIM) [1]. These divergences — a surprising hallmark of the breakdown of many-electron perturbation theory [2] — have been recently observed [3,4] in several contexts, including the dynamical mean-field solution of the Hubbard model. Hitherto, however, a clarification of their origin could be obtained only in the limit of high temperatures and/or large interactions, where the underlying physics is greatly simplified by the absence of low-energy quasiparticle excitations. In this respect, our numerical calculations for the AIM, as well as their comparison with the corresponding results for the Hubbard model, allow us to clarify several open questions about the origin and the properties of vertex divergences occurring in a more interesting context, the correlated metallic regime at low-temperatures.


1:03PM L18.00010: Kondo impurities at the edges of a quantum wire*  
PARAMESHWAR PASNOORI (Presenter), Physics, Rutgers University, COLIN RYLANDS, Joint Quantum Institute, University of Maryland, NATAN ANDREI, Physics, Rutgers University — Quantum impurity systems, where a localized impurity is coupled to a large bath of particles appear naturally in many fields from mesoscopic physics and quantum dot systems to the Kondo lattice of Heavy fermion materials. In this talk we study a miniature Kondo lattice consisting of a one dimensional quantum wire coupled to Kondo impurities at either end. We show that it is exactly solvable by means of Bethe Ansatz for arbitrary values of bulk spin exchange interaction and of the Kondo coupling. The model exhibits both gapped and gapless phases depending on the sign of the bulk interaction and a competition between dynamical mass generation and the Kondo effect. We construct the ground state in all regimes and study the excitations and their finite size corrections as well as the impurity magnetization as function of an applied field.

*Supported by Samuel Marateck Fellowship, NSF grant DMR 1410583.
Dynamics of Densities and Currents in Spin Ladders

JONAS RICHTER (Presenter), Department of Physics, University of Osnabrück, FENGPING JIN, Institute for Advanced Simulation, Forschungszentrum Jülich, LARS KNIPSCHILD, Department of Physics, University of Osnabrück, JACEK HERBRYCH, Department of Physics and Astronomy, The University of Tennessee, HANS DE RAEDT, Zernike Institute for Advanced Materials, University of Groningen, KRISTEL MICHIELSEN, Institute for Advanced Simulation, Forschungszentrum Jülich, JOCHEN GEMMER, ROBIN STEINIGEWEG, Department of Physics, University of Osnabrück — The impact of integrability or nonintegrability on the dynamics of isolated quantum systems is a longstanding issue. For integrable models, a macroscopic set of (quasi)local conservation laws can lead to partially conserved currents and ballistic transport. In generic situations, however, integrability is lifted due to various perturbations and currents are expected to decay. Still, since the dynamics of interacting quantum many-body systems poses a formidable challenge to theory and numerics, it remains open whether nonintegrability as such already implies the emergence of diffusion.

In this context, we study the dynamics of spin and energy in the two-leg spin-1/2 ladder with up to 40 lattice sites, using an efficient pure-state approach based on the concept of typicality. We discuss correlation functions in real and momentum space, and in the time and frequency domain, providing a comprehensive picture of high-temperature dynamics in this archetypal nonintegrable quantum model. Particularly, we unveil the occurrence of diffusion for both spin and energy.


Semiclassical echo dynamics in the Sachdev-Ye-Kitaev model

MARKUS SCHMITT (Presenter), University of California, Berkeley, DRIES SELS, Harvard University, STEFAN KEHREIN, Georg-August-Universität Göttingen, ANATOLI S POLKOVNIKOV, Boston University — The existence of a quantum butterfly effect in the form of exponential sensitivity to small perturbations has been under debate for a long time. Lately, this question gained increased interest due to the proposal to probe chaotic dynamics and scrambling using out-of-time-order correlators. In this work we study echo dynamics in the Sachdev-Ye-Kitaev model under effective time reversal in a semiclassical approach. We demonstrate that small imperfections introduced in the time-reversal procedure result in an exponential divergence from the perfect echo, which allows to identify a Lyapunov exponent \( \lambda \). In particular, we find that \( \lambda \) is twice the Lyapunov exponent of the semiclassical equations of motion. This behavior is attributed to the growth of an out-of-time-order double commutator that resembles an out-of-time-order correlator.

This talk is based on arXiv:1802.06796.

*This work was supported through SFB 1073 (project B03) of the Deutsche Forschungsgemeinschaft (DFG). M.S. acknowledges support by the Studienstiftung des Deutschen Volkes. D.S. acknowledges support from the FWO as post-doctoral fellow of the Research Foundation Flanders and CMTV. A.P. acknowledges support by NSF DMR-1506340 and AFOSR FA9550-16-1-0334

Generalized Hydrodynamics Revisited

JAMES DUFTY (Presenter), JEFFREY WRIGHTON, KAI LUO, Physics, University of Florida — A number of attempts to formulate a continuum description of complex states have been proposed to circumvent more cumbersome many-body and simulation methods. Typically these have been quantum systems and the resulting phenomenologies frequently called “quantum hydrodynamics”. This objective is placed in a formally controlled context using the exact macroscopic conservation laws for number density, energy density, and momentum density, together with standard tools of non-equilibrium statistical mechanics. These continuum equations entail perfect fluid fluxes that are functional of the chosen fields, plus unknown irreversible energy and momentum fluxes. Typically, the latter are obtained from a solution to the Liouville-von Neumann equation for small space and time variations. Instead, here we avoid that restriction by requiring that the unknown irreversible fluxes deliver the exact linear response functions for the fields. In this way, a non-linear generalized hydrodynamic description is obtained, valid across a broad range of length and time scales. The example of electrons in a given ion configuration is described to make contact with current phenomenological "quantum hydrodynamics".

*Research supported by US DOE Grant DE-SC0002139
1:51PM L18.00014: Quantum Fluid Dynamics (QFD) or Bohmian Representation of Schrödinger Equation with Navier–Stokes Type Dissipation Attila Askar Koc University, Sariyer, Istanbul 34450, Turkey  
(Presenter), Koc University — The Quantum Fluid Dynamics (QFD) representation has its foundations in the works of Madelung, De Broglie and Bohm. It is an interpretation of quantum mechanics with the goal to find classically identifiable dynamical variables at the sub-particle level. The approach is partly motivated by Einstein's questioning of the completeness of the quantum theory. Einstein expected the complete theory to have nonlinearity and admit solutions with "particle" nature, similar to solitons in contemporary terminology.

The QFD approach leads to two conservation laws, for "mass" and "momentum", similar to those in fluid-dynamics for a compressible fluid as a set of nonlinear partial differential equations. The QFD formalism is utilized advantageously for solving the time dependent Schrödinger equation for scattering problems.

This paper extends the QFD formalism to include dissipation in the form of Navier–Stokes term in classical fluid dynamics. The introduction of dissipation in the Navier–Stokes sense transform the differential equations from hyperbolic to parabolic type, with nonlinear and dispersive terms. These offer a natural framework for fundamentally new phenomena, in particular possibility of dissipation in quantum mechanics, solitons, vortices and chaos.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L19 DCMP DAMOP DCMP: Precision Many Body Physics VIII  
BCEC 156C - Olga Goulko, Boise State University

11:15AM L19.00001: Entanglement production and information scrambling in a noisy spin system*  
MICHAEL KNAP (Presenter), Department of Physics, Technical University of Munich — We study theoretically entanglement and operator growth in a spin system coupled to an environment, which is modeled with classical dephasing noise. Using exact numerical simulations we show that the entanglement growth and its fluctuations are described by the Kardar-Parisi-Zhang equation. Moreover, we find that the wavefront in the out-of-time ordered correlator (OTOC), which is a measure for the operator growth, propagates linearly with the butterfly velocity and broadens diffusively with a diffusion constant that is larger than the one of spin transport. The obtained entanglement velocity is smaller than the butterfly velocity for finite noise strength, yet both of them are strongly suppressed by the noise. We calculate perturbatively how the effective time scales depend on the noise strength, both for uncorrelated Markovian and for correlated non-Markovian noise.

*We acknowledge support from the Technical University of Munich - Institute for Advanced Study, funded by the German Excellence Initiative and the European Union FP7 under grant agreement 291763, from the DFG grant No. KN 1254/1-1, and DFG TRR80 (Project F8).

11:51AM L19.00002: Real time correlations and spectral functions in numerical linked-cluster expansions*  
EHSAN KHATAMI (Presenter), San Jose State University — Highly precise static properties of strongly correlated fermions at finite temperatures from numerical linked-cluster expansions have been widely used to characterize systems of ultracold atoms in optical lattices. Here, I will discuss how dynamical properties such as various spectral functions of quantum lattice models can be obtained using the method through real time, as opposed to imaginary time, correlation functions at temperatures relevant to current optical lattice experiments. Nichols et al., arXiv:1802.10018

*I acknowledge support from the NSF under Grant No. DMR-1609560.
Interplay of disorder and strong correlations in quantum many-body systems remains an open question despite much progress that has been made in recent years with ultracold atoms in optical lattices to better understand phenomena such as many-body localization or the effect of disorder on Mott metal-insulator transitions. Here we utilize the numerical linked-cluster expansion technique, extended to deal with disordered quantum lattice models in the thermodynamic limit, and study exact thermodynamic properties of the disordered Fermi-Hubbard model on the square lattice. We consider box distributions for the disorder in the hopping amplitude as well as in the onsite energy or the interaction strength and explore how the system properties evolve as the strength of the disorder changes. We compare our results with those obtained from determinant quantum Monte Carlo simulations on finite clusters and discuss the potential applications of the results to experiments with cold fermionic atoms on optical lattices.

*This work is supported by the NSF under Grant No. DMR-1609560.

Computations are performed on the Spartan high-performance computing facility at San Jose State University provided by the NSF under Grant No. OAC-1626645.

Low-energy physics of the bilinear-biquadratic spin-1 chain

Moritz Binder (Presenter), Thomas Barthel, Duke University — The bilinear-biquadratic spin-1 chain features various interesting quantum phases, including the Haldane phase, a dimerized phase, and an extended critical phase. Here, we apply an efficient density matrix renormalization group (DMRG) algorithm utilizing infinite boundary conditions to compute precise dynamic spin structure factors for a comprehensive set of points in the phase diagram. Analyzing both dynamic spin and quadrupolar correlations, we gain detailed insights into the nature of low-lying excitations of the model. We compare our results to Bethe ansatz solutions at the SU(3)-symmetric ULS point and the TB point as well as at the pure biquadratic point, which can be mapped to an anisotropic spin-1/2 XXZ chain in the gapped Néel phase. In the Haldane phase, we relate our results to the approximate description in terms of the non-linear sigma model.
12:27 PM L19.00005: Ground states of a J-Q model with long-range antiferromagnetic interactions*  
SIBIN YANG (Presenter), Boston University, DAO-XIN YAO, Physics, Sun-Yat sen University, ANDERS W SANDVIK, Boston University — We employ large-scale sign-free quantum Monte Carlo and Lanczos exact diagonalization to study the 1D J-Q model (a Heisenberg antiferromagnet with multi-spin couplings added) with long-range interactions. Three phases, an ordered anti-ferromagnet (AFM), a quasi long-range ordered (QLRO state), and a valence bond solid (VBS), are identified by applying Binder-cumulant and level-crossing methods. We investigate different characteristics of these phases and their quantum phase transitions. From our numerical data and for the model we studied, the Binder-cumulant method has advantages in determining the quantum critical AFM-QLRO point and a certain range of the QLRO-VBS transition line, while the level crossing method is more suitable for the other region of QLRO-VBS transition. In addition, there could be a direct quantum phase transition between the AFM and VBS phases, possibly an analog of the 2D deconfined quantum critical point (DQCP) in one dimension.

*S.Y. and D.X.Y. are supported by Grants No. NKRDPC-2017YFA0206203 and No. NSFC-11574404; A.W.S. is supported by NSF DMR-1710170 and the Simons Foundations.

TIGRAN SEDRAKYAN (Presenter), University of Massachusetts Amherst, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, ALEX KAMENEV, University of Minnesota — We study the stability of ordered states in a two-dimensional quantum spin-1/2 J_1-J_2 XY antiferromagnet on a frustrated triangular lattice using composite fermion representation of spins. In the presence of next-nearest-neighbor antiferromagnetic coupling, J_2, the model is shown to undergo a continuous transition from 120° ordered state to a quantum U(1) Dirac spin-liquid (QED_3) at J_2/J_1 \sim 0.089, in accordance with previous variational Monte-Carlo and DMRG studies. In the XY limit, the U(1) gauge field emerges in a narrow parameter interval of 0.089 \lesssim J_2/J_1 \lesssim 0.116, that stabilizes the spin liquid. The transition to the tripe phase at J_2/J_1 \sim 0.116 is found to be of first order. Finite Ising interaction, J_z, pushes the boundaries of the phase transitions to 120° state and the stripe ordered state apart, thus opening a wider interval for the spin-liquid. Our results show an interesting interplay of ordering and the emergence of the gauge field in the vicinity of unconventional criticality.

12:51 PM L19.00007: Anomaly matching and symmetry-protected critical phases in SU(N) spin systems in 1+1 dimensions  
YUAN YAO, CHANG-TSE HSIEH (Presenter), MASAKI OSHIKAWA, Univ of Tokyo-Kashiwanoha — We study (1+1)-dimensional SU(N) spin systems in the presence of the global SU(N) rotation and lattice translation symmetries. By matching the mixed anomaly of the PSU(N)×Z in the continuum limit, we identify a topological index for spin model evaluated as the total number of Young-tableaux boxes of spins per unit cell modulo N, which characterizes the "ingappability" of the system. A nontrivial index implies either a ground-state degeneracy in a gapped phase, which can be regarded as a field-theory version of the Lieb-Schultz-Mattis theorem, or a restriction of the possible universality classes in a critical phase (symmetry-protected critical phase) -- only a class of SU(N) Wess-Zumino-Witten theories can be realized in the low-energy limit of the given lattice model in the presence of the symmetries. Similar constraints also apply when a higher global symmetry emerges in the model with a lower symmetry. Our prediction agrees with several examples known in previous studies of SU(N) models.

1:03 PM L19.00008: Efficient generation of many-body entangled states by multilevel oscillations  
PENG XU (Presenter), Wuhan University — We propose a fast method utilizing multilevel oscillations to generate high-fidelity massive entangled states in an antiferromagnetic spin-1 Bose-Einstein condensate (BEC). Combing the multilevel oscillations with additional adiabatic drives, we greatly shorten the necessary evolution time and relax the requirement on the control accuracy of quadratic Zeeman splitting, from micro-Gauss to milli-Gauss, for a 23Na spinor BEC. The achieved high fidelities over 96% show that two kinds of massively entangled states, the many-body singlet state and the twin-Fock state, are almost perfectly generated. The generalized spin squeezing parameter drops to a value far below the standard quantum limit even with the presence of particle number fluctuations and stray magnetic fields, illustrating the robustness of our protocol under real experimental conditions. The generated many-body entangled states can be employed to achieve the Heisenberg-limit quantum precision measurement and to attack nonclassical problems in quantum information science.
Efficient Two Dimensional Tensor Network Algorithms for Systems with Long-Range Interactions* MATTHEW O’ROURKE (Presenter), ZHENDONG LI, GARNET CHAN, California Institute of Technology — Current state-of-the-art tensor network algorithms in two dimensions, the most predominant being infinite projected entangled-pair states (iPEPS), have not yet advanced beyond the study of local lattice models. In order to utilize the power of these methods to study systems with physically realistic long-range interactions, we discuss a practical and efficient representation of the Hamiltonian of such systems as a projected entangled-pair operator (PEPO). We express the long-range interaction as a linear combination of correlation functions of an auxiliary system with only nearest neighbor interactions. This construction yields a long-range PEPO as a sum of ancillary PEPOs, each of small, constant bond dimension. Applications of this PEPO formulation to iPEPS simulations of model systems will be discussed.

*Primary support for this work was from MURI FA9550-18-1-0095 and an NSF GRFP via grant DEG-1745301. Additional support was from the NSF via grant CHE-1665333 and the Simons Foundation.

Solving constrained counting problems with tensor networks STEFANOS KOURTIS (Presenter), Boston University — In this talk, I will present newly developed physics-inspired methods for the solution of counting constraint satisfaction problems (#CSPs). #CSP instances can be reformulated as models of interacting degrees of freedom, whose zero-temperature partition function represents the volume of the solution manifold. I will introduce practical methods to compute such partition functions based on tensor network contraction. In this formulation, computational complexity can be viewed as a manifestation of quantum entanglement, and controlling the growth of entanglement throughout tensor network contraction can yield a significant computation speedup. Using some hard counting problems as benchmarks, I will demonstrate that tensor network methods can be a useful tool for solving some hard classes of #CSPs. I will conclude with an outline of ongoing work on extensions of this framework.

Non-Abelian symmetries in thermal tensor network states* BIN-BIN CHEN (Presenter), Ludwig Maximillians University, Munich, Germany, WEI LI, Beihang University, ANDREAS WEICHSELBAUM, Brookhaven National Laboratory — The implementation of non-Abelian symmetries in the tensor networks greatly improves efficiency and thus also precision of quantum many-body simulations in quasi-1D systems. Here, in particular, we discuss our general implementation of the SU(2) spin together with U(1) charge symmetry based on the QSpace [1] tensor library in the recently developed thermal tensor network simulations including the series expansion thermal tensor network (SETTN) [2], and exponential thermal renormalization group (XTRG) [3]. We will also show benchmarks of the fermionic Hubbard model on both square and triangular lattice.


*This work is supported by the German Research Foundation, DFG WE4819/3-1.

Exponential Thermal Tensor Network Approach for Quantum Lattice Models ANDREAS WEICHSELBAUM (Presenter), Brookhaven National Laboratory, BIN-BIN CHEN, Ludwig Maximilians University, Munich, Germany, LEI CHEN, ZIYU CHEN, WEI LI, Beihang University, Beijing, China — We speed up thermal simulations of quantum many-body systems in one- (1D) and two-dimensional (2D) models in an exponential way by iteratively projecting the thermal density matrix ρ=e^{-βH} onto itself. We refer to this approach as the exponential tensor renormalization group (XTRG) [1]. It is in stark contrast to conventional Trotter-Suzuki-type methods which employ a linear quasi-continuous grid in inverse temperature β=1/T. By avoiding Trotterization altogether, XTRG can also deal with longer-range interactions in a straightforward algorithmic way. By construction, XTRG can reach exponentially low temperatures by a linear number of iterations, and thus not only saves computational time but also merits better accuracy due to significantly fewer truncation steps. More fine-grained temperature resolution can be achieved via simple interleaving of data sets. We work in an (effective) 1D setting exploiting matrix product operators (MPOs) which allows us to fully and uniquely implement non-Abelian and Abelian symmetries to greatly enhance numerical performance. We show exemplary XTRG results for Heisenberg models on 1D chains and 2D lattices with a finite temperature phase transition down to low temperatures approaching ground state properties. [1] Phys. Rev. X 8, 031082 (2018)
11:15AM L20.00001: Getting to the core of valence excitations from first principles* [invited] DAVID PRENDERGAST (Presenter), Molecular Foundry, Lawrence Berkeley National Laboratory — Excited-state processes in molecules, materials, and at interfaces can reveal intricate details of energy transfer between electronic and nuclear degrees of freedom: photo-induced chemistry, charge transfer, nonthermal melting, etc. Accurate theoretical methods can hypothesize on the ultrafast evolution of these excited states and advanced pump-probe characterization can reveal spectral signatures of the same, however, combining prediction and interpretation of ultrafast phenomena works best when we can simulate both pump and probe to directly connect experiment and theory. To this end, we focus on simulating core-level spectroscopy of ground and excited valence states from first principles. Valence excited states can be modeled in different ways, depending on the context, but here we focus on two approaches based on density functional theory (DFT): constrained-DFT and real-time time-dependent (TD) DFT. Core-excited states are generally modeled with Delta-SCF or linear-response TDDFT, and we outline our approach to combine valence and core excited states for direct interpretation of ultrafast X-ray and XUV probes. An abundance of local physical and chemical detail on valence excitations is evident through probing core-excitations, which we explore, atom by atom, in a predictive fashion.

*Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

11:51AM L20.00002: Ab Initio Simulation of Carrier Dynamics in Electric Fields in Bulk Semiconductors WILLIAM MCCORKINDALE (Presenter), Cavendish Laboratory, University of Cambridge, JIN-JIAN ZHOU, MARCO BERNARDI, Applied Physics and Materials Science, Caltech — Carrier dynamics in the presence of electric fields governs the performance of semiconductor devices. The carrier drift velocity as a function of electric field (so-called velocity-field curve) has been a key material property since the early days of semiconductor physics. Yet, velocity-field curves cannot be computed from first principles, and their simulation still relies on decade-old semiempirical Monte Carlo approaches. We present a first principles method for solving the Boltzmann Transport Equation (BTE) in the presence of electric fields, which allows us to accurately compute velocity-field curves. The approach extends an efficient scheme we recently developed to solve the BTE with ab initio electron-phonon scattering. Including the electric field is nontrivial – it makes the equations computationally ‘stiff’, a challenge we solve by developing an implicit numerical method to time-step the BTE. We demonstrate the stability of the algorithm, and simulate the relaxation of carriers to steady-state distributions in an electric field. Using GaAs as a case study, we obtain the first fully ab initio velocity-field curves, which correctly exhibit the Gunn effect (negative differential resistance at moderate E-fields) and the drift velocity saturation at high field.

12:03PM L20.00003: Ab Initio Radiative Lifetimes in Gallium Nitride VATSAL JHALANI (Presenter), Applied Physics and Materials Science, Caltech, HSIAO-YI CHEN, Physics, Caltech, MAURIZIA PALUMMO, Physics, University of Rome, Tor Vergata, MARCO BERNARDI, Applied Physics and Materials Science, Caltech — Wurtzite GaN is the primary semiconductor for efficient solid state lighting. The radiative recombination and excited carrier dynamics are challenging to measure in GaN due to the ultrafast (fs – ps) timescales at play and the presence of defects and interfaces in devices. Here, we present ab initio calculations of the radiative lifetime as a function of temperature in bulk GaN. We compute the exciton energies and wavefunctions using a combination density functional theory and GW-Bethe Salpeter equation (BSE) method. We derive an equation for the temperature dependent radiative lifetime for an anisotropic bulk crystal within the ab initio BSE framework. The radiative lifetimes in GaN obtained with this approach are in excellent agreement with experiment. We discuss the importance of including spin-orbit coupling, which, though weak in GaN, is essential to obtaining accurate radiative rates. Combined with our previous calculations of excited carrier relaxation in GaN [1], we can obtain from first principles key device parameters such as the hot carrier cooling time and the carrier diffusion lengths, with important technological implications.

12:15PM L20.00004: First-Principles Study of Hot Electron Dynamics on Silicon Quantum Dot-Molecule System*
JIAN CHENG WONG (Presenter), University of North Carolina at Chapel Hill, LESHENG LI, Princeton University, YOSUKE KANAI, University of North Carolina at Chapel Hill — Controlling hot carriers in nanomaterials is an active area of research, central to various optoelectronic applications. In our previous work¹, a short-lived hot electron transfer from a hydrogen-terminated Si(111) surface to the cyanidin molecule was observed during hot electron relaxation within the conduction manifold of the silicon, followed by interfacial electron transfer of picosecond timescale. We expand this study onto a silicon quantum dot attached to a cyanidin molecule to investigate the extent to which these observations change. Hot electron dynamics are investigated using first-principles simulation based on fewest switches surface hopping method combined with first-principles molecular dynamics and GW calculation.


*This work is funded by the UNC Energy Frontier Research Center (EFRC) “Center for Solar Fuels”, an EFRC funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award DE-SC0001011.

12:27PM L20.00005: Rashba effect on spin-resolved carrier dynamics excited by circularly-polarized light from first-principles
SUSHANT KUMAR (Presenter), Rensselaer Polytechnic Institute, FENG WU, University of California, Santa Cruz, ADELA HABIB, Rensselaer Polytechnic Institute, YUAN PING, University of California, Santa Cruz, RAVISHANKAR SUNDARARAMAN, Rensselaer Polytechnic Institute — Recent optical pump/X-ray probe experiments have shown that circularly polarized light can be used to manipulate spin states in materials exhibiting strong Rashba splitting like organo-metallic halide perovskites (OMHPs) and transition metal dichalcogenides (TMDs). The ability to exploit the dynamics of spin makes these materials lucrative candidates for spin-optoelectronic applications [1]. While considerable experimental work has been performed on probing the spin dynamics in TMDs and OMHPs, efforts to model this ultrafast spin-dependent dynamics of charge carriers have so far been limited primarily to effective model Hamiltonians. A key challenge is accounting for electron-phonon scattering effects on the spin dynamics explicitly, due to the requirement of ultra-fine Brillouin-zone sampling arising from the disparate energy scales of electrons and phonons. We present a completely parameter-free ab initio approach to study spin and carrier dynamics, using Wannier functions to facilitate efficient calculation of electron-phonon scattering. Using this approach, we present calculations of spin-resolved photo-excited carrier distributions and phonon-assisted spin relaxation times for TMDs and ferroelectric oxides.


12:39PM L20.00006: Spin-dependent electron transfer dynamics: key role of bandstructure*
DANIEL SANCHEZ-PORTAL (Presenter), MORITZ MÜLLER, Centro de Física de Materiales CSIC-UPV/EHU and DIPC — We investigate theoretically the charge transfer dynamics of core-excited Ar on Co(001) and Fe(110). For these systems, recent core-hole-clock measurements [1] of the lifetime of the photo-excited 4s level of Ar⁺ have shown a clear dependence on the spin of the excited electron. Minority electrons decay significantly faster than majority electrons. We investigate such processes using Green's functions techniques on top of density functional theory calculations, explicitly including the effect of the coupling to the semi-infinite substrate [2, 3]. Our results agree with the observed behavior and allow analyzing in detail the origin of this phenomenon. The key ingredient is the spin-depence of the bandstructure of the substrate and, in particular, the different positions of the Ar⁺ 4s level within the projected band gap appearing around Gamma in the dispersive bands of Co(001) and Fe(110) for both spin channels. A simple model incorporating this effect successfully describes most of the observed phenomenology.


*We acknowledge support from Spanish MINECO Grants MAT2016-78293-C6-4-R and RTC-2016-5681-7.
Ultrafast Excited State Dynamics of Coupled Carriers and Phonons from Ab Initio Calculations

XIAO TONG (Presenter), JIN-JIAN ZHOU, MARCO BERNARDI, Caltech — The out-of-equilibrium dynamics and equilibration processes of excited states in materials are crucial to understanding time-resolved spectroscopies. Several ultrafast phenomena occurring on a sub-picosecond time scale are governed by the coupled dynamics of electrons and atomic vibrations (phonons), including transient structural distortions and excited electron thermalization due to the competing electron-phonon (e-ph) and phonon-phonon (ph-ph) interactions. Here, we show ab initio calculations of the coupled ultrafast dynamics of carriers and phonons. We develop an efficient algorithm to time-step the coupled electron and phonon Boltzmann transport equations, which include both the e-ph and ph-ph scattering on the same footing. Our approach allows us to study the time evolution of the excited electron populations as well as the out-of-equilibrium phonons together with the transient structural distortions they induce. We apply our method to silicon and graphene, and compare the results with time-resolved spectroscopies probing both the structural and the electron dynamics, such as free-electron laser and time-resolved electron diffraction experiments.

Electron-defect interactions and low temperature carrier mobility from first principles

I-TE LU (Presenter), JIN-JIAN ZHOU, MARCO BERNARDI, Caltech — Electron-defect (e-d) interactions control charge and spin transport at low temperature and induce well-known conductance fluctuation and weak localization effects. While established ab initio methods and code exist for treating electron-phonon (e-ph) interactions, ab initio e-d calculations are still in their infancy, mainly due to the formidable computational cost of computing e-d matrix elements and self-energies from calculations on supercells containing the defect. In this talk, we formulate an efficient approach for computing e-d matrix elements using mainly unit cell quantities, and demonstrate its numerical implementation in the PERTURBO code. Using this approach, we can compute and systematically converge the e-d scattering rates for neutral defects such as vacancy and interstitial atom in silicon, and obtain the corresponding defect-limited low temperature mobility. The results deviate in important ways from broadly used empirical approaches to treat e-d interactions, highlighting the shortcomings of these simple models. Efforts on interpolating e-d matrix elements, computing higher-order e-d processes, and releasing the e-d routines in PERTURBO will be discussed.

Simulating Electron Beam – Materials Interactions with Real-Time Electron Dynamics*

JACEK JAKOWSKI (Presenter), DAVID LINGERFELT, PANCHAPAKESAN GANESH, BOBBY G SUMPTER, Oak Ridge National Laboratory — Time-dependent electron dynamics is used to model interaction of electron beam with materials for beam energy and positions relevant to scanning transmission electron microscopy. We investigate the real-time and linear response framework for simulating the response of small molecular systems including benzene and pyrene. The position dependence of selection rules for electron beam induced electronic excitations is discussed. Higher order terms in the multipolar expansion of the electrostatic potential are shown to contribute significantly to the energy loss probability except in the high impact parameter regime where the electric fields emanated by the electron beam are essentially homogeneous over the volume of the material. Results of this study have implications for the prediction of electron energy loss spectra from first principles, and can lead to a more complete understanding of mechanisms underlying both directed nanoscaled materials manipulations and accidental radiation damage sustained by materials subjected to electron beams with energies below the material’s knock-on threshold.

*This work was conducted at the Center for Nanophase Materials Sciences, a US Department of Energy Office of Science User Facility.
Coherent exciton-vibrational dynamics and energy transfer in conjugated organics

TAMMIE NELSON (Presenter), Los Alamos National Laboratory, DIANELYS ONDARSE-ALVAREZ, NICOLAS OLDANI, BEATRIZ HERNANDEZ, LAURA ALFONSO-HERNANDEZ, Universidad Nacional de Quilmes, JOHAN GALINDO, Universidad Nacional de Colombia, VALERIA D KLEIMAN, University of Florida, SEBASTIAN FERNANDEZ-ALBERTI, Universidad Nacional de Quilmes, ADRIAN E ROITBERG, University of Florida, SERGEI TRETIAK, Los Alamos National Laboratory — Excited state dynamics simulations reveal a ubiquitous pattern in the evolution of photoexcitations for a broad range of molecular systems. Symmetries of the wavefunctions define a specific form of the non-adiabatic coupling that drives quantum transitions between excited states, leading to a collective asymmetric vibrational excitation coupled to the electronic system. This promotes periodic oscillatory evolution of the wavefunctions, preserving specific phase and amplitude relations across the ensemble of trajectories. The simple model proposed here explains the appearance of coherent exciton-vibrational dynamics due to non-adiabatic transitions. We demonstrate universality of these phenomena by inspecting photo-induced dynamics in several common cases for organic conjugated materials. These include a linear oligomer, nano-hoop, tree-like dendrimer, and molecular dimer. In all these molecules, ultrafast dynamics and exciton transport is directly simulated using our atomistic nonadiabatic excited-state molecular dynamics (NEXMD) package. Coherent dynamics observed in these systems persists on the timescale of 100s of fs at room temperature and in the presence of a bath, which agrees with experimental spectroscopic reports on various materials.

Modification of excitation and charge transfer in cavity quantum-electrodynamical chemistry*

CHRISTIAN SCHÄFER (Presenter), MICHAEL RUGENTHALER, HEIKO APPEL, ANGEL RUBIO, Max-Planck Institute for the structure and dynamics of matter — Energy transfer in terms of excitation or charge is one of the most basic processes in nature and understanding and controlling them is one of the major challenges of modern quantum chemistry. In this work, we highlight that these processes as well as other chemical properties can be drastically altered by modifying the vacuum fluctuations of the electromagnetic field in a cavity. By using a real-space formulation from first principles that keeps all the electronic degrees of freedom in the model explicit and simulates changes in the environment by an effective photon mode, we can easily connect to well-known quantum-chemical results such as Dexter charge- and Förster excitation-transfer reactions taking into account the often disregarded Coulomb and self-polarization interaction. We find that the photonic degrees of freedom introduce extra electron-electron correlations over large distances, that the coupling to the cavity can drastically alter the characteristic charge-transfer as well as the excitation energy transfer behavior. Our results highlight that changing the photonic environment can redefine chemical processes, rendering polaritonic chemistry a promising approach towards the control of chemical reactions.

*We acknowledge financial support from ERC-2015-AdG-694097.

Non-equilibrium dynamics of spin and charge correlation in strongly correlated systems from pump-probe spectroscopy

CHEN-YEN LAI (Presenter), JIAN-XIN ZHU, Los Alamos National Laboratory — The ultrafast pump-probe techniques are used to probe the elementary excitations in materials. We study the non-equilibrium process of the one-dimensional extended Hubbard model under transient laser pump pulse. In non-polarized cases, the competition between charge and spin results in bond-order-wave between spin-density-wave and charge-density-wave phases in equilibrium. We focus on the regime near the phase boundaries and how those spin and charge correlations affected by different pump pulse frequency and strength. Furthermore, in the spin-polarized systems, the Bethe strings state emerges and the non-equilibrium dynamics of the fractional excitation are investigated. The effects from photoinduced charge carriers near the phase boundaries are investigated by time evolving black decimation. These effects should be measurable by time-resolved angle-resolved photoemission spectroscopy. (LA-UR-18-30001)
Ultrafast decay of low-symmetry photo-induced atomic forces.*

SHANE O’MAHONY (Presenter), JOSE QUERALES-FLORES, IVANA SAVIC, Materials Theory, Tyndall National Institute, ÉAMONN MURRAY, Department of Materials and Department of Physics, Imperial College London, FELIPE MURPHY-ARMANDO, STEPHEN B FAHY, Materials Theory, Tyndall National Institute — Generation and control of atomic forces in optically excited systems is crucial to understanding photocatalysis, renewable energy and laser annealing. Eg-symmetry coherent phonons are excited in group-V semimetals by ultrafast (<100 fs) optical pulses when the radiation is polarised perpendicular to the 3-fold symmetry axis of the crystal. The phonon driving force is consistent with an initially unbalanced occupation of electronic states in symmetry-equivalent regions of the Brillouin zone, which decays to fully-symmetric occupation of the zone on fs timescales. Measured temperature-dependence of the force decay time in Bi and Sb [1] suggests relaxation of the excited electronic distribution by electron-phonon (el-ph) scattering.

We calculate the decay of the Eg-symmetry driving force in Bi, Sb and As within the framework of density functional perturbation theory. We compute the initial excited electronic distribution [2], evolve using el-ph rate equations and calculate the atomic forces at each time-step. We obtain good agreement with experiment, showing that el-ph scattering is a dominant relaxation mechanism for the Eg force.

[1] Li et al PRL 110 047401

*Science Foundation Ireland award 12/IA/1601 and Irish Research Council GOIPG/2015/2784.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L21 DCOMP: Emerging Trends in Molecular Dynamics Simulations and Data Analytics II

11:15AM L21.00001: Overcoming the Time Limitation in Molecular Dynamics Simulation of Crystal Nucleation: A Persistent-Embryo Approach* [Invited] YANG SUN (Presenter), FENG ZHANG, HUAJING SONG, MIKHAIL MENDELEV, Ames Laboratory, ALEX TRAVESSET, Iowa State University, CAI-ZHUANG WANG, Ames Laboratory, KAI-MING HO, Iowa State University — The nucleation of a crystalline phase in liquid is a typical rare event and is usually inaccessible within the limited timescales of conventional molecular dynamics (MD) simulations under experimental conditions. In this talk, we present a “persistent embryo” method to facilitate crystal nucleation in MD simulations, in which a small crystal embryo is inserted into the liquid, with spring forces applied to keep the embryo from melting. The springs are gradually weakened as the embryo grows and are completed removed when the nucleus size remains significantly smaller than the critical size. In this way, one can observe the spontaneous fluctuations of a critical nucleus in an unbiased environment, without any assumptions on the shape of the critical nucleus. We applied this method to simulate crystal nucleation under realistic experimental conditions and obtained results that compare favorably with experiments and other simulation methods. We will show this accelerated dynamic approach provides ample statistics for the critical sampling of the nucleation.

*The work at Ames Laboratory was supported by the US Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division, under Contract No. DEAC02-07CH11358, including a grant of computer time at the National Energy Research Supercomputing Center (NERSC) in Berkeley, CA.

11:51AM L21.00002: TBD [Invited] KLAUS-ROBERT MÜLLER (Presenter), Technical University of Berlin — tbd

12:27PM L21.00003: Cavitation in Water Induced by a SnO2 Nanoparticle and a Strong Electric Field* SHANE JACKSON (Presenter), AIICHIRO NAKANO, PRIYA VASHISHTA, RAJIV KALIA, Physics, University of Southern California — Molecular dynamic simulations are performed to examine the effect of an electric field on a system consisting of a SnO2 nanoparticle embedded in water under ambient conditions. Cavitation is observed in the presence of uniform electric fields ranging from 0.042 to 0.25 V/Angstrom in both the SPCE and the Hydrogen-Bonding Polarizable (HBP) force field models for water. Over at least one order of magnitude, the cavity onset time t is related to the electric field through the Kohlrausch-Williams-Watts form E(t) = E_0 exp(-(t/τ)^β), with b = d^*(d^* + 2) = 3/7, where d^* = d/2, d being the dimensionality of the system. The bubbles are found to rapidly collapse upon removal of the electric field. Results for the structure and dynamics of water along with the electric field distributions in the system will be presented.

* The work was supported by the grant DE-SC0018195 funded by the U.S. Department of Energy, Office of Science. Simulations were performed at the Center for High Performance Computing of the University of Southern California.
12:39PM L21.00004: Interaction Potential for Faceted Nanoparticles.  BRIAN LEE (Presenter), GAURAV ARYA, Duke University — There is a growing interest in studying the assembly of faceted nanocrystals due to the potential of such anisotropic particles to yield unconventional structures with unique electrical, optical, and mechanical properties. While the van der Waals (vdW) interactions between spherical particles can be well-described by analytical functions, no such closed-form expressions are available to describe the vdw interactions between faceted particles. This is especially problematic in molecular simulations of particle assembly, where exact descriptions of interparticle energies in terms of interatomic interactions become computationally prohibitive, requiring a polynomial time algorithm. In this work, we formulate analytical expressions for vdw interactions between faceted particle by taking advantage of available expressions for macroscopic body interactions and by converting the energy integration over the particles' bodies to integration over the particles' facets. We show that the expressions provide reasonably accurate descriptions of the position and orientation dependence of vdw interactions. Since this method is a constant time algorithm, O(1), it could improve the computational efficiency of simulating faceted particles by several orders of magnitude.

12:51PM L21.00005: Atomic Structure of Supported Metal Nano Clusters on MoS2 Monolayer Using Deep Potentials*  WISSAM SAIDI (Presenter), University of Pittsburgh, YONGLIANG SHI, University of Science and Technology of China, LINFENG ZHANG, Princeton University, HAN WANG, Institute and Applied Physics and Computational Mathematics, WEINAN E, Princeton University, JIN ZHAO, University of Science and Technology of China — In nanometer clusters (NCs), the specific arrangement of metal atoms determines the unique size-dependent functionalities of the NCs and hence their potential applications. Here we employ a combined approach utilizing a genetic algorithm and a deep potential (DP) to determine the lowest energy configurations of the NCs including metastable structures. The DP is trained using density functional theory calculations. We discuss the strengths and shortcomings of the DP approach compared to a standard method utilizing density functional theory calculations.

*This work is supported by National Science Foundation (DMR-1809085)

1:03PM L21.00006: Large-Scale Atomistic Simulations of Materials using SNAP Potentials*  AIDAN THOMPSON, MITCHELL A WOOD, MARY ALICE CUSENTINO (Presenter), Sandia National Laboratories — Molecular dynamics (MD) is a powerful materials simulation method whose accuracy is limited by the interatomic potential (IAP). SNAP is an automated quantum data-driven approach to IAP generation that balances accuracy and computational cost. The energy is formulated in terms of a very general set of geometric invariants that characterize the local neighborhood of each atom. The SNAP approach has been used to develop potentials for studying plasticity in tantalum, intrinsic defects in indium phosphide, and plasma surface interactions in tungsten and beryllium. In each case, large quantum-mechanical data sets of energy, force, and stress are accurately reproduced and cross-validation on additional test data is performed. The resultant potentials enable high-fidelity MD simulations with thousands to millions of atoms. The relatively large computational cost of SNAP is offset by the LAMMPS implementation, enabling the efficient use of large CPU and GPU clusters.


1:15PM L21.00007: A mean-field algorithm with decoherence and detailed balance for nonadiabatic molecular dynamics  JUN KANG (Presenter), LIN-WANG WANG, Lawrence Berkeley National Laboratory — Decoherence and detailed balance are two major issues for mixed quantum/classic nonadiabatic molecular dynamics (NAMD) simulations. In this work we introduce a new mean-field dynamics approach with decoherence and detailed balance (MF-DD) for NAMD. This method is able to explicitly treat the decoherence between different pairs of electronic states. Moreover, the energy-increasing and energy-decreasing electronic transitions are distinguished by dividing the density matrix into two parts. The detailed balance correction is then included by a Boltzmann factor applied to the energy-increasing transitions. The MF-DD is applied to study hot-hole cooling and transfer processes in Si quantum dot (QD) systems. The calculated hot carrier relaxation time is in consistent with experiments. In the QD-pair systems, the cooling time shows weak dependence with the QD spacing. However, the charge transfer rate between QDs is found to decreases exponentially as the QD spacing increases, which is attributed to the decreased state anticrossing strength. When the QD spacing is smaller than 1.1 nm, the hot-carrier transfer between two QDs can be quite efficient. It is also shown that the explicit treatment of decoherence time is important.
Multi-Resolution Simulations using the Integral Equation Coarse-Graining Method*

MOHAMMADHASAN DINPAJOOH (Presenter), MARINA GIUSEPPINA GUENZA, University of Oregon — We use the variable-level coarse-grained (CG) description of polymer melts to obtain the effective CG potentials (ECGPs) for multi-resolution simulations of pure polymer melts represented at various CG resolutions. Starting from the Integral Equation Coarse-Graining approach, we obtain the numerical and analytical ECGPs in the multi-resolution simulations that are different from the ECGPs in single-resolution simulations. Therefore, the composition, temperature, and density dependences of such ECGPs can be investigated. In particular, the ECGPs between the polymer melts, represented by $n_{ba}$ blobs, decay slowly with a long tail characteristic scaling exponent of $N_{ba}^{1/4}(\phi_\alpha + (\phi_\alpha - (n_{ba}/n_{b\beta})^3))^{1/4}$, where $\phi_\alpha$ is the volume mole fraction of species $\alpha$, $N_{ba}$ is the number of monomers in a given blob of type $\alpha$, and $\beta$ shows the other species. The ECGPs allow one to avoid any hybrid region in multi-resolution simulations while quantitatively producing the structural and thermodynamical properties of the related atomistic systems such as radial distribution function and pressure.

*The NSF Grant No. CHE-1665466 and the XSEDE COMET resources supported by the NSF Grant No. ACI-1548562.

Development of a universal Electron Force Field*

ISIDRO LOSADA LÓPEZ (Presenter), Condensed Matter Physics, Autonomous University of Madrid, MICHELLE FRITZ, Slalom, Philadelphia, PAULA MORI-SANCHEZ, Chemistry, Autonomous University of Madrid, MARIVI FERNANDEZ SERRA, Department of Physics and Astronomy, Institute for Advance Computational Science, Stony Brook University, JOSE M SOLER, Condensed Matter Physics, Autonomous University of Madrid — In many cases, the unavailability of an adequate classical force field is a major barrier for molecular dynamics simulations. In these cases, density functional theory (DFT) provides a universal but expensive option. We propose an intermediate approach based on an ‘electron force field’ (eFF) [Su and Goddard, PRL 99, 185003 (2007)]. Inspired by VSEPR theory, we expand the electron density as a sum of overlapping spherical electron ‘balls’ (e-balls). The e-balls interact through electrostatic forces, Pauli repulsion, and exchange-correlation. The electronic total energy is calculated as a universal function of the e-ball positions and widths. As in DFT, it is independent of the nuclei, which interact only electrostatically. We parameterize this universal, many-body function by fitting to DFT calculations of a large number of molecules and solids at equilibrium, distorted, and reaction geometries.

*Funded by Spain's MINECO grant FIS2015-64886-C5-5-P

Modeling of La$^{3+}$ doping segregation in nanocrystalline yttria-stabilized zirconia using a combintaion of atomistic MD, Monte Carlo and Nudged Elastic Band calculations*

SHENLI ZHANG, ROLAND FALLER (Presenter), University of California, Davis — The effect of La$^{3+}$ doping on the structure and ionic conductivity change in nanocrystalline yttriasitabilized zirconia (YSZ) was studied using a combination of Monte Carlo and molecular dynamics and Nudge Elastic Band simulations. Simulations of specific grain boundary configurations are developed. Systems with and without La doping are studied and equilibrated using a combintaion of techniques and eventually anaylzed using Voronoi tessellation analysis for the density of the dopants.

The simulation revealed the segregation of La$^{3+}$ at eight tilt grain boundary (GB) structures and predicted an average grain boundary (GB) energy decrease of 0.25 J m$^{-2}$, which is close to the experimental values reported in the literature. Cation stabilization was found to be the main reason for the GB energy decrease, and energy fluctuations near the grain boundary are smoothed out with La$^{3+}$ segregation. Both dynamic and energetic analysis on the S13(510)/[001] GB structure revealed La$^{3+}$ doping hinders O$^2$- diffusion in the GB region, where the diffusion coefficient monotonically decreases with increasing La$^{3+}$ doping concentration. T

*This research was supported by the U.S. Department of Energy, Office of Nuclear Energy, Nuclear Energy University Program under Grant No. DE-NE0000704.
Ultrafast detonation of hydrazoic acid: a case study of the ChIMES model

HUY PHAM (Presenter), NIR GOLDMAN, LAURENCE FRIED, Lawrence Livermore Natl Lab — Understanding the chemical evolution and states of matter of an energetic material under detonation is challenging due to the short time scales of chemical reactions and risk of experimental work. First-principle molecular dynamics simulations can provide valuable insights into such systems. However, the computational cost associated with those simulations limits their applicability to relatively small systems and short time scales. We have developed the Chebyshev Interaction Model for Efficient Simulation (ChIMES), a reactive force field, using force matching to trajectories from density functional theory (DFT). This force field has been shown to be capable of retaining the accuracy of DFT simulation while increasing orders of magnitude in computational efficiency. In this work, we use ChIMES to study hydrazoic acid, an azide energetic material that exhibits an ultrafast detonation during a shock wave. We find that our models are able to accurately reproduce the structural and dynamic properties computed from DFT at different thermodynamic states. The ability to describe charge transfer and chemical reactions is also discussed.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L22 DCOMP DMP: Electrons, Phonons, Electron-Phonon Scattering and Phononics III

Electron-phonon coupling and electronic transport in n-type PbTe: Insights from first principles calculations*

IVANA SAVIC (Presenter), Tyndall National Institute, Cork, Ireland — Exploiting the fascinating properties of materials near soft mode phase transitions is an emerging concept in the quest to increase thermoelectric efficiency [1]. Soft phonons may lead to low lattice thermal conductivity, while preserving high electronic conductivity. Here I will focus on the unusual electronic transport properties of n-type PbTe, which is a classic thermoelectric material that exists near a soft optical mode phase transition. Our first principles calculations show that longitudinal optical phonon scattering dominates electronic transport, while acoustic phonon scattering is relatively weak [2,3]. We find that scattering due to soft transverse optical phonons is by far the weakest scattering mechanism, due to the symmetry-forbidden scattering between the conduction band minima and the zone center soft modes [3]. Soft phonons thus play the key role in the high thermoelectric figure of merit of n-type PbTe: they do not degrade its electronic transport properties although they strongly suppress the lattice thermal conductivity [1].


*This work is supported by Science Foundation Ireland under Investigators Programme No. 15/IA/3160.
11:51AM L22.00002: Predictive calculations of phonon-limited carrier mobilities in semiconductors*  
SAMUEL PONCE (Presenter), Department of Materials, University of Oxford, ELENA ROXANA MARGINE, Department of Physics, Binghamton University-SUNY, MARTIN SCHLIPF, FELICIANO GIUSTINO, Department of Materials, University of Oxford — In this talk, we will probe the accuracy limit of ab initio calculations of carrier mobilities that relies on the electron-phonon coupling, within the framework of the Boltzmann transport equation. In particular, we will show that predictive calculations of electron and hole mobilities require many-body quasiparticle corrections to band structures and electron-phonon matrix elements, the inclusion of spin-orbit coupling, and an extremely fine sampling of inelastic scattering processes in momentum space [1].

Such fine sampling calculation is made possible at an affordable computational cost through the use of efficient Fourier-Wannier interpolation of the electron-phonon matrix elements as implemented in the EPW code [2].

We will discuss recent findings on the mobility of silicon, wurtzite GaN and halide perovskites [3].

References

*Leverhulme Trust (Grant RL-2012-001), UK EPSRC (grant No. EP/M020517/1), Graphene Flagship (Horizon 2020 Grant No. 785219-GrapheneCore2), the Oxford ARC facility, PRACE-15 and PRACE-17 resources MareNostrum at BSC.

12:03PM L22.00003: Stochastic properties of a hot electron gas in a semiconductor from first-principles*  
ALEXANDER CHOI (Presenter), AUSTIN MINNICH, Caltech — Recent advances in ab-initio methods have enabled the routine calculation of the electronic transport properties of crystals. Analogous calculations of stochastic properties, such as the spectral noise power of an electron gas driven by an electric field, have not yet been reported despite their importance in setting fundamental detection limits of microwave electronics. Here, we report an ab-initio treatment of the noise of a driven electron gas using a Boltzmann-Green's function approach. Our approach combines electronic structure and scattering rates from first-principles with a numerically exact solution of the Boltzmann equation, providing a parameter-free description of stochastic transport processes in a semiconductor. The insights derived our ab-initio approach will facilitate the realization of semiconductor devices operating near the quantum noise limit.

*AYC is grateful for support from the National Science Foundation Graduate Student Fellowship.

12:15PM L22.00004: Probing electron-phonon interactions in Weyl semimetal using Raman spectroscopy and anharmonic phonon calculations  
KUNYAN ZHANG (Presenter), Electrical Engineering, Pennsylvania State University, FEI HAN, Nuclear Engineering, Massachusetts Institute of Technology, SHUN-LI SHANG, ZI-KUI LIU, Materials Science and Engineering, Pennsylvania State University, MINGDA LI, Nuclear Engineering, Massachusetts Institute of Technology, SHENGXI HUANG, Electrical Engineering, Pennsylvania State University — TaP, a type of Weyl semimetal (WSM) with noncentrosymmetric space group \( I4_1md \), is a special type of quantum materials that have attracted strong recent interests. The gapless band structure of TaP allows unique optical response and transport phenomena. Although electrical and photoemission characterizations such as Hall measurement and angle-resolved photoemission spectroscopy (ARPES) have been performed on various WSMs, there is insufficient research on the electronic and optical properties using optical spectroscopies as probes. In the present work, the light-matter interactions, including electron-phonon and electron-photon interactions, have been studied comprehensively through phonon-based Raman spectroscopy and first-principles calculations. We demonstrate how the optical spectroscopic responses, such as Raman and absorption, of TaP change under various physical parameters including crystal orientation, temperature, and excitation laser energies. Advanced first-principles calculations of electronic and especially anharmonic phonon properties have been employed to unveil the measured optical spectroscopic responses and their relationship with electronic performance of WSMs.
High Temperature Charge Transport In Strontium Titanate*  
CLEMENT COLLIGNON (Presenter), BENOIT FAUQUE, Institut de Physique, College de France, KAMRAN BEHNIA, LPEM, ESPCI — Strontium titanate quickly becomes metallic upon doping, but while the ferromagnetism of this metallic phase is well understood its transport properties remain elusive [1]. At low temperature, even though the scattering mechanism is not known, the resistivity exhibits a $T^2$ behavior typical of Fermi liquids [1]. With increasing temperature, resistivity rapidly grows and follows an unusual $T^3$ power law [1,2]. At room-temperature, the magnitude of resistivity combined with the effective mass, $m^*$, obtained from quantum oscillations, implies strikingly short mean-free-path and scattering time. The Mott-Ioffe-Regel limit is exceeded, and the scattering time decreases faster than the planckian time ($\tau_P = \frac{h}{2\pi k_B T}$). Nevertheless, the resistivity does not show any sign of saturation.

In this talk, we present new charge transport data extended up to 850 K to follow the fate of this enigmatic metallicity at high temperatures. The system continues to display a metallic behavior without saturation in resistivity and the apparent scattering time (assuming a temperature-independent $m^*$) becomes 10 times lower than $\tau_P$.


*This work was supported by Fonds-ESPCI, the ANR QUANTUMLIMIT and JEIP College de France.

Band structure and optical properties of boron arsenide (BAs): effects of quasiparticle corrections, spin-orbit coupling, and phonon-assisted optical transitions*  
KYLE BUSHICK (Presenter), KELSEY MENGLE, NOCONA SANDERS, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan — The III-V semiconductor BAs is best known for its high thermal conductivity, which was computationally predicted and recently experimentally validated. However, due to a lack of high-quality samples, the electronic and optical properties have not been systematically explored. We use density functional and many body perturbation theory including quasiparticle and spin-orbit coupling corrections to systematically characterize the electronic and optical properties of BAs. Accurate calculations of band gap values, carrier effective masses, and dielectric functions yield insights into the fundamental properties of this new material. We further explore the effect of phonon-mediated transitions across the indirect band gap on the optical properties. We will discuss the implications of our findings on potential applications of BAs to semiconductor technologies.

*This work was supported by NSF DMREF program (1534221). Computational resources provided by DOE NERSC (DE-AC02-05CH11231).

Ab initio studies of electron-phonon coupling to the electron self-energy in organic crystals*  
FLORIAN BROWN-ALTVATER (Presenter), UC Berkeley/Lawrence Berkeley Natl Lab, GABRIEL ANTONIUS, University of California, Berkeley, TONATIUH RANGEL GORDILLO, Lawrence Berkeley Natl Lab, MATTEO GIANTOMASSI, Université catholique de Louvain, CLAUDIA DRAXL, Humboldt-Universität zu Berlin, XAVIER GONZE, Université catholique de Louvain, STEVEN G. LOUIE, University of California, Berkeley, JEFFREY B NEATON, UC Berkeley/Lawrence Berkeley Natl Lab — Organic crystals combine properties of individual molecules and extended periodic systems. They garner much scientific interest due to their high charge carrier mobilities, and because their unique electronic and vibrational properties challenge our understanding of fundamental optoelectronic processes. In this work we use density functional perturbation theory to study the phonon-scattering lifetimes, as well as the temperature dependence of the band structure. We find that a self-consistent approach to the electron self-energy due to electron-phonon coupling yields qualitative differences compared to a conventional approach, and shows much better agreement with experimental results. We discuss efficient methods for self-consistency in organic crystals, and implications on calculating band gap renormalization and quasiparticle lifetimes of these systems.

*This work is supported by DOE and computational resources are provided by NERSC.
The interest in the properties of transition metal dichalcogenides (TMDs) has increased due to the discovery of the coupling between spin and valley degrees of freedom, which can be seen experimentally using a circularly polarised laser. After excitation the newly formed carrier populations must move towards the other valley until balance is reached. However, this relaxation process is not entirely understood in the literature, where the relative importance of the electron-electron (e-e) or electron-phonon (e-p) interactions is still a subject of debate. Previous works on WSe₂ [A. Molina-Sánchez, et al - Nano letters, 2017] have shown that the e-p interaction is a good candidate to describe the relaxation process. Using a fully ab-initio framework based on the Baym-Kadanoff equations [P. M. M. C. de Melo and A. Marini, Phys. Rev. B 93, 155102 (2016)] we study the influence of the e-p interaction on MoSe₂ after its excitation by a laser field. We show how phonons allow carrier relaxation and how the Kerr signal and total magnetisation are affected at different temperatures, with the latter exhibiting a non-monotonic behaviour as the temperature increases.

*Fonds de la Recherche Scientifique - FNRS

1:15PM L22.00009: Ab Initio Electronic $T_1$ Spin Relaxation Times in Silicon and Diamond  JINSOO PARK (Presenter), JINJIAN ZHOU, MARCO BERNARDI, Applied Physics and Materials Science, California Institute of Technology — Spin relaxation in inversion-symmetric crystals primarily occurs through the Elliott-Yafet mechanism, in which the injected spins are scattered by impurities at low temperatures and phonons at higher temperatures. We present an efficient first-principles approach for computing the phonon-limited Elliott-Yafet electronic spin relaxation time $T_1$ in materials ranging from metals to semiconductors and insulators. Our scheme combines fully-relativistic ab initio electron-phonon scattering with a novel approach to correctly treat Kramers degenerate electronic states. Application of our approach to silicon and diamond is discussed in this talk, where we analyze the temperature dependence of the spin relaxation times together with the contributions from intravalley and intervalley processes. The computed spin relaxation times in silicon are in excellent agreement with experiment above 50 K. Our work enables accurate ab initio calculations of the $T_1$ spin relaxation time in a range of materials, including topological ones, providing new microscopic insight into spin relaxation.

1:27PM L22.00010: Quantum-kinetic theory for electron-diffusion and phonon-drag thermoelectric powers from drifting electrons in a quantum wire* RICHARD ZHANG (Presenter), Department of Mechanical & Energy Engineering, University of North Texas, DANHONG HUANG, Space Vehicles Directorate, Kirtland AFB, Air Force Research Laboratory — Thermal conditions during an ultrafast femtosecond-scale laser pulse are difficult to resolve due to phonon vibration drag behind an electron excitation. The motivation behind this study is to establish a ground-up quantum dynamics model to predict elastic wave effects in a confined electron-phonon state. We established transient collision equations from three-phonon coupled anharmonic interactions to obtain the evolution of hot phonon species distribution and thermoelectric response in a confined-size semiconductor material, such as a GaAs nanowire subjected to a spatially uniform DC electric field. A simplified diatomic chain model was chosen to represent longitudinal phonon dispersion. A quasi-steady state was observed in electron-phonon drift-drag response and settling of low frequency phonon-phonon scattering. We also studied the effects from phonon-surface boundary parameters, such as fluctuation strength and interaction length. As new materials with surprising measured transport properties are being found, further development of this unifying theory of carrier-lattice dynamics has potential for capturing ephemeral excitations in various solids.

*US AFOSR, DoD Lab-University Collaborative Initiative (LUCI) Program, and AFRL Summer Faculty Fellowship Program (SFFP).
1:39PM L22.00011: Electron-phonon coupling from ab initio linear-response theory within the GW method: Method and applications to oxide superconductors*  ZHENGLU LI (Presenter), GABRIEL ANTONIUS, MENG WU, FELIPE DA JORNADA, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — We present a first-principles linear-response theory of changes due to perturbations in the quasiparticle self-energy operator within the GW method. This approach, named GW perturbation theory (GWPT), is applied to calculate the electron-phonon (e-ph) interactions with the full inclusion of the GW non-local, energy-dependent self-energy effects, going beyond density-functional perturbation theory. Unlike the frozen-phonon approach, GWPT gives access to e-ph matrix elements at the GW level of all phonons, and the computational cost scales linearly with the number of phonon modes (wavevectors and branches) investigated. We present results of correlation-enhanced superconductivity in Ba$_{0.6}$K$_{0.4}$BiO$_3$ and of e-ph physics in other oxide superconductors where many-electron effects are strong.

*This work was supported by the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) as part of the Computational Materials Sciences Program and by the Theory of Materials Program at the Lawrence Berkeley National Laboratory, both funded by the U.S. Department of Energy, Office of Basic Energy Sciences under Contract No. DE-AC02-05CH11231, and by the National Science Foundation under Grant No. DMR-1508412. Computational resources have been provided by NERSC and XSEDE.

1:51PM L22.00012: First-principles study of electron-phonon interactions in SrTiO3*  NIKOLAUS KANDOLF (Presenter), CARLA VERDI, FELICIANO GIUSTINO, Department of Materials, University of Oxford — The discovery of a two-dimensional electron liquid on the surface of doped SrTiO3 (STO) and the confirmation of high-temperature superconductivity at the FeSe/SrTiO3 interface have attracted considerable interest in the electron-phonon physics of STO. In this work we focus on the polaron satellites observed in the angle-resolved photoelectron spectra of STO, and investigate their origin using the many-body electron-phonon self-energy in the Migdal approximation, augmented with the cumulant expansion formalism. By comparing our first-principles calculations with experiments we investigate the microscopic mechanisms that give rise to the observed polaron satellites.

*Leverhulme Trust (Grant RL-2012-001), UK EPSRC (grant No. EP/M020517/1), Graphene Flagship (Horizon 2020 Grant No. 785219 GrapheneCore2), the University of Oxford ARC facility, PRACE-15 and PRACE-17 resources MareNostrum at BSC, Clarendon Fund

2:03PM L22.00013: Exciton-phonon interactions in organic crystals from first principles many-body perturbation theory*  JONAH HABER (Presenter), Department of Physics, University of California, Berkeley, SIVAN REFAELY-ABRAMSON, Department of Materials and Interfaces, Weizmann Institute of Science, GABRIEL ANTONIUS, Département de Chimie, Biochimie et Physique, Université du Québec à Trois-Rivières, FELIPE DA JORNADA, STEVEN G. LOUIE, JEFFREY B NEATON, Department of Physics, University of California, Berkeley — Molecular crystals are attractive candidates for solar energy conversion applications due to their strong light-matter interactions, nearly endless structural tunability, and the relative inexpense with which they can be synthesized and processed. Acene crystals, such as tetracene and pentacene, possess both strong electron-hole and significant electron-phonon interactions, and a thorough understanding of the photophysics of these materials requires a careful analysis of the interplay between the ionic and excitonic degrees of freedom. In this talk, we present our linear response framework for computing exciton-phonon matrix elements, using ab initio density functional perturbation theory and many-body perturbation theory within the GW plus Bethe-Salpeter equation approach. We apply this method to compute exciton-phonon scattering rates for spin-singlet and spin-triplet excitons in prototypical acene crystals and compare with experimental linewidths. Finally, we discuss the implications of our calculations for exciton diffusion and multiexciton generation in these extended organic systems.

*This work supported by the Department of Energy; computational resources provided by NERSC.
11:15AM L23.00001: Cryogenic Nitrogen-Vacancy Scanning Microscope  URI VOOL, ASSAF HAMO (Presenter), ZIWEI QIU, TONY ZHOU, AMIR YACOBY, Harvard University — The Nitrogen-Vacancy (NV) electron spin is a quantum sensor of magnetic field, with high sensitivity in a wide range of frequencies and extremely high spatial resolution. Most NV magnetometry experiments are performed by stationary NVs in a bulk crystal measuring a nearby sample. This limits the spatial resolution to the optical diffraction limit and strongly limits the sample which can be measured. Recently, a scanning technique was developed to overcome these issues, in which the NV is located on a tip that can be scanned over a sample. In addition, most NV experiments are performed at room temperatures, while many of the unexplored phenomena in condensed matter physics occur at cryogenic temperatures.

Our lab has been working on a setup which aims to address both issues, implementing a cryogenic scanning NV setup. This setup allows us to work in a variable temperature from ~1.7K up to room temperature. In this talk we describe the details of our scanning microscope and its advantages in measuring condensed-matter phenomena, and present preliminary scanning results.

11:27AM L23.00002: Nanoscale CVD Graphene Hall Probes for high resolution Scanning Probe Microscopy* DAVID COLLOMB (Presenter), PENGLEI LI, SIMON BENDING, DANIEL WOLVERSON, University of Bath — Advances in magnetic imaging are one of many improvements in instrumentation which have enabled scientists to pioneer and develop their next big research ideas. One important technique, scanning Hall probe microscopy (SHPM), involves rastering a Hall sensor over a surface to create a magnetic field map across the sample. However, SHPM has typically relied on the low temperature performance of GaAs-based Hall probes, whose figures-of-merit become much worse at room temperature. This tends to exclude SHPM from numerous applications under ambient conditions such as susceptibility for non-destructive evaluation and characterisation of ferromagnetic data storage media. Making use of graphene’s high carrier mobility and facile CVD growth techniques, we have fabricated graphene Hall devices with nanoscale lateral dimensions for sub-100nm spatial resolution imaging while maintaining excellent room temperature minimum detectable fields in the μT/√Hz range. We will illustrate the imaging performance of such probes, including; low frequency noise performance and magnetic sensitivity, for devices with different active areas, carrier densities and drive currents.

*Funding was provided by the Lloyds Register Foundation and the UK EPSRC, with award numbers G0086 and EP/R007160/1 respectively.

11:39AM L23.00003: Near-field correlative nanoscopy accesses physical constants in complex functional materials STEFAN MASTEL (Presenter), TOBIAS GOKUS, ALEXANDER GOVYADINOV, ANDREAS HUBER, Neaspec GmbH — Nanoscale characterization methods play a key role in the analysis, development and optimization of nanoscopic materials and devices. Often several characterization techniques are required to gain a comprehensive understanding of the various material properties of complex functional materials. Here we introduce the combined nanoscale analysis of complex material systems by correlating infrared scattering-type Scanning Near-field Optical Microscopy (s-SNOM) with information obtained by other Scanning Probe Microscopy (SPM) based techniques. For example near-field reflection/absorption imaging at 1500 cm⁻¹ of a only 50 nm thin phase-separated PS/LDPE polymer film allows to selectively highlight the distribution of PS in the blend, while atomic force microscopy modes simultaneously map the mechanical properties like adhesion. Further, results will be presented that correlate the nanoscale near-field optical response of semiconducting samples like SRAM devices in different frequency ranges (mid-IR & THz) to Kelvin Probe Force Microscopy and Electrostatic Force Microscopy measurements. Thus, neaspec s-SNOM systems represent an ideal platform to characterize complex material systems by different near-field optical and SPM-based mechanical and electrical methods at the nanoscale.
11:51AM L23.00004: Magnetic force sensing using a self-assembled GaAs nanowire with a MnAs tip

NICOLA ROSSI (Presenter), BORIS GROSS, University of Basel, FLORIAN DIRNBERGER, DOMINIQUE BOUGEARD, Physics, Universität Regensburg, MARTINO POGGIO, University of Basel — We present a scanning magnetic force sensor based on an individual magnet-tipped GaAs nanowire (NW) grown by molecular beam epitaxy [1]. Its magnetic tip consists of a final segment of single-crystal MnAs formed by sequential crystallization of the liquid Ga catalyst droplet [2]. We characterize the mechanical and magnetic properties of such NWs by measuring their flexural mechanical response in an applied magnetic field [3]. Comparison with numerical simulations allows the identification of their equilibrium magnetization configurations, which in some cases include magnetic vortices. We determine a NW’s performance as a scanning probe [4], by measuring its dynamical response to the magnetic field of a micrometric current-carrying wire. The NWs’ tiny tips and their high force sensitivity make them promising for imaging weak magnetic field patterns on the nanometer-scale, as required for mapping mesoscopic transport and spin textures or in nanometer-scale magnetic resonance.


*Swiss NSF (200020-178863); ERC Starting Grant NWScan (334767); Swiss Nanoscience Institute; Kanton Aargau; NCCR QSIT.

# MICHELLE YOTHERS (Presenter), SOUMYA BHATTACHARYA, LLOYD BUMM, Homer L Dodge Department of Physics and Astronomy, University of Oklahoma — Accurate measurements of structures at the nanoscale are of fundamental importance for nanofabrication. Using alkanethiol self-assembled monolayers (SAMs) as a model system, we demonstrate a way to measure the alkanethiol chain tilt direction from constant-current scanning tunneling microscope (STM) images. These measurements are made with a real-space image post-processing technique that compensates for image distortion using a physical model. Using this measurement, we are also able to establish the chain tilt direction without guest molecules, by using the position uncertainty of molecules about their expected lattice site position. In particular, we will show the direction of maximum position uncertainty is anticorrelated with the alkanethiol chain tilt direction. This anticorrelation is consistent across different STM tips and alkanethiol chain lengths.

*Financial support from the National Science Foundation (CHE-1710102), the Homer L. Dodge Department of Physics, and the OU College of Arts and Sciences, the Carl. T. Bush Fellowship (MPY), and NVIDIA Corporation (donation of a Tesla K-40 GPU) is gratefully acknowledged.

12:15PM L23.00006: A differential photon-rate meter for real-time peak tracking in optically detected magnetic resonance at low photon-count rates

KAPILDEB AMBAL (Presenter), National Institute of Standards and Technology — The optically detected magnetic resonance of the NV− center in diamond provides a mechanism for precise, nanoscale magnetometry. As an alternative to measuring and fitting complete resonance spectra, resonance peak locking and tracking methods provide real-time and continuous measurements of the magnetic field. But the weak photoluminescence from small ensembles of NV− center including single NV− centers poses a problem for peak tracking. The emitted light requires single-photon detection which produces a narrow (≈ 20 ns) voltage pulse per detected photon. The discrete voltage pulses are not amenable for demodulation by regular lockin amplifiers. Here, we address active feedback control and real-time field tracking with photon detection rates in the range of $4 \times 10^3$ s$^{-1}$ to $1 \times 10^6$ s$^{-1}$, which are typical of single NV− centers, and we present a custom differential rate meter with phase sensitive detection. Without compromising signal-to-noise, this real-time data processing scheme provides all the typical functionalities of a lock-in amplifier needed for real-time peak locking and tracking. We demonstrate continuous field measurements at sweep rates exceeding 50 μT/s. This scheme covers a broad magnetic field range, limited by the frequency range of the microwave generator.
The tip shape dependence of the STM-induced luminescence* Songbin Cui (Presenter), Physics, Pohang University of Science and Technology (POSTECH), Ungdon Ham, Caldes, Institute for Basic Science (IBS), Taehwan Kim, Physics, Pohang University of Science and Technology (POSTECH) — Photon signal enhancement due to surface plasmon coupling becomes an important issue in high-resolution microscopy/spectroscopy, such as scanning tunneling microscopy (STM) induced luminescence, surface/tip enhanced Raman spectroscopy, and so on. Such enhancement is significantly varied by modifying the plasmonic nanocavities. The gap-mode plasmonic nanocavity between an STM tip and surface realizes sub-molecular photon spectroscopy. The plasmonic resonant modes are known to be modified by tip indentation. However, the tip shape dependence of the plasmonic nanocavity remains unclear. In this work, we experimentally present the role of tip shape in surface plasmonic light emission. We have used Ag tips and a Ag(100) substrate, and STM-induced photon signals have been measured from the two opposite sides of the STM tip simultaneously. We found that changing small parts of the tip can differ the photon spectrum significantly due to tip shape asymmetry. This finding can help us to tune the plasmonic photon emission spectra more efficiently and give a new insight by using the symmetric or asymmetric STM tip induced luminescence.

*This work was supported by Institute for Basic Science.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L24 DAMOP: Precision spectroscopy of molecules: status and perspectives BCEC 159
- Sergiy Bubin, Nazarbayev University - Tag(s): Focus

11:15AM L24.00001: Precision spectroscopy in few-electron molecules [Invited] Maximilian Beyr, Nicolas Hölisch, Paul Jansen, Luca Semeria, Frederic Merkt (Presenter), ETH Zurich — Few-electron molecules are attractive systems for precision spectroscopy because their properties can be calculated with high accuracy by quantum-chemical methods.\(^1\)\(^2\)\(^3\) The measurements serve to test theoretical predictions, ideally at the level where their accuracy is limited by the uncertainties of the fundamental constants or by unrecognized physical effects. We report on precision measurements of energy intervals in cold samples of H\(_2\) and metastable He\(_2\). In the case of H\(_2\), we determine the ionization energy with a precision (\(\Delta \nu/\nu\)) of 10\(^{-10}\) from high-resolution Rydberg spectra\(^4\)\(^5\) and derive the dissociation energy with an accuracy of 350 kHz, approaching the level where the size of the proton and the uncertainty in the proton-to-electron mass ratio would limit the accuracy of otherwise exact calculations. Comparison will be made to recent theoretical results in the context of a more-than-100-year-long series of experimental and theoretical determinations of the dissociation energy of H\(_2\). In the case of the He\(_2\), we use multistage Zeeman deceleration to prepare slow, cold metastable molecules in selected spin-rotational components of the metastable \(a\) state. We exploit the long transit times of these molecules through microwave and laser fields to measure fine-structure intervals in the \(a\) state, the Rydberg spectrum of He\(_2\), and the energy-level structure of He\(_2^+\).\(^6\)

11:51AM L24.00002: Precision spectroscopy of molecular hydrogen and its ion through molecular Rydberg states and MQDT-assisted extrapolation of Rydberg series  MAXIMILIAN BEYER (Presenter), Department of Physics, Yale University, NICOLAS HOLSCHE, ETH Zurich, CHRISTIAN JUNGEN, Department of Physics and Astronomy, University College London, FREDERIC MERKT, ETH Zurich — H$_2^+$ and H$_2$ are the simplest of all ionic and neutral molecules and as such important systems for the development of molecular quantum mechanics.

The energy-level structure of H$_2^+$ can be calculated extremely precisely and by comparison with the results of precise spectroscopic measurements, fundamental constants or particle properties, such as the proton-to-electron mass ratio or the proton size, may be determined.

Spin-rovibrational intervals in H$_2^+$ are determined with sub-MHz accuracy from high-resolution measurements of Rydberg series of H$_2$ followed by Rydberg-series extrapolation using multichannel quantum defect theory.

For the excitation of Rydberg states, a resonant three-photon excitation scheme was employed, using pulsed VUV and VIS laser sources to reach the intermediate double-well GK state and a continuous-wave near-infrared laser source for the excitation to the Rydberg states. The valence state - Rydberg state intervals could be measured with a relative accuracy of 3E-10 using an optical frequency comb for the frequency calibration of the cw laser and employing a procedure to minimize systematic uncertainties. The measurements were used to determine the spin-rotational intervals of the first three rotational levels of para H$_2^+$ and the fundamental vibrational interval.

12:03PM L24.00003: Geminal-based high-accuracy quantum mechanics for few-body systems*  MARKUS REIHER (Presenter), ETH Zurich — We elaborate on the variational solution of the Schrödinger and Dirac equations of few-body atomic and molecular systems without relying on the Born-Oppenheimer paradigm [1]. The wavefunction is expanded in terms of parameterized explicitly correlated Gaussians with polynomial prefactors. We developed a simple strategy for the elimination of the translational kinetic energy of the total energy carried out in laboratory-fixed Cartesian coordinates [2].

For semi-classical relativistic calculations we devised a kinetic-balance condition for explicitly correlated basis functions [3]. The resulting form of kinetic balance establishes a relation between all spinor components of an N-fermion system to the non-relativistic limit, which is in accordance with modern exact-decoupling methods. In my talk, I will discuss these developments in the light of spectroscopic results.


*Financial support from the Swiss National Science Foundation is gratefully acknowledged.

12:15PM L24.00004: Optical angular momentum induced molecular switching  HAI BI (Presenter), ERIC MAZUR, SEAS, Harvard University — Molecular electronics is a promising route for downscaling electronic devices since organic molecules can play a role in reconfigurable logic operations. The organic molecule can also strongly interact with optical fields provided that the fields are highly concentrated, for instance by the presence of plasmonic nanostructures.

Simultaneously, the plasmonic nanostructures have been demonstrated recently the ability to produce localized angular momentum (LAM), which could further be coupled to a molecular device. By optically transferring angular momentum to a molecular junction, we demonstrate different logic operations. These molecular-scale operations result from the interaction of conducting molecular junction and the plasmonically enhanced electromagnetic field near the tip of the junction. Importantly, this novel investigation of the LAM in the near-field opens the door for characterization of molecular electronics with near-field optical methods.
**12:27PM L24.00005: Positronic beryllium: accurate energies and leading relativistic corrections in the ground and lowest excited states**  
ISTVAN HORNYAK (Presenter), SERGIY BUBIN, Department of Physics, Nazarbayev University, Astana, Kazakhstan — One of the long standing questions of positron physics and chemistry is the existence of electronically stable positron-atom and positron-molecule complexes. From the theoretical and computational viewpoint, reliable identification of states, especially metastable ones, in which a positron can be attached to an atom, is challenging due to very weak binding energies and nontrivial structure of the complexes. A few years ago we predicted the stability against dissociation of an excited P-state of Be. The fact that both the ground and excited states are stable against dissociation in conjunction with their notably different lifetimes opens up an interesting possibility of measuring resonant positron-atom annihilation and providing experimental evidence for the existence of positron-atom complexes. In this work we have undertaken another, more comprehensive study of this system. We have performed considerably more accurate calculations of the binding energies and other relevant properties, such as the electron-positron annihilation rates. In particular, we have computed the leading relativistic corrections and show how they change the tiny binding energies of the ground and first excited states of the $e^+\text{-Be}$ complex.

**12:39PM L24.00006: Precision calculations for four- and five-particle molecular systems**  
EDIT MATYUS (Presenter), Eotvos Lorand University — Solution methods for the few-particle molecular Schrödinger equation are elaborated relying on both the full electron-nucleus Hamiltonian [1] as well as on a perturbative treatment resulting in effective non-adiabatic Hamiltonians for the atomic nuclei [2]. Numerical results are presented for the hydrogen molecule ($\text{H}_2$) and for the helium molecular ion ($\text{He}_2^+$).


*Financial support of the Swiss National Science Foundation through a PROMYS Grant (no. IZ11Z0_166525) is gratefully acknowledged.

**12:51PM L24.00007: Long Baseline Molecular Interferometry**  
YAAKOV FEIN (Presenter), STEFAN GERLICH, PHILIPP GEYER, FILIP KIALKA, LUKAS MAIRHOFER, University of Vienna, KLAUS HORNBERGER, Physics, University of Duisburg-Essen, MARKUS ARNDT, University of Vienna — Interferometry of massive particles can be used to rule out modifications to quantum mechanics [1], test the equivalence principle [2], and measure molecular properties [3].

I present results from the new Long Baseline Universal Matter-wave Interferometer (LUMI) in Vienna. LUMI is a near-field three-grating interferometer with a baseline of two meters. The long baseline makes the experiment compatible with particles beyond 100,000 amu and makes it particularly sensitive for metrology.

LUMI has shown interference and electric deflection of particles ranging from atoms to tailored biomolecules. I will discuss the techniques required to see interference at this scale, such as compensating the Coriolis effect. I will also outline the efforts underway to break the current mass record of matter-wave interferometry [4].


*ERC: PROBIOTIQUS (PN: 320694)
FWF: COLMI (P-30176)
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Counterpropagating light as a means for all-optical phase matching

JEFFERSON MARCIO SANCHES LOPES, Graduate Program in Physics, Federal University of Para, Belem, PA, Brazil — We present novel results on the free base 5,10,15,20-meso-tetrapyridyl-porphyrin (H$_2$TPyP). This molecule presents complex electronic and vibrational properties and in spite of the vast literature reporting the transitions observed in its absorption and fluorescence spectra, a more accurate interpretation has been kept elusive. In particular, we show that the molecule's Q-band is clearly developed into many electronic and vibronic transitions, whose the well-known "four orbital model" finds it difficult to reconcile. Using distinct spectroscopy techniques, we conclude that both $Q_x$- and $Q_y$-bands comprise, in fact, two quasi-degenerated electronic states together with their respective vibronic progressions each. The analysis of the Huang-Rhys factors and complementary time- and polarization-resolved measurements reinforce the need for the proposed Q-band multi features remodeling.

*The authors are grateful to the Professors Waldeci Paraguassu and Sanclayton Moreira, from the Graduate Program in Physics of the Federal University of Para and Prof. Gerard J. Meyer from Department of Chemistry of The University of North Carolina at Chapel Hill, for granting the access to their experimental facilities.

All-optical measurement of molecular spinning dynamics with high-harmonic spectroscopy

PEIXIANG LU (Presenter), LIXIN HE, PENGFEI LAN, Huazhong University of Science and Technology — We demonstrate an all-optical measurement of the spinning dynamics of molecular rotational wave packet (RWP) with an angular high-harmonic spectroscopy. By using a double-pulse excitation scheme, unidirectional rotations (UDR) of the sample molecules are created in experiment. By measuring the time-dependent angular distributions (ADs) of high harmonic generation (HHG), the spatiotemporal evolution of molecular RWP is intuitively visualized. The harmonic ADs also reveal the electronic structure of the sample molecules. Moreover, due to the correlation of HHG and molecular UDR, HHG from the spinning molecules shows obvious nonadiabatic frequency shift at the rotation revivals. The spinning dynamics of molecular RWP can also be revealed from the angle-dependent frequency shift of HHG.

Electronic and Vibrational Anisotropy in Molecular Wavepacket Dynamics

VARUN MAKHIJA (Presenter), Physics and Astronomy, Bowdoin College, ALBERT STOLOW, Physics and Chemistry, University of Ottawa — Resonant excitation of an isolated molecule typically results in an anistropic distribution of molecular axes in the excited state - alignment or orientation of the molecules in the laboratory frame. Femto- or attosecond laser pulses with broad enough bandwidths can potentially excite several electronic and vibrational states in a molecule. By appropriately coupling the angular momentum of these states, we find that an evolving anisotropy (alignment or orientation) develops in the electronic and vibrational probability distributions, in addition to axis alignment. The evolution of the electronic and vibrational alignment is synchronized with vibronic dynamics occurring in the molecular frame, and can be orders of magnitude faster than molecular rotation. This anisotropy can in principal be measured by time and angle resolved scattering. A measurement of the evolving electronic anisotropy in resonantly excited ammonia by time and angle resolved photoelectron spectroscopy confirms the theoretical analysis.
Solving the Helmholtz equation in a fiber with a small axial refractive index variation.* AMALIA SANABRIA (Presenter), PABLO BIANUCCI, Physics, Concordia University — Optical dielectric resonators supporting Whispering Gallery Mode (WGM) represent a class of cavity devices with exceptional properties, like small mode volume, very high power density, and very narrow spectral linewidth [1]. These properties have made them a well-established platform for highly sensitive physical, chemical, and biological sensors [2]. They exist in several geometric structures like cylindrical optical fibers and microspheres, which are the simplest and most common. In this paper we analyze the case of a cylindrical microresonator with a small refractive index variation in the axial direction. We solve the Helmholtz equation assuming a parabolic variation of the refractive index, which allows to obtain harmonic oscillator solutions for the axial component. We derive general transcendental equations to obtain the resonance wavevectors for transverse electric (TE) and transverse magnetic (TM) modes.

*We would like to acknowledge support from the National Science and Engineering Research Council (NSERC) of Canada, through the Discovery Grant program (grant 435875-2013); the Department of Physics of Concordia University and the Physics Summer Research Award.

Wednesday, March 6, 2019 11:15 AM - 1:39 PM

Session L26 DQI: Superconducting Qubits: Noise and Decoherence II

11:15AM L26.00001: Correlating decoherence in transmon qubits: Low frequency noise by single fluctuators* STEFFEN SCHLÖR (Presenter), JÜRGEN LISENFELD, Institute of Physics, Karlsruhe Institute of Technology, CLEMENS MÜLLER, Institute for Theoretical Physics, ETH Zürich, ANDRE SCHNEIDER, ALEKSEY USTINOV, Institute of Physics, Karlsruhe Institute of Technology, MARTIN WEIDES, School of Engineering, University of Glasgow — We report on long-term measurements of a high-coherent, non-tunable transmon qubit, revealing low frequency burst noise in coherence and transition frequency. We present a simultaneous measurement of the qubit’s relaxation and dephasing rates as well as resonance frequency fluctuations, and analyze their correlations. These yield information about the microscopic origin of the intrinsic decoherence mechanisms in Josephson qubits and their fluctuation dynamics. From a spectral noise analysis we obtain further evidence for our presented model of a small number of dominant fluctuators.

*This work is supported by Deutsche Forschungsgemeinschaft (DFG) within Project INST 121384/138-1 FUGG and by the European Research Council (ERC) under the Grant Agreement 648011. We acknowledge financial support by the Helmholtz International Research School for Teratronics.

11:27AM L26.00002: Correlation of Lifetime Fluctuations in Superconducting Qubits* DARIO ROSENSTOCK (Presenter), JOSHUA CAREY, CHEN WANG, University of Massachusetts Amherst — While the energy relaxation times (T1) of superconducting qubits have improved greatly since the birth of the field, much work remains to better understand the limitations on lifetimes and how best to extend them. It is widely observed that qubits exhibit time-dependent fluctuations of their T1 times, but the main sources of this process remain a mystery. Among the leading candidates are spurious resonant two-level systems in the dielectric surrounding the device, which are frequency-specific, and excess quasiparticles near the junction, which are not. We monitor the T1 fluctuations for the first two excited states of 3D flux-tunable transmon and fluxonium qubits and examine correlations between the decay rates. We measure T1 of the |e> state at a flux bias such that the |g> - |e> transition frequency matches that of the unbiased |e> - |f> transition. This allows us to resolve frequency dependence of the T1 fluctuations. We believe this is a helpful general tool to distinguish between the effects of dielectric and quasiparticle loss across a range of devices.

*This research is sponsored by the US Army Research Office and US Air Force Office of Scientific Research.
Cross-correlation noise measurements of a graphene-based SQUID magnetometer

JONATHAN PRANCE (Presenter), MICHAEL THOMPSON, RICHARD HALEY, YURI PASHKIN, Department of Physics, Lancaster University, MOSHE BEN SHALOM, VLADIMIR FALKO, School of Physics and Astronomy, University of Manchester, HARRIET VAN DER VLJET, ANTHONY MATTHEWS, ZIAD MELHEM, Oxford Instruments Nanoscience — Lateral superconductor/graphene structures can be used to make Josephson junctions with low contact resistances and gate-tuneable critical currents [1]. These junctions have the potential to provide new functionality for superconducting devices. For most devices, e.g. transmon qubits and SQUID sensors [2], it is important to quantify the intrinsic noise of the junctions. The voltage noise of low resistance junctions is typically below the noise floor of room temperature amplifiers. By cross-correlating the signals from two parallel amplifiers, we can detect signals down to ~100 pV/√Hz, well below the noise floor of each amplifier.

Using this technique, we characterise the voltage noise of a NbTi DC SQUID with graphene junctions in a frequency range from ~Hz to ~kHz. Combined with measurements of the SQUID's gain, we map its sensitivity across a range of operating conditions and find that the best-case sensitivity of the device is similar to traditional low temperature SQUIDs with oxide tunnel junctions.


*This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 785219.

Reducing energy loss at the interface of superconducting devices

IGOR DINIZ, Instituto de Ciências Exatas, Universidade Federal Rural do Rio de Janeiro, Seropédica, Brazil, ROGÉRIO DE SOUSA (Presenter), Dept. of Physics and Astronomy, University of Victoria, BC, Canada — We present a quantum theory of dielectric energy loss due to the interaction of photons, tunneling two level systems (TTLSs), and phonons in superconducting devices. As each TTLS couple to photons and phonons, it induces a photon-phonon interaction that can be described as an effective piezoelectric effect. We show that most energy loss occurs at the interface, with phonon interference playing an important role, leading to several predictions that can be tested in current experiments. Explicit numerical calculations of the loss tangent in devices demonstrates that dielectric energy loss can be reduced by exploiting destructive interference of the phonon radiation emitted from different interfaces.

*We acknowledge support from NSERC (Canada), through its Discovery (RGPIN-2015-03938) and Collaborative Research and Development programs (CRDPJ 478366-14).

Magneto-Electric Coupling of Noise and Loss-Generating Paramagnetic Spins in Superconducting Circuits

KEITH RAY (Presenter), JONATHAN L DUBOIS, VINCENZO LORDI, Lawrence Livermore Natl Lab — Noise and loss in superconducting circuits caused by fluctuating charge and magnetic flux represent significant challenges for the realization of large-scale quantum computing architectures. Previous experimental [Phys. Rev. Applied 6 041001 (2016), Phys. Rev. Lett. 118, 057703 (2017)] and theoretical [PRL 112 017001 (2014)] work has identified O2, OH, and atomic H surface adsorbates as possible sources of flux noise in superconducting circuits. We report here on an extension to our model for the flux noise generated by the dynamics of an ensemble of paramagnetic spins on adsorbed O2 molecules to include electric charge density differences associated with spin flips. This model combines a thermodynamic ensemble generated with Monte Carlo simulations with Landau-Lifshitz-Gilbert equation simulations for the dynamics and is parametrized with vdW-corrected density functional theory calculations. From this model we evaluate the effects of external electric and magnetic fields on the phases of the spin system, its dynamics, and the charge and flux noise generated.

*Prepared by LLNL under Contract DE-AC52-07NA27344
**12:15PM L26.00006: Non-Gaussian Noise Spectroscopy with a Superconducting Qubit**

YOUNGKYU SUNG (Presenter), Research Laboratory of Electronics, Massachusetts Institute of Technology, FELIX BEAUDOIN, LEIGH NORRIS, Department of Physics and Astronomy, Dartmouth College, FEI YAN, Research Laboratory of Electronics, Massachusetts Institute of Technology, DAVID K KIM, MIT Lincoln Laboratory, JACK YANJIE QIU, UWE VON LUEPKE, Research Laboratory of Electronics, Massachusetts Institute of Technology, JONILYN L YODER, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, Research Laboratory of Electronics, Massachusetts Institute of Technology, LORENZA VIOLA, Department of Physics and Astronomy, Dartmouth College, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, WILLIAM D OLIVER, Department of Physics, Massachusetts Institute of Technology — Most quantum control and quantum error-correction protocols assume that the noise causing decoherence is described by Gaussian statistics. However, the Gaussianity assumption breaks down when a qubit is strongly coupled to a sparse environment or has a non-linear response to environmental degrees of freedom. Here, we experimentally validate an open-loop quantum control protocol that reconstructs the higher-order spectrum of injected non-Gaussian phase noise using a superconducting qubit as a noise spectrometer. This first experimental demonstration of non-Gaussian-noise spectroscopy represents a major step toward the goal of demonstrating a complete noise spectral characterization of quantum devices.

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**12:27PM L26.00007: Sources of decoherence in fixed frequency transmon qubits.**

ANDREAS FUHRER (Presenter), MATTHIAS MERGENTHALER, PETER MUELLER, STEPHAN PAREDES, CLEMENS MÜLLER, MARC GANZHORN, STEFAN FILIPP, THILO STOEFERLE, GIAN SALIS, IBM Research - Zurich — Significant advances in the coherence of superconducting qubits were made possible by clever microwave engineering. For the transmon qubit this was mainly the reduction of its charge dispersion by capacitively shunting the Josephson junction, the increased size of its capacitor pads, filtering of the microwave controls and operation at noise insensitive points. More recently, efforts were made to disentangle the contributions of various material interfaces by engineering participation ratios of the electromagnetic field with different geometries of resonators and qubits in order to pinpoint the sources of noise.

We report on our efforts to measure and understand the noise sources that effect high coherence fixed frequency transmon qubits in a bottom loading dilution refrigerator. We study the effect of various shielding and filtering strategies using fast noise spectroscopy techniques. Furthermore, we present coherence data from devices that were cooled in a UHV package with a controlled atmosphere and discuss the effect of surface adsorbates on qubit performance.

**12:39PM L26.00008: TLS induced decoherence instabilities in superconducting qubits**

ANDREAS BENGTSSON (Presenter), JONATHAN BURNETT, MARCO SCIGLIUZZO, DAVID NIEPCE, MARINA KUDRA, PER DELSING, JONAS BYLANDER, Chalmers University of Technology — We study the temporal stability of relaxation and dephasing in superconducting transmon qubits. By collecting statistics during measurements spanning multiple days, we reveal large fluctuations of qubit lifetimes and find that the main cause of T1 fluctuations is interacting parasitic two-level-systems (TLS). Our statistical analysis also provides useful information about dynamics of TLS which could help identify possible microscopic sources of TLS, which still remain elusive. Moreover, interacting TLS also cause capacitance fluctuations, ultimately leading to frequency noise and dephasing of the qubit state. These discoveries are important for manufacturing stable superconducting circuits suitable as a scalable quantum computing platform where drift and fluctuations lead to unnecessary calibration and downtime.

**12:51PM L26.00009: Charge noise, fluxonium, and all that**

ARI M MIZE (Presenter), YARIV YANAY, Laboratory for Physical Sciences — Fluxonium qubits were designed to eliminate charge offsets. We consider the theory of fluxonium qubits and distill crucial features that reduce vulnerability to charge noise. Our observations prompt a new superconducting qubit design with some attractive features.
Simulations of Magnetic Noise in Classical XY and Heisenberg Spin Models

DANIEL MICKELSEN (Presenter), HUI WANG, Department of Physics and Astronomy, University of California, Irvine, CA, United States, ZHE WANG, Department of Physics, Fudan University, Shanghai, China, RUQIAN WU, CLARE C YU, Department of Physics and Astronomy, University of California, Irvine, CA, United States — Superconducting qubits show great promise but continue to be plagued by flux noise. Experiments show that surface spins are the source of this flux noise, and the noise has a power spectral density of the form $1/f^\alpha$ with the noise exponent $\alpha \approx 1$. Experiments also provide evidence for ferromagnetic exchange. We investigate to what extent ferromagnetic exchange is consistent the observed flux noise exponents. With input from density functional theory calculations of magnetic impurities, we present the results of Monte Carlo simulations of the magnetic noise produced by coupled classical XY and Heisenberg spins in 2D lattices. We find the parameters of the models that result in a noise exponent near 1.

Experimental study of flux noise in nanowire transmons subject to an applied magnetic field

THIJS STAVenga (Presenter), FLORIAN LUTHI, JOEP ASSENDELFT, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, DAVID THOEN, AKIRA ENDO, Department of Microelectronics and Kavli Institute of Nanoscience, Delft University of Technology, PETER KROGSTRUP, Center for Quantum Devices and Station Q Copenhagen, University of Copenhagen, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Flux noise is generally the dominant dephasing mechanism in transmon qubits using SQUID loops as a tunable inductive element. Continuing experimental research ambitions to elucidate the microscopic origin and mitigation of flux noise. In this work, we experimentally investigate flux noise using an unconventional knob for circuit QED: an applied in-plane magnetic field. We first present various changes introduced to our circuit QED system and setup to further extend the field compatibility of resonators and nanowire transmons beyond 70 mT and to reduce extrinsic noise. Next, we use standard coherence measurements and sensitivity analysis on and off flux sweetspots to investigate the dependence of flux noise on field applied along the axis of the two constituent nanowire junctions.

Measuring Quantum Noise Limits in Superconducting Digital Circuits

AARON LEE (Presenter), MICAH STOUTMORe, JOHN X PRZYBYSZ, AARON PESETSKi, OLIVER OBERG, NATHAN MUNGO, JAMES MEDFORD, LEWIS GRANINGER, Mission Systems, Northrop Grumman — A fundamental question in Josephson junction physics is the temperature at which quantum tunneling becomes the dominant source of junction escape as opposed to thermal excitation. This quantum crossover temperature is important to the design of classical superconducting circuits, as it dictates the minimum error rate that can be achieved for a given junction size. This property has been previously described and measured for over forty years, but the measurement technique is limited to single junctions and not extensible to junctions embedded in a larger circuit. Here we demonstrate a technique for measuring the quantum crossover temperature for a superconducting digital circuit by examining the width of the transition from operation to failure in a basic Reciprocal Quantum Logic digital circuit. This transition width is extracted from the broadband noise generated from the circuit errors and further, disambiguates from spectral noise, such as line noise, that can broaden this transition and artificially increase the crossover temperature. Application of this technique to a medium sized circuit demonstrates that the quantum crossover temperature of a junction embedded in a larger circuit is indistinguishable from the crossover temperature extracted from an isolated junction.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L27 DQI: Quantum Error Correction Theory and Experiment

Tag(s): Focus

Fault-tolerant magic state preparation with flag qubits

CHRISTOPHER CHAMBERLAND (Presenter), ANDREW CROSS, IBM Thomas J. Watson Research center — Despite considerable effort, magic state distillation remains one of the leading candidates to achieve universal fault-tolerant quantum computation. However, when analyzing magic state distillation schemes, it is often assumed that gates belonging to the Clifford group can be implemented perfectly. In many current quantum technologies, two-qubit Clifford gates are amongst the noisiest components of quantum computers. In this talk I will present a new scheme for preparing magic states with very low overhead that uses flag qubits. I will then compare our scheme to leading magic state distillation methods and show that the overhead can be reduced by orders of magnitude.
Error correcting Bacon-Shor code with continuous measurement of non-commuting operators*  JUAN ATALAYA (Presenter), Univ of California - Berkeley, ALEXANDER N. KOROTKOV, Univ of California - Riverside, BIRGITTA K WHALEY, Univ of California - Berkeley — We analyze the nine-qubit Bacon-Shor code (smallest Bacon-Shor code capable of correcting any single-qubit error) with simultaneous continuous measurement of non-commuting gauge operators. Error syndromes are determined by cross-correlations of three measurement signals. During continuous operation of the code, such error syndromes can be monitored via running time averages of the measurement signals with a certain weighting function. We investigate how various parameters of the latter affect the performance of the code operation. We calculate the logical error rates due to environmental decoherence, and compare the performances of the continuous and discrete implementation of the nine-qubit Bacon-Shor code.

* This work is supported by IARPA and ARO grant No. W911NF-17-C-0050.

Quantum Error Correction with the Semion Code  GUILLAUME DAUPHINAIS (Presenter), LAURA ORTIZ, SANTIAGO VARONA, MIGUEL ANGEL MARTIN-DELGADO, Complutense University — We present a full quantum error correcting procedure with the semion code: an off-shell extension of the double semion model. We construct open strings operators that recover the quantum memory from arbitrary errors and closed string operators that implement the basic logical operations for information processing. Physically, the new open string operators provide a detailed microscopic description of the creation of semions at their end points. Remarkably, topological properties of the string operators are determined using fundamental properties of the Hamiltonian, namely the fact that it is composed of commuting local terms squaring to the identity. In all, the semion code is a topological code that, unlike previously studied topological codes, it is of non-CSS type and fits into the stabilizer formalism. This is in sharp contrast with previous attempts yielding non-commutative codes.

Disjointness in quantum error correction: Imposing limitations on logical gates [Invited]  TOMAS JOCHYM-O’CONNOR (Presenter), Caltech, THEODORE YODER, IBM, ALEKSANDER M KUBICA, Perimeter Institute — I will introduce the notion of disjointness for stabilizer codes in quantum error correction and discuss its implications for implementing fault-tolerant logical gates. The disjointness, an algebraic quantity, can be used to characterize which level of the Clifford hierarchy is naturally attainable by simple fault-tolerant logical gates such as constant-depth circuits. While the results are applicable to any stabilizer code, when addressing topological code families one can reproduce known bounds on the level of the hierarchy attainable by constant depth circuits, with the addition that the circuits are unconstrained by geometric locality. For instance, symmetric 2D surface codes cannot have non-local constant depth circuits resulting in non-Clifford logical gates.

Stabilizer Slicing: Coherent Error Cancellations in LDPC Codes*  DRIPTO DEBROY (Presenter), Physics, Duke University, MUYUAN LI, School of Computational Science and Engineering, Georgia Institute of Technology, MICHAEL NEWMAN, KENNETH R BROWN, Physics, Chemistry, and Electrical and Computer Engineering, Duke University — In this paper we propose a scheme to cancel coherent overrotation errors when implementing quantum error correcting codes. These are considered to be among the most damaging errors due to the way they grow rapidly when combined. Due to their unitary nature, these errors have inverse operations and through our technique the errors due to different parts of the circuit create pairs of errors which cancel over the logical subspace. When considering a simplified error model and allowing native 3 qubit gates we can completely eliminate error in the purely coherent case for Surface-17, and show 135-fold improvement at 0.99 unitarity. For an ion trap gate set and only two qubit interactions, we can observe an 89-fold improvement in Bacon-Shor-13. This second implementation takes advantage of the prepared gauge of the code, and is the first implementation to our knowledge in which the state of the gauge affects the robustness of our memory.

*This work was supported by the Office of the Director of National Intelligence - Intelligence Advanced Research Projects Activity through ARO contract W911NF-16-1-0082, the ARO MURI on Modular Quantum Systems W911NF-16-1-0349, National Science Foundation Expeditions in Computing award 1730104, and National Science Foundation Phy-1818914.
Continuous Quantum Error Correction with two-qubit Annealing Hamiltonian*

ARMAN BABAKHANI, HERMAN CHAN, JEFFREY EPSTEIN, SONG ZHANG (Presenter), JUAN ATALAYA, BIRGITTA K WHALEY, Berkeley Quantum Information & Computation Center, University of California, Berkeley — Adiabatic quantum computation (AQC) is expected to be robust against dephasing and control errors. Nevertheless, environmental noise on the qubits can cause transitions out of the ground state. Error suppression and correction techniques are needed to remedy this. Using an open quantum system approach, we study the effects of different noise models such as bit-flip errors and more realistic thermal noise on a two-qubit system evolving under an annealing Hamiltonian. By encoding each logical qubit using stabilizer codes, we develop a continuous error correction scheme based on the weakly measured error syndromes and analyze the efficiency of this protocol with different physical parameters. We compare the effectiveness of such error correction with known error suppression techniques.

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Neural Belief-Propagation Decoders for Quantum Error-Correcting Codes*

YE-HUA LIU (Presenter), DAVID POULIN, University of Sherbrooke, Institut Quantique — Belief-propagation (BP) decoders are responsible for the success of many modern coding schemes. While many classical coding schemes have been generalized to the quantum setting, the corresponding BP decoders are flawed by design in this setting. Inspired by an exact mapping between BP and deep neural networks, we train neural BP decoders for quantum low-density parity-check codes, with a loss function tailored for the quantum setting. Training substantially improves the performance of the original BP decoders. The flexibility and adaptability of the neural BP decoders make them suitable for low-overhead error correction in near-term quantum devices.

*Canada First Research Excellence Fund

Demonstration of Channel-Optimized Quantum Error Correction on Cloud-Based Quantum Computers*

HAIMENG ZHANG (Presenter), HANNES LEIPOLD, University of Southern California, ROBERT KOSUT, SC Solutions, Inc., DANIEL A LIDAR, University of Southern California — With the introduction of several cloud-based quantum computers, for example, from IBM and Rigetti, there is a growing interest in experimenting with quantum algorithms and protocols on such platforms. We are specifically interested in testing quantum error correction protocols since noise is an important factor that limits their performance. We demonstrate the channel-optimized quantum error correction protocol [R.L. Kosut, A. Shabani, and D.A. Lidar, PRL 100, 020502 (2008)] on the IBM and Rigetti machines. Our goal is to protect quantum states from noise. The noise on the IBM machine is characterized by standard process tomography. The optimal encoding and recovery map are found numerically by solving a bi-convex optimization problem which maximizes the average channel fidelity. We implement the optimal encoding and recovery maps by decomposing them into directly implementable gate operations. This error correction protocol does not require post-selection and is designed specifically for the physically relevant noise to the platform.

*This work was supported by Oracle Labs and the Lockheed Martin Corporation, and was made possible thanks to the IBM and Rigetti cloud quantum computing platforms.

Demonstration of fidelity improvement using dynamical decoupling with superconducting qubits*

BIBEK POKHAREL (Presenter), NAMIT ANAND, BENJAMIN FORTMAN, DANIEL A LIDAR, University of Southern California — Quantum computers must be able to function in the presence of decoherence. The simplest strategy for decoherence reduction is dynamical decoupling (DD), which requires no encoding overhead and works by converting quantum gates into decoupling pulses. Here, using the IBM and Rigetti platforms, we demonstrate that the DD method is suitable for implementation in today's relatively noisy and small-scale cloud-based quantum computers. Using DD, we achieve substantial fidelity gains relative to unprotected, free evolution of individual superconducting transmon qubits. To a lesser degree, DD is also capable of protecting entangled two-qubit states. We show that dephasing and spontaneous emission errors are dominant in these systems, and that different DD sequences are capable of mitigating both effects. Unlike previous work demonstrating the use of quantum error correcting codes on the same platforms, we make no use of post-selection and hence report unconditional fidelity improvements against natural decoherence.

*This work was supported by Oracle Labs and the Lockheed Martin Corporation, and was made possible thanks to the IBM and Rigetti cloud quantum computing platforms.
1:27PM L27.00010: A family of subsystem codes with only weight two operators  MILAD MARVIAN (Presenter), Massachusetts Institute of Technology — We introduce a family of subsystem codes with the property that their gauge operators, single qubit logical operators and also the product of any two logical operators of the same type can all be implemented using two-local interactions. We discuss their potential applications in error suppression techniques.

1:39PM L27.00011: Higher-dimensional quantum hypergraph-product codes* WEILEI ZENG, LEONID PRYADKO (Presenter), University of California, Riverside — We describe a family of quantum error-correcting codes which generalize both the quantum hypergraph-product (QHP) codes by Tillich and Zémor, and all families of toric codes on m-dimensional hypercubic lattices. Similar to the former, our codes can have finite rates and power-law distance scaling with bounded-weight stabilizer generators. Similar to the toric codes, our codes form m-complexes $K_m$, with $m \geq 2$. These are defined recursively, with $K_m$ obtained as a tensor product of a complex $K_{m-1}$ with a 1-complex parameterized by a binary matrix. Parameters of the constructed codes are given explicitly in terms of those of binary codes associated with the matrices used in the construction.

*This research was supported in part by the NSF Division of Physics via Grants No. 1416578 and 1820939.

1:51PM L27.00012: Continuous parity measurement and error correction* WILLIAM LIVINGSTON (Presenter), MACHIEL BLOK, JUAN ATALAYA, Univ of California - Berkeley, JING YANG, Univ of Rochester, RAZIEH MOHSENINIA, Chapman University, ANDREW N JORDAN, Univ of Rochester, JUSTIN G. DRESSEL, Chapman University, ALEXANDER N. KOROTKOV, Univ of California - Riverside, IRFAN SIDDIQI, Univ of California - Berkeley — In a multi-qubit system, performing continuous measurements of joint properties such as parity permits the study the quantum dynamics of multipartite state evolution and collapse. By performing simultaneous parity measurements in a three qubit system, we can also observe a single qubit flip in real time, providing the basis for quantum error correction. The parity of two superconducting transmons may be directly measured without qubit ancilla by coupling them to a single readout resonator, using identical dispersive couplings much larger than the resonator bandwidth. Using a chip with three qubits and connecting each pair of two to a parity readout resonator, we implement the two parity measurements needed to perform the conventional three-qubit bit-flip code. We control the qubits from a field programmable gate array while continuously monitoring the parity, allowing for low latency correction pulses to be applied when a qubit flip occurs.

*This work was supported by the Army Research Office.

2:03PM L27.00013: Cellular Automaton Decoder for Topological Codes with Boundaries* MICHAEL VASMER (Presenter), DAN BROWNE, Physics & Astronomy, University College London, ALEKSANDER M KUBICA, Perimeter Institute for Theoretical Physics — Topological codes are some of the most widely-studied examples of quantum error-correcting codes. These codes have desirable properties such as low weight stabiliser generators and high error thresholds. To correct errors using a quantum error-correcting code, we must use a classical algorithm (a decoder) to find a correction operator. Recently, a cellular automaton decoder was proposed for a broad family of topological codes defined on lattices without boundaries. This decoder is a local decoder and does not require multiple rounds of syndrome extraction to deal with measurement errors. In this work, we extend this cellular automaton decoder to topological codes defined on lattices with boundaries and compare its performance to other decoding algorithms.

*This work was supported by the EPSRC (grant number EP/L015242/1).

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L28 DQI: Distributed Quantum Computation, Networking and Information Security I BCEC 161 - Stephanie Wehner, Delft Univ of Tech - Tag(s): Focus
11:15AM L28.00001: Linking trapped-ion quantum nodes* [Invited] TRACY NORTHUP (Presenter), Institute for Experimental Physics, University of Innsbruck — Future quantum networks offer a promising route to quantum-secure communication, distributed quantum computing, and quantum-enhanced sensing. The applications of a given network will depend on the capabilities available at its nodes, which may be as simple as quantum state generation and measurement or as advanced as a universal quantum computer. Here, we focus on quantum nodes based on calcium ions confined in a linear Paul trap, an experimental platform with which high-fidelity state preparation, gate operations, and readout have been demonstrated.

By coupling trapped ions to the mode of an optical resonator, we construct a coherent interface between single ions and single photons. I will present ongoing work to transfer photonic quantum states between two remote trapped-ion systems, highlighting the experimental challenges and identifying the key components for scaling up such links into networks.

*This work was supported by the Army Research Laboratory Cooperative Agreement No. W911NF15-2-0060, the Austrian Science Fund (FWF) Project F4019, and the EU Horizon 2020 Project DLV-820445.

11:51AM L28.00002: Diamond quantum networks for distributed quantum computation TIM HUGO TAMINIAU (Presenter), QuTech and Kavli Institute of Nanoscience, Delft University of Technology — A promising approach for quantum computations is to distribute logical qubits and error correction over a quantum network. This approach is naturally extendable to larger sizes by adding independent modules and enables exploring a large variety of error correction codes over different network topologies, including three-dimensional structures and non-nearest neighbor connections.

The NV center in diamond provides a powerful platform to realize such quantum networks. It combines optical entanglement links [Nature 526, 682, 2015] and long-lived multi-qubit nodes that can store and process quantum information [Nature Comm. 7:11526, 2016; Nature Comm. 9:2552, 2018]. In this talk I will present our recent experimental progress towards quantum networks for distributed quantum computations and argue that we are getting close to the point where imperfections can be overcome by quantum error correction, so that logical qubits encoded over the network become increasingly more stable as the network is made increasingly larger.

12:03PM L28.00003: Distributed Quantum Computing Architectures MARTIN SUCHARA (Presenter), YURI ALEXEEV, JOAQUIN CHUNG MIRANDA, RAJKUMAR KETTIMUTHU, Argonne National Laboratory — Despite dramatic improvements in quantum gate fidelities, coherence times and qubit counts, the capabilities of quantum processors will remain modest in the near future. We compare two approaches that use small unreliable quantum processors to solve large computational problems. The first approach uses hybrid quantum-classical architectures where larger quantum circuits are broken into smaller sub-circuits that are evaluated separately, either using small quantum processors or a quantum simulator running on a classical supercomputer. The second approach leverages quantum networks to teleport shared qubits between quantum processors. We compare the suitability of these techniques for various quantum circuits, describe optimizations that enable mapping quantum circuits into sub-circuits, and compare the hardware requirements of the two approaches.

12:15PM L28.00004: Numerical finite-key analysis of quantum key distribution* DARIUS BUNANDAR (Presenter), DIRK R. ENGLUND, Massachusetts Institute of Technology — Quantum key distribution (QKD) is still the only quantum-resistant method of sending secret information at a distance. However, accurate theoretical analysis of QKD that accounts for device imperfections is usually challenging. To circumvent this problem, we have developed an efficient numerical approach to calculate the secret key rates of any QKD protocol. Our approach takes only a brief description of the protocol and the measurement results as inputs. The method outputs the secret key rates by solving a semidefinite program which includes not only practical device imperfections but also statistical fluctuations typically observed in QKD experiments.

*This work is supported by the Air Force Office of Scientific Research and the Office of Naval Research.
Distributed Routing in a Quantum Internet

The aim of Quantum Internet is to enable the transmission of qubits between distant quantum devices, in order to achieve tasks that are impossible using classical information. Due to the losses in communication channel, routers are necessary for long distance quantum communication. In such a network, two distant parties share entanglement using the repeaters and transmit qubits using teleportation. However, due to the technological limitation, establishing long distance entanglement takes time and it increases waiting time. This raises the question whether an advantage can be achieved by distributing entanglement ahead of time. In this article we study distribution of entanglement in advance in a network vs producing it on demand. Here we model this problem as a distributed routing in an undirected simple graph. The nodes and edges in the graph denote the routers and communication links. To share an entangled state, two nodes first find a path in the graph and then use the pre-shared entanglement to perform entanglement swapping along that path. To find a path in the graph we use greedy location based routing algorithms. We have done a comparative study of the waiting time for all of the models.

Quantum Network Simulations

Network simulations are extensively used in the design, operation, and evolution of large-scale classical networks. We expect that simulations will also play a significant role in developing and evolving quantum networks. Our work focuses on developing quantum network simulators at various network layers ranging from the physical layer to applications. We envision the need for three simulators. The lowest-layer simulator allows us to study the physics of optical networks; an intermediate-layer simulator studies quantum networking protocols and the classical control network; and the highest-layer one simulates behavior of distributed quantum systems. The lowest-layer simulator uses Monte Carlo methods to evaluate the effects of Pauli errors and investigate the effectiveness of entanglement purification or error correction in the presence of realistic noise. The intermediate-layer simulator uses traditional techniques such as discrete event simulation to investigate scalability of network topologies and ability to communicate between arbitrary pairs of network nodes. Finally, the highest-layer simulator emulates both quantum computing and quantum networking by using HPC. It can be used for testing and developing new distributed quantum algorithms and applications.

Anonymous transmission in a noisy quantum network using the W state

We consider the task of anonymously transmitting a quantum message in a network. In this task, we are concerned with hiding the identities of the sender and receiver of the message from other nodes of the network. We present a protocol that accomplishes this task using the W state. We analyze its performance in a quantum network where common forms of noise are present, and then compare the performance of our protocol with some of the existing protocols developed for the task of anonymous transmission. We show that, in many regimes, our protocol tolerates more noise and achieves higher fidelities of the transmitted quantum message than the other ones. Furthermore, we demonstrate that our protocol tolerates one non-responsive node, as opposed to other considered protocols. Finally, we prove the security of our protocol in a semi-active adversary scenario, i.e. when the adversary is active and the source of a quantum state is trusted.

Anonymous transmission in a noisy quantum network using the W state

*This work was supported by STW Netherlands, NWO VIDI grant, ERC Starting grant and NWO Zwaartekracht QSC.

Towards a multi-node network with NV centres in diamond

Quantum networks are expected to deliver definitive security for communication, blind quantum computation, improved clock synchronization and more exotic applications such as connecting far apart telescopes. A node of such a network must be capable of running small quantum computations, storing quantum information in memory qubits and generate entanglement with neighbouring nodes.

The nitrogen-vacancy (NV) in diamond is a strong candidate to act as node, as it combines all the mentioned requirements in a solid-state system. Deterministic generation of entanglement between two distant NV centres has been recently shown by our group.

We present our recent progress on the ongoing effort to generate genuine multipartite entanglement between three distant NV centres, as we overcome the obstacles to move beyond two node networks.
Impact of qubit connectivity on quantum algorithm performance

Adam Holmes, Sonika Johri, Gian Giacomo Guerreschi, Jim Clarke, Anne Matsuura (Presenter), Intel — Quantum computing hardware is undergoing rapid development from proof-of-principle devices to scalable machines that could eventually challenge classical supercomputers on specific tasks. On platforms with local connectivity, the transition from one-to-two-dimensional arrays of qubits is seen as a natural technological step to increase the density of computing power and to reduce the routing cost of limited connectivity. Here we map and schedule representative algorithmic workloads - the Quantum Fourier Transform (QFT) relevant to factoring, the Grover diffusion operator relevant to quantum search, and Jordan-Wigner parity rotations relevant to simulations of quantum chemistry and materials science - to qubit arrays with varying connectivity. In particular we investigate the impact of restricting the ideal all-to-all connectivity to a square grid, a ladder and a linear array of qubits. Our schedule for the QFT on a ladder results in running time close to that of a system with all-to-all connectivity. Our results suggest that some common quantum algorithm primitives can be optimized to have execution times on systems with limited connectivities, such as a ladder and linear array, that are competitive with systems that have all-to-all connectivity.

Time-bin and Polarization Superdense Teleportation for Space Applications*

Joseph Chapman (Presenter), University of Illinois at Urbana-Champaign, Trent Graham, Univ of Wisconsin, Madison, Christopher Zeitler, Paul G Kwiat, University of Illinois at Urbana-Champaign —

To build a global quantum communication network, low-transmission, fiber-based communication channels can be supplemented by using a free-space channel between a satellite and a ground station on Earth. We have constructed a system that generates hyperentangled photonic "ququarts" and measures them to execute multiple quantum communication protocols of interest. We have successfully executed and characterized superdense teleportation---our measurements show an average fidelity of 0.94±0.02, with a phase resolution under 7° allowing reliable transmission of >10^5 distinguishable quantum states. Additionally, we have demonstrated the ability to compensate for the Doppler shift, which would otherwise prevent sending time-bin encoded states from a rapidly moving satellite, thus allowing the low-error execution of phase-sensitive protocols during an orbital pass.

* This work was primarily supported by NASA Grant No. NNX13AP35A and NASA Grant No. NNX16AM26G. This work was also supported by a DoD, Air Force Office of Scientific Research, National Defense Science and Engineering Graduate Fellowship (NDSEG).

Simulation of a 1025-node quantum repeater chain of NV centres with NetSquid, a new discrete-event quantum-network simulator

Tim Coopmans (Presenter), Axel Dahlberg, Matthew Skrzypczyk, Filip Rozpedek, Roeland Ter Hoeven, Leon Wubben, Delft University of Technology, Rob Knegjens, Julio de Oliveira Filho, Netherlands Organization for Applied Scientific Research (TNO), David Elkouss, Stephanie Wehner, Delft University of Technology — We simulate quantum repeater chains of up to 1025 nodes holding nitrogen-vacancy (NV) centres as quantum processors. We model qubit decoherence, timing and fidelity of both gates and readout according to experimental data. The model also incorporates scheduling operations on the quantum state as imposed by the physics of NV centres. For example, the presence of a single communication qubit, the electron spin, only allows for entanglement generation with one remote node simultaneously. As a consequence of the accurate modelling, the numerical results indicate directions for future hardware development. In particular, we analyse the sensitivity of hardware parameters on the performance of the entire repeater chain. We also perform optimisation over several parameters and configurations, such as the number of NV centres in a single node and the scheduling for entanglement purification steps.

For these simulations, we have developed a generic quantum-network discrete-event simulator called NetSquid, which is capable of simulating decoherence together with imperfect quantum-state operations and stochastic feedback loops.
11:15AM L29.00001: Fast Parametric Gates with Superconducting Qubits  
X. Y. JIN (Presenter), SHLOMI KOTLER, KATARINA CICAK, FLORENT LECOCQ, JOHN TEUFEL, JOSE AUGMENTADO, RAYMOND SIMMONDS, National Institute of Standards and Technology Boulder — We discuss a system with two transmon qubits coupled parametrically through a shared dc-SQUID coupler. The coupling can be tuned from nominally zero to up to more than 100 MHz. This coupling mechanism can be used to perform a two-qubit controlled Z-gate. We present the latest experiment results on the gate operation.

WEN-LONG MA (Presenter), KYUNGJOO NOH, PHILIP REINHOLD, SERGE ROSENBLUM, STEVEN GIRVIN, ROBERT J SCHOELKOPF, LIANG JIANG, Department of Applied Physics and Physics, Yale University — In circuit quantum electrodynamics (QED), it has been demonstrated that universal control of the cavity states can be realized by quantum control of a transmon coupled to the cavity in the strongly dispersive regime. An important class of quantum gates are the selective number-dependent arbitrary phase (SNAP) gates, which impart arbitrary phases to the different Fock states of the cavity by cyclically driving the transmon. However, the SNAP gate fidelity is limited by the transmon relaxation and dephasing. Here we show that by using a multi-level transmon and conditional evolution on the transmon state after the gate, the SNAP gate can be made fault-tolerant to the dominant transmon relaxation and dephasing errors. The simulations show that the SNAP gate infidelity can be reduced compared to that of non-fault-tolerant SNAP gate. The fault-tolerant SNAP gates combined with the displacement operations on the cavity can realize fault-tolerant quantum computation in circuit QED.

11:39AM L29.00003: High-fidelity conditional two-qubit swapping gate using tunable ancillas*  
NIELS JAKOB LOFT (Presenter), Aarhus University, MORTEN KJÆRGÅRD, Massachusetts Institute of Technology, LASSE BJØRN KRISTENSEN, Aarhus University, CHRISTIAN KRAGLUND ANDERSEN, ETH Zürich, THORVALD W LARSEN, Niels Bohr Institute, Univ of Copenhagen, SIMON GUSTAVSSON, WILLIAM D OLIVER, Massachusetts Institute of Technology, NIKOLAJ T ZINNER, Aarhus University — Scalable quantum computing relies crucially on high-fidelity entangling operations. Here we demonstrate that four coupled qubits can operate as a high-fidelity two-qubit entangling gate that swaps two target qubits and adds a relative sign on the $|11\rangle$ state (ZSWAP). The gate operation is controlled by the state of two ancilla (control) qubits. The system is readily implementable with superconducting qubits, using capacitively coupled qubits arranged in a diamond-shaped architecture. By using realistic device and noise parameters from state-of-the-art superconducting qubits, we show that the conditional ZSWAP operation can be implemented with a fidelity above 0.99 in a time of about 65 ns.

*This work was supported by U.S. Army Research Office Grant No. W911NF-17-S-0008, The Carlsberg Foundation, The Danish National Research Council under the Sapere Aude program, and Microsoft.

11:51AM L29.00004: Implementation of a Walsh-Hadamard gate in a superconducting qutrit*  
MUHAMMET ALI YURTALAN (Presenter), Institute for Quantum Computing, Department of Electrical and Computer Engineering, and Waterloo Institute for Nanotechnology, University of Waterloo, JIAHAO SHI, ADRIAN LUPASCU, Institute for Quantum Computing, Department of Physics and Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo, SAHEL ASHHAB, Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Qatar Foundation, Qatar — We present the experimental demonstration of a generalized Walsh-Hadamard gate, which is a Quantum Fourier Transform gate, for a qutrit embedded in the lowest three energy levels of a superconducting circuit. This circuit is a three Josephson junction flux qubit in which all three junctions are shunted by large coplanar capacitors. We use a decomposition of the quantum gate into two unitary operations, one implemented by an off-diagonal Hamiltonian and the other implemented by a diagonal Hamiltonian. The off-diagonal Hamiltonian is obtained by the simultaneous driving of the transitions between levels 0-1, 1-2, and 0-2, with the latter being a two-photon process. The diagonal Hamiltonian is effectively implemented by appropriately shifting the phases of the driving fields. We find that multi-level ac-Stark shifts play an important role in the dynamics, and we adjust the pulse parameters to correct for these shifts. The gate is characterized using tomography of the generated output states corresponding to a set of input states. The average fidelity exceeds 90%, in good agreement with numerical simulations that take into account the multi-level structure of the system.

*This work was supported by NSERC, CMC Microsystems, and the Joint Waterloo-Technion Cooperation Program
12:03PM L29.00005: Microwave-based CPHASE gates for transmon qubits*  GEORGE BARRON (Presenter), FERNANDO CALDERON-VARGAS, SOPHIA ECONOMOU, Department of Physics, Virginia Tech — Superconducting transmon qubits are of great interest for quantum simulation of quantum chemistry. A key component of these algorithms is breaking up the evolution into small steps, which naturally leads to the need for non-maximally entangling, arbitrary CPHASE gates. Here we design such microwave-based gates using an analytically solvable approach leading to smooth, simple pulses. Our protocol allows for the continuous tuning of the phase. We find CPHASE fidelities of more than 0.999 and typical gate times less than 100ns.

*This research is supported by the Department of Energy, Advanced Scientific Computing Research Quantum Testbed Pathfinder Program under FWP ERKJ332.

12:15PM L29.00006: Limitations and improvements of two qubit gates in superconducting circuit QED*  RAVI NAIK (Presenter), BRADLEY MITCHELL, UNPIL BAEK, DAR DAHLEN, JOHN MARK KREIKEBAUM, VINAY RAMASESH, MACHIEL BLOK, IRFAN SIDDIQI, Physics, Univ of California – Berkeley — Remarkable progress has been made towards creating and operating processors for quantum computation and simulation with superconducting circuits, with respect to qubit count and coherence time. This has allowed for the implementation of a variety of quantum algorithms on small quantum processors, with promising results thus far. However, significant limitations on the fidelity of multi-qubit entangling gates remain, placing constraints on the scalability of current processors with respect to algorithmic circuit depth. We explore the sources of errors in these gates, include designs with employ cross-resonance and parametric interactions, and attempt to correct and/or mitigate the errors with hardware improvements, control sophistication, and algorithmic error suppression.

*This work was supported by the Army Research Office.

12:27PM L29.00007: Novel Two-qubit Gate Through Raman-type Transition  BAPTISTE ROYER (Presenter), Universite de Sherbrooke, SEBASTIAN KRINNER, PHILIPP KURPIERS, PAUL MAGNARD, ANDREAS WALLRAFF, ETH Zürich, ALEXANDRE BLAIS, Universite de Sherbrooke — Two-qubit gates are essential for quantum computing. Presently, the low fidelity of these operations is a major factor limiting the physical implementation of long quantum algorithms. In this talk, we propose an entangling gate for directly coupled superconducting qubits based on a Raman-type transition and numerically show that it is fast and high fidelity. This gate is all-microwave and does not require additional hardware compared to standard cQED experiments.

12:39PM L29.00008: Operation and error budget of the Cross-Resonance gate*  VINAY TRIPATHI (Presenter), University of California, Riverside, MOSTAFA KHEZRI, University of Southern California, ALEXANDER N. KOROTKOV, University of California, Riverside — We analyze operation of the Cross-Resonance (CR) gate, in which control qubit is driven at the frequency of target qubit to realize the CNOT gate after additional single-qubit rotations. Numerical simulations for multi-level transmons and particular pulse shapes are used to find the CNOT time and parameters of single-qubit rotations as functions of the drive amplitude $\epsilon$. To understand these dependences, including saturation of the CNOT time at large $\epsilon$, we develop analytical and semi-analytical theories, which agree well with the numerics. We also calculate intrinsic infidelity of the CR gate as a function of $\epsilon$ and find a minimum, created by the interplay between leakage and imperfect unitary evolution. The error budget of the CR gate can be approximately described analytically or semi-analytically.

*This work was supported by ARO grant No. W911NF-18-1-0178.

12:51PM L29.00009: DEMUXYZ Gate Using Single Microwave Drive Line for Multiple Qubits*  CAROLYN EARNEST (Presenter), JEREMY BEJANIN, EVAN PETERS, MATTEO MARIANTONI, Physics & IQC, University of Waterloo — Superconducting qubits have the potential to lead to large-scale quantum computers with $10^5$ or more qubits in 2D arrays. As the number of qubits increases, finding methods to connect all the necessary control lines to each qubit can become a serious challenge. In this talk, we introduce a new one-qubit gate: DEMUXYZ. This gate makes it possible to decrease the number of microwave control lines from $N^2$ to 1 by allowing multiple qubits to share a single microwave line. The shared line carries a continuous wave (CW) microwave tone, which is initially detuned from the qubits' idle frequency. When a qubit must undergo an arbitrary rotation on the Bloch sphere, the qubit is tuned on resonance with the CW tone and allowed to interact with the drive for the duration required to achieve the desired rotation. The rotation phase is tuned by detuning the qubit frequency away from the drive and idle frequency for the required time length. We demonstrate a first proof of concept for this gate performing experiments on two Xmon transmon qubits.

*This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund (CFREF) and the Discovery and Research Tools and Instruments Grant Programs of the Natural Sciences and Engineering Research Council of Canada (NSERC).
1:03PM L29.00010: Realistic simulations of flux-pulse-based controlled-phase gates in superconducting qubits*  
FRANCESCO BATTISTEL (Presenter), QuTech, Delft University of Technology, MICHEL ADRIAAN ROL, FILIP K MALINOWSKI, BRIAN M TARASINSKI, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, BARBARA TERHAL, QuTech, Delft University of Technology — We study the performance of the controlled-phase gate in flux-pulsed transmons by running extensive numerical simulations. We include thermal relaxation, dephasing due to fast and quasi-static components of the noise, leakage, and pulse-shape distortions, validating our model with experimental data. We first consider the conventional Geller-Martinis pulse and find that the leakage strongly depends on the dephasing times and that there is an optimal tradeoff between fidelity, leakage and pulse length. Also, we show that state-of-the-art distortion correction techniques can sufficiently reduce pulse distortions so that they are not a limiting factor. Finally, we compare the Geller-Martinis pulse with a novel double-sided pulse that we call net-zero, which has a built-in echo effect. We find better performance for net-zero than for the conventional pulse with respect to the same noise parameters.  
*This research is supported by ERC grant EQEC No. 682726 and IARPA (U.S. Army Research Office grant W911NF-16-1-0071).

1:15PM L29.00011: Toward a Universal Gate Set on a Qubit Encoded in Superconducting Cavities*  
JACOB CURTIS (Presenter), BRIAN J LESTER, CHRISTOPHER WANG, YVONNE GAO, YAXING ZHANG, LUIGI FRUNZIO, MICHEL H. DEVORET, LIANG JIANG, STEVEN GIRVIN, ROBERT J SCHOELKOPF, Yale Univ — Superconducting microwave cavities coupled to transmon ancillae are an attractive platform for the storage and manipulation of continuous variable (CV) quantum states. Each cavity is a bosonic mode that provides a long coherence time and a large Hilbert space that can be used to redundantly encode quantum information. The coupled transmon ancilla enables nearly arbitrary control over the state of each mode and can be used to perform high quality quantum nondemolition (QND) measurements of the cavity state. Further, it has been demonstrated that the nonlinearity of these ancilla transmons can be driven to enact parametric operations on the system, such as a bilinear coupling between two modes (Gao, et al., PRX 2018). Performing these operations with high fidelity requires mitigating dephasing effects arising from intrinsic properties of the transmon-cavity system as well as external drives. Here, we present our experimental progress towards mitigating these effects and enabling successive, high-fidelity pumped operations on states stored in these cavities.  
*We acknowledge support from the ARO (W911NF-14-1-0011) and AFOSR (FA9550-15-1-0015); BJL from Yale QIMP Fellowship; SMG from NSF (DMR-1609326); LJ from the Sloan (BR 2013- 049) and the Packard Foundations (2013-39273).

1:27PM L29.00012: Two-Qubit Gates with Fluxonium Circuits.*  
YINQI CHEN (Presenter), KONSTANTIN NESTEROV, University of Wisconsin - Madison, IVAN PECHENIZHSKIY, University of Maryland - College Park, ZHENYI QI, University of Wisconsin - Madison, LONG NGUYEN, YEN-HSIANG LIN, AARON SOMOROFF, RAY MENCIA, VLADIMIR MANUCHARYAN, University of Maryland - College Park, MAXIM VAVILOV, University of Wisconsin - Madison — Among superconducting qubits, the fluxonium offers a unique advantage of the possibility to use different transitions for memory storage and gate realizations [1]. In this talk, we discuss various ways to make entangling gates between fluxoniums using noncomputational levels of the two-qubit system. In one example, a controlled-Z gate is activated by driving a transition leading out of the computational subspace while two qubits are kept at fixed frequencies at their sweet spots [2]. The second example is based on adiabatic tuning of one or both of the qubits away from their sweet spots towards the avoided level crossing between a computational and noncomputational levels [3]. One more possible gate is mediated through a common resonator mode. We compare all the techniques and discuss their advantages and limitations.  
*We acknowledge funding from the U.S. Army Research Office (Grant No. W911NF-18-1-0146).
Superadiabatic Stimulated Raman adiabatic passage in a three-level transmon* ANTTI VEPSÄLÄINEN (Presenter), SERGEY DANILIN, SORIN PARAOANU, Department of Applied Physics, Aalto University — Quantum control by adiabatic pulses presents the advantage of robustness under errors in the control parameters, yet it is inherently slow. Here I present an implementation of the superadiabatic protocol in a three-level system realized with a transmon superconducting circuit, where an additional control pulse is used to cancel the non-adiabatic evolution of the system. This enables the transfer of population from the ground state to the second excited state by stimulated Raman adiabatic passage in only a few tens of nanoseconds, approaching the quantum speed limit. As a bridge between adiabatic and direct methods, superadiabatic concept allows a continuous interpolation between the speed and robustness of the population transfer. As a result, it is possible to choose an optimal protocol speed that meets the given robustness criteria. This is particularly important in the field of circuit quantum electrodynamics, where the acceptable duration of the protocol is limited by the coherence time. Additionally, combination of two superadiabatic passages can be used to form a robust rotation gate in the \(|0\rangle - |2\rangle\) subspace.

*We acknowledge financial support from Väisälä Foundation and the Academy of Finland.

Realization of two-qubit gates with tunable couplers in superconducting circuits* MICHELE COLLODO, JOHANNES HERRMANN, ANTS REMM, JEAN-CLAUDE BESSE, CHRISTIAN KRAGLUND ANDERSEN, SEBASTIAN KRINNER, ANDREAS WALLRAFF, CHRISTOPHER EICHLER (Presenter), ETH Zurich — The realization of two-qubit gates with high fidelity and low crosstalk is a key requirement for the scale-up of quantum processors based on superconducting circuits. Two-qubit gates are typically based on either microwave-controlled interactions or on the in-situ tunability of qubit frequencies. Alternative approaches using tunable coupling elements have also been investigated more recently. Here, we report on the design and implementation of a flux-tunable coupler, featuring small residual qubit-qubit interactions when gates are idle. We study gate operations based on both fast DC flux control and parametric flux modulation.

*We acknowledge support by the US ARO grant W911NF-16-1-0071 and by NCCR QSIT.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L30 GMED: Novel Acquisition Geometries, Radiation Sources, Hardware, and Algorithms for Medical Imaging

The potential of stationary digital tomosynthesis [Invited] EMILIO QUAIA (Presenter), Department of Radiology, University of Padova (Italy) — Digital Tomosynthesis (DT) as a limited angle 3D imaging technique has already demonstrated its clinical superiority compared to planar 2D X-ray. Current systems however, are expensive, lack mobility and are often susceptible to motion breath artifacts due to long acquisition times. Innovative solutions to miniaturize and basically reinvent the X-ray source such as cold-cathode field emitters, allow for the creation of compact array of individual addressable emitters in the form of a flat panel source (FPS). The advantages of a device using an FPS compared to conventional X-rays and DT systems include the ability to acquire images from different angles without any physical movement, the option to create small and compact devices that can be used for bedside imaging and faster acquisition times that will likely reduce the number and severity of motion artefacts. These advantages will likely result in several clinical benefits that will also be discussed. Potential concerns will also be discussed such as a reduced stand-off-distance of the source to the detector, large incidence angles of x-rays and low signal-to-noise ratio of the individual frames which can lead to various effects such as magnification, scattering, and Poisson noise.
11:51AM L30.00002: Cellulose-Based Photonic Nanoparticles for Biomedical Imaging* BERNEY PENG (Presenter), MOHAMMAD ALMEQDADI, Tufts University, FABRICE LAROCHE, Boston University, SHAJESH PALANTAVIDA, MAXIM E DOKUKIN, Tufts University, JATIN ROPER, OMER YILMAZ, MIT, HUI FENG, Boston University, IGOR SOKOLOV, Tufts University — Here we present a fluorescent targeting nanoparticle contrast agent that can serve as an effective companion solution for biomedical imaging and diagnostics of cancer. Particles can be used to label intra- and extracellular biomarkers and provide key information for clinical decisions based on high resolution, real-time optical imaging while mitigating off-target immunogenic effects. We utilize cellulose acetate to develop a class of benign, natural, and chemically inert fluorescent nanoparticles possessing well-defined safety profiles. Particles are generated from supramolecular assemblies of cellulose acetate and guest polymers, producing composite materials with good biocompatibility, tunable morphology, physical encapsulation ability, and excellent luminescence. We demonstrate effective in vivo targeting of sub-mm tumors in zebrafish cervical cancer xenografts as well as topical targeting of colon cancer tumors in mice. We expect a topically administered contrast agent can provide great clinical value especially in the realm of colorectal endoscopies.

*NSF CBET 1745530 is acknowledged by I.S. H.F. acknowledges NIH CA215059 and the St. Baldrick's Foundation. F.J.F.L. acknowledges fellowship from Boston University Innovation Center in Nanotechnology for Cancer.

12:03PM L30.00003: Deformable motion correction for interventional cone-beam CT* SARAH CAPOSTAGNO (Presenter), ALEJANDRO SISNIEGA, Department of Biomedical Engineering, Johns Hopkins University School of Medicine, TINA EHTIATI, Siemens Medical Solutions USA, Inc., J. WEBSTER STAYMAN, Department of Biomedical Engineering, Johns Hopkins University School of Medicine, CLIFFORD R WEISS, Department of Radiology, Johns Hopkins University School of Medicine, JEFFREY SIEWERDSEN, Department of Biomedical Engineering, Johns Hopkins University School of Medicine — Cone-beam CT (CBCT) is a valuable tool for guiding interventional procedures, including embolization and ablation of soft-tissue targets. However, long scan times (5-30 s) make CBCT susceptible to artifacts arising from involuntary motion. This work reports a method to estimate deformable motion from scan data without additional patient monitoring. A motion vector field (MVF) is computed that minimizes a gradient entropy objective function for image sharpness. MVFs describing deformable motion were estimated as a spatial interpolation of M rigid motion trajectories, each with temporal motion modeled by an N-point spline. Abrupt changes were penalized via spatial-temporal regularization, and a modified 3D filtered backprojection approach was used for motion-corrected image reconstruction. The method was evaluated in digital simulation, cadaver, and retrospective clinical studies. Sharpness of edges at soft-tissue boundaries improved by 75% (4.4±1.1 to 1.1±0.1 mm), 77% (2.2±0.1 mm to 0.5±0.0 mm), and 33% (0.9±0.1 to 0.6±0.1 mm), respectively. These initial studies demonstrate feasibility of correcting deformable organ motion, which will increase the utility and precision of CBCT guidance.

*NIH grant R01-EB-017226 and academic-industry research collaboration with Siemens Healthineers.

12:15PM L30.00004: Quantitative vs qualitative evaluation of automatic segmentation JENNIFER PURSLEY (Presenter), GENEVIEVE MAQUILAN, GREGORY SHARP, Radiation Oncology, Massachusetts General Hospital and Harvard Medical School — Automatic segmentation of anatomic regions in medical images has the potential to improve treatment efficiency for image-guided interventions. While many algorithms for automatic segmentation have been developed, evaluation of their clinical usability is largely limited to quantitative metrics such as measures of region overlap (Dice coefficient) or surface distance (Hausdorff distance). Quantitative metrics only tell part of the story; an auto-segmented contour of a small organ, such as an optic nerve, may have a low Dice coefficient but still be clinically acceptable, while a large organ, such as a prostate, may have a high Dice coefficient but be clinically unacceptable. The goal of this work is to explore the use of a qualitative evaluation system for rating the clinical acceptability of auto-segmented contours, and establish the relation between quantitative and qualitative metrics. The qualitative system is designed with 5 levels ranging from “clinically acceptable” to “completely unacceptable” and evaluated by multiple expert observers for pelvic and abdominal structures. If correlation between quantitative and qualitative metrics are found, it would establish scientific basis for the use of quantitative metrics in the evaluation of medical image segmentation.
A Statistical Model Relating Image Quality to Image Registration Accuracy in Image-Guided Surgery

**MICHAEL KETCHA** (Presenter), THARINDU DE SILVA, RUNZE HAN, ALI UNERI, Johns Hopkins University, SEBASTIAN VOGT, GERHARD KLEINSZIG, Siemens Healthineers, JEFFREY SIEWERDSEN, Johns Hopkins University — Image-guided procedures often rely on the ability to accurately register (i.e., align the coordinate systems of) a preoperative image and an intraoperative image. While the accuracy of this registration step is generally thought to increase with improved image quality (in x-ray CT, for example, achieved at the cost of higher dose), there is little quantitative understanding of how registration accuracy relates to image quality. We present a statistical model that relates factors of spatial resolution, noise, and dose to image registration accuracy (viz. root-mean-squared error in the transform parameters). We further show how this framework may be extended to model how rigid registration of bone structures is affected by deformation of surrounding soft-tissue structures. The model is tested in comparison to experiments performed over a range of dose and deformation magnitude showing accurate agreement in general trends and prediction of optimal registration similarity metric. A statistical foundation for understanding the effect of image quality and soft-tissue deformation is an important step in physics-based modeling of imaging systems and guiding the development of new systems for image-guided procedures.

*Research was funded by NIH grant R01-EB-017226 and Siemens Healthineers

Neural network-based delineation of clinical target volumes for glioma patients

**NADYA SHUSHARINA** (Presenter), DAVID EDMUNDS, Harvard Medical School, JONAS SÖDERBERG, FREDRIK LOFMAN, Raysearch Laboratories, HELEN SHIH, THOMAS BORTFELD, Harvard Medical School — Outlining the clinical target volume (CTV) in radiotherapy can be time-consuming and error-prone. We propose a convolutional neural network (CNN)-assisted delineation of the CTV for glioma, aiming to reduce inter- and intra-observer variability and decrease treatment planning time. Microscopic disease spread in the brain is restricted by anatomical barriers that are impenetrable by tumor cells. These brain barrier structures were automatically segmented using a 3D CNN trained on 25 datasets of registered planning CT and diagnostic MR images. Satisfactory results were obtained for segmentation of skull, brainstem, corpus callosum, cerebellum, falx cerebri, brain sinuses, tentorium, and ventricles. Segmentation quality was assessed by comparing CNN-derived and manually drawn structures using an independent dataset. The Dice score ranged from 73% to 96% and did not improve after more patients were added to the training dataset. After segmentation, the CTV was generated by expanding the gross tumor volume (GTV) by a fixed radius, excluding voxels contained in other segmented structures. We will compare CNN-derived CTV quality with manually delineated CTVs for a large set of 100 patients.

*NCI/MGH on C06 CA059267
RaySearch AB

Deep Learning Vessel Segmentation for Microsurgical Free Tissue Transfer

**KATHARINA HOEBEL** (Presenter), Harvard-MIT Division of Health Sciences and Technology, BRANISLAV KOLLAR, Plastic Surgery, Brigham and Women's Hospital, KEN CHANG, Harvard-MIT Division of Health Sciences and Technology, ANDREW BEERS, JAMES BROWN, Athinoula A. Martins Center for Biomedical Imaging, JAY PATEL, Harvard-MIT Division of Health Sciences and Technology, BOHDAN POMAHAC, Plastic Surgery, Brigham and Women's Hospital, JAYASHREE KALPATHY-CRAMER, Athinoula A. Martins Center for Biomedical Imaging —

**Introduction:** Free autologous tissue techniques like DIEP (deep inferior epigastric perforator) are regarded as state-of-the-art for patients undergoing breast reconstruction after oncological mastectomy. However, surgeons have to rely on their experience in the identification of the vascular perforators suitable for flap harvest as there exists no standardized approach to this problem.

**Objective:** To develop a deep-learning method to autonomously segment vessels in the abdominal wall of patients undergoing autologous breast reconstruction to guide pre-surgical planning.

**Methods:** Manual segmentation of vessel perforators was performed on abdominal CTAs of 24 patients (20 training, 4 validation) undergoing autologous breast reconstruction at the Brigham and Women's Hospital by an expert rater. A 3D U-net model implemented in DeepNeuro with Keras backend (Beers et al. 2018) was trained to automatically segment vessels in CTAs.

**Results:** Sensitivity and specificity of the trained model was 0.70/0.70 (training/validation) and 0.99/0.98 (training/validation), respectively.

**Conclusion:** The described model can reliably perform automatic vessel segmentation in CTA. We will further evaluate this result for guidance of pre-surgical decision making.

*GPU computing resources: MGH and BWH CCDS.
1:03PM L30.00008: A Deep Learning Approach to Early Cancer Detection using Near-Infrared Laser Scattering Profiles

MASON ACREE (Presenter), CHRISTOPHER BERNEAU, PORTIA DENSLEY, GUNNAR JENSEN, VERN HART, Utah Valley University — In the early stages of most cancers, before lesions are visible on a CT or MRI, changes begin to occur at the cellular level as nuclei elongate and mitochondria cluster unevenly. As these organelles are responsible for much (>40%) of the optical scattering which occurs in a cell, changes in cell morphology and structure can largely affect the resulting optical signature. Variations in the physical properties of different cancer types leads to a distinct scattering profile unique to each disease. In this study, optical scattering patterns were investigated from five different cancer cell lines, which were irradiated in vitro with a NIR (854 nm) diode laser. The resulting patterns were collected with a CMOS beam profiler and used to train a convolutional neural network. Differences in these profiles were subtle yet significant enough to allow successful classification by the neural network. After being trained with a set of augmented images from each cancer type, the network was able to distinguish cell lines with an accuracy of up to 98.5%. The accurate classification of these patterns at low concentrations could contribute to the early detection of cancerous cells in otherwise healthy tissue. Current methods will also be discussed such as semantics and instance segmentation.

1:15PM L30.00009: Quantitative Cone-Beam CT with High-fidelity Modeling of Imaging Physics

QIAN CAO (Presenter), SISNIEGA ALEJANDRO, MICHAEL BREHLER, SHALINI SUBRAMANIAN, J. WEBSTER STAYMAN, JEFFREY SIEWERDSEN, WOJCIECH ZBJEWSKI, Johns Hopkins University — Bone mineral density (BMD) and bone microstructure are key biomarkers of orthopedic health. Quantitative assessment of these parameters requires high accuracy of reconstructed attenuation values and high spatial resolution. We employ advanced models of x-ray propagation to optimize performance of specialized orthopedic Cone-Beam CT systems in quantitative bone imaging. To achieve accurate measurements of BMD, a model-based reconstruction (MBR) framework utilizing polyenergetic spectral models is used in concert with fast Monte Carlo scatter correction. To advance spatial resolution to a level consistent with trabecular detail (~100 μm), we adopt a customized low-noise CMOS x-ray detector with 400 μm-thick scintillator, optimized through cascaded systems modeling of task-based imaging performance. Studies of BMD accuracy indicate that MBR is able to estimate CaCO₃ concentration with <20 mg/mL error, irrespective of object size and position. The use of optimized CMOS sensor yielded improved correlation with gold-standard micro-CT measurements of bone microstructure compared to current-generation flat-panel detector CBCT, e.g. correlation for trabecular thickness increased from 0.84 with a flat-panel CBCT to 0.96 with CMOS.

*This work was supported by NIH grant 1R01-EB-018896

1:27PM L30.00010: Quantitative evaluation of inflammatory response dynamics in the lung following proton and photon irradiation

YANJING LI (Presenter), MICHAEL DYKSTRA, Department of Radiation Oncology, Massachusetts General Hospital, Harvard Medical School, TILL BEST, Department of Radiology, Division of Thoracic Imaging and Intervention, Massachusetts General Hospital, Harvard Medical School, JENNIFER PURSLEY, NITISH CHOPRA, HARALD PAGANETTI, HENNING WILLERS, Department of Radiation Oncology, Massachusetts General Hospital, Harvard Medical School, FLORIAN Fintelmann, Department of Radiology, Division of Thoracic Imaging and Intervention, Massachusetts General Hospital, Harvard Medical School, CLEMENS GRASSBERGER, Department of Radiation Oncology, Massachusetts General Hospital, Harvard Medical School — We analyzed lung density changes in lung cancer patients receiving stereotactic body radiation therapy with protons (SBPT) or photons (SBRT). Follow-up computer tomography (CT) scans were registered to pre-treatment scans using B-spline based deformable image registration. Dose response curves (DRC) were used to correlate the radiographic change in Hounsfield Units (HU) to the radiation dose and fitted using linear regression to provide a quantitative measure of normal lung response. CTs were also evaluated by a thoracic radiologist. 46 patients (23 SBPT/SBRT) were matched based on patient characteristics, quantitative assessment correlated highly with expert evaluation (p<10⁻¹³, rho=0.6). The maximum response averages 3.8±3.0 (SBPT) versus 3.2±2.4 HU/Gy (SBRT). The lung response after SBRT significantly increases over the observation period (p=0.003), but not after SBPT, indicating an accelerated acute response after SBPT. We demonstrate that quantitative normal lung response evaluation correlates well with established grading systems and differences in response dynamics after SBPT compared to SBRT, that warrant further investigation into their mechanisms of inflammation.

*National Cancer Institute U19CA21239 (PI: Paganetti), American Lung Association LCD-400286 (PI: Willers)
Measurement of In vitro Cancer Tumor Hypoxia* YIHUA ZHAO, Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen 518, ROBERT AUSTIN (Presenter), KE-CHIH LIN, JAMES STURM, Princeton University, JUNLI QU, Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen 518 — Tumors are characterized as swamps: abnormal and disordered tissue masses with highly stressful conditions of hypoxia, low pH, low nutrient conditions due to a combination of rapid cell growth, lack of vasculature and altered metabolism. While for normal cells that combination would be lethal, for cancer cells it provides a genotoxic environment they are adapted to. We show here using a phosphorescence lifetime imaging (PLIM) technology based oxygen sensor to monitor the local \(O_2\) level in a extended two dimensional array of cancer cells with strong and mixed gradients to nutrients and \(O_2\) using a novel pure diffusional three dimensional microfabricated technology the emergence of highly hypoxic dormant cell metapopulations.

*This work was supported by NSF PHY-1659940.

Novel X-ray Sources for Medical Imaging: Making Old Physics Do New Tricks GIL TRAVISH (Presenter), AQUILA MAVALANKAR, Adaptix Ltd — The diagnosis of medical conditions often relies on medical imaging. Imaging applies basic physics and the techniques deployed have often found their origin in experimental methods. While some of these imaging modalities are new and have rapidly evolved, x-ray imaging has remained relatively stagnant since the introduction of Computed Tomography (CT) and more recently digital x-ray detectors. The availability of low-noise detectors, high speed desk-top computers and new algorithms offers incremental improvements on established x-ray imaging, but also challenges the practitioners in optimally deploying these resources as a primary concern is patient lifetime dose. New x-ray sources are often needed for advanced imaging approaches such as digital tomosynthesis, phase contrast imaging or improved interventional radiology. These novel sources often rely on field enhanced emission and carry new challenges into clinically deployed devices including ultra high vacuum, high voltage switching and the need for active feedback controls. I will describe some of these challenges, the regimes of operation under consideration by various groups, and the practical implications of the physics parameters to radiology.

Wednesday, March 6, 2019 11:15 AM - 1:39 PM

Session L31 DCP: Electronic Structure of Quantum Systems II BCEC 203 - Koblar Jackson - Tag(s): Focus

Room-Temperature Magnetoresistance in Single-Molecule Devices [Invited] ELISEO RUIZ (Presenter), Universitat de Barcelona, ISMAEL DÍEZ-PÉREZ, King's College London — The goal of this communication is to present a well-defined experimental/theoretical route map to reach single-molecule devices based on porphyrin systems showing magnetoresistance at room temperature. We have already reported that STM measurements of deposited metal thiocyanate (and selenocyanate) complexes on heavy metal surfaces that have large spin-orbit contributions allows to detect magnetoresistance.[1,2] Such magnetoresistance effect is similar to that reported by Fert and Grünberg in magnetic metal layers used in hard disk heads, just the inversion of the magnetization of the magnetic tip results in an important change in the transport properties of the device and more recently, in magnetic RAM memories as STT-MRAM devices.

In this study, we also provide results for empty porphyrin and metalloporphyrins based devices attached to the electrodes through thiol-pyridine axial ligands. Our study shows a theoretical analysis and the practical implementation through two-terminal devices using STM equipment to achieve the room temperature molecular-based spintronic nanodevices. It is worth noting that such metalloporphyrin devices show larger complexity than the previously studied systems[1,2]: (i) three peaks in the STM conductance histograms (only one in the metal thiocyanate complexes); (ii) magnetoresistance effect was also found if the electrons are injected from the magnetic nickel tip (for the thiocyanate systems only the effect was detected injecting from the gold substrate); (iii) magnetoresistance effect is smaller than in the thiocyanate systems. Non-equilibrium Green functions combined with DFT calculations have been employed in order to rationalize such results.

Problems in the treatment of transition metal magnetism with the SCAN meta-GGA functional* DAVID SINGH (Presenter), YUHAO FU, University of Missouri — We test the SCAN functional for magnetic transition metals including Fe, Co and Ni and the near magnetic elements, V and Pd. We find that while SCAN modestly enhances magnetic moments it very strongly enhances magnetic energies leading to qualitatively incorrect predictions for technologically important systems including steel. The origin of these large errors is discussed.

*The work was supported by grant DE-SC0019114, funded by the U.S. Department of Energy, Office of Science

The calculation of accurate core electron binding energy shifts and absolute core electron binding energies using the SCAN exchange-correlation functional JUHAN MATTHIAS KAHK (Presenter), Department of Materials, Imperial College London, JOHANNES LISCHNER, Department of Materials and Department of Physics, Imperial College London — Core electron X-ray Photoelectron Spectroscopy (XPS) is often used to characterize the elemental as well as the chemical composition of surfaces. However, as experimental practice moves towards the study of increasingly complex systems, the analysis of recorded spectra becomes ever more challenging. First principles calculations of core electron binding energies can substantially alleviate the problems that are commonly encountered in “peak assignment”. Recently, we have found that the SCAN density functional is particularly well suited for the calculation of core electron binding energies using the ΔSCF method. In comparison to gas phase reference data, SCAN yields absolute core electron binding energies that are accurate to within ~0.2 eV for the 1s and 2p core levels of C-F and Si-Cl respectively, without any empirical adjustments.

For calculations of adsorbates on metal surfaces, we have devised a two-step approach in which the geometry of the adsorbate is first relaxed using a slab model of the surface, and then a ΔSCF calculation is performed on a cluster cut from the slab. Analysis of the results for various cluster sizes shows that finite size effects can be minimized to the point where they are smaller than the error due to the DFT functional.

A new generation of effective core potentials from correlated calculations: 3rd row main group GUANGMING WANG (Presenter), ABDULGANI ANNABERDIYEV, CODY MELTON, MICHAEL BENNETT, LUBOS MITAS, North Carolina State University — Recently, we have developed a new generation of effective core potentials (ECP) using valence energy isospectrality with explicitly correlated all-electron excitations and norm-conservation criteria. We extend our correlation consistent effective core potentials (ccECP) to 3rd row main group elements. For K and Ca, we use a Ne core and for the 4p elements we utilize large core potentials with 3d-electrons included in the core and with 4s and 4p in the valence shell. We also incorporate relativity including averaged spin-orbit effects. Our ccECPs reproduce all-electron spectra within about chemical accuracy ≈ 0.05 eV. The transferability of ccECPs is tested on corresponding monohydride and monoxide molecules in a wide range of binding geometries. The ccECPs include also optimized valence basis sets and additional comparisons with previously constructed ECPs.

The Schrödinger-Pauli Theory of Electrons: New Perspectives VIRAHT SAHNI (Presenter), Brooklyn College and The Graduate Center, CUNY — The Schrödinger-Pauli (SP) equation corresponds to a system of $N$ electrons in an electrostatic $E(\mathbf{r}) = -\nabla \nabla \phi(\mathbf{r})$ and a magnetostatic field $B(\mathbf{r}) = \nabla \times A(\mathbf{r})$ in which the interaction of the latter with both the orbital and spin angular momentum is incorporated. The ’Quantal Newtonian’ first law for the SP equation is derived: the sum of the external $F_{\text{ext}}(\mathbf{r})$ and internal $F_{\text{int}}(\mathbf{r})$ fields acting on each electron vanishes. The external field is the sum of the electrostatic and Lorentz fields. The internal field is a sum of fields representative of the Pauli exclusion principle and Coulomb repulsion, kinetic effects, the density, and the magnetic field. From the law, it is shown that the SP equation is intrinsically self-consistent. A Quantal Density Functional Theory of the mapping from the interacting system to one of noninteracting fermions possessing the same density and physical current density is developed.
12:39PM L31.00006: Local embedding/downfolding auxiliary-field quantum Monte Carlo (AFQMC)*

BRANDON ESKRIDGE (Presenter), HENRY KRAKAUER, SHIWEI ZHANG, Department of Physics, William & Mary — A local embedding and effective downfolding scheme has been developed and implemented in the auxiliary-field quantum Monte Carlo (AFQMC) method (Shiwei Zhang and Henry Krakauer, Phys. Rev. Lett. 90, 136401 (2003)). Local embedding in the occupied space (Yudis Virgus, Wirawan Purwanto, Henry Krakauer, and Shiwei Zhang, Phys. Rev. Lett. 113, 175502 (2014)) and local effective downfolding in the virtual space are employed to treat strongly correlated local clusters with an effective Hamiltonian. The accuracy is controlled by two geometric cutoff parameters that define the occupied space embedding and virtual downfolding regions. The systematic cutoff dependence of relative energies of physical and chemical interest is found to converge rapidly to the full AFQMC treatment. Thus, significant computational savings is achieved while maintaining a high degree of accuracy. This significantly increases the system size which can be accurately treated with AFQMC. Applications to transition metal atoms in 1D and in graphitic environments are presented. (Shiwei Zhang also acknowledges the Center for Computational Quantum Physics, Flatiron Institute).

*Supported by DOE and ONR.

12:51PM L31.00007: Benchmark studies for adsorption bond energies to transition metal surfaces*

MANISH KOTHAKONDA (Presenter), JINLIANG NING, YUBO ZHANG, JAMES FURNESS, JIANWEI SUN, Tulane University — The accurate prediction of adsorption energies for molecules on metal surfaces is a challenging subject in condensed matter physics, applied catalysis and physical chemistry research. The use of computational methods such as density functional theory (DFT) calculations to describe surface-adsorbate bond strength is increasing. Often these adsorption energies are used to study heterogeneous catalysis in thermal and electrochemical reactions. Here, we compare the structures and energetics for small gaseous molecules adsorbed to various transition-metal surfaces from density functionals with experimental results [1], with focus on MetaGGAs such as the strongly constrained and appropriately normed (SCAN) [2] density functional that recognizes the different chemical bonds.


*CAROL LAVIN BERNICK FACULTY GRANT

1:03PM L31.00008: An exchange-correlation functional capturing bulk, surface, and confinement physics*

ATTILA CANGI (Presenter), Sandia National Laboratories, FRANCISCA SAGREDO, Chemistry, University of California, Irvine, ANN E MATTSSON, Los Alamos National Laboratory — We present the construction of an exchange-correlation functional which enables us to capture bulk, surface, and confinement physics with a single functional. Using the subsystem functional formalism[1,2,3] and the electron localization function, we interpolate between reference systems representing different physical regimes (homogeneous electron gas, the Airy gas, and the harmonic oscillator gas)[4,5]. The resulting functional can be viewed as a meta-GGA on the Jacob's ladder classification scheme. We report on the initial assessment of this functional, as tested on various materials.


*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
A first-principles study of insulating La$_2$CuO$_4$ and its transition to the metallic state with Sr-doping

KANUN POKHAREL (Presenter), JAMES FURNESS, Tulane University, CHRISTOPHER LANE, Northeastern University, RUIQI ZHANG, Tulane University, BERNARDO BARBIELLINI, Lappeenranta University of Technology, YUBO ZHANG, Tulane University, ARUN BANSIL, Northeastern University, JIANWEI SUN, Tulane University, ROBERT MARKIEWICZ, Northeastern University

Correct prediction of the electronic structure of La$_2$CuO$_4$(LCO), an exemplar half-filled cuprate, has been a long-standing problem where the commonly used exchange-correlation functionals fail to reproduce the experimentally observed insulating state. In contrast, Strongly-Constrained-and-Approximately-Normed (SCAN) functional properly captures not only the ground state antiferromagnetic insulator character of LCO but also its transition to metallic state with Sr doping. We compare and contrast our SCAN-based results with the corresponding results obtained using other meta-GGA's and hybrid functionals. Our analysis suggests that the SCAN functional can provide a new pathway for first-principles modeling of cuprates and other correlated materials.

*carol lavin bernick faculty grant, Tulane University

The Wilson basis applied to electronic structure

JAMES BROWN (Presenter), JAMES WHITFIELD, Department of Physics and Astronomy, Dartmouth College — We present a method to calculate electronic energies using a pruned phase-space grid of Wilson basis functions. Computational scaling of O(N$^{8/3}$) is realized by representing the Coulomb potential in a sum-of-products form and calculating energies using iterative methods. Convergence of the Wilson basis is analyzed in detail for multiple states of H$_2$ and He with and without a strong magnetic field.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L32 DCP: Chemical Physics BCEC 204A - Der-you Kao, NASA Goddard Space Flight Center - Tag(s): Focus

Verification of acoustic mismatching model for sub-THz acoustics in glass

FAN JUN WEI (Presenter), Institute of Physics, Academia Sinica, RICHARD A. MOLE, Bragg Institute, Australian Nuclear Science and Technology Organisation, SUNIL KARNA, Department of Physics & Astronomy, Louisiana State University, JIN-WEI SHI, Department of Electrical Engineering, National Central University, JINN-KONG SHEU, Department of Photonics, National Cheng Kung University, KUNG-HSUAN LIN, Institute of Physics, Academia Sinica — Because of high acoustic attenuation of glass in sub-THz regime, it is difficult to measure the highly damped acoustic waves passing through the media. In theory, the acoustic properties of the media could be experimentally studied by reflection of acoustic waves which do not propagate into the media. Complex acoustic impedance, which includes the information of dispersion relation and frequency-dependence of attenuation, is a parameter in the acoustic mismatching model to describe the phenomena when acoustic waves encounter the interface of media. The mismatch of acoustic impedance results in reflection and transmission of acoustic waves at the interfaces. We report the verification experiments for this model in sub-THz regime. We generated coherent THz acoustic phonons and measured the amplitude and phase of the reflected acoustic phonons from the interface of GaN and silica. Based on the acoustic mismatching model, the frequency dependence of sound speed and the attenuation were obtained up to 0.3 THz. These values were compared with the results from typical method. This verified technique enables the measurement of sub-THz acoustic properties of thick and highly damped materials.

Modulated order and unconventional phase coexistence in a model for lattice mismatched solids

LAYNE FRECHETTE (Presenter), University of California, Berkeley, CHRISTOPH DELLAGO, University of Vienna, PHILLIP L GEISSLER, University of California, Berkeley — Lattice mismatch is a common occurrence in modern materials, but just how it influences the arrangement of atoms in materials is incompletely understood. Here we consider a simple microscopic model for lattice mismatch, in which the difference in natural bond lengths between atoms produces interactions mediated by elastic strain. Monte Carlo simulations reveal that the model exhibits rich phase behavior, supporting structures with modulated order and unusual coexistence scenarios. To explain this phase behavior, we derive an effective pair potential between atoms, revealing preferred spatial arrangements of atoms driven by spatial variations in the interaction energy. Based on this effective interaction, we then develop a mean field theory, which captures the modulated structures observed in our simulations. Finally, we explain the observed coexistence scenarios using a modified Maxwell construction, which is based on the realization that the free energy cost of phase separation in elastic systems is extensive. These results clarify the equilibrium effects of lattice mismatch in macroscopic solids and suggest a role for lattice mismatch in creating spatially heterogeneous compositions in nanoscale materials.

*We acknowledge the NSF for funding under award number 1416161.
substrates by using an organosilane SAM to begin the multilayer growth. AFM tip to create nanowires that span well-defined nanogaps. The second technique seeks to extend nanoshaving to Si assembled monolayers (SAMs). The first technique combines the molecular ruler process with local nanoshaving using an molecular self-assembly. We described two such hybrid techniques based on mercaptohexadecanoic acid (MHDA) self-lithography, the ability to create complex architectures over large areas, to the flexibility and resolution afforded by promise. These hybrid strategies are of particular interest because they couple a key aspect afforded by conventional strategies that combine conventional top-down lithographic techniques with molecular self-assembly show significant promise. These hybrid strategies are of particular interest because they couple a key aspect afforded by conventional lithography, the ability to create complex architectures over large areas, to the flexibility and resolution afforded by molecular self-assembly. We described two such hybrid techniques based on mercaptohexadecanoic acid (MHDA) self-assembled monolayers (SAMs). The first technique combines the molecular ruler process with local nanoshaving using an AFM tip to create nanowires that span well-defined nanogaps. The second technique seeks to extend nanoshaving to Si substrates by using an organosilane SAM to begin the multilayer growth.

*This work is supported by NSF-CMMI-1536528.

11:51AM L32.00004: Fundamental Link between β Relaxation, Excess Wing, and Cage-Breaking in Metallic Glasses* MENGHAO YANG (Presenter), Ames Laboratory, HAIBIN YU, Huazhong University of Science and Technology, YANG SUN, FENG ZHANG, Ames Laboratory, JIANBO LIU, Tsinghua University, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, RANKO RICHERT, Arizona State University, KONRAD SAMWER, Universität Göttingen — In glassy materials, the Johari-Goldstein secondary (β) relaxation is crucial to many properties, as it is directly related to local atomic motions. However, a long-standing puzzle remains elusive: why some glasses exhibit β relaxations as pronounced peaks while others as unobvious excess wings? Using microseconds atomistic simulation of two model metallic glasses (MGs), we demonstrate such a difference is associated with the amount of string-like collective atomic jumps. Relative to that of excess wings, we find that MGs having pronounced β relaxations contain larger numbers of such jumps. Structurally, they are promoted by the higher tendency of cages-breaking events of their neighbors. Our results provide atomistic insights for different signatures of the β relaxation that could be helpful for understanding the low-temperature dynamics and properties of MGs.

*Work conducted at Ames Laboratory was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division, under Contract No. DEAC02-07CH11358, including a grant of computer time at the National Energy Research Supercomputing Center (NERSC) in Berkeley, CA.

12:03PM L32.00005: Ultrafast Conformer Relaxation of Provitamin D Analogs in Lipid Bilayers DANIELLE SOFFERMAN (Presenter), ROSEANNE J SENSION, University of Michigan — Ultrafast photochemical transformations of 7-Dehydrocholesterol (DHC, Provitamin D3), DHC-Acetate and Ergosterol (Ergo, Provitamin D2) to previtamin (D3, D3-acetate and D2) occurs upon a ring-opening reaction in the excited state where a cyclohexadiene (CHD) chromophore embedded within the molecules opens to form a hexatriene previtamin D species. Conformer relaxation back to the ground state of isolated CHD happens on the time scale of picoseconds, therefore it is necessary to use ultrafast techniques such as transient absorption to capture the relaxation. Here we are studying conformer relaxation of DHC and its analogs in liposomes as a simple model for biologically relevant skin membranes. DHC has been studied extensively in isotropic solvents where the molecule is free to relax down to the ground state to form a stable previtamin D3 species. However in the cell membrane the molecule is hypothesized to be locked in an unstable previtamin D3 conformation that thermally relaxes down to form Vitamin D3. To understand the conformer relaxation that takes place in biological membranes we extend our studies to DHC analogs, DHC-Acetate and Ergo in isotropic solvents and in simple lipid bilayers.

12:15PM L32.00006: Probing the Molecular Interactions of Small Molecules with Sapphire* NITYANSHU KUMAR (Presenter), SUKHMANJOT KAUR, The University of Akron, RAJAT KUMAR, Department of Biomedical Engineering, Stony Brook University, SELEMON BEKELE, MESFIN TSIGE, ALI N DHINOJWALA, The University of Akron — Numerous challenges in the field of adhesion, biocompatibility, and purification thrives a persistent need to better understand the interactions of small molecules at any interface. The interaction energy of small molecules at a solid/liquid interface is governed by the surface structure of the solid substrate, the interfacial molecular orientation of the small molecules and their chemical nature. Sometimes, the interaction could be driven by the presence of hydrogen bonding leading to a specific molecular orientation. Here, we seek to understand how small molecules compete for interaction sites, orient and interact at the solid/liquid interface. Using MD simulations, we contemplate and present a model to visualize the interaction of acetone and chloroform molecules on the sapphire. Further, combining the simulation results with experimental data obtained using sum frequency generation (SFG) spectroscopy, we attempt to understand the spectroscopic features and their hidden correlations. This work paves the way for understanding the interaction of molecules at the solid/liquid interface with potential applications in the field of adhesives, coatings, medicines, and water purification.

*This work is supported by the National Science Foundation Grant (NSF-CHE 1506275).
12:27PM L32.00007: Shock Compression Microscopy for Tabletop Detonations in PETN-based Explosives*  
WILL BASSETT (Presenter), Lawrence Livermore Natl Lab, DANA DLOTT, BELINDA PACHECO, LAWRENCE SALVATI, Chemistry, University of Illinois — We have developed a microscope system for performing shock compression experiments with km s⁻¹ impactors and nanosecond-duration shock waves. In the present work, this system is used to study polymer-bound explosive charges (PBXs) 1 mm in diameter and tens to hundreds of microns thick. The microscope diagnostics include particle velocity (Photon Doppler velocimetry) measurements, fast imaging, and optical pyrometry. The PBX under study is a pentaerythritol tetranitrate (PETN)-based PBX (80% PETN, 20% elastomer binder) and has been characterized using x-ray tomography and scanning electron microscopy. At lower shock-pressures we observed sub-detonative behavior and hot spots have structures which evolved over 20 ns and cooled relatively slowly. At higher shock-pressures, the shock wave was supported by fast chemical reactions and the particle velocity remained constant. In this regime the shock wave is detonation-like and the hot spot cooling rate increased dramatically.

*This work was supported by the US Army Research Office under award W911NF-13-1-0217, the US Air Force Office of Scientific Research under award FA9550-16-1-0042. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

12:39PM L32.00008: Quantum Confinement of Helium, Molecular Nitrogen and Molecular Deuterium Clusters in Carbon Nanotubes  
[Invited] MARIA PILAR DE LARA-CASTELLS (Presenter), Consejo Superior de Investigaciones Científicas — NA

1:15PM L32.00009: COARSE-GRAINED SIMULATIONS OF DENDRITIC CARBOHYDRATE NANOPARTICLES*  
EDUARDO MENDEZ (Presenter), MOHAMMAD HASSAN KHATAMI, HENDRICK W DE HAAN, Faculty of Science, University of Ontario Institute of Technology — PhytoSpherix are naturally occurring carbohydrate-polymer dendritic nanoparticles extracted from sweet corn, with branching points at regular intervals. We investigate the structural details of model Px particles via coarse grained strategies (MARTINI forcefield and GROMACS molecular dynamics simulations), and also employ knowledge gathered from small atomistic models to build large structures many thousands of carbohydrate units in size, beyond the typical scales reached by standard atomistic simulations. The scheme used here may be employed to build structures with branched motifs that may not be regular. These structures are produced by other plant species and have a wide degree of applicability due to their sponge-like properties. We present an analysis of various morphologies of these objects and explore their variability depending on the scheme used in their assembly, and thus provide a way to compare models to theories of regular branched dendritic nanoparticles.

*OCE VIP II  
NSERC CRD

1:27PM L32.00010: Designing Interdisciplinary Undergraduate Research Experiences to Increase Diversity in STEM*  
SOLOMON BILILIGN (Presenter), North Carolina Agricultural and Technical State University — The recruitment of undergraduate students, especially minorities, into STEM career paths and in particular into majors in physics continues to be a challenge. One approach for addressing this issue provides an interdisciplinary research opportunity that has societal relevance and uses basic concepts in physics. The program design involves year-round research combined with summer or short visits to major university, national lab, or private research facilities. Other program components include (1) cohort-building activities and effective mentoring; (2) short-course professional development modules focused on research ethics, literature survey, writing, and data management; and (3) student engagement in the creation of personalized professional development plans.

*The Author Acknowledges the funding from NSF under grant number 1600415

1:39PM L32.00011: QPython as mobile computational physics laboratory anywhere, anytime and anyhow  
GODFREY AKPOJOTOR (Presenter), Theoretical and Computational Condensed Matter Physics, Physics Department, Delta State University, Abraka, GODWIN IBEH, Department of Physics, Nigerian Defence Academy, FAMOUS AKPOJOTOR, Department of Physics, University of Benin, SHARON ASEGHELEME EGBORO, Theoretical and Computational Condensed Matter Physics, Physics Department, Delta State University, Abraka — Computational physics (CP) has become an integral part of physics. However, an important choice in deciding the computational approach is accessibility to both the computing device and the programming language. The continuous growth of smartphones in Africa and the availability of the free and open source Python programming capabilities in QPython (QP) meet the accessibility requirement to make them mobile computational physics laboratory (MCPL). We present here one of our current projects under the Python African Computational Science and Engineering Tour Project (PACSETPro) of using QP as MCPL for teaching CP and development of physics Apps to students, new beginners as well as expert programmers anywhere, anytime and anyhow. We examine the third party libraries especially the future of matplotlib in QP.
The triplet state of a two-electron quantum dot in a magnetic field is studied from the perspective of the ‘Quantal Newtonian’ first law. The exact analytical wave function solution of the corresponding Schrödinger-Pauli equation is derived. The anti-symmetric nature of the spatial part of the wave function, and the satisfaction by it of the node electron-electron coalescence constraint is displayed. The quantal sources of the density, pair-correlation density, the Fermi-Coulomb hole charge, the single-particle density matrix, and the current density, and from these the corresponding Hartree, electron-interaction, Pauli-Coulomb, Differential Density, Kinetic, and Effective Magnetic fields are determined. The total energy, and both its external and internal components are obtained from the various fields. The intrinsic self-consistent nature of the Schrödinger-Pauli equation, and thereby the satisfaction of the ‘Quantal Newtonian’ first law is shown.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L33 FIAP: Quantum Devices and 2D Materials

11:15AM L33.00001: Quantum Surfing - Pushing a Particle through a Rough Potential*  
DANIEL MARK (Presenter), SAMUEL F SAVITZ, Physics, Caltech, GIL REFAEL, Institute for Quantum Information and Matter, Caltech — Quantum machines rely on our ability to manipulate the motion of electrons. We investigate the transport of particles by a travelling potential pulse in a one-dimensional system with quenched disorder, dissipation, and thermal noise. We simulate finite temperature and dissipation by applying the Schrödinger-Langevin equation to a single-particle hopping model. The transport is understood as a semiclassical Fokker-Planck diffusion process in the pulse frame. The semiclassical behavior arises from decoherence due to the dissipation and thermal noise. We predict that the “surfing length”, our measure of transport, is exponential with pulse width. Measurements agree with drift velocities and diffusivities from simulations with a constant DC field, in the regime of high disorder and thermal noise. We also introduce an alternative nonlinear dissipative term which allows for generalization to higher dimensions and many-body systems.

*Funding for this research was provided by the Institute for Quantum Information and Matter, a National Science Frontier center partially funded by the Gordon and Betty Moore Foundation. DM was funded by the David L. Goodstein SURF Fellowship, Caltech SFP. SS was funded by a National Science Foundation Graduate Research Fellowship under Grant No. DGE-1745301.

11:27AM L33.00002: Electrical initialization of electron and nuclear spins in a single quantum dot at zero magnetic field  
PIERRE RENUCCI (Presenter), LPCNO, Institut National des Sciences Appliquees de Toulouse, FABIAN CADIZ, Ecole Polytechnique, ADBELHAK DJEFFAL, Institut Jean Lamour, UMR 7198-CNRS-Nancy Université, DELPHINE LAGARDE, ANDREA BALOCCHI, LPCNO, Institut National des Sciences Appliquees de Toulouse, BINGSHAN TAO, Institut Jean Lamour, UMR 7198-CNRS-Nancy Université, BO XU, Institute of Semiconductors Beijing, SHIHENG LIANG, MATHIEU STOFFEL, XAVIER DEVAUX, Institut Jean Lamour, UMR 7198-CNRS-Nancy Université, HENRI JAFFRES, JEAN-MARIE GEORGE, Unité Mixte de Physique CNRS-Thales, MICHEL HEHN, STEPHANE MANGIN, Institut Jean Lamour, UMR 7198-CNRS-Nancy Université, HÉLÈNE CARRERE, XAVIER MARIE, THIERRY AMAND, LPCNO, Institut National des Sciences Appliquees de Toulouse, XIUFENG HAN, Institute of Physics, Beijing, ZHANGUO WANG, Institute of Semiconductors Beijing, BERNHARD URBASZEK, LPCNO, Institut National des Sciences Appliquees de Toulouse, YUAN LU, Institut Jean Lamour, UMR 7198-CNRS-Nancy Université — We demonstrate single quantum dot (p-type InGaAs quantum dot) electroluminescence (EL) with a circular polarization degree up to 35% at zero applied magnetic field, proving highly efficient electrical injection of spin polarized electrons [1]. It is achieved thanks to an ultrathin CoFeB electrode presenting Perpendicular Magnetic Anisotropy on top of a spin-LED. In addition, we measure an Overhauser shift of several micro-eV at zero magnetic field for the positively charged exciton (trion X+) EL emission, which changes sign as we reverse the injected electron spin orientation. This is a signature of dynamic polarization of the nuclear spins [1] in the quantum dot induced by the hyperfine interaction with the electrically injected electron spin. Both EL circular polarization and Overhauser shift follow the hysteresis cycle of the magnetic electrode. This study paves the way for electrical initialization of electron and nuclear spins in a single quantum dot without any external magnetic field. [1] F. Cadiz et al, Nano Letters 18 (4), 2381-2386 (2018)
11:39AM L33.00003: Colloidal Quantum Dot Tandem Photovoltaics Employing a Novel Hole-blocking Injection Layer Concept*  
SUE SHI (Presenter), YIJIN GUO, GILLIAN HAGEN, BENJAMIN A ZANK, ALEXI C ARANGO, Mount Holyoke College — Colloidal quantum dot (CQD) tandem photovoltaics (PV) are of interest as candidates for next-generation PV due to their potential for low-cost fabrication and compatibility with lightweight flexible packaging. In this work, we present a CQD tandem PV device that employs indium tin oxide (ITO) as interconnection layer and a novel injection layer with hole-blocking functionality. A lead sulfide (PbS) CQD heterojunction is formed with C60 in each subcell, yet the traditional BPhen/Ag contact is replaced with ITO. We demonstrate that a hole-blocking injection layer must be inserted between C60 and interconnection layer ITO in order to achieve excellent electrical contact between the two. We obtain a doubling in open-circuit voltage and maintain the high fill factor of the single-junction device. This device structure is particularly suited to multiple-cell tandem PV.

*NSF Award #1744671; Mount Holyoke College Lynk Internship Funds; Marilyn Dawson Sarles Science Internship Fund

11:51AM L33.00004: 0.7 Anomaly, Spin-Mixing and Emergent Spin Gap in Quantum Point Contacts with Strong Spin-Orbit Interaction  
KARINA HUDSON (Presenter), ASHWIN SRINIVASAN, Univ of New South Wales, OLGA GOULKO, Physics, Boise State University, JARROD ADAM, QINGWEN WANG, LAREINE YEOH, OLEH KLOCHAN, Univ of New South Wales, IAN FARRER, Electronic and Electrical Engineering, University of Sheffield, DAVID A RITCHIE, Semiconductor Physics, University of Cambridge, JAN VON DELFT, Arnold Sommerfeld Centre for Theoretical Physics, Ludwig-Maximilians University, ALEX R HAMILTON, Univ of New South Wales — Quantum point contacts (QPCs) are 1D charge constrictions where ballistic conductance through the channel is quantised in integer units, with the exception of the 0.7(2e^2/h) anomaly. The microscopic origin of the 0.7 anomaly remains contentious after over 20 years of study, and the additional influence of spin-orbit interaction (SOI) is even more poorly understood. Here we characterise the 0.7 anomaly for 1D holes with strong interactions and strong SOI. Similarly to electrons, the 0.7 anomaly in 1D holes shares the signature behaviour of evolving to 0.5(2e^2/h) in applied magnetic field. However, while the electron 0.7 anomaly isotropically Zeeman spin-splits in magnetic field, the hole 0.7 anomaly exhibits a weak anisotropic response in in-plane magnetic field. We show the magnetic field orientation dependence of the first 1D hole subband, and demonstrate a new and robust signature for the opening of a spin gap. We compare our measurements to recent theory where the Rashba SOI term predicts the correct anisotropy of the Zeeman spin-splitting in the first hole subband as well as the opening of a spin gap in magnetic field. The opening of a spin gap in 1D hole semiconducting systems has significant implications for the formation of helical spin gaps and Majorana excitations.

12:03PM L33.00005: Ultrasensitive displacement noise measurement of carbon nanotube mechanical resonators  
CHANDAN SAMANTA, SERGIO LUCIO DE BONIS (Presenter), CARLES FLORES, WEI YANG, ICFO, ADRIEN NOURY, CNRS/L2C, QUAN DONG, YONG JIN, Department of Nanoelectronics, CNRS/C2N, ADRIAN BACHTOLD, ICFO — Mechanical resonators based on a single carbon nanotube are exceptional sensors of mass and force. The force sensitivity in these ultra-light resonators is often limited by the noise in the detection of the vibrations. Here, we report on an ultra-sensitive scheme based on a RLC resonator and a low-temperature amplifier to detect nanotube resonators. These advances in detection allow us to reach 0.5 pm/ displacement sensitivity [1]. Thermal vibrations cooled cryogenically at 300 mK are detected with a signal-to-noise ratio as high as 17 dB. We demonstrate 4.3 zN/ force sensitivity, which is the best force sensitivity achieved thus far with a mechanical resonator. This is an important step towards imaging individual nuclear spins and studying the coupling between mechanical vibrations and electrons in different quantum electron transport regimes. We will also present our recent measurements on the coupling between mechanical vibrations and electrons in the Coulomb blockade regime.

Large-area graphene quantized Hall resistance arrays using superconducting interconnections

MATTIAS KRUSKOPF (Presenter), ALBERT RIGOSI, HANBYUL JIN, DINESH PATEL, SHAMITH PAYAGALA, ALIREZA PANNA, DEAN G. JARRETT, DAVID B NEWELL, RANDOLPH E ELMQUIST, Quantum Measurement Division, National Institute of Standards and Technology — Next generation quantum resistance standards based on multiple quantized Hall resistance (QHR) elements will allow tailoring the fundamental value to the needs of a given application. However, scalable resistance networks often suffer from accumulated resistances at metallic interconnections that lead to a deviation from the theoretical value.

This work shows the first results of epitaxial graphene-based, QHR array devices using superconducting contacts and interconnections to minimize parasitic resistances. The applied contact design is optimized for reduced contact resistances and circumvents any possible alteration of the QHR caused by Andreev reflections. For homogenous charge carrier concentrations and high monolayer quality, optimized growth and doping techniques were developed to allow for the realization of complex chip designs on the centimeter scale.

The results show different QHR array devices at exceptionally high currents in the mA range that are utilized to improve the measurement uncertainty of relatively simple, room temperature resistance bridges. To ensure the applicability in quantum resistance metrology, we apply and test new global criteria of quantization and verify the precision using direct current comparators and cryogenic current comparator bridges.

A Metalens Device for Applications of Nitrogen-Vacancy Centers in Diamond

HOPE MCGOVERN (Presenter), JUAN LIZARAZO FERRO, RASHID ZIA, Brown University — There is much interest in using nitrogen-vacancy (NV) centers in diamond for future quantum communication networks. Prerequisite to such advances is a scalable method of focusing light and collecting the resulting emission spectra from the NV centers. Here, we propose a fiber-coupled device that integrates metalenses to excite and collect the photoluminescence from NV centers in diamond. We discuss the design challenges involved in achieving a high numerical-aperture, off-axis metalens and provide detailed simulations evaluating the performance of various optimized metalens systems.

Effects of Wet Transfer on Photoluminescence of WS2*

XIAOTIAN WANG, KYUNGNAM KANG, SHICHEN FU, KYLE GODIN, SIWEI CHEN (Presenter), EUI-HYEOK YANG, Stevens Institute of Technology — Chemical vapor deposition (CVD)-grown transition metal dichalcogenides (TMDs) are often required to be transferred onto another substrate for device applications. The KOH-based wet transfer is the most popular method to transfer TMDs. However, after transfer, PL intensity is heavily quenched due to a combination of trapped water, substrate dope and solvent effects which are introduced during transfer process.

Here, we evaluated the effects of solvents and polymers involved in the wet etching transfer on the PL property of WS2. We used CVD-grown WS2 sample and simulate the transfer process by applying each solvent and polymer to WS2 respectively. The PL mapping results showed there is no significant reduction of PL intensity of WS2 before and after acetone, IPA, DI water and PMMA treatment. We then studied the effect of KOH on the PL intensities by transferring WS2 onto PDMS substrate using the Cu-based transfer method [1]. After 30% KOH solution treatment, the sample showed significant reduction of PL intensity compared to it before KOH treatment. We attribute that KOH molecules are physically adsorbed onto WS2, which can be removed through acid neutralization or high vacuum annealing.


*CFN, BNL, DE-SC0012704
12:51PM L33.00009: Optical verification of H-point exciton in bulk transition metal dichalcogenides*  
SO YEUN KIM (Presenter), Depart of Physics and Astronomy, Seoul National University, HUYEN THI NGUYEN, BYUNG CHEOL PARK, TAE WON NOH, Center for Correlated Electron Systems (CCES), Institute for Basic Science (IBS) — During last decades, transition metal dichalcogenide (TMDC) compounds has been studied extensively. TMDCs provide an excellent platform to investigate many-body physics of exciton, and exciton binding energy increased significantly by reducing thickness. Mostly hydrogen models are used to obtain band gap and exciton binding energy from absorption spectra. On the other hand, recent reports on bulk TMDC claimed an peak previously assigned as \( n=2 \) state of A exciton at K-point is not true, but is an independent \( n=1 \) exciton arising at H-point [J. Kopaczek et al., Jour. Appl. Phys. 119, 235705 (2016)]. Following the argument, previous method to obtain binding energy of bulk TMDC may be incorrect. To verify the existence of H-point, we performed an ellipsometry measurements and two-dimensional correlation spectroscopy on TMDC compounds. We analyzed thermal sequential order of exciton peaks, which may be used to distinguish exciton states that arise from K-point and H-point. In this work, we will discuss on analysis and possible impact in future studies.

*This work was supported by Institute for Basic Science in Korea (Grant No. IBS-R009-G1). S. Y. Kim was supported by Global PH. D Fellowship Program funded by the Ministry of Education (Grant No. NRF-2015H1A2A1034943).

1:03PM L33.00010: Precursor Free Growth of MoS2 Monolayer Devices With Naturally Formed Contacts  
THUSHAN WICKRAMASINGHE (Presenter), GREGORY JENSEN, RUHI THORAT, ERIC A STINAFF, Ohio University — Interest in two dimensional Transition Metal Dichalcogenides (TMDDs) has remained robust due to properties such as their direct band gap, large exciton binding energies, sizeable spin-orbit couplings, and spin-valley interactions. While there are several techniques for developing TMD based devices, in this work we propose a unique, precursor free, Chemical Vapor Deposition (CVD) method in which the device in grown \textit{in situ} with naturally formed contacts. A molybdenum metal pattern, which will form an electrical contact with the TMD, is sputtered on to the substrate prior to the growth. The oxide layer that then naturally forms on the metal surface serves as the precursor for the subsequent growth. In contrast to completely sulfurizing an ultrathin Mo layer, the TMD material grows on, and away from, the thick molybdenum patterns across the Si substrate. Photoluminescence and Raman studies show that the growth can be tuned to produce monolayer and bi-layer Molybdenum Disulfide (MoS2). We also study the self-limiting nature of the growth process and compare it to the growths with the MoO3 precursor.

1:15PM L33.00011: \textit{Ab-initio} Calculations of Electronic Properties of Orthorhombic Tin Selenide (SnSe).*  
YURIY MALOZOVSKY (Presenter), SHAIBU MATHIAS, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Southern University — We present results from \textit{ab-initio}, self-consistent density functional theory (DFT) calculations of electronic properties of tin selenide (SnSe) in the \textit{orthorhombic} \textit{B16} crystal structure. We utilized a local density approximation (LDA) potential and the linear combination of atomic orbital (LCAO) formalism. Our calculations minimized the energy down to the ground state, as required by the second DFT theorem. This process ensures the full, physical content of our findings that include electronic energy bands, total and partial densities of states, and electron and hole effective masses.

*This work was funded in part by the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE- NA0003679), the National Science Foundation (NSF) (Award No. HRD-1503226), LaSPACE, and LONI-SUBR.

1:27PM L33.00012: Microscopic polarization and magnetization fields in extended systems*  
PERRY MAHON (Presenter), Physics, University of Toronto, RODRIGO A. MUNIZ, Electrical Engineering and Computer Science, University of Michigan, JOHN EDWARD SIPE, University of Toronto — We introduce microscopic polarization and magnetization fields at each site of an extended system, as well as free charge and current density fields associated with charge movement from site to site, by employing an approach based on a set of orthogonal orbitals at each site. These microscopic fields are defined using a single-particle electron Green function. For an infinite crystal we choose the orbitals to be maximally-localized Wannier functions, and in the longwavelength limit we recover the expected linear response of an insulator, including the zero frequency transverse conductivity. For a topologically trivial insulator we recover the expected expressions for the microscopic polarization and magnetization in the ground state, and find that the linear response to excitation at arbitrary frequency is described solely by the microscopic polarization and magnetization fields. For very general optical response calculations the microscopic fields automatically satisfy charge conservation, even under basis truncation, and do not suffer from the false divergences at zero frequency that can plague response calculations using other approaches.

*We thank the Natural Sciences and Engineering Research Council of Canada for funding.
Carbon nanotube-quantum dot paper for radiation sensitive Electro-mechanical system

SUKANTA NANDI (Presenter), BUDDHA DEKA BORUAH, ABHA MISRA, Indian Institute of Science — Hybrid nanostructures offer unparalleled properties by coupling different functionalities. Surface modification of multiwalled carbon nanotubes (MWCNTs) by in-situ decoration of zinc oxide quantum dots (ZnO QDs) i.e. ZnO QDs@MWCNTs induces highly sensitive opto-electro-mechanical response. Freestanding paper of ZnO QDs@MWCNTs demonstrated an enhancement of ~122% in the response current upon infrared (radiation) illumination as compared to only MWCNT paper. Moreover, the radiation interaction revealed a comparatively quicker response and recovery time of ~42.4% and ~19.4% respectively. Electro-mechanical measurements revealed a ~349% increment in actuation at 3 V bias owing to increase in net polarization enhancement. Radiation induced actuation further revealed a ~111 ± 4% actuation compared to the electro-mechanical actuation. Through this work we demonstrate MWCNT coupled with dielectric QDs paves extraordinary functionalities altogether for the development of smart micro-opto-electro-mechanical systems.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L34 FIAP: Future of Transportation BCEC 205A - Michael Gordon, IBM Thomas J. Watson Research Center - Tag(s): Invited, Undergraduate

11:15AM L34.00001: Findings of the Governor's Commission on the Future of Transportation in the Commonwealth of Massachusetts [Invited] STEVEN KADISH (Presenter), Harvard Kennedy School — TBD

11:51AM L34.00002: Crowdsourcing inclusive, accessible last-mile transportation with self-driving #AccessibleOlli* [Invited] JOE SPEED (Presenter), IoT Solutions & Technology, ADLINK Technology — #AccessibleOlli is a crowdsourced, open source effort to create the world's most accessible transportation for all including the elderly and those with disabilities. #AccessibleOlli's precursor, Olli developed by Local Motors is an autonomous vehicle enabled by IBM Watson cognitive assistant. Olli can ‘hear’ spoken questions and instructions and respond in familiar conversational language to take people where they need to go. Using a network of embedded sensors, devices, robotics and AI technology, #AccessibleOlli seeks to transform the lives of the world's growing aging population and persons with disabilities. Contributors to #AccessibleOlli include ADLINK Technology, IBM, CTA Foundation, Local Motors, AARP, MIT, PTECH schools, ASU, Local Motors, Ultrahaptics, what3words, Mapbox, Front Porch, LG, Panasonic, BestMile, Mayo Clinic, City of Rochester MN and a worldwide community of volunteer SMEs, designers, developers and engineers.

Why do we need inclusive mobility that is accessible for all? Urban mobility is a $1.5T a year market serving 4 billion people. Existing public transport options don’t serve the elderly or disabled well enough. Currently 1 billion people, around 15 percent of the world's population, experience some form of disability. In the US, over 560,000 people with disabilities never leave home due to transportation difficulties. According to the Journal of Gerontology, seniors outlive their ability to drive safely by an average of 7 to 10 years. By 2050, around 22 percent of the global population will be aged 60 years or older.

Here is a video overview of the program with Joe Speed of ADLINK Technology and IBMers https://youtu.be/KjP6aRtuEv4

*Funding and/or technology has been provided for this program by Local Motors, IBM, ADLINK Technology, CTA Foundation, MIT, Princeton University, Ultrahaptics, Panasonic, LG, what3words, BestMile.

12:27PM L34.00003: State of the art for drone technology [Invited] TIM MEYER (Presenter), IBM — TBD

1:03PM L34.00004: Self-Driving Cars and Lidar [Invited] SIMON VERGHESE (Presenter), Waymo — TBD

1:39PM L34.00005: The Future of Flight [Invited] BRIAN TILLOTSON (Presenter), Boeing — Air and space transportation are advancing in many ways. We describe current and foreseeable advances; their benefits to comfort, capability, and the environment; and the physics challenges that arise in each. Highlights include urban mobility, hypersonic travel, and settling the solar system. Major challenges include acoustics, lightning, thermal control, cosmic radiation, and the short lifetimes of G-type stars.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM
11:15AM L35.00001: Quantum control and entanglement of 6+ spin qubits in diamond  
**CONOR BRADLEY (Presenter), JOE RANDALL, REMON BERREVOETS, MOHAMED ABOBEIH, MAARTEN DEGEN, VIATCHESLAV DOBROVITSKI, TIM HUGO TAMINIAU, QuTech and Kavli Institute of Nanoscience, Delft University of Technology** — The nitrogen vacancy (NV) centre in diamond is a promising candidate for quantum networks. NVs can be entangled remotely [1], and coupling to $^{13}$C nuclear spins in the environment provides qubits for the storage and processing of quantum information [2]. In recent years, basic building blocks for a quantum network have been demonstrated, including quantum error correction [2] and entanglement distillation [3]. A key challenge is to realise high-quality control over multiple $^{13}$C spin qubits.

In this talk, I will show how a novel two-qubit gate - based upon radio frequency driving interleaved with dynamical decoupling - enables quantum entanglement of 6+ spins. The results are the largest entangled state realised on this platform, and are a key step for error correction and larger quantum networks with NV centres.


11:27AM L35.00002: High-fidelity control of a multi-qubit network node in diamond  
**JOE RANDALL (Presenter), CONOR BRADLEY, REMON BERREVOETS, MAARTEN DEGEN, MOHAMED ABOBEIH, VIATCHESLAV DOBROVITSKI, TIM HUGO TAMINIAU, QuTech and Kavli Institute of Nanoscience, Delft University of Technology** — A powerful approach to realise large-scale quantum computations and simulations is to use quantum networks, which are comprised of a number of multi-qubit nodes connected together by photonic links [1]. The nitrogen vacancy (NV) centre in diamond is a promising platform for building such networks, as it combines optical entanglement links through its electron spin [2,3] with long-lived nuclear spin qubits that can store and process quantum information [4,5]. A key requirement is to realise high-fidelity control over multi-qubit nuclear spin registers within each node.

I will present our experimental demonstration of a novel method to perform selective electron-nuclear two-qubit gates. The method uses radio frequency pulses resonant with the target nuclear spin interleaved with dynamical decoupling pulses on the electron spin. This has several key advantages compared to previous control methods, allowing more nuclear spins to be addressed and higher gate fidelities to be reached.


11:39AM L35.00003: Room-Temperature Quantum Error Correction with Nitrogen-Vacancy Centers  
**MO CHEN (Presenter), DAVID LAYDEN, PAOLA CAPPELLARO, Massachusetts Institute of Technology** — In pursuit of near-term quantum devices that either demonstrate a `quantum supremacy' or perform a meaningful algorithm, quantum error correction (QEC) is required. Arguably, fault-tolerance (FT) is not mandatory at this stage. Therefore, instead of traditional FT QEC, we focus on hardware-efficient QEC that demands less redundancy and imposes less overhead penalty. The system of interest is a room-temperature solid-state quantum register consisting of qubits and one ancilla, respectively given by the nuclear spins and the electronic spin associated with the NV center in diamond.

We first studied the decoherence process of the nuclear spins to better characterize the system. The errors on the nuclear spins turn out to be caused by the same source and are thus strongly correlated. We can then proceed to design custom QEC codes for this system, and develop experimental tools for realizing hardware-efficient QEC.
Laser Written Diamond Optoelectronic Devices for use in Quantum Computing*

YASHNA LEKHAI (Presenter), COLIN STEPHEN, Department of Physics, University of Warwick, YU-CHEN CHEN, LAIYI WENG, Department of Materials, University of Oxford, PAUL HILL, Institute of Photonics, University of Strathclyde, SAM JOHNSON, Department of Materials, University of Oxford, ANGELO FRANGESKOU, PHIL DIGGLE, Department of Physics, University of Warwick, MICHAEL STRAIN, ERDAN GU, Institute of Photonics, University of Strathclyde, BEN GREEN, MARK NEWTON, Department of Physics, University of Warwick, JASON M SMITH, Department of Materials, University of Oxford, PATRICK SALTER, Department of Engineering, University of Oxford, GAVIN MORLEY, Department of Physics, University of Warwick — The nitrogen-vacancy (NV) defect within a diamond lattice has been shown as a viable candidate for a quantum register. Using laser writing, these defect centres can be placed with high precision at any depth through a sample, without inducing significant damage to the surrounding lattice [1-3], to create deep solid state qubit arrays. These sites have shown coherence times of 700 µs, as long as the longest achieved for room-temperature spin-echo coherence measurements in non-^{12}C enriched diamond [1]. Additionally, the technique can be used to create conductive graphitic tracks, which are the subject of current investigation for their potential to act as DC circuitry within the diamond. Configuring the wires such that NVs lie between ends of two wires may allow charge state transfer, bringing greater control of defects, and enable sites to be tuned precisely. It is hoped that, combining these aspects, a single diamond could hold many individually addressable qubits leading to a compact quantum processor.


*We acknowledge funding from the UK EPSRC (EP/M013243/1) and the Royal Society.

Nitrogen vacancy (NV) centres in diamond for fun and profit*

COLIN STEPHEN, University of Warwick, SOUGATO BOSE, University College London, ANGELO FRANGESKOU, University of Warwick, ATM ANISHUR RAHMAN, PETER F BARKER, University College London, LAIA GINES, SOUMEN MANDAL, University of Cardiff, MATTHEW W DALE, YASHNA LEKHAI, University of Warwick, LAIYI WENG, University of Oxford, PAUL HILL, University of Strathclyde, SAM JOHNSON, University of Oxford, PHIL DIGGLE, University of Warwick, MICHAEL STRAIN, ERDAN GU, University of Strathclyde, MARK NEWTON, BEN GREEN, University of Warwick, OLIVER A WILLIAMS, University of Cardiff, JASON M SMITH, PATRICK SALTER, University of Oxford, GAVIN MORLEY (Presenter), University of Warwick — We have proposed [1] and begun developing [2-4] an experiment in which a 1 μm diamond containing an NV centre would be put into a superposition of being in two places at once with a superposition distance of 1 μm. This builds on our previous proposals [5-7] and others [8].

Separately, we have shown that laser-writing allows NV centres to be created in chosen locations inside of a diamond, deep enough to allow solid immersion lenses to be made around them, and with spin coherence times at least as long as naturally occurring NV centres [9].

We are also developing a fibre-coupled magnetometer with an NV ensemble towards possible medical applications [10].


*We acknowledge funding from the Royal Society and the EPSRC.
Near-term protocols for deterministic photonic graph state generation*  
ANTONIO RUSSO (Presenter), EDWIN BARNES, SOPHIA ECONOMOU, Virginia Tech — Highly entangled "graph" states of photons have applications in universal quantum computing and in quantum communications. Here we present near-term experimentally realizable protocols for the deterministic production of graph states, with explicit recipes for nitrogen-vacancy centers in diamond and self-assembled quantum dots. We address the scalability of the approach, focusing on arbitrary size "cluster" states, which can support universal quantum computation.

*This research was supported by a NSF (grant nr: EFRI ACQUIRE 1741656).

Mechanical driving of nitrogen-vacancy centers in diamond*  
DOMINICA LYZWA (Presenter), PAOLA CAPPELLARO, Massachusetts Institute of Technology — We theoretically investigate high-frequency phonon-mediated dynamic mechanical driving of spin transitions in nitrogen-vacancy centers in diamond (NV). Mechanical driving is parity non-conserving and can allow quantum control of spin |−1⟩ ↔ |+1⟩ transitions that cannot be addressed using magnetic resonant fields [1,2]. By applying high-frequency mechanical stress, the electronic and nuclear spin interaction is averaged out in the manifold of the |−1⟩ ↔ |+1⟩ spin transition. This dynamic decoupling yields an increase in the nuclear dephasing time. Experimentally, fivefold longer times were demonstrated using a.c. stress generated by a diamond mechanical resonator [1]. We develop a theoretical framework for this increase in the dephasing time for dynamic mechanical driving. Exploring mechanical driving to induce entanglement aims to engineer NV ensemble entanglement at room temperature to increase sensitivity in quantum metrology.

[1] ER MacQuarrie et al., Coherent control of a nitrogen-vacancy center spin ensemble with a diamond mechanical resonator, Optica, 2015  

*Supported by DFG fellowship.

Engineering nitrogen-vacancy center electron-phonon coupling with a semi-confocal diamond acoustic resonator*  
HUIYAO CHEN (Presenter), CORNELL UNIVERSITY, ALEX JIANG, NOAH F ONPOONDO, SUNIL BHAVE, Purdue University, GREGORY FUCHS, Cornell University — Diamond-based microelectromechanical systems (MEMS) provide direct coupling between quantum states of nitrogen-vacancy (NV) center and the phonon modes inside the resonator. As a prime example, diamond thin film bulk acoustic resonators (BARs) feature integrated piezoelectric transducer and high-quality factor resonance modes up to the GHz frequency range. The bulk acoustic modes allow mechanical manipulation of deeply imbedded NV centers with long spin/orbital coherence, as recently demonstrated in experiments. Limited by the resonator size, ~100 um, coherent NV electron-phonon interaction is still scarce in current diamond BAR devices. In this talk, we present the design and fabrication of a semi-confocal diamond BAR device with f*Q product >10^14 [13]. The semi-confocal geometry confines the phonon mode laterally below 10 um. This drastic modal size reduction offers a boost in the NV center electron-phonon coupling with potential applications in spin-mediated resonator cooling and quantum resonator state control.

*Research support was provided by the Office of Naval Research (Grant N000141410812 and N000141712290).

Fabrication of High Quality Quantum Emitters in Diamond Nanostructures*  
MICHAEL WALSH (Presenter), ERIC BERSIN, SARA MOURADIAN, NOEL WAN, DIRK R. ENGLUND, Massachusetts Institute of Technology — As the field of solid-state quantum engineering matures, it is increasingly necessary to produce quantum emitters with narrow optical transitions and long spin coherence times aligned to nanophotonic structures. We demonstrate an emitter-device alignment technique enabling fabrication of photonic devices registered to nitrogen-vacancy centers (NVs). The alignment method relies on autonomously imaging emitters and registering them relative to an on-chip coordinate system. This technique can be performed on a large variety of emitters. The repeatability of this method suggests an accuracy down to 50 nm.

The ability to navigate a sample autonomously while collecting data on a large number of NVs enables statistical analyses. We demonstrate the utility of this by correlating the NVs host nitrogen isotope with the optical linewidth of the emitter to understand the effect of implantation. This technique has implications for investigating the effect on NVs as they go through fabrication processes to understand how the local environment may change.

*This work was supported by AFOSR grants FA12-1-0025, FA9550-14-1-0052, and FA9550-16-1-0391; NSF grants 0551153, 1231319, and 1641064; ARL grant 2875-Z8401005; and DOE grant DE-SC0014664; and a NSTRF grant number: NNH18ZHA007CRFI.
1:03PM L35.00010: Spectral stabilization and indistinguishable photon generation by electromechanical tuning of diamond color centers in nanophotonic devices∗ BARTHOLOMEUS MACHIELSE (Presenter), STEFAN BOGDANOVIC, SRUJAN MEESALA, MICHAEL J BUREK, CLEAVEN CHIA, GRAHAM JOE, Harvard University, SCARLETT GAUTHIER, University of Waterloo, MICHELLE V CHALUPNIK, JEFFREY HOLZGRAFE, LINBO SHAO, HAIG ATIKIAN, MIKHAIL LUKIN, MARKO LONCAR, Harvard University — Silicon-vacancy (SiV) color centers in diamond have excellent optical properties and spin coherence properties, making them ideal candidates for integration into quantum networks. However, their applications are limited by their spectral inhomogeneity and diffusion when implanted within nanophotonic devices. We present a platform for nano-electromechanically stabilizing and tuning the SiV spectral lines inside waveguides and cavities with emitter tuning range 3 times larger than the SiV inhomogeneous distribution. As demonstration of this platform’s capabilities, we tune two, waveguide coupled SiV color centers into resonance using strain and generate an entangled superradiant state between them. We demonstrate that this technique can be used for broad bandwidth suppression of spectral diffusion and to drive spectral lines with 10s of MHz bandwidth. Our platform for cavity coupled, individually tunable solid state quantum emitters with long coherence times should allow for controllable interactions between emitters and is a step towards the creation of a quantum repeater network.

∗STC Center for Integrated Quantum Materials (NSF Grant No. DMR-1231319), ONR MURI on Quantum Optomechanics (Award No. N00014-15-1-2761), NSF EFRI ACQUIRE (Award No. 5710004174) and NSF GRFP.

1:15PM L35.00011: Optical Characterization of Single Tin-Vacancy Centers in Diamond∗ ALISON RUGAR (Presenter), SHUO SUN, CONSTANTIN DORY, JELENA VUCKOVIC, Stanford University — Atom-like defects in diamond have emerged in recent years as candidates for solid-state, optically active qubits. Inversion-symmetric color centers based on group-IV impurities in diamond are of particular interest because of their strong optical properties and relatively good immunity to electric field noise. Phonon-induced transitions resonant with the ground-state (GS) splitting are a major cause of spin decoherence for these color centers but can be mitigated with an increased GS splitting. With a relatively large GS splitting of 850 GHz, the tin-vacancy (SnV) center in diamond holds potential for longer spin coherence times while also possessing good optical properties. In this talk, we will present our recent experimental characterization of the optical and spin properties of single SnV color centers in diamond nanopillars. We measure linewidths <30 GHz, observe a clear polarization dependence of the emission, and experimentally investigate the Zeeman splitting of the SnV. Our results match well the predictions of previous theoretical work.

∗Department of Defense National Defense Science and Engineering Graduate Fellowship
Army Research Office (ARO) (W911NF1310309)
National Science Foundation
Gordon and Betty Moore Foundation
Stanford Graduate Fellowship

1:27PM L35.00012: All-electron calculation of spin-spin interactions∗ KRISHNENDU GHOSH (Presenter), Mechanical Engineering, University of Michigan-Ann Arbor, HE MA, Chemistry, University of Chicago, VIKRAM GA VINI, Mechanical Engineering, University of Michigan-Ann Arbor, GIULIA GALLI, University of Chicago and Argonne National Laboratory — The decoherence time of defect-spin qubits is controlled by the interaction of nuclear and electronic spins and by that between electronic spins. A key quantity determining these interactions is the value of the electronic spin density at the nucleus, which in turn is a crucial ingredient to evaluate the hyperfine interaction (HF) and zero-field splitting (ZFS) tensors of a defect-spin qubit. Here we report all-electron calculations of the HF and ZFS tensors using real space density functional theory (DFT) calculations based on finite elements. While all-electron DFT calculations using localized basis sets (e.g. Gaussians) can be conveniently performed to determine HF and ZFS tensors of molecules and clusters, they become much more demanding for periodic solids, and plane-wave based calculations are prohibitively difficult to converge. We show that real-space, finite element DFT calculations provide robust estimates of ZFS and HF for both molecules and solids and we present results for molecules and the nitrogen-vacancy center in diamond. We also show that coarse-graining capabilities of the real space mesh included in our formulation enable efficient computations, by avoiding redundant mesh refinements far from the nuclei.

∗We acknowledge funding from NSF-MRSEC.
1:39PM L35.00013: Deep-center defects in semiconductors  MARIYA ROMANOVA (Presenter), JELENA SJAKSTE, NATHALIE VAST, Ecole Polytechnique, Laboratoire des Solides Irradiés, CEA-DRF-IRAMIS, CNRS UMR 7642, France — A renewed interest has been recently devoted to the study of deep-center defects in materials for applications in emergent quantum technologies such as quantum sensing. The typical example of a deep-center defect is the nitrogen-vacancy (NV) center in diamond. The spin states of this defect can be optically manipulated at room temperature, which makes it attractive for magnetic sensing [1].

The aim of this work is to obtain a reference method to model the electronic properties of the NV-center in diamond for the purpose of magnetic sensing. Density Functional Theory (DFT) is widely used for the calculation of the electronic structure of defects [2]. However, the single Slater determinant nature of the DFT wavefunctions does not allow for the calculations of the many-body levels of some defects. In the present work I develop a Hubbard model for the NV-center with the model parameters calculated by wannierization of defect levels computed with DFT-GGA and HSE06 calculations in large supercells. I will show that the model enables access to the multideterminant defect levels.


1:51PM L35.00014: Manipulation of electronic defects in hexagonal boron nitride*  ELANA URBACH (Presenter), TAMARA SUMARAC, HELENA KNOWLES, Harvard University, JAVIER D SANCHEZ-YAMAGISHI, University of California Irvine, SOONWON CHOI, University of California Berkeley, BO DWYER, TROND I ANDERSEN, MIKHAIL LUKIN, Harvard University — Hexagonal boron nitride (hBN) provides a regular nuclear spin lattice, which makes it a promising platform for studying models of spin dynamics. This material also hosts numerous electronic defects that have been well-characterized in bulk electron paramagnetic resonance (EPR) spectroscopy. Nitrogen vacancy (NV) centers in diamond are very sensitive local magnetic field probes that can polarize and control single electronic spins and nanoscale volumes of nuclear spins. In this experiment we use an NV center to manipulate electronic defects in and near hBN, and we are working towards utilizing these defects for better initialization and control of local nuclear spins.

*This work was supported by the Defense Advanced Research Projects Agency (QuASAR program), National Science Foundation (NSF), Center for Ultracold Atoms, Army Research Office (ARO) MURI program, National Security Science and Engineering Faculty Fellowship program, and Moore Foundation. E.K.U. acknowledges support by the NSF (Graduate Research Fellowship Program under grant DGE1144152).

2:03PM L35.00015: Auto-Locking Overhauser Field to the Sweet Point for an Electron Spin by Quantum Weak Measurement of Nuclear Spins*  GENGLI ZHANG (Presenter), Physics, The Chinese University of Hong Kong, VINCENT JACQUES, Laboratoire Charles Coulomb, Université de Montpellier and CNRS, PATRICE BERTET, Quantronics group, Université Paris-Saclay, RENBAO LIU, Physics, The Chinese University of Hong Kong — The sweet points such as the clock transitions (CTs) are important for quantum information processing (QIP) and quantum sensing technologies. Being inherently robust to the fluctuations of the environment, they provide almost the best options to counteract the decoherence of the electron spin. The random fields from the environment (Overhauser fields) that lead to the decoherence of the electron spin, however, can also destroy the sweet points, which sets up a big obstacle to the applications. Here we propose a new dynamical nuclear polarization (DNP) scheme that can auto-lock the Overhauser field to the sweet point of the nitrogen vacancy (NV) center. The DNP channel is established by combining the bath state dependent microwave (MW) control, the conditional flipping of the nuclear spins and the optical pumping of the NV center electronic spin. The mechanism can also be understood as sequential weak measurements of the nuclear spins followed by entropy dumping through initialization of the electron spin.

*This work was supported by Hong Kong Research Grants Council ANR/RGC Joint Research Scheme Project A-CUHK403/15.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L36 DMP: Physics of Natural Phenomena  BCEC 205C - Antoinette Taylor, Los Alamos National Laboratory -  Tag(s): Invited, Undergraduate
11:15AM L36.00001: Fire/atmosphere Feedbacks that Control Wildland Fire [Invited] RODMAN RAY LINN (Presenter), Los Alamos National Laboratory — Wildfires pose a threat to life, property and critical infrastructure, but wildland fire is an unavoidable part of the nature. In order to improve our ability to cope with wildfires and anticipate their evolving roles on the earth system we need to better understand how they interact with their environment. Recent fire behavior research illustrates the importance of the two-way feedbacks between fires and the surrounding atmosphere, which is influenced by the vegetation structure and topography as well as ambient winds. The effectiveness and consequences of fuels management activities are tied not only on the removal of combustible fuel, but also on the changes in the ventilation induced by decreased vegetation drag, which can potentially increase fire spread. Safe use of prescribed fires to reduce fire risk while accomplishing ecologic objectives typically depends on fire practitioner's ability to anticipate the interaction of multiple fires. This interaction is controlled by the competition between their fire-induced indrafts. Topographic influences on fire behavior are dominated by terrain-induced changes in entrainment patterns that control the patterns of heat transfer to unburned fuel. Multi-scale two-way fire/atmosphere feedbacks determine heterogeneous fire line dynamics and thus fire spread, the effects of fires on ecology and the near-field lofting and transport of the smoke. Unfortunately, deciphering the complex interaction between fires and surrounding atmosphere through field and laboratory experiments alone has been challenging, but recent advancements in computing power have created new opportunity for the complimentary use of numerical models to provide additional perspectives concerning fire/atmosphere feedbacks that have previously been challenging to explore. Examples of ways that the interactions between fire and surrounding atmosphere dictate fire behavior and the use of numerical models to investigate this coupling will be discussed.

11:51AM L36.00002: The Physics of Climate and Climate Change [Invited] KERRY EMANUEL (Presenter), Massachusetts Institute of Technology — The talk will begin with a broad overview of climate science, including the history of the science itself, and what we have learned about the Earth's climate system through analysis of paleoclimate data, the instrumental record, and, most importantly, the fundamental physics, chemistry, and biology underlying the climate system. Projections of future climates, made using both simple and complex models, will be discussed, with an emphasis on sources of uncertainty together with an assessment of whether and to what extent the level of uncertainty can be reduced. I will end the talk with reflections on how physicists might help find solutions for mitigating climate change.

12:27PM L36.00003: Mixed signals in future climate extremes: understanding counterintuitive results* [Invited] SARAH KAPNICK (Presenter), Geophysical Fluid Dynamics Laboratory, NOAA — If temperatures warm in the future, if everything else remains constant, there should be less snowfall since temperatures will rise above freezing more often. If we know a region will become drier on average in the future, and storms have constant rainfall amounts, the likelihood of extreme events should decline. But these stationarity assumptions do not hold true, resulting in what can appear to be counterintuitive changes in climate phenomena and extremes. We will discuss where snowfall accumulation and blizzards may actually increase and why some glaciers have been expanding. We will also discuss why a region may become drier overall, but also have increased risk for extreme precipitation events. While these regional changes may seem counterintuitive, they can actually be explained by unique conditions, seasonality, and changes in atmospheric moisture.

*Research and computational support from NOAA. A portion of this research is supported by NASA grant #15-HMA15-0016.
1:03PM L36.00004: Physics of Earthquakes: The Real Earthshaking Science [Invited]  RACHEL E ABERCROMBIE (Presenter), Department of Earth & Environment, Boston University — The study of earthquakes is driven by the desire to understand our dynamic planet and to minimize the devastation that earthquakes can cause. Earthquake science spans a huge range of temporal and spatial scales. The largest earthquakes rupture faults that are 100s to 1000s of kilometers long but start from nucleation regions so small that they have never been reliably observed. Earthquake faults move at only millimeters to centimeters a year but earthquake ruptures propagate at speeds of kilometers a second, and most earthquakes last less than a minute.

I will begin by introducing the basic concepts and observations of earthquake occurrence, and the widely-accepted, friction-based physical understanding of fault failure and rupture. I will then discuss how more recent observations and modeling are providing improved insights into this earthshaking science.

Fault rocks obtained from drilling through the San Andreas Fault and other major earthquake ruptures are providing evidence of the frictional strength of these plate boundary faults. Great earthquakes are being recorded by more, better instruments than ever before providing unprecedented resolution of the rupture process. The increase in anthropogenically-induced earthquakes forms an unintentional semi-controlled experiment to probe the triggering process. Improved geodetic observations are revealing that earthquakes are only part of a continuum of fault rupture types, with durations varying from seconds to minutes, days and even months.

Dynamic modeling of individual earthquakes on super computers can now produce realistic simulations of earthquake rupture and shaking. Earthquakes do not occur in isolation but interact as a consequence of both the dynamic and static stress changes they cause. Progress is also being made on modeling earthquakes as part of a complex system of deformation.

* Awards from the National Science Foundation, and the Southern California Earthquake Center.

1:39PM L36.00005: The mechanics of hydraulic fractures in glaciers, volcanoes, and reservoirs [Invited]  BRAD LIPOVSKY (Presenter), Earth and Planetary Sciences, Harvard University — Fractures that interact with fluid are ubiquitous in Earth systems. In the floating ice shelves that fringe the grounded Antarctic Ice Sheet, hydraulic fractures pose a threat to ice sheet stability. Hydraulic fractures in volcanoes transport magma and other fluids through Earth's crust. And hydraulic fractures may be engineered to improve the performance of geothermal energy resources. The mechanical analysis of hydraulic fractures may take several viewpoints, of which I focus on two. First, linear elastic fracture mechanics provides insight into the dynamics of hydraulic fractures at shallow depths above the brittle–ductile transition. Second, active hydraulic fractures may create mechanical vibrations that are observable at distant seismometers. In both instances, geophysical data and mechanical analyses together provide insights into stunning natural phenomena that have direct bearing on human civilization.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L37 GMAG DCMP DMP: Iridates -- Honeycomb Lattice and Other Geometries BCEC 206A - Stuart Calder, Oak Ridge National Laboratory - Tag(s): Focus

11:15AM L37.00001: Anomalous Magnetic Torque Signal in a Kitaev Spin Liquid Candidate [Invited]  VIKRAM NAGARAJAN (Presenter), ALEJANDRO RUIZ, MAYIA VRANAS, GILBERT LOPEZ, Department of Physics, University of California, Berkeley, GREGORY T. MCCANDLESS, Department of Chemistry and Biochemistry, The University of Texas at Dallas, JULIA Y. CHAN, Department of Chemistry, University of Texas at Dallas, NICHOLAS BREZNAY, Department of Physics, Harvey Mudd College, ITAMAR KIMCHI, Center for Theory of Quantum Matter, University of Colorado, Boulder, JAMES G. ANALYTIS, Department of Physics, University of California, Berkeley — The honeycomb iridates have received much attention as potential material realization of Kitaev's exactly solvable honeycomb model, which predicts a quantum spin liquid ground state with fractionalized Majorana excitations. While the presence of magnetic order at low temperature makes the Kitaev nature of the iridates less apparent, it may still be possible to detect high-temperature signatures of the spin liquid state. In this study, we present data on a unique high-temperature phase of lithium iridate as measured by torque magnetometry.

*Supported by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-05CH11231.
A unique feature of 5d materials is the fact that spin-orbit coupling, Coulomb interactions, and crystal electric field effects are of comparable strength. In the edge-sharing honeycomb iridates, this competition of energy scales leads to a strongly anisotropic, Ising-like exchange between neighboring isospin-1/2 moments. Such interactions couple each spin to orthogonal components of the three neighboring spins and, as a consequence, no single exchange direction can be simultaneously satisfied, leading to strong frustration closely approximated by the Kitaev Hamiltonian. So far, most potential Kitaev materials have been found to order at low temperatures, eluding the sought-after QSL state. Nonetheless, experiments suggest that Kitaev exchange is the dominant spin interaction in these systems, with additional small contributions from a direct Heisenberg and a symmetric off-diagonal exchange term. We previously showed that a magnetic field completely suppresses the complex incommensurate spiral order in β-Li2IrO3, while stabilizing a commensurate zig-zag component similar to the ground state observed in Na2IrO3. In this work, we present the magnon excitation spectra of β-Li2IrO3 in zero and finite magnetic field, at zone centers corresponding to both coexisting states.

Spin-Glass Behavior in Hole-Doped Lithium Iridates

*We acknowledge the Department of Energy, National Science Foundation, the Gordon and Betty Moore Foundation, and UC LEADS.

Kitaev iridates in 3D: magnetic and structural instabilities

Here, I will present recent results on the pressurized hyperhoneycomb iridate β-Li2IrO3 and argue that this compound can be tuned to a classical spin liquid state triggered by the reduction in the nearest-neighbor Kitaev term K and the enhancement of the off-diagonal anisotropy Γ. We find that above 1.4 GPa pressurized β-Li2IrO3 separates into a mixture of dynamic and frozen spins representing a partially frozen spin liquid, as expected in a system where spin dynamics is supported by thermal rather than quantum fluctuations.

I will further show how Kitaev magnetism is realized in three-dimensional frameworks of Ir4+ hexahalides that can be chemically tuned even at ambient pressure, thus giving rise to a variety of intertwined structural and magnetic instabilities.

*Financial support by the Alexander von Humboldt Foundation and German Science Foundation (TRR80) is acknowledged.
**12:27PM L37.00005: NQR investigation of low frequency spin dynamics in Kitaev spin liquid candidate material Cu$_2$IrO$_3$ in zero magnetic field**

SEAN K S TAKAHASHI, JIAMING WANG, ALEXANDRE ARSENAULT, Dept. of Physics and Astronomy, McMaster University, MYKOLA ABRAMCHUK, FAZEL FALLAH TAFTI, Dept. of Physics, Boston College, PHILIP SINGER, Dept. of Chemical and Biomolecular Engineering, Rice University, SUNG-SIK LEE, TAKASHI IMAI (Presenter), Dept. of Physics and Astronomy, McMaster University — Cu$_2$IrO$_3$ [1] is a Kitaev spin liquid candidate material with nearly ideal honeycomb planes consisting of Ir magnetic moments, and does not exhibit a bulk magnetic long range order. We report $^{63,65}$Cu Nuclear Quadrupole Resonance (NQR) investigation of Cu$_2$IrO$_3$ in zero external magnetic field [2]. Unlike the case of the celebrated sister compound Na$_2$IrO$_3$ or $\alpha$-RuCl$_3$ with a bulk antiferromagnetic ground state below $T_N$, spin dynamics reflected on the NMR relaxation rate $1/T_1$ does not show a divergent behavior caused by conventional magnons. We can therefore probe the intrinsic low energy spin excitations of the Kitaev planes using NQR in zero magnetic field in a broad window of temperature.


*The work at McMaster was supported by NSERC and CIFAR. The work at Boston College was supported by NSF DMR-5104811.

**12:39PM L37.00006: NMR investigation of Kitaev spin liquid candidate material Cu$_2$IrO$_3$**

JIAMING WANG (Presenter), SEAN K S TAKAHASHI, ALEXANDRE ARSENAULT, Dept. of Physics and Astronomy, McMaster University, MYKOLA ABRAMCHUK, FAZEL FALLAH TAFTI, Dept. of Physics, Boston College, PHILIP SINGER, Dept. of Chemical and Biomolecular Engineering, Rice University, SUNG-SIK LEE, TAKASHI IMAI, Dept. of Physics and Astronomy, McMaster University — Cu$_2$IrO$_3$ is a Kitaev spin liquid candidate material [1]. In this talk, we report $^{63,65}$Cu high-field Nuclear Magnetic Resonance (NMR) measurements of Cu$_2$IrO$_3$ [2]. We probed the intrinsic spin susceptibility based on $^{63,65}$Cu Knight shift, and the magnetic field effects on paramagnetic spin dynamics based on NMR relaxation rate $1/T_1$.


*The work at McMaster was supported by NSERC and CIFAR. The work at Boston College was supported by NSF DMR-5104811.

**12:51PM L37.00007: Competition between static and dynamic magnetism in the Kitaev spin liquid material Cu$_2$IrO$_3$**

ERIC KENNEY (Presenter), Department of Physics, Boston College, CARLO SEGREG, Department of Physics, Illinois Institute of Technology, WILLIAM LAFARGUE-DIT-HAURET, Institut des Sciences Chimiques de Rennes, OLEG I. LEBEDEV, Laboratoire CRISMAT, Ensicaen-CNRS, MYKOLA ABRAMCHUK, Department of Physics, Boston College, ADAM BERLIE, STEPHEN P. COTTRELL, Rutherford-Appleton Laboratory, ISIS Neutron and Muon Source, GEDIMINAS SIMUTIS, Laboratory of Muon Spin Spectroscopy, Paul Scherrer Institute, FARANAK BAHRAMI, Department of Physics, Boston College, NATALIA E. MORDVINOVA, Laboratoire CRISMAT, Ensicaen-CNRS, JESSICA L MCCHESNEY, GILBERTO F L FABBRI, Advanced Photon Source, Argonne National Laboratory, XAVIER ROCQUEFELTE, Institut des Sciences Chimiques de Rennes, MICHAEL JOHN GRAF, FAZEL FALLAH TAFTI, Department of Physics, Boston College — Cu$_2$IrO$_3$ is a new honeycomb iridate without thermodynamic signatures of long-range order. Here, we use muon spin relaxation to uncover the magnetic ground state of Cu$_2$IrO$_3$. We find a two-component depolarization with slow and fast relaxation rates corresponding to distinct regions with dynamic and static magnetism, respectively. X-ray absorption spectroscopy and first principles calculations identify a mixed copper valence as the origin of this behavior. Our results suggest that a minority of Cu$^{2+}$ ions nucleate regions of static magnetism whereas the majority of Cu$^{+}$/Ir$^{4+}$ on the honeycomb lattice give rise to a Kitaev spin liquid.
1:03PM L37.00008: Neutron Scattering Study of Kitaev Spin-Liquid Candidate H$_3$LiIr$_2$O$_6$ — THOMAS HALLORAN (Presenter), COLLIN BROHOLM, Johns Hopkins University, KEMP PLUMB, Physics, Brown University, TOMOHIRO TAKAYAMA, Max Planck Institute for Solid State Research, HIDENORI TAKAGI, Physics, University of Tokyo — A central theme of condensed matter physics in recent years has been the realization of materials that exhibit a quantum spin-liquid state beyond one dimension. The exactly solvable Kitaev model of a quantum spin liquid consists of a 2D honeycomb lattice of $J_{eff} = \frac{1}{2}$ magnetic ions with bond dependant interactions. NMR and bulk sample characterization has suggested that H$_3$LiIr$_2$O$_6$ could be a spin-liquid [1]. The structure consists of a honeycomb lattice of Ir$^{4+}$ ions with strong spin-orbit coupling to support the bond dependent exchange interactions required in the Kitaev model. While previous lithium iridates have all been found to magnetically order at low temperature, specific heat and magnetization measurements show no order in this material down to low temperature. Using inelastic neutron scattering on SEQUOIA at ORNL, we probed the material magnetic excitations in D$_3$Li$^{193}$Ir$_2$O$_6$. We describe features in neutron scattering which are consistent with those of a KSL. Through a first moment analysis of the scattering data we determine the range of interactions and an estimate for the ground state energy.


*EFRC Grant DE-SC0019331

1:15PM L37.00009: Crystal electric field and structural study of $J_{eff} = 1/2$ K$_2$IrX$_6$ (X = Cl, Br) — DALMAU REIG-I-PLESSIS (Presenter), SANGJUN LEE, University of Illinois at Urbana-Champaign, L. HOZOI, MOHAMED SABRY ELDEEB, IFW Dresden, ADAM ACZEL, Oak Ridge Nat. Lab., MARY UPTON, Argonne Nat. Lab., PATRIC CLANCY, McMaster University, JACOB RUFF, Cornell University, JEROEN VAN DEN BRINK, IFW Dresden, PETER ABBAMONTE, GREG MACDOUGALL, University of Illinois at Urbana-Champaign —

Strong spin orbit coupling in 5d materials has been a focus of research due to the wide variety of exotic phases which can exist in these systems. Of particular interest are systems with octahedral coordination, the triply degenerate $t_{2g}$ state will split into the occupied $J_{eff} = 3/2$ and the partially occupied $J_{eff} = 1/2$ states. It is this $J_{eff} = 1/2$ state that can host a large range of exotic phases such as quantum spin liquids and superconductivity. Here we present detailed data on two Iridium halide materials, K$_2$IrX$_6$, X = Cl, Br, which have the antifluorite structure and the Ir atom inside separated halide octahedra. Powder X-ray scattering study show a newly observed structural transition in the Br compound at T$_c$=180K. Resonant inelastic X-ray scattering data and X-ray absorption data are combined with quantum chemistry calculations to study the crystal electric field levels, and show that these materials show record proximity to the ideal $J_{eff} = 1/2$ state at all temperatures down to T=5K.

*This work was supported by the National Science Foundation, grant number DMR-1455264-CAR.

1:27PM L37.00010: Multi-scale Quantum Criticality driven by Kondo-lattice Coupling in Pyrochlore Systems — HANBIT OH (Presenter), EUN-GOOK MOON, KAIST, YONG-BAEK KIM, Department of Physics, University of Toronto, SANGJIN LEE, KAIST —

Pyrochlore systems with local moments and 5d conduction electrons offer excellent material platforms for the discovery of exotic quantum many-body ground states. Notable examples include U(1) quantum spin liquid (QSL) and semimetallic non-Fermi liquid state. Here we investigate emergent quantum phases and their transitions driven by the Kondo-lattice couplings. Using the renormalization group method, we show that weak Kondo-lattice coupling is irrelevant, leading to a fractionalized semimetal phase with decoupled local moments and conduction electrons. Upon increasing the Kondo-lattice coupling, this phase is unstable to the formation of broken symmetry states. The important thing is the opposing influence of the Kondo-lattice coupling and long-range Coulomb interaction. The former prefers to break the particle-hole symmetry while the latter tends to restore it. The characteristic competition leads to multiple phase transitions, first from a fractionalized semimetal phase to a fractionalized Fermi surface state with particle-hole pockets, followed by the second transition to a fractionalized ferromagnetic state. Multi-scale quantum critical behaviors appear at non-zero temperatures and with the external magnetic field near such quantum phase transitions.
1:39PM L37.00011: Observing spin fractionalization of the Kitaev spin liquid via temperature evolution of the K-edge RIXS response

GABOR HALASZ, Oakridge National Laboratory, STEFANOS KOURTIS, Physics, Boston University, JOHANNES KNOELLE, Physics, Imperial College London, NATALIA PERKINS (Presenter), University of Minnesota — A prominent feature of the Kitaev quantum spin liquid is fractionalization of the spin degree of freedom. Here we propose that the temperature evolution of the fractionalization in the Kitaev honeycomb model can be studied by the resonant inelastic X-ray scattering (RIXS). We calculate the RIXS response of the Kitaev honeycomb model and show how the momentum-energy map of the fractionalization varies with temperature. We also suggest that the indirect RIXS process at Ru K-edge which allows for sub-meV resolution can provide important insights about the structure of the excitation spectrum in α-RuCl₃.

*NBP was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award \\#DE-SC0018056.

1:51PM L37.00012: Understanding counter-rotating spiral ordering in three dimensional Kitaev materials

PANAGIOTIS PETER STAVROPOULOS (Presenter), ANDREI CATUNEANU, HAE-YOUNG KEE, University of Toronto — The counter-rotating spiral ordering found in three-dimensional (3D) iridate Kitaev candidates suggest frustration of spin interactions and raise a possibility of nearby spin liquid phases. Understanding the microscopic mechanism of this ordering may provide routes to 3D Kitaev spin liquids. We study a minimal 3D model including Kitaev K and a symmetric off-diagonal bond-dependent Γ interaction on the hyperhoneycomb lattice by using exact diagonalization (ED). An ED cluster was chosen to satisfy a hidden SU(2) symmetry. The magnetic ordering in the transformed basis then generically maps to the counter-rotating noncoplanar spiral order of the original spin when the moment is pinned along a certain direction. When K and Γ are negative, a small positive Heisenberg interaction favours the (1,1,0) direction consistent with the reported spiral order in β-Li₂IrO₃. Our findings offer a relevant set of microscopic parameters, which in turn guides a way to approach possible Kitaev spin liquids.

*This work was supported by NSERC of Canada, CIFAR and SciNet.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L38 GMAG DMP: Spin Chains, Criticality and QPT

11:15AM L38.00001: Magnetic-field induced quantum phase transitions in spin-1/2 XXZ chain materials

THOMAS LORENZ (Presenter), Institute of Physics II, University of Cologne, Germany — Low-dimensional quantum spin systems offer an ideal playground to study the generic behavior close to magnetic-field induced quantum phase transitions. Of particular interest is the XXZ spin-1/2 chain model with anisotropy parameter Δ=Jz/Jxy of the exchange couplings acting either on the z- or the xy-spin components. For Δ=0, 1 and ∞, respectively, the exactly solvable XY, Heisenberg and Ising chain models are covered, but real materials are typically located in between these models and there are additional intra- and/or inter-chain couplings. In this contribution, our recent experimental studies of model materials with field-induced quantum phase transitions will be presented. Cu(C₄H₄N₂)(NO₃)₂, is an almost ideal realization of the Heisenberg chain with weak intra-chain coupling, such that we could study its field induced quantum phase transition in great detail. The experimental data are almost perfectly reproduced by Bethe-Ansatz calculations over a wide temperature and field range and on approaching the quantum critical field the systematic evolution of the generic quantum critical behavior is clearly observed in the experimental data [1]. In BaCo₂V₂O₈, the Co²⁺ ions realize effective spin-1/2 chains with pronounced Ising anisotropy. Here, sizable inter-chain couplings cause long-range, 3D antiferromagnetic order with complex magnetic-field temperature phase diagrams [2]. For a particular transverse-field direction, however, the field-induced suppression of the 3D magnetic order is well separated from the region where we observe the characteristic quantum critical behavior expected for the one-dimensional Ising spin chain in transverse magnetic field [3].


*This work was supported by the Deutsche Forschungsgemeinschaft via CRC 1238, SFB 1143, TRR 80, FOR 2316, and FOR 960.
**11:51AM L38.00002: Impact of pressure on the magnetic order in an S=1/2 quantum antiferromagnet**

TAO HONG (Presenter), Neutron Scattering Division, Oak Ridge National Laboratory, QING HUANG, Department of Physics and Astronomy, University of Tennessee, SACHITH DISSANAYAKE, Department of Physics, Duke University, YIMING QIU, National Institute of Standards and Technology, YAN WU, HUIBO CAO, WEI TIAN, Neutron Scattering Division, Oak Ridge National Laboratory, HAI DONG ZHOU, Department of Physics and Astronomy, University of Tennessee, MARK M. TURNBULL, Carlson School of Chemistry and Biochemistry, Clark University — Here we present a neutron scattering study on a spin-1/2 two-leg ladder antiferromagnet C9D18N2CuBr4 (DLCB for short) under applied hydrostatic pressure. In DLCB, the inter-ladder coupling is sufficiently strong to drive the system to the Néel antiferromagnetic ordering phase below $T_N=2$ K and the analysis of the spin Hamiltonian reveals that DLCB is close to the quantum critical point in two dimensions at zero field and ambient pressure [1]. Single-crystal neutron diffraction measurements under pressures up to 1.3 Gpa suggest that size of the staggered moment becomes suppressed with increase of pressure and the magnetic order breaks down above pressure ~1.0 Gpa.

References:

*A portion of this research used resources at the High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

**12:03PM L38.00003: High pressure and high magnetic field tuning of the S = 1 quantum antiferromagnet system**

DAN SUN (Presenter), Los Alamos National Laboratory, SAM CURLEY, PAUL GODDARD, Warwick University, JACQUELINE VILLA, JAMIE MANSON, Eastern Washington University, JOHN SINGLETON, FEDOR BALAKIREV, Los Alamos National Laboratory — [Ni(HF$_2$)(pyz)$_2$]SbF$_6$ is a quasi-one-dimensional S = 1 antiferromagnet in which the magnetic ground state can be tuned by changing the single-ion anisotropy (D) and the intrachain (J) and interchain (J') exchange interactions, allowing exploration of the Haldane phase diagram close to quantum criticality. With a newly developed pressure cell designed for pulsed magnetic fields of up to 100 T, we tune the above interactions in [Ni(HF$_2$)(pyz)$_2$]SbF$_6$ using hydrostatic pressures of up to 5.4 GPa. The characteristic form of the magnetic susceptibility was measured in pulsed fields of up to 65 T using a Proximity Detector Oscillator (PDO), allowing values of D, J and J' to be inferred at each pressure.

*The National High Magnetic Field Lab Pulsed Field facility is supported by the National Science foundation under cooperative Grant Nos. DMR-1157490 and DMR-1644779, the U.S. DOE, and the State of Florida.

**12:15PM L38.00004: Pressure-Tuning through the $D/J \approx 1$ Quantum Critical Point in an $S = 1$ Antiferromagnetic Chain**

MARCUS K. PEPRAH, PAUL S. EDWARDS, Dept. of Physics and NHMFL, University of Florida, JOHN CAIN, Dept. of Chemistry, University of Florida, ORLANDO TREJO, JAYNISE M. PEREZ, PEDRO A. QUINTERO, Dept. of Physics and NHMFL, University of Florida, JAREDS SINGLETON, LARRY PAUL ENGELHARDT, Dept. of Physics and Astronomy, Francis Marion University, SC, SAUL H. LAPI DUS, X-ray Science Division, Argonne National Laboratory, ERIK CIZMAR, Dept. of Condensed Matter Physics, Institute of Physics, P. J. Safárik University, Košice, Slovakia, JAMIE MANSON, Dept. of Chemistry and Biochemistry, Eastern Washington University, MARK MEISEL (Presenter), Dept. of Physics and NHMFL, University of Florida — Properties of [Ni(HF$_2$)(3-Clpy)$_4$]BF$_4$ (py = pyridine), or NBCT, suggest this S = 1 chain is near the $D/J \approx 1$ quantum critical point with easy-plane anisotropy $D = 4.3$ K, intrachain antiferromagnetic interaction $J = 4.86$ K, and no long-range order to 25 mK [1]. To clarify other work [2], the low field (0.1 T) susceptibility $\chi(2$ K $< T < 300$ K) was studied as a function of pressure ($P < 1.5$ GPa). These data are contrasted with isothermal (300 K) powder XRD studies made with $P < 2.5$ GPa. The pressure evolution of $\chi(T)$ correlates with structural modifications. With no evidence of a structural transition, the $\chi(T)$ data can be simulated by changes of $J$ and $D$ [3]. Complemented by inelastic neutron studies ($P$ and $B = 0$ and $T > 300$ mK) [4], NBCT appears to be the first S = 1 antiferromagnetic chain that can be pressure-tuned from the Haldane phase to the Large-D regime by traversing the $D/J \approx 1$ quantum critical point.


*NSF via DMR-1461019 (UF Physics REU for JMP), DMR-1644779 (NHMFL), DMR-1703003 (JLM), and DMR-1708410 (MWM). XRD at the APS-ANL DOE Contract DE-AC02-06CH11357.*
12:27PM L38.00005: z=2 quantum critical dynamics in spin chain and spin ladder compounds

DOMINIC BLOSSER (Presenter), VIVEK BHARTIYA, ETH Zurich, NOAM KESTIN, Department of Theoretical Physics, Université de Genève, KIRILL POVAROV, ETH Zurich, DAVID J. VONESHEN, ROBERT BEWLEY, ISIS Facility, Rutherford Appleton Laboratory, EMANUELE COIRA, THIERRY GIAMARCHI, Department of Theoretical Physics, Université de Genève, ANDREY ZHELUDEV, ETH Zurich — By means of high resolution inelastic neutron scattering, we investigate finite temperature critical dynamics near the magnetic field induced quantum critical point with dynamical exponent \( z = 2 \) in one dimension.

In the \( S=1/2 \) Heisenberg spin chain compound \( K_2CuSO_4Cl_2 \) at saturation, we find correlations characteristic of the \( z=2, d=1 \) quantum critical point. At the same time we find a novel thermally activated longitudinal mode that remains underdamped across most of the Brillouin zone. By comparison to finite temperature density matrix renormalization group (DMRG) calculations we quantitatively explain the experimental data [1].

In the strong rung quantum spin ladder \( (C_5H_{12}N)_2CuBr_4 \) (BPCB), at the same \( z=2, d=1 \) critical point, as expected we find a similar low energy excitation spectrum. However, making use of the additional symmetry of the spin ladder, here we can separate universal critical and non-universal structure factor contributions. We find universal finite-temperature scaling of the transverse local dynamic structure factor in spectacular quantitative agreement with long-standing theoretical predictions. Already at rather low temperatures, we again observe strong non-universal longitudinal fluctuations [2].


12:39PM L38.00006: The Magnetocaloric Effect in Exotic Spin Chain Compounds

ROBERT WILLIAMS (Presenter), PAUL GODDARD, SAM CURLEY, Physics, University of Warwick, YOSHIMITSU KOHAMA, AKIRA MATSUO, The Institute for Solid State Physics, University of Tokyo, SYDNEY KAECH, ZACHARY MANSON, JAMIE MANSON, Chemistry, Eastern Washington University — The seminal \( S=1/2 \) chain model is highly sensitive to deviations from the ideal Hamiltonian which, together with the intrinsic quantum fluctuations due to low-dimensionality, can induce a range of exotic behaviours. One such perturbation is an alternating local crystal structure, which produces a field-induced gap to solitonic excitations and promotes non-collinear spin structures. The sine-Gordon (SG) model captures this behaviour at low fields, but breaks down as systems approach saturation. We report the results of pulsed-field adiabatic measurements of the magnetocaloric effect in the archetypal SG chain material \( [(pym)-Cu(NO_3)_2(H_2O)_2] \), plus the novel chiral spin-chain compound with four-fold periodicity along the chain axis: \( [Cu(pym)(H_2O)_2]SiF_6.H_2O \), \( (pym=N_2C_4H_4) \). The chiral system displays a rich variety of excitations above a gap which, in contrast to the SG model, has a linear field-dependence and suppressed magnitude. These measurements provide a powerful means of probing both the magnetic entropy across phase diagrams, and the quantum critical behaviour near saturation. Our results highlight similar underlying physics in the compounds, but also indicate intriguing qualitative differences in the quantum phase transitions at high field.

*We thank the ERC and ISSP for funding
Pressure induced magnetic order in the novel 1D magnet K$_2$Cr$_8$O$_{16}$

OLA KENJI FORSLUND (Presenter), ELISABETTA NOCERINO, Royal Institute of Technology, DANIEL ANDREICA, Babes-Bolyai University, YASMINCE SASSA, Uppsala University, HIROSHI NOZAKI, IZUMI UMEGAKI, Toyota Central Research and Development Laboratories Inc., VIKTOR JONSSON, Royal Institute of Technology, ZURAB GUGUCHIA, ZURAB SHERMADINI, RUSTEM KHASANOV, Paul Scherrer Institut, MASAHIKO ISOBE, Max Planck Institute for Solid State Research, YUTAKA UEDA, oyota Physical and Chemical Research Institute, JUN SUGIYAMA, Toyota Central Research and Development Laboratories Inc., MARTIN MÅNSSON, Royal Institute of Technology, HIDENORI TAKAGI, Max Planck Institute for Solid State Research — The title compound, K$_2$Cr$_8$O$_{16}$, belongs to a series of quasi-1D compounds synthesised using a high-pressure/-temperature technique. The channels are formed by zig-zag Cr$_2$O$_4$ chains parallel to the c-axis and K cations occupying the center. Intriguingly, the compound undergoes a metal to insulator transition while maintaining the ferromagnetic order [1, 2], established by a Peierls transition [3]. Pressure dependent studies on this compound is fairly limited and the complete phase diagram of this compound is not fully resolved, especially the low temperature / high pressure region [4]. Here, pressure dependent muon spin rotation/relaxation (μSR) data is presented, which uniquely allow us perform measurements in zero applied field and hereby access the true intrinsic material properties. Finally, neutron diffraction has recently been conducted in order to elucidate the detailed nature of the complex phase diagram.


Magnetic exchange interactions in the BaM$_2$Si$_2$O$_7$(M= Cu, Co, Mn) system

WEIDONG LUO (Presenter), CHENGYANG XU, GUOHUA WANG, JIE MA, Shanghai jiao Tong University — A quasi 1D system with weak exchange coupling between the magnetic chains will exhibit a crossover from 1D magnetic behavior at high temperatures to a 3D ordered state at low temperatures. The BaM$_2$Si$_2$O$_7$(M = Cu, Co, Mn) with layered structure is an excellent system to study low-dimensional magnetic behaviors. BaCu$_2$Si$_2$O$_7$ has an orthorhombic structure with CuO$_4$ plaquettes, while BaCo$_2$Si$_2$O$_7$ and BaMn$_2$Si$_2$O$_7$ have a monoclinic crystal structure with CoO$_4$ and MnO$_4$ tetrahedrons. We have performed local spin-density approximation with onsite Coulomb interaction (LSDA + U) calculations to study the exchange interactions. By computing the total energies of various magnetic configurations and mapping these energies to a Heisenberg model, we extract the magnetic exchange interactions in the three materials. We also discuss the relations between the magnetic exchange interactions with their crystal and electronic structures. In the end, we make comparisons with experimental studies such as single crystal neutron diffraction measurements.

First-principles calculations of the magnetic properties for one-dimensional chains of dihydrated transition-metal oxalates

JUAN HERNÁNDEZ-TECORRALCO (Presenter), Instituto de Física, Benemérita Universidad Autónoma de Puebla, MIGUEL EDUARDO CIFUENTES QUINTAL, Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados del IPN, LILIA MEZA-MONTES, Instituto de Física, Benemérita Universidad Autónoma de Puebla, ROMEO DE COSS, Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados del ipN — Dihydrated transition metal oxalates are crystals composed of quasi one-dimensional (1D) chains which could grow in orthorhombic or monoclinic phases. Their dominant magnetic behavior is a long-range antiferromagnetic order along the metal-oxalate chains. In this work, we have studied the magnetic properties of 1D chains of Co- and Ni-oxalate by means of density functional theory calculations. The intra-chain magnetic interaction is analyzed for ferromagnetic (FM) and antiferromagnetic (AF) orders. The calculated structural parameters along the chain direction are in good agreement with the experimental values for the bulk cases. The magnetic ground state of these systems corresponds to the AF configuration, in agreement with the experimental observations for the bulk. For the Co-oxalate, the calculated local magnetic moment of Co atom is 2.6 μ$_B$ which is in accord with the value obtained from neutron diffraction experiments (2.3 μ$_B$). Thus, 1D chains of transition metal oxalates may be useful systems to implement spin chains for applications in spintronics and quantum computing.

This work was supported by CONACyT-México (grant No. 288344) and VIEP-BUAP 100021244-2018. The authors acknowledge computer resources provided by Laboratorio Nacional de Supercómputo del Sureste de México.
Quantized magnon-excitation continuum in quasi one-dimensional antiferromagnetic S=1 Heisenberg systems
TAKAFUMI SUZUKI (Presenter), SEI-ICHIRO SUGA, University of Hyogo — In recent inelastic neutron scattering measurements on (Ba/Sr)CO_2V_2O_8[1,2], quantization of spinon-excitation continuum has been observed below the Néel temperature. The interesting point is that the excitation energies of the quantized spectra are well explained by negative zeros of the Airy functions (NZAF)[3]. In this study, we investigate the possibility of quantized magnon-excitation continuum in quasi-one-dimensional antiferromagnetic S=1 Heisenberg chains with the single-ion anisotropy, D. We use the infinite time-evolving-block-decimation method to compute dynamical spin structure factors and show that the magnon-excitation continuum is also quantized by the weak inter-chain interaction[4]. We find that the excitation energies agree with NZAF when D is quite large negatively. Although the quantization spectra survive up to D ~ 0, the excitation energies deviate from NZAF. [1] Z. Wang, et al., PRB 91, 140404(R) (2015). [2] B. Grenier, et al., PRL 114, 017201 (2015). [3] H. Shiba, Prog. Theor. Phys. 64, 466 (1980). [4] T. Suzuki, and S. Suga, arXiv:1808.06270.

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Resonant second-order optical resonances in quantum magnets
SHUNSUKE FURUYA (Presenter), RIKEN — Recently, laser control of materials has attracted much attention in various fields of condensed-matter physics. In 2016, Sato, Takayoshi, and Oka proposed an ultrafast way to add to a quantum magnet an effective Dzyaloshinskii-Moriya interaction dynamically. They confirmed their theoretical proposal by calculating the vector chirality to which the Dzyaloshinskii-Moriya interaction is coupled. They also pointed out numerically that there exists a resonance of the dynamically generated vector chirality when the frequency of the applied laser equals to the Zeeman energy of the quantum magnet. This resonance is interesting because the dynamical generation of the vector chirality is the second-order response to the laser but its resonance resembles another linear-response phenomenon to the laser, that is, electron spin resonance. Unfortunately, the resonant second-order response to the laser is yet to be understood. In this presentation, I discuss the origin of the resonant second-order resonance and exemplify it in quantum spin chain systems. I also show that the resonant second-order response can be found in quite a general situation of quantum magnets. For example, the magnetization also exhibits the same resonant second-order optical response.

Lukas Weber (Presenter), Institut für Theoretische Festkörperphysik, RWTH Aachen University, Francesco Parisen Toldin, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Stefan Wessel, Institut für Theoretische Festkörperphysik, RWTH Aachen University — Based on large-scale quantum Monte Carlo simulations, we examine the correlations along the edges of two-dimensional semi-infinite quantum critical Heisenberg spin-1/2 and spin-1 systems. In particular, we consider coupled quantum spin-dimer systems at their bulk quantum critical points, including the columnar-dimer model and the plaquette-square lattice. The alignment of the edge spins strongly affects these correlations and the corresponding scaling exponents, with remarkably similar values obtained for various quantum spin-dimer systems. We furthermore observe subtle effects on the scaling behavior from perturbing the edge spins that exhibit the genuine quantum nature of these edge states.

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Spin-current diode with a monoxial chiral magnet
SHUN OKUMURA (Presenter), HIROAKI ISHIZUKA, YASUYUKI KATO, Department of Applied Physics, University of Tokyo, JUNICHIRO OHE, Department of Physics, Toho University, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo — Chiral magnets often show interesting magnetic and transport properties associated with their peculiar spin textures. For instance, a monoxial chiral magnet CrNb_3S_6 shows a chiral soliton lattice in a magnetic field, accompanied by peculiar temperature and field dependence of resistivity [1]. Such chiral spin textures potentially give rise to nonreciprocal transport phenomena, as they break spatial inversion and time reversal symmetries simultaneously [2]. However, nonreciprocal transport in the monoxial chiral magnets has not been fully understood, especially for spin currents. Here, we investigate the spin-dependent transport properties in a chiral conical magnetic state using a one-dimensional Kondo lattice model. We calculate the conductance of spin current numerically by using the Landauer method based on Green's functions. We show that the system exhibits nonreciprocal spin transport, which depends on the conical angle, the chirality of the magnetic structures, and the polarized direction of the spin current. We discuss the origin of the nonreciprocity by analyzing the spin states near the edges.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L39 GMAG DCMP DMP: Defect Spins in Semiconductors  BSEC 207 - Gregory Fuchs, Cornell University  - Tag(s): Focus

11:15AM L39.00001: Understanding quantum materials using strain-sensitive x-ray diffraction imaging*  [Invited]
JOSEPH HEREMANS (Presenter), Argonne National Laboratory — Understanding the local crystalline strain around point defects, such as the nitrogen vacancy center in diamond and divacancy complexes in SiC, is a critical step toward improving spin coherence and optical properties. These lattice perturbations affect both the charge and the optical transition frequency stability of the defect, limiting their use as nanoscale sensors and quantum bits for quantum communication applications. While local strain can be mitigated using applied electric fields and external static strain, direct observation of inhomogeneous strain fields around these defects at the nanometer length scale remains challenging. Here we present work on the development of synchrotron-based, strain-sensitive x-ray imaging techniques which we use to map the local lattice perturbations within diamond and SiC crystals. These tools can help understand the interaction of defects with dynamically driven strain fields as well as probe the defect creation process to help improve the basic properties of quantum materials. We show two separate techniques: strain-sensitive Bragg coherent diffraction imaging (BCDI) that can measure the three-dimensional lattice strain of individual diamond and SiC nanoparticles as a function of annealing temperature [1,2], and a stroboscopic scanning x-ray diffraction microscopy (s-SXDM) imaging approach that can spatially map acoustic waves in SiC [3] and probe the local strain around crystalline defects. Combining these techniques with growth and implantation protocols could provide a direct means to understand the local crystalline environment surrounding point defect as well as a pathway towards improving their spin properties.


In collaboration with S. J. Whiteley, S. O. Hruszkewycz, M. V. Holt, & D. D. Awschalom.

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ANNEMARIE L EXARHOS (Presenter), Lafayette College — Optically-addressable spins associated with localized defects in wide-bandgap semiconductors are the basis for rapidly expanding quantum technologies in nanoscale sensing and quantum information processing. Whereas most research has focused on three-dimensional host materials such as diamond, the van der Waals material hexagonal boron nitride (hBN) has emerged as a robust host for bright, stable, room-temperature quantum emitters (QEs). However, many questions persist regarding the chemical and electronic structure of the defects responsible for emission as well as the potential role of spin-related effects. Significantly complicating the identification are the heterogeneity of optical characteristics observed for these QEs.

In this talk, I will describe the optical and magnetic properties of QEs in hBN characterized using confocal fluorescence microscopy on suspended hBN films. Qualitative similarities in excitation and emission polarization, spectral shape, and emission statistics are evident among QEs in hBN, even for large variations in emission energy [1]. Significantly, a small percentage of observed QEs exhibit strongly anisotropic photoluminescence modulation in response to an applied magnetic field in ambient conditions [2]. The magnetic-field-induced modulation is consistent with an electronic model featuring a spin-dependent inter-system crossing between triplet and singlet manifolds, suggesting that these defects host optically addressable spin states. This discovery enables the realization of spin-based quantum technologies with van der Waals heterostructures.


*Work supported by the Army Research Office (W911NF-15-1-0589) and NSF MRSEC (DMR-1120901).
12:27PM L39.00003: Diamond Nanomechanical Resonators with Narrow Linewidth NVs* IGNAS LEKAVICIUS (Presenter), THEIN OO, MARK KUZYK, HAILIN WANG, University of Oregon — Nitrogen vacancy centers in diamond are promising qubit candidates which have had recent work focusing on interfacing NVs with acoustic fields. One approach, which is monolithic and doesn't require external driving of phonons, is coupling NVs to high quality factor mechanical resonators in diamond. This approach necessitates low mass, thin membranes which are generally fabricated by thinning down a thicker diamond sample with a plasma etch. However, plasma damage to the diamond results in deep charge defects and poor surface termination which affects the spin and optical properties of the NV center. Here we report on the fabrication of thin mechanical resonators imbedded in a phononic crystal and the measurement of improved optical properties of NVs in those membranes.

*NSF under grant No. 1719396 and AFOSR

12:39PM L39.00004: Mechanical rotation via optical pumping of paramagnetic impurities* PABLO ZANGARA, Physics, City College of New York- CUNY, ALEXANDER A WOOD, Physics, Centre for Quantum Computation and Communication Technology, School of Physics, The University of Melbourne, Melbourne, MARCUS DOHERTY, Physics, Laser Physics Centre, Research School of Physics and Engineering, Australian National University, Canberra, CARLOS MERILES (Presenter), Physics, City College of New York-CUNY — The microscopic understanding of magneto-mechanical processes — involving the inter-convertion between magnetization and angular momentum in a solid — has long been hampered by the complex dynamics governing the spin polarized electrons of a ferromagnetic material, collectively coupled via quantum exchange. Here we use a rotationally invariant Hamiltonian to study the spin dynamics of a pair of paramagnetic centers in an insulator — namely, the so-called P1 and NV centers in diamond — close enough to each other to interact via the dipolar coupling. We examine the interplay between magnetic and mechanical degrees of freedom, and theoretically show that in the presence of continuous optical illumination, cross-relaxation between the NV and P1 spins leads to a rigid rotation of the diamond crystal along with the generation of spin-polarized phonons. The effect should be observable using state-of-the-art torsional oscillators.

*C.A.M. acknowledges support from the National Science Foundation through grants NSF-1619896, NSF-1547830, and from Research Corporation for Science Advancement through a FRED Award. M.W.D. acknowledges support from the Australian Research Council (DE170100169). AAW acknowledges the support of a University of Melbourne ECR mobility fellowship.

12:51PM L39.00005: Observing the charge state of substitutional nitrogen via nitrogen vacancy magnetometry ARTUR LOZOVOI (Presenter), DAMON DAW, JACOB HENSHAW, HARISHANKAR JAYAKUMAR, PABLO ZANGARA, City College of New York, SIDDHARTH DHOMKAR, University College London, HELMUT FEDDER, Swabian Instruments, Germany, MARCUS DOHERTY, Australian National University, CARLOS A. MERILES, City College of New York — Defects in diamond have been widely explored as a potential system for quantum information processing. The negatively charged Nitrogen Vacancy (NV) center is of particular interest because its spin can be operated at ambient conditions and addressed optically with the help of low frequency microwave. It has been suggested that the spin state of the donor electron of the substitutional nitrogen defect (N\textsubscript{s}) can be utilized as a quantum register for a spintronics bus [1]. Here, we use the NV center as a local probe to examine the ionization of small N\textsubscript{s} ensembles in type 1b diamond. To this end, we implement double electron-electron resonance (DEER), [2] which we articulate with multi-color laser excitation to prepare and subsequently probe the local charge state in the N\textsubscript{s} ensemble. We will also discuss the use of polarization transfer techniques from the NVs as a route to probe the spin resilience of photo-generated carriers throughout cycles of ionization from and re-trapping by N\textsubscript{s}.

Polarization transfer between electric and nuclear spins at the level anti-crossing of the NV center in diamond

VIKTOR IVADY (Presenter), Wigner Research Centre for Physics, IGOR ABRIKOSOV, Linkoping University, ADAM GALI, Wigner Research Centre for Physics — Point defect qubits in semiconductors offer new, highly polarizable and controllable electron spin resources to be utilized in nuclear spin polarization experiment. The NV center in diamond holds a great promise for implementing various dynamic nuclear polarization (DNP) mechanisms to achieve high degree of hyperpolarization at elevated temperatures. For example, the level anti-crossing of the electron spin states at moderate magnetic field allows all-optical DNP processes [1] with a mechanism of microwave-free polarization inversion [2]. In my talk, I summarize our most recent theoretical results on all-optical DNP at the level anti-crossing of NV center in diamond of different $^{13}$C nuclear spin concentrations. We demonstrate that the increasing nuclear spin concentration has a negative impact on the efficiency of nuclear polarization transfer that explains the lack of hyperpolarization in $^{13}$C enriched samples. Additionally, I assess the requirements and discuss possible layouts for hyperpolarizing external nuclear spins for sensitivity enhanced NMR and MRI measurements.

References:

First-principle study of spin-strain coupling in defect spin qubits* HE MA (Presenter), Institute for Molecular Engineering and Department of Chemistry, University of Chicago, MENG YE, Institute for Molecular Engineering, University of Chicago, SAMUEL WHITELEY, Institute for Molecular Engineering and Department of Physics, University of Chicago, GARY WOLFOWICZ, DAVID AWSCHALOM, Institute for Molecular Engineering, University of Chicago, GIULIA GALLI, Institute for Molecular Engineering and Department of Chemistry, University of Chicago — Spin defects in semiconductors are promising platforms for quantum information processing and are useful components of hybrid quantum devices. Transition energies between different defect states are sensitive to external perturbations and hence lattice strains can be utilized for mechanical control of qubits. In this work, we use density functional theory to predict the coupling strength between spin and mechanical degrees of freedom for prototypical defect spin qubits including the nitrogen-vacancy centers in diamond and divacancies in silicon carbide, and we compare our results with recent experiments [1].


*This work was supported by the National Science Foundation (NSF) through the University of Chicago MRSEC under award number DMR-1420709.

Exploring solid-state defects with a microwave-modulated spectroscopy technique* DIANA PRADO LOPES AUDE CRAIK (Presenter), PAULI KEHAYIAS, ANDREW GREENSPON, MINA GADALLA, RONALD L WALSWORTH, EVELYN L HU, Harvard University — We have developed a microwave-based spectroscopy technique to determine charge state of nitrogen-vacancy ensembles in diamond. The technique isolates, in situ, the spectral shape of the fluorescence contribution from neutral and negatively-charged defects, producing sample-specific results which take into account the effects of experimental conditions (e.g. illumination intensity and wavelength) and material properties (such as local strain and electric fields). Here, we use this technique to explore how ensemble charge state is affected by experimental and material parameters, and to study the physics of NV ionization from the negative charge state. We also apply a variation of our technique to silicon vacancies (SiV) in 4H silicon carbide. The technique may be used to isolate the spectra of V1 and V2-type defects at room temperature -- these are two silicon vacancies that occur at inequivalent lattice sites but have closely-spaced spectral signatures. We explore the modulation of the SiV signals in both bulk SiC and in nanobeam optical resonators that include the vacancies.

*This work was supported by the NSF STC Center for Integrated Quantum Materials, NSF Grant DMR-1231319, Air Force Office of Scientific Research award FA9550-17-1-0371, and NSF EAGER Grant ECCS 1748106.
Coherent electrical driving of quantum spins via localized magnons

AVINASH RUSTAGI (Presenter), Electrical and Computer Engineering, Purdue University, SHIVAM KAJALE, Electrical Engineering, Indian Institute of Technology Bombay, PRAMEY UPADHYAYA, Electrical and Computer Engineering, Purdue University — Spin-spin interactions in quantum-classical spin hybrids are promising enablers of quantum spintronics. For example, dipolar interactions between classical magnets and quantum dot (QD) spins have enabled electrically driven high-fidelity quantum processors [Nat. Nano 13, 102 (2018)]. Motivated by higher operating temperatures, dipolar interactions in quantum impurity (QI) spin [like Nitrogen vacancy (NV) center]-classical magnet hybrids have been used for quantum sensing of ground state configurations-solitons [Nature 549, 252 (2017); Nat. Commun. 9, 2712 (2018)], as well as, excitations-magnons [Science 357, 195 (2017)]. In addition, magnons have mediated long-distance coherent coupling between NVs and microwave antennas [npj Quantum Info. 3, 28 (2017)]. In contrast to QD spin-magnet hybrids, coherent electrical driving of QI spins is, however, missing. Here, we propose to utilize spin-orbit induced electrical driving of magnons [Nano Lett. 2017, 17, 1, 572], to mitigate this challenge. Specifically, we study coherent and incoherent coupling of QI spins in proximity to electrically controlled localized magnons in nanomagnets-showing coherent electrical driving of QI spins.

*We acknowledge NSF grant DMR-1838513.

Modeling the Quantum Dynamics behind Charge Transport in Photosynthetic Reaction Centers beyond the Spin-Boson Model

KRISTINA LENN (Presenter), EITAN GEVA, University of Michigan — Silicon is one of the most common solar cell materials due to its availability, ideal band gap, and high efficiency but needs to be processed onto glass substrates. Research has turned its attention towards organic materials, which can be processed relatively cheaply onto plastic substrates but are not nearly as efficient as silicon. Modeling the quantum dynamics behind the charge transport process will help elucidate methods to enhance the material’s efficiency. This model can be extrapolated from the transport process in the Fenna-Matthews-Olson complex in green sulfur bacteria.

The photosynthetic process observed in the FMO complex utilizes quantum coherence during electron energy transfer, which has been shown to increase efficiency by offsetting radiative recombination. To model the dynamics of this process, we are using a combination of the Ehrenfest method, which has already been tested on the two-state Spin-Boson model, and Multi-Configuration Time-Dependent Hartree for an eight-state system. However, one of the major drawbacks of quantum calculations is the high computational cost. To circumvent this, we plan to implement the Generalized Quantum Master Equation, which has a much more efficient memory kernel, thus cutting the computational cost of quantum calculations.

Probing Coherent Spin Dynamics of Isolated Exchange Coupled Defects in III-V Semiconductors

STEPHEN MCMILLAN (Presenter), NICHOLAS HARMON, MICHAEL FLATTÉ, University of Iowa — Individual magnetic impurities or small collections of magnetic impurities in III-V semiconductors can be identified via scanning tunneling microscopy (STM) [1,2]. Their exchange interaction can be measured [3], and they can have remarkably long spin coherence times [4]. Through low-field magnetoresistance calculations we find that exchange coupled defects generate a resonance feature in the current at critical values of the applied magnetic field, termed “exchange resistance”. Using a single site approximation [5,6], the signatures of hyperfine interaction and the influence of g-factor fluctuation on exchange resistance are examined. By including a non-trivial spin manifold as the ground state this work becomes applicable to defects like divacancies in silicon carbide and Mn+hole complexes in gallium arsenide.


*We acknowledge support from DOE BES through Grant No. DE-SC0016447.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L40 GMAG DMP: Magnetism and Domain Structures in Complex Oxides
11:15AM L40.00001: Titanate pyrochlores: Growth of stoichiometric crystals below their melting points* [Invited]
SEYED KOOHPAYEH (Presenter), Johns Hopkins University — The pyrochlore rare earth titanates (RE₂Ti₂O₇) have been intensively studied experimentally and theoretically over the past two decades. In the field of magnetism, this class of materials is considered to be ideal hosts for archetypal geometrical frustration, which consists of the quantum spin ice, classical spin ice, and spin liquid behaviors. The energy scales for such magnetic interactions are low; therefore, these systems are expected to be very sensitive to small perturbations of all kinds, including non-stoichiometry and structural defects. In this talk, we report the effects that synthesis and growth conditions can have on the stoichiometry, defect formation, and physical properties. We also describe the process to grow high-quality and stoichiometric pyrochlore titanate single crystals at temperatures below their melting points by changing their composition using the traveling solvent floating zone technique (TSFZ).

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0019331.

11:51AM L40.00002: Topological structural defects and exotic magnetic behaviors in hexagonal TbInO₃ and GdInO₃
JAE WOOK KIM (Presenter), XUEYUEN WANG, FEI-TING HUANG, YAZHONG WANG, Y LI, SANG-WOOK CHEONG, Rutgers University, New Brunswick, XUAN LUO, Pohang University of Science and Technology, EUNDEOK MUN, XIAXIN DING, VIVIEN ZAPF, Los Alamos National Laboratory — Geometrical frustration may induce highly degenerate ground states, complex spin configurations, or exotic ground states. One extreme example is the spin liquid, where magnetic ordering is suppressed even at zero temperature by quantum fluctuations. Spin liquids may host novel properties such as spinon excitations, majorana edge states, etc. Here, we report intriguing examples of coexisting topological ferroelectric domains and exotic magnetism in hexagonal rare-earth (R) indates such as TbInO₃ and GdInO₃. Geometric ferroelectricity is realized in hexagonal RInO₃ and we have unveiled Z₆ vortex domains associated with geometric ferroelectricity in TbInO₃ and GdInO₃, as similar to what has been observed in hexagonal manganites. On the other hand, magnetic properties vary upon different R ions. For example, GdInO₃ shows a phase transition at low temperatures below 2.5 K whereas no signature of phase transition is observed for TbInO₃. We suggest that the topological defects and ferroelectric domain walls serve as an intrinsic playground for the edge states that may exist in frustrated magnets.

12:03PM L40.00003: Imaging antiferromagnetic antiphase domain boundaries using magnetic Bragg diffraction phase contrast*
VALERY KIRYUKHIN (Presenter), MIN GYU KIM, BIN GAO, SANG-WOOK CHEONG, Rutgers University, New Brunswick, HU MIAO, CLAUDIO MAZZOLI, ANDI BARBOUR, STUART B WILKINS, IAN KEITH ROBINSON, MARK DEAN, BNL — Manipulating magnetic domains is essential for many technological applications. Recent breakthroughs in Antiferromagnetic Spintronics brought up novel concepts for electronic device development. Imaging antiferromagnetic domains is of key importance to this field. Unfortunately, some of the basic domain types, such as antiphase domains, cannot be imaged by conventional techniques. Herein, we present a new domain projection imaging technique based on the localization of domain boundaries by resonant magnetic diffraction of coherent x rays. Contrast arises from reduction of the scattered intensity at the domain boundaries due to destructive interference effects. We demonstrate this approach by imaging antiphase domains in a collinear antiferromagnet Fe₂M₀₂O₈, and observe evidence of domain wall interaction with a structural defect. This technique does not involve any numerical algorithms. It is fast, sensitive, produces large-scale images in a single-exposure measurement, and is applicable to a variety of magnetic domain types.

*Supported by the DOE, Grant No. DOE: DE-FG02-07ER46382.
12:15PM L40.00004: Imaging scale-invariant magnetic textures in a strongly correlated oxide  JIARUI LI (Presenter), JONATHAN PELLICIANI, ABRAHAM LEVITAN, Department of Physics, Massachusetts Institute of Technology, CLAUDIO MAZZOLI, National Synchrotron Light Source II, Brookhaven National Laboratory, SARA CATALANO, Department of Quantum Matter Physics, University of Geneva, FORREST SIMMONS, Department of Physics and Astronomy, Purdue University, JERZY T. SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory, MARTA GIBERT, Department of Quantum Matter Physics, University of Geneva, ERICA CARLSON, Department of Physics and Astronomy, Purdue University, JEAN-MARC TRISCONE, Department of Quantum Matter Physics, University of Geneva, STUART B WILKINS, National Synchrotron Light Source II, Brookhaven National Laboratory — The electronic ground state of correlated electron systems, often manifests a granular texture across a broad range of length scales. Antiferromagnetic order is a common instability of these materials, however, its nanoscale spatial organization has not been systematically studied. In this talk, I will present our recent result using a resonant soft X-ray scattering nanoprobe to image the bulk magnetic landscape in NdNiO₃ thin films. Our measurements provide direct evidence for a highly textured magnetic fabric, that further exhibits return memory effects across the Neel transition. The scale-free distribution of antiferromagnetic domains and its non-integral dimensionality, together reveal an unprecedented magnetic fractal geometry near criticality, which reflects the interplay between electronic correlations and an intrinsic local parameter. Our observations expose new essential details of the nanoscale anatomy of strongly correlated electronic systems.

12:27PM L40.00005: Capturing Dynamics of Incommensurate Antiferromagnetic Domains with Coherent Soft X-ray Scattering  JOHN BOWLAN (Presenter), Physical Chemistry and Applied Spectroscopy, Los Alamos National Laboratory, RICHARD L SANDBERG, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, VIVIEN ZAPF, XIAXIN DING, National High Magnetic Field Laboratory, Los Alamos National Laboratory, SHIZENG LIN, Theoretical Division, Los Alamos National Laboratory, COLBY WALKER, BENJAMIN A POUND, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, NARA LEE, YOUNG JAI CHOI, Yonsei University, ANDI BARBOUR, WEN HU, STUART B WILKINS, CLAUDIO MAZZOLI, NSLS-II, Brookhaven National Laboratory — The observation of antiferromagnetic (AFM) domains and the dynamics of their interfaces remains an elusive problem. The physical origin and dynamics of AFM domains are different from ferromagnetic domains and are largely unexplored. In this work, we have studied the frustrated AFM, Lu₂CoMnO₆, with the brilliant, coherent, soft X-ray flux of the 23ID-1 beamline at NSLS-II [1]. Lu₂CoMnO₆ is a double perovskite with frustrated AFM order leading to incommensurate ordering and dynamic time scales ranging from seconds to days [2-4]. We have probed the AFM domain structure and dynamics of this material with X-ray photon correlation spectroscopy (XPCS). The motion of the domains is revealed by the motion of a speckle pattern in the scattered X-ray beam. We observed faster domain fluctuations below onsets of hysteresis at (35K) and explained these observations within the Axial Next-Nearest-Neighbor Ising (ANNNI) model.

References

12:39PM L40.00006: Magnetic Domain wall resistance in Half-metallic CrO2*  LIJUAN QIAN (Presenter), WENZHE CHEN, GANG XIAO, Brown University — The half-metallic CrO₂ is experimentally confirmed to have the highest spin polarization of nearly 100%. It is an ideal system to study magnetic domain-wall resistance (DWR), which differs from the resistance (or resistivity) inside a single-domain. We design and prepare a CrO₂ epitaxial nanostructure with an asymmetrical weak link to localize a single DW, using the techniques of chemical vapor deposition and selective-area growth. The weak link design provides us the capability to generate /annihilate a single DW by applying a moderate/strong reversing magnetic field. By contrasting the resistance between a single-domain state and a DW state under zero field, we obtain the domain wall resistance in half-metallic CrO₂. Using the Levy-Zhang model of DWR and simulated domain wall contour, we further obtain the spin asymmetry ratio between resistivities in the two spin channels. The ratio, 4256 ± 388 at 5.0 K, is 2 to 3 orders larger than that of conventional ferromagnetic metals, attesting the half-metallicity of CrO₂.

*We acknowledge the financial support by National Science Foundation through Grants No. DMR-1307056 and by research funding from King Abdullah University of Science and Technology (KAUST).
12:51PM L40.00007: Domain reversal dynamics and avalanches in a model insulating Ising ferromagnet  
DANIEL SILEVITCH (Presenter), CHRISTOPHER TANG, THOMAS F ROSENBAUM, Caltech — 100 years ago, Barkhausen's noise experiments provided evidence for discrete domains within ferromagnets and magnetization reversal occurring as a set of discrete events. By characterizing individual avalanche events, the underlying mechanisms for domain reversal can be studied. Many materials show a drag effect which appears in the statistical distribution of avalanche event shapes. In typical metallic ferromagnets, this drag is believed to be due to eddy currents induced during magnetization reversal. Whether this is only significant source of drag is an open question which we address by studying the model Ising system LiHo$_{0.65}$Y$_{0.35}$F$_4$, an insulating rare-earth, dipole-coupled ferromagnet with $T_C$ of 0.98 K. The LiHo$_{x}$Y$_{1-x}$F$_4$ family combine strong quantum fluctuations, random-field pinning, and a lack of eddy currents, extending the study of domain dynamics to an entirely new regime. We find symmetrical scaled distributions near $T_C$, indicative of a drag-free environment. By contrast, strong asymmetries appear for long-duration events at lower temperatures, suggesting the presence of drag without eddy currents. A thermal-driven crossover between random-field effects and a quantum-fluctuation regime suggests that the latter act as the source of this additional drag mechanism.

1:03PM L40.00008: Domain Structure and Reversal Dynamics of Magnetoelectric Antiferromagnets*  
ARUN PARTHASARATHY (Presenter), SHALOO RAKHEJA, Electrical and Computer Engineering, New York University — The single domain state of magnetoelectric (ME) antiferromagnet like Cr$_2$O$_3$ can be switched isothermally at room temperature by simultaneous application of electric and magnetic fields (He, et al., Nat. Comm. 2010; Kosub, et al., Nat. Comm. 2017). However, studies pertaining to switching dynamics, especially in thin-film systems, have been limited.

Domain reversal involves switching between saturated single-domain states. This constraint does not limit the dynamic process of reversal, which can exhibit single or multi-domain switching mechanisms, or a mix of both. In general, the mechanism of domain reversal depends on material parameters like the exchange interaction and magnetic anisotropy, size and shape of the sample, structure of defects, and strength of the excitation including thermal fluctuations.

In this work, we theorize the spatial and temporal limits of ME-induced reversal of antiferromagnet domain for nucleation, domain wall propagation and coherent rotation. We also address the formation of non-trivial domain structures in equilibrium in thin film Cr$_2$O$_3$ (Wu, et al., Phys. Rev. Lett. 2011), despite the absence of magnetostatic interaction in the bulk.

*This work was supported in part by the SRC and the NSF through ECCS 1740136.

1:15PM L40.00009: Non-Reciprocal Directional Dichroism of THz Radiation in LiCoPO$_4$: Read-out of Magnetoelectric Domains*  
TOOMAS ROOM (Presenter), URMAS NAGEL, National Institute of Chemical Physics and Biophysics, SANDOR BORDACS, JAKUB VIT, Department of Physics, Budapest University of Technology and Economics and MTA-BME, ISTVAN KEZSMARKI, Experimental Physics 5, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany, JUDIT ROMHANYI, Okinawa Institute of Science and Technology, Okinawa, Japan, KARLO PENC, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary, VILMOS KOCSIS, YUSUKE TOKUNAGA, YASUJIRO TAGUCHI, YOSHINORI TOKURA, RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan — Magnetoelectric (ME) effect in multiferroic materials is the cornerstone of new electronic devices allowing the electric field control of magnetization. Here we demonstrate the optical read-out of magnetoelectric domains in LiCoPO$_4$ exploiting the absorption difference between ME domains [Kocsis et al., PRL 121, 057601 (2018)]. Domains absorb differently because of non-reciprocal directional dichroism of spin wave resonances coupled to electric polarization. Single ME domain can be selected by poling with crossed electric and magnetic fields from the magnetically disordered state. LiCoPO$_4$ is the realization of a ME memory effect in an insulator with coupled anti-ferroelectric and anti-ferromagnetic orders.

*Part of the work was supported by The Estonian Ministry of Education and Research under Grant No. IUT23-03, and the European Regional Development Fund project TK134.
1:27PM L40.00010: Inhomogeneous magnetic order in T'-La$_4$Ni$_3$O$_8$* OSCAR BERNAL (Presenter), Physics and Astronomy, California State University, Los Angeles, Los Angeles, CA 90032, DOUGLAS E. MACLAUGHLIN, Physics and Astronomy, University of California, Riverside, Riverside, CA 92521, GERALD D MORRIS, Center for Molecular and Materials Science, TRIUMF, Vancouver, BC V6T 2A3, Canada, LEI SHU, CHENG TAN, JIAN ZHANG, ZHAOFENG DING, State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, China, KEVIN HUANG, National High Magnetic Field Lab, Florida State University, Tallahassee, Florida 32310, VIKTOR V. POLTAVETS, Department of Chemistry and Advanced Materials Research Institute, University of New Orleans, New Orleans, Louisiana 70148 — We report a muon spin rotation (μSR) study of the magnetic properties of the cuprate-analog nickelate La$_4$Ni$_3$O$_8$. The crystal structure of this compound involves square planar NiO$_2$ layers, potentially isoelectronic (Ni$^{1+}$) to the Cu$^{2+}$O$_2$ layers of the cuprates. The material has a magnetic phase transition at 105 K, the structure of which has remained elusive. Zero-field μSR confirms the antiferromagnetic nature and commensurate character of this transition, and sheds light on the most likely configuration of Ni spins below the Néel temperature. Comparison of spectra of observed muon precession frequencies to lattice calculations of Ni dipolar fields at candidate muon stopping sites suggests a spin configuration consistent with the stripe charge order observed previously by x-ray diffraction [1]; in particular, the number of observed frequencies is greater than calculated for homogeneous spin structures without stripes. The frequency magnitudes suggest reduced Ni ordered moments of less than or about 0.5μB. We briefly discuss models of magnetic-stripe order based on alternative charge stripe configurations (cf. Ref. [1]).


*Work at Cal State LA supported by the National Science Foundation under DMR-PREM grant 1523588.

1:39PM L40.00011: Unravelling Giant Exchange bias in the single layered Ruddlesden-Popper compound SrLaCo$_{0.5}$Mn$_{0.5}$O$_4$: A combined studies of Experimental and Density Functional Theory* RANJANA RANI DAS, PRIYADARSHINI PARIDA, Indian Institute of Technology Madras, A.K. BERA, Solid State Physics Division, Bhabha Atomic Research Centre, T. CHATTERJII, Institut Laue-Langevin, B.R K NANDA, SANTHOSH NAGAPPAN NAIR (Presenter), Indian Institute of Technology Madras — Discovering exotic magnetism due to competing magnetic interactions in layered perovskites with 3d hetero-species B-site ions has remained an intriguing topic with many unexplained features. Here we study Exchange bias (EB) phenomena in a single layered Ruddlesden-Popper SrLaCo$_{0.5}$Mn$_{0.5}$O$_4$ using state of art measurement such as susceptibility, neutron diffraction and training effect along with density functional calculations. EB as large as ~5.5 kOe is observed in SrLaCo$_{0.5}$Mn$_{0.5}$O$_4$ which is the highest ever found in any layered transition metal oxides including Ruddlesden-Popper series. Neutron diffraction measurements and together with dc magnetic measurements suggest formation of short range magnetic domains. By carrying out density functional calculations on several model configurations we propose that EB is originated at the boundary between Mn rich antiferromagnetic and Co rich ferromagnetic domains at the sub-nanoscale. Our analysis infers that presence of competing magnetic interactions is sufficient to induce exchange bias and thereby a wide range of materials exhibiting EB can be engineered.

*PNS acknowledge the project support by CSIR, India (03 (1214)/12/EMR-II)).

1:51PM L40.00012: Potts transition in coupled XY models* VICTOR DROUIN-TOUCHETTE (Presenter), Rutgers University, New Brunswick, PETER ORTH, Physics, Iowa State University, PREMALA CHANDRA, PIERS COLEMAN, Rutgers University, New Brunswick, TOM CARL LUBENSKY, Physics, University of Pennsylvania — Motivated by the long standing experimental mystery of the observation of a melting transition seemingly in the 3-state Potts universality class in thin films of liquid crystals, we revisit a model of coupled XY models. In these compounds, the interplay of the bond-orientational and herring-bone packing degrees of freedom, respectively invariant under rotation by π and by π/3, may lead to emergent discrete variables through the resulting anisotropic coupling. Using both large scale Monte-Carlo algorithms, with an adapted Wolff step and parallel tempering, and analytical methods, such as RG, we study the phase diagram of such a coupled XY model with global U(1) × Z$_3$ symmetry. The presence of the discrete order can highly frustrate the possible binding of vortices, and we investigate how this non-trivial interaction can lead to unconventional arrangements of the vortices. Our extensive numerical study focuses on the regime where both XY variables are equally present, and we discuss the possibility of a 3-state Potts transition at higher temperature than the BKT transition, as well as the nature of the meeting point between the BKT and Potts phase transition.

*We acknowledge financial support by the DOE, Basic Energy Sciences grant DE-FG02-99ER45790, and the Quebec FRQNT.
2:03PM L40.00013: Inelastic Neutron Scattering Investigation of Quantum Order-by-disorder in Bi$_2$CuO$_4$  BO YUAN (Presenter), Physics, University of Toronto, NICHOLAS BUTCH, GUANGYONG XU, National Institute of Standards and Technology, YOUNG-JUNE KIM, Physics, University of Toronto —

Order by disorder (ObD), where ground state is selected from a continuous manifold of classically degenerate states by either thermal or quantum fluctuation has been intensively studied theoretically. However, experimental realizations of ObD in real materials are still very rare. In this talk, we present strong evidence from neutron scattering for quantum ObD in tetragonal cuprate Bi$_2$CuO$_4$. With high resolution inelastic neutron scattering, we observed a gapless and a gapped magnon mode due to in-plane and out-of-plane spin fluctuation. By studying field dependence of the in-plane mode and magnetic Bragg peak, we directly observed a spin-flop transition at $\sim 0.4T$ and demonstrated the existence of a small magnetic anisotropy within the ab plane. Since any in-plane anisotropy is prohibited by symmetry in Bi$_2$CuO$_4$ on a classical level, we attribute its existence to quantum ObD. We investigated quantum ObD in Bi$_2$CuO$_4$ theoretically by spin-wave analysis. By taking into account quantum zero-point fluctuation of the spin wave modes in Bi$_2$CuO$_4$, we found a small in-plane anisotropy favouring an ordered moment 45 degrees from the crystallographic a and b directions. Our model quantitatively explained the size of critical field for spin-flop transition in our data.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L41 GMAG DMP: Heterostructures and Thin Films for Skyrmions  BCEC 209 - Andrew Kent, New York Univ NYU - Tag(s): Focus

11:15AM L41.00001: Hybrid chiral domain walls and skyrmions in magnetic multilayers* [Invited] WILLIAM LEGRAND (Presenter), Unité Mixte de Physique CNRS/Thales, Univ. Paris-Sud, Université Paris-Saclay, 91767 Palaiseau, France, NATHAN RONCERAY, Ecole Polytechnique, 91128 Palaiseau, France, JEAN-YVES CHAULEAU, Synchrotron SOLEIL, L'Orme des Merisiers, 91192 Gif-sur-Yvette, France, DAVIDE MACCARIELLO, FERNANDO AJEJAS, SOPHIE COLLIN, K BOUZEHOUANE, NICOLAS REYREN, Unité Mixte de Physique CNRS/Thales, Univ. Paris-Sud, Université Paris-Saclay, 91767 Palaiseau, France, NATHAN RONCERAY, Ecole Polytechnique, 91128 Palaiseau, France, JEAN-YVES CHAULEAU, Synchrotron SOLEIL, L'Orme des Merisiers, 91192 Gif-sur-Yvette, France, VINCENT CROS, ALBERT FERT, Unité Mixte de Physique CNRS/Thales, Univ. Paris-Sud, Université Paris-Saclay, 91767 Palaiseau, France — Aiming at reducing the radius of individual magnetic skyrmions below 10 nm without making compromises between room-temperature stability and current-induced mobility, a multilayered magnetic system is often privileged. However, dipolar interactions can overcome the essential chiral properties of magnetic skyrmions stemming from the Dzyaloshinskii-Moriya interaction (DMI), for multilayers with too large magnetization or number of layers. Using circular dichroism in X-ray Resonant Magnetic Scattering, we demonstrate a reorientation of chirality along the vertical direction of magnetic domain-walls and skyrmions, leading to the formation of hybrid chiral skyrmions. We next establish an extensive micromagnetic model of magnetic skyrmions, which allows obtaining their equilibrium profiles with an accurate and layer-resolved description of both size and chirality. The resulting magnetization profiles allow predicting, within the Thiele formalism, the expected velocity of skyrmions under current-induced spin-orbit torques in different spin injection geometries. We find the requirements on the DMI magnitude to ensure an efficient motion, and observe a regime of compensation of the skyrmion Hall effect for hybrid chiral skyrmions. Beyond such issues related to the chirality of ferromagnetic skyrmions, we finally present our recent progresses in the study of multilayers hosting synthetic antiferromagnetic skyrmions, whose alternation of polarity enables a way to circumvent all issues related to dipolar interactions in skyrmion multilayers.


*French ANR grant TOPSKY (ANR-17-CE24-0025), DARPA TEE program grant (MIPR#HR0011831554) and EU grant MAGicSky (FET-Open-665095) are acknowledged.
Surprisingly, they were all at least several tens of nanometer in diameter. Their large size has a fundamental origin: these skyrmions are stabilized by a competition of classical long range fields, namely stray fields and externally applied fields. Based on accurate analytical modeling, we could show that this is a general property of ferromagnets due to their overwhelming stray fields [5].

In ferri- and antiferromagnetic materials, stray fields play no significant role. We predicted theoretically [5] and confirmed experimentally [6] that a different type of skyrmion can exist in these materials at room temperature, stabilized by all-quantum interactions. These skyrmions are insensitive to classical fields, exist even at zero external field, and can be as small as ~10 nm in diameter. Finally, they are also created by quantum spin-orbit torques [7].


12:03PM L41.00003: Structural Imprinting of Target Skyrmions in Magnetic Multilayers* NOAH KENT (Presenter), UC Santa Cruz/ LBNL, ROBERT STREUBEL, MSD, Lawrence Berkeley National Laboratory, CHARLES-HENRI LAMBERT, ETH Zurich, SCOTT DHUEY, MI-YOUNG IM, MSD, Lawrence Berkeley National Laboratory, FELIX BUETTNER, Massachusetts Institute of Technology, PETER FISCHER, UC Santa Cruz/ LBNL — We will report on a recent study of topological spin textures that were imprinted due to coupling between a 30nm thin permalloy (Py) nanodisk with diameters from 250-1000nm and a multilayer Ir/Co/Pt film with strong DMI. Using element-specific magnetic soft x-ray microscopy we were able to image the magnetic structure of the Py nanomagnets and the spin texture in the DMI film independently. We found a significant increase of the imprinted domain period (240nm) in the film under the disks compared to the free film (180nm), which can be traced back to a locally varying stray field energy. We stabilize extended target skyrmions in the film with up to four \( \pi \) rotations of the z component of magnetization. This is due to the reduced stray field energy and enforced radial symmetry caused by the Py disk. We confirm that these structures have a uniform chirality enforced by the DMI of the thin film by observing an asymmetric expansion of the domain walls as a function of applied magnetic field pulses. We also observe the overall structural stability of target skyrmions in an external magnetic field has no dependence on topological charge.

*Work supported by DOE MSE BES DE-AC02-05-CH11231, Non-Equilibrium Magnetic Materials Program

12:15PM L41.00004: Realization of magnetic skyrmions in thin films at ambient conditions* LISA DEBEER-SCHMITT (Presenter), RYAN DESAUTELS, Oak Ridge National Laboratory, SERGIO MONTOYA, Space and Naval Warfare Systems Center Pacific, JULIE BORCHERS, NIST Center for Neutron Research, National Institute of Standards and Technology, SOONG-GEUN JE, MI-YOUNG IM, Center for X-ray Optics, Lawrence Berkeley National Laboratory, MICHAEL R. FITZSIMMONS, Oak Ridge National Laboratory, ERIC FULLERTON, Center for Memory and Recording Research, University of California, San Diego, DUSTIN GILBERT, Department of Materials Engineering, University of Tennesse, Knoxville — Magnetic skyrmions present interesting physics due to their topological nature and hold significant promise for future informational technologies. A key barrier to realizing skyrmion devices has been stabilizing these spin structures in ambient conditions. I will discuss how we exploited the tunable magnetic properties of amorphous Fe/Gd films to realize, for the first time, skyrmion lattices in continuous amorphous thin-films, stable at room temperature and zero magnetic field. These Bloch-type skyrmions are stabilized by dipolar interactions rather than traditional Dzyaloshinskii-Moriya interactions. Small angle neutron scattering was used in combination with soft x-ray microscopy providing a unique, multi-scale probe of the local and long-range order of these structures. Key to this work was to prepare an artificial stripe phase, which evolves into the hexagonally ordered skyrmion lattice structure under increasing magnetic field. These results identify a pathway to engineer controllable skyrmion phases in thin film geometries which are stable at ambient conditions.

*This research used resources at the High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.
12:27PM L41.00005: SP-STM Studies of B20 MnGe* JACOB REPICKY (Presenter), JOSEPH CORBETT, TAO LIU, ADAM AHMED, Ohio State University, JONATHAN GUERRERO-SANCHEZ, National Autonomous University of Mexico, ROLAND KAWAKAMI, JAY A GUPTA, Ohio State University — Materials in the B20 crystal structure have broken bulk inversion symmetry, which can lead to the formation of chiral magnetic textures. MnGe is an example with the smallest magnetic period (~3 nm) and largest topological Hall signals observed among B20 chiral magnets. Here, we present spin-polarized scanning tunneling microscopy (SP-STM) characterization of thin MnGe(111) films grown by molecular beam epitaxy. Atomic resolution images show a triangular lattice with a lattice parameter of 6.85 Å in good agreement with the bulk. Three of four possible surface terminations are observed in STM images of different terraces on the surface. Tunneling spectroscopy with a bulk Cr tip shows a pronounced dependence on magnetic field, which we compare to the spin-resolved local density of states calculated by DFT. Counter-intuitively, we observe the largest spin signal from one of the Ge-terminated surfaces, due to their antiferromagnetic coupling to the underlying Mn layer. We also examine magnetic field dependence in topography and spectroscopic maps to probe for surface magnetic structures.

*Funding for this research was provided by the Defense Advanced Research Projects Agency Grant No. 18AP00008

12:39PM L41.00006: Stability of Skyrmions and Topological Hall Effect in Mn2CoAl thin films GUY DUBUIS (Presenter), YAO ZHANG, SIMON GRANVILLE, Victoria University of Wellington — Skyrmions are magnetic quasi-particles that have the potential to help resurrect Moore’s Law.[1] Due to their topological protection, they could be used as non-volatile memory,[2] while also allowing the design of logic gates[3] that could be used in magnonic devices. The presence of skyrmions can be detected by observing the topological contribution to the Hall resistance, due to the time-varying magnetic field experienced by an electron travelling through a material hosting skyrmions. We observe skyrmions in thin films of the ferromagnetic spin-gapless semiconductor Heusler alloy Mn2CoAl capped by Pd.[4] We can engineer our thin films to make the skyrmions stable from 3K to above room temperature. By careful control of the magnetic and thermal history of the sample, we can condition various forms of skyrmions in this material. In order to understand their stability, we have measured time dependent Hall resistance and magnetization in the skyrmion regions. We observe skyrmions that are stable for at least hours at room temperature in the absence of a magnetic field.

References:
1 D. Chandler, *MIT News.*, 2017
3 S. Luo et al., *Nano Lett.*, 2018, 18, 1180-1184

12:51PM L41.00007: Determining Chirality of Non-Centrosymmetric FeGe and MnGe Thin Films via STM JOSEPH CORBETT (Presenter), JACOB J REPICKY, Department of Physics, Ohio State University, JONATHAN GUERRERO-SANCHEZ, Centro de Nanociencias y Nanotecnologia, Universidad Nacional Autónoma de México, TIANCONG ZHU, ADAM S AHMED, STEVEN TJUNG, TAKAHIRO TAKEUCHI, ROLAND KAWAKAMI, JAY A GUPTA, Department of Physics, Ohio State University — Recent interest in the 'B20' phase of FeGe and MnGe stems from noncollinear magnetic states, such as magnetic Skyrmions. Here we present a joint STM and DFT study of FeGe and MnGe films grown by molecular beam epitaxy. An average surface lattice constant of ~6.8 Å (FeGe) and of ~6.9 Å (MnGe), in agreement with the bulk values, was observed via LEED, as well as in situ RHEED during the MBE growth. Atomic resolution images of each of the four possible chemical terminations in the FeGe films were characterized by distinct image contrast and corrugation, as well as local density of states in tunneling spectra. Likewise, three of the four possible chemical terminations of MnGe were identified in atomic resolution STM images. These assignments were confirmed by the good agreement between the STM images and DFT-simulated images using the Tersoff-Hamann approximation. Having determined the surface terminations, STM images of the atomic layering order and registry across step edges allows us to uniquely determine the stacking order, and hence chirality of these films, which is difficult with conventional crystallography techniques.
1:03PM L41.00008: Skyrmions in Monolayer van der Waals 2D Magnets*  
AROOP BEHERA (Presenter), Kansas State University, SUGATA CHOWDHURY, Physical Measurement Laboratory, NIST, SUPREM DAS, Kansas State University — In this work, using Landau-Lifshitz Gilbert (LLG) model and first-principle calculations we demonstrate the occurrence of skyrmions in monolayer CrI$_3$. We considered a paramagnetic state and apply a range of magnetic fields from 0 T to 1.5 T. We found the system evolves under normal conditions (i.e., the time evolution under the influence of exchange and anisotropic interactions) to energetically favourable skyrmionic ground state. We derive the Heisenberg exchange ($J$), uniaxial magnetocrystalline anisotropy ($K$) and Dzyaloshinskii-Moriya interaction (DMI) parameters for monolayer CrI$_3$. Our calculations revealed that the isolated skyrmionic spin textures evolved in the order of a few picoseconds for a wide range of magnetic field. We found the chiral domain walls or helical states in the 2D monolayer CrI$_3$ along with the presence of skyrmions at low magnetic field strengths. However, with increasing strength of the magnetic field, the density of occurrence of chiral domains reduces converging and forming skyrmions. It is also observed that with the increase in the field strength the size of stable skyrmions reduces.

*This work is funded by Kansas State University. Authors thank to Nikolai Kiselev and Gideon Muller of Forschungszentrum Jülich, Germany.

1:15PM L41.00009: Large terahertz resonance in MnGe thin films  
YOSHIHIRO OKAMURA (Presenter), YUDAI HAYASHI, NAOYA KANAZAWA, University of Tokyo, ATSUSHI TSUKAZAKI, Tohoku University, MASASHI KAWASAKI, MASAKAZU ICHIKAWA, University of Tokyo, YOSHINORI TOKURA, RIKEN CEMS, YOUTAROU TAKAHASHI, University of Tokyo — Topological nature of matters often plays an important role in transport phenomena such as Hall effect. For example, the large anomalous Hall effect (AHE) and topological Hall effect (THE) have been observed in bulk MnGe [1]. In this study, we investigate the optical Hall conductivity by means of terahertz time domain spectroscopy in MnGe thin films. While the diagonal conductivity can be well described by the conventional Drude model, the Hall conductivity spectra show the large resonance structure at ~1.2 meV, which is significantly enhanced and dominates the DC Hall conductivity at low temperatures. We further analyze the Hall conductivity spectra based on the Karplus-Luttinger model, which indicates that the resonance structure consists of two interband transitions corresponding to AHE and THE.


1:27PM L41.00010: Detecting Crystallographic Lattice Chirality using Resonant Inelastic X-ray Scattering  
TRINANJAN DATTA (Presenter), SEAN KEVIN MONGAN, Chemistry and Physics, Augusta University, GA, ZENGYE HUANG, School of Physics, Sun Yat-Sen University, China, TAKUJI NOMURA, Synchrotron Radiation Research Center, National Institutes for Quantum and Radiological Science and Technology, SPring-8, Japan, DAO-XIN YAO, School of Physics, Sun Yat-Sen University, China — The control and detection of crystallographic chirality is an important and challenging scientific problem. Chirality has wide ranging implications from medical physics to cosmology including an intimate but subtle connection in magnetic systems, for example Mn$_1-x$Fe$_x$Si. We demonstrate using theoretical calculations the feasibility of indirect K-edge bimagnon resonant inelastic X-ray scattering (RIXS) spectrum as a viable experimental technique to distinguish crystallographic handedness. We apply spin wave theory to the recently discovered $\sqrt{5} \times \sqrt{5}$ vacancy ordered chalcogenide Rb$_{0.89}$Fe$_{1.58}$Se$_2$ for realistic X-ray experimental set up parameters (incoming energy, polarization, and Bragg angle) to show that the computed RIXS spectrum is sensitive to the underlying handedness (right or left) of the lattice. A Flack parameter definition that incorporates the right- and left- chiral lattice RIXS response is introduced. It is shown that the RIXS response of the multiband magnon system RbFeSe arises both from inter- and intra- band scattering processes. The extinction or survival of these RIXS peaks are sensitive to the underlying chiral lattice orientation. This in turn allows for the identification of the two chiral lattice orientations.

1:39PM L41.00011: Numerical study of skyrmion-string dynamics  
WATARU KOSHIBAE (Presenter), NAOTO NAGAOSA, RIKEN CEMS — Magnetic skyrmion is a swirling emergent particle in two-dimensions characterized by the topological index called skyrmion number. The skyrmion in three dimensional chiral magnets forms a string, end points of which are monopole and antimonopole. This meandering one-dimensional object has many internal degrees of freedom including the rotation and breathing. The skyrmion string is driven by the current through the spin transfer torque effect, and the collision with the disorder induces a variety of phenomena. Here we show theoretically by the numerical simulation of a skyrmion string under current that the four distinct behaviors: (i) pinned string, (ii) depinned motion with the excitation of breathing mode, (iii) resonant excitation of breathing mode leading to the creation of monopole and antimonopole, and (iv) motional narrowing to recover the straight string, as the current density increases.
1:51PM L41.00012: Skyrmions Driven by Intrinsic Magnons  CHRISTINA PSAROUDAKI (Presenter), DANIEL LOSS, Department of Physics, University of Basel — We study the dynamics of a Skyrmion in a magnetic insulating nanowire in the presence of time-dependent oscillating magnetic field gradients [1]. These ac fields act as a net driving force on the Skyrmion via its own intrinsic magnetic excitations. Making use the generalized micromagnetic equations of motion for the quantum propagation of a skyrmion in a magnetic insulator [2], we include the unavoidable coupling of the external field to the magnons, which gives rise to time-dependent dissipation for the Skyrmion. We demonstrate that the magnetic ac field induces a super-Ohmic to Ohmic crossover behavior for the Skyrmion dissipation kernels with time-dependent Ohmic terms. The ac driving of the magnon bath at resonance results in a unidirectional helical propagation of the Skyrmion in addition to the otherwise periodic bounded motion.


2:03PM L41.00013: Relaxation dynamics in magnetic skyrmions with quenched disorder*  BART J BROWN (Presenter), UWE CLAUS TAUBER, MICHEL PLEIMLING, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — Magnetic skyrmions are topologically protected spin textures of nanometer size found in certain chiral magnets. Skyrmions can be moved by very low current densities which makes them ideal for applications in spintronics such as data storage devices and logic gates. A thorough understanding of the relaxation processes for systems of interacting skyrmions far from equilibrium could prove invaluable in real world applications. We use a particle based model derived from Thiele’s approach to study the relaxation dynamics of thin film skyrmions in the presence of randomly distributed defects. The particle model differs most notably from similar models which describe vortices in type-II superconductors by the addition of the Magnus force which always acts perpendicular to the forces in the plane. The interplay between the Magnus force, repulsive skyrmion-skyrmion interaction and Gaussian noise yields different regimes during non-equilibrium relaxation depending on the strength of the defects.

*This research was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Grant No. DE-FG02-09ER46613.

Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L42 DQI: Quantum Annealing: Algorithms and Applications  BCEC 210A - Lin Tian, University of California, Merced - Tag(s): Focus

11:15AM L42.00001: Benchmarking coherent Ising machines and quantum annealers with MAX-CUT and SK problems*  RYAN HAMERLY (Presenter), Research Laboratory of Electronics, Massachusetts Institute of Technology, TAKAHIRO INAGAKI, NTT Basic Research Laboratories, PETER MCMAHON, E. L. Ginzton Laboratory, Stanford University, DAVIDE VENTURELLI, Quantum Artificial Intelligence Laboratory (QuAIL), NASA Ames Research Center, ALIREZA MARANDI, TATSUHIRO ONODERA, EDWIN NG, E. L. Ginzton Laboratory, Stanford University, ELEANOR RIEFFEL, Quantum Artificial Intelligence Laboratory (QuAIL), NASA Ames Research Center, MARTIN FEJER, HIDEO MABUCHI, E. L. Ginzton Laboratory, Stanford University, SHOKO UTSUNOMIYA, National Institute of Informatics, HIROKI TAKESUE, NTT Basic Research Laboratories, YOSHIHISA YAMAMOTO, E. L. Ginzton Laboratory, Stanford University — We benchmark the performance of two types of physical annealing machines -- coherent Ising machines (CIMs) built from coupled optical parametric oscillators, and a commercial quantum annealer (QA) by D-Wave Systems -- on a range of NP-hard Ising problems including MAX-CUT and ground-state computation of Sherrington-Kirkpatrick (SK) spin glasses. Connectivity and embeddability play a central role in the performance differences between the machines, as the QA's connections are defined on a Chimera graph while the CIM is all-to-all. The QA outperforms the CIM for MAX-CUT problems on sparse graphs, while for dense-graph MAX-CUT and SK problems, the QA exhibits an exponential performance penalty relative to the CIM. This performance difference persists in an optimal anneal-time analysis. The strong correlation between hardness and graph edge density when solving problems on the QA, which is absent in the CIM, motivates future work to increase the connectivity in quantum annealers. [arXiv:1805.05217]

*Impulsing Paradigm Change through Disruptive Technologies (ImPACT) Program of the Council of Science, Technology and Innovation (Cabinet Office, Government of Japan). R.H. is supported by an IC Postdoctoral Research Fellowship at MIT, administered by ORISE through U.S. DOE and ODNI.
Benchmarking Portfolio Selection with Adiabatic Quantum Optimization*  
ERICA GRANT  
(Presenter), Bredesen Center, University of Tennessee, TRAVIS HUMBLE, Oak Ridge National Laboratory, NADA WAEL SAMIR ELSOKKARY, FAISAL SHAH KHAN, Khalifa University, GREG QUIROZ, Applied Physics Laboratory, Johns Hopkins University — Portfolio selection is a constrained optimization problem to choose a set of financial assets that maximizes returns while staying under budget and minimizing risk. Markowitz portfolio theory strategically uses correlated behaviors between assets to mitigate financial risk, which we formulate as a quadratic unconstrained binary optimization problem with frustrated stoquastic form. We benchmark the probability of success with the D-Wave 2000Q quantum annealer using problems derived from cryptocurrency market data. We retrieve the lowest energy result from the quantum annealer and compare to the ground truth of a brute force solver. We observe a weakly sub-exponential decay in the probability of success for up to 20 assets, which we extrapolate to estimate the samples required for larger problems. We also find that the relative contributions of the positive diagonal and negative off-diagonal elements have minor influence on the performance as described by the risk. We further investigate performance improvements due to changes in annealing duration, spin-reversal transformations, and reverse annealing post-processing techniques.

*Circuit fault diagnosis using quantum annealing and other spin glass solvers*  
BRENDAN REID  
(Presenter), Information Sciences Institute, University of Southern California, ELIZABETH CROSSON, Department of Physics and Astronomy, University of New Mexico, ITAY HEN, Information Sciences Institute, University of Southern California — In this work we present a novel approach to solving circuit fault diagnosis (CFD) problems using quantum annealers and other spin glass solvers, such as simulated annealing and parallel tempering. The cost function we construct does not minimize the number of faults but rather the distance between real and model circuit outputs: as such it has the attractive property of processing multiple circuit input/output pairs contrary to existing schemes. By showcasing the algorithms' performance through comparison of various metrics, such as time-to-solution, we aim to offer a fresh perspective on using real world-applicable problems in order to understand the nature of quantum annealing optimizers.

*Forward-reverse error mitigation algorithm for quantum annealers*  
NIC EZZELL  
(Presenter), MISSISSIPPI STATE UNIVERSITY — We propose a novel way to try to improve ground-state sampling statistics on quantum annealers with no cost in ancilla qubits—“forward-reverse error mitigation” (FREM) sampling. FREM starts by partitioning a Hamiltonian such that \( H = H_F + H_R \) and proceeds by forward annealing \( H_F \) while backward annealing \( H_R \). While there are no strict requirements on how \( H \) should be partitioned, one should have a good approximation of the ground-state of \( H \) projected onto the qubits in \( H_R \) for the reverse anneal. We study the efficacy of FREM using numerical simulations. In particular, our simulation is modelled after the annealing processes on a D-Wave 2000Q, and we use it to compare the ground-state sampling success of forward, reverse, and FREM annealing by comparing their Kullback-Leibler divergence with respect to direct diagonalization. Overall, this work provides an interesting new method to attempt to mitigate errors on near-term quantum annealers with limited qubit numbers.

*Based on work supported by the Air Force Research Laboratory (AFRL) under agreement number FA8750-18-1-0096. The views and conclusions herein are those of the authors, and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of AFRL or the US Government.
12:03PM L42.00005: Minor embedding: an application in quantum annealing*  
YAN-LONG FANG (Presenter), SIMONE SEVERINI, PAUL A. WARBURTON, University College London — Minor embedding is the embedding of a logical graph as a minor of another graph representing a real quantum annealing device. In the embedded graph each logical qubit is represented by a tree of ferromagnetically-coupled physical qubits. Choi's work gives bounds on the magnitude of the ferromagnetic coupling needed to preserve the ground state spin configuration. We have developed a new method for determining tighter bounds on this magnitude, which in turn should result in fewer errors from thermal noise. Moreover, we prove that our bound is the best bound under some conditions. We have confirmed this result by experimenting on the D-Wave annealer. Since this machine is an open quantum system, the probability of finding the ground state of the embedded problem is maximized when the ferromagnetic coupling strength is set to be equal to the calculated best bound. Our result will likely lead to improved performance for a wide variety of optimization problems with higher degree than can be directly implemented on quantum annealing hardware.

*This research is supported in part by Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office Contract No. W911NF-17-C-0050; and by EPSRC (EP/R020159/1).

12:15PM L42.00006: Performance Improvement of a Quantum Annealer Using Optimized Quantum Control  
GREGORY QUIROZ (Presenter), Johns Hopkins University Applied Physics Lab — Adiabatic quantum computation (AQC) relies on controlled adiabatic evolution to implement a quantum algorithm. Properly designed time-optimal control has been shown to be particularly advantageous for AQC. Grover’s search algorithm is one such example where analytically-derived time-optimal control leads to improved scaling of the minimum energy gap between the ground state and first excited state and thus, the well-known quadratic quantum speedup. Recently, the D-Wave Systems quantum processing unit (QPU) -- a system designed to implement quantum annealing (a non-universal, finite-temperature version of AQC) -- has been upgraded with the ability to manipulate the annealing schedule; thus, enabling an evaluation of the effect of optimized control on computational accuracy. Here, we evaluate the new control features of the device for a range of optimization techniques, assessing the potential benefits of control for enhancing QPU performance for hard problem instances. Specifically, we employ closed-loop control optimization protocols based on stochastic gradient ascent and Bayesian optimization to optimize QPU performance. We focus on engineered hard problem instances for the QPU that exhibit small energy gaps and strong susceptibility to noise.

12:27PM L42.00007: Quantum magnetism on a chip [Invited]  
RICHARD HARRIS (Presenter), D-Wave Systems Incorporated — D-Wave Systems builds superconducting quantum annealing processors that are primarily intended to be used for solving classical computation problems such as optimization and sampling. However, recent publications in Science (Vol. 361, Issue 6398, pp. 162-165) and Nature (Vol. 560, Issue 7719, August 22, 2018) have shown how this computing platform can be used as a programmable quantum magnet that can be used to simulate physical systems relevant to the field of condensed matter physics. This lecture will provide a brief review of the aforementioned results and an update on related experiments.

1:03PM L42.00008: Reverse Quantum Annealing on D-Wave 2000Q*  
DAVIDE VENTURELLI (Presenter), Quantum Artificial Intelligence Laboratory, USRA:RIACS and NASA — We review results to date obtained by the usage of the quantum reverse annealing feature introduced in the latest model of the D-Wave machine - especially comparatively with forward annealing protocols. Results suggest that there is sizable advantage in hybridizing runs with classical initialization algorithms. Particular attention will be devoted in combinatorial optimization problems connected to applications, with examples taken from several different industrial domains, where a large ferromagnetic structure is present in the spin systems due to minor embedding.

*NASA Academic Mission Service contract number NNA16BD14C. National Science Foundation award number 1648832 and 1824470.
1:15PM L42.00009: Quantum Annealing XORSAT on Dilute Square Lattices*  PRANAY PATIL, CLAUDIO CHAMON, STEFANOS KOURTIS, ANDREI E RUCKENSTEIN, Boston University, EDUARDO R MUCCILO (Presenter), Physics, University of Central Florida — Here we show how we can embed the 3-regular 3-XORSAT on a square lattice made out of gates which couple the bits in a manner that recreates the constraints. This system can be annealed to the solution by tuning a transverse field to zero. We explore ways to avoid two potential obstacles that limit how fast one can anneal this system; the first is the nature of the phase transition as we tune the transverse field and the second is the avoided level crossings for small transverse field strength. We discuss how the second pitfall can possibly be avoided in the lattice and other embeddings which have already been studied. We also present Quantum Monte Carlo results on the nature of the phase transition for the embedding of XORSAT on the square lattice. We compare the results to the embedding on a random regular graph, where the phase transition is known to be first order. We also show that different XORSAT problems result in lattice arrangements which exhibit a phase transition whose order is closely related to the classical complexity of the particular problem.

*E.R.M. was supported in part by the NSF Grant No. CCF-1525943.

1:27PM L42.00010: Solution planting scheme for fully-connected spin glasses  CHRISTOPHER PATTISON (Presenter), Texas A&M University, FIRAS HAMZE, JACK RAYMOND, D-Wave Systems Inc., HELMUT KATZGRABER, Texas A&M University — The advent of new specialized hardware designed to tackle spin-glass-like problems on dense graphs has resulted in a renewed interest in planted solutions for spin-glass Hamiltonians. Here we present a method for planting solutions in fully-connected spin-glass systems with tunable hardness. In particular, the hardness of the problems undergoes a complexity transition. Using both analytical and numerical techniques, we characterize the behavior of these new planted systems.

1:39PM L42.00011: Testing the D-Wave 2000Q as a quantum Monte Carlo simulator*  ZOE GONZALEZ IZQUIERDO (Presenter), Physics and Astronomy, University of Southern California, ITAY HEN, TAMEEM ALBASH, Information Sciences Institute, USC — With recent advances in quantum annealing technologies allowing for ‘measurement in the middle’ protocols, present-day experimental quantum annealers have been suggested as practical quantum simulators in lieu of quantum Monte Carlo algorithms. To put this assertion to the test, we have studied the prospects of a D-Wave 2000Q device to function as a simulator of simple one-dimensional chains, in particular to measure thermal expectation values. Here we will present the results of our work along with some interesting conclusions.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050

1:51PM L42.00012: Theoretical survey of unconventional quantum annealing methods applied to a difficult trial problem*  ZHIJIE TANG (Presenter), ELIOT KAPIT, physics, colorado school of mines — Adiabatic quantum annealing is a promising method to solve optimization problems. In our work, we define an artificial trial problem inspired by "transverse field chaos" in larger systems where classical and quantum methods are steered toward a local false minimum and the minimum gap to the true ground state is exponentially small. (all N spins must be flipped from the local minimum to the global minimum, which makes the problem exponentially difficult to solve.) We numerically study this problem by using a variety of new methods from the literature: ramping the transverse field down one by one; adding transverse couplers between qubits; adding local oscillating transverse field. We show that the standard adiabatic quantum annealing method can be improved with these methods, and comparison of these methods could help identify the most promising routes to a quantum speedup in future quantum hardware.

*National Science Foundation, via grant PHY-1653820

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L43 DCMP: New Developments in the FQHE in Half-filled Landau Levels BCEC 210B -
Tag(s): Invited
The universality of the quantum of measurements not trivial, and inter-mode equilibration is not fully understood.

thermal conductance is more challenging as heat flow is not conserved, accurate and noninvasive temperature measurements not trivial, and inter-mode equilibration is not fully understood.

Unlike the relative ease in determining accurately the quantization of the electrical conductance, measuring accurately the thermal conductance, agreeing in good accuracy with numerical works.

We first focused on the Integer, Laughlin's, and hole-conjugate \((\frac{1}{2} < \nu < 1)\) states \([6]\) - proving the universality of \(k_0\). We extended our studies to the fractional states in the first-excited Landau level \((2 < \nu < 3)\), and in particular on the \(\nu=5/2\) state.

We find in the latter a deviation from the quantization of the thermal conductance, suggesting the non-abelian character of the state \([7]\). This topological order was not expected in previous numerical works.

Even denominator fractional quantum Hall physics in higher order Landau levels of graphene

[Invited] JURGEN SMET (Presenter), Max Planck Institute for Solid State Research — An important development in the field of the fractional quantum Hall effect has been the proposal that the 5/2 state observed in the Landau level with orbital index \( n = 1 \) of two-dimensional electrons in a GaAs quantum well originates from a chiral \( p \)-wave paired state of composite fermions which are topological bound states of electrons and quantized vortices. This state is theoretically described by a `Pfaffian` wave function or its hole partner called the anti-Pfaffian, whose excitations are neither fermions nor bosons but Majorana quasiparticles obeying non-Abelian braid statistics. This has inspired innovative ideas for computation and has also instigated a quest for other states with exotic quasiparticles. Here we report experiments on monolayer graphene that show clear evidence for unexpected even-denominator fractional quantum Hall physics in the \( n = 3 \) Landau level. We numerically investigated the known candidate states for even-denominator fractional quantum Hall effect, including the Pfaffian, the particle-hole symmetric Pfaffian, the 221-parton, and several valley/spin singlet states. We conclude that, among these, the 221-parton state is a possible candidate to explain the experimentally observed state and that this incompressible ground state is distinct from the 5/2 state in GaAs. Like the Pfaffian, this state is also believed to harbour quasi-particles with non-Abelian braid statistics.

This work has been carried out with Youngwook Kim, Ajit Balram, Takashi Taniguchi, Kenji Watanabe and Jainendra Jain.

The Dirac Composite Fermion of the Fractional Quantum Hall Effect

[Invited] DAM THANH SON (Presenter), University of Chicago — TBD

Wednesday, March 6, 2019 11:15 AM - 1:39 PM

Session L44 DCMP GSNP: Onsager, Kadanoff, Davisson-Germer Prize Session BCEC 210C - Greg Huber - Tag(s): Invited

11:15AM L44.00001: Lars Onsager Prize Talk: Scaling down the laws of thermodynamics [Invited] CHRISTOPHER JARZYNSKI (Presenter), University of Maryland, College Park — Thermodynamics provides a robust conceptual framework and set of laws that govern the exchange of energy and matter. Although these laws were originally articulated for macroscopic objects, it is hard to deny that nanoscale systems also exhibit “thermodynamic-like” behavior – for instance, biomolecular motors convert chemical fuel into mechanical work. To what extent can the laws of thermodynamics be “scaled down” to apply to individual microscopic systems, and what new features emerge at the nanoscale? I will describe some of the recent progress and challenges associated with addressing these questions.

11:51AM L44.00002: Dissertation Award in Statistical and Nonlinear Physics Talk: The emergence of collective modes, ecological collapse and directed percolation at the laminar-turbulent transition* [Invited] HONG-YAN SHIH (Presenter), Department of Physics and Carl R. Woese Institute for Genomic Biology, University of Illinois at Urbana-Champaign — How a laminar flow becomes turbulence has been an unsolved problem for 130 years and is important in various industrial applications. Only since a decade ago, precise measurements in pipe flow experiments showed non-trivial spatio-temporal complexity at the onset of turbulence where lifetime and splitting time of metastable turbulence do not diverge asymptotically as would have been expected in a sharp transition. Based on numerical evidence in the Navier-Stokes equations, we discovered the surprising fact that the fluid behavior at the transition is governed by the emergent predator-prey dynamics of the important long-wavelength mode, leading to the mathematical prediction that the laminar-turbulent transition is a non-equilibrium phase transition in the directed percolation universality class. This prediction explains the universal scaling laws in experimental observations, and provides a unified picture of transition to turbulence emerging in systems ranging from turbulent convection to magnetohydrodynamics.

*This work was partially supported by NSF-DMR-1044901.
M CRISTINA MARCHETTI (Presenter), University of California, Santa Barbara — Active matter is the named coined to describe collections of interacting self-driven entities that spontaneously organize in active fluids and solids, with nonequilibrium transitions between ordered and disordered states. Examples include subcellular structures, groups of motile organisms, and chemical and mechanical analogues with life-like properties. The distinguishing property of active systems is that they are driven out of equilibrium by a forcing that acts independently on each unit, breaking detailed balance at the micro-scale and resulting in behaviors that challenge our intuition. For instance, active fluids flow with no externally applied forces and active gases do not fill their container. After highlighting some of these behaviors, I will focus in this talk on the self-sustained flows of active nematics where the proliferation of motile topological defects mediates the transition to spatiotemporal chaotic dynamics. I will conclude by identifying some of the challenges that lie ahead.

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RANDALL FEENSTRA (Presenter), Carnegie Mellon University — Over the past decade, much research world-wide has focused on two-dimensional (2D) materials, in which the electrons are localized within a single atomic plane. Obtaining μm-size flakes of 2D material by “exfoliating” (peeling apart) layers using adhesive tape has been a standard practice for decades, but only recently has this method been applied to produce small, microfabricated electronic devices on the flakes (Geim and Novoselov, Nobel Prize 2010). However, for practical electronics of the future, such devices must be produced on grown (deposited), large-area 2D layers, rather than on flakes. In this talk, studies of the structure of grown 2D layers will be described, focusing on heterobilayers of MoS2 on WSe2. The method of scanning tunneling microscopy is used to obtain detailed, atomic-scale views of the structure of the layers. Additionally, through spectroscopic measurements with the tunneling microscope, band gaps of the materials and band offsets between neighboring layers are determined. We find, in particular, the occurrence of localized electron states associated with the moiré pattern that forms when one layer of a 2D material (MoS2) is placed on another layer (WSe2) with different lattice constant.

*Work performed in collaboration with D. Waters, F. Lüpke, Y. Pan, S. Fölsch, Y. Nie, Y.-C. Lin, B. Jariwala, K. Zhang, K. Cho, and J. A. Robinson, and supported in part by the Center for Low Energy Systems Technology (LEAST, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA), the National Science Foundation, and the A. von Humboldt Foundation.

Wednesday, March 6, 2019 11:15 AM - 1:51 PM

Session L45 DCMP: Surface Studies of Transition Metal Chalcogenides

GUANNAN CHEN (Presenter), SEAN T HOWARD, SOMESH CHANDRA GANGULI, VIDYA MADHAVAN, WACLAW SWIECH, Physics, University of Illinois at Urbana-Champaign — TMDC provide a unique platform exhibiting ground states from CDW, to ferromagnetism and superconductivity. Among the TMDC family, bulk 1-T VSe2 is known as a typical 3D CDW material with a transition temperature of 105 K. But there have been two interesting observations in a few layers VSe2. First, while bulk VSe2 is paramagnetic, VSe2 a few layers limit was shown ferromagnetism. Second, multiple CDW patterns with different Q-vectors have been observed. In this work, we grow VSe2 thin films at two growth temperatures (Tg) by a home-built MBE and study the samples in a 4K STM. In the samples grown at low Tg, we found different 2D CDW patterns in the first and second layer. The high Tg films show stripe-type topographies in the first and second layer with different periodicity. The STM scans and RHEED images indicate that the second layer grown at high Tg is 1T' phase VSe2. Based on this we conclude that two different Tg produce distinct polymorphs of VSe2. We further compare the dI/dV spectrums of the two polymorphs as a function of layer thickness and discuss the evolution of the electronic properties with thickness.

*The work was supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4860 and NSF-DMREF program through Grants 1629382 and 1629068.
Transport properties of high-mobility InSe in Quantum Hall regime.*

DMITRY SHCHERBAKOV (Presenter), PETR STEPANOV, JIAWEI YANG, Ohio State University, SHAHRIAR MEMARAN, WENKAI ZHENG, National High Magnetic Field Laboratory FSU, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Namiki Tsukuba Ibaraki, Japan, LUIS BALICAS, National High Magnetic Field Laboratory FSU, CHUN NING LAU, Ohio State University — Among the modern two-dimensional (2D) semiconductors, InSe is a promising candidate for future electronics due to its large thickness-dependent bandgap and high mobility. We have fabricated high mobility ultrathin InSe devices, and observed quantum Hall states in high magnetic field. Transport properties of InSe at low temperatures and high magnetic fields will be presented.

*This research was supported by grants NSF-DMR 1807928 (Lau) and NSF-DMR 1807969 (Balicas)

New Mechanical Exfoliation Technique for Preparing Large Area 2D Materials and Special Structures

YUAN HUANG (Presenter), WEN JUAN ZHAO, LIN ZHAO, GUO DONG LIU, National Laboratory for Superconductivity (NLSC), Institute of Physics, CAS, PETER SUTTER, Engineering, University of Nebraska, Lincoln, XINGJIANG ZHOU, National Laboratory for Superconductivity (NLSC), Institute of Physics, CAS — Mechanical exfoliation method has been widely used to study the intrinsic properties of 2D materials. Even though the exfoliated 2D materials show high quality, the size of monolayer samples are usually quite small, which has limited the investigation progress of 2D materials. Recently, we developed a new mechanical exfoliation technique for preparing large area and high quality 2D materials[1]. Many monolayer 2D materials with millimeter to centimeter size have been successfully exfoliated through this method, including graphene, TMDCs et al. The key of this technique is to enhance the van der Waals interaction between the layered materials and the substrates, which can be realized by optimizing the exfoliation process, such as substrate types, temperature and vacuum. Besides, some special structures (like bubble and wrinkle) can be prepared by using different parameters. Therefore, many unique properties can be observed on these structures, e.g., standing wave induced Raman oscillation was first discovered on the exfoliated graphene bubbles[2]. The new mechanical technique will show great potential for exploring new properties of 2D materials.

References

Epitaxial Growth and Structure Phase Transition of monolayer 1T'-WSe2 thin film*

WANG CHEN, TONG CHEN, DONGJIN LIN, XUEDONG XIE, JUNYU ZONG, FAN YU, SHAOEN JIN, LINGJIE ZHOU, JINGYI ZOU, JIAN SUN, XIAOXIANG XI, YI ZHANG (Presenter), Nanjing University — The emerging two-dimensional (2D) materials are playing more and more important roles in both fundamental research and practical application potentials in recent years. The 2D transition metal dichalcogenides (TMDCs) have attracted extensive interest due to their remarkable fundamental properties distinct from those of their bulk counterparts. Its 2H phase possesses an indirect to direct bandgap transition in 2D limit. The 1T' phase transition can drive the monolayer MX2 to be a 2D topological insulator. Using molecular beam epitaxial (MBE) method, we realized the growth of both the 1T' and 2H phase monolayer WSe2 thin films. The crystalline structure of these two phases was characterized using the in-situ scanning tunneling microscopy (STM) technique. The monolayer 1T'-WSe2 was found to be metastable, and can transform into 2H phase under post-annealing procedure. This thermo-driven crystalline phase transition makes the monolayer WSe2 to be an possible platform for controlling of topological phase transition.

*This work was supported by the National Key R&D Program of China (No.2018YFA036800), and the National Natural Science Foundation of China (Grant Nos. 11714154, 11790311 and 11774151).
Distinct ultrafast carrier dynamics governed by spin filtering in bulk and single-layer WSe$_2$*

RO-YA LIU (Presenter), Institute of Physics, Academia Sinica, MENG-KAI LIN, PENG CHEN, Physics, University of Illinois at Urbana-Champaign, TAKESHI SUZUKI, Institute for Solid State Physics, University of Tokyo, PHILIPPA CLARK, NATHAN LEWIS, Photon Science Institute, University of Manchester, CEPHISE CACHO, Diamond Light Source, STFC Rutherford Appleton Laboratory, EMMA SPRINGATE, Central Laser Facility, STFC Rutherford Appleton Laboratory, CHIA-SENG CHANG, Institute of Physics, Academia Sinica, KOZO OKAZAKI, Institute for Solid State Physics, University of Tokyo, WENDY FLAVELL, Photon Science Institute, University of Manchester, IWAO MATSUDA, Institute for Solid State Physics, University of Tokyo, TAI-CHANG CHIANG, Physics, University of Illinois at Urbana-Champaign — Carrier dynamics in a semiconductor following pulsed optical excitation is relevant to ultrafast optoelectronic applications. We report herein a comparative study of bulk WSe$_2$ and single-layer (SL) WSe$_2$ grown on bilayer-graphene-terminated SiC. Subtle dimensional effects lead to substantial differences in the transient response as revealed by time-resolved angle-resolved photoemission spectroscopy (TRARPES) measurements. The conduction band minimum in bulk WSe$_2$, populated by optical pumping, decays promptly. The corresponding decay for SL WSe$_2$ is more complex but overall much slower due to spin filtering arising from the lack of space inversion symmetry. Concurrent measurements of the valence bands show longer but different response times arising from lattice excitation, carrier transport, and dissipation. These results illustrate the various time scales and processes at work for carrier and band structure evolution.

*This work is supported by the U.S. DOE, Office of Science, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under Grant No. DE-FG02-07ER46383 (TCC). The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

A Gate Free Monolayer WSe$_2$ pn Diode

CHUNG-LIN WU (Presenter), JHIH-WEI CHEN, Department of Physics, National Cheng-Kung University, CHIA-HAO CHEN, National Synchrotron Radiation Research Center (NSRRC), YI-CHUN CHEN, TSE-MING CHEN, SHUN-TSUNG LO, SHENG-SHONG WONG, Department of Physics, National Cheng-Kung University — Interest in bringing p- and n-type monolayer semiconducting transition-metal dichalcogenides (TMD) into contact to form rectifying pn diode has thrived since it is crucial to control the electrical properties in two-dimensional (2D) electronic and optoelectronic devices. Usually this involves vertically stacking different TMDs with pn heterojunction or, laterally manipulating carrier density by gate biasing. Here, by utilizing a locally reversed ferroelectric polarization, we laterally manipulate the carrier density and created a WSe$_2$ pn homojunction on the supporting ferroelectric BiFeO$_3$ substrate. This non-volatile WSe$_2$ pn homojunction is demonstrated with optical and scanning probe methods and scanning photoelectron micro-spectroscopy. A homo-interface is a direct manifestation of our WSe$_2$ pn diode, which can be quantitatively understood as a clear rectifying behavior. The non-volatile confinement of carriers and associated gate-free pn homojunction can be an addition to the 2D electron-photon toolbox and pave the way to develop laterally 2D electronics and photonics.

Investigation of charge density wave transitions in a proximally coupled single-layer TiTe$_2$/TiSe$_2$ system

MENG-KAI LIN (Presenter), JOSEPH HLEVYACK, PENG CHEN, RO-YA LIU, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign — TiSe$_2$, a prototypical charge density wave (CDW) system with a 1T structure in the bulk, undergoes a (2×2×2) CDW transition at 205 K. By comparison, a single layer of TiSe$_2$ prepared on a bilayer-graphene-terminated SiC(0001) undergoes a (2×2) CDW transition at 232 K. The bonding of the single layer to the substrate is expected to be of the van der Waals type. Furthermore, the structures are incommensurate, which makes the interfacial bonding even weaker. A reasonable premise is that the single layer is nearly freestanding with minimal influence from the substrate on its (2×2) CDW. TiTe$_2$, by contrast, shows no CDWs in the bulk or in films grown on the same bilayer-graphene-terminated SiC; the only exception is a (2×2) CDW transition at 92 K in the single layer. The unique behavior of the single layer is an anomaly. To explore the physics further, we have grown a composite system made of a single layer of TiTe$_2$ on a single layer of TiSe$_2$ on a bilayer-graphene-terminated SiC. The crystal structures of TiSe$_2$, TiTe$_2$, and graphene are all incommensurate. Questions abound: Is there a CDW transition in this composite system? Or, are there actually two transitions? Results of band structure mapping by angle-resolved photoemission spectroscopy will be presented to address these issues.
12:39PM L45.00008: Electronic and structural properties of the phase transitions in TaTe$_{2-x}$Se$_x$* CHEN CHEN (Presenter), HEUNG SIK KIM, ALEMAYEHU S ADMASU, WENHAN ZHANG, FEI-TING HUANG, SANG-WOOK CHEONG, KRISTJAN HAULE, DAVID VANDERBILT, WEIDA WU, Department of Physics and Astronomy, Rutgers University — Charge density wave (CDW) is a spontaneous modulation of electron density, which is usually associated with periodic lattice distortion with the same wavelength. Such phenomenon is often observed in layered transition metal dichalcogenides (TMD), although its origin is still under debate. 1T-TMD TaTe$_2$ shows a CDW like phase transition around 170 K where new modulation of 3×3 superstructure forms. Magnetic susceptibility and resistivity show abnormal behavior at the phase transition, which is inconsistent with conventional model or example. Here, we use combination of scanning tunneling microscopy/spectroscopy, low energy electron diffraction, and density functional theory calculations to study the temperature dependence of CDW in undoped and Se doped TaTe$_2$ single crystals. We have observed a hidden phase with a distinct modulation, which can be stabilized by Se doping, and is less metallic than the 3×3 low temperature phase. Our results suggest a possible explanation to the mystery in transport properties, which provides new insight on the electron-lattice coupling associated with CDW phase transitions.

*NSF-DMREF-1629059

12:51PM L45.00009: Confining electronic states with domain walls in ferroelectric SnTe monolayers* KAI CHANG (Presenter), Max-Planck Institute of Microstructure Physics, BRANDON J MILLER, Department of Physics, University of Arkansas, HAO YANG, Max-Planck Institute of Microstructure Physics, HAICHENG LIN, QIKUN XUE, XI CHEN, SHUAIHUA JI, Department of Physics, Tsinghua University, SALVADOR BARRAZA-LOPEZ, Department of Physics, University of Arkansas, STUART S P PARKIN, Max-Planck Institute of Microstructure Physics — Electronic standing wave patterns at surfaces are usually generated by edges, atomic steps or adatoms that introduce large potential barriers. However, in multi-valley semiconducting 2D materials, quasiparticle confinement and suppressed transmission can be created from mismatched electronic structures through domain walls, with a neglectable built-in bias at the interface. Here, we report the first observation of electronic standing waves near the valence band maximum in a SnTe monolayer that is generated by the reflection from ferroelectric domain walls. Despite of the nearly flat potential barrier at the domain walls, the reflectivity is found to be 68+-9% at 4.7 K, and no sign of transmission was seen. Such a strong confinement of electronic states is due to a large change of valley positions between the neighboring domains arising from a 90 degree rotation of the Brillouin zone. These results show potential for polarization-tuned valleytronics in 2D ferroelectrics.

*DFG PA 1812/2-1. National NSF of China (Grant No. 51561145005). Ministry of Science and Technology of China (2016YFA0301002). U.S. DOE, Office of Basic Energy Sciences DE-SC0016139. Calculations at Cori (NERSC) and Trestles (Arkansas).

1:03PM L45.00010: Electrical and Optical Characterization of Ultrathin Tellurium Nanostructures Synthesized by Vapor Phase Deposition* KESHAB SAPKOTA (Presenter), DOUGLAS L. MEDLIN, PING LU, TING-SHAN LUK, TZU-MING LU, GEORGE T. WANG, Sandia National Labs — Tellurium (Te) is a semiconductor with a slightly indirect bulk bandgap of 0.35 eV. The trigonal crystal structure of Te consists of 1D helical chains of Te atoms stacked together by van der Waals type bonds arranged on 2D hexagonal lattice. Each Te atom is covalently bonded with its two nearest neighbors on the same chain. This unique crystal structure allows a stable 1T-MoS$_2$-like α-Te, a metastable tetragonal β-Te, and a 2H-MoS$_2$-like γ-Te structures. The α- and γ-Te phases are expected to have nearly direct band gaps and high carrier motilities suggesting potential applications in electronic and optoelectronic devices. Here we present the vapor phase synthesis and characterization of novel ultrathin Te nanostructures having thickness down to 3.5 nm. Room temperature (RT) electrical measurements exhibit p-type semiconductor with field effect hole mobility of ~350 cm$^2$/V.s. The low-temperature transport properties, RT micro-photoluminescence, and structural properties of the Te nanostructures will also be presented.

*Sandia National Laboratories is a multi-program laboratory managed and operated by NTiSS Corporation, a wholly owned subsidiary of Honeywell Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.
1:15PM L45.00011: Biexcitons in Monolayer Transition Metal Dichalcogenides Tuned by Magnetic Fields

CHRISTOPHER E STEVENS, VARUN MAPARA (Presenter), JAGANNATH PAUL, TIMOTHY COX, PRASANA SAHOO, HUMBERTO RODRIGUEZ GUTIERREZ, Dept. of Physics, University of South Florida, VOLODYMYR TURKOWSKI, Dept. of Physics, University of Central Florida, DIMITRY SEMENOV, STEPHEN A MCGILL, National High Magnetic Field Laboratory, Florida State University, MYRON KAPETANAKIS, ILIAS PERAKIS, DAVID J. HILTON, Dept. of Physics, University of Alabama Birmingham, DENIS KARAISKAJ, Dept. of Physics, University of South Florida — Time-Integrated Four Wave Mixing measurements were performed on CVD grown MoSe$_2$ monolayers. The dephasing lifetime was investigated in magnetic fields up to 25T. Additionally, the effects of valley selection on the lifetime was explored through varying polarization schemes. The results were then modeled using time-dependent density function theory revealed the dephasing lifetime is dominated by the inter-valley biexcitons.

*The research at USF and UAB is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DESC0012635. This work was in part supported by the National Science Foundation under Grant no. DMR-1409473. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement no. DMR-1157490 and the State of Florida. S.M. acknowledges funding through NSF DMR-1229217. H.R.G acknowledges support from the National Science Foundation (NSF) grant DMR-1557434. V.T. acknowledges the Department of Energy for partial support under Grant no. DOE-DE-FG02-07ER46345.

1:27PM L45.00012: Controlled and Tunable Light Emission of Heat Treated Black Phosphorus: Towards Tunable Optoelectronic Devices

SARAH ALODAN (Presenter), FADHEL ALSAFFAR, King Abdulaziz City for Science and Technology, JUSTIN M. GORHAM, FRANK W. DELRIO, Material Measurement Laboratory, National Institute of Standards and Technology, MOHAMMED R AMER, King Abdulaziz City for Science and Technology — Layered black phosphorus (BP) has shown exceptional optical properties due to its layer-dependent band gap, which ranges from 0.3 to 1.7 eV for bulk to monolayer, respectively. However, instability of black phosphorus nanosheets can be a major hurdle in controlling this light emission and requires various passivation methods. Moreover, the tunablility of the emitted light can only be controlled by changing the nanosheet thickness, which in turns changes the band gap energy. Here, we show for the first time a well-controlled tunable light emission from heat treated black phosphorous nanosheets. We show tunable wideband photoluminescence (PL) between 590nm to 720nm, with a tunablility resolution of 5nm. This tunable PL is found to be anisotropic and can last for at least 10 days when nanosheets are properly stored. We attribute the origin of this light emission to the formation of stable black phosphorus oxide on the surface of black phosphorus, as confirmed with i-XPS measurements. Our findings unlock doors for optoelectronic applications of layered black phosphorus nanosheets.

*King Abdulaziz City for Science and Technology

1:39PM L45.00013: Reversible Thermally Driven Phase Transformation in Ultrathin Ferroelectric In$_2$Se$_3$ Layers

FAN ZHANG (Presenter), Department of Physics, Virginia Tech, ZHE WANG, Department of Physics, University of Science and Technology of China, ANMIN NIE, JIANYONG XIANG, State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, China, WENGUANG ZHU, Department of Physics, University of Science and Technology of China, ZHONGYUAN LIU, State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, China, CHENGGANG TAO, Department of Physics, Virginia Tech — Phase transformation in emerging two dimensional (2D) ferroelectric materials is crucial for their applications, such as in nonvolatile memory devices. We combined STM, STEM, Raman spectroscopy and first-principles calculation to investigate ultrathin layered In$_2$Se$_3$ syntheszed by chemical vapor deposition (CVD). At room temperature, we observed that ultrathin In$_2$Se$_3$ ranging from ~20 layers to monolayer, stabilized at the $\beta$ phase with a superlattice. Strikingly, at around 210 K the $\beta$ phase converted to a novel and more stable $\beta'$ phase, which has never been revealed in 2D In$_2$Se$_3$ with atomic resolution. The thermally driven kinetics of the reversible $\beta$-$\beta'$ phase transformation was studied with temperature dependent STEM and Raman spectroscopy, which corroborated with the expected minimum-energy pathways for the transformation obtained from our DFT calculation. The calculated energy difference between the $\beta$ phase and the $\beta'$ phase is 0.033 eV/In$_2$Se$_3$, with an energy barrier of 0.006 eV/In$_2$Se$_3$. The DFT calculation further suggested in-plane ferroelectricity in the $\beta'$ phase, and in contrast, both in-plane and out-of-plane ferroelectricity in the $\beta$ phase.

*F.Z. and C.T. acknowledge the financial support provided by the U.S. Army Research Office under Grant W911NF-15-1-0414.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM
11:15AM L46.00001: Shedding light on materials out of equilibrium: Ultrafast control of magnetism in complex oxide thin-films* [Invited] NICOLE BENEDDEK (Presenter), Department of Materials Science and Engineering, Cornell University — The recent development of intense ultrashort mid- and far-infrared laser sources has created an opportunity for functional materials based on the direct excitation of infrared active phonons. Strong excitation of infrared active phonons can produce sizable unidirectional distortions of crystal structure through non-linear couplings between various lattice modes. Complex oxides provide an important test-ground for this experimental approach due to their chemical diversity, strong coupling to optical fields, and demonstrated connection between subtle structural changes and functional properties. Early experiments in complex oxides are intriguing, suggesting that non-linear phonon coupling is responsible for transiently induced insulator-metal phase transitions and enhanced superconductivity in optical experiments. In this talk, I will describe our recent theoretical efforts exploring selective control of functional properties in perovskite oxides that exploit non-linear lattice dynamics. Using first-principles techniques we show that optical control of various properties is experimentally feasible and that, when combined with epitaxial strain, it is possible to transiently stabilize and explore phases inaccessible in the equilibrium phase diagram.

*This work was supported by the National Science Foundation (NSF) under awards DMR-1550347 and DMR-1719875 (Cornell Center for Materials Research, an NSF MRSEC). This work made use of high-performance computing facilities provided by the Cornell Center for Advanced Computing and the NSF through XSEDE allocation DMR-160052.

11:51AM L46.00002: Ultrafast Carrier Dynamics in La_{1-x}Sr_xMnO_3/SrTiO_3 Heterostructures* KUN ZHAO (Presenter), JOEL E TAYLOR, Department of Physics & Astronomy, Louisiana State University, RAMI A KHOURY, Department of Chemistry, Louisiana State University, MOHAMMAD SAGHAYEZHIAN, Department of Physics & Astronomy, Louisiana State University, LOUIS H HABER, Department of Chemistry, Louisiana State University, JIANDI ZHANG, E WARD PLUMMER, Department of Physics & Astronomy, Louisiana State University — Transition metal oxide thin films and heterostructures have attracted interest of community due to manifestation of broken symmetry and dimensional confinement, which create new forms of coupling and consequently new functionality. An important challenge is to probe the excited states of these artificially structured materials. Ultrafast reflectivity measurements can be used to study the highly non-equilibrium exited states and observe subsequent dynamical behavior. We grew La_{1-x}Sr_xMnO_3/SrTiO_3(001) heterostructures using different growth conditions, being able to control structural and compositional modulation near the interface, which profoundly changes electronic and magnetic properties of these thin films. Using ultrafast reflectivity measurements, we show novel excited-state relaxation dynamics and phonon oscillations in these heterostructures. The changes in these relaxations will be discussed relevant to the growth conditions. With specific growth condition, we observed the relaxations of electron-phonon coupling and phonon-phonon coupling with larger than expected lifetimes as well as the oscillations of two phonon modes. Furthermore, pump-power dependent reflectivity and lifetimes were also studied.

*Supported by the U.S. Department of Energy under Grant No. DE-SC0002136.

12:03PM L46.00003: Atomic-Resolution Studies of Radiation-Induced Defects In High Conductivity Delafossite Oxide Metals* CELESTA CHANG (Presenter), Cornell University, VERONIKA SUNKO, PHILIPPA MCGUINNESS, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, DAVID ANTHONY MULLER, Cornell University — Delafossite metals are known for having the highest in-plane conductivity in the oxide family. Room temperature resistivity of PdCoO_2 is 2.6μΩ, and at low temperature it drops down to 0.0075μΩ, with a mean free path of 20μm. Such long mean free path raises the question of the nature of the defects – is the density truly that low, or are defects present but somehow hidden from scattering channels? Using scanning transmission electron microscopy (STEM) we deliberately introduced defects at a specific atomic plane of PdCoO_2 and PtCoO_2 using a high electron dose of 520×10^{-3}C/mm^2, then imaging at lower doses. Our results show that damage from an electron beam focused on the Pd (Pt) atomic layers creates local metallic chains and clusters. A beam placed on the O-Co-O layer damages more dramatically by cutting the Co layers off, resulting in Pd (Pt) layers to be pulled towards the neighboring Co layer position.

*Work supported by the U.S. DOE BES, Award #DE-SC0002334 and PARADIM, an NSF MIP (DMR-1539918). EM Facility support from the NSF MRSEC program (DMR 1120296).
Interfaces of complex oxides can exhibit properties not realized in the constituent materials. The chemistry that occurs at such interfaces has received relatively little attention, yet can be very influential and permit control of interfacial properties, if it is well understood. Here we focus on a dramatic interface chemical effect: the apparent dissolution of an entire atomic plane during WO₃ heteroepitaxy on TiO₂-terminated SrTiO₃(001). Transmission electron microscopy indicates that the first subsurface SrO monolayer is completely removed, resulting in the formation of a TiO₂ bi-layer at the interface. In combination with x-ray photoelectron spectroscopy measurements, these data suggest that at least a fraction of the Sr from this layer dissolves into the WO₃ film. To assist interpretation of the TEM data, we determined the thermodynamic stability of candidate interfacial structures using ab initio (density functional theory) simulations and linked these stabilities to the growth conditions. The analysis of near-interface diffusion pathways suggests ways in which SrO dissolution takes place, and how manipulation with the growth conditions can shift the thermodynamic preference from one structure to another.

*US DOE, BES/MSE Award 10122, Early Career Research Program Award 68278

12:27PM L46.00005: Defects and transport in oxide heterostructures* [Invited] CHRIS VAN DE WALLE (Presenter), University of California, Santa Barbara — Complex oxide heterostructures have been intensively investigated in recent years. However, the widely used transition-metal oxides suffer from low carrier mobility, which limits device applications. For applications in electronics, attention has shifted to materials such as BaSnO₃ and Ga₂O₃. They have large band gaps, rendering them suitable for transparent conductors and high-frequency and power electronics, but can be highly n-type doped and exhibit good transport properties. Better control of dopants and point defects is still needed in order to improve materials quality and enable further applications. I will show how cutting-edge first-principles modeling, using advanced hybrid functional calculations within density functional theory, can shed light on the multiple aspects of this problem: band alignment and confinement of two-dimensional electron gases [1,2,3,4], carrier scattering and mobility [5,6], doping [7,8], point defects and their impact on carrier concentrations [8], energetics and electronic structure of alloys [3,4], and optical properties [9,10].


*Work supported by AFOSR, ONR, and NSF.
1:03PM L46.00006: Structural Goldstone modes in 111-strained perovskite SrMnO$_3$*

ASTRID MARTHINSEN,
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Norwegian University of Science and Technology, TOR GRANDE, Department of Materials Science and Engineering, NTNU Norwegian
University of Science and Technology, THOMAS TYBELL, Department of Electronic Systems, NTNU Norwegian University of Science and
Technology, SVERR SELBACH (Presenter), Department of Materials Science and Engineering, NTNU Norwegian University of Science and
Technology — Epitaxial strain has been extensively explored to enhance existing and enable new functional properties in perovskite thin films. While most of this work has been done on 001-oriented heterostructures, 111-oriented films can have very different properties. Here we use DFT calculations to predict structural Goldstone modes in the (111)-strained perovskite SrMnO$_3$. Massless Goldstone modes are found in high energy particle physics as well as in low energy systems like superconductors and superfluid helium, while structural Goldstone modes are rare. Here we predict acoustic Goldstone phonon modes under compressive strain resulting from coupling between two in-plane rotational instabilities, giving the characteristic Mexican hat shaped energy surface. Large tensile strain is found to induce in-plane polar instabilities giving rise to a continuous polar ground state. Such phonon modes with U(1) symmetry could emulate structural condensed matter Higgs modes, where the mass of this boson is given by the shape of the Mexican hat energy surface, which is tunable by epitaxial strain.

*Research Council of Norway, Grants 231430 and 231290. US Department of Energy DE-AC02-05-CH11231. Swiss National Science Foundation Early Postdoctoral Mobility Program. UNINETT Sigma2 NN9264K and NN9301K.

1:15PM L46.00007: Designing Optimal Perovskite Structure for High Ionic Conduction*

RAN GAO (Presenter), Materials Science and Engineering, University of California, Berkeley, ABHINAV JAIN, Materials Science and Engineering, University of Illinois, Urbana-Champaign, SHISHIR PANDYA, Materials Science and Engineering, University of California, Berkeley, YONGQI DONG, X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, YAKUN YUAN, Materials Science and Engineering, Pennsylvania State University, HUA ZHOU, X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, LIV R DEDON, Materials Science and Engineering, University of California, Berkeley, VINCENT THORÉTON, WPI international Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, SAHAR SAREMI, RUIJUAN XU, AILEEN LUO, Materials Science and Engineering, University of California, Berkeley, TING CHEN, WPI International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, VENKATRAMAN GOPALAN, Materials Science and Engineering, Pennsylvania State University, ELIF ERTEKIN, Mechanical Science and Engineering, University of Illinois, Urbana-Champaign, JOHN KILNER, TATSUMI ISHIHARA, WPI International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, NICOLA PERRY, DALLAS TRINKLE, Materials Science and Engineering, University of Illinois, Urbana-Champaign, LANE MARTIN, Materials Science and Engineering, University of California, Berkeley — There has been an incomplete understanding of the structure-property relationships that would enable the rational design of better ion-conducting electrolytes for SOFC. Here, using epitaxial thin-film growth, synchrotron X-ray diffraction, impedance spectroscopy, and density-functional theory, we delineate the impact of structural parameters (i.e., unit-cell volume and octahedral rotations) on ionic conductivity in La$_{0.9}$Sr$_{0.1}$Ga$_{0.95}$Mg$_{0.05}$O$_{3-\delta}$. As compared to the zero-strain state, compressive strain reduces the unit-cell volume while maintaining large octahedral rotations, resulting in a strong reduction of ionic conductivity, while tensile strain increases the unit-cell volume while quenching octahedral rotations, resulting in a negligible effect on the ionic conductivity. Calculations reveal that larger unit-cell volumes and octahedral rotations decrease migration barriers and create low-energy migration pathways, respectively. The desired combination of large unit-cell volume and octahedral rotations is normally contraindicated, but through the creation of superlattice structures we experimentally realize both expanded unit-cell volume and strong octahedral rotations which result in an enhancement of the ionic conductivity by ~250% at around 600°C.

*NSF Grant OISE-1545907
Epitaxial strain effect on site occupancy and conductivity of titanomagnetite*  
TIFFANY KASPAR (Presenter), Pacific Northwest Natl Lab, STEVE MICHAEL HEALD, Argonne National Lab, MARK BOWDEN, PETER SUSHKO, SCOTT CHAMBERS, Pacific Northwest Natl Lab — Magnetite, Fe$_3$O$_4$, exhibits metallic conductivity via electron hopping between Fe$^{2+}$ and Fe$^{3+}$ occupying octahedral sites in the spinel lattice. As Ti$^{4+}$ is doped into the octahedral sites of magnetite (the titanomagnetite series), an equal fraction of Fe$^{3+}$ is reduced to Fe$^{2+}$ to maintain charge neutrality. The site occupancies of Fe$^{2+}$ and Fe$^{3+}$ determine the transport properties of the titanomagnetite series; the end-member ulvöspinel, Fe$_2$TiO$_4$, exhibits $p$-type semiconducting transport properties. The Fe$^{2+}$/Fe$^{3+}$ site occupancy remains controversial, but is likely in part a function of the lattice strain induced by doping smaller Ti$^{4+}$ into the lattice. Here, we have deposited titanomagnetites and ulvöspinel as well-defined epitaxial thin films on both MgO and MgAl$_2$O$_4$ substrates. We have characterized the Fe valence state and site occupancy with XPS, XANES, and EXAFS, and related them to the epitaxial strain induced by the substrate. The impact of these factors on the electrical transport properties of the films will be discussed.

*U.S. Department of Energy (DOE), Basic Energy Sciences (BES), Division of Materials Sciences and Engineering, under Award No. 10122.

Electronic and Catalytic Behavior of Mn-based Spinels Grown by Molecular Beam Epitaxy*  
MILES BLANCHET (Presenter), SHALINEE CHIKARA, ALEXANDRIA BREDAR, Auburn University, TIFFANY KASPAR, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, BYRON FARNUM, RYAN COMES, Auburn University — Previous research on manganese-based spinel structures has shown that some exhibit strong oxygen reduction reaction catalytic behavior for water splitting in hydrogen fuel cells. However, there have been limited efforts to study these materials as epitaxial thin films which can be used for surface catalysis studies. With this in mind, thin films of spinel structures such as MnFe$_2$O$_4$, CoMn$_2$O$_4$, NiMn$_2$O$_4$ and Mn$_3$O$_4$ were synthesized to study the relationship of electronic properties and catalytic behavior. Films were grown using a molecular beam epitaxy system which allowed for precise control of sample stoichiometry. After growth, films were transferred to an in-situ x-ray photoelectron spectroscopy system to be examined without exposure to atmosphere. In addition, measurements characterizing the films’ electronic and catalytic properties such as ellipsometry and cyclic voltammetry were also performed. The combination of these studies allows for a greater understanding of these spinels and how they might be used in future catalytic applications.

*This work is funded by the National Science Foundation, Division of Materials Research, Solid State and Materials Chemistry program under award number 1809847 with additional funding from EPSCOR.

Fluorination of Epitaxial Thin Films of Functional Metal Oxides*  
JOSEPH CARTELLI (Presenter), FRANCIS WALZ, ANTON WIGGINS, DAVID HUSTON, SANEDYA HERNANDEZ, AZRIEL WEINREB, RAJESWARI M KOLAGANI, Towson University — The goal of this project is to investigate the effects of incorporating fluorine into epitaxial thin films of functional metal oxides including Lanthanum Calcium Manganese Oxide (LCMO), Calcium Manganese Oxide (CMO), and Strontium Titanate (STO), with emphasis on electrical resistivity and structural changes. Electrical resistivity is a property of interest for many technical applications of these advanced and emerging materials. Fluorination of similar perovskite oxide materials including SrFeO$_{3-d}$ in thin films has yielded many interesting results. These results include altering the crystal structures and altering the electrical properties. Fluorine alters the anionic composition of these materials thus providing a way for extending the range of functional properties realizable. Fluorine introduction has the potential for charge doping the materials and altering the cation valence states. This would lead to changing structural order and symmetry through ionic size differences in the cation, and changes in the charge carrier concentration and mobility.

*We acknowledge support from the NSF grant DMR 1709781 and support from the Fisher General Endowment grant from the Jess and Mildred Fisher College of Science and Mathematics at Towson University.
2:03PM L46.00011: Nanoscale Visualization of the Au/HfO2/Si(001) Interface Electrostatics with BEEM  
JACK ROGERS (Presenter), DANIEL PENNOCK, HYEONSEON CHOI, STEVEN GASSNER, WESTLY NOLTING, VINCENT LABELLA, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute — Understanding carrier transport through the electrostatic potential of monolayer-thick oxide layers is important for nanoscale devices. Ballistic electron emission microscopy (BEEM) is an STM-based technique which allows for the visualization of nanoscale fluctuations of metal / insulator / semiconductor interface electrostatics [1]. In this work, the electrostatic barrier of an Au/HfO2/Si(001) interface is examined with BEEM to nanoscale dimensions. Thousands of spectra are taken at equally spaced points in a grid over a square micron. Barrier heights consistent with the band offsets for SiO2, HfO2, and the Schottky barrier for gold on p-type silicon are observed. This suggests that the monolayer-thick HfO2 layer is transparent to the ballistic electrons. X-ray photoemission spectroscopy confirms the presence of native SiO2 formation, which is further supported by computational modeling.


Wednesday, March 6, 2019 11:15 AM - 2:03 PM

Session L47 GERA: Photovoltaics -- Solar Energy Conversion II  
BCEC 213 - John Mintmire, Oklahoma State University-Stillwater - Tag(s): Focus

11:15AM L47.00001: Hybrid functional studies of electronic properties of Cu2MgSnS4 (CMTS) for photovoltaics*  
KIN FAI TSE (Presenter), MAN HOI WONG, JUNYI ZHU, The Chinese University of Hong Kong — Cu2ZnSnS4 (CZTS) is a promising photovoltaic absorber material, efficiency is however largely hindered by potential fluctuation and band tailing problem due to abundance of defect and their complexes. Our previous work has establish CMTS should have a stable chemical potential range and desirable optical properties similar to CZTS. In this work, we examine the electronic properties of CMTS using HSE06 functional, our results shows 1) a general increase in formation energy in most defects except MgSn in CMTS, mainly due to the change of ground state structure, 2) qualitative similarity of defect thermodynamics and electronic properties in CMTS to CZTS and 3) identified CuMg as the main contribution to p-type carrier. These findings suggest CMTS may suppress potential fluctuation due to formation of detrimental CuZn+ZnCu defect complex in CZTS, and alleviate the band tailing near CZTS and CdS interface, and further confirm the feasibility of CMTS as an alternative absorber material to CZTS, suggesting potential for tuning. Implications to alloy with CZTS will be discussed.

*We are grateful for the support from Research Grants Council of Hong Kong (GRF/14319416) and Direct Grant from the Chinese University of Hong Kong (No. 4053233).

11:27AM L47.00002: First-principles structural studies of polythiophene isomeric systems*  
JOHN MINTMIRE (Presenter), Oklahoma State University-Stillwater — Recent experimental work has been reported for the synthesis of poly-ortho-thiophenes, in particular helical poly(5-alkyl-2,3-thiophene)s. These polythiophenes differ from the poly(3-alkyl-2,5-thiophene)s studied over for the past several decades as electroactive polymers similar to the polypyrroles, and which have had application in bulk heterojunction photovoltaics. We have carried out first-principles, density functional simulations for the electronic structure and total energy of a range of polythiophene systems using Gaussian-function-based orbitals in a band structure approach using helical symmetry. We have examined the hydrogen, methyl, ethyl, and propyl substituted poly(5-alkyl-2,3-thiophene)s and poly(3-alkyl-2,5-thiophene)s, optimizing the geometry as a function of twist angle in the helical backbone. We have also looked into other possible polymer conformations such as the poly(5-alkyl-2,4-thiophene).

*This work was supported in part by a sabbatical period at the ORNL Center for Nanophase Materials Science funded through the ORAU ORNL-HERE program.
11:39AM L47.00003: A New Family of Plasmonic Photocatalysts without Noble Metals* DONGYANG WAN (Presenter), BIXING YAN, NUSNNI, National University of Singapore, XIAO RENSHAW WANG, Nanyang Technological University, THIRUMALAI VENKY VENKATESAN, NUSNNI, National University of Singapore — Efficient photocatalysis is important for sustainable energy. Recently, an unconventional photocatalyst based on intrinsic plasmon, called intrinsic plasmonic photocatalyst (IPP), seems promising for higher efficiency in hydrogen evolution. This catalyst seems to benefit from the advantages of visible light absorption, plasmon-assisted hot carrier generation over conventional photocatalysts. Here, we report the relative hydrogen evolution efficiency under visible light irradiation of a family of IPP based on alkaline earth niobates (MxNbOy, where M=Ca, Sr or Ba), with efficiency of CaNbO3 > SrNbO3 > BaNbO3. The contributions of electron-phonon coupling time and solar energy absorption to the hydrogen evolution efficiency are identified as keys based on our comprehensive characterization of carrier density (10²² cm⁻³), plasmon absorption, carrier dynamics and surface area. This study demonstrates a generic approach to create a family of IPP and validates the solar energy absorption of intrinsic plasmon as an additional knob to enhance the photocatalytic efficiency.


*We thanks to Singapore National Research Foundation under the CRP project ‘Oxide Electronics on Silicon beyond Moore’ (NRF-CRP15-2015-01)

11:51AM L47.00004: Influence of microstructure on resistance, photovoltaic response and piezoelectric voltage of Colemanite CHANDRIMA CHATTERJEE, Department of Physics and Astronomy, University of Mississippi, BHASKAR ROY BARDHAN (Presenter), Department of Physics and Astronomy, SUNY Geneseo — Colemanite belongs to the class of prismatic monoclinic crystals. It is a hydrous compound and the water molecules contribute to conduction mechanisms at high temperature. The material contains interstitial and substitutional point defects which form intraband energy levels. These energy levels trap electrons and at high temperature the electrons gain enough energy to move to the conduction band. This phenomenon shows up as peaks in the current-voltage characteristics of colemanite. When excited with near ultraviolet light, colemanite exhibits ohmic resistance. The presence of photovoltaic microstructures such as grain boundaries, ferroelectric domains and others is responsible for this kind of behavior. The results show that colemanite may be used to generate higher photocurrent than conventional semiconductors. This opens up new possibilities of replacing semiconductors in photovoltaic device with colemanite. The piezoelectric response from different positions of colemanite varies in order of magnitude. These variations are due to the presence of point defects. The results may be used in the nondestructive testing of the uniformity of surfaces of piezoelectric crystals in general.

12:03PM L47.00005: Inexpensive Solar Tracking for Developing Regions* BETH PARKS (Presenter), Colgate University — A solar tracking system for photovoltaic cells was built and tested in sub-Saharan Africa. The cell was suspended from a mount, and weights were hung on the two ends. One of the weights was a water bucket with a controllable leak. The water bucket was hung from the east end of the cell, and the weights were adjusted so it was heavier in the morning. Over the course of the day, as it lost water, the cell rotated to track the sun. The system was tested for 20 days, and collected 32% more energy than would have been collected by a horizontal solar cell in the same location. The cost of the frame is less than the savings in purchasing a smaller PV cell, so it has the potential to make solar energy more affordable to households and small businesses in the developing world.

*This project was supported by the Fulbright Scholar program.

12:15PM L47.00006: Simulation-Optimized ZnSₓSe₁₋ₓ Contacts on Si for Photovoltaic Carrier-Selective Contacts* REBECCA GLAUDELL (Presenter), HARRY ATWATER, Caltech — ZnSₓSe₁₋ₓ films are promising materials for front carrier-selective contacts in silicon photovoltaics given their wide bandgaps and low resistivities compared to amorphous silicon, with the potential to capture more photo-generated current than a traditional heterojunction with intrinsic thin layer (HIT) solar cell. X-ray photoelectron and ellipsometric spectra of ZnSₓSe₁₋ₓ (x ranging from 0 to 1) films grown on Si by molecular beam epitaxy were used to measure band offsets of ZnSₓSe₁₋ₓ with respect to Si for purposes of accurate optoelectronic simulations of photovoltaic devices incorporating ZnSₓSe₁₋ₓ carrier-selective contacts. Further experimentally determined parameters including complex refractive index and resistivity were also included in the simulation of a HIT-style cell to determine the ZnSₓSe₁₋ₓ top contact mole fraction x, doping level, and thickness for optimal device performance.

*This material is based upon work supported by the NSF and the DOE under NSF CA No. EEC-1041895, by the DOE under Award Nos. DE-E0006335 and DE-E0004946, and by the NSF Graduate Research Fellowship under Grant No. 1144469.
12:27PM L47.00007: Modeling of PV/TPV devices using analytical solution of generalized Shockley – Queisser model* ANDREI SERGEEV (Presenter), HARRY HIER, CHRISTOPHER MIKE WAITS, US Army Rsch Lab - Adelphi — The generalized Shockley-Queisser (gSQ) model takes into account the frequency dependent absorption (emission), photon trapping and recycling, photocarriers multiplication, and nonradiative recombination processes. Exact analytical solution of gSQ model allows one to present the conversion efficiency and other photovoltaic (PV) and thermophotovoltaic (TPV) characteristics in convenient form via the Lambert W function, which is well approximated by logarithmic functions [1]. Analytical equations for useful energy, emission losses, thermal losses and optimal photocarrier collection time provide effective, convenient, and flexible tool for modeling of modern devices with effective photon trapping and recycling. We discuss analysis of experimental characteristics and optimization of PV/TPV devices based on gSQ solution. [1] Sergeev and Sablon, Exact Solution, Endoreversible Thermodynamics, and Kinetics of the Generalized Shockley-Queisser Model, Phys. Rev. Appl. 2018.

*This work is supported by ORAU (AS) and Army Research Laboratory.

12:39PM L47.00008: Density Functional Theory calculations of optical properties of Hybrid Halide Perovskite Bio-Solar Cells SUBHABRATA DAS (Presenter), Langmuir Center of Colloids and Interfaces, Columbia University, BERNARDO BARBIELLINI, Physics, Lappeenranta University of Technology, PONISSERIL SOMASUNDARAN, Langmuir Center of Colloids and Interfaces, Columbia University, VENKATESAN RENUGOPALAKRISHNAN, Chemical and Chemical Biology, Northeastern University — The photovoltaic performance of hybrid halide perovskite is related to the atomic and electronic structure at the interface between the carrier generating perovskite layer and the electron transport layer (ETL). Based on ab-initio density functional theory (DFT) calculations, we studied the interfacing of the ETL layer, bacteriorhodopsin (bR) protein with Methylammonium lead triiodide CH$_3$NH$_3$PbI$_3$ based organic-inorganic hybrid perovskite to fabricate Perovskite Biosolar Cells, which demonstrated a high ambient stability and an optical bandgap extending into the visible range. The dielectric spectrum of the Perovskite thin films is evaluated and validated with spectroscopic ellipsometry data. We further model the dielectric function according to the established Drude model with coupled harmonic oscillators. Our results agree well with reported data of the optical absorption coefficient and consistent with Kramers–Kronig transformations thus demonstrating band alignment between the protein and the perovskite. Hence, we comment on the structural, electronic, and transport properties at the br/perovskite/ETL interface.

12:51PM L47.00009: The Influence of Imperfect Band-edges on the Maximum Efficiency of a Solar Cell JOESON WONG (Presenter), STEFAN OMELCHENKO, HARRY ATWATER, Caltech — The theoretical maximum efficiency of a solar cell is given by the Shockley-Queisser Limit, which assumes a step-function absorbance near the band-edge. However, real materials always have an imperfect band-edge, which is usually characterized by an Urbach tail. In this work, we utilize optoelectronic reciprocity relations to develop a modified detailed balance limit of solar cells with imperfect band-edges. We find that for band-edges that are not sharper than the thermal energy, an effective renormalized band-gap is given by the quasi-Fermi level splitting within the solar cell. This renormalized bandgap creates a Stokes shift between the onset of absorption and the photoluminescence peak position, which drastically lowers the maximum achievable efficiency. The band-edge density of states therefore has important implications for the performance of photovoltaic devices.

1:03PM L47.00010: Heterocyclic halides as passivating layer improves photovoltaic properties and intrinsic stability in perovskite solar cells* MANUEL SALADO (Presenter), Materials science, BC Materials, ALEXANDER D. JODLOWSKI, University of Cordoba, CRISTINA ROLDAN-CARMONA, EPFL, GUSTAVO DE MIGUEL, University of Cordoba, SAMRANA KAZIM, Materials science, BC Materials, MOHAMMAD KHAJA NAZEERUDDIN, EPFL, SHAHZADA AHMAD, Materials science, BC Materials — Perovskites solar cells have improved in the photovoltaic field with no precedent. Rising from ~4% to 23.2% the power conversion efficiencies (PCE), however long term stability together with the lack of a fully understanding of intrinsic processes are still issues which need to be undertaken. To improve the intriguing challenges, compositional engineering of perovskites as well as molecular engineering of hole transport materials (HTMs) were adopted. Furthermore, an optimized interface between the different layers of the perovskite device is paramount to improve the problems aforementioned. In this regard, an optimized surface passivation layer is seen as an ideal approach to protect the surface from extrinsic factors, without altering the electro-optical properties.

In this work, we present the utilization of a passivation layer, which protect the perovskite layer from atmospheric attack. An improved PCE (20%) was also obtained compare with reference devices (18%), as the passivation layer will restricts the flow of electron towards the HTM layers and reduce recombination processes.

*This project has received funding from the COST action [MP1307] and European Research council grant [MOLEMAT, 72630]. MSM thanks the support of Juan de la Cierva grant [FJCI-2017-31761]
**1:15PM L47.00011:** An *ab-initio* study of water interactions in the hybrid perovskite MAPbI$_3^*$  
ARVIN KAKEKHANI (Presenter), ANDREW RAPPE, Chemistry, University of Pennsylvania — Hybrid (organic-inorganic) perovskites have recently received great attention as candidates for commercially viable and efficient conversion of solar energy. Nevertheless, the performance and stability of these materials gets affected by water and moisture in the environment. Here, using density functional theory (DFT) simulations, and taking MAPbI$_3$ as our case study, we investigate the nature of water interactions in hybrid perovskite MAPbI$_3$. Changing water concentration over 2 orders of magnitude, we study the process of water infiltration and the surface and bulk chemistry that follows and leads to first reversible, and then irreversible changes to the material's structure. We discuss, based on electronic-structure analyses, how water changes the optical properties of the material in different concentrations. Such understanding of the nature of water--hybrid-perovskite interactions, can then be used to design better and more stable solar cells.

*ONR N00014-17-1-2574

**1:27PM L47.00012:** Synthesis and optoelectronic properties of Perovskite nanowire*  
ATIKUR RAHMAN (Presenter), GOKUL M. A., Department of Physics, Indian Institute of Science Education and Research (IISER)-Pune — We have developed a simple solution based synthesis method of CsPbI$_3$ nanowire. This method produces high yield nanowire with controllable length and diameter. We studied in details the effect of various growth conditions, such as temperature and time on the morphology of these nanowires. Single nanowire devices were made to investigate their individual property. To understand different mechanisms that play a major role in determining the performance and stability of these nanowire devices, we studied optoelectronic and noise characteristics under various conditions. These nanowires are structurally stable under ambient condition and show stable photoresponse. We will discuss in details the possible growth mechanism and the observed optoelectronic properties of these nanowires.

*The authors acknowledge funding support from IISER Pune.

**1:39PM L47.00013:** A density functional theory study (GGA+U) of the electronic and optical properties of Sn doped acanthite Cu$_2$S*  
SAJIB BARMAN (Presenter), MUHAMMAD NURUL HUDA, Physics, University of Texas at Arlington — Cu$_2$S is earth abundant, non-toxic and an important semiconductor with many applications. Previously it sought wide attention to scientific community as a promising photovoltaic material since Cu$_2$S based thin film solar cells demonstrated nearly 10% conversion efficiency. Despite excessive Cu vacancy formation tendency, studies on Cu$_2$S based thin film solar cells didn't lose its importance in decades. Our recently published theoretical study (J. Phys.: Condens. Matter 30 165701) on the acanthite phase of Cu$_2$S showed that Cu vacancy formation tendency can be reduced with Ag alloying. Hence, alloying with other materials needs to be studied systematically, as well. Here, we report a systematic first principle study on Sn doped acanthite Cu$_2$S. We have showed that Sn doping in this structure is even thermodynamically more favorable. Even though excessive Sn doping makes the material metallic, the Cu vacancy formation tendency decreases with high doping concentration. With suitable low doping the material undergoes electronic intraband transition which extends the optical absorption to the infrared region. In addition, detail electronic structures and optical properties will be presented for pure and Sn doped cases.

*All the computational work was done at Lonestar5 at TACC in Austin, TX.

**1:51PM L47.00014:** Screening of Metallic Single-Replacements for Lead-free Perovskites with Intrinsic Photovoltaic Functionalities  
CLARK ZHANG (Presenter), XUAN LUO, National Graphene Research and Development Center — Methylammonium lead triiodide perovskites, CH$_3$NH$_3$PbI$_3$ (MAPbI$_3$), are solution-processable materials with photovoltaic properties capable of surpassing those of silicon solar cells. However, concerns over lead toxicity and lack of exploration into transition metal perovskites drove this ab initio Density Functional Theory screening for environmentally friendly perovskite materials by incorporating transition and post-transition metals at the B-site of MAPbI$_3$. This revealed fourteen replacements to be suitable: their band structures are highly dispersive while band gaps of such materials fall within ideal ranges for single-junction and tandem cells. Transition metal monoreplacements are shown to be viable perovskites after reducing the size of the halide, corroborating that tunability of the band gap is observed in halide replacement at the X-site. Strong peaks in the imaginary output of the dielectric function below 3.5 eV indicate high sunlight absorption efficiency for select materials. Excellent carrier mobility is expected of studied materials as their effective mass is low. This work helps gain further insight into the viability of plentiful transition metals for lower toxicity and higher absorption divalent perovskites.

*Wednesday, March 6, 2019 11:15 AM - 2:15 PM*
11:15AM L51.00001: Max Delbruck Prize in Biological Physics Talk: The Physics of Cellular Proteostasis [Invited]  KEN DILL (Presenter), Stony Brook University — In order for cells to function, their proteins must be folded and not aggregated. This healthy state is maintained by a complex energy-expensive system of chaperones, and synthesis and degradation machinery. This is among the most central and complex ‘decision-making’ processes of simple cells. We model proteostasis by combining the dynamics of the chaperone binding and trafficking with the kinetics of protein folding and aggregation. We also explore the rates of evolution of protein sequences and how the chaperones modulate those rates.

11:51AM L51.00002: Max Delbruck Prize in Biological Physics Talk: Exploring the Energy Landscape for Protein Folding and Function: Integrating Structural Models and Sequence Coevolution Information. [Invited]  JOSE ONUCHIC (Presenter), Center for Theoretical Biological Physics, Rice University — Energy landscape theory and the funnel concept have been a powerful approach to study protein folding dynamics and function. The discovery that an accurate estimate of the joint probability distribution of amino acid occupancies in protein families provides insights about residue-residue coevolution and concrete details about protein folding landscapes has also advanced structural biophysics. Our realization that the collection of couplings and local fields as parameters of such distribution is inherently connected with the thermodynamics of sequence selection towards folding and function demonstrates the importance of coevolutionary methods to understand stability and function of biomolecules. The synergy between structure based models and coevolutionary information has spearheaded the field of structure prediction, including protein and RNA, as well as accelerating the discovery of functional structural states and the prediction of protein complexes. Coevolution signals can also be used to create protein recognition metrics, which led to successful experimental efforts, and the uncovering of novel molecular interactions. This idea has opened the door to encode recognition in protein pairs. Coevolved interfaces can also be combined with small molecule hot spot estimation methods to improve the discovery of druggable interfaces. Recently this approach has been used to predict extremely large protein assemblies consisting of structural maintenance of chromosones (SMC) and kleisin subunits which are essential for the process of chromosome segregation across all domains of life. While limited structural data exist for the proteins that comprise the (SMC)–kleisin complex, using an integrative approach combining both crystallographic data and coevolutionary information, we have predicted an atomic-scale structure of the whole condensing complex in prokaryotes.

*Supported by the NSF and the Welch Foundation

12:27PM L51.00003: Using evolutionary repair to learn about biological functions [Invited]  MARCO FUMASONI, YU-YING HSIEH, ANDREW MURRAY (Presenter), Harvard University — Although many biological processes, such as DNA replication and chromosome segregation, are universal and many of the proteins that mediate them have persisted since the last common ancestor, other components have appeared and disappeared during evolution. We have removed important, but non-essential components from two different processes, DNA replication and chromosome segregation, allowed cells to accumulate mutations that restore reproductive fitness to nearly wild-type levels, and studied how these mutations affect DNA metabolism. In both cases, mutations alter multiple aspects of DNA metabolism with the effects of the different mutations being approximately additive and at least one of the adaptations is to slow an aspect of DNA replication. We discuss the trade-off between the speed of DNA replication and the accumulation of harmful intermediates in wild-type and mutant cells and how mutations can regulate the trade-off to improve reproductive fitness.

*NIH/NIGMS GM043987

1:03PM L51.00004: Fitness Landscapes of Ribozymes [Invited]  IRENE CHEN (Presenter), Chemistry and Biochemistry, UCSB — Evolutionary outcomes are difficult, if not impossible, to predict, largely because the effect of any possible mutation is unknown. In other words, understanding evolution requires detailed knowledge of the relationship between sequence and activity, or the fitness landscape. Molecules explore the fitness landscape in sequence space during evolution, much as proteins explore the folding landscape in conformational space. Inspired by the RNA World theory of early life, in which RNA would carry information and also perform catalytic functions, we study the emergence and evolution of functional RNAs. Our experimental efforts focus on mapping complete fitness landscapes of ribozyme activity. We also study how confinement in a vesicle affects RNA activity and structure. These studies inform our understanding of the likelihood of emergence of function and the roles of chance vs. natural selection in prebiotic evolution.
1:39PM L51.00005: From Tunneling Pathways to Essential Biological Function* [Invited] DAVID BERATAN (Presenter), Duke University — Energy capture, storage, and conversion in living systems relies, fundamentally, on the flow of electrons and protons. The transport of electrons through proteins uses cofactors, special chemical groups that sequester electrons as they hop among these sites through otherwise insulating proteins. These cofactors trade electrons with one another via electron tunneling. Electrons thus move across membranes, generating a proton gradient, and leading to the synthesis of energy storing chemical bonds. Electron transfer reactions also participate in essential reaction of biosynthesis, damage repair, and signaling. Electrons flow in biology on time scales from picoseconds to seconds, and the trick for insuring that the electrons get to the right places at the right times is to employ electron tunneling pathways between the charge localizing cofactors. I will describe the theoretical framework for describing how proteins control these reactions with tunneling pathways, and will discuss research frontiers in that have become accessible to theoretical analysis as a consequence of the tunneling pathways framework. Examples will include the repair of DNA damage by the protein photolyase, the micrometer length scale flow of electrons through extracellular bacterial nanowires that enable respiration in some aerobic bacteria (when deprived of oxygen) through the use of biotic-abiotic charge exchange (i.e., electron transfer to rocks), and electron bifurcation - a reaction that couples electron flow between two-electron donors and single-electron carriers.

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Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L53 GSOFT: Controlling Local Structure With Time-Dependent External Fields BCEC
253C - Craig Maloney, Northeastern University - Tag(s): Invited

11:15AM L53.00001: Symmetric and Asymmetric Time-Varying Magnetic Fields to Control and Drive Paramagnetic Colloidal Assemblies* [Invited] SIBANI BISWAL (Presenter), Rice University — Micron-sized superparamagnetic colloids placed in time-varying magnetic fields can provide us with rich dynamic behavior depending on the magnetic field applied and the particle concentration. In symmetric magnetic fields, a long-range attractive potential is induced resulting in the formation of colloidal clusters, which assemble into circular shapes that exhibit fluid-like behavior at relatively low fields, while becoming crystallized and highly ordered at higher field strengths. These systems exhibit interesting coarsening and spinodal decomposition structural transitions for larger particle systems.

In asymmetric time-varying fields, the colloids assemble into directed collective motion. The simplest case of two bodies by which a smaller arm particle can be driven in an asymmetric orbit in the proximity of a larger torso particle using an eccentric rotating magnetic field (ERM), resulting in both bodies swimming in a directed motion. Furthermore, adding additional particles the arm leads to overlapping orbits and arm synchronization, resulting in faster swimming speeds. This new methodology for being able to achieve nonreciprocal motion at low Re offers insight into directing the motion of collective active systems.

*National Science Foundation CBET-17055703

11:51AM L53.00002: Driving and assembling magnetic particles with incoherent fields* [Invited] RANDY ERB (Presenter), RASAM SOHEILIAN, HAMED ABDI, CRAIG MALONEY, Northeastern University — Magnetic particles in suspension can chain under static applied magnetic fields or be transported to target sites with static magnetic field gradients. This is clear and has led to innovations from magnetorheological fluids to magnetic targeting of tumors to magnetic delivery of drugs. But how do magnetic particles behave in more complicated fields and field gradients? Can we use these complications to our advantage? Can we understand the physics? There has been significant research toward these questions for coherent (simple rotating) fields by many research groups including ours. Dynamically tuning the direction (but not magnitude) of the field will disrupt the simple chaining of particles. For two isolated particles, this disruption is found to be an elegant systematic dance between particle pairs. For large populations of particles, fascinating group dynamics occur. We have looked at these dynamics for chains as well as for multipolar ring formations. In addition, we have been investigating the behavior of magnetic particles under incoherent fields, in which there is a mismatch in the frequency domain for x, y, and z field functions. Surprisingly, we find that incoherent fields can generate coherent assemblies! We apply our findings to the realms of magnetic assembly, magnetic drug delivery and magnetic rheology in an attempt to enhance current practices through complicating the applied fields.

*This material is based in part upon work supported by the National Science Foundation under Grant Number CPS-1329649.
12:27PM L53.00003: A touch of non-linearity in fluid fields: where spheres “think” collectively and swim together*
[Invited] DAPHNE KLOTSA (Presenter), University of North Carolina at Chapel Hill — From crawling cells to orca whales, swimming in nature occurs at different scales. The study of swimming across length scales can shed light onto the biological functions of natural swimmers or inspire the design of artificial swimmers with applications ranging from targeted drug delivery to deep-water explorations. In this talk, I will present experiments and simulations of how oscillating spheres, universally simple geometric objects, can utilize non-linearities to demonstrate complex pattern formation in a granular system, or different swimming behaviors in a spherobot (robot made out of spheres) when placed in a fluid at intermediate Reynolds numbers, 1<Re.

*National Science Foundation, grant award DMR-1753148

1:03PM L53.00004: Deck the walls with tunable energy fields for colloidal particles in nematic liquid crystals*
[Invited] KATHLEEN STEBE (Presenter), University of Pennsylvania — Confined nematic liquid crystals provide new opportunities to direct colloidal motion and assembly. Nematic liquid crystal director fields molded by confinement can present domains of bend, splay or twist with associated elastic energies. Colloidal particles also distort the nematic director field, and are repelled or attracted to these domains to minimize the elastic energy cost in these systems. We have been studying colloids adjacent to a wavy wall in a nematic liquid crystal with a smoothly varying, non-singular director field that features bend and splay distortions. Colloids within this field can have multi-stable states. Wall-colloid equilibrium distances and ranges of interaction can be tuned by varying wavy wall geometry. Colloids move toward and dock at attractive sites and away from repulsive loci; this repulsion can propel objects in the domain. Extensions to anisotropic colloids are discussed. Manipulation by application of external fields to complement the nematic director fields are discussed in the context of reconfigurable systems and microrobotics.

*U.S. Army Research Office under Grant W911NF1610288

1:39PM L53.00005: Emergent dynamics and self-assembly of colloids in time-dependent magnetic fields*
[Invited] ALEXEY SNEZHKO (Presenter), Argonne National Laboratory — Strongly interacting colloids subject to an external periodic forcing often exhibit nontrivial collective dynamics and self-organization. Driven magnetic colloids proved to be an excellent model system to explore emergent collective behavior and out-of-equilibrium self-assembly. New self-assembled structures emerging in time-dependent magnetic fields are often not accessible under equilibrium conditions. In this presentation I will demonstrate that dispersions of magnetic particles suspended at a liquid-air, liquid-liquid interfaces or in the bulk and driven out-of-equilibrium by an alternating magnetic field develop nontrivial dynamic self-assembled phases and structures. Experiments reveal new types of nontrivially ordered phases and collective dynamics emerging in such systems in a certain range of excitation parameters. These remarkable non-equilibrium structures emerge as a result of the competition between magnetic and hydrodynamic forces. The dynamic phases are reversible and fine-tuned by the parameters of the driving magnetic field. Above certain frequency threshold or on external perturbation some of the dynamic structures spontaneously break the symmetry of self-induced flows and turn into swimmers, spinners or can be used as robotic manipulators at microscale. Furthermore, collective motion of self-assembled dynamic structures at interfaces often generates chaotic fluid flow reminiscent of two-dimensional turbulence - active turbulence. In case of a rotational magnetic field two-dimensional active spinner materials can be realized.

*The research was supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering.

Wednesday, March 6, 2019 11:15 AM - 1:51 PM

Session L54 DCMP: 2D Heterostructures -- Transport BCEC 254A - Jianhao Chen, Peking University - Tag(s): Focus
11:15AM L54.00001: Perfectly gate-tunable graphene-WSe₂ van der Waal’s heterostructure at the Schottky-Mott limit  
SAMUEL LAGASSE (Presenter), PRATHAMESH DHAKRAS, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, JI UNG LEE, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute — Recently, the Schottky-Mott (SM) limit has been studied through measurements on many metal-semiconductor junctions with various metals [1]. Here, we probe the SM limit using a single, gate-tunable, hexagonal boron nitride encapsulated graphene-WSe₂-graphene heterostructure. One-dimensional edge contacts are made to the graphene and buried split-gates are used to separately tune the electrical properties each graphene-WSe₂ junction. By making one graphene-WSe₂ junction Ohmic, we perform electrical measurements of the Schottky barrier (SB) formed in the other junction. Electrical measurements of the SB show striking agreement with the ideal-diode equation, with over thirteen decades of drain current modulation via the gate voltage. Arrhenius activation energy measurements reveal one-to-one electrical control of the SB height by the gate voltage. These measurements indicate a stark absence of Fermi-level pinning at the graphene-WSe₂ interface, resulting in a tunable SM limited heterojunction. Our findings are of broad significance, enabling fundamental studies of the SM limit and the ability to make superior electrical contact to two-dimensional materials.


11:27AM L54.00002: Naturally formed contacts between assorted metals and 2D TMD materials*  
RUHI THORAT (Presenter), THUSHAN WICKRAMASINGHE, GREGORY JENSEN, MARYAM BIZHANI, ERIC A STINAFF, Ohio University — Novel technologies built on the properties of two dimensional transition metal dichalcogenides (TMD) require the ability to pattern, process, and contact the material in a scalable manner. However, reproducibly making quality contact to 2D materials remains a significant challenge. We have developed a technique which uses bulk transition metal contacts which act as nucleation sites and a source of material for the growth of 2D TMDs. The bulk metal remains after growth, establishing a naturally formed electrical contact with the TMD material. In the original manifestation of this technique, the contact material was limited to the transition metal of the subsequently grown TMD, however, it has been reported that various elemental metal contacts exhibit reduced Schottky barriers. We will present results from a modification of our growth process which allows for different metal contacts to be produced. A comparison between various metal contacts such as Ti-MoS₂ and Mo-MoS₂ will be presented and transport measurements will be discussed. This modification to our technique opens up the possibility of producing more complex device architectures with tailored contact properties.

*Nanoscale and Quantum Phenomena Institute, Ohio University

11:39AM L54.00003: Direct reversible writing of nanoscale doping patterns in van der Waals heterostructures*  
WU SHI (Presenter), SALMAN KAHN, Lawrence Berkeley National Laboratory and UC Berkeley, LILI JIANG, SHENG-YU WANG, HSIN-ZON TSAI, UC Berkeley, DILLON WONG, Princeton University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, FENG WANG, MICHAEL F CROMMIE, ALEX ZETTL, Lawrence Berkeley National Laboratory and UC Berkeley — Spatially controlled modification of charge density is essential to explore exotic physics and enable new device applications. Conventionally, this has been achieved using lithographically defined local gates or by employing molecular self-assemblies on surfaces. However, these methods face limitations in applications necessitating spatial re-writability and complex circuit designs. Recent progress has demonstrated alternative ways to induce rewritable doping patterns in van der Waals (vdW) heterostructures without complex processing masks or resist by optical illumination or applying an STM tip voltage pulse. In this work we introduce a more flexible electron beam doping technique to induce controllable and erasable doping effect in (vdW) heterostructures. With this new doping technique, we can accumulate high carrier density and reversibly write complex doping patterns with nanoscale spatial resolution while preserving the high quality of the vdW heterostructures. The technique can be an ideal approach to study a variety of superlattice physics in vdW heterostructures and to create on-demand circuits for device applications.

*This work was supported in part by the U.S. Department of Energy under Contract No. DE-AC02-05-CH11231, within the sp2-Bonded Materials Program (KC2207).
11:51AM L54.00004: Effect of Remote Surface Optical Phonon Scattering in Ferroelectric-Gated Single- and Bi-layer Graphene*  
HANYING CHEN (Presenter), ZHIYONG XIAO, ANIL K RAJAPITAMAHUNI, YIFEI HAO, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science - Japan, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln — We investigate the effect of the remote surface optical (RSO) phonon scattering on the transport properties of single and bi-layer graphene gated by ferroelectric Ba$_{0.6}$Sr$_{0.4}$TiO$_3$ (BSTO) thin films. Graphene flakes were exfoliated on epitaxial 100-300 nm BSTO thin films grown on Nb-doped SrTiO$_3$ substrates. Single and bi-layer samples were then identified via optical microscopy and characterized by atomic force microscopy and Raman spectra. Selected flakes were fabricated into field effect transistor (FET) devices via e-beam lithography. At low temperature, these ferroelectric-gated FETs (FeFET) exhibit resistivity hysteresis induced by ferroelectric switching, which evolves to anti-hysteresis at ~40 K. The graphene FETs exhibit high field effect mobility up to $\mu_{FE}$~19,000 cm$^2$/Vs and quantum Hall at 10 K, from which we deduced a dielectric constant of ~60 for BSTO. We examined the temperature dependence of the resistivity, which reveals dominant RSO phonon scattering from the interface with BSTO. We also discuss the effect of capping these samples with a top h-BN layer. Our study facilitates the development of high-performance FeFETs based on graphene.

*This work was primarily supported by the U.S. Department of Energy, BES, under Award No. DE-SC0016153.

12:03PM L54.00005: Quantifying thermal boundary conductance of 2D-3D interfaces  
CAMERON FOSS (Presenter), ZLATAN AKSAMija, Electrical and Computer Engineering, University of Massachusetts Amherst — Heat dissipation in next-generation electronics based on two-dimensional (2D) materials is a critical issue in their development and implementation. A bottleneck for heat removal from the 2D layer into its supporting substrate is the thermal boundary conductance (TBC) of the 2D-3D interface, which is impacted by their structure and composition. Here we investigate the temperature-dependent TBC of 42 interfaces formed between a group of six 2D materials and seven crystalline and amorphous substrates. Our results show that the TBC can be varied by nearly two orders of magnitude, from 0.6 MW.m$^{-2}$.K$^{-1}$ (h-BN on diamond) to 40 MW.m$^{-2}$.K$^{-1}$ (h-BN on SiO$_2$), for the same 2D layer by changing the substrate material. We find that amorphous materials boost the TBC due to the low-frequency Boson peak feature in their vibrational density of states (vDOS) relative to their crystalline counterparts, whose vDOS follows a Debye model at low frequency, assuming the two interfaces have the same adhesion. For crystalline substrates, we correlate constituent material properties with the calculated TBCs and find that TBC depends on a combination of the speed of sound, Debye temperature, density of the substrate, and bandwidth of the flexural branch in the 2D material.

12:15PM L54.00006: Towards the Mechanism of Protonic Transport in Graphene Oxide*  
VLADIMIR SAMUILOV (Presenter), Department of Mat. Sci & Eng., SUNY at Stony Brook, NIKOLAI POKLONSKI, Department of Physics, Belarus State University — Graphene oxide (GO) has been considered as a good ionic conductor and an electronic insulator simultaneously [1,2]. The mechanism of the protonic conductivity in GO has not been studied carefully yet. This report presents new experimental data of the protonic conduction in GO in a wide temperature range with the humidity as a parameter. The activation energy of the protonic transport (approx. 0.7 eV) was obtained from the Arrhenius plots. Applications of GO membranes to the humidity sensors [2] and to solid-state electrolyte energy storage devices [1] have been considered.  

*The work was partially supported by Belarusian Scientific Program “Convergence”, Belarusian Republican Foundation for Fundamental Research (Grant No. F18R-253) and by Sensor CAT at Stony Brook University, NY
12:27PM L54.00007: AC Josephson effect in a capacitively shunted graphene Josephson junction  FAN YU (Presenter), SANDESH S KALANTRE, University of Maryland, College Park, GLEB FINKELSTEIN, Physics, Duke University, FRANCOIS AMET, Physics and Astronomy, Appalachian State University, JAMES R WILLIAMS, University of Maryland, College Park — The AC Josephson effect is being used to detect signatures of novel modes in Josephson junctions. However, complex behavior of these junctions under RF radiation can also from trivial effects, like the presence of a large shunting capacitance. Here we study the AC Josephson effect on a junction made of graphene encapsulated in boron nitride and contacted by electrodes made of a superconducting molybdenum-rhenium alloy. In regions where chemical potential is close to the charge-neutrality point and the RF drive current is comparable with critical current, this device demonstrated a bi-stability between the first Shapiro steps, indicating the Josephson junction is in a chaotic regime. A full description of the chaotic physics observed is presented. These observations cast doubt over arguments that AC Josephson effect in the low RF drive amplitude region would offer the opportunity to observe 4-π current phase relation in topological Josephson junctions.

12:39PM L54.00008: Superconductivity in Graphene NbSe₂ heterostructures* SATRIO GANI (Presenter), Physics Department, College of William & Mary, HADAR STEINBERG, The Racah Institute of Physics, The Hebrew University of Jerusalem, ENRICO ROSSI, Physics Department, College of William and Mary — We study van der Waals heterostructures formed by graphene and monolayer NbSe₂. We show that despite the large mismatch between the lattice constant of graphene and NbSe₂ in these structures a large superconducting pairing can be induced into the graphene layer. In addition, we show how such pairing depends, both in nature and structure, on the stacking configuration. Our results are relevant also to heterostructures formed by graphene and other monolayer of transition metal dichalcogenides such NbS₂, TaS₂, and TaSe₂, that have also been shown to be superconducting at low temperature, and suggest a way to probe the nature of the multiband superconducting gap in these systems.

*Work supported by NSF and BSF.

12:51PM L54.00009: Superconducting contact to 2D transition-metal dichalcogenide superconductors* MICHAEL SINKO (Presenter), SERGIO DE LA BARRERA, Carnegie Mellon University, OLIVIA LANES, MICHAEL HATRIDGE, University of Pittsburgh, BENJAMIN MATTHEW HUNT, Carnegie Mellon University — Two-dimensional transition-metal dichalcogenide superconductors have unique and desirable properties for integration with conventional superconducting circuits. These properties include the ability to form atomically clean and flat interfaces with stable tunnel barriers (such as boron nitride), increased kinetic inductance due to the atomically-thin geometry, and resilience to very high in-plane magnetic fields. Integrating 2D superconductors into superconducting circuits requires a fully superconducting contact be made between the 2D material and a conventional superconductor. By means of an in situ process of etching and angled Al evaporation, we present evidence of robust superconducting edge contact to NbSe₂ fully encapsulated by insulating hBN. A critical current density Jc = 7x10⁸ A/m² is achieved in the contacts. In a second set of samples, two contacts are connected with an Al loop to form a SQUID. A Fraunhofer pattern is observed in each of these samples, whose periodicities can be modeled by using an effective area for the SQUID loop equal to the physical loop area plus an area from the thin NbSe₂ flake that is uniformly penetrated by the applied magnetic field.

*This project was supported by the National Science Foundation PIRE program under award number 1743717

1:03PM L54.00010: Magnetotransport studies in hybrid 2D/0D nanostructures* ETHEL PEREZ-HOYOS (Presenter), YUNQIU (KELLY) LUO, Physics, The Ohio State University, ABHILASHA DEHANKAR, Chemical and Biomolecular Engineering, The Ohio State University, JINSONG XU, ROLAND KAWAKAMI, Physics, The Ohio State University, JESSICA WINTER, Chemical and Biomolecular Engineering, The Ohio State University — We present a device fabrication strategy that takes advantage of stacking techniques developed for van der Waals heterostructures to construct hybrid 2D/0D composite nanostructures, with potential application in the study of spin and charge disorder as well as magnetic-proximity effects. The structures in this study are comprised of superparamagnetic iron oxide nanoparticles (SPIONs) and monolayer graphene. The SPIONs are deposited first using a Langmuir-Blodgett technique, yielding rafts of highly ordered nanoparticles. Characterization via magnetic force microscopy (MFM) reveals magnetic order at multiple length scales and SQUID magnetometry identifies both glassy antiferomagnetic and ferromagnetic response. Single graphene monolayers are mechanically stacked on the SPION layer, and are found to maintain relatively high mobility and gate sensitivity, as indicated by quantum Hall effect (QHE) measurements.

*Funding for this research was provided by the Center for Emergent Materials: an NSF MRSEC under award number DMR-1420451.

1:15PM L54.00011: Transport measurements on 2D material devices [invited] YU HUANG (Presenter), UCLA — Selected by Focus Topic Organizer John Schaibley
Wednesday, March 6, 2019 11:15 AM - 1:51 PM

Session L55 DMP: Devices from 2D Materials -- Optical Spectroscopy BCEC 254B - Nick Vamivakas, University of Rochester

DAVOUD HEJAZI (Presenter), SARAH OSTADABBAS, SWASTIK KAR, Northeastern University — We created a vector of low-cost filters for estimating the wavelength of a light source in the range of 300nm-1100nm using gradually differing mixtures of nano-flakes of semiconducting materials, Molybdenum-Disulfide (MoS2) and Tungsten-Disulfide (WS2). The nano-flakes were produced by method of Liquid-Phase Exfoliation and Sonication. We studied the incident and transmitted intensities of light passing through these filters and derived a statistical model for the behavior pattern of the filters for incident light. By employing machine learning techniques we estimated the wavelength distribution of incident light with accuracy of ≤ %1 using the incident and transmitted sensor readings for intensity of light.

11:27AM L55.00002: Interface-Driven Nonlinear Optical Response at MoS2/Ferroelectric Composite Structures*  
DAWEI LI (Presenter), Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln, XI HUANG, Department of Electrical and Computer Engineering, University of Nebraska - Lincoln, ZHIYONG XIAO, HANYING CHEN, LE ZHANG, DING-FU SHAO, EVGENY Y TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln, YONGFENG LU, Department of Electrical and Computer Engineering, University of Nebraska - Lincoln, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln — Integrating layered van der Waals materials such as the transition metal dichalcogenides with ferroelectrics offers the opportunity to introduce new functionalities to the 2D platform, including nonvolatile memory and programmable junctions. In this work, we report a novel nonlinear optical response emerged at the interface between monolayer MoS2 and ferroelectric thin films. We have pre-patterned ferroelectric domain structures with polarization up and down domains on epitaxial PbZr0.2Ti0.8O3 (PZT) thin films using piezoresponse force microscopy, and then transferred on the top MoS2 flakes. We then carried out second-harmonic generation (SHG) microscopy studies on the composite structures. In the reflection mode, we find that the SHG intensity on the ferroelectric domain wall (DW) is highly modulated compared with those on both polar domains, either significantly enhanced or suppressed depending on the chirality of the DW. Stacking angle dependence demonstrates that MoS2 also tunes the polarity of the SHG response on the DW. Our study points to a new strategy to achieve tailored light polarity and intensity modulation via nanoscale ferroelectric control.

*This work was primarily supported by the DOE, BES, under Award No. DE-SC0016153.

11:39AM L55.00003: Investigation of Intrinsic Optical Characteristics in MoS2 Phototransistors using Van der Waals Heterostructure  
JINSU PAK (Presenter), Seoul National University, ILMIN LEE, Electronic and Electrical Engineering, Sungkyunkwan University, KYUNGJUNE CHO, WANG-TAEK HWANG, JAE-KEUN KIM, KEEHOON KANG, Seoul National University, WOO JONG YU, Electronic and Electrical Engineering, Sungkyunkwan University, SEUNGJUN CHUNG, Photoelectronic Hybrids Research Center, Korea Institute of Science and Technology, TAKHEE LEE, Seoul National University — Since the photodetectors based on molybdenum disulfide (MoS2) emerged, diverse researches have been conducted to obtain high performance as the photodetectors.[1] However, it is not trivial to study the intrinsic optical properties of MoS2 because of the reflected incident light by the generally used opaque substrate such as SiO2. Here, we report our study of the intrinsic optical characteristics in MoS2 phototransistor through the transparent device structure fabricated by 2D materials-based heterostructure. The internal photo-responses (corresponding to the photo-response generated by absorbed photons in a MoS2 sheet) such as responsivity, detectivity, and quantum efficiency were carefully investigated. The measured results indicated that the internal quantum efficiency was not strongly dependent on the wavelength of the incident light, whereas the external quantum efficiency was. Our study helps to understand the intrinsic optical characteristics of 2D-based photodetectors, and will provide an insight for the realization of 2D-based transparent photodetectors.

References  
11:51AM L55.00004: Nonlinear Plasmonics with 2D Excitons*  
BEKELE BADADA (Presenter), MATTHEW KLEIN, Physics, University of Arizona, Tucson, Arizona 85721, USA, ROLF BINDER, College of Optical Sciences, University of Arizona, Tucson, Arizona 85721, USA, ADAM ALFREY, MAX MCKIE, Physics, University of Arizona, Tucson, Arizona 85721, USA, MICHAEL KOEHLER, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan, BRIAN LEROY, JOHN SCHAIBLEY, Physics, University of Arizona, Tucson, Arizona 85721, USA — We investigate the interactions between propagating surface plasmon polaritons (SPP) in a metallic waveguide and excitons in WSe2 monolayer. The WSe2 monolayer was encapsulated by few layer thick hBN and transferred onto a lithographically defined gold waveguide using dry transfer technique. SPPs were launched by focusing a tunable laser onto an integrated input grating coupler and scattered out using another grating coupler. Both linear and nonlinear response of SPP-exciton interactions were measured. We report a very large linear absorption of SPP ~ 73% when the SPP is tuned to the exciton energy. For the nonlinear response, we report both optical-pumped and SPP-pumped differential SPP transmission measurements. For the SPP-pumped case, we report a large differential transmission (DT/T) over 4%. These results are highly consistent with a theoretical model of the linear and nonlinear SPP-exciton response. In our model, the SPP-exciton wave is based on an eigenmode analysis in the linear response regime, which is then perturbatively extended to the nonlinear regime. We believe that our device architecture and analysis could pave the road towards all-plasmonic modulators, amplifiers and transistors.

*This work is mainly supported by AFOSR-YIP through award No FA9550-17-1-0215.

12:03PM L55.00005: Low-frequency Raman signature of Ag-intercalated MoS2: A first-principles study.  
NATALYA SHEREMETYEVA (Presenter), DRAKE NIEDZIELSKI, DAMIEN TRISTANT, Physics, Rensselaer Polytechnic Institute, LAUREN E. KERSTETTER, AMA AGYAPONG, ANNA C. DOMASK, SUZANNE MOHNEY, Materials Science and Engineering, Pennsylvania State University, VINCENT MEUNIER, Physics, Rensselaer Polytechnic Institute — Two-dimensional layered materials (2DMs) are promising candidates for novel electronic devices as their electronic properties can be tuned e.g. by controlling their layer number. Precise characterization of 2DMs' is crucial for exact property control. Raman spectroscopy is a nondestructive technique that can identify even small structural/electronic changes.

Recent advances in Raman spectroscopy hardware made resolution of low-frequency (LF) Raman response in 2DMs possible. This response has a low intensity compared to the high-frequency (HF) Raman signature and is located close to the strong Rayleigh line making the detection challenging. However, as LF interlayer modes are rigid motions of each layer as a whole unit within the 2DM with restoring forces governed by the weak interlayer interactions, they are more sensitive to structural parameters than their HF intralayer counterparts (Liang L. et al., ACS Nano Article ASAP, DOI:10.1021/acsnano.7b06551).

Motivated by experiment, we present a Density Functional Theory based study of LF Raman modes of few-layer MoS2 intercalated with silver. We predict a noticeable red shift of LF modes with increasing Ag concentration. This shift is confirmed experimentally and can be used for confirmation of successful silver diffusion into MoS2.

12:15PM L55.00006: Tailoring the electroluminescence of dual-gated monolayer p–n diodes*  
ERIK LENFERINK (Presenter), Physics and Astronomy, Northwestern University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, NATHANIEL STERN, Physics and Astronomy, Northwestern University — Owing to their direct bandgaps and atomic-scale thickness, monolayer transition metal dichalcogenides have been heavily investigated for optoelectronic applications. Their potential for atomically-thin visible frequency light sources can be realized by lateral monolayer p–n diodes defined by local electrostatic gates. Control over the spectral distribution and polarization of the electroluminescence is desirable for integrating these prototypical monolayer LEDs into optoelectronic and nanophotonic devices with tunable coupling. The high electric fields near the p–n interface in these single-monolayer devices provide a route for in situ control of emission. Here, we discuss electrical tuning of the electroluminescence from the electrostatically-induced interface of gate-defined monolayer WSe2 p–n diodes. We observe strong linear polarization (~50%) of the electrically-pumped luminescence and a gate-tunable emission energy shift originating at this interface. Current-induced valley polarization, a possible avenue to achieving electrically-controlled circularly polarized emission, is also investigated with spatially-resolved Kerr rotation at cryogenic temperatures.

*Work supported by the Office of Naval Research (N00014-16-1-3055).
12:27PM L55.00007: Characterizing the low doping regime and charge fluctuation in graphene using Raman spectroscopy.*  
ZHUOFA CHEN (Presenter), NATHAN JEAN CARL ULLBERG, DAVID BARTON, ANNA K SWAN, Department of Electrical and Computer Engineering, Boston University — Graphene without charge impurities is essential for high-quality transport-based devices. Here we propose using Raman spectroscopy, as opposed to labor-intensive transport measurements, to monitor low-level accidental doping and charge fluctuation in graphene. At low doping level, monitoring the 2D band splitting reveals a whole host of information on charge density screening in graphene [1]. This method provides orders of magnitude higher precision than the reported results using the G-band shift. Our work provides a simple, noninvasive way to explore doping levels and charge fluctuation in graphene, which is important to evaluate the quality of graphene before fabricating graphene-based devices.


*This work is supported by NSF DMR grant 1411008

12:39PM L55.00008: Low-Temperature Interfacial States of MoS2-Pentacene Heterojunctions*  
TEODOR STANEV (Presenter), TREVOR LAMOUNTAIN, VINOD SANGWAN, HADALLIA BERGERON, MARK HERSAM, NATHANIEL STERN, Northwestern University — Layered 2D materials such as transition metal dichalcogenides are fundamental components for building more complex heterostructures using organic molecules, nanostructures, or other layered materials. Organic thin film solids of pentacene, a well understood polycyclic aromatic hydrocarbon used commonly for photovoltaics and thin-film FETs, has been used to form mixed dimensional p-n heterojunctions with 2D MoS2, wherein the type II band alignment leads to ultrafast hole transfer across the junction. Here, we report low temperature optical spectroscopy showing distinct optical features that emerge in the pentacene-MoS2 heterostructure. We observe the quenching of pentacene singlet/triplet-emission and of MoS2 defect photoluminescence as well as the emergence of a narrow emission feature at low temperatures. The power dependence and lack of response to local back-gating suggest these effects are not from charge doping or bound excitons. These results demonstrate the diverse control over opto-electronic properties obtainable by combining low-dimensional materials.

*Work supported by the NSF MRSEC program (DMR-1720139).

12:51PM L55.00009: Engineering photoluminescence in thin-layer WSe2 by ionic gating*  
LEI LIU (Presenter), Department of Materials Science and Engineering, College of Engineering, Peking University, ERIK J. LENFERINK, Department of Physics and Astronomy, Northwestern University, GUOHUA WEI, Applied Physics Program, Northwestern University, TEODOR STANEV, NATHANIEL STERN, Department of Physics and Astronomy, Northwestern University — Electron-double-layer gating with ionic liquid introduces extreme doping level, compared with the conventional solid dielectric approach. For transition metal dichalcogenides (TMDCs) atomic crystal, ionic gating has been demonstrated as a powerful tool to tuning the lattice and electronic properties, e.g., the transition between the 2H and 1T’ phase of MoTe2 and Ising superconductivity in MoS21,2. The tuning of TMDCs’ optical properties by ionic liquid gating so far has remained largely unexplored. Here we show the voltage-tunable photoluminescence (PL) of monolayer and bilayer WSe2 in the ambipolar devices. With the Fermi level sweeping from the conductance and valence band, the PL strength varies continuously (down to zero) and the valley polarization can be controlled, while the Raman results reveal no phase transition. The emission from indirect optical transition can be enhanced by applying appropriate gating in bilayer WSe2. The efficient electrical tuning of thin-layer TMDC photoluminescence opens new possibilities for the opto-electronic functional devices.


*This work is supported by the ONR (N00014-16-1-3055), the NSF MRSEC program (DMR-1720139), and the U.S. DOE (BES DE-SC0012130).
1:03PM L55.00010: Rapid and High Sensitivity Imaging of Two-dimensional Materials by Stimulated Raman Scattering Microscopy*  
JIWEI LING (Presenter), XIANCHONG MIAO, MINBIAO JI, Fudan University — 
Raman microscopy has been widely used to characterize phonon vibration in two dimensional materials. It enables us to gain insight into the information of sample thickness, doping and strain effect. However, Raman mapping by spontaneous Raman microscopy is often hindered by limited sensitivity and imaging speed. Here, we bring the stimulated Raman scattering (SRS) for the first time in characterizing two dimensional hexagonal-boron nitride. We found that SRS offers background free and greater sensitivity imaging than spontaneous Raman scattering (SR), second harmonic generation (SHG) and four-wave-mixing(FWM). The SRS signal shows good linearly dependence on layer number. What is more, it enables rapid imaging that is thousand times faster than SR mapping. Our result shows great potential of SRS in the study of two dimensional materials.

* National Key R&D Program of China (2016YFC0102100,2016YFA0203900); National Nature Science Foundation of China (81671725); Shanghai Raising Star Program (15QA1400500); Shanghai Action Plan for Scientific and Technological Innovation Program (16441909200); and Shanghai Municipal Science and Technology Major Project (2017SHZDZX01) National

1:15PM L55.00011: Electrostatic control of exciton flux in van der Waals heterostructures  
DMITRII UNUCHEK (Presenter), ALBERTO CIARROCCHI, AHMET AVSAR, Ecole polytechnique federale de Lausanne, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ANDRAS KIS, Ecole polytechnique federale de Lausanne — Large exciton binding energy in recently discovered two-dimensional semiconductors makes exciton physics accessible even at room temperature in these materials. Particular interest has been given to the interlayer excitons in van der Waals heterostructures based on transition metal dichalcogenides (TMDCs) with type-II band alignment. Whereas individual two-dimensional materials have short exciton diffusion lengths, the spatial separation of electrons and holes in different layers in heterostructures increases exciton lifetime and thus helps to overcome this limitation. In addition, this charge separation realizes built-in out-of-plane electric dipole moment, allowing exciton manipulation via an external electric field, showing promise for next-generation photonic devices relying on excitonic effects. Here, we present van der Waals devices made of TMDCs heterostructures encapsulated in h-BN with graphene control gates, which allow us to manipulate exciton dynamics by creating electrically reconfigurable potential profiles for the exciton flux. Our excitonic device demonstrates electrically controlled transistor actions at room temperature, that holds great promise for realizing small and efficient interconnects between optical data transmission and electrical processing systems.

1:27PM L55.00012: Directional coupling of valley exciton emissions from monolayer MoS2 on periodic plasmonic nanostructures  
CHIEN-JU LEE (Presenter), CHIH-LUN WU, LI-SHUAN LU, WEN-HAO CHANG, Department of Electrophysics, National Chiao Tung University — The unique coupled spin-valley physics in two-dimensional (2D) transition metal dichalcogenides (TMDs) has triggered abundant research activities in realizing valleytronic applications. Due to the valley contrast optical selection rule, excitons in monolayer TMDs formed at two degenerate but inequivalent K and K' valleys can couple to light with different helicities. Here, we demonstrate the spatial separation of valley-polarized excitons at room temperature by coupling monolayer MoS2 with the surface plasmon polariton (SPP) of a periodic metallic structures. Due to the spin-orbit coupling of light, the SPP waves excited by exciton emissions with opposite helicities interacting with the periodic metallic structures can be separated into different directions. When the exciton emissions are on resonance with the SPP modes, we observe the valley-dependent directional coupling of exciton emissions in both real and momentum space by polarization-resolved photoluminescence imaging. Our results demonstrate a route for controlling and detecting the valley polarization of TMDs by optical means.
1:39PM L55.00013: Generating Strain in 2D Materials using Microelectromechanical Systems*  MOUNIKA VUTUKURU (Presenter), JASON W CHRISTOPHER, ZHUOFA CHEN, DAVID JOHN BISHOP, ANNA K SWAN, Boston University — 2D materials are unique in that many of their material properties, such as doping and band-gap, are dynamically tunable. Strain engineering is a promising way to access and tune their electronic properties. We integrate 2D materials with MEMS technology which offers tremendous control over the strain field and is readily compatible with modern electronics. We have previously achieved success in straining MoS2 to 1.3% using MEMS [1]. Here we report on the use of electrothermal MEMS actuators to uniaxially strain monolayer graphene, as confirmed through micro-Raman spectroscopy. This was achieved through the development of gold micro-riveting to anchor the 2D material in place. We also examine two terminal electrical transport through MEMS-strained graphene. The application of controlled strain using MEMS therefore allows for the investigation of electrical and mechanical interplay in strained 2D materials, opening the door to the development of strain-based 2D electronics.


*This work is supported by NSF DMR grant 1411008.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L60 FED FGSA: Launching a Successful Career as a Physicist  BCEC 258A - Chuhee Kwon, Cal State Unv- Long Beach - Tag(s): Careers, Education , Industry, Invited, Undergraduate

11:15AM L60.00001: Launching a Successful Legal Career as a Physicist?  [Invited]  LARISSA BIFANO (Presenter), DLA Piper — Physics degree holders are highly employable in a variety of settings. With a physics training, a potential hire has acquired a broad problem-solving skill set that translates to almost any environment, as well as an ability to be self-guided and -motivated so that they can learn the skills are needed to achieve. Patent law presents an interesting opportunity for physicists to apply their technical skills to the legal field. As a patent lawyer, you have the opportunity to work with researchers, innovators, start-ups, and large Fortune 500 companies to protect their ideas with patents, and potentially enforce those patents against competitors.

11:51AM L60.00002: Transitioning from Physical Science to Data Science  [Invited]  CHRIS RYAN (Presenter), TrialSpark — In the past decade, data science has emerged as an indispensable part of many engineering organizations at technology companies. Physical scientists have a great background for this kind of work, and this has been appreciated since this still-evolving role was originally defined. Expectations for the role have continued to clarify and can differ from company to company—from product feature experiments, focused analytics work, open-ended research projects, machine learning feature development, to all of the above and more. This talk will focus on how to efficiently overcome the possible hurdles faced when making this transition. I will talk about what to do and what to avoid when leveraging your research experiences, skills to know and learn, resume and interview tips, what to look for in job descriptions, what "data science" means at different kinds of companies, and other topics. I will also discuss examples of recent projects I have worked on as a data scientist at a healthcare startup.

12:27PM L60.00003: Why I Teach: High School Physics Teaching as a Career  [Invited]  AARON OSOWIEKI (Presenter), Science, Boston Latin School — What can you do with a degree in physics? You can teach others about the joy in understanding the world around them. Teach students how to think critically and solve problems. Come to this session to learn why I became a physics teacher and you should to.

1:03PM L60.00004: What do physics students need for career success? Findings from the Phys21 report*  [Invited]  LAURIE MCNEIL (Presenter), University of North Carolina at Chapel Hill — In October 2016 the Joint Task Force on Undergraduate Physics Programs published a report, Phys21: Preparing Physics Students for 21st-Century Careers. Based on information supplied by employers of physics graduates in the private sector and in government laboratories as well as in academia, the report summarizes the knowledge and skills that physicists need to succeed in a wide range of contemporary careers. In this presentation I will discuss those findings as well as ways in which students can prepare themselves for successful careers and how physics departments can help.

*The preparation of the Phys21 report was supported by the NSF under grants DUE-1540570 and -1540574.
1:39PM L60.00005: The Value of Curiosity [Invited] JOSEPH DAY (Presenter), Research, Bridgewater Associates — As physicists we are all driven by a deep curiosity to better understand the world. In this talk I'll share how curiosity has taken me on a journey from a public high school in Los Angeles, to a particle physics PhD, Stanford, the Ivy League, and the world's biggest hedge fund.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L62 DAMOP: Topological and Non-Hermitian Photonics BCEC 258C - Wladimir Benalcazar, Pennsylvania State University - Tag(s): Invited

11:15AM L62.00001: Topological Photonics [Invited] MARIN SOLJACIC (Presenter), Massachusetts Institute of Technology — TBD

11:51AM L62.00002: Nontrivial topology from simple photonic structures [Invited] SHANHUI FAN (Presenter), Stanford University — Within the emerging area of topological photonics, which seeks to discover novel topological physics effects in photonic systems, much of the efforts have been devoted to discover non-trivial topology in photonic band structures. On the other hand, there are also interesting topological effects in other aspects of photonics. In this talk, as one of the examples, we discuss the non-trivial topology that arises from the dependency of the scattering matrix of a photonic crystal slab on the angles of incidence. We show that these scattering matrices can exhibit non-trivial topology, which leads to complete polarization conversion, as well as the capability for generation of arbitrary polarization by varying only the input angles. Being topological, these effects are robust to frequency variation, and thus is naturally broad-band.

12:27PM L62.00003: Exceptional points, coherent perfect absorption and disorder scattering in non-Hermitian media* [Invited] STEFAN ROTTER (Presenter), Institute for Theoretical Physics, Vienna University of Technology (TU Wien) — In my talk I will discuss the physics of exceptional points (EPs) and how encircling them creates a robust and asymmetric switch between the two resonant modes that meet at such an EP. In particular, I will focus on the topological aspects of this state transfer protocol that has meanwhile been implemented in a number of different experimental setups [1-3]. I will then point out that EPs can not only be obtained by merging two resonant states, but also by the coalescence of two S-matrix zeros giving rise to a perfect chiral absorber [4]. By studying the movement of such perfectly absorbing S-matrix zeros in a disordered system, we recently achieved the first experimental demonstration of a "random anti-laser" - a disordered system that perfectly absorbs a suitably shaped incoming wave state [5]. If time permits, I will also report on scattering states in disordered media with constant intensity and perfect transmission [6]. Implementing these states using several loudspeakers with gain and loss allows us to steer an incoming sound wave across a strongly disordered waveguide without any reflection or variation in its pressure [7].


*We acknowledge funding by the Austrian Science Fund (FWF) through project numbers SFB-NextLite F49-P10 and I 1142-N27 (GePartWave).

1:03PM L62.00004: Topological photonics in open systems [Invited] BO ZHEN (Presenter), University of Pennsylvania — Topological order has raised great research interests in optical systems over the past years, while most of the efforts have been focused on closed and lossless (Hermitian) systems. Here, I will present some of the recent progresses in studying topological states in optical systems with open boundary conditions. On the one hand, radiation losses in these non-Hermitian systems give rise to new topological states that are not possible in Hermitian ones. On the other hand, the concept of topological invariants gives us new means to control the radiation fields, both in their amplitudes and polarization states.
Photonic Topological Insulators in Synthetic Dimensions

Topological phases enable protected transport along the edges of materials, offering immunity against scattering from disorder and imperfections. These phases were suggested and demonstrated not only for electronic systems, but also for electromagnetic waves, cold atoms, acoustics, and even mechanics. Traditionally, the underlying model of these systems is a spatial lattice in two or three dimensions. However, it recently became clear that many lattice systems can exist also in synthetic dimensions which are not spatial but extend over a different degree of freedom. Thus far, topological insulators in synthetic dimensions were demonstrated only in cold atoms, where synthetic dimensions have now become a useful tool for demonstrating a variety of lattice models that are not available in spatial lattices. Recently, efforts have been directed towards realizing topological lattices with synthetic dimensions in photonics, where they are connected to physical phenomena in high-dimensions, interacting photons, and more. We will describe our recent results demonstrating experimentally the first photonic topological insulator in synthetic dimensions. The ability to study experimentally photonic systems in synthetic dimensions opens the door for a plethora of unexplored physical phenomena ranging from PT-symmetry, exceptional points and unidirectional invisibility to Anderson localization in high dimensions and high-dimensional lattice solitons, topological insulator lasers in synthetic dimensions and more. Our study here paves the way to these exciting phenomena, which are extremely hard (if not impossible) to observe in other physical systems.

Wednesday, March 6, 2019 11:15 AM - 2:15 PM

Session L69 CSWP: Creating Inclusive Environments for Working and Learning

Tag(s): Diversity, Invited

11:15AM L69.00001: Sexual Harassment Reported by Undergraduate Women in Physics*

LAUREN AYCOCK (Presenter), AAAS Science & Technology Policy Fellow, Department of Energy, ZAHRA HAZARI, STEM Transformation Institute, Department of Teaching & Learning, and Department of Physics, Florida International University, ERIC BREWE, Department of Physics and School of Education, Drexel University, KATHRYN B. H. CLANCY, Department of Anthropology, University of Illinois at Urbana-Champaign, THEODORE W HODAPP, RENEE MICHELLE GOERTZEN, American Physical Society APS — Sexual harassment occurs frequently in male-dominated fields including physics which is more male-dominated than most other science, technology, engineering and mathematics (STEM) fields. I will present results on the incidence of sexual harassment and its impact on our sample of women in physics. Our work focused on undergraduate women, who attended a conference for undergraduate women in physics, and took an online post-conference survey. Approximately three quarters (74.3%; 338/455) of survey respondents experienced at least one type of sexual harassment in physics. We find that more frequent/less severe types of sexual harassment predict a negative sense of belonging and exacerbate the imposter phenomenon. Prior work has found that sense of belonging and the imposter phenomenon are related to students' persistence in STEM fields. Our results have implications for understanding and improving persistence in physics. Informing the community about the occurrence of sexual harassment in physics can enable work toward reducing its occurrence and mitigating its impact.

*This work was supported in part by the National Science Foundation (NSF) (PHY-1346627) and by the Department of Energy (DOE) (DE-SC0011076). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the NSF, DOE, APS, or AAAS STPF Program.

11:51AM L69.00002: An honest look at why women are underrepresented in competitive technical leader roles; strategies to create inclusive environments to bridge the gap

JOANNA PERKINS (Presenter), Intel Corporation — In this talk I will share my insight on key practices that have helped to create inclusive environments at each stage of my career: studying undergraduate Physics at a small liberal arts college, teaching high school Physics in the Mississippi Delta, completing my Physics PhD at a large university, and finally in an extremely competitive Technology Development career in industry. Attendees should walk away with strategies for navigating career opportunities in all sectors and ideas to help build strong communities for women in technical roles.
Inclusion, Equity, and Program Improvement with the APS/AAPT Guide to Effective Practices in Physics Programs (EP3)

Courtney Lannert (Presenter), Smith College — In light of the numerous challenges faced by Physics programs in the United States, along with feedback from the physics community, the Council of the American Physical Society formed a national blue-ribbon task force charged with creating a living guide to equip undergraduate physics programs to address these challenges. Developed in partnership with AAPT, the Effective Practices for Physics Programs (EP3) Guide will assist physics programs nationwide by providing a practical set of practices, approaches, and tools deemed effective by the community or informed by current research. Topics covered by the Guide span the areas of curricula, pedagogy, mentoring, recruitment, retention, career/workforce preparation, resources, and faculty professional development. Considerations of inclusion and equity are woven throughout the Guide and also appear as stand-alone sections within the Guide to motivate broader discussions of inclusion.

The work of the task force is underway and the first release of the Guide is expected in Spring 2020. This talk will outline and introduce the Guide, highlighting how it can be an effective tool for individuals and departments to improve their programs by adopting practices that are inclusive and equitable.

*This material is based upon work supported by the National Science Foundation under Grant Nos. 1738311, 1747563, and 1821372. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

Creating environments where women of color can thrive

Angela Johnson (Presenter), St. Mary's College of Maryland — I have been exploring where women of color complete physics degrees. Despite the fact that women of color (Black, American Indian, Asian and Asian American women and Latinas) are clustered in women's colleges and minority-serving institutions, most women of color nonetheless study physics at large, predominantly White institutions where they are deeply isolated. Thus, it is imperative that all physics professors know how to create departments where women of color can thrive.

I will begin with some theory to help understand the experiences of women of color in physics, including intersectionality and implicit bias. Next I will present data about the extreme under-representation of women of color in physics and patterns in where they are completing physics degrees. I will also present what little is known about these women's typical experiences, which, unfortunately, are often discouraging and alienating.

Next, I will describe the findings from an ethnography I conducted at a physics department where women of color reported a strong sense of belonging. I will describe typical student experiences in this department (for all students, not just the women of color) and then pinpoint the actions taken by physics faculty that I believe created this positive environment. Typical experiences of the women of color (and all students, for that matter) include having a lot of friends among physics majors, feeling comfortable asking other students for help, and trusting their professors for help both with physics and with handling racism and sexism. Typical actions by professors including insisting that students collaborate and support one another during group work and emphasizing that success in physics comes from hard work rather than innate ability.

*This research was funded in part by NSF IUSE grant #1712531, “Centering Women of Color in STEM: Identifying and Scaling Up What Helps Women of Color Thrive.”

Gender Research in PER: A Binary Past and Complex Future

Ramon S Barthelemy (Presenter), EAB — Gender research in physics education research (PER) has become common in the last three decades. This work, however, has focused heavily on the differences between men and women in introductory physics courses. Known as gender gap research, these studies create a deficit model comparing women to men, and do not account for other identities and factors. This talk will present a “gapless” study that upends this trend by focusing on the contextualized experiences of women in graduate physics and astronomy using qualitative interviews. Data will include an exploration of their gendered experiences through the forms of microaggressions and hostile sexism. A concluding vignette will show an example of “gapless” research using quantitative methods, focused on the experiences of transgender physicists.

Wednesday, March 6, 2019 11:15 AM - 11:15 AM

Session L70 : Poster Session II (11:15am-2:15pm) BCEC Exhibit Hall - Tag(s): Poster

L70.00001: POLYMER PHYSICS —
L70.00002: Thermal Properties of Polyvinyl Alcohol by Fast Scanning Calorimetry

DAVID THOMAS, Physics and Astronomy, Tufts University, EVGENY ZHURAVLEV, ANDREAS WURM, CHRISTOPH SCHICK, University of Rostock, PEGGY CEBE (Presenter), Physics and Astronomy, Tufts University — Polyvinyl alcohol crystallizes from the melt so rapidly that it is difficult to obtain fully amorphous glassy polymer. To study thermal properties of fully amorphous PVA, we use fast scanning calorimetry (FSC) to heat and cool at rates ranging from 1000 K/s up to 600,000 K/s. We determine the critical cooling rate, $\beta_c$, needed to quench PVA from the melt into an amorphous glass as $|\beta_c| = 20,000$ K/s. Using FSC in combination with conventional differential scanning calorimetry (DSC), we evaluate the temperature dependent liquid state heat capacity, $c_p^{\text{Liquid}}(T) = (0.0016 \pm 0.0002^* T + (2.3 \pm 0.2)) J/(gK)$. The specific heat capacity increment at $T_g$ for fully amorphous PVA is $\Delta c_p^{\text{amor}}(T_g) = (1.005 \pm 0.002) J/(gK)$. For the semi-crystalline samples used in this study, PVA obeys a two phase model in which the rigid amorphous fraction, $\varphi_{RA} \sim 0$. The approaches used in this work are applicable to any semicrystalline polymer or biopolymer which degrades upon heating, or crystallizes so rapidly from the melt that a fully amorphous material cannot be realized at conventional DSC rates.

L70.00003: A new concept of electrodes for ambipolar carrier injection in organic semiconductors

KATSUMI TANIGAKI (Presenter), THANGAVEL KANAGASEKARAN, WPI-AIMR, Tohoku University, SYUN ONUKI, TAIKI MIURA, HIDEKAZU SHIMOTANI, Department of Physics, Graduate School of Science, Tohoku University — Organic semiconductors (OSCs) have attracted much attention for low cost, flexible and human friendly optoelectronics. However, achieving high electron injection efficiency is difficult from air stable electrodes and cannot be equivalent to that of holes. Here, we present a novel concept of electrode composed of a bilayer of tetratetracontane (TTC) and polycrystalline organic semiconductors (pcOSC) covered by a metal (M) thin film layer. Field effect transistors of single crystal organic semiconductors (scOSCs) with the new electrodes of M/pcOSC/TTC (M: Ca or Au) show both highly efficient electron and hole injection. Contact resistances of electron and hole injection from Ca/pcOSC/TTC and Au/pcOSC/TTC are fascinatingly lower than those from pure Ca for electrons and Au for holes, respectively. Equivalent high field effect mobilities of holes (22 cm$^2$V$^{-1}$s$^{-1}$) and electrons (5.0 cm$^2$V$^{-1}$s$^{-1}$) can be observed in a rubrene single crystal, which are the highest among field effect transistors so far proposed. Highly efficient light emission will be demonstrated via amipolar carrier injection.

L70.00004: Water-Mediated Mixed Ionic-Electronic Conduction in Polythiophene-Derived Polyelectrolytes

GARRETT GROCKE (Presenter), BAN DONG, SHRAYESH PATEL, Institute for Molecular Engineering, University of Chicago — Conjugated polyelectrolytes that can conduct both ionically and electronically are attractive candidates for next-generation electrochemical devices, yet little is known about the impact of polymer processing and morphology on mixed conduction characteristics. This work reports the influence of water on the structure and conduction of poly[3-(potassium-n-alkanoate) thiophene-2,5-diyl]s (P3KnTs) in thin film. These materials were found to be highly resistive under anhydrous conditions but exhibited mixed ion-electron conduction as a function of increasing relative humidity. UV-Vis-NIR measurements provide evidence for water-assisted formation of alkanoate-anion-stabilized polythiophene bipolaron states and thus electronic conductivity, wherein dissociation of potassium-alkanoate bonds leads to the enhanced ionic conductivity. Additionally, using in-situ humidified scattering experiments, it was shown that increasing side-chain stacking distance coincides with the improvement in ionic conductivity as a function of relative humidity, suggesting that ionic transport occurs through regular pathways formed by the flexible side-chains. Our results show strong influence of water on mixed ion-electron conduction characteristics of conjugated polyelectrolytes in undoped conditions.
In this study, focusing on polymer / fullerene-free type PTB7 / ITIC complex, we obtain the electronic structure of complex and absorption spectrum at donor / acceptor interface using time dependent density functional theory method. In addition, from the viewpoint of electronic structure, absorption spectrum, and HOMO–LUMO gap, we consider the mechanism of charge transfer in polymer / fullerene-free type organic solar cell.

We compared the amounts of D/A transition contribution in absorption spectra, charge transfer (CT) and CT distance of the PTB7/ITIC complex with those of the fullerene PTB7/PC71BM complex. It turns out that any of these quantities were larger for the former. In addition, PCE is reported to be larger for fullerene-free OSC than for fullerene OSC and to be higher when CT distance becomes longer in fullerene OSC. Therefore, we have found that the CT distance is a descriptor for assessing PCE in the fullerene-free type OCS as well.

L70.00007: Excimontec: An Open-Source Software Tool for Kinetic Monte Carlo Simulations of Organic Electronic Devices* MICHAEL HEIBER (Presenter), Center for Hierarchical Materials Design, Northwestern University — Kinetic Monte Carlo (KMC) simulations are a powerful computational tool that have been used in concert with experiments and theory to understand and optimize organic semiconductor devices. However, despite over 30 years of applying KMC simulations to organic semiconductors, no standardized software tools have emerged. Instead, many research groups around the world have maintained private codebases of varying complexity, efficiency, and reliability. As a result, there have been large barriers to entry for new researchers and a lot of repetitious efforts that would be much better off applied to further refining the physical models. Excimontec is a new well-tested, reliable, and accessible open-source software tool for performing KMC simulations of organic electronic devices, and this presentation will highlight some of the main features currently available, including time-of-flight charge transport simulations, excited state dynamics simulations, and internal quantum efficiency simulations.

*Financial assistance award 70NANB14H012 from U.S. Department of Commerce, NIST as part of the Center for Hierarchical Materials Design (CHiMaD).

L70.00008: Variable Resolution Coarse-Graining of Ion-Coupled Electron Transport in Electrochemically Active Polymers BRET SAVOIE (Presenter), Purdue University — Conducting polymers that exhibit reversible mass and ion exchange with aqueous media have potential for sensing applications when implemented in organic electrochemical transistors (OECTs). However, the degree to which ion motion is coupled with electron transport and morphology changes, and the range of polymer chemistries that can exhibit and be optimized for electrochemical response in aqueous media is unknown. To address these challenges we have developed the first variable resolution model of hydrated PEDOT:PSS, the archetypical electrochemically active system, with several simple salts. Using this variable resolution model we are able to characterize both long-timescale morphology reorganizations and the corresponding short-timescale evolution of the conducting polymer electronic structure and develop design rules for optimal doping and hydration levels in PEDOT-based systems. The generality of this approach creates an opportunity to establish to what degree PEDOT:PSS is representative of other OECT polymers and address the lack of materials diversity in OECT applications.
Absorption enhancement in evanescently-coupled waveguides

In this project the main goal is to construct various thin films of different thicknesses of CYTOP and PMMA in a glass substrate using the spin coating. A glass, CYTOP and PMMA substrate was proposed. Although this substrate was bio-imaging oriented in order to enhance resolutions and get better signals when working with bio-samples, is also a good platform for luminescence cooling. In a Matlab simulation, we find that the best thicknesses that will enhance the electrical field on the films surface at a resonant angle between 65-70 degrees are ~600-750 nm and ~350-450 nm, respectively. Then, Glass/CYTOP/PMMA substrate were successfully spin-coated with an optimal thickness achieved between ~700nm (for CYTOP) and ~400nm (for 1wt% of Lumogen Red L305 with PMMA). Photoluminescence (PL) spectra was enhanced and absorption is stronger on thicker films. The reflectivity spectrum shows that the resonant angle was ~47 degrees. The idea of cooling a solid-state optical material by simply shining a laser beam onto it, the advantages of compactness, the absence of vibrations and moving parts or fluids, high reliability and the ability to operate without cryogens is rapidly becoming a promising technology for future cryocoolers.

*Interdisciplinary Materials REU program at Penn State University

Optical Super-Resolution Imaging of Block Copolymer Thin Film Surface Morphology Using Fluorescent Silica Nanoparticles

Block copolymers (BCPs) are of tremendous academic and industrial interest, as they exhibit myriad tunable properties useful across a broad range of applications. This is particularly true for BCP thin films. Traditionally, imaging mesostructured BCP surfaces of such films has been dominated by electron and scanning probe microscopies. In recent years, however, high-resolution optical imaging in the far field has provided exciting opportunities for alternative approaches. Here, we report the optical super-resolution imaging of BCP thin film surface mesostructure through stochastic optical reconstruction microscopy (STORM). To that end, we introduce a new class of functionalized silica nanoparticles to enhance the brightness of encapsulated dyes for STORM, offering distinct advantages over conventional sample labeling with organic dyes. These nanoparticles are simply mixed with or attached to specific blocks of the BCPs, thereby enabling selective block staining and optical visualization. This allows for facile imaging of morphological features on the near-molecular scale, thus providing a versatile method for BCP surface morphology assessments using optical imaging.

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Ion transport properties of block copolymer electrolytes comprising mixed ionic liquids

Ionic conductivity and mechanical properties of block copolymers comprising various ionic liquids has been extensively studied lately to develop future solid-state polymer electrolytes. It has been found that the independent control of cation and anion in ionic liquid can improve ion transport properties of such materials given that the type of cation and anion determines swelling behavior of ionic domains and interfacial properties of ionophilic/ionophobic phases. In the present study, we investigate ion transport properties of block copolymers comprising different ionic liquids. In particular, by employing mixed ionic liquids, markedly improved ionic conductivity was obtained, far higher than simple sum of known values. The results were understood by dissimilar ion distributions in the substructure of self-assembled morphology, as quantified by combining scattering and spectroscopy techniques.

Nanofabrication for Probing Ionic Conductivity Mechanisms in Thin-Film Polymer Electrolytes

These devices are fabricated so that a percentage of the trenches, which model the conducting pathway of a BCP, are blocked by additional SiO₂. A PEO/LITFSI solution is spincoated and reflowed onto the devices then measured using AC impedance spectroscopy to calculate the conductivity. We report a decrease in conductivity with increasing percent hindered pathways. By eliminating the effects of grain boundaries and interfacial blurring between blocks of a block copolymer, this study elicits a direct relationship between structure and conductivity.
L70.00013: Ion Transport in Polymer Blend Electrolytes* BILL WHEATLE (Presenter), VENKATRAGHAVAN GANESAN, University of Texas at Austin — In conventional small-molecule battery electrolytes, high ionic conductivity is achieved through blending of high polarity and low viscosity components. One may simply assume that the conductivities of these blended electrolytes will be an average of the intrinsic conductivities of each host, each of which is weighted by its volume fraction. However, it has been shown that the ionic conductivity is instead a nonmonotonic function of the volume fraction of each host, maximizing at some intermediate blend composition.

Inspired by these results in small molecule electrolytes, we hypothesize similar nonlinearities may occur in polymeric blend electrolytes. In this work, we seek to examine the effect of blending polymeric hosts by using the Stockmayer polarity model in a coarse-grained molecular dynamics framework, which we have previously used to describe the role of host polarity on ionic conductivity. We first investigate the role of host polarity contrast (measured by the difference in monomeric dipole strength) and blend composition on blend phase stability and segmental dynamics. We then correlate these properties with the resultant ionic conductivities of these electrolytes.

*The authors acknowledge the Welsh Foundation and the National Science Foundations for funding this work.

L70.00014: Simultaneous Transient Gel Behavior and Multivalent Ionic Mobility in Polymeric Ionic Liquid-Ligand Gels* SEAMUS JONES (Presenter), Department of Chemical Engineering, University of California, Santa Barbara, NICOLE MICHENFELDER-SCHAUSER, Materials Department, University of California, Santa Barbara, GLENN FREDRICKSON, RACHEL SEGALMAN, Department of Chemical Engineering, University of California, Santa Barbara — Polymeric ionic liquids form labile metal-ligand bonds with cations to delocalize and conduct multivalent metal ions in the solid state. These multifunctional interactions transiently cross-link the polymer network, leading to dramatic enhancements in the storage modulus on some timescales. Correlating the relationship between metal-ligand interaction energies, timescales, and continuum-level mechanical and conductivity properties leads to design rules for multivalent ion-conductive polymers. Oscillatory rheology experiments are used to elucidate metal-ligand coordination timescales while ionic conductivity measurements are used to both understand the timescale of crosslink motion and the mechanism of ion motion in a telechelic poly(methyl acrylate) with imidazole endgroups.

*This work was supported by the MRSEC Program of the National Science Foundation under Award DMR 1720256 (IRG-2).

L70.00015: Mechanism of pattern formation in polymer ionic liquid blends under the influence of an electric field* VANDANA RAJPUT (Presenter), ANUBHA AGRAWAL, PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Formation of controllable self-assembled patterns in soft materials can be used to design a variety of multifunctional materials with tunable properties. Here, we utilize unique properties offered by the blends of polymers and ionic liquids (PIL) to reveal the mechanism behind the formation of intricate morphological patterns that emerge in these blends in the presence of an external electric field (EF). In particular, we perform stability analyses to identify key parameters that can be used to lock a pattern of a particular wavenumber in PILs. In addition, we reveal that under the effect of an external stimulus, which in our case is the strength of the EF, both ordered and disordered phase morphologies can co-exist. We also show that the increased strength of EF in PIL system results in the formation of alternating layers of polymer-rich and IL-rich phases of different widths. The reason for this behavior is attributed to cation-anion, polymer-anion, and polymer-cation interactions present in the blends. Thus, the effect of EF can drive new patterns and allows the control of these patterns through wavenumber locking. We believe that our approach can be extended to a variety of soft matter blends containing constituents with stark different properties.

*IIT Gandhinagar
Gel polymer electrolyte membranes have many advantages over their liquid counterparts, such as high energy density and flexible geometry. However, one of the major challenges in using the polymer electrolytes is their low ionic conductivity at ambient temperature that limits their practical applications. The development of heterogeneous electrolytes, comprising ion-rich and ion-poor regions, has enabled the decoupling of electrical and mechanical properties. However, ILS possess delocalized charges and are composed of ionic species that are generally large and asymmetric. These characteristics hinder the formation of well-ordered ionic domains and result in low conductivity. The emerging challenge is how to design heterogeneous polymer electrolytes with different shapes of continuous nanochannels to maximize the decoupling of ionic conductivity and mechanical strength. We propose that this challenge can be addressed through the polymerization of mesophases of monomer, ionic liquid, and amphiphilic block copolymers. Our results show that high mechanical strength without sacrificing the ionic conductivity can be obtained by the mesophase templating method.

*This research is funded by NM NASA EPSCoR Research Infrastructure Development (RID), Grant No: NNX15AK41A.
MINJUNG LEE (Presenter), RYAN HAYWARD, Polymer Science and Engineering, University of Massachusetts Amherst — The formation of complex coacervates has been a subject of great interest in the field of charged polymers, with a focus almost exclusively on aqueous systems. Herein, we studied the phase behavior of two polymerized ionic liquids, namely poly(1-ethyl-3-methyl imidazolium (3-sulfopropyl) acrylate) and poly(1-(2-acryloyloxy-ethyl)-3-buthyl-imidazolium bis(trifluoromethane) sulfonimide), representing a polyanion and a polycation, respectively, in non-aqueous solutions. By controlling the concentration of the polymers and added salt composed of the two counterions, we studied the conditions for one vs. two phases, which provides useful information for further applications of polymerized ionic liquids, as well as providing an interesting comparison with the phase behavior of other charged polymers such as polypeptides and polysaccharides in aqueous media.

RITUPARNA SAMANTA (Presenter), VENKATRAGHAVAN GANESAN, University of Texas at Austin — We study the effect of pH of the solution on the structural characteristics of a system of weakly charged spherical particles in oppositely charged, dissociable polyelectrolyte solutions. The pH dependent dissociation of weak polyelectrolytes is known to affect the adsorption and bridging of polymers on the particles. We have used a hybrid method of single chain in mean field theory and the solution of general Poisson’s equation in a semi-grand canonical framework. We study the effect of charge of particles, volume fraction of particles and polymers, concentration of polymers on the structural characteristics of the suspension.

ALAN NAKATANI (Presenter), LYNDASY LEAL, NIHIL FERNANDES, KATHLEEN MICHELS, JENNIFER M KOENIG, CATHRYN JACKSON, Dow Chemical Company — Two sets of Hydrophobically modified Alkali Soluble Emulsion (HASE) polymers were investigated using steady shear viscosity and dynamic frequency measurements. One set of HASE polymers contained a fixed ratio of ethyl acrylate (EA) to methacrylic acid (MAA) and a hydrophobe (C12, C18, or C22) containing monomer (macromonomer). The second set of HASE polymers contained a fixed amount of MAA but the amount of C18 macromonomer was varied (1%, 5%, or 10% by mass). Aqueous solutions of the polymers (1% by mass) were tested at pH = 3, 5, 7 and 10. The neutralization process is known to impact the solution viscosity, therefore, samples “back-titrated” from pH = 10 to pH = 7 were also tested. The samples at pH = 3 and 5 had the lowest viscosities. Samples directly adjusted to pH 7 had a much higher viscosity and a yield stress, which increased with increasing hydrophobe size. The samples at pH = 10 had the highest viscosity and yield stress values. Samples back-titrated to pH = 7, were lower in viscosity than the samples directly adjusted to pH = 7. The dynamic frequency results at pH = 10 show additional characteristic timescales which shift as a function of the hydrophobe size.

SUPRIYA GUPTA (Presenter), PARESH CHOKSHI, Chemical Engineering, Indian Institute of Technology Delhi — Incorporation of nanofillers in polymer melt produces composites with extra-ordinary properties due to enhanced surface to volume ratio of the fillers. Fillers are functionalized by grafting polymeric chains on the surface inducing steric stabilizing preventing particle agglomeration. Here, we address the dispersion of clay nanosheets in polymer matrix. We use self-consistent field theory to theoretically construct the polymer mediated interparticle potential curve. The interaction potential is obtained from the inhomogeneous composition field for the polymer segments. First, we examine the interparticle interaction between two grafted nanosheets immersed in the matrix of polymeric chains of dissimilar chemistry to that of the grafted chains. The interaction potential is repulsive at short separation and shows depletion attraction for moderate separations. Further, we construct the interaction potential between two nanosheets grafted with polymeric chains of varying architectures, like star polymer and diblock copolymer. Nanosheets disperse better in the matrix of star polymer than linear polymer. In surfaces grafted with diblock copolymers, the interplay between the enthalpic and entropic interaction gives rise to a rich behavior in the interparticle interaction potential curve.
L70.00024: Novel Properties of Mesostructured Superconductors Synthesized via Block Copolymer Self Assembled Nanocomposites*  RANDAL THEDFORD (Presenter), SOL MICHAEL GRUNER, ULRICH WIESNER, Cornell University — The effect of mesoscale confinement or ordering on the properties of superconductors is an active area of study, but to date this work has largely been done using 2D materials. Three-dimensionally mesostructured superconductors are expected to behave very differently than their 2D or bulk analogues, but exploration of such materials has been limited by the lack of available methods for their synthesis. We demonstrate multiple routes to superconductors with mesoscale order and porosity though the self-assembly of block copolymer nanocomposites. This represents a versatile, robust, and tunable platform for the investigation of 3D mesostructured superconductors. Our results show changes in the superconducting properties of multiple materials when synthesized in block copolymer derived 3D periodic structures such as the bicontinuous double gyroid and the alternating gyroid, suggesting quantum metamaterials behavior.

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L70.00025: In-Situ Monitoring Polymer-graft Functionalization on Gold Nanoparticles and Influences on Assembly Formation  YIWEN QIAN (Presenter), TING XU, Department of Materials Science and Engineering, University of California, Berkeley — Controlled assemblies of polymer grafted nanoparticles can lead to a unique class of material with distinct advantages due to the programmability and diversity endowed from polymer-based-ligands. Surface functionalization of nanoparticles (NPs) with polymer-based ligands plays a critical role in controlling the effective size and ‘interaction softness’. To this end, it is requisite to quantity the attached polymer ligands. Here we present the (in situ) proton nuclear magnetic resonance ($^1$H NMR) study on the ligand exchange of oleylamine by thiol end-functionalized polystyrene as a function of the ligand concentration and particle size on Au NPs. As the extensive overlap of the polymer ligands impede the direct evaluation, we examine the pristine chemical shifts of the oleylamine to characterize the ligand modification. We show that the surface functionalization efficacy depends on the ligand/particle ratio, size of NPs and molecular weight of the polymeric ligands. These quantitative studies enabled us to investigate the influences of the ligand modification and solvent quality on the ordering of the self-assembled polymer grafted nanoparticles with a focus on a polycrystalline assembly to hexagonally ordered superlattice transition.

L70.00026: Fabrication of polymer-brush modified Ba-Ti oxide/poly(vinylidene fluoride) nanocomposites thin film*  MAIKO NISHIBORI (Presenter), KOHEI NOSUE, AYUMI HAMADA, YUKO KONISHI, ATSUSHI TAKAHARA, Kyushu University — Polymer composite with high dielectric constant have attracted attention in the micro-electronic industry due to their easy-processing and low cost. In the composite thin film, the surface properties of the ceramics nanoparticle and the volume fraction of polymer to ceramics particles are quite important in order to increase in their functionality. In this study, the surface modification of Ba-Ti oxide nanoparticles (BT) with high-density poly-methyl methacrylate (PMMA) brushes was conducted to improve its dispersibility in poly(vinylidene fluoride) (PVDF) and the fabrication of nanocomposites thin film of PMMA-BT and PVDF was investigated. PMMA brushes on the surface of BT particles were fabricated by Atom Transfer Radical Polymerization with (2-bromo-2-methyl) propionyloxyhexyltriethxysilane as a silane coupling agent. PMMA-BT particles showed high dispersibility in PVDF-DMF and almost no voids and clacks were observed in the composite film of BT-PMMA mixed with PVDF even if the volume fraction of PMMA-BT particles was high to PVDF. The results indicated that the surface modification by polymer-brush could be a promising method to fabricate the composite film having good quality and high dielectric property.

*This work was supported by JSPS KAKENHI Grant Number 18K04706.
L70.00027: Morphological behavior of ABC mikto-arm terpolymer with a C60*  
HYEYOUNG KIM, University of Massachusetts Amherst, MATTHIAS ML ARRAS, Oak Ridge National Lab, SERGEY CHERNYY, Technical University of Denmark, DUK MAN YU, University of Massachusetts Amherst, GREGORY S SMITH, Oak Ridge National Lab, THOMAS RUSSELL (Presenter), University of Massachusetts Amherst — We observed the morphological behavior of ABC mikto-arm terpolymer with a C60 additive. ABC mikto-arm terpolymers, consisting of polystyrene, polyisoprene and poly(2-vinylpyridine) (PS-PI-P2VP), with various P2VP volume fractions were examined. The role of C60 on the morphological behavior of mikto-arm terpolymer was studied by small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). The affinity of C60 to PS or P2VP was examined by neutron reflectivity. C60 can form charge-transfer complexes with electron donating pyridine groups in P2VP blocks. Before and after charge-transfer reaction, C60 showed different effects on the self-assembly of mikto-arm polymers. The domain spacing, interfacial width, and morphology of mikto-arm terpolymers were changed depending on the concentration of C60.

*This research was supported by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy (DOE). The Research at Oak Ridge National Laboratory's Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. This work was supported by the Air Force Offices of Scientific Research under Contract 16RT1602.

L70.00028: Desorption of Water Collected on Hygroscopic Polymer Nanofibers  
ZHIHAO SHANG, D RENEKER (Presenter), The University of Akron — The high surface area-to-mass ratio make nanofibers an optimal material structure for water absorption from humid ambient air. Water molecules were concentrated on the surface of hygroscopic nanofibers. Strong nanofibers withstood the forces from the flowing air that carried water molecules to within about 100 nm of the fiber surfaces. Nanofiber surfaces became saturated with water molecules. Microwave energy with frequency of 2.45 GHz caused rapid evaporation and formation of a bolus of steam in the air stream. The bolus was collected and the water condensed in an external condenser. Alternatively, high voltage DC was applied to two edges of a thin mat of hygroscopic nanofiber to evaporate water from the nanofiber mat. The apparatus provides a useful method to test water absorption ability of different hygroscopic nanofibers. It also provides other information needed to design large scale water collectors.

L70.00029: A Colloidal Model to describe the effects of mixing time on filler dispersion in industrial nanocomposites*  
VISHAK NARAYANAN (Presenter), KABIR RISHI, GREG BEAUCAGE, Chemical and Materials Engineering, University of Cincinnati, VIKRAM K KUPPA, Nonstructural Materials Division, University of Dayton Research Institute, ALEX MCGLASSON, MICHAEL CHAUBY, Chemical and Materials Engineering, University of Cincinnati — The properties of industrial nanocomposites such as tires depend on the degree of filler dispersion under high-shear mixing. Conventionally, the dispersion is quantified through an index based on the reduction in micron-scale agglomerate size observed in micrographs and bulk electrical conductivity measurements. An alternate nano-scale dispersion technique based on x-ray scattering has been proposed.1 The impact of mixing time on dispersion is investigated taking advantage of the van der Waals equation to describe excluded volume and interaction energy in the dispersion. Herein, an analogy is made between thermally driven true colloidal dispersions and total accumulated strain in nanocomposites. The excluded volume depends only on the filler type and seems insensitive to bound rubber whereas the interaction energy is strongly dependent on viscosity and polymer chemistry. Moreover, the wetting time for nano-scale incorporation of elastomer into filler can be predicted. The description of nano-scale dispersion via a pseudo- second virial coefficient offers the additional possibility of determining the interaction potential that can be used for coarse grained simulations.

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Entropy driven assembly in multicomponent nanocomposite

DENIZ RENDE, Center for Materials, Devices, and Integrated Systems, Rensselaer Polytechnic Institute, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute, FUCHUAN DING, JINGJING LIU, LUYI SUN (Presenter), University of Connecticut — Large-Large Scale One-Step Co-assembly

*This work was supported by the Department of Energy, Office of Basic Energy Science, under Contract DE-AC02-05CH11231 through the “Organic−inorganic Nanocomposites” program at Lawrence Berkeley National Laboratory. The tomography was performed at the National Center for Electron Microscopy.

Nafion Nanocomposite Fuel Cell Membranes for Improved High Temperature Performance

DONOVAN WEIBLEN (Presenter), KRISTA BIGGS, ALIANGNA MAGUIRE, Materials Science and Engineering, Rensselaer Polytechnic Institute, DENIZ RENDE, Center for Materials, Devices, and Integrated Systems, Rensselaer Polytechnic Institute, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Proton exchange membranes represent an active area of fuel cell research. Current work seeks a membrane with excellent proton conductivity, minimal permeability of oxygen and fuel, and stable physical properties. At temperatures above 90 °C, traditional Nafion membranes experience decreased proton conduction, decreased water uptake, and softening. Although the performance is still being improved, addition of silica nanoparticles to Nafion membranes is known to improve conduction and water uptake at high temperatures. Recent work shows a new polymer nanocomposite system that stiffens repeatably and reversibly with increasing temperature via interfacial heterogeneous dynamics between a matrix polymer with low glass transition temperature (Tg) and high Tg polymer modifier adsorbed to silica nanoparticles. Studies were completed to investigate the applicability of this phenomena to Nafion using silane coupling agents to achieve improved high temperature performance. The effects of silica nanoparticle and grafted modifier concentration, and grafted chain structure and dynamics on Nafion nanocomposite structure and properties, particularly thermal stiffening, were studied.

Growth and Bulk Effects of Irreversibly Adsorbed Layers in Polymer Nanocomposites

KATELYN RANDAZZO (Presenter), RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — Recent studies have demonstrated that the formation of irreversibly adsorbed layers at the polymer-substrate interface can significantly affect the overall properties in thin films. However, little attention has focused on the polymer nanocomposites, where irreversibly adsorbed layer growth is expected to be an important parameter due to the amount of surface area and high temperature processing. In this work, we characterize the growth of irreversibly adsorbed layers of polystyrene atop silica nanoparticles, which we correlate to the resulting bulk properties of polystyrene-silica nanocomposites. Our approach compares bulk properties measured via traditional means such as DSC with a direct measurement of local properties achieved by fluorescence spectroscopy. We expect the characterization of irreversibly adsorbed layers and their bulk effects to be useful in engineering new polymer nanocomposite materials.

Biomimetic Nanocoatings with Exceptional Mechanical, Barrier, and Flame Retardant Properties from Large Scale One-Step Co-assembly

FUCHUAN DING, JINGJING LIU, LUYI SUN (Presenter), University of Connecticut — Large-scale biomimetic organic/inorganic hybrid nanocoatings with a nacre-like microstructure were prepared via a facile co-assembly process. Different from conventional polymer nanocomposites, such nanocoatings contain a high concentration of nanosheets, which can be well aligned along the substrate surface. Moreover, the nanosheets and polymer matrix can be chemically co-crosslinked. As a result, the nanocoatings exhibit exceptional mechanical properties (high stiffness and strength), barrier properties (to both oxygen and water vapor), and flame retardancy, but meanwhile they are highly transparent (maintaining more than 85% of their original transmittance to visible light). The nanocoatings can be applied to various substrates and regular or irregular surfaces (e.g., films as well as foams). Because of their excellent performance and high versatility, such nanocoatings are expected to find widespread application.
Metal-polymer nanocomposites are an interesting material class, which allows combining the superior plasmonic, electrical and thermal properties of metal-nanoparticles with the good processability of polymers. To achieve stable nanoparticles in a polymer matrix, the nanoparticle surface has to be modified with a polymer brush, which is commonly done by a ligand exchange approach.

By using Brillouin light scattering (BLS), we elucidate the nanomechanical properties of this hybrid material and combine these measurements with finite element modeling and thermography. We found a counterintuitive decrease of the speed of sound with increasing Ag content and a strong influence of the hybrid material composition. The mesoscopic order of this material can be varied drastically by thermal annealing going from a dispersed phase to a clustered state and back. Finally, the strong light absorption and thermalization of the Ag nanoparticles results in a pronounced local heating effect. Consequently, this thermoplasmonic heating can be used to change the acoustic and, therefore, mechanical properties locally.

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Coassembly of binary nanoparticle systems  
JIULING WANG (Presenter), BRIAN LEE, GAURAV ARYA, Duke University — The spatial distribution of nanoparticles (NPs) in polymer nanocomposites plays a critical role in governing their mechanical and optical properties. Although there have been many studies focusing on the assembly of uniform-sized NPs in polymers, relatively few studies have investigated the coassembly of NPs of different sizes and surface properties. Using a lattice Monte Carlo approach, we investigated the morphology of heterogeneous NP structures assembled from NPs of different sizes and surface properties. Our results indicate that these particles assemble into networks with different pore sizes, fractal dimensions and local aggregation interfaces depending on the particle sizes and sticking probabilities between them. The effects of the initial distribution of NPs on the assembly will also be discussed. Our findings provide guidance for controlling NP assembly and could help us design nanocomposites with superior mechanical and optical properties.

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Hybrid computer simulations of block copolymer/nanoparticle systems  
MARCO PINNA (Presenter), JAVIER DIAZ, Centre for Computational Physics, University of Lincoln, IGNACIO PAGONABARRAGA, Departament de Fisica Fonamental, Universitat de Barcelona, ANDREI ZVELINDOVSKY, Centre for Computational Physics, University of Lincoln — Polymer nanocomposites have been shown to display improved properties over their purely polymeric counterparts. Furthermore, block copolymers (BCP) are perfect candidates to control the localisation of nanoparticles. Nonetheless, the presence of nanoparticles can distort the BCP properties such as morphology and thus colloids act as more than just passive fillers. A systematic study of the co-assembly of block copolymers and nanoparticles is presented. Using a hybrid Cell Dynamic/Brownian Dynamic Simulation method we study the mesoscopic properties of the system. The phase behavior of the block copolymer after the inclusion of nanoparticles is studied, finding phase transitions along with the appearance of new phases due to the effect of colloids in the system [1]. Similarly, the nanoparticles are found to segregate within the block copolymer depending on chemistry, size and anisotropy. The conditions for the formation of aggregates is studied, both in the case of isotropic particles as in the case of anisotropic colloids (Janus, rods, squares, among others).

Influence of PVAc/PMMA/Silica Nanocomposite Structure on Properties

CHEN GONG (Presenter),
Materials Science and Engineering, Rensselaer Polytechnic Institute
DENIZ RENDE, Center for Materials, Devices and Integrated Systems, Rensselaer Polytechnic Institute
RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute —
Rheological properties of poly(vinyl acetate), PVAc, and silica composites were previously studied as a function of silica concentration and silica surface chemistry. In the current work, we investigate the effect of poly(methyl methacrylate), PMMA, coated silica nanoparticles on the properties of PVAc. PVAc and PMMA are known to form a miscible blend, however, the addition of silica nanoparticles, which forms hydrogen bonds with PVAc might alter the blend morphology and therefore, the blend properties. In addition, by selectively adsorbing PMMA onto silica nanoparticles first, and then embedding them into PVAc might lead to a phase separated interface at the nanoparticle surface. The morphology and rheological properties of PVAc/PMMA/silica nanocomposites were investigated as a function of composition and silica nanoparticle surface chemistry.

This material is based upon work supported by NSF under Grant No. CMMI-1825254

Energy dissipation of elastomer nanocomposites at large strains and high strain-rates

KEITH DUSOE (Presenter), ALFRED CROSBY, Polymer Science and Engineering, UMass Amherst — Characterization of the mechanical behavior of rubbery materials at high strain rates is a nontrivial challenge. Many of the physical properties of rubbers are strain-rate dependent and therefore necessitates the understanding of the high-strain rate response of rubbery materials. Current methods to characterize the mechanical properties of rubbers typical probe the material response under low strain-rate, quasi-static conditions or dynamic conditions at low strain. A highly strained rubber undergoes free retraction when the material is suddenly released from one end. The resulting speed of the retracting material can be very fast, approaching the speed of sound in the material, and is related to the material's molecular structure, modulus and internal friction. In this work, large strain, high strain-rate mechanical response of elastomer and elastomer-matrix nanocomposite materials are investigated by free retraction of highly-stretched samples. High-speed videos of rubber retraction are acquired and analyzed to characterize the mechanical properties of these materials at high strain rate, large strains. Furthermore, the role of filler-matrix interactions in elastomer nanocomposites in minimizing viscoelastic energy losses at large strain and high strain-rates are considered.

Nanoparticle Diffusion in Athermal And Attractive Entangled Polymer Melts

ERIC BAILEY (Presenter),
RUSSELL JOHN COMPOSTO, KAREN WINEY, Materials Science and Engineering, University of Pennsylvania — Understanding the mechanisms by which nanoparticles (NPs) diffuse in a polymer melt remains an experimental challenge. In this study, we combine Rutherford backscattering spectrometry (RBS) and X-ray photon correlation spectroscopy (XPCS) to probe the diffusion of (i) enthalpically attractive silica (SiO2) NPs in poly(2-vinyl pyridine) melts and (ii) athermal phenyl-capped SiO2 NPs in polystyrene melts. In both systems, RBS shows NP diffusion in reasonable agreement with recent theoretical predictions where the athermal NPs diffuse faster than the attractive NPs. XPCS show quantitative agreement with RBS in weakly entangled polymer melts but in well-entangled polymers, XPCS shows unexpected hyperdiffusive behavior that is not observed in RBS. Our direct comparison of these techniques probes NP diffusion between ~30 and 800 nm, isolates the effect of NP-polymer interaction, and highlights the different sensitivities and observations of these experimental methods.

The Study of Mechanical Property of Block Copolymer Composites Tuned by Nanoscale Polymeric Morphology and Nanoparticles

JUNPYO KWON (Presenter), ROBERT OLIVER RITCHIE, TING XU, University of California, Berkeley — The Understanding of structure-property relationships in block copolymer nanocomposites is one of the main challenges. Especially, the study of mechanical properties tuned by compositional and structural variables is significant to the applications of the nanocomposites. Here, we focus on the fundamental analysis with regard to the mechanical properties changed by the block copolymer morphologies, the volume fractions of nanoparticles and the strength of interactions between the polymeric matrix and fillers. In addition, we studied thermal annealing effects on the nanoscale structural rearrangements which link to the mechanical behavior changes.

This work was supported by the Jane Lewis Fellowship and the Department of Energy, under Contract DE-AC02-05CH11231 through the “Organic–Inorganic Nanocomposites” program at Lawrence Berkeley National Laboratory.
L70.00041: Elucidating Synthetic Pathways in the Synthesis of Block Copolymer Self-Assembly Derived Mesostructured Nitrides with in situ Multimodal Synchrotron Characterization  PETER BEAUCAGE (Presenter), FRANCIS J DI SALVO, SOL MICHAEL GRUNER, ULRICH WIESNER, Cornell University — Block copolymer-inorganic hybrid co-assembly has recently emerged as a scalable, tunable route to crystallographically ordered, mesoporous, highly crystalline inorganics relevant to catalysis, energy conversion and storage, and other areas. The successful synthesis of these materials, however, often relies on heavily tuned thermal processing in order to crystallize a functional inorganic material without crystal growth-induced mesostructure collapse. For example, in our recent efforts to produce gyroidal niobium nitride (NbN) superconductors, a two-step thermal treatment process was needed with temperature sensitivity ca. ± 1%. To enable the rapid discovery and optimization of these synthesis routes, we developed an in situ apparatus capable of measuring small- and wide-angle x-ray scattering (SAXS/WAXS) during annealing at temperatures up to 1200°C in reactive gases. In a first application, we have explored the transformation pathways from block copolymer-oxide nanocomposite to nitride, resulting in the first synthesis of a mesostructured nitride from a Pluronics ABA block copolymer. We expect that this system will enable the rapid screening of a variety of block copolymer-derived oxide, nitride, and carbide materials with applications in catalysis, energy, and beyond.

L70.00042: Probing the Morphology of Hydrocarbon-Based Anion-Exchange Membranes via Scattering and Computational Methods*  ERIC SCHIBLI (Presenter), BARBARA J FRISKEN, Department of Physics, Simon Fraser University, STEVEN HOLDCROFT, Department of Chemistry, Simon Fraser University — While perfluorinated polymers dominate the commercial fuel cell industry, hostility to catalysts, difficult and expensive synthetic routes, and challenging disposal hamper wide adoption of fuel cell technology and impede further development. Hydrocarbon-based membranes utilize simple, well-developed synthetic routes that allow for rapid material development. We have investigated a promising series of methylated (benz)imidazole-based ionenes utilizing a combination of lab-scale X-ray scattering and molecular dynamics simulations, based on the united-atom DREIDING model with targeted optimizations to quickly elucidate the morphology of these materials. Derived structure-property relationships may motivate further material development.

*Financial support for this study was provided by Natural Sciences and Engineering Research Council of Canada (NSERC). Research described in this work made use of the 4D LABS shared facilities at SFU supported by the Canada Foundation for Innovation (CFI), British Columbia Knowledge Development Fund (BCKDF), Western Economic Diversification Canada (WD), and Simon Fraser University (SFU). This research was enabled in part by support provided by WestGrid and Compute Canada/Calcul Canada.

L70.00043: Investigation of microdomain deformation of thermoplastic elastomer based on in situ synchrotron radiation X-ray scattering  NATTANEE DECHNARONG (Presenter), Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, KAZUTAKA KAMITANI, Institute for Materials Chemistry and Engineering, Kyushu University, CHAO-HUNG CHENG, SHIORI MASUDA, SHUHEI NOZAKI, CHIGUSA NAGANO, Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, NOBUHISA TAKAYAMA, Institute for Materials Chemistry and Engineering, Kyushu University, KEN KOJIO, ATSUSHI TAKAHARA, Kyushu University — Microphase separation occurs in polystyrene (PS)-b-poly(ethylene-co-butylene)-b-PS (SEBS), leading PS domains to serve as physical crosslinking points. To investigate behaviors of PS domains, well-ordered SEBS films with low PS content were measured during uniaxial, biaxial and compression testing using in situ SAXS in SPring-8, Japan. After annealing, characteristics of spherical microdomain of PS packed in body-centered cubic lattice were observed in structure and form factors. During uniaxial testing, a shift of structure factor reveals an increase in domain spacing in parallel to stretching direction (SD) while it decreased in the perpendicular to SD. Furthermore, the shift of form factor implies to the deformation of PS spherical domains to egg-like ellipsoidal shape. For biaxial testing, a shift of structure factor indicates an increase in domain spacing as strain increased. In compression testing, the experiment was observed from the edge of sample. It was found that structure factor indicates a decrease in domain spacing in the parallel to compressing direction (CD) while it increased in the perpendicular to CD. The results of form factor observed in biaxial and compression testing suggest the deformation of PS domain, which the sphere became asymmetry in three dimension.
**L70.00044: Quantification of Nanocomposite Dispersion for Weakly Correlated Systems**

ALEX MCGLASSON (Presenter), GREG BEAUCAUGE, MICHAEL CHAUBY, KABIR RISHI, University of Cincinnati, VIKRAM K KUPPA, University of Dayton Research Institute — Nanocomposites such as carbon black dispersions in elastomers can be described by a mean-field approach and the RPA equation. [1,2] However, dispersion of nanoparticles influenced by surface potentials or entropic and steric interactions, such as for surface-grafted nanoparticles, often cannot be described using the mean-field approach since the particles are weakly organized. For these cases it is necessary to consider a discrete correlation function and an associated structure factor in scattering. Recently Oberdisse and Genix [3] have developed an approach to model scattering from nanocomposites of precipitated silica in elastomers. In this talk an approach similar to Oberdisse is used but with a simpler structure factor based on the Born-Green approach of Guinier and Fournet. [4] The result is a simple parameterization of correlations that can be used to determine the second virial coefficient for direct comparison with uncorrelated systems such as fumed silica or carbon black in elastomers.


*NSF grants CMMI-1635865 and CMMI-1636036.

**L70.00045: Electrospun fiber deposition using the gap method alters fiber moduli**

CHRISTINE HELMS (Presenter), MIMI TRAN, GARRETT LANG, NICOLE BIALICK, University of Richmond — Applications of electrospun nanofibers often require precise mechanical properties and fiber deposition. One common way to control fiber deposition is to use parallel collectors separated by a gap (gap method). In this work, we investigate the effect of gap method deposition on fiber modulus.

We formed electrospun fibers using collectors spaced at various gaps ranging from 2 cm to 10 cm and fiber moduli were measured by AFM using 3-point bending.

The gap between the collector plates had an inverse relationship with the diameter of the fibers; larger gaps produced smaller fibers. In agreement with previous data, the small fibers created by the larger gap distance had higher average moduli (67 +/- 9 GPa for a 10 cm gap) than larger fibers (10 +/- 2 GPa for a 4 cm gap). Therefore, fiber deposition directly influenced individual fiber moduli. Additionally, when we compared fibers of similar diameter we found larger gap distances produces fibers with higher moduli independent of fiber diameter. Fibers with diameters between 150 nm and 250 nm had an average modulus of 18 +/- 3 GPa for an 8 cm gap and 12 +/- 2 GPa for a 4 cm gap. Preliminary data using polarized-FTIR suggest molecular alignment is increased by the gap method.

*This research was supported by the Jeffress Memorial Trust.

**L70.00046: Evolution of CTAB/NaSal Micelles: Structural Analysis by SANS**

CHRISTOPHER LAM (Presenter), WEI-REN CHEN, CHANGWOO DO, Oak Ridge National Laboratory — Surfactants self-assemble into micelles in aqueous solution and exhibit structural polymorphism. Under certain conditions, long and flexible structures referred to as wormlike micelles (WLMs) can develop and entangle to form a transient network, leading to spectacular viscoelastic properties. The salt concentration—in particular, the molar ratio of salt (Cs) to surfactant (Cd), Cs/Cd—has been shown to have a significant influence on the viscoelastic properties of WLMs. Salicylate (Sal-) has a strong affinity for the cationic surfactant cetyltrimethylammonium bromide (CTAB) and can promote the growth of WLMs even at very dilute surfactant concentration. We investigate the structure of CTAB/NaSal micelles at relatively low concentration over a wide range of Cs/Cd. Using small-angle neutron scattering and the most advanced scattering function for WLMs, we characterize the development and structural evolution of wormlike micelles both qualitatively and quantitatively, culminating in an understanding of the phase behavior of CTAB/NaSal within this region of phase space.

*The research at the Spallation Neutron Source of Oak Ridge National Laboratory was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.
decorated with a lower frequency component. We will discuss possible mechanistic causes for these distinct patterns.

In the thinnest films (10 nm ~ 50 nm) the high wavenumber mode is throughout the bulk of the pattern. In intermediate thickness films (50 nm ~ 600 nm), the bulk wave mode cascades into wrinkle pattern in three different thickness regimes: In the thickest films (600 nm ~ 1 μm) a single wave number is seen of the floating film. When a large range of film thickness is used (10 nm to 1 μm) we observe a qualitative change in the previously studied, this wrinkle pattern is generated by the capillary force exerted by a water droplet placed at the center polymer (PS, PMMA, and Cytop™ (poly(perfluoro(1-butenyl vinyl ether)) films, floating on an air-water interface. As

MENON, THOMAS RUSSELL, University of Massachusetts Amherst — We investigated capillary force induced wrinkling of MENON, THOMAS RUSSELL, University of Massachusetts Amherst — We investigated capillary force induced wrinkling of polymer (PS, PMMA, and Cytop™ (poly(perfluoro(1-butenyl vinyl ether)) films, floating on an air-water interface. As

neutron scattering. It is demonstrated that structural screening, and the associated virial coefficient, has an increasing impact on scattering with increasing surfactant concentration. A linear relationship between the second virial coefficient, $A_2$, and the salt to surfactant ratio, $\Theta_{s-s}$, is derived based on SANS results. The $\Theta_{s-s}$-dependency is described via association/dissociation kinetics of salt ions between the bulk and an ion cloud surrounding the WLMs. An ion-cloud model for the high ionic strength condition is proposed and verified based on this work. It is also demonstrated that a virial approach can be used to understand and predict WLM stability.


*P&G

L70.00048: Classes of radial wrinkle patterns in capillary wrinkling* JOOYOUNG CHANG (Presenter), NARAYANAN MENON, THOMAS RUSSELL, University of Massachusetts Amherst — We investigated capillary force induced wrinkling of polymer (PS, PMMA, and Cytop™ (poly(perfluoro(1-butenyl vinyl ether)) films, floating on an air-water interface. As

previously studied, this wrinkle pattern is generated by the capillary force exerted by a water droplet placed at the center of the floating film. When a large range of film thickness is used (10 nm to 1 μm) we observe a qualitative change in the wrinkle pattern in three different thickness regimes: In the thickest films (600 nm ~ 1 μm) a single wave number is seen throughout the bulk of the pattern. In intermediate thickness films (50 nm ~ 600 nm), the bulk wave mode cascades into higher wavenumber close to the contact line. In the thinnest films (10 nm ~ 50 nm) the high wavenumber mode is decorated with a lower frequency component. We will discuss possible mechanistic causes for these distinct patterns.

*W.M. Keck Foundation

L70.00049: Influence of Side Chain Isomerism on the Conformation of Poly(3-alkylthiophenes) in Solutions Revealed by Neutron Scattering* KUNLUN HONG (Presenter), YANGYANG WANG, CHANGWOO DO, CHRISTOPHER LAM, WEI-REN CHEN, Oak Ridge National Laboratory — Using small angle neutron scattering, we conducted a detailed structural study of poly(3-alkylthiophenes) dispersed in deuterated dichlorobenzene. The focus was placed on addressing the influence of spatial arrangement of constituent atoms of side chain on backbone conformation. We demonstrate that by impeding the π - π interactions, the branch point in side chain promotes torsional motion between backbone units and results in greater chain flexibility. Our findings highlight the key role of topological isomerism in determining the molecular rigidity and are relevant to the current debate about the condition necessary for optimizing the electronic properties of conducting polymers via side chain engineering.

*The research at Oak Ridge National Laboratory was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences. The work conducted at the Spallation Neutron Source of Oak Ridge National Laboratory was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy. Work was also performed at the Center for Nanophase Materials Sciences of Oak Ridge National Laboratory, which is a DOE Office of Science User Facility.

L70.00050: Relaxation behavior of biodegradable aliphatic-aromatic block copolymers as revealed by dielectric spectroscopy I. IRSKA, Institute of Material Science and Engineering, ZUT Szczecin, Poland, A. LINARES, A. NOGALES, IEM-CSIC, Serrano 121, Madrid 28006, Spain, E. PIESOWICZ, S. PASZKIEWICZ, Z. ROSLANIEC, Institute of Material Science and Engineering, ZUT Szczecin, Poland, TIBERIO EZQUERRA (Presenter), IEM-CSIC, Serrano 121, Madrid 28006, Spain — Thermoplastic elastomers are copolymers composed of a hard block, typically a polyester, and a soft block, typically a polyether. Most commercially available poly(ether-ester) thermoplastic elastomers are produced based on petrochemical monomers. The increasing necessity of eco-friendly polymers has driven the interest for the production of thermoplastic elastomers fully or partially based on monomers from renewable sources. Poly(lactic acid) (PLA) is a biodegradable aliphatic polymer which can be obtained from natural products. Here we present dielectric relaxation results of a series of thermoplastic elastomers based on poly(tetramethylene oxide), as soft segment, and on a multiblock of poly(buthylene terephthalate) (PB) and poly(lactic acid) (PLA) as hard segment. The results indicate the existence of a single alpha relaxation, associated to the segmental motions above the glass transition temperature, regardless of the PB/PLA ratio of the hard segment pointing towards an absence of phase segregation between the two blocks within the hard segment. In addition, different local dynamic processes are revealed below the glass transition temperature contributing to a multimodal beta relaxation that can be assigned to different bonds of both hard and soft blocks.
**L70.00051: Polymer Dynamics in Poly(styrene-isoprene-2,vinylpyridine) miktoarm terpolymers**

THOMAS KINSEY (Presenter), EMMANUEL MAPESA, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, KUNLUN HONG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JOSHUA SANGORO, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — In this study we employ broadband dielectric spectroscopy to probe the motion of several poly(styrene-isoprene-2,vinylpyridine) (PS-PI-P2VP, respectively) miktoarm star terpolymers with constant “PS” and “PI” block molecular weights, and we vary the molecular weight of the “P2VP” block. A strong but significantly faster secondary, dipolar relaxation is observed over wide temperature and frequency ranges for the terpolymers compared to homopolymers. This process is attributed to local dynamics of the “P2VP” heterocyclic segments. Additionally, to probe the end-to-end dipole vector timescales of the Type-A polymer chains in the “PI” block, lithium salts were added to suppress the β-process of the “P2VP” block due to coordination of the nitrogen in the heterocycle with the Li+ cation. These data for the “PI” chain relaxation are compared the dynamics of poly(isoprene) in phase separated linear diblock and homopolymer systems. We show that this unique miktoarm star architecture greatly affects the dynamics in these polymers, and discuss the results in terms of polymer dynamics in well-studied phase separated systems.

*The authors acknowledge financial support through the National Science Foundation, Division of Chemistry through grant CHE-1753282.

**L70.00052: Low frequency complex dielectric response of dilute clay suspensions**

LING FENG (Presenter), CHANG-YU HOU, NIKITA SELEZNEV, DENISE FREED, Schlumberger-Doll Res Ctr — In this work, we measured the low-frequency complex dielectric dispersion of dilute clay suspensions using a four-point impedance measurement, which can be reliably calibrated in the frequency range between 0.1 Hz and 10 kHz. Complex dielectric spectra of smectite and illite suspensions in brine with different weight fractions were obtained. The brine salinities ranged from 100 to 3000 ppm. We fit our results to an effective medium model incorporating the dielectric response of a charged oblate spheroid immersed in an electrolyte. We found reasonable agreement between our measurements and the model; they both exhibited the same trends when the brine salinities and weight fractions of the clays were varied. When the clay grains have a narrow size distribution, we expect that the dispersion of the complex conductivity phase exhibits a near-resonance peak associated with the size of the particles. In our case, because the clay grains have a broad size distribution, the phase peak is broadened. The parameters obtained from the fit agree reasonably well with independently measured quantities, including the size distribution and cation exchange capacity of the clays.

**L70.00053: Entanglement Effect on Mechanical Properties in Ultra-thin Glassy Polymer Films**

CYNTHIA BUKOWSKI (Presenter), REED BAY, ALFRED CROSBY, University of Massachusetts Amherst — Entanglement density can influence the large strain and failure responses of ultra-thin glassy polymer films. For model films of high molecular weight polystyrene (PS), recent results show severe embrittlement as film thickness decreases below the average size of an unconfined chain. The hypothesized cause for this effect is the loss of interchain entanglements as polymers statistically interact with themselves more than neighbors in dimensionally-confined geometries. Introducing polymer chains shorter than the entanglement molecular weight can also lower the entanglement density, effectively swelling the entanglement network. Here, we blend short (10 kDa) and long (151.5 kDa) PS chains and measure the changes in mechanical properties using the recently developed TUTTUT (The Uniaxial Tensile Tester for Ultra-Thin films). We measure the complete uniaxial stress-strain response of 100 nm PS films as a function of blend concentration. We observe a decrease in yield stress and strain with increasing diluent concentration. Above a critical diluent concentration, the entanglement density reaches a limit where films are too brittle to manipulate. These results establish the framework of how entanglement density affects mechanical properties of ultra-thin polymer films.

*NSF DMR-1608614*
L70.00054: Effect of Topological Constraints on the Glass Transition Behaviors of Polyrotaxanes* KAZUAKI KATO (Presenter), AKIHIRO OHARA, HIDEAKI YOKOYAMA, KOHZO ITO, Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo — We report here peculiar glass transition behaviors attributed to the topological interactions between two different components of a mechanically interlocked polymer. A new class of polymer glasses were recently materialized from polyrotaxanes, which are necklace-like supramolecules composed of a linear polymer and threaded cyclic molecules. Some of the glasses were ductile and extensible to more than four-folds in length because of the slipping of threading chains through the rings in the region where the stress is concentrated. The unique structural change forced by large deformation seems to relate to the molecular dynamics. In the glass transition regime, the relaxation mode is almost an Arrhenius dependence on temperature, suggesting negligible cooperativity of molecular motions. In addition, a new viscoelastic relaxation at slightly slower than the glass transition regime is generated, when the number of rings in a single threaded chain (so-called “coverage”) is increased. The slower relaxation is significantly prolonged by the increase in coverage. It suggests that the increased topological constraints between different components restrict the translational motions of the rings dragging the threading chain.

*This work was supported by a JSPS KAKENHI Grant (16H06050).

L70.00055: Alternation of thin film morphology with monomer modifications QIMING HE (Presenter), DEAN MASTROPIETRO, WEI CHEN, MATTHEW TIRRELL, University of Chicago — The morphologies of a group of well-defined fluorine-containing copolymers, poly(methyl methacrylate)-b-poly(perfluoroalkyl methacrylate) (PMMA-b-PFMA) with chemical compositions on silicon substrates have been investigated. Thin polymer coatings were prepared on silicon substrates by spin coating from polymer solutions of varying composition and suspended in varying solvents and characterized using atomic force microscopy (AFM) tapping mode height and phase traces. By varying the chemical compositions slightly in the copolymers, alternation of morphologies can be achieved, which provides a unique way to engineer the polymeric coatings on substrates with varying mechanical and surface properties.

L70.00056: Self-assembled Copolymer Adsorption Layer-Induced Block Copolymer Nanostructures in Thin Films DONG HYUP KIM (Presenter), SO YOUN Y KIM, Ulsan National Institute of Science and Technology — Generally, a very thin adsorption layer originated from the irreversible chain adsorption on solid substrates exists in polymer thin films, which often governs the macroscopic property of the polymer films. Thus, even in microphase separated block copolymer (BCP) films, an adsorption layer can be present playing a critical role in BCP self-assembly. However, understanding on the adsorption layer in BCP films has not yet been elaborated, and therefore its effective control has not been discussed. Herein, we employ self-assembled copolymer adsorption layers (SCALs), transferred from the self-assembly of BCPs at the air/water interface, as an effective way to control adsorption layers in BCP thin films. SCALs are irreversibly adsorbed onto substrates and can replace the natural adsorption layer when other BCP is additionally coated. We further show that SCALs can guide the film nanostructures as it provides topological restrictions and enthalpic/entropic preferences for additionally coated BCP self-assembly. Thus various novel nanostructures of SCAL-induced self-assembly are introduced such as arrays of spacing-controlled hole/dot pattern, dotted-line pattern, dash-line pattern, anisotropic cluster pattern, and etc.

L70.00057: Morphological Evolution of Poly(solketal methacrylate)-block-polystyrene in Thin Films* DUK MAN YU (Presenter), University of Massachusetts Amherst, DARREN SMITH, Univ. at Buffalo, The State Univ. of New York, HYEYOUNG KIM, University of Massachusetts Amherst, JOSE KENNETH D. MAPAS, JAVID RZAYEV, Univ. at Buffalo, The State Univ. of New York, THOMAS RUSSELL, University of Massachusetts Amherst — The morphological evolution of the lamellar microdomains for the thin films of symmetric poly(solketal methacrylate-b-styrene) (PSM-b-PS) copolymers that can be converted into poly(glycerol mono-methacrylate-b-styrene) (PGM-b-PS) copolymers by the hydrolysis reaction was investigated. This simple hydrolysis was performed in the solid state using an acid vapor and markedly improves the segmental interaction parameter (χ) from 0.035 to 0.438 at 25 °C. For the perpendicular orientation of the lamellar microdomains, the hydroxyl-terminated random copolymer (PSM-r-PS) with χ_{PSM} = 0.5 was used to tune the interfacial interactions at the substrate as a neutral and it can also be transformed into PGM-r-PS with the block copolymers. Scanning force microscope (SFM) and grazing-incidence small angle X-ray scattering (GISAXS) measurements as a function of the exposure time to an acid vapor were conducted to characterize the transition from the disordered state as well as the perpendicular orientation and features of the lamellar microdomains. As a result, sub-10 nm full pitch lamellar patterns in the thin films were achieved after full conversion and thermal annealing.

*This work was supported by the Air Force Office of Scientific Research under contract 16RT1602.
Highly Ordered, Complex Morphologies in Block Copolymer Films Obtained by Spatial Confinement Using Topographical Substrates

ELISHEVA MICHAM, Institute of Chemistry, The Hebrew University of Jerusalem, ROLAND STENGER, MARCEL LANGENBERG, MARCUS MUELLER, Institute for Theoretical Physics, Georg-August-University Göttingen, ROY SHENHAR (Presenter), Institute of Chemistry, The Hebrew University of Jerusalem — Block copolymers microphase separate into periodic arrays of nanostructures. Thin films of these self-assembled BCPs are finding increasing use as platforms for nanofabrication, either as lithography masks or as templates for the patterning of nanowires and particles. Directed self-assembly, using a chemical or topographical pre-pattern, increases the long range order of BCP thin films and can be used to introduce diversity to the BCP morphology. However, the ability to pattern BCPs in a variety of morphologies in close confinement usually requires multiple fabrication steps and is limited in scope.

We present a simple, one-step process for obtaining complex, highly ordered morphologies in ultra-confined films in a controlled fashion. Our approach utilizes topographically patterned silicon substrates to guide the assembly of block copolymer domains. Remarkably, different local morphologies of the block copolymer are observed on the plateaus and inside the trenches. This behavior is explained in terms of the variation in the local film thickness and the selectivity of the substrate towards one of the copolymer domains.

*EM thanks the Cambr Charitable Foundation for financial support. This research was supported by an Israel Science Foundation, grant number 229/17.

Quasi-Two-Dimensional Assembly of Bottlebrush Block Copolymers with Nanoparticles in Ultrathin Films: Combined Effect of Graft Asymmetry and Nanoparticle Size

YARON AVIV, Institute of Chemistry, The Hebrew University of Jerusalem, ESRA ALTAY ESRAALTA@BUFFALO.EDU, Department of Chemistry, University at Buffalo, LEA FINK, URI RAVIV, Institute of Chemistry, The Hebrew University of Jerusalem, JAVID RZAYEV, Department of Chemistry, University at Buffalo, ROY SHENHAR (Presenter), Institute of Chemistry, The Hebrew University of Jerusalem — Block copolymer guided assembly of nanoparticles leads to the formation of nanocomposites with periodic arrangement of nanoparticles, which are important for applications, such as photonic devices and sensors. However, linear block copolymers offer limited control over the internal arrangement of nanoparticles inside their hosting domains. In contrast, bottlebrush block copolymers possess unique architectural attributes that enable additional ways to control the local organization of nanoparticles. In this work, we studied the co-assembly of 8 and 13 nm gold nanoparticles with three bottlebrush block copolymers differing in the asymmetry of their graft lengths in ultra-confined films, where assembly occurs quasi-two-dimensionally. Our results indicate that graft asymmetry could be used as an additional tool to enhance nanoparticle ordering by forcing them to localize at the center of the domain regardless of their size. This behavior is analyzed in terms of the influence of the graft asymmetry on the average conformations of the blocks.

*Financial support for this work was provided by the National Science Foundation (DMR-1409467).

Kinetic Pathway Dependent Supramolecular Nanocomposite Assembly on Patterned Substrates

KATHERINE EVANS (Presenter), TING XU, University of California, Berkeley — Block copolymer (BCP)-based supramolecular nanocomposites are promising materials to create hierarchically structured materials and incorporate and organize nanoparticles (NPs). Assembling these materials on lithographically patterned substrates combines the advantages of “bottom-up” and “top-down” assembly to yield materials where the exact ordering and placement of NPs can be controlled. However, for traditional BCP self-assembly on patterned substrates, the width of the underlying pattern must be commensurate with the periodicity of the BCP due to thermodynamic constraints. Here, supramolecular nanocomposites are assembled onto several different geometrically patterned substrates, including lines and concentric circles. On these patterns, incommensurability between the pattern and the supramolecule periodicity was not observed. Instead, the supramolecule self-adjusts to a smaller, non-equilibrium periodicity in the trench. This phenomenon is attributed to the kinetic pathway taken during assembly.
L70.00061: Protein-Polymer Block Copolymer Thin Films for Detection of Small Proteins in Biological Matrices via Size-Exclusion*  

JUSTIN PALONI (Presenter), BRADLEY DAVID OLSEN, Massachusetts Institute of Technology — While biosensors have been developed to allow sensitive detection of biomolecules, limit of detection (LOD) is often increased by several orders of magnitude in biological matrices due to nonspecific binding events from off-target molecules. Here, we demonstrate the self-assembly of protein-polymer conjugate thin films into lamellar structures containing alternating domains of proteins and polymer meshes that can exclude molecules based on particle size. By comparing the diffusion of two analytes, streptavidin (52.8 kDa) and monomeric streptavidin (15.6 kDa), it is found that the larger protein streptavidin experiences greater resistance to diffusion into the films and is largely excluded from the film structure. Furthermore, by decreasing the polymer molecular weight and therefore the spacing of the polymer nanodomains, the thin films can be tuned to enhance selectivity for smaller molecules. When compared against a traditional surface-immobilized protein biosensor, the conjugate films achieve a two order of magnitude reduction in LOD when detecting monomeric streptavidin, resulting from both the greater density of binding sites within the thin films as well as the size-based exclusion of larger proteins.

*This work was funded by the NSF.

L70.00062: Interfacial Interaction Effects on Phase Transition Behavior of Block Copolymer Thin Films  
YEONGSIK KIM (Presenter), Yonsei University, DAESEONG YONG, Ulsan National Institute of Science and Technology, HYUNGJU AHN, Pohang University of Science and Technology, JAEUP KIM, Ulsan National Institute of Science and Technology, DU YEOL RYU, Yonsei University — Confined in a film geometry, the preferential interaction of the polymer/air and polymer/substrate interfaces generates cylindrical and lamellar microdomains oriented parallel to the substrate. We presented the thickness dependent phase diagram of BCP films using ex-situ grazing incidence small-angle x-ray scattering (GISAXS) and transmission electron microscopy (TEM). With decreasing film thickness (t) when t < t₀, where t₀ is an onset thickness above which the ODT temperatures (T_ODTs) of the films are independent of film thickness, the T_ODTs of cylinder- and lamella-forming polystyrene-b-poly(2-vinylpyridine) (PS-b-P2VP) films supported on preferential substrates remarkably increase. Consistent between cylinder- and lamella-forming PS-b-P2VP films, this effect is so intense in very thin BCP films.

L70.00063: Top Coats: Control of Orientation, Alignment and Morphologies of Sub-10 nm Block Copolymer Microdomains  
EUNJIN KIM, EUNKYOUNG YOON, IN HYU RYU, JINWOO OH, JEONG GON SON (Presenter), Photo-electronic Hybrids Research Center, Korea Institute of Science and Technology — Achieving sub-10 nm high-aspect-ratio patterns from diblock copolymer self-assembly requires both a high interaction parameter (χ, determined by the incompatibility between the two blocks) and a perpendicular orientation of microdomains. However, these two conditions are extremely difficult to achieve simultaneously because the blocks in a high-χ copolymer typically have very different surface energies, favoring in-plane microdomain orientations. We introduce top coat for the control of orientation, alignment and morphology of a high-χ block copolymer, poly(styrene-block-dimethylsiloxane) (PS-b-PDMS). Using partially hydrolyzed PVA top coats with a solvent annealing, perpendicular orientation of PS-b-PDMS can be obtained despite the large surface energy differences between PS and PDMS. Extremely straight and laterally aligned cylindrical microdomain of BCP films were prepared by simply covering the BCP films with a top coat and dewetting the latter via thermal annealing to generate shear flow in the BCP underlayer. We also observed the gyroid-cylinder phase transition using interfacial-energy-tailored top-coat. At the optimized top-coat composition, gyroid nanostructures with sub-10 nm strut width were achieved down to ~125 nm.
Thin Films of Block Copolymer-Based Supramolecules with Feature Size Over 50 nm

KATHERINE EVANS, EMMA VARGO (Presenter), TING XU, University of California, Berkeley — Block copolymer-based supramolecular self-assembly offers a simple method to overcome issues with incommensurability, surface chemistry, and assembly kinetics to access nanostructures in thin films. Much work has been focused on creating nanostructures with periodicities between 10-50 nm. However, for some applications, including the interaction with visible light, larger periodicity features are necessary. Creating thin films with feature sizes larger than 100 nm is challenging. Large MW nanocomposites have differing kinetic and thermodynamic considerations when compared to the low MW analogs. Thermodynamically, incorporation of particles does not have the same entropic penalty when the polymer chain length increases. Kinetically, the diffusions of nanoparticle and supramolecule may play a more critical role in determining the NP placement and NP packing within supramolecular microdomains. Here, we demonstrate that nanocomposites with controllable morphology can be created with a periodicity of up to ~100 nm. The size and loading of nanoparticles, as well as the solvent annealing condition, determines the final morphology as well as the periodicity, grain size, and packing of nanoparticles.

*This work is funded by DOE Contract DE-AC02-05-CH11231 (Organic-Inorganic Nanocomposites KC3104).

Influence of salt additives on unconfined melt electrospinning of thermoplastics

NEELAM SHEORAN (Presenter), BRENTON BOLAND, Department of Physics, North Carolina State University, ELNAZ SHABANI, RUSSELL E GORGA, Fiber and Polymer Science Program, North Carolina State University, JASON BOCHINSKI, LAURA CLARKE, Department of Physics, North Carolina State University — Incorporation of ionic or salt additives into thermoplastic melts can effect both viscoelastic properties and ionic conductivity. Such an approach might usefully alter the process of melt electrospinning where jet diameter (and subsequent fiber size) is influenced by melt viscosity as well as ionic motion within the melt under the influence of a strong applied electric field. These changes have the potential of producing mesoscale thermoplastic nanofibers which are important for filtration and biological applications where high strength nanofibrous materials are required. We report ionic conductivity measurements obtained using broad-band impedance spectroscopy of commercial linear low-density polyethylene (ASPUN 6850A) as a function of temperature, salt type, and concentration, along with corresponding information on viscosity changes. The salt-doped melts were electrospun in an unconfined geometry; changes in jet formation time, number of jets, jet and cone widths, and the resulting fiber diameters were determined. We discuss results and current understanding of the changes in melt properties due to salt additives.

*Support from National Science Foundation CMMI-1635113

A facile route to calculate the effective volume fractions in block copolymers during solvent vapor annealing

SAEED BEHZADINASAB (Presenter), JULIE ALBERT, Chemical & Biomolecular Engineering Department, Tulane University — The nano-scale domains obtained from self-assembly of block copolymers (BCPs) have attracted significant attention. In a BCP system, solvents are oftentimes used to plasticize the polymer molecules and reduce the unfavorable interactions in between to facilitate the microphase separation. However, it is not straightforward to predict the final morphology of a BCP system due to the critical impacts of the annealing condition on the nanostructure. The effective volume fraction of each block remains constant when a neutral solvent is used, while selective solvents can significantly change this parameter and encourage the formation of a distinct morphology. To monitor morphology changes, advanced in-situ techniques, such as X-ray or neutron scattering, which are not readily accessible, are required. In this work, we present a facile route to predict the morphology of BCPs during solvent vapor annealing by simultaneous calculation of the Flory-Huggins theory coupled with mass conservation. This results in the prediction of effective volume fractions of each block, which can significantly reduce the number of required experiments in morphological studies.

*The authors are grateful for the support of this work by the National Science Foundation through NSF CAREER grant, CBET-155 45 55.
**L70.00067: Reactive Processing of 3D Printed ABS Structures Formed by Fused Deposition Modeling to Reduce Structural Anisotropy**  
KAIZHONG GUAN (Presenter), MARK DADMUN, University of Tennessee, Knoxville — Fused deposition modeling (FDM) is one of the most common additive manufacturing methods, which allows the fabrication of complex structures and customization. However, due to its layer-by-layer nature, the resultant structures exhibit anisotropic properties. A primary reason for the anisotropy is weak interactions and poor entanglement between subsequently deposited layers. Methods to increase inter-layer adhesion include post-deposition heating, which results in loss of fidelity of the fabricated shape to the target structure. To address this shortcoming, our group has modified an FDM printer to allow for the reactive processing of the interlayer interface as a part of the deposition. This is realized by adding a UV-LED optical fiber to an FDM 3D printer, which is designed to initiate a reaction at the inter-layer interface. This presentation will present results that examine the success of this novel processing scheme. Samples of ABS that include a photo-initiator and a crosslinker to form covalent bonds across the interlayer interface are printed with this modified printer, and its tensile properties and anisotropy monitored. This presentation will report the impact of the loading of photo-initiator and crosslinker on the mechanical properties of the printed sample.

**L70.00068: Droplet-Jet Shape Parameters Predict Electrospun Polymer Nanofiber Diameter**  
SUQI LIU (Presenter), D RENEKER, The University of Akron — The relationships between observable features of the droplet-jet shape and the diameter of electrospun nanofiber were studied. Three shape parameters were derived from optical images of the jet emerging from a droplet. They are: Left-Right (L-R) curvature, initial jet diameter, and transition slope. Fiber diameter increased as each shape parameter increased. The relation between initial jet diameter and fiber diameter, as well as the relation between transition slope and fiber diameter, were not affected by the variation of voltage or viscosity of the polymer solution. Ambient temperature and humidity were controlled. Day-to-day variations in other ambient conditions that might have occurred in the laboratory do not invalidate these relationships.

**L70.00069: Solvent Effects on the Crystallization Order and Morphology in PEO-b-PCL Copolymers**  
RYAN VAN HORN (Presenter), Lafayette College, COLE TOWER, NATASHA BRIGHAM, KRISTI M ALLEN, ALLISON CARANDANG, Allegheny College — Physical structure of block copolymer films plays an important role in the macroscopic properties of the material. Where applicable, crystallization is one important aspect of the physical structure. PEO-b-PCL copolymer films have two crystalline components that makes for rich hierarchical assembly. Using various solvents for film casting has allowed for the opportunity to control this hierarchical assembly. Films were made using various molecular weight samples at varying drying temperatures in an attempt to manipulate the crystallization process. The crystallization order and morphology was monitored via DSC, FTIR, and optical microscopy. It was determined that the relative solubilities of the two blocks influences the film's final structure.

*This work was supported by funding from NSF (DMR-1606532).*

**L70.00070: Morphology and crystallization kinetics of poly(ethylene brassylate)**  
DAOKUN SONG (Presenter), RUFINA G ALAMO, Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, IRMA FLORES, ALEJANDRO J MÜLLER, POLYMAT and Polymer Science and Technology Department, University of the Basque Country — Poly (ethylene tridecane dioate), also known as poly(ethylene brassylate) (PEB), is a long-spaced aliphatic polyester obtained from a renewable source. PEB in a range of molar mass between 27,000 and 188,000 Dalton crystallize rapidly as single peaks at ~55 C and display two major melting peaks (60 -70 C). The two melting peaks are associated with crystallites that differ in the packing of the crystalline ester layer. Although the WAXD patterns are undistinguishable, differences in the ester layer packing lead to the effect of self-poisoning at the growth front, and hence to a deep depression of the growth rate at temperatures approaching the transition between both forms, from above. This minimum of the rate, first described for n-alkanes, is also observed in the overall crystallization kinetics obtained by DSC, and follows a general behavior of precision polyethylenes that develop different crystalline polymorphs by changing undercooling.

**L70.00071: Tunable Liquid Crystallinity of Graphene Oxide by Polymer Crystallization**  
SOHJIN MUN (Presenter), SO YOUN KIM, Ulsan National Institute of Science and Technology — Graphene oxide (GO) can form liquid crystals (LC) in aqueous solution, which can be a valuable method for many applications using GO. One of the attractive applications is GO based polymer nanocomposites where GO can act as an effective nanofiller in semicrystalline polymer matrix. Previous studies have shown that polymer can be crystallized on GO surface and thus adding GO controls the polymer crystallinity and changes the macroscopic property of GO. However, less attention has been paid to how crystallizable polymers can conversely alter the liquid crystallinity of GO. Herein, we show that GO LC can be correlated with polymer crystallization. We found that the stability and directionality of GO LC can be affected by the rate of polymer crystallization. The microstructure and rheological property of GO LC are extensively investigated with small-angle X-ray scattering and rheometry experiments at a given temperature profile for polymer crystallization.
Controlling of Chain-Level Structure of Polymer via Freeze-Drying

TOSHIKAZU MIYOSHI (Presenter), The University of Akron — Freeze-drying (FD) method may potentially control chain-level structures of polymer with varying entanglement densities. In this work, we investigated phase structure, chain-to-chain distance, \(<R>\) and self-assembled chain structure of \(^{13}\text{C}\) labeled poly(L-Lactic Acid) (PLLA) formed via FD from both good and poor solvents, by solid-state (ss) NMR. It is found that the FD-PLLA from the good solvent adopts an amorphous state while the FD one from the poor solvent forms a semicrystalline state with a crystallinity of \(~40\%\). By comparisons of the \(^{13}\text{C},^{13}\text{C}\) Double Quantum (DQ) experimental and simulated curves, it is demonstrated that i) FD-PLLA chains from both poor and good solvents adopt the same \(<R>\) value of \(6.2\ \AA\), ii) FD-PLLA chains in the latter adopts much larger nanoclusters via folding than those in the former, and is slightly smaller than those in the single crystals. While the FD-PLLA chains obtained from good solvent exhibited similar structure with the bulk glassy state. It is concluded that different solvent-polymer affinities do not affect \(<R>\) and significantly affect self-assembly structure of individual chains.

**NSF DMR 1708999**

Liquids That Freeze When Mixed: Co-Crystallization and Liquid-Liquid Equilibrium in Polyoxacyclobutane-Water Mixtures

JOYITA BANNERJEE, PETER KORONAIOS, ERIC BECKMAN, ROBERT ENICK, JOHN KEITH, SACHIN VELANKAR (Presenter), University of Pittsburgh — We show that liquid polyoxacyclobutane –\([\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{O}]_n\)– when mixed with water at room temperature, precipitates solid co-crystals of the polymer and water. Such co-crystals are formally known as a clathrate hydrate. Hydrate co-crystals can also be formed by simply exposing the liquid polymer to saturated humidity. Outside of metal alloys, this is a rare example of an co-crystal whose melting point exceeds that of the pure species, and the only known example of non-reacting liquids that combine to form a solid co-crystal at room temperature. At high temperatures, the same polymer-water mixtures phase separate into two co-existing liquid phases. This combination of co-crystal hydrate formation and LCST-type liquid-liquid equilibrium (LLE) gives rise to an unusual, possibly unique, type of phase diagram. We examine the effects of polymer molecular weight on the phase behavior and show that at molecular weights exceeding \(~2000\) g/mol, nearly the entire composition-temperature space is split between regions of solid-liquid equilibrium and liquid-liquid equilibrium. Furthermore, this unusual phase diagram produces distinct crystallization pathways depending on whether the mixture is single-phase or two-phase prior to crystallization.

**MCSI, U. Pittsburgh**

Crystallization behavior, morphology and mechanical properties of copolymers of syndiotactic polypropylene with branched monomers

CLAUDIO DE ROSA, MIRIAM SCOTI (Presenter), FINIZIA AURIEMMA, Chemical Sciences, University of Napoli Federico II — We report a study of the structure and mechanical properties of copolymers of syndiotactic polypropylene (sPP) with different comonomers from ethylene to branched a-olefins. The effect of the presence of short or long branches on the crystallization behaviour and elastomeric properties of sPP has been analyzed. Incorporation of long branched comonomers, as 1-octadecene and 1-eicosene, allows fast decrease of the glass transition temperature and development of interesting elastomeric materials. The relationships between structure and stress-induced phase transformations and mechanical properties have been clarified. In samples with low comonomer content the elastic properties are associated with a reversible polymorphic transition that occurs upon stretching and releasing the tension, which provides an enthalpic contribution to the elasticity. Samples with higher comonomer concentrations show very low crystallinity and a typical thermoplastic elastomeric behavior. The study of the crystal morphology shows the presence of small bundles of rod-like lamellar crystals in all copolymers whose size decreases with increasing content and size of comonomeric units. The small needle-like crystals act as knots of an elastomeric lattice, explaining the development of elastic properties.

Fractionated and confined crystallization of polybutene-1 in immiscible polypropylene/polybutene-1 blends

CHENGUANG LIU (Presenter), YAO XU, HUARONG NIE, AIHUA HE, Qingdao University of Science and Technology — The crystallization of immiscible polypropylene (PP)/polybutene-1 (PB) blends, in particular the effect of crystal morphology of PP (HTC) on the subsequent crystallization behavior of PB (LTC) was studied. We firstly deemed that PP/PB blends are not complete compatibility but characterized as the LCST-like phase diagram above the melting temperature of PP. Crystallization of PP at different crystallization temperatures brought different PP crystal morphologies and PB was segregated and confined at different locations. Much larger-sized domain of PB component appeared in PP spherulites resulting from the effects of non-negligible phase separation and the slower PP crystallization rate as PP crystallized at high temperature. As temperature continued to fall below Tm of PB, the fractionated and confined crystallization of PB occurred in the framework of PP spherulites reflecting as the decreased crystallization temperature (Tc) of PB and the formation of form I beside form II. If PP previously crystallized at high Tc, fractionated crystallization of PB became prominent and confined crystallization of PB became weak due to the much wider droplet-size distribution of PB domains.

*Supported by Shandong Provincial Key R&D Program (2015GGX102019) and the Taishan Scholar Program.
L70.00076: Crystallization of trans-1,4-polyisoprene* HUARONG NIE, XIAO HAN (Presenter), AIHUA HE, HUICHENG REN, Qingdao University of Science and Technology — Isothermal crystallization of TPI from its solutions and melt were both studied to attain the kinetic parameters and polymorphic behavior. The solubility curves of TPI in solvents and the conversion temperatures between isothermal and non-isothermal crystallization were supplied to propose the available concentrations and temperatures for TPI isothermal crystallization. In most cases, the kinetics of TPI crystallization was subject to the Avrami-equation though few deviations arising from the influence of non-isothermal crystallization and transient nucleation were also observed under several special conditions. When TPI melt recrystallization was observed, β-TPI (metastable form) exhibited stronger melting memory effect than α-TPI. Irrespective of the pre-existed crystal modification, the reduced energy barrier for nucleation favored the formation of α-TPI. Furthermore, an increase in crystallinity was also observed if recrystallization occurred at low temperatures.

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L70.00077: Thermodynamic Concepts of the First-Order Prefreezing OLEKSANDR DOLYNCHUK (Presenter), MUHAMMAD TARIQ, THOMAS THURN-ALBRECHT, Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg — An interaction with a solid surface can induce crystallization in liquids by either heterogeneous nucleation or prefreezing. The latter is seen as the crystalline layer formation at an interface to a solid substrate at temperatures higher than that of a bulk crystal. Most recently, it was ascertained that prefreezing is a first-order transition, since the formation of the crystalline phase is abrupt and reversible.

We introduce a phenomenological theory of prefreezing and analyze such equilibrium properties as the temperature dependent crystal thickness, the maximum melting temperature $T_{\text{max}}$, and the mesoscopic jump of thickness during melting or crystallization. The theory enables a clear first-principles explanation of the abrupt formation of a crystalline layer, i.e., the first-order nature of prefreezing and defines the corresponding transition temperature $T_{\text{max}}$ as a function of the interfacial free energies. We show that it is the difference of the interfacial energies that controls $T_{\text{max}}$ and acts as a driving force for prefreezing. The analytical outcomes are congruent with recent experimental results for poly(epsilon-caprolactone) crystallized on graphite via prefreezing.

L70.00078: In Situ Electron Microscopy of Polyethylene Glycol Crystallizing in an Ionic Liquid SATYAM SRIVASTAVA (Presenter), ALEXANDER RIBBE, THOMAS RUSSEL, DAVID HOAGLAND, University of Massachusetts Amherst — In this study, the nonvolatile room temperature ionic liquid (IL) 1-ethyl-3-methylimidazolium ethyl sulfate ([EMIM][ETSO4]) was chosen as a suitable solvent to study the thermally induced solution crystallization and gelation of polyethylene glycol (PEG) by electron microscopy and electron diffraction. For both phenomena, key features occur at the nanoscale. PEG-IL samples were prepared as thin freestanding or supported liquid films on TEM grids, with crystallization observed upon cooling of heated films to room temperature. In free-standing films, crystals predominantly resided at the liquid surface, and in supported films, on the solid substrate, varied by use of different support films on TEM grids. Crystalline morphologies were observed in the form of rods (width <100 nm), fibers, spherulites (80-500 nm diameter), compact faceted single crystals (<100 nm), and interconnected networks. Electron diffraction patterns on the rod- and fiber-like crystals reveal single crystal order at length scales greater than one micron. Electron microscopy and electron diffraction were also performed on fiber-like PEG crystals grown from mixtures of [EMIM][ETSO4] with the less polar ethyltributylphosphonium diethyl phosphate ([P2444] [DEP]).


Tentative results on the MEM analysis for the X-ray powder diffraction data of Polymer crystal will be explained in my poster presentation.

*The synchrotron radiation experiments were performed at BL44B2 in Spring-8 with the approval of RIKEN (Proposal No. 20160041, 20170094, 20180039).
L70.00080: Gelatinization and Gelation Process of Japanese sweets -Warabi-mochi-  
AKANE NAGASAKI, GO MATSUBA  
(Presenter), Grad Sch of Organic Materials Engineering, Yamagata University — Fig. 1 Chemical structure of amylopectin.

"Warabi-mochi" is one of Japanese traditional sweets and is made from mainly starch and water (and sugar and so on). The way to make Warabi-mochi is to heat and stir the mixed suspension of starch and water then to cool down the gelatinized “mixed starch and water”. Fig.1 shows the chemical structure of starch (amylopectin). The amylopectin has a lot of branches because of both \(\alpha(1-4)\) bond and \(\alpha(1-6)\) bond. Warabi-mochi is safe for human and quite significant for our daily life such as boiling rice (making “gohan”), making noodle, baking breads and so many foods. Recently, it has been used as a supporting medicine of swallowing for preventing aspiration in aged persons. It’s well known that a texture and feel of Warabi-mochi depend on various parameters such as the contents (ratio) of starch and water, heating for time and temperature, and cooling process. However, the processes of making Warabi-mochi are unclear from the view point of molecular structure. In order to control these properties, we focus on the structural change during gelatinization and gelation processes with X-ray and viscoelastic measurements.

L70.00081: Mesoscale Simulations for Micellization of Diblock Copolymers*  
CHU-YUN HUANG (Presenter), Chemical Engineering, National Taiwan University, MING-TSUNG LEE, Chemical Engineering and Biotechnology, National Taipei University of Technology, HSIU-YU YU, Chemical Engineering, National Taiwan University — Polymeric filomicelles have been considered as drug carriers in nanomedicine for their structural stability and long circulation time in the blood flow. Literature (Geng, Y., et al., Nat. Nanotechnol. 2007) suggests that filomicelles formed by poly(ethylene oxide)-b-poly(ε-caprolactone) (PEO-PCL) copolymers have high capacity for paclitaxel (TAX) which could suppress tumor growth. We investigate the micellization of PEO-PCL copolymers using a mesoscale method called dissipative particle dynamics (DPD). Force fields are parameterized to best reproduce the equilibrium configurations of micelles. Inter-species parameters are chosen to reproduce the bulk properties of bead components. The stiffness of the bonds that connect copolymer beads is determined to satisfy the average distance of composing monomers at the same system density. The obtained equilibrium micellar morphologies are simulated in relevant blood flow conditions to characterize the corresponding dynamical response of filomicelles.

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L70.00082: Anti-biofouling polymer surfaces by a top-down approach  
ZHIXING HUANG (Presenter), DANIEL SALATTO, WEIYI LI, Stony Brook University, LEIO KOGA, Ward Melville High School, YIZHI MENG, MAYA ENDOH, TADANORI KOGA, Stony Brook University — Polymer have been used to develop alternative antifouling coatings against primary protein adsorption. Antifouling polymers have very diverse chemical, structural, and surface topological properties, but they share common physical characteristics: hydrophilic, electrically neutral, or highly hydrated, causing strong interactions with water molecules while reducing interactions with proteins. To stabilize polymer coating under various environmental conditions, chemical end-grafting of polymer chains have been utilized. However, challenges remain in developing a universal non-fouling material that contains the necessary attributes for the next generation of polymer-based anti-biofouling coating technologies. Here we report a radically new paradigm of designing a polymeric coating that is a few nanometers thick (“polymer nanocoating”) with an anti-biofouling property. The nanocoating is composed of homopolymer chains physically adsorbed onto solid surfaces. The results demonstrate that the polymer nanocoatings composed of high surface energy hydrophobic polymers exhibit an antifouling property against a model protein, bovine serum albumin (BSA), while counterpart spin-cast thin films still exhibit adsorption of the protein.

L70.00083: Knot untying in elongational fields*  
BEATRICE SOH (Presenter), ALEXANDER KLOTZ, PATRICK DOYLE, Massachusetts Institute of Technology — Knotting is a prevalent phenomenon which occurs in long polymer chains. We perform Brownian dynamics simulations and single-molecule DNA experiments to investigate knot untying in elongational fields that is induced by the knot being convected off the chain. The change in knot size as the knot moves off the chain and unties causes a change in the effective Weissenberg number, which in turn leads to a change in chain extension. Large-scale chain conformational changes are observed in both simulations and experiments for complex knots at low Weissenberg numbers (Wi). We investigate the knot untying time and untying-induced change in extension for a range of knot types and field strengths.

*This work was supported by the Agency for Science, Technology and Research (A*STAR), Singapore-MIT Alliance for Research and Technology (SMART) and National Science Foundation (NSF) grant CBET-1602406.
L70.00084: Polymer Diffusion Under Cylindrical Confinement  JAMES PRESSLY (Presenter), ROBERT RIGGLEMAN, KAREN WINEY, University of Pennsylvania — Measuring the center of mass diffusion of polymers under confinement is critical for understanding polymer dynamics in applications including semiconductor manufacturing, separation membranes, and polymer nanocomposites. Recent simulations of polymers confined to cylindrical pores reveal non-monotonic changes in the polymer diffusion coefficient, D, as the pore size decreases due to competition between increasing disentanglement and chain segregation. In this study, we use elastic recoil detection to examine the diffusion coefficients of linear polystyrene (M_w = 100-800 kg/mol) confined to cylindrical anodic aluminum oxide (AAO) nanopores (diameter, d = 10-80 nm). The experimental results are compared to the previous coarse grained molecular dynamics simulations to interpret the measured diffusion coefficient in terms of the competition between chain disentanglement and segregation.

L70.00085: Theoretical Study of Polymer-Grafted Nanoparticle Translocation*  GABRIELA T JUSTINO (Presenter), MICHAEL HORE, Case Western Reserve University — Typically, translocation -- the movement of polymers or particles from one region through a channel into another -- is studied by observing changes in ionic current through the channel as a function of time. As the particle moves through the channel, blockage of the pore results in a decrease in the current. Here, we combine self-consistent field theory (SCFT) and Poisson-Nernst-Planck (PNP) theory to investigate the translocation of both bare and polymer-grafted nanoparticles as a function of the ratio of channel diameter to nanoparticle diameter, polymer grafting density, and electric field strength by computing the expected ionic current traces that would be observed experimentally.

*This work was supported by an academic partnership between CAPES (Brazil) and Case Western Reserve University.

L70.00086: Prediction of Stable Morphology of Block Copolymers by using SCF Calculation and Deep Learning*  Takeshi Aoyagi (Presenter), Sadato Yamanaka, CD-FMat, National Institute of Advanced Industrial Science and Technology, Japan — Block copolymers show various microphase separated structure depending on the chain architecture, and miscibility (chi parameter) between different segment type. Various stable phase such as lamellar, double gyroid, hexagonal cylinder and bcc sphere are known, and phase diagram has been studied for simple block copolymers by SCF calculation. However, it is not simple to find equilibrated morphologies even by the calculation, because many metastable morphologies are obtained. Usually, it takes large computational resource to obtain stable structure from many possible metastable structures by real space SCF calculation. We applied 3D CNN deep learning technique to predict stable morphology from metastable morphology obtained from the SCF calculation without initial constraint. Metastable morphology of diblock copolymer and stable morphologies derived from well-known phase diagram are used for training sample. The optimized deep learning network can predict stable morphology of diblock copolymers of arbitral volume fraction and chi parameter.

*This work was supported by JSPS Grant-in-Aid for Scientific Research on Innovative Areas "Discrete Geometric Analysis for Materials Design": Grant Number 17H06464

L70.00087: Evaluation of Accelerated Aging of Cross-Linked Polyethylene Pipes by Applying Machine Learning Concepts to Infrared Spectra  Melanie Hiles, Michael Grossutti, John Dutcher (Presenter), University of Guelph — Cross-linked polyethylene (PEX) pipes are emerging as promising replacements for traditional metal or concrete pipes used for water, gas and sewage transport. Infrared (IR) spectroscopy is well suited to the characterization of PEX pipes and additives that are used to achieve long term stability. We have developed a methodology based on IR absorbance peaks to track crystallinity, degree of degradation and the presence of stabilizing additives across the wall thickness of PEX pipes. We observed that, in response to accelerated aging protocols such as heating and UV exposure, the intensities of many IR peaks corresponding to functional groups of both polyethylene and the stabilizing additives are interdependent and highly correlated. We have used principal component analysis to identify and track the IR peaks that are most relevant to pipe degradation. We used these results, together with machine learning techniques such as support vector machines and cluster analysis, to identify and classify different modes of degradation. Our approach highlights the advantages of using machine learning techniques to understand the effects of accelerated aging of PEX pipes, which can be used to refine the pipe manufacturing process to maximize pipe durability.
L70.00088: Mobile Doubly Grafted Polymers and their Interaction  MIN CHU, DIETER HEERMANN (Presenter), Heidelberg University — Doubly grafted polymers can, for example, be found in viral membrane proteins. The interaction between doubly grafted polymers, essentially ring polymers, on a two-dimensional substrate differs from the singly grafted polymer due to the entropic repulsion. What does this entail as the grafting density increases and what are the consequences for the viral membrane proteins? We study various quantities of interest such as the order parameter, density profiles etc. varying the maximal distance between the anchor points in the range \([d_{\text{min}},d_{\text{max}}]\) (otherwise the anchor points are mobile), the chain length and the grafting density. We show that there is no phase transition from the disordered (isotropic) phase to an ordered (nematic) phase. However, due to the interaction of loops, i.e. the entropic repulsion, an increasing tendency for locally orientational order without long range order is observed. As the grafting density is increased, the transition from the mushroom regime to an almost upright conformations is observed.

L70.00089: Non-monotonicity in the knotting probability of semiflexible rings: numerical and analytical prediction  ERICA UEHARA, Physics, Ochanonizu University, Tokyo, LUCIA CORONEL (Presenter), CRISTIAN MICHELETTI, International School for Advanced Studies, TETSUO DEGUCHI, Physics, Ochanonizu University, Tokyo — Polymers in canonical equilibrium are prone to become knotted, and the knotting probability for a specific type of knot depends on several conditions, among these we found interesting to study on the effect of bending rigidity of self-avoiding polymers. We use a simple physical mapping to adapt the known asymptotic expressions for the knotting probabilities of self-avoiding polygons to the case of semiflexible rings of beads. We thus obtain analytical expressions that approximate the abundance of the simplest knots as a function of the length and bending rigidity of the rings. We validate the predictions against previously published data from stochastic simulations of rings of beads showing that they reproduce the intriguing non-monotonic dependence of knotting probability on bending rigidity. The mapping thus provides a useful theoretical tool not only for a physically-transparent interpretation of previous results, but especially to predict the rigidity-dependent knotting probabilities for previously unexplored combinations of chain lengths and bending rigidities. In particular, our mapping suggests that for rings longer than 20,000 beads, the rigidity-dependent knotting probability prole switches from unimodal to bimodal.

L70.00090: Dynamics of Biodegradation*  RYAN SAYKO (Presenter), ZILU WANG, MATTHEW BECKER, ANDREY DOBRYNIN, The University of Akron — Biodegradable polymers are widely used in drug delivery and tissue engineering. However, direct experimental observation of the degradation process of such polymers is limited. To address this issue, we have developed a coarse-grained model to mimic degradation dynamics of L-valine and L-phenylalanine based poly(ester urea)s (PEUs) in vitro. Simulations show that the rates of hydrolysis and chain diffusion control the degradation process. In particular, it is found that PEUs experience a combination of surface and bulk erosions, which both contribute to the degradation of the material. By tuning the reaction parameters in our simulations, we determine the crossover between degradation-controlled and swelling-controlled regimes. Using these results, we established a general framework for modeling competition between degradation and swelling-controlled mechanisms in biodegradable materials. To test model predictions and to map coarse-grained parameters, we compare the time evolution of the molecular weight distributions of the polymer chains obtained in simulations with those obtained experimentally from size-exclusion chromatography.

*ODSA TECG20180022

L70.00091: A Computational Method for Inverse Design Problem in Directed Self-Assembly of Block Copolymers  DANIIL BOCHKOV (Presenter), FREDERIC GIBOU, Mechanical Engineering, University of California, Santa Barbara — Directed Self-Assembly is an important process used in the semi-conductor industry. It uses confinement masks to drive the self-assembly of block copolymers towards targeted nano-templates for subsequent optical or e-beam lithography. The shape of such confinement masks must be carefully designed as it is one of the primary factors determining the final polymeric structures. In this talk, we present a computational approach, within the self-consistent field theory framework, for finding confinement shapes that lead to a-priori chosen self-assembled structures of block copolymers. The method is based on a constrained optimization formulation described by partial differential equations: we define a cost functional that measures the discrepancy between the target and the actual self-assembled configurations, and analytically derive the sensitivity of the functional to changes in shape, which in turn enables an efficient minimization of the functional with respect to the confinement shape. We provide simulation results that demonstrate the ability of our approach to design mask geometries that successfully guide the self-assembly to the desired targets.
L70.00092: Coarse-Grained Simulations to Understand the Effect of Grafting on Methylcellulose* VAIDYANATHAN SETHURAMAN (Presenter), KEVIN DORFMAN, University of Minnesota — Methylcellulose is a biopolymer derived from sugar, and it has a wide range of industrial applications. Recent experiments on methylcellulose solutions showed that they undergo fibril formation above the lower critical solution temperature. However, on grafting the methylcellulose polymer with polyethylene oxide (PEG), experiments show that the fibril structure is destroyed. We use coarse-grained molecular dynamics simulations to provide molecular insights into the effect of grafting on fibril formation. Our results showed that the radius of gyration of the polymer increases with increasing grafting density, in qualitative agreement with the experimental results. We also show that the loss in fibrillar structure arises from a steric repulsion between the grafted PEG monomers and the methylcellulose backbone.

*Materials Science Research and Engineering Center Award No. DMR-1420013

L70.00093: A Coarse-Grain Model for Efficient Simulation of Self-Assembling Amyloidogenic Peptide Systems* MURRAY SKOLNICK (Presenter), ROBERT RIGGLEMAN, ZAHRA FAKHRAAI, University of Pennsylvania — Prior experiments with amyloid forming peptides have demonstrated that short peptides exhibit distinct self-assembly behavior when constrained to a surface resulting in rapid formation of amyloid fibrils. Molecular dynamics simulations of such systems can provide key insights into this self-assembly process. However, the size and time scales associated with such systems is too large for atomistic approaches to study self-assembly. Thus, we are developing an implicit-solvent coarse-grained model of amyloidogenic peptides for the investigation of their surface mediated self-assembly in these systems using MD. The model consists of three CG beads per residue where the central bead has either hydrophobic or hydrophilic character depending on the amino acid it represents. The two side-chain beads form a dipole which replicates that found in an all atom amide backbone. The simulations of initially randomly oriented peptides demonstrate rapid self-assembly into fibrillar structures upon adsorption to a surface. Additionally, the simulations show that fibrillar structures are favored at lower peptide concentrations while surface covering films are favored at high peptide concentrations which is in agreement with experimental evidence.

*MRSEC grant (NSF DMR-1720530)

L70.00094: A Model for Hyaluronan Secretion into Biological Fluids JAN SCRMGEOUR (Presenter), Clarkson University — Hyaluronan (HA) is an essential biopolymer in joint tissues and synovial fluid, and changes in its molecular weight distribution have been linked to debilitating inflammatory joint conditions such as arthritis. Despite this, there is limited understanding of the physical mechanisms behind its secretion into biological fluids. HA is unique among biological polymers, as the polymer is synthesized at, and directly extruded through, the cell membrane. Current models for HA secretion have largely focused on a single enzyme, hyaluronan synthase, although no governing mechanism has been identified. In tissue observations point toward a more complex regulatory system involving additional enzymes, such as cell surface hyaluronidase, which is responsible for HA cleavage. This work presents a simple model for the synthesis and release of HA. The model makes predictions for the equilibrium molecular weight distributions of surface tethered and secreted HA. In addition, it describes the time-dependent growth and degradation of surface tethered HA. The model provides guidance for experimental investigation into rates of HA synthesis and release from the cell surface, and may act as a basis for understanding how the environment in the joint affects HA secretion into synovial fluid.
L70.00095: Predicting the linear stress and dielectric relaxations of polydisperse linear polymers* DANIEL READ (Presenter), CHINMAY DAS, School of Mathematics, University of Leeds — We present a generic algorithm to predict the linear relaxation spectrum for polydisperse linear polymers. As common in the tube theory descriptions of linear polymers, we assume that the stress relaxation is affected by both constraint release and tube escape modes. But unlike most existing descriptions, we consider how these two modes of relaxation affect each other and argue that the proper description for relaxation in an arbitrary blend of linear polymers requires consideration four embedded tubes affecting the different relaxation pathways: the thin tube, the tube for fastest reptation, the constraint release "supertube" and the fully diluted tube. We derive the scaling level descriptions of these relaxation pathways and use a large number of existing experimental results on the stress and dielectric relaxations to validate our model. For the particular case of binary blends of long and short polymers, our model is successful at predicting the linear stress and dielectric response for blends throughout the two dimensional space (constraint release rate and degree of entanglement) mapped by the Viovy diagram.

*Supported by EPSRC grant ref EP/P005403/1

L70.00096: Impact of divalent ions on the rheology and aggregation of semidilute polyelectrolyte solutions CARLOS LOPEZ (Presenter), WALTER RICHTERING, RWTH Aachen University — We report rheology and light scattering data for the Na+, Mg2+, Ca2+, Mn2+, Co2+, Ba2+ salts of carboxymethyl cellulose in aqueous solutions. The viscosity as a function of molar polymer concentration falls into a single curve for all divalent salts. Compared NaCMC, divalent salts display a lower viscosities at low concentrations (in the non-entangled regime), suggesting less expanded chains. Above the entanglement crossover, solutions with divalent counterions display viscosities an order of magnitude larger than NaCMC because interchain crosslinks form by electrostatic bridging.

DLS measurements on semidilute reveal a bimodal decay function, where the relative amplitudes of the two modes vary with counterion valence, size as well as with the filter size employed and the time after filtration. These variables (except for counterion valency) do not affect the solution viscosity, indicating that polyelectrolyte clusters contain a small fraction of the total number of chains in solution.

L70.00097: Viscoelastic Relaxation Behavior of Polyelectrolyte Complexes from Coacervate to Precipitate SAMIM ALI (Presenter), ANAND RAHALKAR, National Institute of Standards and Technology, JUAN DE PABLO, Institute for Molecular Engineering, The University of Chicago, VIVEK PRABHU, National Institute of Standards and Technology — The relaxation dynamics of polyelectrolyte complexes slows down while transitioning from coacervate to precipitate upon decreasing salt concentration. However, knowledge of such changes over full relaxation spectrum is still limited. This presentation will describe the relaxation behavior of complexes probed over a wide timescale by measuring viscoelastic spectra and zero-shear viscosities at varying temperatures, salt concentrations and molecular weights using a set of model polyelectrolytes. Our studies show that the complexes exhibit time-temperature superposition (TTS) at all salt concentrations, while the range of overlapped-frequencies for time-temperature-salt superposition (TTSS) strongly depends on the salt concentration and gradually shifts to higher frequencies as the complex approaches precipitate phase. Further understanding of this transition using the sticky Rouse model and simulations studies will be presented.

L70.00098: Free Surface Flows and Extensional Rheology of Polymer Solutions JELENA DINIC (Presenter), LEIDY NALLELY JIMENEZ, VIVEK SHARMA, University of Illinois at Chicago — Free-surface flows -- jetting, spraying, atomization during fuel injection, roller-coating, gravure printing, several microfluidic drop/particle formation techniques, and screen-printing -- all involve the formation of axisymmetric fluid elements that spontaneously break into droplets by a surface-tension-driven instability. The growth of the capillary-driven instability and pinch-off dynamics are dictated by a complex interplay of inertial, viscous and capillary stresses for simple fluids. Additional contributions by elasticity, extensibility and extensional viscosity play a role for complex fluids. We show that visualization and analysis of capillary-driven thinning and pinch-off dynamics of the columnar neck in an asymmetric liquid bridge created by dripping-onto-substrate (DoS) can be used for characterizing the extensional rheology of complex fluids. Using a wide variety of complex fluids, we show the measurement of the extensional relaxation time, extensional viscosity, power-law index and shear viscosity. Lastly, we elucidate how polymer composition, flexibility, and molecular weight determine the thinning and pinch-off dynamics of polymeric complex fluids.
L70.00099: Electronically excited states in p/p stacking compounds  AYAKA TERAUCHI, ATSUNE MITSUI, AZUSA MURAOKA (Presenter), Japan Women’s University — In particular, p/p stacking compounds have become of interest in new materials for photocatalysis, solar energy and phosphorescent organic light-emitting diodes. We investigate theoretically the photo-induced charge transfer in supramolecular chemistry such as a bowl-shaped polycyclic hydrocarbon and helical ortho-position linked phenylenes (OPs). The electronically excited states and absorption spectra of these materials were first studied by using TD-DFT calculations with various functionals. The functional that best reproduced the experimental results was found to be wB97XD, and the assignment of the experimentally observed UV-Vis absorption spectrum was successfully performed in comparison with the theoretically obtained one. We especially performed spectral assignment of the carbazole (Cz)-modified OP complexes. The results showed that the absorption spectrum of the complexes consisted of (i) an n–p* charge-transfer type transition from Cz to OPs units of longer wavelength at around 290 nm and the p–p* transition of a shorter wavelength at around 230 nm, and (ii) the components of three isomers which coexist with three kinds of substitution of Cz to OPs, such as ortho, meta and para linkage of Cz, to interconnect the aromatic units of the Ops.

L70.00100: Deformation of Hybrid Networks  MICHAEL JACOBS (Presenter), HEYI LIANG, ANDREY DOBRYNIN, The University of Akron — Mimicking the mechanical properties of soft materials and biological tissues is crucial for novel materials development for medical implants, tissue engineering, soft robotics, and wearable electronics. Bottlebrush and comb networks are shown to be able to replicate the required combination of softness, strength and toughness in solvent-free elastomers. Such networks are made by crosslinking the side chains which results in the formation of the hybrid networks which have two types of strands of different rigidity and extensibility. We use a combination of analytical calculations and coarse-grained molecular dynamics simulations of hybrid network deformation to establish universal features. In our approach we first study an idealized system which preserves the network topology and represents the difference in the strands’ bending rigidities by considering the network strands as linear polymer chains with different Kuhn lengths and degrees of polymerization. The developed model is used to describe deformation of bottlebrush and comb networks in the linear and nonlinear network deformation regimes.

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L70.00101: Comparison of Mullins Effect between Tough Double Network Hydrogels and Filled Elastomers under Various Types of Deformation  THANH-TAM MAI (Presenter), Kyoto Institute of Technology, TAKAHIRO MATSUDA, TASUKU NAKAJIMA, JIAN PING GONG, Hokkaido University, YOSHIHIRO MORISHITA, Bridgestone Corporation, Tokyo, KENJI URAYAMA, Kyoto Institute of Technology — The distinctive features of the Mullins effect between the double network (DN) hydrogels (Mai et al., Macromolecules 51, 5245–5257, 2018) and filled elastomers (Mai et al., Soft Matter 13, 1966–1977, 2017) are revealed by cyclic stretching measurement with various extension modes, i.e., uniaxial, planar, unequal and equal biaxial stretching. The modulus reduction, energy dissipation (D), and dissipation factor (Δ, the ratio of dissipated energy to input strain energy) in each loading-unloading cycle are evaluated. The result indicates that the cross-effect of strains (λij; ij = x,y,z and i ≠ j) on Δ is pronounced in the DN gels whereas it is minimal in the filled elastomers. Interestingly, the modulus reduction relative to initial modulus and Δ in each cycle almost agree with each other in the DN gels, but they are considerably different in filled elastomers. This discrepancy reflects that the modulus reduction and dissipation factor are different in the main origin for the filled elastomers, while both of them totally stem from the purely elastic fracture of the chains in rigid and brittle DN gels networks.

L70.00102: Effect of miscibility on shape memory characteristics of Polymer Blends  SURBHI KHEWLE (Presenter), PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology, Gandhinagar, Gujarat — Designing programmable shape shifting materials has been a grand challenge for science and engineering. Shape Memory Polymers (SMPs) are smart materials that have the ability to transform back to their intended shape when the external conditions are reversed. One of the strategies for synthesizing SMPs is to bond soft and rigid chemical moieties with one another through polymerization. Although polymer blending offers a simple strategy, it has not been used as a preferred technique to design SMPs. As most of the polymer blends are immiscible, synthesizing SMPs through blending route introduces a new set of challenges. Here, we use the equilibrium phase diagram to examine the role of compatibility of the constituent polymers on the characteristics of SMP blend. Specifically, we use Flory-Huggins theory in conjunction with the phase-field theory to capture the amorphous-amorphous and crystal-amorphous interactions in the SMP blends, respectively. Subsequently, we use the thermo-mechanical constitutive model to demonstrate the effect of miscibility on shape fixity and shape recovery of the SMP blend. Our approach can be utilized to design SMP blends with tunable properties and allows a mechanism to establish structure-property relationships in these systems.

*IIT Gandhinagar
L70.00103: Ion Specific, Odd-Even Glass Transition Temperatures in Precise Network Polymerized Ionic Liquids

CHRISTOPHER EVANS (Presenter), CHENTIAN SHEN, QIUJIE ZHAO, University of Illinois at Urbana-Champaign — Relationships between \( T_g \), fragility, nanostructure, electrostatics and conductivity are investigated in precise network polymerized ionic liquids (n-PILs). These n-PILs contain an exact number of carbon atoms (C\( x \)) between charges in the backbone and can be exchanged to various anionic forms. The \( T_g \) exhibits an odd-even effect with the non-spherical, bulky bis(trifluoromethane sulfonamide) (TFSI) counter ion with a maximum jump of 45 K between C4 and C5 networks. In contrast, the same n-PIL networks with the smaller and spherical BF\(_4\) anion show no odd-even \( T_g \) effect. Small angle X-ray scattering of TFSI networks suggests that ionic aggregation is not the primary cause of the odd-even effect. The amorphous halo exhibits a weak odd-even dependence indicating a minor role of backbone-backbone correlations and packing on the observed effects. However, odd-even effects appear to be largely dynamical in n-PILs with only minor variations in structure. Due to the large changes in \( T_g \), the room temperature ionic conductivities of the TFSI n-PILs exhibit odd-even effects greater than an order of magnitude between adjacent C\( x \) networks. Finally, dynamic fragility shows odd-even fluctuations with higher fragility corresponds to lower \( T_g \) opposite to what is typically observed.

L70.00104: Efficient Shockwave Energy Dissipation in Dynamic Covalent PDMS Rubber

CHRISTOPHER EVANS (Presenter), JAEJUN LEE, BRIAN JING, LAURA E PORATH, NANCY SOTTOS, University of Illinois at Urbana-Champaign — Polymer networks containing transient bonds require some amount of energy to undergo an exchange process. We hypothesize and demonstrate that dynamic bonds in polydimethylsiloxane (PDMS) networks can be used as an effective mechanism for dissipating shockwave energy. By controlling the diol molecular weight, the density of dynamic boronic ester linkages can be controlled while the network chemistry is invariant. Using a classical laser induced shockwave technique, we demonstrate superior energy dissipation in a PDMS boronic ester dynamic rubber (PDMS-B-DR) compared to the benchmark polyurea and covalent PDMS (cured via thiol-ene click chemistry). A monotonic improvement in dissipation performance (monitored as a reduced peak pressure of the shockwave) is observed with increasing density of dynamic boronic ester bonds. In all cases, the Tg is invariant in the different networks (-125 °C) implying a minimal role of segmental dynamics on dissipation in these specific networks. Our results indicate that dynamic networks are a promising route to engineering improved SWED materials which are lightweight, flexible, and able to withstand repeated shocks. X-ray scattering and rheology have also been performed to relate dissipation performance to structure and relaxation of the material.

L70.00105: Approaches to Modification of Maleic Anhydride Copolymers with Applications to Antifouling and Water Purification

STEVEN ZBORAY (Presenter), KIRILL EFIMENKO, JAN GENZER, North Carolina State University — Precise control over structure and tailoring of chemical moieties along the chain are the keys to creating polymeric materials with advanced functionality. We present an approach based on maleic anhydride copolymers allowing facile modification with various chemical groups as embodied in two systems: a polymer network capable of catalytic degradation of organophosphates and antibiofouling coatings. Through the use of crosslinking, which could be controlled via several synthetic pathways, hydrogels containing hydroxamic acid groups were made that allowed the gel to be used for water purification applications. Kinetic studies of the performance of the gels in degrading the model compound dimethyl nitrophenyl phosphate (DMNP) were performed. For antifouling purposes, a systematic study of the structure-property relationships of several sulfobetaines and the ability to resist fouling by fluorescent-labeled proteins was conducted. It was also found that by varying the comonomer in the system, it was possible to control hydrophobic/hydrophilic interactions and adhere the polymers to substrates as thin-layer coatings.

L70.00106: Elastocapillary-driven Deposition of Liquid Drops in Polymer Gels

HONGBO FU (Presenter), CHRISTOPHER BARNEY, XUDONG LIANG, ALFRED CROSBY, University of Massachusetts Amherst — The deposition of a finite volume of liquid at a specific location within an elastic gel offers novel opportunities for device fabrication and materials properties measurement. We present a systematic study of the controlled deposition of liquid droplets within a polymer hydrogel. With parameters, such as pressure and viscosity of the liquid, the size and spacing of deposited liquid droplets can be controlled. To understand this process, we propose an elastocapillary-based mechanism that balances the surface tension and viscosity of the liquid with the elasticity of the gel.

*Human Frontier Science Program (HFSP) RGP0019/2017
L70.00107: Finite element modelling of polymer gels that exhibit temperature induced volume phase transitions*  
PRIYANKA NEMANI (Presenter), Department of Chemical Engineering, Indian Institute of Technology Gandhinagar, RAVI SASTRI AYYAGARI, Department of Mechanical Engineering, Indian Institute of Technology Gandhinagar, PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Temperature-induced volume phase transitions are one of the mechanisms by which large-scale deformations are manifested in biological systems. Polymer hydrogels that undergo spontaneous volume change upon variations in temperature are, therefore, perfect candidates for designing bioinspired self-oscillating materials that can reversibly sustain large deformations. Here, we present a computational framework to design the dynamical system based on chemical reactions, that undergoes large mechanical oscillations via external loading and thermally induced volume phase transitions, simultaneously. Specifically, our model is based on a nonlinear finite element framework that essentially combines reaction-diffusion phenomena with nonlinear elastic deformations of the gel under nonisothermal conditions. Through modelling and simulation, we capture large deformations and volume changes represented by swelling/shrinkage of the gels at varied temperatures. Our major findings not only complement the existing features of polymer gels and facilitates the design of a variety of complex biomimetic systems like thermosensitive actuators but also provides a mechanism to predict their complex nonlinear phenomena.

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L70.00108: Diffusion of Gold Nanoparticles in Entangled Poly (vinyl alcohol) Solutions and Gels.  
KAVINDYA SENANAYAKE (Presenter), ASHIS MUKHOPADHYAY, Wayne State University — Dynamical studies of nanoparticles in concentrated polymer solutions have importance in industrial and medical applications. We study the diffusion of gold nanoparticles (AuNPs) in high molecular weight poly (vinyl alcohol) (PVA) entangled solutions and gels. Using fluctuation correlation spectroscopy, diffusion coefficients of different sized AuNPs in different volume fractions above the entanglement volume fraction of PVA were determined. Comparison of results with the recent scaling theories will be presented.

L70.00109: Computational investigation of cavitation phenomena in physically assembled gels*  
SATISH MISHRA (Presenter), Mississippi State University, THOMAS E. LACY, JR, Mechanical engineering, Texas A&M University, SANTANU KUNDU, Mississippi State University — Cavitation rheology is a novel technique to probe local mechanical properties of soft materials. In this experiment, a defect is introduced in the gel by inserting a needle connected to a syringe pump. The growth of defect subjected to a pressure load is recorded. At critical pressure, the defect becomes unstable and suddenly expands into a cavity leading to a drop in pressure. For physically assembled gels, experimental studies demonstrate critical pressure as high as ten times of that calculated analytically using hyperelastic models. We present a finite element modeling approach to capture the coupled effect of material modulus, viscous dissipation, surface tension, and geometry confinement in determining the critical pressure. Our results indicate that a portion of pressure applied to expand the defect dissipates through stress relaxation mechanism, thus, pumping rate influences the critical pressure. Surface tension restricts the expansion of defect while the confinement introduces an artificial stiffening response to the gel, hence, increase the critical pressure. We will also compare the finite element analysis results with that obtained from cavitation experiments.

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L70.00110: Polyethylene Cross-link Density Effects on Crystallization and Shape Memory Performance*  
DEAN PENNER (Presenter), CHESTERTON B SCHUCHARDT, AUDREY T YOUNG, DAVID D HSU, Wheaton College — In pursuit of a model of microstructure-property relationships in cross-linked, semi-crystalline Shape Memory Polymers (SMPs), we investigate the effect of cross-link density on thermally-activated SMP performance characteristics. Specifically, we aim to establish a relationship between crystal size distribution and shape fixity, shape recovery rate, and shape recovery temperature. United-atom Molecular Dynamics (UAMD) simulations of the shape memory cycle for cross-linked polyethylene are carried out at varying cross-link densities between 150 and 800 g/mol. Crystal size distribution is investigated as a function of cross-link density using order parameter and a density-based clustering algorithm. Both shape fixity and shape recovery rate are found to increase with lower cross-link density down to 150 g/mol, due to the uniform crystal size distribution resulting from unimpeded crystal growth.

*D.P., C.S., A.Y., and D.H. acknowledge support from the Wheaton College Alumni Association and Wheaton Summer Research Grant.
While plants are traditionally regarded as static, some plants are able to move at accelerations thousands of times the acceleration of gravity. Engineered systems seek to achieve the high accelerations and high speeds observed in nature for use as fast and adaptable materials. Using the inspiration of plant seed pods, we aim to demonstrate that adhesion may act as self-releasing latch when sufficient bending energy is applied to overcome the adhesion of the latch, causing rapid energy release in the form of a bending motion. We prepare a bilayer beam made of polydimethylsiloxane (PDMS) layers with different crosslinking densities, which provides a mechanism for asymmetric swelling and bending when placed in good solvents. Our actuator approaches accelerations 20 times that of gravity and with total response times on the order of 10 ms over cm-scale distances. This work is one step towards increasing the abilities of soft actuators and robots capable of fast motion that are not limited by the requirements of mechanical motors.

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**L70.00112: Water Dynamics in Poly(N-isopropyl acrylamide) Solutions at Ambient and High Pressure Probed with Quasi-elastic Neutron Scattering**  
BART-JAN NIEBUUR, Physics Department, TU Munich, WIEBKE LOHSTROH, Heinz Maier-Leibnitz Zentrum (MLZ), TU Munich, MARIE-SOUSAI APPAVOU, Jülich Centre for Neutron Science at MLZ, TU Munich, ALFONS SCHULTE (Presenter), Physics Department, University of Central Florida, CHRISTINE M. PAPADAKIS, Physics Department, TU Munich — We investigate the dynamic behavior of hydration water in a 25 wt% aqueous Poly(N-isopropyl acrylamide) (PNIPAM) solution in dependence on temperature (25 – 50 °C) and pressure (0.1 – 130 MPa) employing quasi-elastic neutron scattering (QENS). The susceptibility spectra span the frequency range from 2 GHz to 2 THz at momentum transfers between 0.7 to 1.7 A⁻¹ and reveal the relaxation peak of the hydration water near 10 GHz, in addition to the known diffusive and effective local and vibrational processes of bulk water. Evaluating the temperature dependence, we find that, at atmospheric pressure, the relative population of (bound) hydration water sharply decreases upon heating from the one-phase to the two-phase state, i.e. the chains dehydrate strongly. In contrast, at 130 MPa, no sharp decrease is observed, i.e. the dehydration takes place over a much broader temperature range. This suggests an enhanced hydrophobic hydration at high pressure.

**L70.00113: Biomimetic wet-applicable adhesive as a stiffness-tunable binding interface for on-skin sensors and self-locking actuators**  
SONG CHEN, South China University of Technology, SONGSHAN ZENG, University of Connecticut, LAN LIU, South China University of Technology, LUYI SUN (Presenter), University of Connecticut — Both stimuli responsive strain sensors and actuators have drawn significant attention because they are promising in a wide span of applications, including wearable devices, stretchable electronics, and soft robotics. However, there are few researches focusing on achieving a wet-applicable, ultra-conformable, and stiffness-tunable interface, which is highly critical in these fields. Herein, we develop a novel wet stretchable adhesive that shows high binding strength to various substrates. Furthermore, by introducing hygroscopic calcium chloride (CaCl₂) into the system, the Young's modulus of the adhesive film can be easily adjusted from higher than 1.5 GPa to lower than 0.01 MPa under ambient environment (ca. 25 °C, 70% relative humidity) because of the water uptake and the corresponding plasticizing effect. We further use this adhesive to fabricate a soft (skin-like modulus, 0.1-10.0 MPa), thin (~50 μm), highly sensitive (a gauge factor of ~2000 under 20% strain), and ultra-compliant on-skin strain sensor and a multi-responsive (heat, near infrared (NIR) light, voltage, and humidity) self-locking actuator. A new avenue has been created to address both sensing and actuating bottlenecks by introducing a wet-applicable adhesive as a versatile and robust binding interface.

**L70.00114: Spinodal Decomposition-Induced Surface Wettability Modification of Thermo-Responsive Nanoemulsion Films**  
HYEMIN SEO (Presenter), JIN WOONG KIM, Hanyang University — Functional polymer thin films with a multilayer structure have been constructed with nanometer scales typically by using the sequential adsorption of oppositely charged polyelectrolytes onto a solid substrate. Tight control over phase separation is essential for providing the film with structured surface heterogeneity as well as surface functionality. Herein, we fabricate nanoscale emulsion thin films by utilizing the layer-by-layer deposition. Their thickness was tunable to micrometer scales by solely changing the number of alternate emulsions and polyelectrolytes layers. Interestingly, the nanoemulsion films exhibited a thermoresponsive heterogeneous phase separation behavior, which is typically referred as Spinodal decomposition. We observed that surface wettability of the Nanoemulsion films was critically dependent upon the pattern of the Spinodal decomposition, which enables development of thin film-based smart drug delivery patches.
L70.00115: Towards Optimizing Synthesis Temperature for Microgels with Large Degree of Deswelling* KIRIL STRELETZKY (Presenter), KRISTA G FREEMAN, JACOB ADAMCZYK, Cleveland State University — Polysaccharide microgels have been synthesized at various temperatures (Tsyn) above the LCST of the parent polymer. Microgel structure and dynamics below and above the corresponding volume phase transition have been studied with light scattering. All microgels were found to undergo a reversible 15-50-fold deswelling in volume. However, the size distribution, structure, dynamics, and deswelling ability of microgels were found to strongly depend on synthesis temperature. In this work, the attempt was made to optimize the synthesis temperature to yield more monodisperse microgels with a larger degree of deswelling. The results suggest that Tsyn influences the density distribution of microgels and, therefore, their structure and dynamics.

*USRA program of CSU and REU Award #1659541

L70.00116: Effect of Elasticity, Viscosity, External Dissipation and Structures on Impulsive Elastic Energy Release in Polymers* XUDONG LIANG (Presenter), ALFRED CROSBY, Polymer Science and Engineering, Univ of Mass - Amherst — Impulsive elastic energy release in materials have been widely adopted in small organisms and engineered micro-robotic devices to achieve high speed motion. The kinematics of impulsive motion are well characterized through high speed camera imaging, but the mechanics of the materials under large deformation and high strain-rate deformation is not yet established. Here, we present a theoretical and experimental study about the effects of material properties, environmental interactions and structures of synthetic polymers for the performance of a free retraction. Building upon the 1D elastodynamics and nonlinear mechanics, we discover that kinematics of impulsive recoiling can be described through a power-law constitutive model, and the residual strain after retraction determines the maximum center-of-mass velocity. The viscous losses in the materials and frictional force in the environment are shown to significantly affect the center-of-mass velocity. Finally, we explore how topologies in mechanical metamaterials can lead to control of impulsive elastic energy release.

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L70.00117: Microballistic Deformation Behavior of Carbon Nanotube Mats WALE LAWAL, Eglin Air Force Base, JINHO HYON, Rice University, RAMATHASAN THEVAMARAN, University of Wisconsin, EDWIN THOMAS (Presenter), Rice University — We investigate the energy absorption characteristics of 2D isotropic multiwall carbon nanotube (MWCNT) mats using a micro-projectile impact test at velocities ranging from 300 m/s to 900 m/s. The quasi-static properties of the 2D isotropic network of meandering MWCNT nanofibers are quite modest but at the extreme strain rates and large strains of ballistic impact, the deformation behavior of the mat results in unprecedented energy absorption per unit mass of the target mat. The mat is comprised of a network of ultra high aspect ratio interconnected tubes and tube bundles with many branches and cross-overs leading to increasing retarding forces from the interacting tubes and tube bundles with the silica sphere projectile. As the projectile rotates and moves forward, the MWCNT tubes and tube bundles are straightened and pulled into the impact region. The increased friction associated with the amplified surface interactions occurring between the translating principal tubes raises the load on those portions of the tubes adhering to the sphere surface and the subsequent large back-deflection of the impact region slows the advancing projectile as KE is converted into elastic stretching energy of the network and ultimately fracture of many principal tubes.

L70.00118: Slicing of soft materials STEVEN RHODES (Presenter), ERIC WEEKS, Emory University — We experimentally study the slicing of soft materials. We use a rheometer to press a circular cutting tool into materials (a steel “cookie cutter”). This allows us to measure the normal force required to press the cutter and the torque required to rotate the cutter, while controlling the shear rate. Our soft materials are Styrofoam and PDMS. We find rotating the cutter makes it easier to cut into the material. In particular, without rotation, the cutter only indents the Styrofoam rather than slicing it.

L70.00119: Optimizing random heteropolymers to improve protein folding in cell-free synthesis ZHIYUAN RUAN (Presenter), TAO JIANG, TING XU, Materials Science and Engineering, UC Berkeley — Membrane proteins play key roles in biological activities, and represent one of most prevailing drug targets. Functional and structural analysis of membrane proteins remain intriguing but challenging due to the protein misfolding and aggregation. Here, we show that four-meronmer random heteropolymers (RHPs) can assist membrane protein folding during translation in cell free synthesis. Two types of membrane proteins, Aquaporin Z (water channel, helices) and OmpT (protease, barrel) were examined, and demonstrated tunable polymer performance by controlling the composition of RHPs. The results indicated that the extent of folding assistance of various RHPs for the membrane proteins was different due to the chemical heterogeneity along the length of RHP chains. An in-house program for chemical heterogeneity analysis was developed to investigate the sequences of various RHPs and proteins. The current data suggests that RHPs act as artificial chaperones and that their ability to aid in the proper folding of membrane proteins can be easily tuned by changing their composition.
L70.00120: Thickness-dependent elastic modulus of spin-coated PDMS films*  PAK MAN YIU (Presenter), HAILIN YUAN, OPHELIA TSUI, Department of Physics, Hong Kong University of Science and Technology — Poly(dimethyl siloxane) (PDMS) elastomer is one of the most commonly used substrate materials for stretchable electronics and artificial skin. Many fundamental studies of soft interface mechanics use PDMS. It is therefore important to understand the factors affecting the mechanical properties of this material. A previous study revealed that the elastic modulus, $E$, of spin-coated PDMS increased almost three-fold when the PDMS thickness, $h$, was decreased from 108 to ~30 μm. The enhancement in $E$ had been attributed to the alignment of PDMS chains during spin-coating. In this study, we measured the elastic modulus of spin-coated PDMS with various $h$ from 15 to 110 μm. We found that $E$ increased with decreasing $h$ initially, but on reaching $h \sim 20$ μm, $E$ decreased with decreasing $h$. We verified that this phenomenon was universal regardless of the curing condition. We discuss a possible origin for the phenomenon with supporting measurement data.

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L70.00121: Force Balance at Contact Lines of Soft Substrates*  HEYI LIANG (Presenter), Department of Polymer Science, University of Akron, ZHEN CAO, Department of Materials Science and Engineering, Massachusetts Institute of Technology, ZILU WANG, ANDREY DOBRYNIN, Department of Polymer Science, University of Akron — We use coarse-grained molecular dynamics simulations to show that the force balance analysis at the triple-phase contact line formed at an elastic substrate must include a quartet of forces: three surface tensions (surface free energies) and an elastic force per unit length. In the case of the contact line formed by a droplet on an elastic substrate, the elastic force is due to substrate deformation generated by formation of the wetting ridge. The magnitude of this force $f_{el}$ is proportional to the product of the ridge height $h$ and substrate shear modulus $G$. Similar elastic line force should be included in the force analysis at the triple-phase contact line of a solid particle in contact with an elastic substrate. For this contact problem elastic force obtained from contact angles and surface tensions is a sum of the elastic forces acting from the side of a solid particle and an elastic substrate. By considering only three line forces acting at the triple-phase contact line, one implicitly accounts the bulk stress contribution as a part of resultant surface stresses. This “contamination” of surface properties by a bulk contribution could lead to unphysically large values of the surface stresses in soft materials.

*L70.00122: Effects of force on facilitated protein dissociation  JING ZHAO (Presenter), KATELYN DAHLKE, CHARLES E. SING, University of Illinois at Urbana-Champaign — Protein-DNA interactions depend on the conformation of DNA, so binding/unbinding kinetics may be altered by applied forces; classically, protein unbinding is accelerated and binding is inhibited as force increases. Additionally, certain proteins exhibit concentration-dependent dissociation rates, where proteins in solution compete to facilitate protein dissociation from DNA. Together, facilitated dissociation (FD) and force can lead to diverse dissociation behaviors including “slip bonds”, where dissociation rates decrease with force, and “catch bonds”, where dissociation rates increase with force. We investigate these combined effects via coarse-grained simulation. We reproduce concentration-dependent rates that are observed experimentally and explore how force can alter these binding kinetics. We observe catch bonds when protein binding is strongly coupled to the force, while the force dependence of protein unbinding is relatively weak. Slip bonds occur under opposite conditions. Transitions between these different bonds occur when force effects on binding and unbinding compete. Thus, applied force may regulate protein-DNA interactions by inhibiting FD by coupling protein exchange rates to DNA conformations.

L70.00123: Melt-Electrospinning of Poly(ether ether ketone) Fibers to Avoid Sulfonation*  NELAKA DILSHAN GOVINNA (Presenter), THOMAS KELLER, PEGGY CEBE, Department of Physics and Astronomy, Tufts University — We have successfully electrospun un-sulfonated fibers of poly(ether ether ketone), PEEK, from the molten state. A high temperature furnace was used to melt electrically grounded PEEK pellets at 350 °C, and the electric force caused fibers to be deposited onto the high voltage collector. Whereas solution electrospinning of PEEK results in sulfonation of the polymer chain and reduction of thermal stability, direct melt electrospinning produced PEEK fibers which are chemically unaltered from as-received pellets, as shown by their Fourier transform infrared spectra. Thermogravimetry demonstrated electrospun PEEK fibers have similar thermal decomposition temperature, $T_d = 600$ °C as the pellets. Melt electrospun fibers had a large range of diameters, ranging from 1.5 μm to 8.5 μm, and were smooth, defect-free, and round in cross-section. As-spun amorphous fibers, with thicknesses less than 10 μm and masses ~200 ng, were selected for fast scanning calorimetry (FSC) experiments. Using heating and cooling rates from 50 to 2000 K/s, FSC studies were made of the glass transition, melting and crystallization behavior of electrospun PEEK fibers.

*NSF DMR 1608125
L70.00124: Structural differences in regenerated cellulose fibers produced using Viscose and Lyocell techniques*  
AAKASH SHARMA (Presenter), GURUSWAMY KUMARASWAMY, National Chemical Laboratory, SHIRISH THAKRE, Aditya Birla Science and Technology Company Pvt. Ltd. — We compare the structural features of regenerated cellulose fibers manufactured using Viscose and Lyocell processes. It is known that these fibers possess different surface morphologies. However, there is not much information on nanoscale structural features e.g. microvoids, lamellar structure etc. We show using small angle x ray and ultra-small angle neutron scattering that the fibers possess elongated microvoids, oriented in the fiber direction. We analyse 2D SAXS data using Ruland’s equatorial streak method and obtain average length and average misorientation of the microvoids in both fibers. Using Porod’s law and invariant calculated from the combined SAXS and USANS measurement, we evaluate the radius. We show that Lyocell fibers have bigger, better orientated voids than Viscose fibers. There are also differences in the crystal structure of these two fibers. Scattering from Viscose fibers show evidence for lamellar stacking in the fiber direction whereas, that from the Lyocell fibers is qualitatively different and does not show stacking. This shows that process differences strongly affect the microstructure of the fibers at length scales of few nanometres.

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L70.00125: A molecular model for ductility (T< Tg) and drawability (T>Tg) of semicrystalline polymers*  
SHIQING WANG, MASOUD RAZAVI (Presenter), Department of Polymer Science, University of Akron — We make oversimplifications to construct a tractable molecular model for mechanics of semicrystalline polymers that takes into account of the mechanical interplay between crystalline and amorphous regions connected by tie chains. The idea can be reformulated to address the origin of yielding or breaking in semicrystalline polymers that form spherulites. Our goal is to understand the brittle failure of fully crystallized glassy polymers such as PLA and PET and whether or not various semicrystalline polymers are highly drawable above their glass transition temperatures.

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L70.00126: Semiflexible Polymers in Spherical Confinement  
ARASH NIKOUBASHMAN (Presenter), Johannes Gutenberg University Mainz, ANDREY MILCHEV, Institute for Physical Chemistry, Bulgarian Academy of Sciences, MIHIR KHADILKAR, Johannes Gutenberg University Mainz, SERGEI EGOROV, Chemistry, University of Virginia, DANIEL VEGA, Physics, Universidad Nacional del Sur-IFISUR-CONICET, KURT BINDER, Johannes Gutenberg University Mainz — Semiflexible macromolecules find various applications as versatile materials, in particular due to their possible liquid crystalline order, and are also important constituents of living matter. We studied the ordering of such stiff macromolecules confined in spheres by molecular dynamics simulations, and found that densely packed semiflexible polymers cannot exhibit uniform nematic order when their contour length is of the same order as the sphere radius. Instead, the confinement leads to the emergence of topological defects on the sphere surface with competing ordering in the interior of the sphere. Each of the configuration variables including chain length, chain stiffness, packing density, and shell thickness uniquely affect the ordering, including the nature and relative orientation of the defects on the surface. For example, at high densities, a thin shell of polymers close to the surface exhibits a quadrupolar tennis ball texture due to the confinement-induced gradual bending of polymer bonds. Systemic trends observed could pave the way for better understanding the links between topological defects and elastic properties of polymers. Further, controlling the defect locations is promising for designing patterned colloids in experiments by functionalizing defect sites.

L70.00127: Replicating Chiral Structures with Common Polymers and the Study of Surface Changes under VOC’s  
THOMAS STOKE (Presenter), PETR SHIBAYEV, Fordham University — Liquid crystals are known to have interesting surface patterns, characterized by focal conic domains patterned across their surface. These chiral structures can be observed through Atomic Force Microscopy, and replicated on the surfaces of common polymers. When exposed to certain Volatile Organic Compounds (VOC’s), the surface structures of chiral polymers are seen to break down. However, on these replica polymers, no such changes can be seen. The applications of these traits are discussed.
L70.00128: Dynamic Relaxation and Glass Transformation of Electrospun Fibrous Membrane with Confined Chain Configuration: for Physical Aging and Shape Function Control and Delivery  BIN XIAO, CHENHONG WANG, NUOZI ZHANG, HERAN WANG, XUHONG CHEN (Presenter), SHANSHAN XU, CHARLES C HAN, Institute for Advanced Study, Shenzhen University — The thermodynamic glass transformation processes of electrospun membranes are firstly introduced to study the dynamic relaxation nature of this not always in equilibrium transformation process. The relaxation modes of the electrospun membrane are slow but measurable in the vicinity of the Tg and even above the Tg due to the stretched chain in long distance. Based on the differential scanning calorimetry (DSC) experiments and the general principle of mode-coupling theory (MCT), the endothermic peak temperature and the relaxation enthalpy were used to analyze the relaxation process by capturing these instantaneous "arrested" structures. With different annealing time and annealing temperatures relative to DSC measured T for E-spun membrane with different molecular weight, the short and long wavelength relaxation modes could be identified. These results clearly show the dynamic nature of the glass transition in polymeric materials which can be explained by the general principle of MCT type of dynamic theory.

L70.00129: Terahertz Dynamics of Carboxymethyl Starch*  WAKANA TERAO, LEONA MOTOJI (Presenter), TATSUYA MORI, Division of Materials Science, University of Tsukuba, KAROLINA KACZMARSKA, BEATA GRABOWSKA, Faculty of Foundry Engineering, AGH University of Science and Technology, YASUHIRO FUJII, AKITOSHI KOREEDA, Department of Physical Sciences, Ritsumeikan University, MIKITOSHI KABEYA, Division of Materials Science, University of Tsukuba, JAE-HYON KO, Department of Physics, Hallym University, SEIJI KOJIMA, Division of Materials Science, University of Tsukuba — We performed terahertz time-domain spectroscopy on microwave-treated sodium carboxymethyl starch (CM-Starch), to detect the boson peak and fracton. Starch is a natural polymer formed by polymerization of a number of D-glucose molecules by glycosidic linkage and CM-Starch is produced by carboxymethylating the starch. The obtained spectral shape of boson peak plot $\alpha(\nu)/\nu^2$ of the CM-Starch, where $\alpha(\nu)$ is the absorption coefficient, is different from vitreous glucose. It suggests the existence of the fracton in the CM-Starch.

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L70.00130: Contrasting rubber-toughen mechanisms for glassy polymers*  MASOUD RAZAVI (Presenter), SHIQING WANG, Department of Polymer Science, University of Akron, HAILAN GUO, Dow Chemical — We perform standard pre-yield and post-yield stress relaxation to probe molecular mobility in various rubber-toughened polymer glasses and to differentiate between "apparent" and true yielding. The rubber-toughened PS and SAN, e.g., HIPS and ABS, show apparent yield at high strains whereas a new generation of PMMA based nanocomposites from Dow Chemical is transparent, truly ductile and shows enhanced molecular mobility in post-yield deformation at different draw rates, form a sharp contrast with the conventional materials such as HIPS and ABS.

*This work is supported, in part, by NSF-DMR 1609977.

L70.00131: The morphology and flowing behaviors of TEMPO-oxidized cellulose nanofibers dispersed in non-aqueous solutions*  RUIFU WANG (Presenter), TOMAS ROSEN, CHENGBO ZHAN, BENJAMIN S HSIAO, Chemistry, Stony Brook University — Cellulose nanofibers (CNF), sustainable and possessing good mechanical properties, is a good reinforcement agent for polymer composites. However, pure CNF is hard to disperse in common organic solvents due to the strong interfibrillar H-bondings and $van der Waals$ interactions. In this study, we investigated the dispersion behavior of CNFs having different charged density, prepared by the TEMPO-oxidation and nitro-oxidation methods, in two different non-aqueous solvents: ethylene glycol and propylene glycol. The morphologies of CNF was first characterized by combined AFM, TEM and solution SAXS methods, whereby the results showed that the fiber cross-section dimensions were closely related to the oxidation conditions that also led to different charge density. The rheological results indicated that the overlap concentration of the suspension is solvent independent. Moreover, the CNF/glycol suspensions behave very similarly to polymer solutions, exhibiting shear thinning behavior beyond the overlap concentration. We postulate that the solvent exchanging method could also be used to disperse CNF into other non-aqueous solvent for better mixing with hydrophobic polymers.

*The presenter would like to thank the National Science Foundation (DMR-1409507)
L70.00132: Polymer physics and flow dynamics of thermodynamically pure ring polymers*  
MICHAEL TU (Presenter), CHING-WEI LEE, CHRISTOPHER RUDOLPHI, SIMON ROGERS, CHARLES SCHROEDER, Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign — Ring polymers have fascinated polymer chemists and physicists for decades, yet achieving a complete understanding of the dynamics of pure ring polymer systems has remained elusive due to major challenges in residual linear polymer contamination. Despite recent advances in purification methods, trace amounts of linear polymers are thought to remain in existing ring polymer samples, greatly affecting the mechanical properties of these materials. Here, we study the equilibrium and non-equilibrium flow properties of synthetic rings based on cyclic poly(phtalaldehyde) (cPPA), a low-temperature polymer whose linear chain analogues are thermodynamically unstable at room temperature due to depolymerization at free ends. The polymerization reaction yields high molecular weight cyclic polymers with no free ends, thereby providing highly pure and thermodynamically stable ring polymers. Using this approach, we study the linear viscoelastic properties, zero-shear viscosity, and nonlinear flow response of cPPA samples as a function of polymer molecular weight and weight fraction. Overall, these results give insight into the dynamics of ring polymer systems with unprecedented purity.

*This work is supported by the NSF Grant CBET-1604038 to CMS.

L70.00133: Nonlinear melt rheology explored by molecular dynamics simulations*  
YEXIN ZHENG (Presenter), MESFIN TSIGE, SHIQING WANG, The University of Akron — We apply bead-spring based molecular dynamics simulation to study both shear and extensional responses of entangled melts. Shear creep is carried out to show the emergence of entanglement-disentanglement transition (EDT) previously observed in experiment [1], confirming that EDT can take place in absence of edge instability. At high Rouse-Weissenberg numbers (larger than ca. 5), entangled melt is observed to undergo melt rupture independent of whether Filament stretching rheometry or Sentmanat extensional rheometry is employed. The lack of yielding suggests intriguing lockup of chain entanglement in melt stretching [2]. Such extreme tensile strain localization is observed for the first time in MD simulation, corresponding to the threshold of full chain disentanglement in absence of the chain scission mechanism that in reality triggers the unzipping of chain entanglement.


*This work is supported, in part, by NSF-DMR 1609977.

L70.00134: Melt Blown Cross-linked Fibers from Thermally Reversible Diels-Alder Polymer Networks*  
KAILONG JIN (Presenter), SUNG-SOO KIM, JUN XU, FRANK BATES, CHRISTOPHER ELLISON, University of Minnesota — Melt blowing is a process in which liquid polymer is extruded through orifices and then drawn by hot air jets to produce nonwoven fibers. Melt blown nonwovens constitute more than 10% of the $50 billion global nonwovens market. Thermoplastic feedstock, such as polyethylene, polypropylene, and poly(butylene terephthalate), have dominated melt blown nonwovens because of their combined cost, good chemical resistance and high-temperature performance. Cross-linked nonwovens from other commodity polymers (e.g., (meth)acrylates, styrenics, silicones, etc.) could be attractive alternatives; however, no commercial cross-linked nonwovens currently exist. Here, cross-linked fibers were produced via one-step melt blowing of thermoreversible Diels-Alder polymer networks comprised of furan- and maleimide-functional methacrylate-based polymer backbones. These dynamic networks decross-link and flow like viscous liquids under melt blowing conditions, then revert to a network via cooling-induced cross-linking during/after melt blowing. Finally, the resulting cross-linked fibers can be recycled because of their reversible dynamic nature, which may help address the microfiber pollution problem.

*The authors thank Cummins Filtration for financial support.
L70.00135: Properties of chemically crosslinked methylcellulose gels  PETER SCHMIDT (Presenter), Department of Chemical Engineering and Materials Science, University of Minnesota, Twin Cities, SVETLANA MOROZOVA, Department of Chemistry, University of Minnesota, Twin Cities, MCKENZIE COUGHLIN, Department of Chemical Engineering and Materials Science, University of Minnesota, Twin Cities, S. PIRIL ERTEM, THERESA M. REINEKE, Department of Chemistry, University of Minnesota, Twin Cities, FRANK BATES, Department of Chemical Engineering and Materials Science, University of Minnesota, Twin Cities, TIMOTHY LODGE, Department of Chemistry, University of Minnesota, Twin Cities — Methylcellulose (MC) is used in an impressively wide variety of commercial products due to its ability to reversibly form fibrous networks upon heating. To investigate the effect of crosslinking on these materials, we have prepared two types of gels and compared their thermodynamic and elastic properties. First, crosslinked methylcellulose gels were prepared at room temperature using a thiol-ene click reaction. Allyl methylcellulose was crosslinked with dithiol poly(ethylene glycol) ($M = 1500$ g/mol) and allowed to swell to equilibrium as a function of temperature and strand length. Upon heating, instead of forming fibrous networks, crosslinked methylcellulose gels experience volume change. By measuring the polymer volume fraction and modulus of gels in equilibrium we identify the thermodynamic parameters that drive the gel volume change using a modified Flory-Rehner theory. Second, crosslinked methylcellulose fiber gels were prepared by crosslinking allyl methylcellulose solutions at 80 °C, after the full conversion of chains to fibrils. The swelling and thermodynamic properties of crosslinked chain gels and crosslinked fiber gels will be compared and discussed.

L70.00136: Gel Point Determination of a Diffusive Photopolymer via $^1$H NMR Relaxometry*  CASEY LEE-FOSS (Presenter), ANTHONY V LYNCH, GRETCHEN HOFMEISTER, Dept. of Chemistry, Carleton College, MARTHA-ELIZABETH BAYLOR, Dept. of Physics and Astronomy, Carleton College — Diffusive photopolymers can simplify the fabrication of “lab on a chip” devices. Knowledge of the gel point of the photopolymer, defined as the exposure time when an infinite macromolecule is formed, is required to create complex coplanar features via UV exposure. Because instrumentation for traditional gel point determination techniques is not locally accessible, we sought to develop a locally available method of gel point quantitation for a two-stage methacrylate/thiol-ene formulation. Since methacrylate chain growth and increasing cross-linking during the sol-gel transition reduces the mobility of diluent monomers, we hypothesized that the gel point can be found using NMR inversion-recovery to measure how polymerization affects the mobility-dependent $T_1$ relaxation time of an added “spectator” molecule. We present results showing a correlation between the rheological gel point and the time when the slope of $T_1$ versus exposure time changes, demonstrating $^1$H NMR relaxometry is a feasible method of gel point determination.

*This material is based upon work supported by the National Science Foundation under CHE-1428752 as well as the Harry A. and Margaret D. Towsley Foundation Fellowship at Carleton College.

L70.00137: Self-Moving Polymer beads*  ANKUR MITTAL (Presenter), PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Self-propelled motion through internalized chemical reaction, a characteristic of living systems, has led to the design of various synthetic bio-inspired systems. Here, we design a self-moving macroscopic system through careful use of self-oscillating chemical reaction inside a polymeric gel. Specifically, we use poly-N-isopropylacrylamide (NIPAAm) gel bead as a miniaturized reactor and harness chemical oscillations of the Belousov Zhabotinsky (BZ) reaction to produce sustained motion. In a typical experiment, the gel beads are charged with BZ reagents and placed on an oil-covered substrate. Due to the porous nature of the gel beads, the intermediates of BZ reaction ooze out of the gel and react with oil, thereby producing spontaneous motion of the bead via Marangoni effect. We further demonstrate that the velocity of the beads can not only be controlled by tuning the kinetics of BZ reaction but also by varying the external stimuli. In particular, we show that by using Ru decorated graphene nanosheets as catalysts the velocity of the beads can be enhanced significantly compared to the traditional solution based catalysts. Our findings can be used to design self-propelled conveyor belts that can deliver cargo from micron to mm length scale.

*DST-SERB (EMR/2016/007778)
Self-oscillating polymer gels that intrinsically utilize Belousov-Zhabotinsky (BZ) reaction have emerged as an interesting class of smart materials due to their biomimetic characteristics. Here, we synthesize polymer gels using imidazolium-based ionic liquid as a precursor and immobilize the catalyst of the BZ reaction onto the backbone of the gel. Further, we replace the protonating agent in the BZ reaction with Ethyl Ammonium Bisulfate (EABS)—a protic ionic liquid. In essence, we demonstrate that through careful replacement of BZ reagents with their ionic liquid counterparts, the chemical oscillations in the BZ system can be manifested into mechanical swelling and deswelling of the polymer gel, just like the conventional BZ gels. Our approach, however, offers significant advantage over the BZ gels synthesized through the conventional route. Specifically, due to the presence of ionic bonds the dynamics of the mechanical oscillations in our self-oscillating ionic gels can be controlled via electric and magnetic fields. Thus, our approach opens up new avenues for designing multi-functional biomimetic systems that can be controlled by application of variety of external stimuli.

*L70.00138: Design of Self Oscillating Ionic Gels*
SAIRAM S (Presenter), Department of Chemical Engineering, Indian Institute of Technology, Gandhinagar, ARNAB DUTTA, Department of Chemistry, Indian Institute of Technology, Gandhinagar, ARVIND KUMAR, Salt and Marine Chemicals Division, Central Salt and Marine Chemicals Research Institute, Council of Scientific and Industrial Research (CSIR), G.B Marg, Bhavnagar 364002, PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology, Gandhinagar —

L70.00139: Salt and Water Diffusivities in Polymer Electrolyte Membranes
DIPAK ARYAL (Presenter), VENKATRAGHAVAN GANESAN, University of Texas at Austin — Motivated by experimental observation where transport properties of salt ions and water in charged polymer membranes exhibit an intriguing dependence on salt concentration, we have probed a series of atomistic molecular dynamics simulations of non-cross linked membranes in aqueous mono and divalent salt solutions along with mesoscale dissipative particle dynamics (DPD) simulations for crosslinked membranes at concentrations ranging from 0.06 to 1 M. We investigate the molecular level understanding the effects of both multi-component salt solutions and crosslinking of polymers on fundamental salt and water transport properties. Our finding shows that the diffusion of salt ions and water are influenced by cation sizes and salt concentrations. Divalent ions are more strongly coupled with ionic groups which reduce their motions as increasing concentration in fixed charged membranes. In crosslinked membranes, diffusion of salt ions and water are reduced significantly relative to non-crosslinked systems. However, the trends exhibited by the salt concentration dependence of diffusivities, and the coordination of the cations with anions, and with the polymer backbone remain qualitatively similar to those observed in non-crosslinked membranes.

L70.00140: Effect of doping ratio on lithium-ion conductivity in nanostructured self-doped block polymer electrolytes
MELODY MORRIS (Presenter), Department of Chemical and Biomolecular Engineering, University of Delaware, THOMAS H EPPS, Department of Chemical and Biomolecular Engineering, Department of Materials Science and Engineering, University of Delaware — Self-doped polymers, in which the salt anions are attached covalently to the polymer, are promising alternatives to salt-doped polymer electrolytes because concentration polarization is reduced and stability is enhanced in the electrolyte. A self-doped diblock terpolymer electrolyte was synthesized such that one block was composed of a high modulus material and the other block consisted of both ion-conducting and self-doping monomer segments. The self-doped block polymers were made with a series of self-doped lithium concentrations (by altering the relative amounts of ion-conducting and self-doping monomer segments). Small-angle X-ray scattering results suggested that all self-doped block polymers exhibited ordered nanostructures. AC impedance spectroscopy and DC polarization were used to evaluate the conducting properties of the electrolyte (ionic conductivity and transference number), and the conductivities increased with self-doping ratio. Thus, with the framework for nanostructured self-doped block polymer electrolytes realized, the ion content can be manipulated to design improved electrolyte systems.

*SERB:EMR/2016/007778*

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L70.00141: Tailoring Ionic Conductivity of Block Copolymer Electrolytes with End-functionalyzed Homopolymers
JIHOON KIM (Presenter), MOON JEONG PARK, Pohang University of Science and Technology — Block copolymer electrolytes based on poly(ethylene oxide) (PEO) have been regarded as promising candidates of solid electrolyte materials for lithium ion batteries. This is attributed to their ability to dissolve lithium salts and high ionic conductivity of the resultant polymer/salts complexes. However, PEO crystallization below its melting temperature has been tied to a radical reduction in ionic conductivity, especially at room temperature, various attempts have been made to reduce the PEO crystallinity. Herein, we propose a new method to modulate crystallization behavior of PEO-based block copolymers with embedded end-group-functionalyzed PEO homopolymers. Intriguing, the morphology and ionic conductivity of the resultant block copolymer/homopolymer blends were sensitive function of the type of end group in PEO homopolymers at the same blend ratio. Our approach offers a platform for the development of efficient solid-state polymer electrolytes by controlling intermolecular interactions in PEO phases via a simple end-group chemistry.

L70.00142: Ion clustering behavior of “precise” phosphonated polymers
SE JONG KANG (Presenter), MOON JEONG PARK, Pohang University of Science and Technology — Polymers functionalized with phosphonic acid groups are promising candidates of proton exchange membranes for fuel cells that can be operating at high temperatures. This is owing to the amphoteric nature and self-dissociation ability of phosphonic acid groups, unlike sulfonic acid counterparts, thereby allowing acid groups to form hydrogen-bond networks in the absence of moisture. In the present study, we report the synthesis of polymers bearing phosphonic acid groups at the precise position. For this purpose, controlled radical polymerization of styrene phosphonate was carried out, where the substitution positions were varied based on ortho, metal, para directing groups. It has been revealed that polymers tethered with phosphonic acid groups at meta and ortho positions display suppressed ion clustering behavior than those with para position acid group, attributed to the dominant hydrogen bonding interactions of neighboring acid groups.

L70.00143: Self-Assembled Shape-Anisotropic Diblock Copolymer Particles from Evaporative Emulsions: Experiment and Theory*
KANG HEE KU (Presenter), YOUNG JUN LEE, YONGJOO KIM, BUMJOON KIM, KAIST — We report the systematic design of shape-anisotropic diblock copolymer (dBCP) particles based on a new theoretical model that embodies entropic penalty associated with bending of the cylindrical and lamellar dBCP chains upon deformation of the particles. First, we produced the convex-lens shaped (oblate) and football-shaped (prolate) PS-b-PDMS particles, where the aspect ratios (AR) were tunable over a broad range from 1 to 10. Of note, the AR of oblate particle increased almost linearly up to 10 as the particle size increased, whereas the increase of AR for the prolate particle was limited to 2.0. To understand this discrepancy, we developed the theoretical model that includes the bulk elastic and bending energies of dBCP cylinders and lamellae, and the surface energy between the particle/ surrounding medium. For oblate particles, the high excessive bending energy of the curved cylinders at the periphery of particle can be released by increasing the AR of particle. However, the relatively low excessive bending energy of curved lamellae of prolate particles prevents the particles from having a high AR.

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L70.00144: Coupling between mean curvature and texture in thin block copolymer film
GABRIEL CATALINI (Presenter), ALDO DANIEL PEZZUTTI, DANIEL VEGA, Departamento de Física, Universidad Nacional del Sur (UNS), Instituto de Física del Sur (IFISUR), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) — Using a phase field approach we study the orientational coupling between the pattern developed by a lamellae forming block copolymer thin film and a topographically patterned substrate. Utilizing the Brazovskii free energy functional for a conserved order parameter, we perform a Taylor series expansion on the film thickness to obtain an effective geometric potential that correlates the smectic texture orientation to the curvature of the underlying surface. The results of this expansion are in good agreement with numerical results obtained through a Cahn-Hilliard model and experimental data on curved monolayers of asymmetric diblock copolymers.
L70.00145: Modelling Silica in Aggregates of Block Copolymers

PALLABI HALDAR (Presenter), ALESSANDRO PATTI, FLOR R. SIPERSTEIN, University of Manchester — There is developing interest in the use of Periodic Porous Materials (PPMs) synthesized from silicic acid and amphiphilic block copolymers in drug delivery and catalysis. Existing studies of the formation of PPMs have not drawn a clear conclusion as to the formation mechanism. In the prior studies two formation mechanisms were suggested; Liquid Crystal Template (LCT), where silicic acid plays no active role in the formation, and Cooperative Mechanism, where silicic acid plays a role in the formation.

In this study, we have investigated how the presence of silicic acid affects the self-assembly of these block copolymers by employing molecular dynamics simulations of coarse-grained (CG) models of Polyethyleneoxide-b-polybutylmethacrylate (PEO-b-PBMA) with silicates in water and tetrahydrofuran. An existing CG silicic acid model could not reproduce the water-silicic acid interaction observed experimentally. We have developed a more effective silicic acid CG model by comparing the solvation free energy of silicic acid in solvents with the values obtained from DFT calculations, which will allow for the determination of the correct formation method of PPMs.


*MSCA, MULTIMAT, Horizon 2020

L70.00146: Thermally Induced Phase Transitions in Amorphous-Crystalline Brush Block Copolymers

GAYATHRI KOPANATI (Presenter), BENJAMIN M YAVITT, HUAFENG FEI, University of Massachusetts Amherst, RUIPENG LI, MASAFUMI FUKUTO, Brookhaven National Lab, Upton, JAMES J WATKINS, University of Massachusetts Amherst — Temperature resolved small angle x-ray scattering (SAXS) and wide-angle x-ray scattering (WAXS) were used to investigate the temperature dependent phase transitions of five lamellae forming poly(styrene)-block-poly(ethylene oxide) (PS-b-PEO) brush block copolymers. Asymmetric lamellar morphologies were observed for all the PS-b-PEO series irrespective of their volume fraction and backbone length. The temperature dependent SAXS and WAXS reveal the presence of long-range order up to 140 °C. Unlike their linear counterparts, the primary peak position (q*) and full-width half maximum (FWHM) of q* remain constant, indicating no order-disorder transition (ODT) up to 200 °C. The melting and crystallization of the PEO side chains co-exists within the lamellar morphology. Isothermal crystallization studies were conducted to investigate the crystallization kinetics of the PEO domain. The results indicate a two-stage crystallization process with Avrami exponents of 1 and 2, suggesting a one-dimensional initial stage followed by two-dimensional growth at later times.

*NSF Center for Hierarchical Manufacturing at UMass Amherst

L70.00147: The Systematic Study of Porous Monoliths to Measure Diffusion Induced by Hydrochloric Acid

PAOLA LO-EZ (Presenter), Lehigh University — There is the open question of the effect of loaded and non-loaded hydrogels with CaCO3 on diffusion kinetics. Formulations of PEDGA solutions were created containing varying concentrations of CaCO3 since higher concentrations would result in the material to develop yield stresses. The formulation was polymerized into flat monoliths using UV light rays. The 200 µm monoliths were swelled in H2O for 24 hours. Then, were subjected to a diffusive dissolution experiment and submerged into different concentrations of HCl (1 M/L to 0.06 M/L) and CaCO3 (0% to 25%). Time measurements were taken assuming that the longer the hydrogel was soaked in HCl the less CaCO3 and the more porosity. Pictures taken with an SEM of the porous dissolution fronts measured over time show the diffusion reaction scheme fits a model of diffusion of the square root of time. Also, a pH sensitive dye experiment was carried out in the porous hydrogels. The methyl orange soaked hydrogels were put in an aqueous HCl bath, and the movement of the concentration front was measured assuming the dye is trapped and the reaction is limited by diffusion of the acidic front. Rearranging the diffusion equations, diffusion coefficients were retrieved for the reactions.

*Ilaccoca Internship Program
University of Bordeaux
Solvay, S.A
L70.00148: Effect of Partial Saturation on Thermodynamic Interactions in Polydiene/Polyolefin Blends* JIALIN QIU
(Presenter), MEGAN L ROBERTSON, RAMANAN KRISHNAMOORTI, University of Houston — Polymer blends exhibit properties
that are highly dependent on interactions between components, typically quantified by the Flory-Huggins interaction
parameter, χ. Polyolefins and polydienes are important materials with commercial relevance in elastomer applications.
The majority of previous studies on the thermodynamics in polyolefin and polydiene systems have focused on polymer
pairs within the same class, which generally exhibit a small and weakly temperature dependent χ. There is little
quantitative information on thermodynamic interactions of polydienes and polyolefins. In our previous work, we
characterized the χ parameter in a model polydiene/polyolefin blend based on 1,2-polybutadiene (1,2-PBD) by small angle
neutron scattering (SANS). We observed an unusually large χ parameter in blends of 1,2-PBD and saturated 1,2-PBD that
exhibited a strong temperature dependence. We also studied the impact of partial saturation on χ of polydiene/polyolefin
blends. The χ(T) behavior in blends of fully saturated 1,2-PBD with partially saturated 1,2-PBD, at varying levels of
saturation, was characterized. The applicability of the random copolymer theory to predict χ(T) behavior in these blends
was evaluated.

*This work was supported by ExxonMobil Chemical Company.

L70.00149: Temperature-induced coil-globule transition of polypropylene oxide in aqueous solutions* RASIKI
DAHANAYAKE (Presenter), UDAYA R DAHAL, ELENA DORMIDONTOVA, Polymer Program - Institute of Material Science and Physics
Department, University of Connecticut — Polypropylene oxide (PPO) is a biocompatible polymer which is used in a wide range
of industrial to biomedical applications, e.g. as a component of the commercial family of Pluronics. Using all-atom
molecular dynamics simulations with modified OPLS forcefield we study the conformational changes of PPO in aqueous
solutions as a function of temperature. We analyzed the temperature induced change in the PPO radius of gyration and
 correlate it with the polymer hydration properties, such as hydrogen bonding, hydration number, solvent accessible
surface area, etc. We found that the coil-globular transition is accompanied by a noticeable reduction in polymer-water
hydrogen bonding. We also estimate the heat capacity change as a function of temperature, which exhibits a maximum at
the transition point and compare it with experimental data.

*This work was supported by the National Science Foundation under Grant No.DMR-1410928

L70.00150: Simulating Diblock Copolymer Micelles in Binary Explicit Solvents JING ZONG (Presenter), DONG MENG,
Mississippi State University — Amphiphilic block copolymers form nanoscale assemblies when dissolved in a selective
solvent. Such self-assembled structures have wide-ranging applications as drug delivery vehicles and nanoreactors, etc. A
powerful method to manipulate the assemblies is to vary the composition of solvent mixtures. Unlike single solvent
solution, computational studies of amphiphilic block copolymers in solvent mixtures are rarely reported due to high
computational cost associated with the necessity of treating solvents explicitly. Here, the Field-Accelerated Monte Carlo [1]
simulation is employed in the expanded grand canonical ensemble to study the micelle formation of diblock copolymers in
binary solvent: one selective solvent and one good solvent for both blocks. We investigate effects of molecular weight and
solvent composition on micelle morphology, critical micelle concentration, and micelle size and aggregation number. It is
found that distribution of the good solvent is highly inhomogeneous, concentrating at micelle interface and partitioning
unevenly outside/inside micelle cores. Solvent intake by micelle cores increases with polymer molecular weight, affecting
the way micelle size and aggregation number change with solvent composition.


L70.00151: Local Structure and Relaxation Dynamics in the Brush of Polymer-Grafted Silica Nanoparticles* YUAN
WEI (Presenter), MICHAEL HORE, Case Western Reserve University — Polymer chains are grafted to nanoparticle (NP) surfaces
for a variety of purposes, including altering NP solubility or dispersion within a polymer matrix. At high grafting densities,
high molecular weight polymers adopt two primary conformations on the NP surface. Polymer chains near the NP core are
stretched in the concentrated polymer brush region (CPB). Farther away from the core, polymer chains are less confined
and the conformation becomes more ideal in the semi-dilute polymer brush region (SDPB). Using a combination of small-
angle neutron scattering (SANS) and neutron spin echo (NSE) spectroscopy, we directly characterized both the structure
and dynamics of the CPB and SDPB on poly (methyl acrylate) (PMA) grafted SiO2 NPs by selectively deuterating each region
separately. Analysis of SANS measurements using a new core-chain-chain (CCC) model confirmed that the portion of the
polymer chains in the CPB region are stretched, and transitions to a more ideal conformation in the SDPB region. From
NSE, we found the dynamics in the CPB region were found to be much slower than the SDPB region across all length
scales, and followed the Zimm model.

*This work was supported by a National Science Foundation CAREER Award from the Polymers program (DMR-1651002).
L70.00152: Thermodynamics of Binary and Ternary Polymer Blend Nanocomposites

SHAWN MAGUIRE (Presenter), NADIA KROOK, University of Pennsylvania, PATRICE RANNOU, MANUEL MARECHAL, CEA-CNRS-University Grenoble Alpes, KOHJI OHNO, Kyoto University, RUSSELL JOHN COMPOSTO, University of Pennsylvania — Polymer nanocomposites (PNC), which are a combination of organic and inorganic fillers and a polymer matrix, have found great scientific interest due to the fact that the material properties of the PNC are largely determined by the chemical composition of the polymer as well as the type of fillers. While the fundamental physics governing the phase space of polymer blends is mature, there is a significant lack of understanding of the thermodynamics and kinetics that govern PNCs. In this work, we investigate model binary and ternary nanocomposites of poly(methyl methacrylate) grafted silica nanoparticles (PMMA NP), poly(styrene-ran-acrylonitrile) (SAN), and poly(methyl methacrylate) as a platform to elucidate the governing thermodynamic contributions. The thermally annealed films were characterized using electron microscopy and x-ray scattering, revealing lower critical solution temperature (LCST) behavior in the binary composite and an increased miscibility window in off-critical compositions for the ternary. These results extend the current understanding of PNC phase behavior and allow for greater control over NP dispersions.

*NSF PIRE, Grant #1545884, ANR-15-PIRE-0001-7: University of Pennsylvania, ANR-15-PIRE-0001-1: SyMMES

L70.00153: Vinyl Imidazole Sulfonate-based Zwitterionic Copolymers with Tuneable Adsorption on Carbonates

MOHAMMED KAWELAH (Presenter), MARIAM F. ALGHAMDI, S. SHERRY ZHU, AYRAT GIZZATOV, Aramco Research Centre - Boston, Aramco Services Company, YUAN HE, TIMOTHY M SWAGER, Department of Chemistry, Massachusetts Institute of Technology — Polymer injection in hydrocarbon reservoirs has been of great interest in petroleum engineering as an enhanced oil recovery (EOR) method. Injection of aqueous solutions of polymers into reservoirs increases the fluid viscosity and reduces its relative permeability in the reservoir, and hence improves volumetric sweep efficiency for EOR applications. However, the flow of polymeric solutions in porous media is subject to some particular effects such as non-Newtonian flow, degradation (thermal, physical, bacterial, and chemical), retention and inaccessible pore volume that are key to evaluating the success of a polymeric flooding. Significant polymer adsorption on the rock surface under high salinity and high temperature reservoir conditions is one of the most major challenges in polymer flooding EOR. Here we report the dynamic adsorption studies of four brine-soluble zwitterionic copolymers containing vinyl imidazole sulfonate using a Quartz Crystal Microbalance and core flooding at high temperatures. Our results indicate that the dynamic adsorption of the polymers on carbonates correlates to their structure variation and fluid properties, and a small presence of certain functional co-monomers on the polymers dramatically changes their dynamic adsorption.

L70.00154: Nonmonotonic glass transition behavior of polystyrene film in contact with polystyrene brushes

WOOSEOP LEE (Presenter), HOYEON LEE, Yonsei University, VAIDYANATHAN SETHURAMAN, University of Texas at Austin, DU YEOL RYU, Yonsei University, VENKATRAGHAVAN GANESAN, University of Texas at Austin — The interplay between a polymer melt the substrate grafted with 'chemically identical' polymer brushes has attracted attention due to the possible applicability to slip, adhesion, wettability, and lubrication. In this study, we controlled grafting density (σ) and chain length of polystyrene (PS) brushes on substrates to investigate their effect on the glass transition temperature ($T_g$) of overlaying PS films. To our surprise, we observed a nonmonotonic change of the $T_g$ of PS film as a function of $σ$ with the maximum value that exceeds the $T_g$ of bulk PS. A computer simulation supports our experimental results in terms of the local segmental dynamics in overlaying PS film, which is related to the enhanced friction by interpenetration between the melt (PS film) and the grafted layer.

L70.00155: Ion-Conducting Polymers as Interfacial Layers in Solid Electrolytes

ARVIN SOOKEZIAN, PRIYADARSHINI MIRMIRA (Presenter), SHRAYESH PATEL, STUART J ROWAN, Institute for Molecular Engineering, University of Chicago — The development of safe lithium/lithium ion batteries is of interest for large-scale energy storage applications such as electric vehicles. The use of solid-electrolytes (SE) is a promising alternative to commonly used liquid electrolyte based batteries, which have safety and electrochemical stability concerns. Notably, solid-state systems are bottlenecked in performance due to inadequate solid-to-solid contact between the SE and the electrode that leads to high interfacial impedance. To address this challenge, we have developed a class of ion-conducting polymers that can be utilized as thin interfacial layers that help mitigate the poor adhesion between the solid interface while still permitting lithium ion-transfer across the interface. We specifically report on the lithium-ion conductivity, mechanical, and adhesive properties of our materials. Lastly, we report the electrochemical stability and performance of the ion-conducting interfacial layers in normal lithium-ion battery operating conditions.

*Our research is supported through NSF DMR 1609076.
L70.00156: Brushes of Peptide Coiled Coil Bundle Chains  MATTHEW LANGENSTEIN (Presenter), DARRIN POCHAN, University of Delaware — Through solution self-assembly, computationally designed peptide coiled coil bundles (CCBs) have shown the ability to produce 2-D lattices, nanocages, nanotubes, and 1-D supramolecular polymers. However, to date no studies have been performed on the impact of substrate interactions on the structure of CCBs. Successful preservation of the coiled coil motif during surface conjugation could provide a robust pathway towards the computational design of stimuli-responsive latticed self-assembled monolayers and serve as a template for layer by layer growth of complex brushes with exact sequence control. In this poster the use of atomic force microscopy (AFM), angle resolved X-ray photoelectron spectroscopy (ARXPS), and quartz crystal microgravimetry (QCM) to characterize peptide layer thickness, surface topography, orientation, and deposition rate will be discussed. Additionally, the impact of temperature, solvent, and pH on the structure of cysteine terminated CCBs on planar gold substrates will be examined.

L70.00157: Impact of casting conditions on mechanical properties of polynorbornene membranes under typical biobutanol operating conditions. * MEETA TRIVEDI (Presenter), BRYAN VOGT, Department of Polymer Engineering, University of Akron — Poly(butylnorbornene)-ran-poly(hydroxyhexafluoroisopropyl norbornene) (BuNB-r-HFANB) is a promising material for biobutanol membrane with Tg’s for both segments exceeding 300°C to provide the potential for highly stable membranes. During operation, the BuNB-r-HFANB is swollen by the aqueous butanol in the broth that impacts its properties. The membrane performance is dependent on how it is cast. Here we investigated effect of four different casting solvents (THF, Toluene, DMF and Butanol) on the mechanical properties of these membranes using DMA. The change in mechanical properties in the butanol broth was enabled by using a submersion cell with DMA. The effect of temperature in both the dry and swollen state was also examined to provide insights into how the mechanical properties of these membranes would be expected to change during operation.

*This work was financially supported by the National Science Foundation under grant no. CMMI-1462284.

L70.00158: Oligomeric Cellulose Co-Crystallization with DMSO SEULGI KIM (Presenter), JI EUN KIM, JEONG YI KANG, JIN WOONG KIM, Hanyang University — Oligomeric cellulose nanofibers (BCNFs), known as bacteria-derived celluloses, are attractive biomaterials, since they are biocompatible and can be easily chemically modified for a variety of biomedical treatments. When primary hydroxyl groups on the BCNFs are substituted to carboxylic groups by 2,2,6,6-tetramethylpiperidine-1-oxyl radical (TEMPO)-mediated oxidation, they are able to physicochemically interact with biomolecules. Herein, we propose a new BCNF-based bioadhesion system for dermal therapy. The essence of our approach is that the antibody-conjugated BCNFs are bound to involucrin in the corneocyte of stratum corneum. The BCNF bioadhesives were fabricated by 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC)/N-hydroxysulfosuccinimide (sulfo-NHS) coupling reaction of antibody. Then, the adhesion force between the antibody-conjugated BCNFs and porcine skin was characterized by using the axial rheometer measurement. Finally, we demonstrated that our BCNF bioadhesives exhibited such a strong interaction with the skin tissue even under wet conditions, thus promising a variety of biological applications in the field of dermal therapy.

L70.00159: Oligomeric Cellulose Co-Crystallization with DMSO XIN ZHANG (Presenter), FENG JIANG, YIMIN MAO, DOUG HENDERSON, University of Maryland, College Park, YOSHIHARU NISHIYAMA, CERMAV, CNRS, Grenoble, Isère, France, ROBERT M BRIBER, HOWARD WANG, University of Maryland, College Park — Oligomeric cellulose with a median degree of polymerization of 7 (DP7) is produced by hydrolysis of cellulose in phosphoric acid. DP7 molecular weight distribution was characterized by NMR, MALDI-TOF, and GPC. DP7 is soluble in hot DMSO and crystallizes in the form of spherulites upon cooling. The spherulite morphologies and crystallization kinetics was characterized by polarized optical microscopy. The structure of the crystal has been studied by synchrotron radiation XRD, TEM and MD simulation. The oligomeric cellulose and DMSO co-crystallize. After removing excessive solvent, the crystal is metastable in dry air but transforms into the cellulose II crystal structure when exposed to humidity.

L70.00160: Synthesis and Self-Assembly of Oligomeric Cellulose-block-Poly(ethylene glycol) Diblock Copolymers FENG JIANG (Presenter), XIN ZHANG, DOUG HENDERSON, WONSEOK HWANG, HOWARD WANG, ROBERT M BRIBER, University of Maryland, College Park — Block copolymers containing cellulose have not been well studied or understood partly due to the poor solubility of cellulose in common solvents. In this study, well-defined oligomeric cellulose-block-poly(ethylene glycol) diblock copolymers, Cell1.1k-b-PEG1.7k (Mn = 2.8 kD, PDI = 1.04) and Cell1.1k-b-PEG5k (Mn = 6.1 kD, PDI = 1.02), have been synthesized via coupling reactions. The volume fractions of oligomeric cellulose in Cell1.1k-b-PEG1.7k and Cell1.1k-b-PEG5k diblock copolymers are 0.32 and 0.14, respectively. Due to the incompatibility between the cellulose and PEG, Cell-b-PEG diblock copolymers can separate at a local scale forming cellulose-rich and PEG-rich nano-domains, which further organize into larger scale structures, both in solutions and in the bulk. Small-angle X-ray scattering, atom force microscopy, and electron microscopy show hierarchical structures of Cell-b-PEG from nanometers to microns.

L70.00161: SOFT CONDENSED MATTER —
New coarse grained model for the study of the dynamics of the Worm Like Chain

ANGELO SETARO (Presenter), Rensselaer Polytechnic Institute — Semiflexible polymers display rich and varied behavior, distinct from both their rigid and flexible counterparts. This diversity arises from the interplay between bending energetics and conformational entropy. This energetic balance manifests as correlations between orientations along the polymer backbone, which depend on the flexibility of the polymer. Typically, the Kratky-Porod model is used to study semiflexible polymer systems, however, it is of limited utility when attempting to study non-equilibrium polymer dynamics, particularly over long timescales in flow. Currently, coarse grained models exist which allow for the study of polymers over longer time scales than the Kratky-Porod model, but at the cost of much fine grained information. To address this deficiency and bridge the gap between models, we propose a new coarse grained model for semiflexible polymers that reproduces some key behaviors of the Kratky-Porod model while simultaneously allowing for study of polymeric systems on a longer time scale. In this work, we have used Brownian dynamics to quantify and assess the accuracy of other key features of the model.

Dynamic and Structural Critical-like Behaviors in glassy monolayers of colloidal ellipsoids

ZHONGYU ZHENG (Presenter), Center for Soft and Living Matter, Institute for Basic Science, YILONG HAN, Department of Physics, The Hong Kong University of Science and Technology — Whether the glass transition is a purely dynamic transition or a thermodynamic one is a long-standing debate in condensed matter physics. Critical behaviors have been found in translational degree of freedom in glasses composed of spheres with local polycrystalline structures, but it is not clear if criticality exists in more general glassy systems without crystalline orders or composed of non-spherical particles. Here, we show rich critical behaviors in both translation and rotation in monolayers of monodispersed colloidal ellipsoids lacking crystal-like structures. We found an Ising criticality at the ideal glass transition point $\phi_0$ for the static glassy structures, local structural entropies and dynamic slow-moving clusters. These structural and dynamic quantities sharing the same Ising criticality are a direct evidence of the critical phenomena and thermodynamic nature of the glass transition at $\phi_0$. A different criticality is found at the mode-coupling point $\phi_C$ for the fast-moving clusters reflecting a dynamic glass transition. These results may explain the theoretical puzzles that the dynamic correlation length diverges at two different temperatures and the relaxation mechanism changes around $T_C$.

*This work was supported by NSFC grants, 11372314.

Measure particle diffusion in cytoskeletal networks with light-sheet and differential dynamic microscopy

CHRISTELLE MATSUDA (Presenter), SYLAS ANDERSON, RAE ROBERTSON-ANDERSON, RYAN J. MCGORTY, University of San Diego — Filamentous actin and microtubules contribute to the crowded environment of the cytoplasm. Modeling the cytoplasm, we create networks of varying crosslinking motifs and varying ratios of actin and microtubules. We crosslink either actin to actin, tubulin to tubulin, or tubulin to actin. We add micron-sized fluorescent beads to the various networks, record videos of the samples using light-sheet microscopy, and perform differential dynamic microscopy (DDM) analysis. We compare DDM and single-particle tracking results to examine differences between ensemble and single-particle transport properties. We find varying degrees of anomalous diffusion and significant heterogeneity in the dynamics, particularly in actin environments.

*National Institutes of Health (1R15GM123420)

Particle-tracking reveals heterogeneous subdiffusion in in vitro cytoskeleton composites

SYLAS ANDERSON (Presenter), CHRISTELLE MATSUDA, RYAN J. MCGORTY, RAE ROBERTSON-ANDERSON, University of San Diego — The diffusion of microscopic particles through the cell, important to processes such as transcription, viral infection, transfection and gene delivery, is largely controlled by the complex cytoskeletal network that pervades the cytoplasm. The cytoskeleton is predominantly made up of thin semiflexible actin filaments and thicker, more rigid microtubules, as well as binding proteins that can crosslink each filament. By varying the relative concentrations of actin and microtubules, as well as the degree to which each filament is crosslinked, the cytoskeleton can display a host of different structural and dynamic properties that in turn impact the diffusion of particles through the network. Here we use single particle tracking methods to quantify the mean-squared displacements of microspheres diffusing in custom-designed in vitro composites of actin and microtubules. We show that particles exhibit subdiffusion, with scaling exponents and transport coefficients that decrease as the relative fraction of actin in composites increases. By evaluating the distributions of bead displacements, we also find that composites induce unique non-gaussian diffusion characteristics and substantial heterogeneities in particle trajectories.

*This work was funded by NIH NNIGMS Grant No. R15GM123420.
L70.00166: Colloidal diffusion and viscoelasticity in blended solutions of supercoiled, ring and linear DNA*  
MEGAN LEE (Presenter), KARTHIK REDDY PEDDIREDDY, SYLAS ANDERSON, RAE ROBERTSON-ANDERSON, University of San Diego — DNA, which has been widely studied as a model polymer system, naturally exists in different topological forms including linear, relaxed circular (ring) and supercoiled. While the reptation model can be used to understand molecular transport and interactions in systems of entangled linear polymers, it is far less successful in describing the dynamics of entangled supercoiled or ring polymers. The properties of entangled polymer blends of different topologies and polymer solutions near the critical entanglement concentration are also still poorly understood. Here, we address these problems by creating blended solutions of (1) entangled linear and ring DNA of varying blend ratios and (2) supercoiled and ring DNA of varying overall concentrations from the semidilute to entangled regime. We use particle-tracking methods to measure the diffusion of colloids embedded in these solutions as well as the corresponding linear viscoelastic properties. We reveal previously unobserved and unpredicted dependences of transport and viscoelasticity on the ratio of linear to ring DNA in blends as well as the overall solution concentration.

*This work was funded by AFOSR Grant No. FA9550-17-1-0249 and NSF-CBET-1603925.

L70.00167: Tuning dynamics of moisture responsive wrinkling surfaces  
SONGSHAN ZENG, RUI LI, DIANYUN ZHANG, LUYI SUN (Presenter), University of Connecticut — The wrinkle dynamics (such as reversibility and stability) of human skin are affected by the external stimuli, as well as the skin's structure and mechanical properties. Inspired by these tunable responses, three types of moistureresponsive wrinkle dynamics are achieved, for the first time, through a single film-substrate system. These dynamics include: (1) completely reversible wrinkles formation; (2) irreversible wrinkles formation I: the initially formed wrinkles can be permanently erased and never reappear; and (3) irreversible wrinkles formation II: once the wrinkles form, they can no longer be erased. The key to success is to control the stiffness and thickness ratios of the film and the substrate, and tailor the crosslink degree/gradient of the film to allow for moisture-dependent changes of modulus and swelling degree. These unique responsive dynamics motivate the invention of a series of optical devices triggered by moisture, including anticounterfeit tabs, encryption devices, water indicators, light diffusors, and antiglare films. This study also paves the road for further understanding of the skin wrinkling dynamics and manipulation.

L70.00168: How crosslinking actin filaments influences the microscale viscoelastic properties of actin-microtubule composites*  
MADISON FRANCIS (Presenter), RAE ROBERTSON-ANDERSON, SHEA RICKETTS, University of San Diego, JENNIFER ROSS, Physics, University of Massachusetts Amherst — The strength and mobility of cells is dependent upon the interactions between two protein filaments that comprise the cytoskeleton: actin and microtubules. These proteins form entangled networks that can also be chemically crosslinked to enable a wide range of mechanical properties. Here, we use optical tweezers microrheology to determine how varying concentrations of actin crosslinkers influences the viscoelastic properties of actin-microtubule composites. We create equimolar co-entangled networks of actin and microtubules with varying concentrations of actin crosslinkers. We use optical tweezers to apply both oscillatory and constant speed microscale strains over a range of rates and distances while simultaneously measuring the force the networks exert to resist these strains. We quantify the frequency-dependent complex viscosity, the nonlinear stress response, and the relaxation dynamics following strain. Surprisingly, we find that increasing the concentration of crosslinkers yields a decrease in network elasticity and stiffness.

*Funding: This work was funded by a NSF CAREER Award #1255446, a NIH NNIGMS Award #R15GM123420, and a W.M. Keck Foundation Research Grant.

L70.00169: Mechanism of reinforcement in soft composites: random fiber networks with inclusions*  
MOHAMMAD ISLAM, CATALIN PICU (Presenter), Rensselaer Polytechnic Institute — The mechanical behavior of athermal random fiber networks embedding particulate inclusions is studied in this work. Composites in which the filler size is comparable with the mean segment length of the network are considered. In presence of inclusions, the small strain modulus increases, while the ability of the network to strain stiffens decreases relative to the unfilled network case. The reinforcement induced by fillers is most pronounced in sparse networks of floppier filaments that deform in the bending-dominated mode in the unfilled state. As the unfilled network density or the bending stiffness of fibers increase, the effect of filling diminishes rapidly. Fillers lead to a transition from the soft, bending-dominated, to the stiffer, axial-dominated, deformation mode of the network, transition which is primarily responsible for the observed overall reinforcement. These results provide a justification for the broadly observed difference in reinforcement in sparsely versus densely cross-linked networks at given filling fraction, and provide guidance for the further development of network-based materials.

*This work was supported in part by the NSF through grant No. CMMI-1634328.
L70.00170: Characterization of Aqueous Hyaluronate Solutions using Static and Quasielastic Light Scattering*

DAVID WALLS (Presenter), LAUREL HUNTER, VINGNESH VENKATARAMANI, DAVID ROSS, SCOTT FRANKLIN, MOUMITA DAS, GEORGE THURSTON, Rochester Institute of Technology — Human vitreous humor contains a hydrogel made up of a network of dilute collagen and hyaluronic acid. Liquefaction of the vitreous gel with age and in other conditions has been associated with retinal pathologies.

We use static and quasielastic light scattering to study the osmotic compressibility and local dynamics of aqueous hyaluronate solutions, in preparation for studying model vitreous gels. Buffered solutions prepared from commercial sodium hyaluronate were filtered to minimize light scattering heterogeneity. Refractometry was used to assess sample concentration post-filtration. Excess Rayleigh ratios from cleaned low-concentration samples gave molecular weights compatible with manufacturer's data. Higher concentration data give osmotic compressibilities that indicate repulsive intermolecular interactions, which we compare with theoretical models. At all concentrations, quasielastic light intensity autocorrelation functions show two well-separated slower decays and a faster decay. With increasing concentration, the slow component that has a characteristic decay time of tens of microseconds becomes faster as concentration increases, while the slowest component becomes more prominent.

*This research is funded by the National Science Foundation via the award NSF/CBET-1604712.

L70.00171: Nonlinear mechanics of composite fiber networks*

SADJAD ARZASH (Presenter), JORDAN SHIVERS, FRED C. MACKINTOSH, Department of Chemical & Biomolecular Engineering, Rice University — Fibrous networks such as collagen are ubiquitous in biological systems. Although the mechanical behavior of single fiber networks has been, both experimentally and theoretically, well studied, understanding the effect of the interplay between different biopolymer networks remains unclear especially under large deformations. In this work, we model a rigid fiber network inside a soft and flexible underlying matrix. This double network model enables us to study the effect of internal interactions of different networks on their overall mechanics. We find that the linear shear modulus of the composite system is greater than the sum of the individual linear shear moduli. Moreover, by calculating the non-affine fluctuations, we see clear suppression of fluctuations in the rigid fiber network. We also find a mechanical phase transition between matrix-dominated and fiber-dominated states.

*This work was supported in part by the National Science Foundation (Grants DMR-1826623 and PHY-1427654).

L70.00172: Classification and prediction of the mesophases of block copolymers*

SADATO YAMANAKA (Presenter), TAKESHI AOYAGI, CD-FMat, National Institute of Advanced Industrial Science and Technology — Self-organization and the resultant mesoscopic structures in block copolymer systems are of great advantage to applications such as nanolithography. Nevertheless, the whole phase behaviors still have not understood well even in ABC triblock copolymers. We study on classification problem on the classical phase diagram of AB diblock copolymers by means of supervised machine learning. We compare three model: kernel support vector machine (SVM), random forest, and k-nearest neighbor method. The prediction accuracy of kernel SVM is 94.5%, which is higher than the other two methods. This indicates that kernel SVM can be a candidate of classification model that is applicable to more complex architectures, such as linear/star ABC triblock copolymers.

*This work was supported by JSPS Grant-in-Aid for Scientific Research on Innovative Areas "Discrete Geometric Analysis for Materials Design": Grant Number 17H06464.

L70.00173: Using an autoencoder to reduce experimental noise*

NANCY THOMAS (Presenter), JORDAN HOFFMANN, LISA LEE, PARKER LAMASCUS, SHMUEL RUBINSTEIN, CHRISTOPHER RYCROFT, Harvard University — Experimental noise is ubiquitous in the sciences. Some of this noise is random, however some is systematic. We use machine learning to try to remove the systematic noise in experimentally found scans of crumpled sheets of paper in order to be able to study this classical disordered system. Properties that were previously uncovered using other denoising mechanisms were that crease mileage is a state variable of crumpling, is independent of crumpling history, and has a logarithmic scaling property. Through the use of an autoencoder, we were able to recover the scaling properties of crease mileage while improving the automation of the denoising process. This denoiser is able to outperform other methods on extremely noisy sheets. The removal of noise from our data is essential in order to be able to further explore the characteristics of the crease networks in a crumpled sheet.

*This work was supported by the National Science Foundation through the Harvard Materials Research Science and Engineering Center (DMR-1420570).
L70.00174: Probing mechanical properties of particle shells formed on droplets by electric field-induced wrinkling*  
ALEXANDER MIKKELSEN, Physics, Adam Mickiewicz University, ZBIGNIEW ROZYNEK (Presenter), Harvard University —  
Fabricating curved monolayers that mimic the properties from natural shells can help researchers to develop lighter,  
stronger and more flexible materials, better drug delivery and encapsulation systems, etc. Here we investigate  
synthetically made particle shells formed on droplets in a bulk fluid, in context of their mechanical properties. We used  
induced compressive stress on the particle shells by applying electric fields. In response to the stress, the particle  
monolayers folded and formed wrinkles with characteristic wavelengths. By deriving a simple model for particle shell  
wrinkling, we used these wavelengths to estimate the Young modulus and bending stiffness of the shells. Our results  
indicate that the elasticity of particle shells decreases with particle and shell size. We also show that deformation cycles  
induced by electric fields can be used to increase particle packing of monolayers on droplets and reduce wrinkle  
formation. These results suggest that in addition to probing mechanical properties, our approach can also be used to  
tailor the surface properties of shells, i.e. their permeability and roughness.

*Polish National Science Centre - OPUS program 2015/19/B/ST3/03055 and EU's Horizon programme under the MSCA  
grant agreement no. 752896.

L70.00175: Emergent Dynamics of Paramagnetic Suspensions under Toggled Magnetic Fields  
HOJIN KIM (Presenter), ERIC M FURST, Department of Chemical and Biomolecular Engineering, University of Delaware —  
Suspensions of superparamagnetic colloidal particles are subjected to toggled magnetic fields by switching on and off the field repeatedly.  
At sufficiently high field strengths, the microstructure of the suspension begins in a solid, gel-like state and anneals to  
droplet-like domains governed by time-averaged bulk and surface energies. Here, we study the effect of the toggled-field  
duty cycle. At frequencies range investigated in this study (0.33-5Hz) and high duty cycle ratio (0.8), the suspensions form  
column-like microstructures that do not evolve into energetically favorable states. In this case, the period the field is off is  
shorter than the particle characteristic diffusion time scale. As duty cycle decreases, however, microstructures grow to  
ellipsoidal-shape as a result of the sufficient time for particle diffusion. Under a small range of conditions (1.5-3.5 Hz, 0.2  
duty cycle ratio), we observe a new class of wavy-shaped microstructures with dynamics that exhibit a strong and  
continuous process of rotation, coalescence, and breakup. We attempt to understand these dynamics by considering the  
hydrodynamic forces exerted by a collection of thermal ratchets composed of particles in an asymmetric process of  
ballistic approach and diffusive relaxation.

L70.00176: ABSTRACT WITHDRAWN —

L70.00177: ABSTRACT WITHDRAWN —

L70.00178: Quantifying the surface tension of non-equilibrium colloidal fluids*  
CAROLINE RIEDSTRA (Presenter), JING  
WANG, RYAN J. MCGORTY, University of San Diego — Through the use of a colloid-polymer system employing temperature-  
sensitive pNIPAM microgel colloidal particles, we observe the nucleation and dissolution of colloid-rich liquid droplets. We  
use light-sheet microscopy to observe the formation and dissolution of colloid-rich droplets in three-dimensions and with  
optical sectioning. Our colloid-polymer system allows us to precisely tune the equilibrium state--mixed or demixed--by  
adjusting the sample temperature. With videos obtained from the light-sheet microscope, we perform image analysis of  
fluctuating droplets to extract the surface tension.

*American Chemical Society Petroleum Research Fund (57326-UNI10)

L70.00179: Probing viscoelasticity of dilatant fluid by solid projectile impact*  
KAZUYA EGAWA (Presenter), HIROAKI  
KATSURAGI, Nagoya University — Dilatant fluids offer complex rheological properties such as discontinuous shear  
thickening (DST). In recent years, various solid-impact experiments onto a dilatant fluid have been performed to reveal the  
physical properties of DST. Interesting phenomena such as dynamic jamming[S. R. Waitukaitis & H. M. Jaeger,Nature 487,  
205(2012)] and dynamic fracturing[M. Roche et al., Phys. Rev. Lett. 110 148304(2013)] have been reported in previous  
reserches. In addition, peculiar surface deformation of the vibrated dilatant fluid has also been found[F. S. Merkt et al.,  
Phys. Rev. Lett. 92 184501(2004)]. In this study, we perform a simple solid-projectile impact to a dilatant-fluid target to  
observe the penetration and rebound dynamics. In addition, to investigate the effect of vibration to the rheological  
properties of dilatant fluid, mechanical vibration is also applied to the dilatant fluid. From these results, the rebound  
timescale and restitution coefficient are measured. To characterize the viscoelasticity, we assume a simple attenuating-  
n oscillation model. Using the model, the effects of impact inertia, boundary conditions, and mechanical vibration to the  
rheological properties are systematically studied.

*JSPS KAKENHI No.18H03679
**L70.00180: Cratering and collapse of an inclined granular layer by oblique impact of a spherical projectile**

SHINTA TAKIZAWA (Presenter), RYUSEI YAMAGUCHI, HIROAKI KATSURAGI, Nagoya University — The oblique impact of a solid sphere onto an inclined granular layer is experimentally studied. The inclination angle of the target granular layer is varied from 0 to 33 degrees. The incident angle is also varied from 10 to 170 degrees. The range of impact velocity is 10 - 100 m/s. As a result, we observe following behaviors. When the incident angle is 90±10 degrees (almost normal impact), simple penetration of the projectile is observed. However, rebound or ricochet of the projectile occurs when the incident angle is smaller than 70 degrees (or larger than 110 degrees). When the target granular layer is steep enough, the transient crater produced by the impact is significantly modified by the asymmetric collapse of crater wall. Due to these complex effects, the final crater shape becomes complex. In this study, the characteristic dimensions of the crater (diameter, depth, and cavity volume) are measured and scaled by the effective impact kinetic energy transferred to the target by the projectile impact. While the crater volume can be scaled with a universal exponent, the specific volume value depends on the inclination angle.

*JSPS KAKENHI No. 18H03679

**L70.00181: Granular flow dynamics in a vibrating system from multiple points of view: Laboratory experiments, continuum modeling, and numerical simulations**

DAISUKE TSUJI (Presenter), Department of Earth and Environmental Sciences, Nagoya University, MICHIO OTSUKI, Graduate School of Engineering Science, Osaka University, HIROAKI KATSURAGI, Department of Earth and Environmental Sciences, Nagoya University — This study investigates granular flow dynamics in a vibrating system from multiple directions: laboratory experiments, continuum modeling, and numerical simulations. In the experiment, a conical granular pile is subjected to vertical vibration. Depending on its strength, granular particles are fluidized, and the shape of the pile is gradually relaxed. During the vibration, the relaxing pile is observed by a high-speed laser profiler. Based on those data, we have proposed a continuum model, which can predict how the flux of granular particles is determined. This model has only one fitting parameter that indicates the conversion efficiency from inputted vibration energy into granular transport energy. By comparing the experimental data obtained under various conditions, we have confirmed that the continuum model is satisfied and the conversion efficiency does not change in numerical simulations. We have also found that the velocity decreases exponentially from the surface of a pile, which suggests the presence of shear-band structure.

**L70.00182: Reversible Sol-Gel Transition of Silicone Complex Oils Using Hydrophobically Modified Attractive Hectorite Nanoplatelets as Rheology Modifiers**

DOYEON KIM (Presenter), DAEHWAN PARK, YEONG SIK CHO, JIN WOONG KIM, Hanyang University — Hectorite nanoplatelets (HNPs) have truly intriguing surface properties such as high specific surface area, high cation exchange capacity. Herein, we introduce a facile but robust approach to fabricate attractive hectorite nanoplatelets (AHNPs), in which the surface of HNPs was hydrophobically modified by using a cationic surfactant, dimethyl dioctadecyl ammonium chloride. We could finely disperse the AHNPs in the silicone oil by repeated high pressurized homogenization. The suspension rheological studies revealed that the AHNPs interacted to form a strong gel phase that exhibits the reversible shear stress-responsive sol-gel transition. Based on the chemical and structural characterization of AHNPs by using XRD, FT-IR, AFM, and TEM analyses, we interpreted this is attributed to the weak but long-range edge-to-edge interaction of AHNPs in the silicone oil, which is induced by the hydrogen bonding between small amounts of hydroxy groups at the edge of AHNPs. The AHNPs fabricated in this study are expected to be widely used as rheology modifiers for various oil-based complex fluids.

**Keywords:** Sol-gel transition, hectorite nanoplatelets, suspension rheology, rheology modifiers
L70.00183: Using Pressure Sensors To Characterize Avalanche Dynamics On A Conical Bead Pile*  
KATIE SHIDELER (Presenter), SUSAN LEHMAN, College of Wooster — A system of pressure sensors is used to characterize the dynamics of avalanches as they occur on a conical bead pile. The bead pile is a slowly driven critical system of roughly 20,000 steel beads, 3 mm in diameter, atop a circular base. We slowly drive the pile by dropping one bead at a time on the pile apex, and we record avalanches (the change in mass as beads leave the pile) occurring over the course of 60,000 bead drops. To complement this statistical information about the avalanche size probability distribution, we recently modified the base of the pile to add a system of eight pressure sensors that are monitored continuously during the data run. The sensors respond to shifting of forces within the pile during the avalanche, providing a way for us to characterize the types of bead motions occurring on the pile at different places on the pile and at different stages of the avalanche. With these sensors, we can characterize surface motion of beads on the pile independently from motion of beads off the pile. We are developing analysis techniques to characterize avalanches not just by the number of beads involved but also by the area of the pile participating in the avalanche; we propose an experimental definition for a system-spanning avalanche.

*Supported by NSF DMR 1560093.

L70.00184: Controlling Interactions in Active Matter Systems*  
JOSHUA STEIMEL (Presenter), SAGE MORELAND, University of the Pacific, ALFREDO ALEXANDER-KATZ, MIT — It has been demonstrated in a 2D colloidal monolayer composed of active spinning ferromagnetic and passive colloids that an ultra-long range attractive interaction emerges between active colloids. This interaction was induced by the activity of the spinning particles and mediated by the elasticity of the passive colloidal monolayer. We demonstrate through experiments and simulations that the range and dynamics of this emergent attractive interaction can be tuned or reversed by changing the mode of activity or the composition of the passive monolayer. With a 3D Helmholtz-coil like apparatus we can change the mode of activity from spinning to a top-like motion. These tops exhibit a similar attractive interaction at long-range, however they repel at distances less than four particle diameters, unlike the spinners. The tops also effectively anneal the passive monolayer into almost perfect crystal grains while the tops occupy sites on the grain boundaries effectively functioning as dislocation sources. Additionally, by doping the passive colloidal monolayer with small concentrations of passive particles of different sizes the monolayer behaves more elastically. This increases the range of the interaction but the dopants impede dislocation motion so the rate of attraction decreases.

*UOP

L70.00185: A Method to Measure Drag Coefficient of An Active Particle  
CHONG SHEN (Presenter), H DANIEL OU-YANG, Lehigh University — The drag coefficient of an active particle is important because it reveals the energy cost of swimming of an active particle, i.e., micro-organisms or swimming colloids. We introduce a method to obtain the drag coefficient for an active particle by separately measuring diffusion and sedimentation. We test this method on an active Brownian particle (ABP) that is driven by induced-charge electrophoresis of Janus particles. The diffusion is measured by tracking the single-particle motion and calculating the slope of mean squared displacement at long times. An effective temperature, $T_{\text{eff1}}$, can be calculated from diffusion. The particle density distribution in sedimentation is measured by counting the number of particles at different heights in the dilute region, where it obeys Boltzmann distribution with an effective temperature, $T_{\text{eff2}}$. With the assumption that the effective temperatures measured from the two methods are the same, the drag coefficient of ABP could be solved.

L70.00186: Macro and Micro Phase Separation in Mixtures of Active and Passive Particles  
RYAN TOLLEFSEN, Oregon State, JONATHAN LU, MIT, JOSHUA STEIMEL, University of the Pacific, ALFREDO ALEXANDER-KATZ (Presenter), MIT — Active spinning particles have been shown to phase separate when mixed with inactive particles. Here we present our work on controlling such phase separation to obtain microphase separation apart from the typical macrophase separation as a function of the reversal of the torque on the particles. Using this technique we can achieve control over the domain size as a function of the activity. We further show that the systems displays hysteresis as one changes the driving force. These results extend our knowledge of phase separation in mixtures of active and passive particles.
L70.00187: Snapping induced by controlled drying of polymer gels: from moving bonito flakes to jumping shells*

YONGJIN KIM (Presenter), University of Massachusetts Amherst, JAY VAN DEN BERG, Delft University of Technology, ALFRED CROSBY, University of Massachusetts Amherst — Dynamic changes in swelling states can induce life-like motions in bonito flakes placed on a hot Okonomiyaki. The shape transitions of these thin polypeptides films not only happen smoothly but also occur abruptly. Inspired by these generally occurring, but random events, we developed novel design principles for inducing self-repeating snapping motions during the drying process of swollen polymer disks that can persist until the depletion of the solvent. We demonstrate the ability to tune the system performance of these polymer devices to achieve either higher jumping kinetics (t ~ 2ms, Power ~ 370W/kg) or greater total energy output (Eout ~ 2J/kg) by controlling the geometry and boundary conditions. The performance of the snapping shells under different conditions was modeled with finite element analysis results. The systematic study on the snapping mechanism and its incorporation into engineered systems will bring great advantages for designing micro-scale, high-efficiency robots.

*This material is based upon work supported by, or in part by, the U. S. Army Research Laboratory and the U. S. Army Research Office under contract/grant number W911NF-15-1-0358

L70.00188: Temperature-invertible gel for manipulation of colloidal particles*

CATHY ZHANG (Presenter), SEAS, Harvard University, YA LIU, University of Pittsburg, CINDY WANG, University of Waterloo, XIAOGUANG WANG, STEFAN KOLLE, SEAS, Harvard University, ANNA CHRISTINA BALAZS, University of Pittsburgh, JOANNA AIZENBERG, SEAS, Harvard University — We develop an actuatable, responsive gel surface with a set of periodically spaced, temperature-invertible ridges and demonstrate that this surface enables us to create large, dynamic arrays of a range of colloidal particles through multiple physical mechanisms. The surface is constructed from a responsive gel that is spatially patterned on a topographically ridged surface to form gel ridges that collapse to form valleys. Using both experiments and numerical simulations, we show that we can obtain fine-grained control over the amplitude of surface topography, where the exact trajectory of the surface change depends on the rate and direction of temperature change. We then sediment particles on the surface and quantitatively demonstrate how the dynamic features of this gel enable us to pattern colloidal assembly and release under low Reynolds number shear flow. Finally, we introduce biological particles on the surface and show how such a multifunctional surface provides opportunities in creating antifouling surfaces whose properties can be tuned on demand.

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L70.00189: Competition and Cooperation among Chemically Active Sheets and Particles

ABHRAJIT LASKAR (Presenter), OLEG SHKLYAEV, ANNA CHRISTINA BALAZS, University of Pittsburgh — Using theory and simulation, we model the interactions among different, chemically active objects in a fluid-filled microchamber to establish conditions that drive these synthetic objects to display biomimetic competitive or cooperative behavior. The first objects are catalyst-coated, flexible sheets that generate buoyancy-driven fluid flows. The second objects are mobile tracer particles that move via diffusiophoresis towards higher reactant concentrations. We vary the sheets’ size and areal concentration of catalyst to tune the rate of reaction at this layer. Through these studies, we determine regions in phase space that lead to “aggressive” competition or “beneficial” cooperation within this dynamic, non-equilibrium system. As an example of competition, we show that when a low concentration of reactants is introduced into the solution, the larger sheet “catches” more tracers than a smaller sheet with a higher areal concentration of catalyst. Furthermore, we isolate conditions where single sheets acting alone do not capture tracers, but can trap the motile particles through cooperative interactions. These studies illustrate how purely physicochemical factors can promote behavior highly reminiscent of biological systems among active objects in fluidic environments.

L70.00190: Self-propelled Nanoparticles

JOHANNES SACHS (Presenter), PEER FISCHER, Micro Nano and Molecular System, Max Planck Institute for Intelligent Systems — Chemically active particles that self-propel due to catalytic reactions have been demonstrated at various length scales. It has, however, not yet been experimentally established how the propulsion of very small chemical motors scales with size. For this reason, we use a unique physical nanofabrication technique, based on physical vapor deposition, to grow catalytically-active Janus particles. These can be grown at defined lengths ranging from 20nm to 500nm, and can contain photocatalytic materials. This allows us to switch the particle between its passive and active state and thereby potentially from Brownian to enhanced diffusion. The observation of the particles’ motion is, however, far from trivial. We report our latest experimental results from a variety of analytical techniques, some of which can be used in situ.
L70.00191: Seal Zone Mechanics: Mechanical Stability of the Endograft/Aorta Interface  LUKA POCIVAVSEK (Presenter), University of Chicago, ENRIQUE CERDA, Universidad de Santiago de Chile, CHRISTOPHER SKELLY, ROSS MILNER, University of Chicago — Endovascular surgery (EVAR) has nearly replaced open aortic aneurysm repair. The long-term stability of EVAR repairs has come into question especially concerning graft endoleaks. Adhesion between the endograft and aortic wall is poorly understood and differs substantially from the traditional approach of kinematic fastening (suturing) utilized in open reconstructions. We provide a first general computational and theoretical approach to characterize and study seal zone mechanics. Our analysis (computational and analytical) shows that in the limit of no adhesion (or very weak adhesion) the endograft is always unstable relative to its position in the non-aneurysmal aorta. The energy driving graft displacement is the stored elastic energy in the aortic wall that comes from the oversizing of the stent graft. Adhesion between the aorta and endograft balances this stored elastic energy. This balance of adhesive energy to elastic energy is the central control parameter in the stability of the endograft. We develop a toy model for graft stability and apply it to patient specific geometries. Our work provides the first steps towards a robust physical understanding of the mechanics involved in EVAR stability that will allow for more durable future devices.

L70.00192: Controlling the strength of network materials: insights into failure mechanisms of random soft networks and composites*  SAI S DEOGEKAR, MOHAMMAD ISLAM, CATALIN PICU (Presenter), Rensselaer Polytechnic Institute — Fiber networks occur abundantly at all length scales in biological and artificial materials. In most cases, the network has structural role and hence its failure defines the strength of the material. Since these materials are structurally stochastic, heterogeneity plays a major role in determining the dominant failure mechanism. In this work we establish relationships between network strength and various parameters defining the network structure and properties of fibers and bonds [1]. These provide guidelines for network design. Further, we explore the role of heterogeneity in defining the strength and consider structures in which the fluctuations in the mechanical fields are controlled by adjusting various network parameters. Specifically, we consider networks with rigid inclusions (composite networks) and networks with stochastic structural perturbations of increasing amplitude. The results are discussed against insights related to stochastic continua, from the literature.


*L70.00193: In Situ TEM Imaging of Nanoscale Bubble Collapse and the Resulting Damage in Soft Matter*  GARTH EGAN (Presenter), XAVIER LEPRO CHAVEZ, EDMOND LAU, ERIC R SCHWEGLER, Lawrence Livermore Natl Lab — In recent years, it has been suggested that micron and sub-micron scale cavitation can occur in the human brain during explosive pressure wave, blunt trauma, or sports collision type events and that the resulting bubble collapse could be the main cause of damage leading to traumatic brain injuries. However, the behavior of sub-micron bubbles and their damagae potential to soft mater is not yet well understood. This is in part a result of the challenges associated with imaging on the necessary length and time scales. Here, we present the direct imaging of bubble collapse in a liquid cell using the Movie-Mode Dynamic Transmission Electron Microscope (MM-DTEM) at Lawrence Livermore National Laboratory. Bubbles were induced in ~1-3 µm of water using laser heating of 60 nm gold particles and typically found to collapse within 200 ns. Various polymers coated on the liquid cell substrates served as witnesses to potential damage. The experiments were performed in conjuncture with molecular dynamic (MD) simulations to further explore the dynamics of the system.

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L70.00194: Characterization of Novel Surfactant Molecules for Liquid Crystal Phase Triggering*  LINDA OSTER, BENJAMIN STRAIN (Presenter), University of Massachusetts Amherst, JESSICA SLEATOR, Springfield College, JAKE SHECHTER, FNU MANISHA, SANKARAN THAYUMANAVAN, JENNIFER ROSS, University of Massachusetts Amherst — Liquid crystal systems have the potential to produce macroscopic reactions from microscopic stimuli, making them exciting systems for triggered assemblies. Such triggerable systems are a cornerstone of biological systems’ ability to respond to their environment. Here, we use a novel surfactant composed of a trimer of amphiphilic molecules. These trimeric surfactants have three hydrophobic tails, with one tail varying in length. We have characterized the phase of the liquid crystal, 5CB, in spherical droplets as a function of surfactant type, surfactant concentration, and the diameter of the 5CB droplet. We find that small droplets, less than 11 µm in diameter, with high surfactant concentration, are more likely to be in the radial phase. We also find that the concentration and droplet sizes for the phase transition depended on the variable tail length.

*DoD ARO MURI 67455-CH-MUR
L70.00195: A Generalized Interfacial Structure Analysis Model for the Crystal Morphology: β HMX  JUNBEOM CHO (Presenter), WON BO LEE, Seoul National University — We studied the spiral growth mechanism of β-cycloctetramethylenetetranitramine (β-HMX) crystals with (0 2 0), (0 1 1), (1 1 0), and (1 0 1) faces, both experimentally and theoretically. In this work, a generalized interfacial structure analysis model is suggested to elucidate the morphology of β-HMX. There are two significant factors on crystallization procedure; 1) Molecular concentration near the surface of crystal 2) Whether pre-ordering of growth units occur during adsorption on the surface of each crystal faces. We investigated these through the Molecular Dynamic approach and metadynamics simulation, respectively. However, due to high conformational free energy barrier, pre-ordering of the growth unit does not occur and the factor 1 plays critical role in crystal growth, so the result of present work indicates that anisotropic local concentration of the growth units at the interface is the main factor determining relative growth rates, which was consistent with those of previous studies.

L70.00196: Computer simulations of associating liquid crystals*  DIMITRI BAPTISTE (Presenter), ELENA DORMIDONTOVA, Polymer Program Institute of Materials Science and Physics Department, University of Connecticut, Storrs, CT 06269 — Liquid crystals possess a range of interesting properties and are actively used in various technological applications. Reversible association, such as hydrogen bonding or metal-ligand complexation can provide additional mechanisms to control their properties leading to new applications including responsive functional materials. We employ Monte Carlo simulations using a spherocylinder model to predict the phase diagram for formation of the different ordered liquid crystalline phases in the presence of reversible associations. In particular we investigate the inter-relation between the strength of reversible association and the aspect ratio of liquid crystalline mesogens. The effect of confinement on system behavior will be discussed well.

*This work was supported by the Research Excellence Program (REP) of the University of Connecticut

L70.00197: Static and Dynamic properties of self-assembled hybrid wormlike surfactant micelles: Molecular Dynamics Study*  HARI SHARMA (Presenter), ELENA DORMIDONTOVA, Polymer Program, Institute of Material Science, Department of Physics, Storrs CT 06269, USA, University of Connecticut — Self-assembled wormlike surfactant aggregates have attracted considerable interest in both fundamental research and in practical applications due to their rich viscoelastic behavior and dynamic responsiveness to external conditions. Incorporation of polymer within wormlike micelles is shown to have enhanced stability and potentially superior viscoelastic properties. Co-assembly of polymers with surfactants in hybrid micelles is studied using coarse grained MD simulation with MARTINI force field and by united atom MD simulation with GROMOS53a6 force field. Simulations are carried out using GPU accelerated version of GROMACS 4.6.5. The change in micelle properties due to the presence of polymer is analyzed and the results are compared with available experimental data

*This research is supported by the ACS PRF#56803-ND6 and NVIDIA GPU grant.

L70.00198: Simulating the Response of Liquid Crystalline Elastomer Microposts to Light  JAMES WATERS (Presenter), University of Pittsburgh, JOANNA AIZENBERG, Harvard University, ANNA CHRISTINA BALAZS, University of Pittsburgh — Liquid crystalline elastomers (LCEs) represent a realizable physical system that can exhibit a large, non-linear response to an environmental stimulus. By adding light-sensitive moieties to the mesogens responsible for liquid crystalline order, one can create elastomers that will change shape in response to ultraviolet light. This provides a basis for a “write once, read many times” (WORM) memory. Information is encoded in an array of LCE microposts through a magnetic field during cross-linking, and then read out by introducing a light source. The system will return to its initial state upon removal of the stimulus, allowing the reading process to be repeated without altering the system. We developed a finite element simulation code to study components of such a system. Using our simulation method, we can predict the micropost deflection as a function of the preset nematic director and the incident angle of the light. We make comparisons to available experimental results and describe new findings that reveal how light can be used regulate the structure of an array of multiple, interacting LCE microposts. These studies point to new ways of utilizing the LCE arrays for technological applications.
Finally, we construct a phase diagram and correlate it w.r.t various phase diagrams of F127 available in the literature. 

The glass transition behavior is also observed at high temperature during gel melting. This illustrates the rate dependence of glass transition. The temperature associated with the glass transition decreases on increase in F127 concentration. Interestingly, the maxima in tan $\delta$ with $\omega$, followed by a glass transition as characterized by a peak in tan $\delta$. Interestingly, the maxima in tan $\delta$ shifts to lower temperatures with an increase in $\omega$, which illustrates the rate dependence of glass transition. The temperature associated with the glass transition decreases with increase in F127 concentration. The glass transition behavior is also observed at high temperature during gel melting. Finally, we construct a phase diagram and correlate it w.r.t various phase diagrams of F127 available in the literature.

In stationary state, the torque produced by friction force in the contact area balances that due to the external force generated by the active beads and the shell sticks to the substrate. In steady rolling state, rolling friction force balances the driving force, and the shell maintains a constant rolling velocity. Theoretical analysis shows a universal scaling relationship between the magnitude of driving force and shell velocity. This is a manifestation of viscoelastic nature of shell skin deformation dynamics during rolling motion. In accelerating state, energy supplied to the system by active beads exceeds the energy dissipation due to viscoelastic shell deformation in the contact area. Furthermore, the contact area of the shell with substrate decreases with increasing shell instantaneous velocity.

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L70.00200: Phase Behaviour of Block Copolymer Pluronic: A Rheological Perspective

KHUSHBOO SUMAN (Presenter), SAGAR SOURAV, YOGESH M JOSHI, Indian Institute of Technology Kanpur — We study temperature induced phase change of a block copolymer Pluronic F127 (PEO$_{100}$-PPO$_{65}$-PEO$_{100}$) over a concentration range of 20-35 wt%. While this temperature dependent phase change visually appears like a liquid-soft solid transition, termed as gel in the literature, there is a debate regarding precise microstructure of the soft solid state. In this work, we conduct frequency ($\omega$) sweep at various temperatures on F127 solution. We observe that irrespective of the concentration, F127 solution shows all the rheological characteristics of sol – gel – glass transition. This suggests the transition of a liquid-like sample to a space spanning percolated network, whose rheological characteristic is increase in tan $\delta$ with $\omega$, followed by a glass transition as characterized by a peak in tan $\delta$. Interestingly, the maxima in tan $\delta$ shifts to lower temperatures with an increase in $\omega$, which illustrates the rate dependence of glass transition. The temperature associated with the glass transition decreases with increase in F127 concentration. The glass transition behavior is also observed at high temperature during gel melting. Finally, we construct a phase diagram and correlate it w.r.t various phase diagrams of F127 available in the literature.

L70.00201: Anomalous apparent Poisson ratios in stiff semiflexible polymer networks

JORDAN SHIVERS (Presenter), SADJAD ARZASH, FRED C. MACKINTOSH, Department of Chemical and Biomolecular Engineering, Rice University — Fibrous networks of stiff athermal biopolymers such as collagen, a major structural component of the extracellular matrix, have been shown to exhibit anomalously large apparent Poisson ratios, i.e. significant transverse contraction under small applied longitudinal extension. Here we show that this effect can be understood in the context of a macroscopic mechanical phase transition from a bending-dominated regime to a stretching-dominated regime at a critical applied extension controlled by the network connectivity. We measure this effect using a variety of 2D and 3D model network structures and propose a phase diagram governing the transition as a function of connectivity and strain.

*This work was supported in part by the National Science Foundation (DMR-1826623 and PHY-1427654).

L70.00202: Computationally modeling the use of digital holographic microscopy to characterize colloidal fractal aggregates

JEROME FUNG (Presenter), Department of Physics & Astronomy, Ithaca College, SAMANTHA HOANG, Department of Physics, Wellesley College — Recent experiments suggest that digital holographic microscopy can be used to determine the average fractal dimension of an ensemble of colloidal fractal aggregates [1]. We present computational results that clarify the range of validity of this approach. In the experiments, an aggregate in solution is illuminated with coherent light, and the interference pattern formed between scattered and unscattered light, or hologram, is recorded. Fitting an effective-sphere scattering model to a hologram allows an effective radius $r_{\text{eff}}$ and effective refractive index $n_{\text{eff}}$ to be determined for each aggregate. Once $r_{\text{eff}}$ and $n_{\text{eff}}$ are determined for an ensemble of aggregates, a scaling relationship between $r_{\text{eff}}$ and $n_{\text{eff}}$ derived from the Maxwell Garnett effective medium theory yields the average fractal dimension. In our study, we computationally generate holograms of aggregates of known geometry (and hence, fractal dimension) and fit effective-sphere models to those holograms. We then determine whether the scaling relationship between $r_{\text{eff}}$ and $n_{\text{eff}}$ correctly determines the fractal dimension. Our results suggest that this approach is useful for loosely-packed aggregates whose extent does not greatly exceed the wavelength of the incident light.

L70.00203: Charge Transport and Electrode Polarization in Phosphonium Ionic Liquids Bearing Sulfonate and Carboxylate Anions*  MATTHEW HARRIS (Presenter), JAMES T COSBY, University of Tennessee, DURGESH WAGLE, GARY BAKER, University of Missouri, JOSHUA SANGORO, University of Tennessee — The impact of chemical structure on mesoscale organization and dynamics in a series of ionic liquids based on the tetradecyltrihexylphosphonium cation with various sulfonate and carboxylate anions has been studied using broadband dielectric spectroscopy and wide-angle X-ray scattering. The effects of anion structure on the mesoscale organization in the liquid and ion transport properties were interpreted based on current theoretical understanding. In addition, the phenomena of electrode polarization arising due to accumulation of ions at the electrode surface was analyzed with regard to mesoscale organization and bulk transport properties. Evidence of slow dynamics at the electrode/ionic liquid interface is observed and attributed to electrosorption.

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L70.00204: Charge transport and structural dynamics in deep eutectic mixtures (DEMs)*  STEPHANIE SPITTLE (Presenter), JAMES T COSBY, JOSHUA SANGORO, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — Charge transport and structural dynamics in choline chloride and glycerol mixtures were studied by broadband dielectric spectroscopy (BDS), dynamic mechanical spectroscopy (DMS), and differential scanning calorimetry (DSC). Slow sub-α relaxations are observed with BDS and DMS spectra. With decreasing choline chloride concentration, the sub-α dielectric relaxation, that is coupled to ion diffusion becomes much slower, while the slower mechanical relaxation is unaffected. This unexpected result is discussed within the framework of recent theories of ion transport and sub-α dynamics in small-molecule liquids.

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L70.00205: Charge Transport and Ion Dynamics in Imidazolium-Based Homo- and Tri-Block Poly(Ionic Liquid)s*  ALEXANDRE HORTON (Presenter), EMMANUEL MAPESA, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, MINGTAO CHEN, Chemistry, Macromolecules Innovation Institute (MII), Virginia Tech University, MAXIMILIAN F HERES, MATTHEW HARRIS, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, YANGYANG WANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, TIMOTHY LONG, Chemistry, Macromolecules Innovation Institute (MII), Virginia Tech University, BRADLEY LOKITZ, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JOSHUA SANGORO, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — Broadband Dielectric Spectroscopy (BDS) and Differential Scanning Calorimetry (DSC) are used to probe ion dynamics in a series of imidazolium-based tri-block copolymers, and compared to their homopolymer analogues. Two calorimetric glass transitions are observed and assigned to the charged and uncharged (polystyrene) blocks. Exchanging bromide with bis(trifluoromethylsulfonyl)amide counter-ion, a change of the glass transition temperature by over 50 K is realized, bringing forth an increase in the room-temperature dc-ionic conductivity by over six (6) orders of magnitude. By systematically varying the volume fraction of the charged block, we demonstrate that the choice of counter-ion is the key parameter influencing charge transport in these systems.

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L70.00206: Charge Transport and Dynamics of 2D-Conﬁned Polymerized Ionic Liquid Blends* KAITLIN GLYNN
(Presenter), THOMAS KINSEY, JOSHUA SANGORO, Chemical and Biomolecular Engineering, University of Tennessee, Knoxville —
The impact of geometrical conﬁnement on ion transport and dynamics in molecular and polymerized is investigated by broadband dielectric spectroscopy. The monomers of ammonium based ionic liquids are ﬁlled into unidirectional silica nanopores with mean diameters of 7 nm and studied by Raman spectroscopy in situ to monitor the progress of monomer conversion. Ionic conductivity is also probed at different degrees of polymerization and compared to bulk blends of molecular and polymerized ionic liquids. In agreement with similar systems recently published, it is found that the ionic conductivity in polymerized ionic liquids in nanopores is enhanced compared to their bulk counterparts. The results are discussed within the current theoretical frameworks for describing dynamics and transport in conﬁned polymers.

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L70.00207: Molecular Dynamics in Poly(Methyl Methacrylate)/Silica Nanoparticle Composites* EMMANUEL MAPESA
(Presenter), MICHAEL KILBEY, DAYTON STREET, JOSHUA SANGORO, University of Tennessee — Broadband Dielectric Spectroscopy (BDS) and Differential Scanning Calorimetry (DSC) are employed to study molecular dynamics and glass transition temperature (Tg) in poly(methyl methacrylate) (PMMA)/Silica-nanoparticle (NP) composites. By systematically probing the case of bare (non-functionalized) Si-NPs dispersed in PMMA matrix and that of PMMA grafted Si-NPs in PMMA matrix, we isolate the effects of each of these cases on dynamics and Tg. Furthermore, we show – for the structural relaxation process – that in addition to slowed down mobility, which is commonly reported in literature and assigned to dynamics at the NP-matrix interface, faster modes also arise due to conﬁnement effects. Scanning Electron Microscopy (SEM) is used to conﬁrm uniform dispersion of the NPs.

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L70.00208: 3D Printing Water-In-Water GANHUA XIE, University of Massachusetts Amherst, JOE FORTH, YU CHAI, PAUL ASHBY, BRETT HELMS, Lawrence Berkeley National Lab, THOMAS RUSSELL (Presenter), University of Massachusetts Amherst — One of the hallmarks of biology is the ability to compartmentalize and coordinate system functions, which has been difﬁcult to reproduce even in the most sophisticated synthetic mimics. We show how to fabricate ﬂexible, 3D structured water-in-water systems embodying both principles by using the interface of immiscible polymer solutions to generate tubular membranes held in shape by an elastic polyanion-polycation complex. Using a 3D printer, the length, shape, and diameter of printed tubules water-in-water systems can be controlled. We demonstrate directional diffusion and separation of ionic species conﬁned to each liquid phase according to their preferential afﬁnity for the polyelectrolyte in the opposite phase. By coupling compartmentalization with ﬂow-driven directed material transport, continuous molecular separation can be achieved in such water-in-water systems. A layer-by-layer strategy is also used to further strengthen and functionalize the ﬂexible tubules, signiﬁcantly extending the potential applications of these all-aqueous 3D printed tubular systems.

L70.00209: The Manipulation of Granular Media Flow Properties to Produce Stable, Uphill, Low Mass Bipedal Locomotion JONATHAN GOSYNE (Presenter), DANIEL GOLDMAN, Georgia Institute of Technology — Unlike multileg robots which are typically close to the ground and generally statically stable, bipedal robots must maintain balance in potentially shifting terrain. We performed a series of systematic experiments to enable a 7 degree-of-freedom planar biped walker (45cm tall) to robustly traverse granular inclines of 0 to 10 deg of 1 mm poppy seeds. Through gait optimization, center of mass (CoM) variation, and contact-based control, a robust open-loop (OL) system for low mass biped robotic locomotion on granular media (GM) was developed. This was achieved through manipulation of step length, L, and vertical CoM to minimize GM ﬂow at the foot-media boundary. Because of nonlinearities involved in GM deformation, typical body and joint stabilization techniques used in biped robotics over hard ground are insufﬁcient. Thus, we developed a control scheme encompassing static inertial changes through torso position, and contact area variation through dynamic expansion of the feet, to redistribute slip forces (characterized by foot intrusion or material ﬂow). This allows for robust, steady gait over GM, and have found that this scheme enables the robot to remain upright for the duration of a trial (5 gait cycles) 90% of the time, compared to consistent OL failure within 1 gait cycle.

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L70.00210: Versatile and Robust Soft Untethered Robots with Tight Integration of Soft Actuators and Flex Circuitry that Navigating Through Unstructured Terrains  
XIAONAN HUANG (Presenter), KITTY KUMAR, Carnegie Mellon University, MOHAMMAD KHALID JAWED, University of Los Angeles, California, ZISHENG YE, CARMEL MAJIDI, Carnegie Mellon University — Soft legged robots require robust walking dynamics and untethered functionality to approach the capability of their natural mammalian and reptilian counterparts to swiftly maneuver through unstructured environments. Achieving a soft robotics platform capable of biologically-relevant locomotion speeds depends on careful selection of actuators and electronics with soft materials and integration of power and control electronics. We demonstrate this with two untethered soft robotic testbeds that are both composed of flexible printed circuit board that integrates power and control electronics and electrically-powered soft limbs. The first implementation is a quadruped that is capable of walking at a maximum speed of 0.56 body length per second (3.2cm/s) and making 90 degree turns in two complete gait cycles (~5s). The second is a caterpillar-inspired robot capable of crawling with multiple gait at a speed of ~10mm/s over 25min. These robots are versatile and robust and have the capability of walking on a variety of surfaces, including up inclines, rocky terrain and poppy seeds, climbing over a half body height step, and maintaining continuous forward locomotion through confined space or after being dropped from an elevated height.

L70.00211: Self-Organization of Confined Binary Active Particles  
WILSON LUO (Presenter), MINGFEI ZHAO, XIN YONG, Mechanical Engineering, Binghamton University — The emergent behavior of active systems with self-propelled particles can be found in nature at many length scales, from bird flocking to bacteria swarming. Most previous studies investigate the collective behavior of systems with uniform morphology. However, many biological systems function via the interactions between multiple distinct organisms, often with differing geometries. In this study, we investigate the interactions between active particles of differing morphology. Our system consists of a mixture of self-propelled rod-like and sphere-like particles which exert pairwise repulsive forces and torques on each other in a 2D confined domain. Segregation of rods and spheres into distinct clusters can be observed without any adhesion. Our study will provide important insight in phase separation and cell sorting in co-cultured organisms.

L70.00212: Stress Localization of Thin Sheets in a Cylindrical Geometry  
NICOLE VOCE (Presenter), KLEBERT B FEITOSA, James Madison University, MARCELO AZEVEDO DIAS, Aarhus University — The ability to manipulate surface elastic instabilities finds many applications in engineering smart interfaces. We study the buckling phenomena of a thin cylindrical shell under axial compression that is constrained to slide onto an inner non-deformable pipe. Surface buckling is induced by immobilizing one end of the cylindrical shell and applying force to the other end. We study the geometry of the surface pattern, which is composed of rhombus shaped unit cells. We characterize the stress localization through shell thickness dependence and the out-of-plane deformation of the pattern after compression. Analysis of the curvature radii around the vertices of the unit cell shows that for thinner shells, the features get sharper suggesting that the stress is becoming more localized. Furthermore, as the thickness decreases, the distribution of the measured Gaussian curvature on the surface narrows around the zero mean indicating that the cylindrical shell is approaching the classical origami Yoshimura pattern.

L70.00213: Crystals and Liquids in Monolayers of Heavy particles  
NISHA LAMA (Presenter), ERIC WEEKS, YIJUN DONG, Physics, Emory University, PEIYAO WU, JAMES T KINDT, Chemistry, Emory University — We use brightfield microscopy to observe a dense monolayer of heavy colloidal particles sedimented to the bottom of a sample chamber. In our system, we control two parameters: particle concentration and Peclet number (Pe). Pe measures the relative importance of the gravitational force over the thermal effects and is directly proportional to the particle diameter. We are trying to find how Pe and particle concentration influence the packing structure of the sedimented monolayer. When we compared our simulation data with our experimental results, we found that our experiments were significantly less ordered than the simulations. This led us to investigate the influence of polydispersity in our samples and experimental issues created by the unintended influence of gravity when the slide has a slight tilt away from the horizontal.
L70.00214: Compressible Colloidal Clusters from Pickering Emulsions and Their DNA Functionalization* IN-SEONG JO (Presenter), School of Chemical Engineering, Sungkyunkwan University, JOON SUK OH, Center for Soft Matter Research, New York University, SHIN-HYUN KIM, Department of Chemical & Biomolecular Engineering, KAIST, DAVID J PINE, Center for Soft Matter Research, New York University, GI-RA YI, School of Chemical Engineering, Sungkyunkwan University — In this study for DNA-mediated colloidal assembly with pre-assembled clusters, DNA sequences, areal density of DNA, particle number density and size ratio are key parameters for determining equilibrium structures. We developed a simple and facile method to produce compressible colloidal clusters were prepared by assembling azide-functionalized non-crosslinked polymer particles using fluorinated oil-in-water emulsion droplets. The particles were adsorbed onto the droplet interface, which were packed to form clusters during slow evaporation of the oil. Because we use non-crosslinked polystyrene particles for colloidal clusters instead, which can be merged partially through solvent annealing, the compression ratio can be precisely controlled. Then, the clusters were coated by DNA using an strain-promoted alkyne-azide cycloaddition reaction. As the particles are not crosslinked, the shape of the DNA-coated clusters can be further modified to control the compression ratio through plasticization.

*We acknowledge support from the National Research Foundation of Korea (NRF-2017M3A7B8065528, NRF-2017R1A5A1070259 and NRF-2014M3A9B8023471). DP acknowledges partial support from the US National Science Foundation under Award Number DMR-1610788.

L70.00215: Tuning the Temperature-Dependent Thermal Conductivity via Complex Colloidal Superstructures* FABIAN NUTZ, MARKUS RETSCH (Presenter), Department of Chemistry, University of Bayreuth, 95447 Bayreuth, Germany — The ability to precisely tune the temperature dependence of the thermal conductivity possess a vital challenge to develop and conceive future heat management devices. In this contribution, we demonstrate the vast potential of polymer colloidal crystals to address and master these challenges. We achieve this goal based on the constriction-controlled thermal transport through well-defined colloidal crystal superstructures. These colloidal superstructures are specifically built by tailor-made latex particles with distinct glass transition temperatures. We exploit their multiresponsive film formation at various temperatures to demonstrate unprecedented control over thermal conductivity at temperatures between 25 °C and 200 °C. Based on the film formation process, we can irreversibly increase the thermal conductivity by a factor of about three. We show how to control:

i) the temperature, where the increase in thermal conductivity happens
ii) the sharpness of the thermal conductivity increase
iii) the height of the increase in thermal conductivity
iv) the incorporation of a multistep increase in thermal conductivity

*This project was funded by the Volkswagen Foundation (Lichtenberg professorship). Additional support was provided by the SFB 840.

L70.00216: WITHDRAWN ABSTRACT

L70.00217: de Gennes Narrowing in Colloidal Discs NAMITA SHOKEEN (Presenter), ASHIS MUKHOPADHYAY, Wayne State University — We studied the wave vector (q) dependence of relaxation time (τ) for different volume fractions of aqueous solutions of microspheres and microdiscs in concentrated regime. We observed characteristic peaks in τ(q) at certain q values. Such peaks indicate slow relaxations of structural rearrangements. These peaks match very well with the peaks in structure factor S(q) and radial distribution function g(r) calculations. This phenomena is called as de Gennes narrowing.

L70.00218: Dynamics of Polydisperse Emulsion Systems in a T-Shaped Chamber KENNY NGUYEN (Presenter), XIN DU, Department of Physics, Aquinas College — Emulsions consist of droplets of one liquid mixed into another immiscible liquid. Our samples are oil-in-water emulsion droplets flowing through a T-shape chamber. By means of microscopy, we studied the influence of the polydispersity on the dynamics of emulsion droplets, analyzed the deformation profile of the droplets and compared the emulsions flow with stratified liquid flow. Our experimental results indicate that (1) monodispersed sample exhibited more jammed behavior than the polydispersed samples; (2) particles near the boundary move differently from those in the middle at the T-junction; (3) The flow of emulsion system exhibit more turbulence comparing with stratified flow; (4) smaller droplets moved faster and are less affected by cooperative motion of neighbor droplets.
Effect of Interfacial Rheology on the Properties of Polymerized High Internal Phase Emulsions

MUCHU ZHOU (Presenter), REZA FOUDAZI, Chemical and Materials Engineering, New Mexico State University — High internal phase emulsions (HIPEs) can be created when the volume fraction of dispersed phase exceeds 74%. Porous polymer materials can be produced through HIPE-templating approach. Polymerized high internal phase emulsions (polyHIPEs) are formed by polymerization of the continuous phase of HIPEs that contains the organic monomers and subsequent extraction of the dispersed phase. The porous interconnected structure of polyHIPE is achieved through the formation of small holes (also known as windows) on the polymer wall between droplets. The polyHIPEs can be used as adsorbents, ion-exchange resins, separation membranes, and scaffolds in tissue engineering due to their high porosity and low density. In order to meet the requirements of the specific applications, strategies to control the pore size and window size of the polyHIPEs are necessary to be investigated. In this study, different surfactant systems and mixing methods are employed to prepare the polyHIPEs with different pore and window sizes. We also study the effect of interfacial rheological properties of different surfactant systems at the interface of the aqueous and oil phases on the morphology, and thus, mechanical properties of final polyHIPEs.

Foam-templated macroporous polymers

RYAN ZOWADA (Presenter), REZA FOUDAZI, Chemical Engineering, New Mexico State University — Foam templates were produced by rapid gas dispersion into an aqueous monomer solution at various dispersion concentrations. Then, the templates were cured through free radical polymerization to obtain polydispersed solid foams. The foams were analyzed for their stability by measuring coarsening rates and drainage times to quantify and compare the effect of gas dispersion concentration. The foams exhibited yield stress with pseudoplastic behavior, so their flow curve was fitted using Herschel-Bulkley model to calculate the required foaming energy. The benefits of using a gas dispersion phase instead of a liquid phase is an increase in starting material efficiency and eliminating typical removal step of the disperse phase in foam-templating compared to emulsion-templating. We investigated the morphological characteristics and mechanical properties of obtained porous polymers from foam- and emulsion-templating methods.

Foamability of Aqueous Solutions of Charged Surfactants and of Surfactant-Polymer Mixtures

CARINA MARTINEZ (Presenter), Chemical Engineering, University of Illinois at Chicago, SOPHIA HOROWICZ, University of Chicago, MATTHEW WAGENER, VIVEK SHARMA, Chemical Engineering, University of Illinois at Chicago — Dynamic adsorption of a freshly created interface is intimately linked with the rate of mass transfer of surfactant from liquid sub-phase to the interface, and this adsorption-limited kinetics is said to impact the stability of the newly formed interface. Addition of polymer to a surfactant solution affects the dynamic adsorption and the rheological response due to the formation of association complexes. Dynamic surface tension refers to the time dependent variation in surface tension, which is related with the rate of mass transfer of a surfactant from liquid sub-phase to the interface. In this study, we apply the method of maximum bubble pressure tensiometry for the measurement of dynamic surface tension effects at extremely short (1-50 ms) timescales. We discuss the overall adsorption kinetics of charged surfactants and the influence of added polymer on dynamic surface tension. Finally, we examine how pinch-off dynamics and rheological properties are modified in the presence of added polymers by including a critical examination of shear and extensional rheological responses.

Viscous fingering in lyotropic chromonic liquid crystals

SHUANG ZHOU (Presenter), University of Massachusetts Amherst, QING ZHANG, IRMGARD BISCHOFBERGER, Massachusetts Institute of Technology — We studied the Saffman-Taylor instability in a Hele-Shaw cell containing nematic lyotropic chromonic liquid crystals. The coupling between the flow field and director field changes the effective viscosity of the liquid crystal, and therefore influences the patterns formed by the injected liquid. In particular, the hugely different viscosities for different distortion modes in chromonic liquid crystals play important roles in determining the patterns. Besides changing the viscosity of injected fluid and the injection rate, we can also control the pattern by changing the concentration of chromonics in water solution, which tunes the anisotropic viscosities. By quantitatively comparing the local director field with flow field, we show that the intrinsic anisotropy of the displaced liquid can lead to rich and controllable patterns in a Hele-Shaw cell setup.

*New faculty start-up fund of UMass Amherst
L70.00223: Omnidirectional optical band gap for circularly polarized light in a nanocomposite cholesteric elastomer. Guillermo Reyes (Presenter), Adrian Reyes, National Autonomous University of Mexico — In recent years, Liquid Crystal Elastomers (LCE) have become very important in research, due to its possible applications to manufacture many optical devices as filters, actuators or transducers.

LCE combine properties of liquid crystals and elastic properties of polymers, these materials are composed by mesogens joined into a chain of polymers, their orientations may be changed by action of mechanical forces. Due to orientation change of mesogens in LCE, optical properties, as reflectance or transmittance can be modified. Reflectance and transmittance in LCE can be substantially modified by the effect of a particulated medium.

In this work we have studied a nano-composite consisting of a chiral elastomer doped with metallic nano spheres. We show that Bragg phenomenon occurs in this chiral media, hence this composite works as a complex circular polarization optical controller handle by the filling factor of nano spheres, incidence angle of light and stretching of the sample.

L70.00224: Fast electro-optical switching of dichroic dye-doped antiferroelectric liquid crystals without polarizers. Veridiana Garcia Guimarães, Department of Physics, Universidade Estadual de Maringá, Junren Wang, Liquid Crystal Institute, Kent State University, Steven Planitzer, Department of Physics, Kent State University, Rafael Soares Zola, Department of Physics, Universidade Estadual de Maringá, Antal Istvan Jakli (Presenter), Liquid Crystal Institute, Kent State University — In this work we investigate alignment and electro-optical properties of a room temperature dye-doped antiferroelectric liquid crystal mixture. We achieved extremely uniform alignment on macroscopic scale of thin cells with the combination of proper surface alignment and electric field treatment. We have also successfully demonstrated that two films of dye-doped antiferroelectric liquid crystals in their antclinic chiral smectic C (SmC*) phase can be used to switch the transmitted light intensity between dark and bright states without the need of polarizer filters. We also demonstrate that one could get either normally dark or bright states. Normally dark states can be useful in number of applications such as in privacy windows or smart refrigerators. A normally transparent display has applications in plethora of other areas, such as navigation systems built in windshields, in goggles, or smart windows.

*This research was supported by Valeo Lightning Systems and by CAPES Foundation – PDSE [88881.133505/2016-01].

L70.00225: Amplification of chirality of lyotropic chromonic liquid crystals confined to capillaries. Sujin Lee (Presenter), Elsa Reichmanis, Jung Ok Park, Mohan Srinivasarao, Georgia Institute of Technology — Lyotropic chromonic liquid crystals (LCLC) molecules are achiral, that have plank-like rigid aromatic cores and hydrophilic ionic groups at the peripheries. Upon confinement of LCLCs in cylindrical capillary, the director adopts a doubly twisted director configuration, due to unusually small twist elastic constants in LCLCs. Since the LCLC is achiral, they possess multi domain with equal probability of both handedness which is separated by Neel walls. In this work, we report that by adding minute amounts of chiral molecules to LCLCs with a doubly twisted director configuration possessing both handedness, the whole system can be transformed into a single handedness. The structure and charge of the chiral molecules were also studied. By investigating the effect of various chiral molecules within this LCLCs in capillary system, we expect to understand chirality amplification mechanisms.

L70.00226: Repeated rehydration of lipid films as a method to mix phospholipids without the use of organic solvents. Eric Oropeza-Guzman (Presenter), Soft & Bio Lab, CINVESTAV Monterrey, México — A technically simple method for mixing phospholipids of different species without using organic solvents or additives has been developed. Based on the reported literature regarding aqueous lamellar systems, phospholipid interaction parameters, and lipid diffusion coefficients, we hypothesized that the repeated drying and rehydration of a multispecies phospholipid sample, using only deionized water, should produce a uniform distribution of phospholipid molecules. Different lipid films of binary mixtures of zwitterionic and anionic glycerophospholipids were prepared using this method. The resulting films were reconstituted in vesicular form and compared to controls prepared with organic solvents by differential scanning calorimetry. The calorimetric scans revealed no significant differences between samples and controls for any of the tested mixtures. This finding suggests that the proposed technique creates a product with equivalent compositional homogeneity than the conventional method. From an environmental, health and safety standpoint, we are confident that this technique can contribute to the implementation of sustainable chemical practices, especially in industrial settings where organic solvents are tightly regulated.
L70.00227: Self-assembly of cyclic polygon shaped fluid colloidal membranes through pinning  

LACHIT SAIKIA (Presenter), PRERNA SHARMA, Department of Physics, Indian Institute of Science, Bangalore, India — An isotropic mixture of rod-like viruses self-assembles into 2D fluid monolayer membranes in presence of non-adsorbing polymer through depletion attraction. These membranes are circular in shape due to surface tension. Surprisingly, cyclic polygon shaped colloidal membranes form when isotropic mixtures of two kinds of geometrically different rods are mixed with depleting polymer. Long rods form faceted core of the cyclic polygon whereas short rods phase separate into lobes that are connected through pinning points. We demonstrate that the origin of this stable out of equilibrium anisotropic shape of the membranes lies in the phenomenon of how one fluid membrane spreads over another in presence of disorder/pinning sites. We show that the pinning sites are not topological defects rather accumulation point of rods that are significantly different. Our results show a unique counter-intuitive scenario where disorder leads to self-assembly of ordered structure.

L70.00228: Structure of Lung-Mimetic Multilamellar Bodies with Lipid Compositions Relevant in Pneumonia*  

DYLAN STEER (Presenter), SHERRY LEUNG, HANNAH MEISELMAN, University of Illinois at Urbana-Champaign, DANIEL TOPGAARD, Division of Physical Chemistry, Lund University, CECILIA LEAL, University of Illinois at Urbana-Champaign — Pneumonia is the leading cause of death amongst captive dolphins. While the pathology of pneumonia is understood at a macroscopic level, recent results show that changes in material chemistry at the lung-air interface plays an important role in symptoms, though the physical basis is unknown.[1] Healthy lungs are coated by a thin, hydrated biological composite composed primarily of amphiphilic lipids and a small amount of proteins. These self-assemble into liquid-crystalline phases which can reduce the fluid-air interfacial surface energy to near 0. In diseased lungs abnormally high concentrations of cardiolipin, a highly charged and highly unsaturated lipid, and Ca^{2+} can be found. Here we observe using small angle X-ray diffraction (SAXS) that addition of cardiolipin dehydrates the lipid membranes, contrary to predictions of pure electric double layer theory. The physical cause for these effects and the influence of Ca^{2+} is studied using wide angle X-ray diffraction (WAXS) and solid state nuclear magnetic resonance (ssNMR).


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L70.00229: Colloidal Gelation of Thermo-Responsive Microgel Mixture Suspensions*  

SAORI MINAMI (Presenter), Kyoto Institute of Technology, TAKUMI WATANABE, DAISUKE SUZUKI, Shinshu University, KENJI URAYAMA, Kyoto Institute of Technology — Concentrated suspensions of microgels composed of thermo-responsive polymer such as poly(N-isopropylacrylamide) (PNIPA) exhibit various states, i.e., repulsive glass, dispersion, (attractive) colloidal gel, depending on temperature (T), particle concentration, surface charge density. The heating reduces the volume of the microgels, and also substantially changes the type of interparticle interaction from repulsive to attractive when T across the LCST, resulting in the formation of colloidal gel. Present work focuses on the dense suspensions of the microgel mixtures of PNIPA and the homologue with different LCSTs. We show that the rheological properties of the mixture suspensions are pronouncedly affected by the mixing ratio. The T-dependent viscoelastic properties of the mixture suspensions are interpreted by considering the T-dependence of the volume fraction and the type of interparticle interaction of each component.[1] [1] S. Minami, T. Watanabe, D. Suzuki, K. Urayama, Soft Matter, 14, 1596-1607, 2018

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L70.00230: Thermoelastic heterogeneity in a model metallic glass from molecular dynamics calculations*  

BAOSHUANG SHANG (Presenter), Laboratoire Interdisciplinaire de Physique, PENGFEI GUAN, Beijing Computational Science Research Center, JEAN-LOUIS BARRAT, Laboratoire Interdisciplinaire de Physique — It is well known that the elastic properties of amorphous systems are heterogeneous, leading to peculiarities in vibrational spectra and thermal properties. In this work, we investigate the heterogeneity in thermoelastic properties, and more precisely in the thermal expansion coefficient, in a model metallic glass. We find heterogeneities that are similar - in terms of length scales - to those in elastic constants. It has been suggested that such heterogeneities could be the reason for "cryogenic rejuvenation" processes observed under thermal cycling in several experiments. We investigate this hypothesis by comparing the values of the local yield stresses with the stresses generated by heterogeneities in thermal dilation.

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**L70.00231: Terahertz Time-Domain Spectroscopy and Low-Temperature Specific Heat Investigation of Vitreous Glucose**

TATSUYA MORI (Presenter), MIKITOSHI KABEYA, Division of Materials Science, University of Tsukuba, SUGURU KITANI, Laboratory for Materials and Structures, Tokyo Institute of Technology, YASUHIRO FUJII, Department of Physical Sciences, Ritsumeikan University, JAE-HYON KO, Department of Physics, Hallym University, AKITOSHI KOREEDA, Department of Physical Sciences, Ritsumeikan University, HITOSHI KAWAJI, Laboratory for Materials and Structures, Tokyo Institute of Technology, SEIJI KOJIMA, Division of Materials Science, University of Tsukuba — The boson peak is a low energy excitation universally observed in the THz region of the amorphous materials. The boson peak of infrared spectra appears in the spectra of $a(v)/v^2$ [$a(v)$ is the absorption coefficient]. In this study, we performed terahertz time-domain spectroscopy on glassy glucose to investigate the boson peak dynamics. Moreover, we determined infrared light-vibration coupling coefficient using the $a(v)$ and vibrational density of states obtained from the low-temperature specific heat measurement.

*This work was partially supported by JSPS KAKENHI Grants No. 17K14318, No. 18H04476 and No. 26287067, and the Asahi Glass Foundation.

**L70.00232: Mechanics of filamentous growth in soft materials**

NICOLAS BRUOT (Presenter), NINO KUKHALEISHVILI, Institut de Physique de Nice, CNRS, Université Côte d’Azur, CHARLES PUERNER, D. THOMPSON, Institut de Biologie de Valrose, CNRS, INSERM, Université Côte d’Azur, AGNESE SEMINARA, Institut de Physique de Nice, CNRS, INSERM, Université Côte d’Azur, MARTINE BASSILANA, ROBERT ARKOWITZ, Institut de Biologie de Valrose, CNRS, INSERM, Université Côte d’Azur, XAVIER NOBLIN, Institut de Physique de Nice, CNRS, Université Côte d’Azur — Candida albicans is a yeast that grows in the shape of a filament with a tip continuously moving forward in the nutritious medium. The forces at the tip are driven by the internal pressure of the cell and are strong enough to induce indentation and penetration in materials such as the human tissues. This allows *C. albicans* to invade a host, with possibly lethal consequences, especially in immunodeficient individuals. How the growth rate and direction depend on the material properties provide indications of the internal behaviour and response of the organism to its environment. These can be better understood by growing filaments in controlled substrates, and even reducing experiments to observing the penetration of thin solids in soft materials. We present here experiments of both the indentation of PDMS by a micrometric-sized sphere, and the observation of *C. albicans* growing in PDMS substrates containing fluorescent particles where the deformations of the material can be monitored. We expect with such experiments to improve and develop models of the mechanics of penetration in brittle and elastic materials depending on their mechanical properties such as the Young modulus, the viscosity and the adhesive properties.

*We acknowledge funding from the ANR 2016 project "FORFUNIGO".

**L70.00233: DNA-Functionalized 100 nm Polymer Nanoparticles from Block Copolymer Micelles**

JEONGHOON YOON (Presenter), SAEROM LEE, IN-SEONG JO, School of Chemical Engineering, Sungkyunkwan University, JOON SUK OH, Department of Physics and Center for Soft Matter Research, New York University, DAVID J PINE, Department of Chemical & Biomolecular Engineering, New York University, TAE SOUP SHIM, Department of Chemical Engineering and Department of Energy Systems Research, Ajou University, GI-RA YI, School of Chemical Engineering, Sungkyunkwan University — DNA-mediated self-assembly of colloidal particles is one of the most promising approaches for constructing colloidal superstructures. For nanophotonic materials and devices, DNA-functionalized colloids with diameters of around 100 nm are essential building blocks. Here, we demonstrate a strategy for synthesizing DNA-functionalized polymer nanoparticles (DNA-polyNPs) in the size range of 55~150 nm using block copolymer micelles as a template. Diblock copolymers of polystyrene-b-poly(ethylene oxide) with an azide end group are first formed into spherical micelles. Then, micelle cores are swollen with styrene monomer and polymerized, thus producing PS nanoparticles with PEO brushes and azide functional end groups. DNA strands are conjugated onto the ends of the PEO brushes on the surface of PS particles through a strain-promoted alkyne-azide cycloaddition reaction (SPAAC). The DNA-polyNP with complementary sequences show thermally-responsive association and dissociation behavior.

*This work was supported by grant nos. NRF-2010-0029409, 2017M3A7B8065528 and 2016R1C1B2016089 through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and Future Planning (MSIP). J.S.O. and D.J.P. were funded by the US Department of Energy (DOE) grant no. DE-SC0007991.
**L70.00234: Geometry-driven self-assembly of interfacial sheets**  
ZACHARIAH SCHRECENGOST (Presenter), JORDAN V BARRETT, Physics, Syracuse University, VINCENT DÉMERY, Physics, Université de Lyon, JOSEPH D PAULSEN, Physics, Syracuse University —  
When a linear elastic material is made sufficiently thin, the energy required to bend the sheet is orders of magnitude lower than the energy required to stretch it. Placing this sheet on a liquid interface introduces another energy scale. In the case of an inextensible sheet with zero bending cost – an asymptotic limit that is readily achieved in experiments using ultrathin polymer films – the sheet will bend and wrinkle in such a way as to minimize the exposed liquid surface area [1]. However, predicting the overall shape of the film is a nontrivial optimization problem that is highly sensitive to the curvature of the interface or the boundary conditions. We use Surface Evolver simulations and analytic calculations to study the energetic cost of placing an ultrathin elastic disc on an arbitrary local topography of moderate curvature, from spherical to ellipsoidal to saddle-shaped interfaces. We establish scaling laws that relate the system energy to the principal radii of curvature, which capture our measurements spanning nearly three decades in curvature. This work paves the way for designing curved interfacial topographies that promote self-assembly via energy minimization. [1] Paulsen et al., Nat. Mater. 14 (2015).

**L70.00235: Hierarchical Self-assembly, Spongy Architecture and Phase States of Laponite in water-Alcohol mixtures**  
RAVI KUMAR PUJALA (Presenter), Physics, University of Hyderabad —  
We propose an alternative method to tune the electrostatic interactions to obtain a transition from a repulsive to an attractive system of nanoplatelets by increasing the alcohol concentration, i.e. increasing the Bjerrum length. A phase diagram of Laponite® in alcohol solutions has been proposed, which clearly demarcates regions of stable sol, unstable sol, transparent gel, turbid gel, glass, and flocculation. A new class of soft materials, called nanoclay-organogels, was deeply explored using confocal and scanning electron microscopy that depicted spongy architecture and presence of nano and micron size pores inside the gel matrix indicating the hierarchical self-assembly of the nanoplatelets in the binary solvent. Universal power-law scaling of storage modulus and yield stress with alcohol concentration was observed. We have extensively examined the dispersion stability, aggregation and gelation behaviour of Laponite nanoplatelets in different alcohol -water binary solvents, thereby proposing a universal description of nanoclay dispersion in alcoholic solutions, which is poorly probed and marginally understood in the literature.

*RKP acknowledges receiving the Department of Science and Technology INSPIRE Faculty Award grant [DST/INSPIRE/04/2016/002370].

**L70.00236: Liquid Magnets**  
XUBO LIU (Presenter), Beijing University of Chemical Technology, NOAH KENT, ALEJANDRO CEBALLOS, JOE FORTH, Lawrence Berkeley National Lab, SHAOWEI SHI, DONG WANG, THOMAS RUSSELL, Beijing University of Chemical Technology —  
Dispersions of carboxylated iron oxide magnetic nanoparticle (Fe₃O₄-COOH MNP) with a diameter of 30nm are a type of ferrofluid that is superparamagnetic under normal conditions. Here, we demonstrate a simple approach to reversibly transform a paramagnetic ferrofluid droplet into the ferromagnetic state by immersing it into an immiscible liquid containing ligands, that can interact with the particle to form MNP-surfactants that subsequently are brought into the jammed state. As a result, a novel ferromagnetic liquid device, namely a liquid magnet, is generated in one step. The liquid magnet is a functional core-shell structure, with a superparamagnetic fluid core wrapped by a monolayer shell of jammed ferromagnetic MNPs-surfactants, where the thermal energy of the active MNPs is weakened significantly by anchored ligands. The magnetic dipole moment of the ferrofluid is able to be maintained indefinitely. There is a measurable coercivity and remnant magnetization of the ferromagnetic liquid droplet. Under the influence of a rotating permanent magnet, the liquid droplets are seen to rotate at an angular velocity that increases with decreasing droplet size. The angular velocity is also found to increase with increasing time and reach a limiting velocity.
L70.00237: Dimerization of Annular Sector Particles*  
ELYSE ROOD (Presenter), SCOTT FRANKLIN, Rochester Institute of Technology, THEODORE ANTHONY BRZINSKI, SYKES CARGILE, Haverford College — We study annular sector particles (ASPs), open semi-circular rings characterized by two dimensionless numbers: the subtended opening angle and the ratio of inner and outer radii. The ASPs are placed in an annulus with a rotating, ridged ring above them. Applying a torque to this ring exerts a shear stress on the quasi-2D packing of ASPs. Within the annulus, if two ASPs are within the outer radius distance from each other they have the potential to intersect with each other. This entangled pair of ASPs is defined as a dimer. The movement of ASPs results in the formation as well as annihilation of dimers, known as dimerization and de-dimerization. From images of the annulus and computational analysis, the location and orientation of each ASP is determined. From this information, we can identify dimers and classify them based on the dot product of ASP orientations. Opposite facing dimers, which have the ability to form chains, are defined by a negative dot product; similar facing dimers are defined by a positive dot product. We investigate the distribution of structure types and how they evolve with shear.

*This material is based upon work supported by the National Science Foundation under Grant No. CBET-#1438077

L70.00238: STATISTICAL AND NONLINEAR PHYSICS —

L70.00239: Predicting Network Edge Count and Fragmentation under Vertex Percolation Processes*  
NICHOLAS BRUNK (Presenter), Intelligent Systems Engineering, Indiana University Bloomington, WILLIAM BUTSKE, Department of Mathematics, Rose-Hulman Institute of Technology, JAMES ALEXANDER GLAZIER, Intelligent Systems Engineering, Indiana University Bloomington — Network and graph-based percolation theory are applicable to a broad range of disciplines throughout the natural, life, and social sciences. We present a graph-based vertex (site) percolation study empirically quantifying – as a function of vertex occupation fraction – the number of edges (bonds) formed, the extent of fragmentation of the network, and the scaling of percolation thresholds with the mean vertex degree of the graph. The edge count is shown to be quadratically dependent upon the vertex occupation fraction with no unknown fitting parameters, thus applying universally - that is, to all networks - with minimal error. It may be used to predict, for example, the number of nearest neighbor bonds remaining in a lattice (e.g. translational degrees of freedom in a spatial lattice) or the number of friendships remaining as a social network is deconstructed (e.g. due to account closure on social media or mortality). For well-behaved networks with a reasonably low variance in the vertex degree distribution, the latter relations may be used to predict fragmentation: both the percolation threshold and, subsequently, the number of distinct connected components in the network at a given occupation fraction.

*This work was partially supported by NIH R01-AI118933 and NSF 1720625.

L70.00240: Optimal deployment of resources for maximizing impact in spreading processes  
ANDREY LOKHOV (Presenter), Los Alamos National Laboratory, DAVID SAAD, Aston University — The effective use of limited resources for controlling spreading processes on networks is of prime significance in diverse contexts, ranging from the identification of “influential spreaders” for maximizing information dissemination and targeted interventions in regulatory networks, to the development of mitigation policies for infectious diseases and financial contagion in economic systems. Solutions for these optimization tasks that are based purely on topological arguments are not fully satisfactory; in realistic settings, the problem is often characterized by heterogeneous interactions and requires interventions in a dynamic fashion over a finite time window via a restricted set of controllable nodes. The optimal distribution of available resources hence results from an interplay between network topology and spreading dynamics. We show how these problems can be addressed as particular instances of a universal analytical framework based on a scalable dynamic message-passing approach and demonstrate the efficacy of the method on a variety of real-world examples.

L70.00241: Electromechanical Instability of a Dielectric Elastomer Balloon  
SHENQIANG CAI (Presenter), University of California, San Diego — As an electroactive polymer, dielectric elastomer has been recently intensively explored in different engineering applications, ranging from soft robot, haptic devices, artificial muscle to energy harvesting system. In the applications, inflated dielectric elastomer balloons of various shapes have been widely adopted. Some recent experiments have shown unusual instability modes in dielectric elastomer balloon, when it is subjected to an internal pressure and electric voltage. In the talk, I will present our theoretical analysis of electromechanical instability of dielectric elastomer balloons with considering electromechanical coupling effect, hyperelasticity and viscoelasticity of the material. Our theoretical results have indicated that the electromechanical instability of the dielectric elastomer balloon may dramatically affect its performance or even determine its failure mechanism. Our results further show that by controlling the electromechanical loading path, we may achieve or avoid the electromechanical instabilities of the balloon. Our theoretical predictions agree very well with experimental observations.
L70.00242: Cross-Influence of Thermodynamic Driving Forces in Confined Environment  YU QIAO (Presenter), MENG WANG, University of California, San Diego — The second law of thermodynamics dictates that under a certain condition, the cross-influences of thermodynamic driving forces (tdf) must be balanced. For a galvanic cell, it is equivalent to the well-known Nernst equation; for a double-layer supercapacitor, it is consistent with the classic Gouy-Chapman model. In our recent experiment on confined large pivalate ions in carbon nanopores, however, it was measured that the cross-influences of the electromotive force and the chemical potential were different from each other by an order of magnitude. We attribute this remarkable phenomenon to the confinement effect of the electrode inner surfaces, which forbids the formation of diffuse layer. We argue that in general, in a low-dimensional environment, in the large dimension(s), the laws of classic statistical physics can be applied; but in the small dimension(s) wherein two tdf interact, the governing equations can be distinct. With this unique mechanism, the second law of thermodynamics may break down, in a dissimilar manner to “Maxwell's demon”. The concept of unbalanced cross-influence of tdf is further examined through a theoretical analysis on a model system comprising of randomly moving elastic particles restricted in a two-dimensional transition zone in a gravitational field.

L70.00243: Fractional Langevin equation with reflecting barrier* SARAH SKINNER (Presenter), THOMAS VOJTA, Physics, Missouri University of Science and Technology — The Fractional Langevin equation describes a the motion of a particle under the influence of a random force with long-time correlations. This stochastic differential equation is a common model for anomalous diffusion. We investigate the fractional Langevin equation in the presence of a reflecting wall using Monte Carlo simulations. The mean-square displacement shows the expected anomalous diffusion behavior, $x^2 \sim t^{2-\alpha}$, as in the unconfined case. However, the probability density close to the wall shows highly non-Gaussian behavior. For reference, we compare our results to reflected fractional Brownian motion for which the probability density shows a power law singularity at the barrier [1].


*L This work is supported in part by the NSF under Grant No. DMR-1506152 and DMR-1828489.

L70.00244: Fractional Brownian Motion with an Absorbing Wall* ALEX WARHOVER (Presenter), THOMAS VOJTA, Missouri University of Science and Technology — Fractional Brownian motion, a random walk with long-time power-law correlations between its steps, is a prototypical model for anomalous diffusion. We employ large scale Monte Carlo simulations to investigate fractional Brownian motion in the presence of an absorbing wall. In the limit of vanishing correlations, our findings reproduce the well-known results for normal diffusion. In contrast, the interplay between the absorbing wall and the long-range power correlations leads to a singular probability density close to the wall. We compare our results to those of Brownian Motion in the presence of a reflecting wall [1], and we discuss implications of our results. [1] A.H.O Wada and T. Vojta, Phys. Rev. E 97, 020102 (2018)

*L This work was supported in part by the NSF under Grant No. DMR-1506152 and DMR-1828489.

L70.00245: Oscillatory force generation in nonequilibrium systems from peaked energy spectra.* ANTHONY BONFILS (Presenter), WOOSOK MOON, DHRUBADITYA MITRA, Nordic Institute for Theoretical Physics, Sweden, JOHN WETTLAUFER, Yale university — A key to force generation in non-equilibrium systems is encoded in their energy fluctuation spectrum. A non-equipartition of energy, which is only possible in active or forced systems, can lead to a non-monotonic fluctuation spectrum. Recently, it has been shown that for a narrow, unimodal spectrum, the force exerted by a non-equilibrium system on two walls embedded in a system with such a spectrum oscillates between repulsion and attraction as a function of wall separation [1]. These results are consistent with the Maritime Casimir effect, which is driven by wind-water interactions, and with recent simulations of active Brownian particles. The spectrum is believed to be the solution of a specific class of Fokker-Planck equations. Taking a hydrodynamic perspective of Janssen [2], we construct a theory and a numerical basis for the observed Pierson and Moskovitz spectrum, which underlies the Maritime Casimir effect.


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L70.00246: Counterintuitive asymmetry of transition times in the Brownian asymmetric simple exclusion process
DOMINIK LIPS (Presenter), University of Osnabrück, ARTEM RYABOV, Department of Macromolecular Physics, Charles University, PHILIPP MAASS, University of Osnabrück — Driven diffusion of hard spheres (rods) in a one-dimensional cosine potential under a static bias should reflect properties of the asymmetric simple exclusion process (ASEP) on a lattice, if the amplitude of the cosine potential is considered to be large compared to the particles' thermal energy. For this Brownian asymmetric exclusion process (BASEP) [1], we study transition times of a tagged particle between potential wells against and along the bias direction in non-equilibrium steady states. These transition times exhibit a counterintuitive asymmetry: While one may expect that the mean transition time in bias direction is shorter, the opposite is true. We relate this surprising asymmetry to the collective motion of the particles. Differences in the distributions of the times in and against bias direction depend sensitively on the filling factor (number of particles per potential well) and the rod length. Our analysis sheds light on the transport behavior of the model, which, compared to the ASEP, shows richer properties due to the additional length scale given by the rod length.


L70.00247: Imperfections by Design: Interactive Buckling and postbuckling in Architected Materials*
YINGHAO ZHAO, Department of Civil, Environmental and Geodetic Engineering, The Ohio State University, AMAL JERALD JOSEPH MARIA JOSEPH, Department of Mechanical and Aerospace Engineering, The Ohio State University, CHUNPING MA (Presenter), MEGAN SKIBINSKI, BURAK GUL, ANDREW SCHELLENBERG, NAN HU, Department of Civil, Environmental and Geodetic Engineering, The Ohio State University — Harnessing elastic instabilities in materials has recently enabled new classes of tunable systems and devices, such as gating mechanisms, artificial muscles, and soft robotics, etc. The common feature of those instability-induced smart systems is the amplification of force and motion compared to their traditional stiff counterparts. Achieving these amplifying effects usually relies on harnessing tailor able architected materials as the building block. One of the challenges is how defects change the properties of architected materials to achieve targeted functions with aperiodic materials. In response to such need, we introduce a class of shell structures which undergoes interactive buckling. By combining finite-element simulations and desktop-scale experiments, we found that the interactive buckling can be induced by strategically controlling the number and the distribution of defects, leading to a deterministic actuation response compared to the one without geometric defects. Our study thereby opens avenues for the design of next-generation actuators and robots with high fidelity and low sensitivity over a wide range of length scales.

*N.H. acknowledges the start-up fund from the College of Engineering at the Ohio State University.

L70.00248: Scaling Features as Universal Hallmark of Physiological Dynamics across Systems, States and Clinical Conditions*
PLAMEN IVANOV (Presenter), Physics Department, Boston University — We will present a review of linear and nonlinear scaling characteristics in physiological dynamics, their universality across systems, phase transitions across physiological states, relation to underlying control mechanisms and their relevance for diagnosis and prognosis of disease.

*We acknowledge support from W M Keck Foundation, National Institutes of Health (NIH Grant 1R01-HL098437), the Office of Naval Research (ONR Grant 000141010078), the US-Israel Binational Science Foundation (BSF Grant 2012219).

L70.00249: Discrete Bound States in a Floquet-Bloch Active Spinning System
SHAHRZAD YAZDI (Presenter), ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Inspired by electronic systems, we explore the transport of an active spinning particle in a lattice of posts using a periodic driving protocol akin to a Floquet system. In our 2D Floquet-Bloch system, coupling of hydrodynamic and electrostatic interactions leads to hybridization of localized states of the spinning particle that are able to diffuse through the medium, or in some cases move ballistically. More interestingly, we find a set of discrete localized states at quantized applied frequencies that delimit regions of diffusion. These states have typical orbits much larger than the original localized states. They occur approximately at fractional frequency values of the two frequencies for the localized trivial states. Our results may be an interesting new view on transport in active colloidal systems and their counterparts in solid state physics.
L70.00250: Tunable Failure in Non-periodic Architected Materials Inspired by Slime Mold Growth*  
CHUNPING MA (Presenter), Department of Civil, Environmental and Geodetic Engineering, The Ohio State University, HANQING ZHANG, DAOBO ZHANG, PENG FENG, Department of Civil Engineering, Tsinghua University, BURAK GUL, NAM HU, Department of Civil, Environmental and Geodetic Engineering, The Ohio State University — The field of architected materials has been explored in many disciplines over the past decade, it has yet to be fully explored in civil engineering and architecture. From the perspective of material constitution, most existing efforts on metamaterials primarily use the elastic buckling of soft materials, while common infrastructure materials lack the ability to undergo such large deformation/strain. In addition, most studies to date have maintained the symmetry of material and studied the simple periodic form. Inspired by slime mold growth, we explored a new class of non-periodic cellular materials and conducted proof-of-concept experiments on 3D-printed specimens. We found that simple changes on the architectures of material can lead to significant differences in failure mechanism. Therefore, this study paves the road for the future design of resilient infrastructure involving the ability to rebound from extreme events and the corresponding repair approaches to recover capacity after those events.

*N.H. acknowledges the start-up fund from the College of Engineering at the Ohio State University.

L70.00251: Predicting shear transformation events in glasses via energy landscape sampling*  
BIN XU (Presenter), Beijing Computational Science Research Center, MICHAEL FALK, Johns Hopkins University, JINFU LI, LINGTI KONG, Shanghai Jiaotong University — Shear transformation (ST) events, as the elementary process for plastic deformation of glasses, are of vital importance to understand the mechanical behavior of glasses. Here, by characterizing first-order saddle points in the potential energy landscape, we develop a framework to characterize and to predict the triggering (i.e. locations, triggering strains, and local structural transformations under different shear protocols) of ST events. Verification undertaken with a model Cu-Zr glass reveals that the predictions agree well with athermal quasistatic shear simulations. The proposed framework is believed to provide an important tool for developing a quantitative understanding of the deformation processes that control mechanical behavior of metallic glasses.

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L70.00252: Machine Learning on Lithium Sulfur Materials*  
YING LI (Presenter), Argonne National Laboratory — Materials properties are collective phenomena in a nonlinear relationship of compositions and interatomic configurations, which are difficult to acquire from computations. Interactions between the constituent particles (atoms) are so complicated which only the limited scale of the problem is analytically solvable with descriptive theory (e.g., density functional theory, molecular dynamics, etc.) combining with current high-performance computing technology. To generalize materials simulation and properties prediction, data-driven approaches (e.g., machine learning, neural network, etc.) are much needed. Here, we provide an example showing how the cohesive energy, Fermi energy and band structures of lithium-sulfur materials as intrinsic collective behaviors are learned via Machine Learning methods, such as random forest, K-nearest neighbor algorithm, LASSO, Neural Networks, etc, and the performance comparison of the different methods will be demonstrated, which provides a general design guidance for lithium-sulfur batteries.

*This work was supported by the Margaret Butler Postdoctoral Fellowship at Argonne National Laboratory. The computational work used resources of U.S. Department of Energy Office of Science User Facility operated under Contract DE- AC02-06CH11357.
L70.00253: Behavior of a Non-equilibrium Self-Organizing System: A Potential Means to Enhance Energy Efficiency in Systems with Functional Intelligence*  
GAO(ZACHARY) SUN (Presenter), ZHOU XU, KUN WANG, BUQIN WANG, MARK T. TUOMINEN, University of Massachusetts Amherst — Research and development efforts in so-called artificial intelligence has increased dramatically. However, designing AI with energy efficiency is becoming an important priority. It is not yet clear how this should be done. One possible inspiration is to study the physics of self-organizing systems, both non-living and living, as guidance for future designs with functional intelligence. Irreversible processes at non-equilibrium can drive a system to self-organize and exhibit characteristics shown in systems known as dissipative structures. Our research explores the characteristics of experiments that use electrically conductive beads in an applied electric field. The setup resembles a primitive dissipative structure that can be interpreted as a possible bridge between behaviors in non-living and living systems. Using video and electrical measurements, we investigate the transient and steady-state behavior of self-organizing worm-like behavior under a range of initial and driving conditions. The non-equilibrium processes of a non-living system exhibiting characteristics that also exist within a living system are a possible way to explore biomimetic structures that exhibit intelligence.

*National Science Foundation Center for Hierarchical Manufacturing Award Number CMMI-1025020.

L70.00254: Dynamics of Driven Diffusive Systems with Interactions and with Langmuir kinetics  
TRIPTI MIDHA (Presenter), Department of Mathematics, Indian Institute of Technology Ropar, ANATOLY BORIS KOLOMEISKY, Department of Chemistry and Centre for Theoretical Biological Physics, Rice University, ARVIND KUMAR GUPTA, Department of Mathematics, Indian Institute of Technology Ropar — Driven diffusive system belongs to a special class of nonequilibrium systems that has wide applications in biological and vehicular transport processes. During intracellular transport of vesicles along microtubules, motor proteins interact among each other as well as frequently associate and dissociate from the tracks. Motivated by the above phenomenon, we develop a model that assimilates the interactions along with the nonconserved Langmuir kinetics in a totally asymmetric simple exclusion process [1]. We find that the continuum version of the simple mean-field (SMF) approach fails to handle strong correlations in the system. To incorporate the effect of correlation, we analyze the model using the correlated cluster mean-field theory. We compute the stationary phase diagrams, density, current and correlation profiles along the lattice for the various strength of attractive and repulsive interaction energy. Our results are in excellent agreement with the Monte Carlo computer simulations. For the case of attractions, we find the two-point correlation function to be stronger at the position of localized shocks.

References

L70.00255: Least Rattling Feedback from Strong Time-scale Separation*  
PAVEL CHVYKOV (Presenter), JEREMY L ENGLAND, Massachusetts Institute of Technology — Many interesting dynamical systems in the world have a hierarchical structure. Here we explore how to leverage this structure to better understand and predict such systems. We assume that the dynamics on different scales can be viewed as independent, except for a clearly defined feedback loop: the slow motion defines the environment that fast dynamics live in, while fast motion maintains the rules governing effective slow dynamics. Focusing on this feedback loop, rather than the details of the fast or slow motion, may pave the way for generalizable insights about hierarchical systems. We illustrate on toy examples.

*We thank the Gordon and Betty Moore Foundation Grant GBMF4343 for making this work possible

L70.00256: Janus Colloidal Crystal, a New Model System for Spin Ice and Glass  
MYEONGGON PARK (Presenter), STEVE GRANICK, Ulsan National Institute of Science and Technology — Questions like the dynamics of magnetic monopole in spin ice and the translation -rotation coupling in molecular glass have long puzzled scientists in different communities, mainly because it is hard to monitor the dynamics of these systems on microscopic level. Here we try to address these questions using Janus colloidal crystals, in which both the translational and rotational motions of particles can be tracked by video microscopy and the particle interaction can be finely tuned by electric field. as one of the results, we find that glasslike dynamics for rotational motion appears when the area fraction is so high that the system is crystalline. Our experimental system paves the way for modeling a wide range of phenomenon in spin ice and molecular glasses.
L70.00257: Jamming with Pins: How do different pin geometries affect jamming?*  
BRIAN JENIKE (Presenter), TRISTAN CATES, AMY GRAVES, Physics and Astronomy, Swarthmore College — We simulate two-dimensional, zero temperature systems of soft disks with harmonic repulsive pair potentials. The pin lattices contain disks that employ the same potential, but are of negligible size. We study square, triangular, honeycomb, and random lattices. That is, it has been known for several years that the jamming threshold, $\phi_j$, decreases with pin density, $\rho$. At low pin densities, all lattice geometries produce the same $\phi_j(\rho)$ which decreases linearly with $\rho$, but pin lattice geometry begins to matter as $\rho$ increases further. At low densities, as expected, all lattices are equivalent with a linear dependence on $\rho$. At moderate densities, the square lattice supports jamming better than the random lattice; but interestingly, at higher densities the situation is reversed. We present data on $\phi_j$ parameterized by lattice constant and lattice density; and on structural features such as distributions of contacts and angular ordering of bonds between particles.

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L70.00258: Relaxation Dynamics after the Removal of a Static Force: Binary Operators and Impact of Eigenstate Thermalization  
JONAS RICHTER (Presenter), Department of Physics, University of Osnabrück, JACEK HERBRYCH, Department of Physics and Astronomy, The University of Tennessee, JOCHEN GEMMER, ROBIN STEINIGEWEG, Department of Physics, University of Osnabrück — We study the relaxation dynamics of expectation values under unitary time evolution for a certain class of initial states. The latter are thermal states of the quantum system in the presence of an additional static force which, however, become nonequilibrium states when this force is eventually removed. While for weak forces the dynamics is well captured by linear response theory (LRT), the case of strong forces, i.e., initial states far away from equilibrium, is highly nontrivial.

Employing a combination of analytical arguments as well as numerical calculations for interacting quantum lattice models, we unveil that the nonequilibrium dynamics at high temperatures can, in various cases, be universally generated by a single correlation function in the entire regime close to and far away from equilibrium. Specifically, we consider so-called binary operators and study, as an example, the dynamics of spinless fermions in a random potential. In addition, we discuss the role of the eigenstate thermalization hypothesis (ETH) and establish a connection between ETH and LRT.


L70.00259: Disruption and Recovery of Reaction-Diffusion Wavefronts Colliding with Obstacles*  
REBECCA GLASER (Presenter), NATHANIEL SMITH, VINCENT W.H. HUI, JOHN LINDNER, NIKLAS MANZ, The College of Wooster — We study the damage to and restoration of planar reaction-diffusion wavefronts colliding with convex obstacles in narrow two-dimensional channels using finite-difference numerical integration of the Tyson-Fife reduction of the Oregonator model of the Belousov-Zhabotinsky reaction. We characterize the obstacles' effects on the wavefront shape by plotting wavefront delay versus time. Due to the curvature dependent wavefront velocities, the initial planar wavefront (or iso-concentration line) is restored after a relaxation period that can be characterized by a power-law. We find that recovery times are insensitive to obstacle concatenation or to the upstream obstacle shape but are sensitive to the downstream shape, with a vertical back side causing the longest disruption. Delays vary cyclically with obstacle orientations. The relaxation power-laws confirm that larger obstacles produce larger wavefront delays and longer recovery times, and for a given area larger obstacle width-to-length ratios produce longer delays. Possible applications include elucidating the effect of inhomogeneities on wavefront recovery in cardiac tissue.

*This work is supported by the National Science Foundation [NSF-REU grant number DMR 1560093] and The College of Wooster.
Many-Body Dynamic Localization Effect in Periodically Driven Finite Clusters of Spins 1/2 without Disorder* BORIS FINE (Presenter), Skolkovo Institute of Science and Technology, KAI JI, Department of Physics, Shanghai Normal University — We investigate numerically and analytically the heating process in ergodic clusters of interacting spins 1/2 subjected to periodic pulses of an external magnetic field. Our findings indicate that many-body dynamic localization manifests itself as a cluster-size-dependent threshold for the pulse strength below which the heating is suppressed. This threshold decreases with the increase of the cluster size, approaching zero in the thermodynamic limit. Nevertheless, it should be observable in clusters with fairly large Hilbert spaces. We obtain the above threshold quantitatively as a condition for the breakdown of the golden rule in the second-order perturbation theory.

References:

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The thermodynamics of computing with finite automata* DAVID WOLPERT (Presenter), ARTEMY KOLCHINSKY, Santa Fe Institute — Recent breakthroughs in stochastic thermodynamics have greatly enriched our understanding of the thermodynamics of computation. To date, these analyses have concentrated on the “computation” of erasing a single bit. One of the idiosyncratic characteristics of such computation is that we know ahead of time when it will finish, and so do not need to continually observe it to tell whether it has finished - thereby avoiding the thermodynamic costs of such observation. Here we show how to analyze the thermodynamic costs of running a computer without continually observing it even though its finishing time is random, e.g., because it depends on the random input to the computer. We then use this to analyze the thermodynamics of finite automata (FA), one of the most important types of computational system. In particular, we show that due to the variability in the number of iterations it takes a given FA to finish, the Landauer cost of running that FA is a sum of novel information theoretic quantities, which we call “partial entropies”.

*We would like to thank the Santa Fe Institute and Grant No. CHE-1648973 from the U.S. National Science Foundation

Spatiotemporal tiling of the Kuramoto-Sivashinsky equation* MATTHEW GUDORF (Presenter), PREDRAG CVITANOVIC, Georgia Institute of Technology — Numerical simulations play a very important role in the study of chaotic partial differential equations due to the lack of analytic solutions. In the limit of strong chaos and or turbulence, these computations become very challenging if not completely intractible. In an attempt to circumvent these difficulties, we recast time dynamical systems as purely spatiotemporal problems in (d+1) dimensional spacetime. Specifically, the focus of this study will be on the spatiotemporal Kuramoto-Sivashinsky equation, a (1+1) dimensional system. Our main hypothesis is that spatiotemporal recurrences resultant from shadowing of invariant 2-tori are of critical import. This intuition is a spatiotemporal parody derived from the theory of cycle expansions [1]. By developing a (1+1) dimensional symbolic dynamics with invariant 2-tori as the fundamental building blocks, we hope to quantitatively characterize infinite spacetime solutions.


*P.C. thanks the family of the late G. Robinson Jr. and NSF DMS-1211827 for support.

Propagation of light-sensitive reaction-diffusion waves in inhomogeneously illuminated systems* DANIEL BLAIKIE (Presenter), SPENCER L. KIRN, NIKLAS MANZ, College of Wooster — The propagation dynamics of reaction-diffusion (RD) waves in illuminated quasi-2-dimensional systems was investigated, using various light-sensitive chemical Belousov-Zhabotinsky (BZ) reactions. Illuminating the BZ waves from below with visible light with a checkerboard pattern was used to change the light intensity in a repeating pattern, thus changing the speed of the light-sensitive waves. In our system, BZ waves slow down at higher illumination levels. Using a Ruthenium based catalyst, a light-sensitive BZ solution was made and absorbed by a filter paper to create the quasi-2D system. As the wave propagated over the checkerboard pattern of the illuminated system, the changes in speed would cause the wave to curve forward (dark area) and backward (bright area). The curvature should alternate and increase the overall speed of the wave as shown numerically by Schebesch and Engel in Phys.-Rev.-E 60(6) 1999. We used various catalysts, light intensities, illumination patterns, and BZ-component concentrations to determine how different excitation waves propagate through non-homogeneous excitation pattern.

*This work is supported by the National Science Foundation [NSF-REU grant number DMR 1560093] and The College of Wooster.
L70.00264: Structural Vulnerability of Quantum Networks
ANGKUN WU (Presenter), Physics and Astronomy, Rutgers University, New Brunswick, LIANG TIAN, YANG-YU LIU, Channing Division of Network Medicine, Brigham and Women's Hospital and Harvard Medical School — Quantum networks allow for the transmission of quantum information between physically separated quantum processors. They play a very important role in quantum computing and quantum communication. Previous studies show clear advantages of establishing long-distance entanglement between two nodes in a quantum network for communication. Yet, the general structural vulnerability of such quantum networks has not been studied. Here we systematically examine two key notions in graph theory: articulation points (APs) and bridges, which ensure the connectivity of a network and naturally represent potential targets of attack if one aims for immediate damage to a network. We offer an analytical framework to calculate the fraction of APs and bridges for quantum networks with arbitrary degree distribution. We find that quantum networks with swap operations have lower fractions of APs and bridges than their classical counterparts. Moreover, we find that quantum networks under low degree swap operations are substantially more robust against AP attacks than their classical counterparts. These results help us better understand the structural vulnerability of such quantum networks.

L70.00265: Human Information Processing in Complex Networks*
ARI E KAHN, CHRISTOPHER LYNN (Presenter), LIA PAPADOPOULOS, DANIELLE BASSETT, University of Pennsylvania — A curious aspect of information is its relativity: the amount of information contained in a message depends not just on its content, but also on the expectations of a receiver. Nowhere is this observation more evident, nor are the implications more important, than in the context of human cognition. Here, we develop an analytical framework for measuring information relative to human expectations, and we demonstrate its utility in two distinct ways. First, we verify that our framework predicts aspects of human behavior that cannot be accounted for by traditional information theoretical measures such as entropy. Second, we apply our framework to characterize the network structure of designed information sources, such as the network topology of natural languages and the structure of note transitions in music. Across a range of real-world networks, we discover that their inherent complexity is high while their divergence from human expectations is low, thereby allowing for the efficient communication of information. We find that this competition between high complexity and low divergence from expectations is driven by hierarchically modular organization, which, interestingly, has been observed in many evolved and designed networks.

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L70.00266: Coarse-graining of Dynamics in Weakly Non-linear Processes on Networks
NIMA DEHMAMY (Presenter), YANCHEN LIU, Northeastern University — It is known that if the graph has a hierarchical structure, many dynamical processes exhibit transient states in which the dynamics synchronizes or stabilizes at communities in one level of hierarchy. In linear and weakly non-linear processes these transient states appear at time scales associated with inverse of the so-called community eigenvectors of the quadratic piece of the Hamiltonian. We show that these transient states can be exploited to coarse-grain the network during the dynamics and reduce the time complexity of estimating the outcome of a dynamical process from $O(N^3)$ down to a lower complexity in most hierarchical networks, and possibly to $O(N^2 \log N)$ in tree-like networks. We outline the coarse-graining procedure, which relies on spectral methods and can be computed efficiently. We also discuss potential relations with graph learning and regression on graphs.

L70.00267: Global and microstructural ergodic properties of financial markets*
JACK SARKISSIAN (Presenter), Managing Director, Algostox Trading — In finance everyone is concerned about future expectations. Whether it’s pricing or risk evaluation - current models always involve some form of time averaging. Understanding the ergodic properties of the markets allows to replace the time average with ensemble average. Since calculation of ensemble average requires only one step in time, this approach allows much faster computation, and therefore a much faster reaction to changing market conditions. In this work we will explore market ergodicity from various points of view. First, we will consider market properties as a global dynamic system made of individual securities. Second, we will discuss ergodicity of individual securities represented by a dynamic limit order book. We will show how concepts of ergodicity can be applied to determine current market volatility, and introduce the new eVOL and eVAR indices that measure current volatility as opposed to traditional realized and implied volatilities. We will demonstrate real-life examples highlighting the capabilities of these new indices for trading and asset management.

*This work was not funded by external sources
L70.00268: Classical Dimer Model on the Square Bilayer Lattice*  NISHEETA DESAI (Presenter), University of Kentucky, KEDAR DAMLE, Tata Institute of Fundamental Research, SUMIRAN PUJARI, Indian Institute of Technology, Bombay — We study the Classical Dimer Model (CDM) on the square bilayer lattice with the fugacity of interlayer dimers as a tuning parameter. The square monolayer CDM is one of the paradigmatic model of a “Coulomb” phases whose distinct signatures are a) power law correlations in real space, and b) “pinch points” in the “transverse” form of structure factors in momentum space. Here we find that for low fugacity, the square bilayer CDM again hosts Coulomb phases with power law correlations. The pinch point phenomenology is however crucially different than the monolayer. This is integrally related to presence of longitudinal modes and Coulomb correlations together in the bilayer CDM ensemble. For high fugacity, it hosts a featureless phase with predominantly interlayer dimers and exponentially decaying correlations. Remarkably, even though the two phases are not symmetry related, numerical evidence from system sizes upto 512 × 512 points to a continuous transition rather than first-order. We provide an effective “electrostatic” description of the numerical data for low fugacities with the interlayer dimers interpreted as spontaneously fluctuating charged dipole defects.

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L70.00269: Influence of correlated temporal disorder on an extinction phase transition*  MATTHEW SMALL (Presenter), ALEXANDER H ONIWA WADA, THOMAS VOJTA, Missouri University of Science and Technology — We employ large-scale Monte Carlo simulations to investigate the effect of long-range correlated temporal disorder (i.e. external noise) on extinction phase transitions in the logistic evolution equation. Uncorrelated temporal disorder is known to cause an unusual phase transition controlled by an infinite-noise critical point [1]. It features diverging density fluctuations at criticality, implying that the typical population decay is much faster than the ensemble average. Our results demonstrate that correlated temporal disorder enhances these effects; the correlations further accelerate the decay of a typical population while slowing the decay of the ensemble average. We also establish a relation to reflected fractional Brownian motion [2] which yields a conjecture for the critical behavior of the population.


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L70.00270: Universal quantum Hawking evaporation of integrable two-dimensional solitons*  CHARLES ROBSON, DI MAURO VILLARI LEONE (Presenter), FABIO BIANCALANA, Heriot-Watt University — In a work published in 1976, Abdus Salam and his student John Strathdee proposed a connection between two different fields, namely general relativity and the theory of nonlinear evolution equations. Their conjecture was simple: a black hole is nothing else than a soliton. We show that any soliton of an arbitrary two-dimensional integrable equation has the potential to evaporate and emit the analogue of Hawking radiation from black holes. From the AKNS matrix formulation of integrability, we show that it is possible to associate a real spacetime metric tensor which defines a curved surface, perceived by the classical and quantum fluctuations propagating on the soliton. By defining proper scalar invariants of the associated Riemannian geometry, and introducing the conformal anomaly, we are able to determine the Hawking temperatures and entropies of the fundamental solitons of the nonlinear Schrödinger, KdV and the sine-Gordon equations. The mechanism advanced here is simple, completely universal and can be applied to all integrable equations in two dimensions, and is easily applicable to a large class of black holes of any dimensionality, opening up totally new windows on the quantum mechanics of solitons and their deep connections with black hole physics.

*EPSRC
MPG
L70.00271: Exotic quantum statistics from a many-body theory of Majorana fermions  JOSHUAH HEATH (Presenter), KEVIN SHAWN BEDELL, Boston College — Starting with a simple counting argument, we construct a statistical and thermodynamic model of free Majorana fermions at low temperature. Originally defined as a fermion identical to its own antiparticle state, Majorana particles often appear in the contemporary many-body literature as non-Abelian zero energy modes in topological superconductors. We deviate from the usual anyonic description and instead consider a gas of non-interacting, spin-1/2 Majorana fermions as Ettore Majorana first envisioned them. A combinatorial analysis of the many-body Majorana ensemble leads to a configurational entropy which deviates from the fermionic result with an increasing number of available microstates. A Majorana distribution function is derived which shows signatures of a sharply-defined Fermi surface at finite temperatures. The Majorana distribution is then re-derived in the context of a modified Kitaev chain with bosonic pair interaction. The thermodynamics of the free Majorana system is found to be nearly identical to that of a free Fermi gas, except now distinguished by a two-fold ground state degeneracy and, thus, a residual entropy at zero temperature. Experimental realization of the Majorana thermodynamics is then discussed in the context of real materials and cosmological phenomena.

L70.00272: BIOLOGICAL PHYSICS —

L70.00273: A numerical method for detecting and classifying multi-channel and multi-state binding events in single-molecule TIRFM experiments* JOSEPH TIBBS, University of Northern Iowa, ELIZABETH BOEHM, Harvard University, FLETCHER BAIN, COLLEEN CALDWELL, TODD WASHINGTON, MARIA SPIES, University of Iowa, ALI TABEI (Presenter), University of Northern Iowa — Biomolecular binding may be observed using Total Internal Reflection Fluorescence Microscopy. By using multiple channels, which corresponds to different colors of fluorescence, the real-time interaction of multiple proteins can be observed. Although for many of these interactions the bound state is binary, for some the binding is more complex, with discrete states demonstrating intermediate levels of fluorescence. We will explain a numerical method for extracting these fluorescence traces from microscope data and then organizing and classifying traces from single-molecule experiments. With multiple channels and multiple binding states possible, the possible binding patterns are numerous. The data is organized in groups by these binding patterns and the statistics of each interaction is displayed. Which combinations are most likely, the binding duration of each protein or the probable binding/dissociation order of each subunit are all data which can inform on the underlying mechanism behind the interaction. We show how our method determines cooperative or inhibitory binding in multi-protein systems, or observe the construction of protein complexes.

*1) UNI CHAS Faculty Grant for Research Activity
2) University of Iowa, FUTURE Program
3) UNI, Graduate College, Summer Fellowship Program

L70.00274: Activity and Effects of Retroelements in Bacteria* DAVNEET KAUR (Presenter), GLORIA LEE, NICHOLAS SHERER, NEIL KIM, ELLIOT URRIOLA, CHI XUE, K. MICHAEL MARTINI, NIGEL GOLDENFELD, University of Illinois at Urbana-Champaign, THOMAS KUHLMAN, Physics, University of California at Riverside — Retroelements (RTEs) are abundant in eukaryotic genomes but less numerous in bacteria as group II introns. It has been hypothesized that eukaryotic spliceosomal introns and retrotransposons may have evolved as a result of invasion by bacterial group II introns. However, it remains unclear what limits RTE proliferation in bacteria and archaea and what enables it in eukaryotes. We quantify the effects of the human RTE LINE-1 and the bacterial group II intron Ll.LtrB in Escherichia coli, Bacillus subtilis and Enterococcus faecalis. We find that RTE expression is detrimental to all species, that LINE-1 successfully integrates into the chromosomes, and that the ability to repair DNA breaks with bacterial non-homologous end joining systems increases retrotransposition efficiency. Our results show that RTEs place a significant burden on organisms poorly equipped to handle their effects, and that the capacity of the last eukaryotic common ancestor for NHEJ may have enabled the proliferation of RTEs and the evolution of eukaryotes.

*This work was supported by the NSF Center for the Physics of Living Cells (PHY 1430124), the Alfred P. Sloan Foundation (FG-2015-65532), and the Institute for Universal Biology, through partial support by the NASA Astrobiology Institute (NAI) (NNA13AA91A).
L70.00275: Understanding protamine-induced DNA folding in sperm  HILARY BEDIAKO (Presenter), ADAM D. SMITH, OBINNA UKOGU, ANDREA BOSKOVIC, MOUMITA DASGUPTA, ASHLEY CARTER, Amherst College — We examine how protamine causes DNA folding within the sperm nucleus. Specifically, we are interested in how protamine loops the DNA into toroids that allow for tight packaging of the paternal genome. The formation of toroids have implications in epigenetics and fertility. Toroids may be formed in a single step (collapse model) or multistep (sequential model) manner. In the collapse model, all loops form along the DNA at once and then collapse into the toroid. In the sequential model, loops stack sequentially into a toroid. To decipher between these two models, we perform an in vitro Tethered Particle Motion (TPM) assay. In a TPM assay, an individual DNA molecule is attached to a bead and tethered to a cover-slip. By observing the position of the bead over time, we can measure the DNA length to a precision of about 10 nm and infer the folding trajectory of our DNA. We observe that as the length of the DNA increases, the number of folding events increases, suggesting that toroid formation is multistep (sequential model). If DNA folding is multistep, the location of nucleation loops is important as they may indicate where histones, and thus epigenetic tags, may be present. Moreover, the ratio of different protamine proteins may affect how toroids form and play a role in fertility.

L70.00276: Characterizing Protamine-Induced DNA Loop Formation Using a Tethered Particle Motion Assay  KYLIE JONES (Presenter), ASHWIN BALAJI, HILARY BEDIAKO, ANDREA BOSKOVIC, ASHLEY CARTER, Amherst College — Protamine is a protein found in sperm cells. It folds DNA into compact toroids by first forming it into loops and then stacking those loops. This compaction plays an important role in reproduction, ensuring that sperm are hydrodynamically efficient and protecting the DNA they carry. We use a tethered particle motion assay to examine the mechanics of loop formation in this process. By tracking the Brownian motion of a bead tethered to a length of DNA, we can detect changes in DNA conformation through changes in the bead’s motion. We find that loop formation is a multi-step process with intermediate states.

*This work was supported by a Research Corporation Cottrell Science Award (23239), a National Science Foundation CAREER Award (1653501), and Amherst College.

L70.00277: Characterizing the Mechanism of DNA Loop Formation by Protamine  ASHWIN BALAJI (Presenter), ASHLEY CARTER, Amherst College — DNA compaction in sperm cells by the protein protamine represents an extreme case of polymer folding, approaching crystalline packing of the molecule. This high compaction is necessary for creating viable sperm, yet the physical mechanism of folding is unknown. In this study, we investigate how protamine folds DNA into a loop. One hypothesis is loop formation occurs through entropic folding where protamine binds and neutralizes the negative charge of the DNA backbone, increasing flexibility and allowing the molecule to fold into a loop. Another hypothesis is loop formation occurs as each protamine binds and bends DNA, changing its enthalpy. Using single-molecule force spectroscopy, we measure force-extension curves and fit them with a worm-like chain model. This model obtains the entropic and enthalpic portions of the folding, allowing us to differentiate between our two hypotheses. Specifically, we pull on DNA tethers biochemically attached on one end to a glass slide and on the other to a polystyrene bead. We then flow protamine over the tethers and measure the force-extension curve. We use a centrifuge force microscope to apply force and to image the tethers to track their extension. Here we report progress in building the instrument and measuring force-extension curves.

L70.00278: Expressing, Purifying, and Characterizing a Flavodoxin from the Solvent-Producing Clostridium Acetobutylicum  ALYSSA ALVAREZ (Presenter), Undergraduate Physics, St. Mary's University, San Antonio, TX, ANDREA PADRON, ANNA GUSEVA, Biochemistry and Cell Biology Graduate Program, Rice University, Houston, TX, JONATHAN SILBERG, Department of Biosciences, Rice University, Houston, TX — Flavodoxins (Fld) are relatively small redox proteins responsible for facilitating the transport of electrons in certain types of bacteria and algae. In order to understand how these proteins control the flow of electrons between different redox partners in organisms with multiple electron transfer proteins, we must understand their structure and partner specificity. While structures have been reported for Flds, we do not understand their structural properties sufficiently enough to predict electron flow in cells. This project aims to overexpress a flavodoxin from Clostridium acetobutylicum (CacFld1) in E. coli cells, purify it using chromatography techniques, screen for conditions that yield CacFld1 crystals, and acquire structural data using the crystals. To express CacFld1, the gene encoding this protein was synthesized and placed under a T7 phage promoter which is inducible by IPTG. Optimal expression conditions of CacFld1 were found and purification of the protein by anion exchange chromatography was attempted. Future studies entail finding the conditions in which CacFld1 crystallizes and analysis of its structure through x-ray crystallography techniques.

*This work was supported by the National Science Foundation BioXFEL STC award No. 1231306
L70.00279: A three-dimensional analytical pathway to smoothly connect successive nucleosomes along DNA*
SEYED AHMAD SABOK-SAYR (Presenter), WILMA K OLSON, Rutgers University, New Brunswick — Most DNA in the human genome is wrapped on nucleosomes. The nucleosome is an assembly of eight proteins and about 150 base pairs of DNA. Understanding the biological processing of DNA requires knowledge of how the nucleosomes are arranged in space. We have developed a new analytical model to describe the three-dimensional pathways of long stretches of nucleosome-bound DNA. Given the positions and orientations of a set of nucleosomes, we can find a smooth connector that joins the ends of successive nucleosomes along the DNA. Our studies show that the simplest equation which can smoothly connect any two nucleosomes is a quadric function which is uniquely determined by the position and orientation of each pair of successive nucleosomes. Since the equation for the connector only depends on the boundary conditions, our method can be used to connect either theoretical curves describing the nucleosomal pathway or the protein-bound DNA in known high-resolution structures. This treatment makes it possible to study the effect of elastic and electrostatic energies of the connectors on the stable structure of the nucleosomal arrays and to examine the influence of nucleosomal pathways, such as the length of bound DNA, on the global folding of the arrays.

*Supported in part by USPHS GM 34809

L70.00280: Effects of Protein Conformation on Charge Regulation  JACOB PALMERIO (Presenter), DAVID ROSS, GEORGE THURSTON, Rochester Institute of Technology — Proteins change charge in response to their electrostatic environments, by changing protonation patterns of titratable residues. This charge regulation is important for modeling protein interactions, including proteins that undergo conformational change, such as intrinsically disordered proteins, and enzymes that are allosterically controlled. We construct grand canonical partition function models that take account of flexibility by incorporating it into the relevant partition functions for each proton occupancy pattern. We use this model to analyze titration data for selected small molecule sequences, including dicarboxylic acids, diamines, and peptides.

L70.00281: Investigating Protamine-Induced Toroid Formation*  ANDREA BOSKOVIC (Presenter), KYLE JONES, HILARY BEDIAKO, ASHWIN BALAJI, ASHLEY CARTER, Amherst College — In somatic cells, DNA is folded by histones, forming chromatin. However, protamine, a small, arginine-rich protein that allows DNA to fold in mammalian sperm cells. Protamine allows DNA to form loops, which are then condensed into toroids that are stacked within the sperm cell. In order to investigate protamine-induced toroid formation in DNA, we performed a tethered particle motion (TPM) assay. Due to the fact that we see multiple states present in our visualizations of standard deviation over time, toroid formation in DNA due to the binding of protamine is a multi-step process. Understanding how DNA folds has applications in biomaterials, epigenetics and infertility.

*I would like to thank the Gregory Call Fund at Amherst College for providing funding to attend this conference.

L70.00282: Improved Molecular Dynamic Simulation of Protein Devices: PEGylated Proteins and Protein Microarrays  ADDISON SMITH (Presenter), THOMAS KNOTTS IV, Brigham Young University — Protein-based devices have great potential to change how we harness the power of biology. PEGylated proteins and protein microarrays are two such devices. PEGylation covalently bonds polyethylene glycol (PEG) chains onto a protein's primary structure to increase a protein's stability in the body. Protein microarrays covalently tether proteins onto a solid surface and has transformative applications for detection assays. However, for both devices, functionalization often renders it inactive.

We have developed a coarse-grain molecular simulation model that has been shown to accurately predict optimal functionalization sites. This presentation explains this model and reports its use on a the commercially-relevent protein β-lactamase. The in silco screen reveals the best candidate sites for PEG and surface attachment. Experiments then validate these results.

The results for both protein devices are presented and indicate that device attachment site strongly affects thermostability and that configurations more stable than wild type are possible. Moreover, by using the same protein for both devices, we show that optimal site locations for one device is not predictive for the other. Finally, PEGylation simulation indicate stabilizing PEG/protein structures contradict current theory
**L70.00283: Effect of substrate viscosity on stick-slip dynamics of migrating cells**  
RUMI DE (Presenter), Department of Physical Sciences., Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India — Migration is central to many cellular processes such as wound healing, morphogenesis, embryonic development, tissue regeneration to name a few. 'Stick-slip' motion, observed during cell crawling, has been found to be strongly sensitive to the substrate stiffness. The stick-slip behaviour has been investigated before typically using purely elastic substrates. For a more realistic understanding of this phenomenon, we propose a theoretical model to study the dynamics on a viscoelastic substrate. Our model based on a reaction-diffusion framework, incorporates known important interactions such as retrograde flow of actin, myosin contractility, force dependent assembly and disassembly of focal adhesions coupled with cell-substrate interaction. We show that consideration of a viscoelastic substrate not only captures the usually observed stick-slip patterns, but also predicts the existence of an optimal substrate viscosity corresponding to a maximum traction force and minimum retrograde flow which was hitherto unexplored. Moreover, our theory predicts the evolution of individual bond force which provides insights into the stick-slip jumps on soft versus stiff substrates. Our analysis also elucidates the dependence of the duration of stick-slip cycles on various system parameters.

**L70.00284: Actomyosin contractility depends on the load-dependent binding kinetics of myosin motors**  
PASHA TABATABAI (Presenter), DANIEL S. SEARA, IAN LINSMEIER, MICHAEL MURRELL, Yale Univ — Within the cytoskeleton, myosin motor proteins consume chemical energy and generate mechanical work within the filamentous actin network essential for diverse cell functions like migration, division, and shape change. Myosin unbinding kinetics are force dependent exhibiting "catch-bond" behavior which decreases the probability of unbinding under load. Altering the binding kinetics of proteins is prohibitively difficult, thus the impact of load dependent binding kinetics on the dynamics and mechanics of actomyosin contractility are unclear. To this end, we use coarse grained molecular dynamics simulations to explore the effect of catch bonds on the accumulation and dissipation of mechanical energy in the actomyosin cytoskeleton. We find that motor binding that increases under load sensitizes the network to myosin motor concentration, increasing the rate of contractility while simultaneously increasing network toughness, or the storage of mechanical energy.

*We acknowledge funding ARO MURI W911NF-14-1-0403.

**L70.00285: Actin-microtubule co-formation inside of a giant unilamellar vesicle**  
SUNGWOO JUNG (Presenter), C. H. KIM, A SETIAWATI, HUONG NGUYEN, Sogang University, M. C. CHOI, KAIST, KWAN SHIN, Sogang University — Microtubule and actin cytoskeletons are physically contacted in a cell, and dynamically coordinated to play vital roles in many cell functions, from migration, growth, and division. These structural dynamics of cytoskeletal proteins are of interest, the physical roles of cross-linking proteins between two filaments have been identified. Yet most studies were performed in a highly controlled interface or a bulk. Recently, we developed to simulate a cytoskeleton formation through ATP-dependent actin polymerization in a giant unilamellar vesicle. Optical stimulation initiated ATP synthesis and induced ATP-dependent actin polymerization, leading to growth of three-dimensional highly curled actin filament network. In this study, we further added the ingredients for microtubule formation into the actin polymerizable GUV system, and initiated the filament formations of those two cytoskeleton proteins simultaneously. We will discuss how these highly curled actin filaments in the single vesicle affects the structural environment in the presence of highly straight microtubule filaments. We will discuss how these two filaments are interacting in a highly confined, cell-like space where they are mutually restricted.

**L70.00286: Building Towards Single Particle Characterization of Nanoparticle Bioconjugates**  
MOHAMMAD ABDULMOQUEET (Presenter), LEEANA TOVAIS, KATHRYN MAYER, Physics and Astronomy, University of Texas at San Antonio — Development of functional nanoparticle bioconjugates has been an important research area for nearly the last decade. Functionalized nanoparticles of various self-assembled monolayers (SAM-layers) have been used for biological and medical applications. Determining the exact spatial distribution of functionalized antibodies on the surface of the nanoparticles will provide necessary information to fully characterize and optimized nanoparticle bioconjugates for the preclinical stages of research. Gold bipyramids have been synthesized and then coated with a SAM-layer of various ligand types. Current and future work consists of conjugating these functionalized nanoparticles with fluorescently labeled anti-EGFR antibodies, which will enable imaging of the number and spatial arrangement of antibodies around the gold bipyramid using Total Internal Reflection Fluorescent (TIRF) Microscopy. EGFR is chosen as the target for future applications in cancer therapy.

*I would like to acknowledge the NIH Score program for supporting this research project.*
Correlation of hatchling mass and egg volume in extant birds from Archilochus colubris to Struthio camelus

JOSHUA THOMAS (Presenter), Clarkson University, SCOTT LEE, MAX COOLEY, RICHARD IRVING, University of Toledo — Observations suggest that birds hatch when they are near the maximum size that can be contained in their egg. In order to test this hypothesis, we have measured the volume of eggs of nineteen bird species from Archilochus colubris (the ruby-throated hummingbird) to Struthio camelus (the ostrich). The hatchling mass of these birds vary by more than three orders of magnitude. The volume of the eggs were measured by using scaled pictures of the eggs. The OpenCV library, and a custom python code was used to detect the edges of the eggs. We assumed the images were taken at right angles to the eggs, and that the eggs have cylindrical symmetry around the long axis. The points along the edges of the egg were fit with a polynomial to avoid resolution-induced calculation issues. The surface area and volume were calculated as if the points were a solid of revolution. Our method reproduces the volumes of ellipsoids with known dimensions with errors of less than 1%. The hatchling mass is found to depend on the egg volume via a power law with an exponent of 1.01 (standard deviation = 0.04), in support of the hypothesis. This relationship predicts a hatchling mass of 8.0 kg for the extinct Aepyornis maximus (the giant elephant bird), the largest known bird for which intact eggs exist.

Humeral bone strength and flight in eumaniraptoran dinosaurs

SCOTT LEE (Presenter), University of Toledo, JOSHUA THOMAS, Clarkson University — Flight requires that the animal be able to generate sufficient lift and thrust to support its weight in air. This requires that the humerus have a sufficiently strong section modulus to withstand the applied stresses. In order to study the possibility of flight in extinct dinosaurs, the humeral section modulus of 17 species of extant volant birds with masses ranging from 5.8 grams in Regulus calendula to 8.959 kg in Cygnus olor has been measured. The humeral section modulus is related to the mass of the animal via a power law with an exponent of 1.14 (standard deviation 0.02). The humeral section modulus is evaluated for 19 extinct dinosaurs from Dromaeosauridae, Troodontidae and Avialae. Comparing to the data for extant volant birds allows for the determination of those dinosaurs whose humeri were too weak to support powered flight. All five species of Avialae are found to have had humeri sufficiently strong for flight. Four dromaeosaurids (Microraptor gui, Graciliraptor lujiahunensis, Buitreraptor gonzalezorum, and Changyuraptor yangi) and one troodontid (Jianianhualong tengi) are also found to have had humeri that were strong enough for flight. This is a necessary, but not necessarily sufficient, condition for flight.

On the kinetics and dynamics of apatite crystallization at amyloid-solution interfaces found during enamel biomineralization

SUSRUT AKKINENI (Presenter), University of Washington, JINHUI TAO, Pacific Northwest National Laboratory, STEFAN HABELITZ, University of California, San Francisco, JAMES J DE YOREO, Pacific Northwest National Laboratory — Mammalian enamel has a remarkable structure made of interwoven apatite filaments. Recent in vivo and in vitro evidence suggests amyloid-like amelogenin nanoribbons act as a scaffold for apatite growth. However, the correlation between amyloid structure and apatite crystallization is unclear. Parts of this relationship are unraveled by the kinetics of calcium phosphate nucleation and growth at the amyloid-solution interface through in situ atomic force microscopy. Using peptide analogs of amelogenin, films of oriented nanoribbons with 3-fold symmetry stabilized by Van der Waals's forces were self-assembled on graphite. They shared similar amyloidal properties even after addition of charged residues at C-terminus or with phosphorylated serine-16. Their role during apatite crystallization was then determined using physiologically-relevant solutions, favorable to heterogenous apatite nucleation. Quantitative analysis reveals that the peptide films, with or without additional charged residues, cannot independently promote apatite nucleation over time, but can provide an interface for growth of nuclei.


*Funded by NIH/NIDCR R01DE025709-01A1

ABSTRACT WITHDRAWN
L70.00291: Biomechanics of the peafowl's crest reveals frequencies tuned to social displays*  SUZANNE KANE, DANIEL VAN BEVEREN (Presenter), Physics & Astronomy, Haverford College, ROSLYN DAKIN, Migratory Bird Center, Smithsonian Institute — Feathers can act as vibrotactile sensors of mechanical stimuli during avian flight and tactile navigation, suggesting they may also detect stimuli during social displays. Here we present the first measurements of the biomechanical properties of bird feather head crests. We show that in Indian peafowl (Pavo cristatus), crest feathers are coupled to mechanosensory filoplume feathers. We also determined that peafowl crests are driven at resonance by their main social display frequency, but that other peacock feathers and crest of other birds have resonant frequencies that vary over a wide range (seven times that of the peafowl's crest). Peafowl crests were also driven to vibrate near resonance when we played back audio recordings of their displays in geometries that mimicked the acoustic near-field geometry found during these behaviors in vivo, but not when we played back control audio. These results suggest that mechanosensory stimuli could complement acoustic and visual perception and/or proprioception of social displays in peafowl and other bird species.

*This work was supported by Haverford College and a National Sciences and Engineering Research Council of Canada (NSERC) Postdoctoral Fellowship to R.D.

L70.00292: Mechanical principles of biofilm formation revealed by single-cell resolution imaging  JING YAN (Presenter), FARZAN BEROZ, HOWARD A STONE, NED WINGREEN, BONNIE BASSLER, Princeton University — Biofilms are surface-associated bacterial communities embedded in an extracellular matrix. Biofilm cells are more resistant to antibiotics than their planktonic counterparts, which is a major problem in the context of chronic infections. We still lack a fundamental biophysical understanding of how bacteria, in time and space, build these three-dimensional structures that attach to surfaces and resist mechanical and chemical perturbations. During this talk, I will present a technique to image living, growing bacterial biofilms from single founder cells to ten thousand cells at single-cell resolution. Using the human pathogen Vibrio cholerae as a model biofilm former, we discovered that the biofilm develops from a disordered, two-dimensional layer of founder cells into a three-dimensional structure with a vertically aligned core. Using computer simulations, we found that verticalization proceeds through a series of localized mechanical instabilities on the cellular scale. By modulating cell lengths and osmotic conditions, we quantitatively tested the predictions made from the agent-based simulations.

L70.00293: Application of RLGC Models in Addressing Hospital Acquired Infections*  JESUS PEREZ (Presenter), California State University, San Marcos, YAW OBENG, National Institute of Standards and Technology — In this presentation, I will discuss the application of RLGC models to extract the electrical(RLGC) properties of modeled pathogens in the context of Hospital Acquired Infections (HAIs). HAIs can occur from antibiotic-resistant pathogen contaminants in either the medical procedures, devices, or from the overall hospital circumstance. It is known that exposure to UV light can prevent bacteria from reproducing. However, there is no reasonable quick-turn metrology for evaluating the efficacy of such treatments. Thus, our project is aimed at providing a module for acquiring the electrical properties of pertinent materials to help quantify the amount or intensity of UV light required kill bacteria. In our study, we investigated the changes in the capacitance and resistance of pertinent thin films in response to broad-band UV light irradiation. The results from this study demonstrate the feasibility of using our RLGC model to interpret the radio frequencies’ response of biological systems.

*Society of Physics Students

L70.00294: Myosin V executes steps of variable length via structurally constrained diffusion  DAVID HATHCOCK (Presenter), Cornell University, RIINA TEHVER, Denison University, MICHAEL HINCZEWSKI, Case Western Reserve University, DAVE THIRUMALAI, University of Texas, Austin — Myosin V is a molecular motor that performs intracellular transport by moving along actin filaments and generating energy through ATP hydrolysis. By alternating head detachment, myosin V steps hand-over-hand with the free head executing a random diffusive search for actin binding sites. Recent experiments suggest that the joint between the myosin lever-arms is not freely rotating, as indicated by previous studies, but instead has a preferred angle giving rise to structurally constrained diffusion. We address this controversy by developing a comprehensive model of myosin V, combining a polymeric description of the diffusive search with the kinetic network of states occupied during the stepping cycle. When the joint is constrained, our model predicts diffusion similar to that recently observed, allowing us to estimate bounds on the constraint energy. We also analyze the consistency of constrained diffusion with previous measurements of step distributions and the load dependence of the forward-to-backward step ratio, run length, and velocity, finding good agreement for each. The theory lets us address the biological significance of the constrained joint and provides testable predictions of new myosin behaviors, including a stomp distribution and the run length under off-axis force.
**L70.00295: Label-free visualization of cellular uptake and trafficking of nanoparticles by interferometric scattering microscopy**  
**JIN-SUNG PARK (Presenter), IL-BUEM LEE, Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science, HYEON-MIN MOON, KYOUNG-HOON KIM, SEOK-CHEOL HONG, Department of Physics, Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science, MINHAENG CHO, Department of Chemistry, Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science — Interferometric scattering (iSCAT) microscopy is a new label-free optical imaging technique, recently developed to identify the nano-sized particles beyond a diffraction limit at a high temporal resolution. Here we report on the direct iSCAT visualization for the moment of cellular uptake of nanoparticles which are diffused in the plasma membrane of a live cell. After initial docking onto the plasma membrane, nanoparticles undergo abnormal sub-diffusion, characterized by simple Brownian motion, local confined diffusion, or Hopf diffusion in their long trajectories. During these processes, we sometimes observed that the scattering signals from nanoparticles in the plasma membrane are suddenly disappeared after exhibiting the oscillating motion in the vertical direction of a flat membrane. Such signal loss indicates that these nanoparticles escape from the focal plane of the microscope as they transport rapidly into the cytoplasmic area after cellular uptake. Our experimental results demonstrate that the label-free iSCAT microscopy can be used as a powerful tool to shed interferometric light on dynamic biophysical processes of various intracellular phenomena.  
*This work was supported by IBS-R023-D1*

**L70.00296: The Effect of Intracellular Crowding on the Diffusion Dynamics of Neurofilaments and Microtubules**  
PETER JUNG (Presenter), NILAJ CHAKRABARTY, Department of Physics and Astronomy, Ohio University — Neurofilaments are a class of cytoskeletal proteins which are essential for providing structural support for axons and for regulating axon diameter. Neurofilaments are primarily synthesized in the cell body of neurons and are cargoes of slow axonal transport. Several studies have established that neurofilaments are transported as assembled polymers along microtubule tracks driven by motor proteins. The transport kinetics of neurofilaments have been explained by a “Stop-and-go” model where neurofilaments move intermittently in a bidirectional manner. However, the established models do not take into account the intracellular crowding which can severely limit the diffusion kinetics and in turn affect the reaction rates. We model the neurofilament and microtubules as a bi-disperse population of hard disks in a circular domain representing the cross section of the axon. We find that both cellular confinement and steric repulsion play important roles in modulating the diffusion dynamics and in turn the reaction rates. We are also using our model to study whether phase transition effects at high crowding densities can explain the segregated neurofilament and microtubule populations typically found in some neurodegenerative diseases.

**L70.00297: A Nonlinear Dynamical System Approach to Bird Song Analysis**  
**XIAO ZENG (Presenter), EVE ARMSTRONG, VIJAY BALASUBRAMANIAN, University of Pennsylvania — Songbird vocal production is a complex nonlinear phenomenon. However, acoustic studies of bird vocalization have mostly been based on linear spectral analysis. Such analysis methods necessarily fail to capture the information content of song, and for that reason are not effective probes of the means by which songbirds communicate. We present a novel approach to the analysis and classification of songbird vocalization using nonlinear time series analysis techniques. Time-delay embedding is used to construct a new coordinate system in which to view the song time series. The number of coordinates required to unfold the dynamics represents the dimensionality of a new geometric space, wherein the song's attractor can be visualized. We show that the reconstructed phase space representation of bird vocalization can reveal information that is absent in traditional linear approaches.**

**L70.00298: Spots to stripes: using machine learning to navigate pattern formation space**  
**REBECKAH K FUSSELL, AYESHA BHIXHA, SUZANNE KANE (Presenter), Haverford College — Current models of pattern formation (e.g., Turing reaction-diffusion theory) can generate many observed animal pigmentation patterns. However, their dependence on many interacting parameters makes it difficult to explore their full phase space of patterns. This is an important problem because research in cell signaling and developmental biology allows us to generate increasingly accurate pattern formation models. In this study, we first defined a "measure space" using 25 different measures of pattern geometry (e.g., feature circularity, compactness, intensity variance). We mapped photographs of pigment patterns in measure space and classified them using k-means clustering. We found that three measures were sufficient to group patterns into distinct classes (e.g., spots, stripes, labyrinthine, etc.) The next phase involves using this measure space as a guide for navigating the complex parameter space of a new pattern formation theory. For example, all known patterns generated by the model and a new test pattern (for which the model parameterization is unknown) first are mapped onto measure space. To determine the parameters needed to form the test pattern, a guided search can be performed in parameter space using the measure space distance between the test and known patterns.**
**L70.00299: Self-organized Pattern Formation in Bacterial Colonies**

SIYU LIU (Presenter), The Chinese University of Hong Kong — Pattern formation is ubiquitous in living organisms. In bacterial colonies, pattern formation generally relies on chemical signalings, such as in the case of chemotactic ring formation. Here we study how mechanical interactions between cells in a colony may promote self-organized pattern formation in bacterial colonies. The results may provide new insights into the development of structured bacterial communities, such as biofilms.

*This work was supported by the Research Grants Council of Hong Kong SAR (RGC Reference numbers 14303918, 14322316 and 14301915) and the National Natural Science Foundation of China (NSFC 21473152)*

**L70.00300: Building a Custom Microscope to Study Brownian Motion and Active Matter**

HUNTER SEYFORTH (Presenter), WYLIE AHMED, California State University, Fullerton — Our goal is to build an optical microscope, calibrate it, and make precise measurements of Brownian motion and diffusion using multiple approaches such as mean squared displacement (MSD) analysis and differential dynamic microscopy (DDM). These methods of analysis were applied to quantify the motility of active matter and standardize the process to develop an advanced module for the graduate program. We constructed a microscope based on the design by Kemp et al.(arXiv:1606.03052). Then, the Brownian motion of 1 micron colloidal particles were studied and both single particle tracking and image correlation techniques were implemented to analyze colloidal diffusion. To do this, publicly available matlab codes for particle tracking, MSD analysis, and DDM analysis were applied to calculate the diffusion coefficient. These methods were utilized to quantify the diffusion of two different types of active matter: janus particles and swimming microorganisms. This was done to quantify the motility of active matter. This project is being developed into an advanced lab module to be an introduction to physics research, fortify concepts from optics and statistical physics, and give students experience in building optical systems and analyzing noisy data.

*Dan Black Fellowship, Eiker-Adams Award*

**L70.00301: Analysis and Modeling of Mitochondrial Fission and Fusion Processes in Cells From Healthy and Trisomy Patients**

JOHANNA PAINE (Presenter), California Lutheran University, CARLOS PEREZ, GHANIM ULLAH, Computational Biophysics, University of South Florida, JORGE BUSCIGLIO, Neuroscience, University California Irvine — Mitochondria play a vital role in many cell functions, including ATP production, modulation of Ca2+ signaling and apoptosis. The homeostasis of the fission and fusion of the mitochondrial network allow for healthy cellular function. If the homeostasis of fission and fusion processes becomes unbalanced, the mitochondria can no longer supply enough ATP nor process the calcium ions which leads to apoptosis. Mitochondria’s role in apoptosis makes it a possible target for curing neurodegenerative diseases. The causes behind the progressive degeneration of neurons are not yet understood, beyond a correlation with age, an understanding of the details of mitochondrial function and structure is crucial for better treatments for neurodegenerative diseases. Mitochondrial reticulum structure and function are altered due to conditions like Trisomy 21. We investigate the difference rates of fission and fusion, cluster size and mean degree of healthy and Trisomy mitochondria reticulum. We present a model of the dynamic mitochondrial reticulum, and deduce fission and fusion rates from a single image. This process can be used to deduced the fission and fusion rates of mitochondrial networks with different neurological disease to understand the exact mechanisms these diseases.

*NSF Grant: 1560090*

**L70.00302: Time cells in the mouse dentate gyrus: An apparent instance of traveling waves in the brain**

WEI ZHONG GOH (Presenter), MARC HOWARD, Boston University — The role of standing brain rhythms in cognition has been well investigated, but traveling waves have only recently attracted interest for their potential role in memory and attention. A manifestation of traveling waves in the brain may be "time cells". In animal experiments, a task-relevant event triggers a reliable sequence of neural firing. Each “time cell” fires during a circumscribed period of a delay interval; different events can trigger different sequences. As the time interval since the event increases, the proportion of active time cells decreases. We present evidence of time cells in the mouse dentate gyrus whose activity spans a 20 s delay interval. We describe how information encoded about the time interval since the event is characteristic of a propagating wave traveling in a medium with graduated index of refraction. This framework allows us to characterise how the brain is continually aware of its orientation with respect to events in the world unfolding in time.
L70.00303: Modularity and flexibility quantify unique processing of music and speech stimuli in the human brain*
MELIA BONOMO (Presenter), Department of Physics & Astronomy, Rice University, CHRISTOF KARMONIK, Magnetic Resonance Imaging Core, Center for Performing Arts Medicine, Houston Methodist Hospital, J TODD FRAZIER, Center for Performing Arts Medicine, Houston Methodist Hospital, MICHAEL DEEM, Department of Bioengineering, Department of Physics & Astronomy, Rice University — Music has been shown to have therapeutic benefits for mental health, though few studies have quantified the impact on the brain. We investigated neural network changes from fMRI data while subjects actively listened to a variety of auditory pieces that varied in cultural familiarity and emotivity. We applied theory derived in our group showing that the extent to which modularity and flexibility of the network are selected for depends on the complexity and timescale of the activity being carried out. We found a strong negative correlation between modularity and flexibility while subjects listened to speech; this relationship decreased during self-selected and culturally familiar music, and it became random during culturally unfamiliar music and speech. We also found that modularity during a self-selected song was predictive of the neural network architecture during other pieces. These novel quantifiers of neural activity pave the way for creating individualized predictions of response to music engagement and tailoring therapy interventions to individual patients.

*This work was supported by the Center for Theoretical Biological Physics at Rice University and The Welch Foundation.

L70.00304: Modelling Axon Growth Using Driven Diffusion
NIMA DEHMAMY (Presenter), YANCHEN LIU, Northeastern University — Axon growth has been studied at small scales using models based on diffusion. An important part of the guidance of axons during their growth is following gradients of concentration of special chemicals called axonal guiders. We show how a model of coupled random walkers in a background potential derived from a the concentration guiders can lead to realistic paths for axons, exhibiting a high level of parallelism and following reasonably short paths. We propose a simple mechanism by which using a handful of axonal guiders, a brain could accurately assign target addresses for hundreds of brain regions and grow axons from any brain region to any other using a small alphabet. We also present some preliminary analysis of axon trajectories in the mouse brain.

L70.00305: Overcome Competitive Exclusion in Ecosystems
XIN WANG (Presenter), YANG-YU LIU, Harvard Medical School — Explaining biodiversity in nature is a fundamental problem in ecology. An outstanding challenge is embodied in the so-called Competitive Exclusion Principle: two species competing for one limiting resource cannot coexist at constant population densities, or more generally, the number of consumer species in steady coexistence cannot exceed that of resources. The fact that competitive exclusion is rarely observed in natural ecosystems has not been fully understood. Here we show that by forming chasing triplets among the consumers and resources in the predation process, the Competitive Exclusion Principle can be naturally violated. Our model can be broadly applicable to explain the biodiversity of many consumer-resource ecosystems and deepen our understanding of biodiversity in nature.

L70.00306: A chemical basis for metabolic cooperation in microbial communities*
AKSHIT GOYAL (Presenter), SANDEEP KRISHNA, Simons Centre for the Study of Living Machines, National Centre for Biological Sciences (NCBS-TIFR) — What distinguishes autonomous and cooperating metabolic networks in microbes? How does the underlying universal chemical network constrain metabolic cooperation between individuals? Answering these questions remains a conceptual roadblock given the dearth of culturable, sequenced microorganisms: only about 1% of the expected diversity. Here, we attempt to sidestep this experimental limitation by algorithmically generating reaction networks from the repertoire of chemical reactions in KEGG. We generate a large set of reaction networks, both autonomous and cooperating (cross-feeding). We survey their size, energy (ATP) and biomass yields, as well as their response to a variety of perturbations. We find that while rare, cross-fed pairs can best even the most productive autonomous networks without an obvious compromise to stability. This central result is robust to changing environmental conditions, biomass compositions and the precise method to calculate yields. As a proof-of-concept that a “productivity boost” is possible by cross-feeding, our study provides a chemical basis for the prevalence of metabolic diversity and cooperation in naturally-occurring microbial communities.

*This work was supported by the Simons Foundation.
Heterogeneous Absorption of Antimicrobial Peptide LL37 in Escherichia coli Cells Enhances Population Survivability

Paul Talledo (Presenter), Physics and Astronomy, California State University, Northridge, MEHDI SNOUSSE, Nathan Del Rosario, Biology, California State University, Northridge, BAE-YEUN HA, Physics and Astronomy, University of Waterloo, ANDREJ KOSMRLJ, Mechanical and Aerospace Engineering, Princeton University, SATTAR TAHERI-ARAGHI, Physics and Astronomy, California State University, Northridge — Antimicrobial peptides (AMPs) are broad-spectrum antibiotics that selectively target bacteria. Here, we present our recent investigations on the activity of human AMP LL37 against Escherichia coli by integrating quantitative, population and single-cell level experiments with theoretical modeling. Our data indicate an unexpected, rapid absorption and retention of a large number of LL37 by E. coli cells upon the inhibition of their growth, which increases the chance of survival for the rest of the population. Cultures with relatively high cell density exhibit two distinct subpopulations: a non-growing population that absorb peptides and a growing population that survives attributable to the sequestration of the AMPs by other cells. Comparatively, we screened several common antibiotics for their MIC as controls to juxtapose AMPs' effects on E. coli. A mathematical model based on this binary picture reproduces a quite surprising behavior of E. coli culture in the presence of LL37, including the increase of the MIC with cell density—even in dilute cultures—and the extended lag duration of growth introduced by sub-lethal dosages of LL37.

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Survival chances of a prey swarm: selfish runaway versus cooperative interaction

Rumi De (Presenter), Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India — Cohesive group formation has been observed in diverse species, for example, flock of birds, school of fishes, herd of zebras, huddle of penguins to name a few. In nature, swarming behaviour has generally been found in search of food, for breeding, or to avoid predators etc. However, swarming could also thought to be unfavourable for preys as the predator could easily track and attack the whole group. Here, we investigate the effect of cooperative interaction within a prey group based on a simple theoretical prey-predator model framework incorporating short range repulsion and long range attraction between preys. Moreover, the range of interaction of preys, as in real scenario, may be limited due to their sensitivity, vision, age, or even physical structure; hence, in our model, we consider that each prey interacts with other neighbouring preys within a certain range of interaction radius. Our analysis shows that varying range of interaction vastly influences the trajectory of preys when chased by a predator and also strongly affects the survival probability of the prey group. Interestingly, we find that the survival of number of preys increases within an intermediate regime of interaction radius. These findings could also be qualitatively mapped with observations in nature.

Consecutive seeding and transfer of genetic diversity in metastasis

Alexander Heyde (Presenter), Harvard University, Johannes Reiter, Stanford University, Martin A Nowak, Harvard University — The transfer of genetic diversity between spatially separated growing populations is relevant to a wide range of biological applications, including clonal diversity in cancer metastasis, clonal hematopoiesis in stem cell biology, and species diversity in ecology. We study a multitype branching process of population growth that originates from a single individual but over time receives additional migrants. We derive a surprisingly simple expression for the fraction of genetic diversity transferred between populations as a function of the immigration rates that connect them. Additionally, we calculate statistics for the fixation index FST between populations. Using this model framework, we analyze single-cell sequencing data from ovarian, breast, and colorectal cancer samples collected from 15 patients. For these genetically diverse cell populations, we find an average seeding rate of 1-10 migrant cells per cellular generation time. Under typical metastasis growth conditions, this estimate suggests that 16-130 cells seeded each metastasis and left surviving lineages. Since primary tumors are often surgically removed, the genetic diversity of these metastases determines the probability for treatment efficacy.

*This material is based on work supported by NSF Grant DGE 1144152 (A.H.).

Tracking motion and sleep in Astyanax fish

Adam Patch (Presenter), Yaouen F Fily, Physics, Wilkes Honors College, Florida Atlantic University — Astyanax or tetra fish, as a genus, contain more than 150 species, many of which have migrated into coastal caves around the Gulf of Mexico, convergently evolving sleeplessness, blindness and more sensitive lateral lines. Social behavior is also affected, which may in turn affect sleep patterns. We analyze Astyanax tracking data from the labs of Alex Keene and Erik Duboué at Florida Atlantic University and Wilkes Honors College to characterize motion and sleep patterns and their variations across species.

*Wilkes Honors College of Florida Atlantic University
L70.00311: Directed self-organization through thermoregulation in ant colonies* FAZIL USLU ( Presenter ), Institute of Mechanical Engineering, Ecole polytechnique federale de Lausanne, SEAN MCGREGOR, LAURENT KELLER, Department of Ecology and Evolution, University of Lausanne, MAHMUT SELMAN SAKAR, Institute of Mechanical Engineering, Ecole polytechnique federale de Lausanne — The nest of social insects is a complex architecture housing a multitude of individuals in a highly structured hierarchical network. At the heart of each of these spontaneously organized colonies, are the brood. Given the great lengths that social insects invest in their nest design and the spatial fidelity that individuals present, it stands to reason that the location of brood may regulate the dynamics of the social network and in turn, influence division of labor. We aim to test this prediction in colonies of C. fellah by taking advantage of the inherent thermosensitivity of the colony members. We discovered that the workers repeatedly transport the brood to locations within a certain temperature range. We then developed a robotic heat regulation system that allows us, for the first time, to directly control the position of the brood pile within an ant colony by subtly altering fine thermal gradients under the nest surface floor, while simultaneously, gathering precise behavioral data for all individuals within the colony using automated visual tracking. Analysis of spatial and social interaction network reveals novel insight on how spatial reorganization within the colony drives changes in population dynamics and collective decision making.

*Swiss National Science Foundation

L70.00312: Morphology of interacting proteins (CorA) by a coarse-grained Monte Carlo simulation WARIN JETSADAWISUT, Chemistry, Chulalongkorn University, SUNAN KITJARUWANKUL, Kasetsart University Sriracha Campus, PANISAK BOONAMNAJ, PORNTHEP SOMPORNPIISUT, Chemistry, Chulalongkorn University, RAS PANDEY ( Presenter ), University of Southern Mississippi — A transmembrane protein such as CorA performs selective transport of magnesium across the membrane with specific functions of its inner (iCorA) and outer (oCorA) membrane segments and known to exist as a homo-pentamer. The thermal response of iCorA is found [1, 2] to differ from that of oCorA in both native and denatured phases. Self-organized structures of proteins (CorA and iCorA) are examined by a coarse-grained model as a function of protein concentration at a range of temperatures. The collective structures show clear distinctions in morphology visually in its dilute concentration from that in the crowded (dense) protein matrix both at low and high temperatures. The effective dimension $D$ of CorA assembly is found to be lower ($D \leq 2$) than that of iCorA segments which remain globular ($D \approx 3$) at almost all length scales in its native phase. Based on the higher structural response, (i.e. structure factor and radius of gyration) in its native phase, the inner-segments may be more conducive to transient channel pathways due to cooperative protein-protein interactions.


L70.00313: Exploring the structure of single amylose chains using molecular dynamics* MASON SULLIVAN ( Presenter ), MOHAMMAD HASSAN KHATAMI, HENDRICK W DE HAAN, University of Ontario Institute of Technology — Amylose is a polymeric chain consisting of glucose molecules bound through $\alpha$-1,4 glycosidic linkages. Amylose can assume a variety of conformations in water – the structure and dynamics of which are of primary interest in this research. Despite well-defined secondary structures of amylose chains in experimental studies, the structures obtained through MD simulations lack such well-defined conformations (i.e. helical structures). Presented are results from all-atom MD simulations of single amylose chains (V-amylose) in water. From these simulations, criteria for helix-like structures is developed and the prevalence of these structures is explored. Dynamics such as bond flipping and other structural changes and their effects on helices are also discussed.

*OCE VIP II
NSERC CRD
oscillating swimmer which is capable to chemotax.

In presence of the gradient, the restricted oscillatory motion of the squirmer is altered due to the modification of the slip coefficients of the slip velocity and it starts to move towards the direction of the gradient. Here we have studied, how the net displacement of the body at the end of a complete cycle of oscillation towards the direction of the gradient depends on the strength of the gradient and the frequency of oscillation. This study can be helpful to design an artificial oscillating swimmer which is capable to chemotax.

1. R. Maity and P. S. Burada, to be submitted

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L70.00318: Collective dynamics of 2D self-propelled semiflexible chains  GIMOON NAM (Presenter), CHANGBONG HYEON, Korea Institute for Advanced Study — Collective behavior is an emergent dynamics in active systems. This behavior often involves a hydrodynamic transition between coherent and turbulent flows, which occurs spontaneously even in the absence of an external driving. While the coherent flow state is theoretically well described as a polar and nematic phase, the turbulent state is rather difficult to describe as a single phase due to the existence of many complex local structural patterns such as vortices and spirals. So far, most of the studies have focused on such transition in self-propelled particles system, but the corresponding polymers system is rarely studied. In recent simulation studies on self-propelled chains, it has been implicated that the transition could take place near the boundary between the coherent flow and spiral phases, where each phase is characterized by different values of the stiffness and Peclet number of a single chain. To reveal the underlying mechanism, we have studied the collective dynamics of 2D active semiflexible chains. By means of coarse-grained modeling and Brownian Dynamics simulation, we modeled self-propelled chains melt and monitored its structural dynamics. In this poster session, we report our recent progress on the collective behaviors of 2D active polymer system.

L70.00319: Compressing a Swarm of Multicellular Magnetotactic Bacteria with an Applied Magnetic Field  ALEJANDRA ROSSELLI (Presenter), CAMERON MITCHELL, BENJAMIN ROQUE, ALEXANDER PETROFF, Clark University — Bacteria of the species Magnetoglobus multicellularis live in spherical colonies composed of 10-50 individual bacteria. The colony swims as a single unit parallel to the Earth's magnetic field. Here we investigate the collective dynamics of a swarm of these colonies under an applied magnetic field. We orient the magnetic field towards a wall and measure the spatial distribution of the colonies. We track the motion of individual colonies as they align with the field and collide with one another and the chamber walls. We show that the distribution of colonies is the same as that of an ideal gas in a harmonic potential. We present a simple model to explain how this similarity arises and how it breaks down.

L70.00320: Control of Multicellular Magnetotactic Bacteria with a Magnetic Field  BENJAMIN ROQUE (Presenter), ALEJANDRA ROSSELLI, CAMERON MITCHELL, ALEXANDER PETROFF, Clark University — Bacteria of the species Magnetoglobus multicellularis form spherical colonies composed of tens of cells. A colony moves as a single unit as each cell rotates its flagella. Magnetic minerals within each cell cause the direction of the colony’s motion to align with the ambient magnetic field. Here we characterize the motion of these large, fast-swimming colonies both individually and collectively in an oscillating magnetic field. First, we observe the dynamics of individual colonies. We measure their swimming speed, magnetic moment, and diffusion coefficient. Next, we observe the collective motion of dense swarms of colonies in a rotating magnetic field. We compare the these observations to the predictions of a simple model. We use these results to propose a method to direct swarms of swimming colonies to perform tasks, such as sorting tracer particles in a fluid.

L70.00321: Mechanism of Reentrant Liquid Condensation in Arginine-rich Low Complexity Domains*  TARANPREET KAUR (Presenter), IBRAHEEM ALSHAREEDAH, PRIYA R. BANERJEE, Department of Physics, University at Buffalo, The State University of New York — Arginine-rich (R-rich) low complexity domains (LCDs) are ubiquitous in eukaryotic RNA binding proteome, act as multi-valent RNA/protein-binding elements for liquid-liquid phase separation, and implicated in c9orf72-related ALS disease etiology. Recently, we showed that RNA mediates a remarkable reentrant liquid condensation of R-rich LCDs1, a phenomenon that is also observed in the cell2. Combining biophysical experiments and polymer physics theories, here we study the mechanism of the reentrant phase behavior of R-rich LCDs in ALS-associated protein FUS. We show that charge regulated electrostatic forces (long range) control condensation and de-condensation thresholds, whereas short-range attractions determine the stability of the condensates. Importantly, conditions promoting homotypic LCD-LCD and/or RNA-RNA interactions result in a more complex phase behavior, such as the formation of distinctive condensates with orthogonal physical properties. Together, our experiments and free-energy surface modeling suggest a highly tunable phase behavior of R-rich LCDs.


*College of Arts and Sciences, UB
L70.00322: Modularity Promotes Adaptation in a Model of Exploratory Evolution* SHUBHAM TRIPATHI (Presenter), MICHAEL DEEM, Rice University — Biological systems are modular. They are composed of distinct components that function almost independently of one another. Studies have shown that modularity can spontaneously emerge in systems evolving under changing environmental conditions if the goals of evolution are varying in a modular manner or if horizontal gene transfer is present. Here, we examine a model that relaxes these constraints. We analyzed the effect of adding modular organization to a previously characterized model of evolution in gene regulatory networks. In this model, the topology of regulatory interactions is fixed while the regulatory strengths evolve to satisfy a linear constraint on the levels of different regulatory factors. We observed that the probability of successful adaptation within a fixed time period was higher when the regulatory topology was modular. The probability varied non-monotonically with the modularity of the regulatory topology. There are neither modularly-varying goals nor horizontal gene transfer in our model. Our model thus represents a previously uncharacterized scenario wherein modularity can be beneficial in evolving biological systems.

*This work was supported by the National Science Foundation (PHY-1427654).

L70.00323: Bio-energy Transport as a Dressed Vibrational Exciton in Protein Molecules* PEIGHTON BOLT, THEJA DE SILVA (Presenter), Physics, Augusta University — Following the ideas of Davydov's soliton theory, we study the bio-energy transport in protein molecules. By using a quantum Brownian motion model for a phonon dressed vibrational exciton, we calculate the time-dependence on the mean square distance, diffusion coefficient, and energy of the vibrational exciton. We find the time-dependence by solving the quantum Langevin equation and find oscillatory behaviors due to the super-diffusive non-ohmic dissipation. We find that the vibrational exciton gains an overall energy due to the coupling to the phonon bath, it also dissipates its energy to the environment as it propagates. The amount of energy gain and the oscillatory features depend on both temperature and the phonon-vibron coupling.

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L70.00324: Continue study of nano-Co synthesized by pea (Pisum Sativum L.) and lucerne (Medicago Sativa L.). NEREIDA AVENDAÑO GAVIRA (Presenter), ELIZABETH CHAVIRA, GUADALUPE ZAVALA, ADRIANA TEJEDA, National Autonomous University of Mexico — Our research group reports the synthesis on nano-Co using Co3O4 (STREM CHEMICALS) reagent, analyzed by X-ray powder diffraction, (XRD) with concerning a hexagonal unit cell (PDF 43-1003) and 3% of iron oxides (PDF: 8-0097) impurities.

Lucerne oxidizes Co3O4 by its growing process; all vegetables need oxygen to grow (we are working in the mechanism by which lucerne do that). The lucerne is a natural nano-synthesizer; by HRTEM it is visualized Co shape and size of the nano-crystals in lucerne. Co is distributing in small highly symmetric complex similar to virus structure in infected cells. In pea the results are not that clear, we visualized the Co agglomerate by HRTEM in the root.

Due to the interest in the structural properties of nano-cobalt synthesized, the contaminated samples were allowed to dry under room conditions during 29 days. Then plats were grind, and as we know we have metallic Co inside the plat, so using a magnet we separated the organic part which contained it. Finally they were analyzed with XRD, one study for lucerne and other for pea.

Because of in the XRD analysis the proportion of Co were less than 1% (plants were contaminated with 0.05 g of Co3O4) result showed us only the diffraction of the organic part.
Technologies such as microalgae cultures and nanotechnology have been developed for water purification systems. In this work we continue using the silver nanocrystals that were synthesized from garlic (Allium sativum) and onion (Allium cepa) with two different solvents (water and ammonium hydroxide) plus a precursor agent in solution and polycrystals; obtaining a cubic crystalline structure for garlic (Allium sativum) PDF 00-001-1236 of AgCl and onion (Allium cepa) PDF 00-001-1167 obtained with X-ray diffraction analysis (XRD). In addition, a mass loss process of 90% at 100 °C corroborated by thermogravimetric analysis (TGA) and simultaneous analysis (SDT), crystalline cubic conglomerates of silver nanocrystals between 100 and 200 nm with crystal morphology have order diameters of 2-10 nm. Obtained by SEM and HRTEM. To be able to mix the nanocrystals with a microalgae and determine the reactions between them; The first stage is carried out, consisting of the production of microalgae using 10, 20 and 30 ml of liquid humus obtained from the California red worm (eisenia foetida) in 600 ml of water with growth conditions at a temperature of 23-26 °C and a humidity of 45-55% after the first 192 h of diatomaceous microalgae observed at 10x in the optical microscope.

Identification of a Model Organism for Giardia Lamblia by Raman Spectroscopy* JOSEMARIA SORIANO (Presenter), Physics and Environmental Science, St. Mary's University, CHENGLONG ZHAO, FARZIA KARIM, Physics, University of Dayton — Giardia Lamblia is a protozoan parasite which causes Giardiasis, the most common intestinal protozoan infection in the world. Several studies show the presence of blackish pigment granules in retinal layers due to Giardiasis, making of Giardia a pigment-related parasite. In the following work, Raman spectroscopy will be used for the identification of Euglena gracilis, model organism chosen because of its physical similarity, low cost and biosafety. In this study, Euglena samples were excited at 785 nm and signal optimization was performed using Surface-Enhanced Raman spectroscopy (SERS) utilizing gold (Au) nanoparticles as substrate. Our results indicate that SERS provides a four-fold signal enhancement for peaks at 1188 cm⁻¹ and 1530 cm⁻¹, corresponding to the β-carotene conjugated double-bond system present in Euglena, pigment concentrated in the light sensitive eyespot. Thus, we have shown the effectiveness of Raman and SERS Spectroscopy on the identifying of microbial pigments, constituting a robust method to detect and characterize pathogenic microbes such as Giardia, which will have significant downstream diagnostic implications.

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Single Molecule Localization and Orientation Mapping Using a Joint Inversion Technique ANTHONY MAUTINO (Presenter), ABHISHEK KUMAR, University of Maryland, College Park, JAMES M MARR, MARK MCLEAN, STEPHAN STRANICK, Materials Measurement Laboratory, National Institute of Standards and Technology, VERONIKA SZALAI, JAMES LIDDLE, Physical Measurement Laboratory, National Institute of Standards and Technology — For rotationally-constrained molecules, single molecule (SM) localization based super-resolution imaging can incur losses in accuracy when not accounting for the effect of SM orientation on the point spread function. It is important to determine molecular orientation both to maximize localization accuracy and also because orientation provides information about the local molecular environment, which determines features such as chemical reactivity, biomolecular interactions, local polymer mobility, etc. To map the 3D orientation of SMs, we collect the intensity projected onto four different polarization orientations simultaneously and use the intensities in the different channels to reconstruct each dipole's 3D orientation. These data provide 1) information on the SM's local environment, and 2) constraints for image point spread function-fitting and localization. SM images acquired from a second objective positioned on the opposite side of the sample versus the four-channel collection system are utilized for a joint inversion technique for position. We present techniques of registration, localization, and polarization analysis, along with an uncertainty analysis and assessment of the developed methods.
We monitored γ-H2AX formation using ChIP-qPCR after creating a site-specific break on Chromosome III. Experimentally measured γ-H2AX profiles by the two kinases are significantly different from each other suggesting that different mechanisms are used to reach H2A histones around the break. We consider four modes of phosphorylation propagation: (a) 3D diffusion of a kinase initially bound to the break, (b) looping of chromatin to bring a kinase tethered to the break to distant sites along the chromatin, (c) directed sliding of a kinase along the chromatin, and (d) 1D diffusion of a kinase along the chromatin. Using Bayesian model selection, we determined that the activity of Mec1 is best described by looping while Tel1 is best described by directed sliding.

*Funding provided by R35 GM127029-01

JING XIA (Presenter), School of engineering and applied science, Harvard University, FRED C. MACKINTOSH, Chemical and Biomolecular Engineering, rice university, LIHENG CAI, Materials Science and Engineering, university of virginia, HUAYIN WU, DAVID A WEITZ, School of engineering and applied science, Harvard University — Fibrin are the main constituent during the hemostasis due to its unique mechanical properties resulting from its hierarchy structure, malfunction of fibrin can lead to diseases such as thrombosis. Here we show Zn can tune the fibrin network and its mechanical properties. In the presence of Zn2+, fibrin protofibrils form huge fiber bundles which are intrinsic loosely coupled. By further comparing with theoretical model, we show that under low stress, the mechanical properties of Zn modified fibrin network are contributed by the thermal fluctuation of the network; at high stress, the mechanical properties are contributed by single protofibril mechanics.
Finally, we examine the influence of resulting network structures on dynamics of molecular motor motion. Using tools from graph computational methods utilizing kinetic Monte Carlo and Brownian dynamics simulations to study the organization of such as plant villin influence cytoskeletal organization and intracellular transport in plant cells. In this work, we use hybrid computational methods utilizing kinetic Monte Carlo and Brownian dynamics simulations to study the organization of actin networks as a function of system size, system shape, and density of crosslinking proteins. Using tools from graph theory, we gain insight into cytoskeletal architecture by analyzing graphs characterizing the connectivity of actin networks. We analyze how the connectivity, as described by the Flory-Stockmayer theory, changes as a function of the concentration of non-neuronal microtubules have been evaluated in several reported studies. However, our knowledge about dielectric factors of non-neuronal microtubules is still limited. In our study, we quantified the normalized polarization coefficient of Tau-MCF7 microtubules by implementing the electro-orientation method. The result was then compared with the one we previously reported for MCF7 microtubules in the absence of Tau protein. This study is significant, as MCF7 microtubules are structurally different from neuronal microtubules in terms of the distribution of beta tubulin isotypes. The polarization factor and, consequently, negative charge of those microtubules is smaller than MCF7 polymerized from MCF7 tubulin. This can potentially be an underlying mechanism for many intracellular functions.

Finally we compare this result with actin networks containing Arp2/3. We expect our results to give an insight into how the concentrations of linker and motors than those required to observe contractions in the mechanochemical simulations. We find that the sol-gel transition in the system occurs at lower concentrations of linker and motors than those required to observe contractions in the mechanochemical simulations. Finally we compare this result with actin networks containing Arp2/3. We expect our results to give an insight into how the connectivity of the network affects its dynamic behavior.

*This work was supported by the Center for Theoretical Biological Physics sponsored by the National Science Foundation (PHY 1427654) and by the National Institute of General Medical Sciences (R01 GM44557).
Single Wall Carbon Nanotube (SWCNT) as an Intracellular Gene Delivery Cargo*  
(ADEYINKA ADESINA (Presenter), NANOSCIENCE, UNIVERSITY OF NORTH CAROLINA AT GREENSBORO — A SWCNT is truly one-dimensional nanoscale object, possessing unique optical, electronic, and mechanical properties. Earlier works on SWCNT toxicity and size allowed for widespread use of SWCNTs in biological studies. SWCNTs bind to biomolecules, proteins and nucleic acids via Coulomb and other interactions, both on the specific and nonspecific level, this motivated many drug and gene delivery studies which demonstrated that SWCNTs, functionalized with polymers and biological molecules may serve as highly efficient and easily targeted delivery agents.

In this study, ssDNA labeled with Alexa Fluor 546 dye was used to functionalize SWCNT. This hybrid matched a complementary ssDNA which was labeled with Alexa Fluor 488 dye. Double-stranded DNA hybridization on the solvent-exposed sticky ends was monitored by Forster Resonance Energy Transfer technique. The modulation of the SWCNT optical response due to DNA conformational charge motion before and after hybridization was also investigated.

*Acknowledgement
UNC Inter-institutional Planning Grant A19-0079-001

Mining recombination algorithms in modular biosynthetic gene clusters  
(ZHIYUAN LI (Presenter), DONIA MOHAMED, Princeton University — Non-ribosomal peptide synthetases (NRPSs) are ubiquitous in micro-organisms and produce large varieties of metabolites with pharmaceutical potentials. Its modularity structure inspired de-novo designing efforts by recombining desired modules. However, past efforts in this direction are largely unsuccessful. The difficulty in re-engineering new products raise questions on the modulized view: are there unknown functional constraints between different parts of NRPS that favor/disfavor certain combinations of modules or subunits?

In large database, correlations between different subunits of NRPS can be uncovered by statistic techniques. However, as subunits in the same gene cluster are correlated by sharing the same lineage history, the correlation induced by functional constraints usually get blurred.

A unique marine bacteria described in our previous research reveals important design principles of NRPS. In this bacteria, 20 NRPS pathways generate chemical diversity though extremely frequent recombination. Genetic exchange between NRPSs is so intensive that it largely erases the correlation by lineage history, leaving correlation by function clearly observable. In this system, we revealed previously undescribed constraints between different types of subunits of NRPS.

Probing the Cell-Fate Decision During Infection of E. coli by the Virus Lambda  
(SETH COLEMAN (Presenter), RICE UNIVERSITY; IDO GOLDING, BAYLOR COLLEGE OF MEDICINE; OLEG A IGOSHIN, RICE UNIVERSITY — Lambda is a virus which infects E. coli bacteria, and its infection serves as a paradigm for cell-fate decisions, processes where cells select and transition to stable states. Infected cells can proceed along one of two developmental pathways: lysis, characterized by rampant viral replication and eventual cell death, or lysogeny, characterized by viral dormancy. Despite the decades of research done on this system, fundamental questions remain about what factors drive the decision and the mechanisms by which they act.

We are developing models which, calibrated by single-cell resolution experimental data, will be able to shed light on how currently known factors (such as gene copy number, both as an initial condition and as a function of time due to replication, as well as cell volume) influence the decision process, and predict additional factors.  We are also investigating explanations for a surprising observation in lambda – the scaling of the probability of a lysogenic outcome with viral concentration exhibits a complicated structure, which can be understood by positing that viruses independently decide their fates. We are developing simple models to test this hypothesis and propose a possible physical mechanism for this intracellular individuality.
A game-theoretic approach to model the transmission of Chikungunya on Reunion Island.

DAVID FEAGINS (Presenter), Department of Physics and Environmental Science, St. Mary's University, Texas, SYLVIA KLEIN, Department of Mathematics, St. Mary's College of Maryland, Maryland, ALEX FOSTER, Department of Mathematics, Coastal Carolina University, South Carolina, JONATHAN ROWELL, IGOR EROVENKO, Department of Mathematics, University of North Carolina at Greensboro, North Carolina — Chikungunya is a viral infection that is spread by mosquitoes of the genus Aedes. Chikungunya victims experience symptoms similar to those caused by the Dengue and Zika viruses but are less likely to die from it. Chikungunya was not a major research interest up until 2004 when a third of the population on Reunion Island, located in Africa, was infected by the disease. This outbreak inspired the creation of mathematical models to study how Chikungunya is transmitted. Driven by these studies, we constructed a game-theoretic model that considers how rational individuals decide to use mosquito repellent to prevent the disease. In our model, individuals make their decision based on a payoff function that takes into account the consequences of being infected and the perceived cost of using mosquito repellent. We found that the usage of mosquito repellent is negatively correlated with the perceived cost of mosquito repellent while keeping the consequences of contracting the disease constant. However, setting the perceived cost of mosquito repellent to zero does not guarantee the eradication of Chikungunya. With this in mind, governments and disease control programs can better understand how to manage the transmission of this mosquito-borne disease.

(Supported by NSF Grant DMS-1659646)

Critical level of epistasis separates trajectories toward evolution of mutational or drift robustness in small populations

CHRIS ADAMI (Presenter), Microbiology and Molecular Genetics, Michigan State Univ, DARIYA SYDYKOVA, Department of Integrative Biology, University of Texas at Austin, THOMAS LABAR, Department of Molecular and Cellular Biology, Harvard University, CLAUS WILKE, Department of Integrative Biology, University of Texas at Austin — High mutation rates select for the evolution of mutational robustness, where populations inhabit flat fitness peaks with little epistasis [1]. Recent evidence shows that a different effect shields small populations from fitness declines. In drift robustness [2], populations occupy peaks with steep “flanks”, and positive epistasis. But what happens when mutation rates are high and population sizes are small at the same time? Using a fitness model with both variable epistasis and mutational effect size, we show that the equilibrium fitness has a minimum as a function of the parameter that tunes epistasis, implying that this critical point is an unstable fixed point for evolutionary trajectories. In agent-based simulations of evolution at finite mutation rate, we demonstrate that when mutations can change epistasis, trajectories with a subcritical value of epistasis evolve to decrease epistasis, while those with supercritical initial points evolve towards higher epistasis. These two fixed points can be identified with mutational and drift robustness, respectively.


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Structured Active Fluids via Interfacial Nanoparticle Assembly

PAUL KIM (Presenter), JOE FORTH, Lawrence Berkeley National Laborabory, ZVONIMIR DOGIC, POOJA CHANDRAKAR, University of California, Santa Barbara, THOMAS RUSSELL, Lawrence Berkeley National Laborabory — The transport of ordinary liquids tends to be driven by pressure difference, whereas for active fluids (or biological matters), the transport is autonomous and/or isotropic, governed by the gradient in specific chemical. Wu et al. recently discovered the emergence of spontaneous directional flow of active fluids, consisting of microtubule filaments and kinesin molecular motors, upon their confinement in a variety of microfluidic channels [Science 24 Mar 2017: Vol. 355, Issue 6331]; when confined in loops of toroidal and cylindrical channels, the flow persisted in one direction, either clockwise or counterclockwise. Here, we observed the same active fluid confined in channels of similar geometries, which are made of a thin layer of nanoparticles. By extruding or molding a dispersion of charged nanoparticles in an immiscible solution of oppositely charged surfactants, liquids can be mechanically stabilized (or structured) in an arbitrary shape by jamming of nanoparticle surfactants at the liquid interface. The flow of active fluid and its consequence to overall structures are observed in situ by fluorescent microscopy. The interactions between the liquid interface and active fluid is also studied.
**L70.00343: Emergence of E. coli Critically Buckled Motile Helices Under Antibiotic Stress**

TRUNG PHAN, Princeton University, RYAN MORRIS, Physics, University Edinburgh, ROBERT AUSTIN (Presenter), MATTHEW BLACK, Princeton University, JULIA BOS, Institute Pasteur

— Bacteria under external stress can reveal unexpected emergent phenotypes. We show that the intensely studied bacterium E. coli can transform into long, highly motile helical filaments poised at a torsional buckling criticality when exposed to minimum inhibitory concentrations of several antibiotics. While the highly motile helices are physically either right- or left-handed, the motile helices always rotate with a right-handed angular velocity \( \omega \) which points in the same direction as the translational velocity \( \nu_T \) of the helix. Furthermore, these helical cells do not swim by a 'run and tumble' but rather rather synchronously flip their spin \( \omega \) and thus translational velocity \( \nu_T \) backing up rather than tumbling. By increasing the translational persistence length, these dynamics give rise to an effective diffusion coefficient up to 20 times that of a normal E. coli cell. Finally, we propose an evolutionary mechanism for this phenotype's emergence whereby the increased effective diffusivity provides a fitness advantage in allowing filamentous cells to more readily escape regions of high external stress.

*This work was supported by NSF PHY-1659940.

**L70.00344: Simple Stochastic Simulations for Visualizing and Testing Models of Gene Expression and Proofreading**

KEVIN Y CHEN, Chemistry, University of Cambridge, DANIEL ZUCKERMAN, Biomedical Engineering, Oregon Health & Science University, PHIL NELSON (Presenter), Physics and Astronomy, University of Pennsylvania — To better visualize the stochastic nature of cellular processes and how they unfold over time, we developed a simple Gillespie algorithm to simulate two important non-equilibrium statistical processes, gene expression and translation error correction.

For example, our simulations demonstrate the concept of kinetic proofreading, generating proteins with error fractions predicted by Hopfield's rate-equation analysis, but also providing illustrative time courses for the reaction. Animations derived from simulation help build intuition. Furthermore, our simulations show that a ribosome with only kinetic proofreading, i.e. only a difference in unbinding rates between right and wrong charged tRNA, must sacrifice speed for accuracy. Simulating translation with recently measured rate constants shows how the ribosome combines kinetic proofreading, which relies on sequential, quasi-equilibrium steps, with internal discrimination, which allows for unequal forward rates, to efficiently translate mRNA with few misreadings. The stochastic simulation algorithm used here requires only a few lines of code and can easily be adapted for other biomolecular processes.

Details are available at http://biorxiv.org/cgi/content/short/418772v1

*National Science Foundation PHY--1601894.

**L70.00345: Modeling the collective behaviour of Dictyostelium discoideum under directed migration**

VIKTOR TESHOME BELAY (Presenter), Department of Physics, American University, WOLFGANG LOSERT, Department of Physics, University of Maryland — Cellular migration is a function that is ubiquitous across a vast number of organisms. This phenomenon is observed in many biological functions such as embryogenesis, tissue regeneration, tumor metastasis, muscle contraction, and more. Cellular migration is influenced by various factors; principally, by chemical, mechanical, and electrical cues. We utilize the model organism Dictyostelium discoideum to study the effects of nanotopographical guidance and electrostatic fields on the motion of cells. We develop a cell-scale stochastic model of the influence of nanotopography, electrostatic fields, and chemical signaling by the secondary messenger cyclic adenosine monophosphate on the motion of D. discoideum cells. Model simulations show that unidirectional guidance by nano-ridges allows for D. discoideum streaming and aggregation, while bidirectional nanotopography creates a cell bifurcation in which there is little to no streaming or aggregation. In addition, simulations indicate that D. discoideum cells exhibit directed collective motion when under the influence of a unidirectional electric field.

*This project was fully funded by the National Science Foundation, award number: PHY-1756179.
L70.00346: Designing Compact Microfluidic Structures to study Cancer Cell Metastasis via Flow-less Spatial and Temporal Gradients*  
ARTURO RUBEN DIAZ (Presenter), ILEENE ASHLEY DIAZ, Physics and Astronomy, Georgia Southern University, DWAYNE G. STUPACK, Moores Cancer Center, University of California San Diego, DRAGOS AMARIE, Physics and Astronomy, Georgia Southern University — Metastasis, the migration of cancer cells away from an original tumor to other tissues, is the primary cause of morbidity and mortality in cancer patients. This migration is controlled by complex biomechanical processes and triggered by diverse stimuli. We seek to develop a set of microfluidic tools to investigate metastasis that will allow us to analytically pinpoint triggering factors by studying changes in cell migration as prompted by as few simultaneous stimuli as possible. These devices are microfluidic structures that produce stable, controlled gradient flows across and along a microfluidic gradient chamber. They will allow us to study how extracellular chemical gradients of various compositions and/or concentrations drive ovarian carcinoma cell migration. These tools follow our previous work and use the concept of splitting and recombining flows through a series of bifurcations and trifurcations, while introducing a gradient chamber separate from the cell culture chamber. Bright field and epi-fluorescence microscopy will be used to characterize these devices.

*This work was supported in part by the Office of the Provost and Vice President for Academic Affairs of Georgia Southern University

L70.00347: Bacterial Physiology during Intercellular Signaling*  
SHIQI LIU (Presenter), The Chinese University of Hong Kong — Cell-cell communication plays an important role in many biological processes. The communication is often mediated by diffusing chemical signals released by cells. Here we study how the bacterial physiological state responds to the intercellular signals and how individual cells benefit from those signaling-related processes. A better understanding of bacterial physiology during intercellular signaling could enable us to manipulate the behavior of cells and may help to understand biofilm formation.

*This work was supported by the Research Grants Council of Hong Kong SAR (RGC Reference numbers 14303918, 14322316 and 14301915) and the National Natural Science Foundation of China (NSFC 21473152)

L70.00348: Propagation of Wall-Less Bacteria*  
YISEN LI (Presenter), The Chinese University of Hong Kong — Normally bacterial growth relies on the peptidoglycan cell wall. However, cells in a wall-free state can propagate in a wall-independent manner, which remains poorly understood. We will present our recent work on continuous propagation of wall-less bacteria and colony formation. The underlying mechanism is relevant to antibiotic resistance of pathogens.

*This work was supported by the Research Grants Council of Hong Kong SAR (RGC Reference numbers 14303918, 14322316 and 14301915) and the National Natural Science Foundation of China (NSFC 21473152).

L70.00349: Anomalous flip-flop of DMPC in lipid membranes*  
NETI BHATT (Presenter), URSULA PEREZ-SALAS, University of Illinois at Chicago, LIONEL PORCAR, Institut Laue–Langevin, YANGMINGYUE LIU, MICHAEL STANFIELD, University of Illinois at Chicago — Although the study of the passive movement of lipids between and within membranes can give insight into lipid transport regulation by providing a way to gauge the energetic cost on active metabolic pathways, published work on the spontaneous transfer of lipids report a wide variation in the rates of transfer between and particularly within membranes. Non-invasive approaches like time resolved small angle neutron scattering or sum-frequency vibrational spectroscopy have shown that the movement of lipids is extremely sensitive to chemical structures of molecules finding that the transfer rates of unaltered lipid molecules are dramatically different from their chemically tagged counterparts. My group performed Neutron Scattering experiment and found that DMPC flip-flop rates display two Arrhenius states well above DMPC’s melting temperature. I will report on measurements of the flip-flop rates in DMPC using nuclear magnetic resonance spectroscopy and membrane order and fluidity using Laurdan generalized polarization, DPH anisotropy respectively, to reveal the nature of this intriguing behavior.

*We thank CAREER award DMR-1753238 as well as University of Illinois at Chicago Chancellor’s undergraduate award and Honors college research grant for providing funding for the experiment
L70.00350: Deterministic and stochastic analysis of an oncolytic infection model* KARAN BUNTVAL (Presenter), Bard College at Simon’s Rock, HANA M DOBROVOLNY, Departments of Physics and Astronomy, Texas Christian University — Mathematical models of biological processes have had a history of high predictive power of both experimental data and preliminary drug tests. Models that aim to predict the dynamics of oncolytic virus infections have previously focused solely on 3 populations, i.e., the cancer cells, virus-inflicted cancer cells, and the virus itself. Considering that most tumor populations have a substantial proportion of healthy cells, an oncolytic model that rightly adjusts for this increased fraction would provide insight into dual cell dynamics. Our findings elucidated that certain parameter variations with the tumor proliferation, infection, virus replication, and infected cell dissolution rates eventually allowed for the negation of cancer cells while simultaneously keeping the healthy cells alive. A stochastic interpretation of the model was further utilized to more authentically characterize the probabilistic events during an infection. In addition to preventing the oscillatory behavior observed with the deterministic model, it also confirmed the initial denouement of an extinct cancer population and thriving non-cancerous cells.

*This work was supported by NSF REU grants NSF-1358770 & NSF-1659444.

L70.00351: Assessing tumor treatment modalities using an allometric model JENNIFER FIREHAMMER, ALLEN GARNER (Presenter), Purdue University — Allometric growth models apply universal growth laws to predict growth of organisms and structures from very small to very large and have accurately modeled avascular tumor growth. These models have been extended by coupling the allometric growth law to a reaction-diffusion equation for nutrient transport to model necrotic core formation [A. L. Garner, Y. Y. Lau, T. L. Jackson, M. D. Uhler, D. W. Jordan, and R. M. Gilgenbach, J. Appl. Phys. 98, 124701 (2005).] and incorporated vascularization by applying energy arguments to incorporate vascularization [A. B. Herman, V. M. Savage, G. B. West, PLoS ONE 6, e22973 (2011).]. Recent developments of artificial, 3D tumor in vitro models that can incorporate vasculature provide a future means to assess chemical, physical, and combined treatments [R. Michna, M. Gadde, A. Ozkan, M. DeWitt, and M. Rylander, Biotech. Bioeng., https://doi.org/10.1002/bit.26778] for eventual clinical use. In this study, we modify the allometric growth model to assess the implications of dosage profiles on tumor growth. For a constant dosage, we observe that a subthreshold treatment reduces the steady-state tumor size while a suprathreshold amount destroys the tumor. The therapeutic implications of these results and future experiments will be discussed.

L70.00352: Tracking the Kinematics of Zebrafish Startle Responses Following Ablation of Sensory Hair Cells PETER JAEOH CHO (Presenter), MOHAMED AHMED RAMY, YAGMUR I. OZDEMIR, RANA BARGHOUT, JOSEF TRAPANI, ASHLEY CARTER, Amherst College — The survival of a zebrafish depends on its ability to detect and respond to external stimuli. Indeed, to avoid predators, zebrafish startle when subjected to sudden mechanical stimuli. Here our goal is to characterize the kinematic properties of the zebrafish startle response following ablation of sensory hair cells to determine the role of these cells as well as observe whether differences in the neural circuitry lead to measurable physical changes in the kinematic properties. To measure these kinematic properties, we head mounted a single larval zebrafish, induced a startle, and took videos of tail movement with a high-speed camera. Videos were analyzed in MATLAB to find the tail midline, allowing us to measure the kinematic differences in tail angle, velocity, acceleration, and curvature. Further work could observe twist and out of plane motion of the tail. Differences in these kinematic parameters would highlight how zebrafish behavior is affected by an altered neural circuit.

L70.00353: Scale-dependent relationships in human language AAKASH SARKAR (Presenter), MARC HOWARD, Psychological and Brain Sciences, Physics, Boston University — Many models of human language extract statistical regularities of natural language to estimate “meaning”. Mutual information between words in natural language has been shown to decay as a power law (Lin and Tegmark, 2017). Despite this evidence for scale-invariant statistics, statistical models of language typically impose a strong scale. We study the scale-dependence of language using Word2Vec (Mikolov et al., 2013), a shallow neural network model which generates a vector embedding of words by training over a corpus of text. We modify the Word2Vec algorithm to choose neighbors of a target word with an exponentially decaying distribution, and look at the embedding generated for a broad spectrum of scale parameters. It seems to appear that different syntactic and semantic relations (as classified in several tests developed by Mikolov et al.) seem to be best expressed at different word scales. Word similarities between neighbors seem to capture qualitatively different behavior across a range of word-scales, often peaking at distances that would not be captured by an embedding sampled at a single, particular scale. These results point toward the importance of developing scale-free models of semantic meaning.
L70.00354: Temporal contingency and informativeness in Laplace domain  KONSTANTIN TIUREV (Presenter), MARC HOWARD, Boston University — Associative learning in conditioning protocols is traditionally thought to depend on temporal contiguity between the stimuli. However, recent proposals suggest that temporal contingency rather than temporal contiguity is responsible for associative learning. That is, associations to the unconditional stimulus develop whenever it provides meaningful information about the expected time of reinforcement. Such information-theoretic framework has recently been considered in the context of Pavlovian conditioning, operant conditioning, and behavioral neuroscience. Here we develop information-theoretic approach to the long-range temporal credit assignment subject to several cognitively-inspired constraints. First, we assume that the system cannot possibly measure the joint statistics of the past combinations of stimuli. Second, our method assumes that the approximate stimuli history is available in the form of the inverse Laplace transform, which makes the method time-local and scale-invariant and helps to overcome major drawbacks of traditional approaches to the long-range credit assignment problem. The result is a biologically-plausible, computationally efficient model of associative learning, one of the fundamental processes in neural function.

L70.00355: An Electro-Mechanical Model of the Axon*  JOHN LEVENTIS (Presenter), GARY PENNINGTON, Towson University — Recent research into the electro-chemical effects of neural damage have provided evidence for interactions between deformations of the axonal membrane and the flow of charges thru its ion channels. Furthermore, traveling mechanical membrane waves in the axon have been shown to accompany the action potential. It seems possible that a more complete understanding of the true phenomena governing the transmission of an electric signal along a myelinated axon must incorporate more than just the electro-chemical mechanisms. We report simulation of signal transport in neural axons incorporating both electro-chemical and mechanical strain-related membrane deformations. Myelinated axons under normal and abnormal stressed conditions are compared. The results are used to investigate interdependencies between strain-related membrane deformations and electrical signals along the membrane. We model electro-mechanical behavior due to cell damage, disease, and abnormal ionic concentrations around the cell. We hope that making explicit the interdependencies between mechanical waves and electrical signals within the axon will prove useful to further biophysical research.

*We would like to gratefully acknowledge funding support from the Fischer College for Science and Mathematics at Towson University.

L70.00356: Development of a Behavioral Assay using Fluidic Devices to Study Learning and Memory in Cuttlefish Larvae*  COLTON SELLARS (Presenter), Physics and Astronomy, Georgia Southern University, JESSICA BOWERS, VINOTH SITTARAMANE, Biology, Georgia Southern University, DRAGOS AMARIE, Physics and Astronomy, Georgia Southern University — We developed behavioral assays to investigate the behaviors of cuttlefish hatchlings. Despite their behavioral complexity, little is known about cuttlefish behavior due to chemical stimuli. Current work done in 6-well plates shows the need for designing new fluidic device to manipulate chemical flow, delivery times, and allow event recording. Since behavioral assays for aquatic species require a flow-through design, our chip consists of joined channels, while diffusion coefficient calculation allowed us to evaluate flow rates. Our fluidic device provides more control thus creating a complex environment for cuttlefish hatchlings to explore. Using this device and tracking software, we can quantify the movement of cuttlefish in response to different stimuli. In these trials we aim to determine how prey cues have an effect on the cuttlefish navigation throughout the new environment. By providing food rewards for performing tasks, we can determine cuttlefish ability to learn to discriminate specific chemical information. This work presents a novel method for studying animal behavior in a dynamically changing chemical environment.

*This work was supported in part by a COUR award from the College of Science and Mathematics, and FRC Seed funding from the Georgia Southern University.

L70.00357: Investigating material properties of fish schools with dynamic light fields  PRANAV KAYASTHA (Presenter), AAWAZ POKHREL, JAMES PUCKETT, Gettysburg College — Many social animals, such as birds, fish and insects, exhibit complex group behavior. Models have shown that simple local interactions between individuals gives rise to the emergent self-organized macroscopic states such as flocks, swarms, or schools. We investigate the material properties of laboratory fish schools by exploiting the negative phototaxicity of Rummy-Nose Tetra (Hemigrammus blehri) to strain the school using projected dynamic light field. To do this, we use an overhead high speed camera to record individual fish trajectories in a quasi-two-dimensional tank. The strain is generated by projecting two dark regions moving in opposite directions, where fish use both social and environmental information to determine their behavior. We find that schools can undergo large deformations before collapsing back to one of the regions. We show that the school exhibits a linear stress-strain relationship, analogous to the Hooke's law.

L70.00358: CHEMICAL PHYSICS
Quantum Chemical Investigations on Heavy Ligand Atom Induced Large Magnetic Anisotropy in Mn(II) Complexes.*

SABYASACHI ROY CHOWDHURY (Presenter), SABYASHACHI MISHRA, Chemistry, Indian Institute of Technology Kharagpur — In Single Molecule Magnets (SMM) metal ions are considered pivotal towards achieving large magnetic anisotropy barriers. A metal ion with strong spin-orbit coupling constant and low coordination number results in the retention of unquenched metal-orbital angular momentum, produces large magnetic anisotropy (1-2). In this context, the influence of ligands with heavy elements, showing large spin-orbit coupling, on magnetic anisotropy barriers was investigated using a series of Mn(II)-based complexes, in which the metal ion did not have any orbital contribution. The mixing of metal and ligand orbitals was achieved by explicitly correlating the metal and ligand valence electrons with Complete Active Space Self-Consistent Field (CASSCF) calculations. The CASSCF wave functions were further used for evaluating spin-orbit coupling and zero-field splitting parameters for these complexes. For Mn(II) complexes with heavy ligand atoms, such as Br and I, several interesting inter-state mixings occur via the spin–orbit operator, which results in large magnetic anisotropy in these Mn(II) complexes(3).


*IIT Kharagpur

Modeling X-ray Absorption Spectroscopy with Relativistic TDDFT*

XIAOSONG LI (Presenter), University of Washington — X-ray absorption spectroscopy (XAS) is an element specific probe that has been used to understand the local electronic and binding environment around metal centers. Electronic structure theory has become an important aid in interpreting XAS spectra. While K-edge spectra have been investigated in great detail, the modeling of L-edge spectra poses several unique challenges. First, the L-edge spectrum is composed of multiple features: L₁ corresponding to the 2s orbital, and L₂,3 corresponding to 2p orbitals, which are split into 2p₁/₂ and 2p₃/₂ levels by spin-orbit coupling. Additionally, with density functional theory (DFT) it also becomes necessary to make modifications to handle non-collinear spin densities in the presence of spin-orbit coupling. We model the L₂,3 spectra for several molecules with variety of model chemistries using exact two component TDDFT (X2C-TDDFT). With the X2C-TDDFT method we are able to include the one-electron spin-orbit coupling terms variationally from first principles. An analysis of the molecular orbitals involved in the transitions yields valuable theoretical information that can be used to connect the local electronic structure with experimental observables.

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Excited State Time-Resolved Vibrational Dynamics: the Challenge of Charge Transfer Complexes

FEDERICO COPPOLA (Presenter), Chemical Sciences, University of Naples Federico II, PAOLA CIMINO, Pharmaceutical Sciences, University of Salerno, UMBERTO RAUCCI, MARIA GABRIELLA CHIARIELLO, NADIA REGA, Chemical Sciences, University of Naples Federico II —

Charge transfer -CT- reactions are ubiquitous processes in nature. Photoexcited systems can be monitored to modulate the process and to rationally design photosensitive materials. Current vibrational spectroscopies provide experimental data with high time resolution, although the interpretation at molecular level requires the help of theory and computation. In this context, the atomistic description provided by theoretical analysis and ab initio molecular dynamics (AIMD) are a valid support. Isolated molecular systems are a good starting point to disentangle the complexity of anharmonicity and for the method's assessment. This contribution focuses on photoinduced CT reactions of benchmark systems showing a complex photophysical behaviour both in ground and excited state. To unravel the vibrational dynamics of key vibrational modes we use a theoretical approach² combining the AIMD simulations to the Wavelet Analysis in both electronic state. We focused vibrational relaxations of several vibrational modes moving towards quantification of the anharmonic coupling especially between high and low frequencies modes.

L70.00362: Speeding-up \textit{Ab Initio} Simulations: Novel Approaches for Extended Lagrangian Molecular Dynamics
FULVIO PERRELLA (Presenter), ALESSIO PETRONE, NADIA REGA, Chemical Sciences, University of Naples Federico II — Modern theoretical chemistry is prompted to give insight into ultrafast phenomena from an atomistic point-of-view and to give an interpretation of the experimental data from time-resolved spectroscopies. \textit{Ab initio} molecular dynamics (AIMD) is the prominent approach to capture both electronic and nuclear relaxation events.\textsuperscript{1} Among different approaches to molecular simulations, the Extended Lagrangian AIMD techniques appear to give best performances with respect to the accuracy/cost ratio. The fictitious electronic mass is a crucial parameter, because it has to ensure an efficient propagation of the electronic degrees of freedom, while keeping a strong degree of adiabaticity.\textsuperscript{2} Current implementations are based on a uniform or an energy-based weighting of atom centered basis functions and often cannot capture their core or valence-like character. A novel mass weighting scheme, based upon a rational classification of the atomic functions, will be proven to be consistently more reliable, while avoiding errors typically occurring with fixed energy thresholds. Such an approach may allow larger time-steps, while ensuring a strong physical soundness to the simulation.


L70.00363: Using geometric phases to separate overall rotation and internal motions in classical and quantum molecular dynamics\textsuperscript{*}
F. J. LIN (Presenter), F. J. Lin Research — In 1959, Aharonov and Bohm pointed out that electrons could be affected by vector potentials without an external magnetic field. To make the wave functions in vector potentials single-valued, an \textit{ad hoc} phase shift is required. This phase shift exemplifies a geometric phase (or Berry's phase). Similarly, Mead and Truhlar described an \textit{ad hoc} phase shift required for nuclear wave functions describing three-body molecular dynamics in the Born-Oppenheimer approximation. In their "molecular Aharonov-Bohm effect," Mead and Truhlar \textit{assumed} decoupled overall rotation and internal motion and considered the effects of a conical intersection. Instead of neglecting coupled overall rotation and internal motion, now this coupling is used to create a frame with \textit{decoupled} overall rotation and vanishing classical and quantum geometric phases. An extension of the classical dynamics describes the quantum dynamics of a three-body molecular system in the Born-Oppenheimer approximation. This theoretical approach agrees with observations of spectra of rare gas-diatomic molecule complexes and observations of triatomic photodissociation dynamics.

\textsuperscript{*}Travel support by a Douglas C. Basil Award from the University of Southern California Emeriti Center is gratefully acknowledged.

L70.00364: Calculations of small molecules using the Highly Accurate N-DEterminant (HANDE) quantum Monte Carlo software package\textsuperscript{*}
HAYLEY PETRAS (Presenter), TINA MIHM, JAMES SHEPHERD, University of Iowa — We use calculations of small molecules and the uniform electron gas to illustrate the capability of HANDE, an open-source software package that calculates stochastic estimates for high accuracy quantum chemistry methods. We choose to focus on full configuration interaction and its finite temperature variant, density matrix quantum Monte Carlo. We describe how strong correlation and other phenomena manifest in the context of this and the initiator approximation to these methods.

\textsuperscript{*}We thank the University of Iowa for funding.

L70.00365: Theoretical Insights into the Mechanisms of Aggregation-Induced Emission of a Tetraphenylethylene\textsuperscript{*}
NORIFUMI YAMAMOTO (Presenter), Chiba Institute of Technology — The aggregation induced emission (AIE) of tetraphenylethylene (TPE) was studied theoretically. The TPE has been known to exhibit the AIE, which is non-emissive in dilute solutions but becomes highly emissive in solid or aggregated state. In this study, the AIE mechanism of TPE was investigated by using electronic structure calculations, together with molecular dynamics (MD) simulations. The results of electronic structure calculations showed that potential energies of TPE for electronic ground (S\textsubscript{0}) and first excited (S\textsubscript{1}) states are degenerated at a conformation with the twist angle of 90° around its ethylenic C=C bond, which can lead the fluorescence quenching of this molecule in dilute solutions. The results of MD simulations revealed that the TPE in aggregated state tends to assemble in close contact, where the ethylenic C=C bond rotation is markedly restricted, preventing the fluorescence quenching via the S\textsubscript{0}/S\textsubscript{1} conical intersection; the TPE in THF solution, however, proceeds the barrierless non-radiative transition. These results gave a clear picture of the AIE mechanism of TPE.

\textsuperscript{*}This work was supported by the Japan Society for the Promotion of Science (JSPS) KAKENHI (Grant-in-Aid for Scientific Research (C) 17K07315).
L70.00366: Single-electron excitations from thermally-assisted-occupation reference* SHU-HAO YEH, AADITYA MANJANATH (Presenter), Institute of Chemistry, Academia Sinica, JENG-DA CHAI, Department of Physics, National Taiwan University, CHAO-PING HSU, Institute of Chemistry, Academia Sinica — The linear response time-dependent density functional theory (LR-TDDFT) has been broadly used to investigate excited-state properties of various molecular systems. However, current LR-TDDFT methods heavily rely upon outcomes from ground-state DFT calculations. For systems with small HOMO-LUMO gaps, single-determinant ground-state DFT may be prone to non-dynamical correlation, and hence, LR-TDDFT results can be inaccurate. Traditionally, nearly degenerate orbitals require proper treatment of non-dynamical correlation, which usually involves active-space treatments. Recently, the thermally-assisted-occupation (TAO) DFT scheme was proposed, which explicitly incorporates the non-dynamical correlation effect in the ground-state simulation, but retains the low computational complexity of conventional DFT. The aim of this work is to combine ground-state TAO-DFT with LR-TDDFT framework to study excited-state phenomena. The preliminary simulations successfully capture the dissociation feature of the first triplet excited state of hydrogen molecule, which is not the case for conventional TDDFT.

*Academia Sinica Investigator award AS-IA-106-M01 and Ministry of Science and Technology of Taiwan with project 105-2113-M-001-009-MY4, and Academia Sinica Distinguished Postdoctoral Fellowship.

L70.00367: Bicarbonate charging of hydrophobic/water interfaces* FRANCOIS GANACHAUD (Presenter), COMPASS, JULIEN BERNARD, XIBO YAN, IMP, INSA Lyon, ANTONIO STOCCHO, Institut Charles Sadron, CNRS — Most surfaces in contact with water are negatively charged. The reason for that has long been debated in the physics community as arising either from hydroxide ion adsorption or water reorganization towards a hydrophobic interface. We have recently proposed another explanation coming from the carbonate of water. Bicarbonates, which in distilled water are the most present ions at intermediate pHs (from 5 to 10), are catatropic ions that stick to interfaces. We made use of a combination of interfacial tension measurements of oil droplets in water, and nanoprecipitation assays of polymers in a large range of pH, to show such affinity of HCO3⁻ for hexadecane oil and PMMA. This preferred adsorption of bicarbonate allows also explaining why freeze/thaw cycles contribute to emulsifying oil/water mixtures.

*ANR PREPROPOSAL ANR-15-CE09-0021
ANR LimOuzInE ANR-10-BLAN-0942

L70.00368: Computational Study of the Intermolecular Interactions Hg and Hg (II) With Thiols in Aqueous Environments. JICLI ROJAS (Presenter), Departamento de Química, Universidad Nacional de Colombia, JUAN CAMILO GALVIS, ALFREDO LORA, CARLOS PINILLA, Departamento de Física y Geociencias, Universidad del Norte, NEIL ALLAN, School of Chemistry, University of Bristol — Hg water contamination is one of the most common problems of gold mining. It is known that Hg has a great capacity to form compounds, especially when it reacts chemically with aquifer sources transforming it into methylmercury [CH₃Hg]⁺; a powerful neurotoxic that tends to accumulate, through the trophic chain, in fish, humans and wildlife that feed on them, causing irreversible effects on health. Currently there are no efficient methods for the treatment of water contaminated by Hg. In this work we systematically study the interaction energies between Hg, Hg (II) and methylmercury species with the -SH (thiol) group of the compounds Cysteine C₃H₇NO₂S (1), 3-mercaptop-3-methylbutan-1-ol C₅H₁₂OS (2), Silanol C₃H₇O₂SSi (3) and Dimercaprol C₃H₈OS₂ (4) in aqueous medium, using DFT in order to identify the compound with the most favorable interactions, which can be used for functionalization and so to produce new materials for the extraction of Hg. The results show that interactions with elemental mercury (Hg) are thermodynamically favored. However, with mercury in its ionic form (Hg II), the interactions that are favored are those when compound (2) and compound (4) were used. Our study hints on the possiblity to use thiols extracted from local vegetables and fruit sources.
A Theoretical Study of Novel Composite Clusters of Platinum Metals*  
AJIT HIRA (Presenter), JOSE PACHECO, RUBEN RIVERA, MATILDA FERNANDEZ, ALEXANDRA VALDEZ, Math and Physics, Northern New Mexico College — Material shell composites of platinum (Pt) and palladium metals have great stability and remarkable physical and chemical properties. In light of our previous work on the small atomic clusters on metallic clusters, we present here an Ab-initio quantum-mechanical study of the Ptn, Irn, and Osn (n = 1-9) clusters, their hybrids MiNj (M= Pt, Ir, Os; N= Pt, Ir, Os; i= 1-6; j= 1-6), and their composites of these metal clusters with palladium (Pd) clusters. Our theoretical approach is to utilize the ab initio methods of quantum chemistry to derive optimal geometries for the clusters of interest. Of particular interest in this research are the Pt6 and Pt8 rectangular parallelepipeds, and the Pt8, Pt9, Pt8Pd8, Pt8Pd9 cubic clusters. We examine the implications of this research for the self-assembly of metallo-supramolecular structures, by the directional bonding approach. Also, of interest here is the recent experimental work that showed that Pt clusters deposited on Pd shell over Au core nanoparticles (Au@Pd@Pt NPs) exhibit unusually high electrocatalytic activity for the electro-oxidation.

*Financial support from the New Mexico Alliance for Minority Participation (NM-AMP) program of the National Science Foundation (NSF)

Structure and optical properties of In1-xRExTaO4 (RE= Er, Yb) and their oxynitrides, an evaluation as photocatalysts for water splitting*  
JUAN CRUZ PUERTO (Presenter), CRISTINA RAMÍREZ, Facultad de Química, Universidad Nacional Autonoma de Mexico, PABLO DE LA MORA, Facultad de Ciencias, Universidad Nacional Autonoma de Mexico, GUSTAVO TAVIZÓN, Facultad de Química, Universidad Nacional Autonoma de Mexico — Ta2O5 based photocatalysts show a band gap of about 4.0 eV, this implies that they should be used under UV electromagnetic radiation, this condition limits its applications. Zou, Z. et al. [1] prepared visible-light active photocatalyst with formula InTaO4: NiO, with a wolframite structure and a band gap of 2.6 eV; more recently this system was reviewed by Malingowski, A. et al. [2] and they found a direct band gap of 3.96 eV for the nickel doped InTaO4 compound. In this work, we studied the In1-xRExTaO4 (RE= Er, Yb, 0.0≤x≤2.0) solid solution with a wolframite structure and we found that for the Yb case the system it does not exhibit absorption in the visible region of the electromagnetic spectrum, while the Er system it shows a rich absorbance spectrum in the visible region. Probably this absorbance signals are associated to internal f-f electronic transitions and could be active in photocatalysis under visible radiation.


*Authors of this work acknowledge support from PAPIIT-IN115618 (UNAM).

Theoretical modeling of coherent proton transfer dynamics and pump probe spectroscopy simulation*  
LUHAO ZHANG (Presenter), GREG SCHOLES, Princeton University — Proton transfer reaction is ubiquitous in chemistry and biology. Pump probe spectroscopy shows general feature of fast rising and oscillation signal of excited state proton transfer which can only be explained by quantum mechanics. However, due to the interplay of electron rearrangement, nuclear vibrations, skeletal torsion and molecule-solution interaction, it’s difficult to use ab-initial quantum dynamics calculation to illustrate pump probe signal. Here, we adopt the a vibronic coupling Hamiltonian and used methods of open quantum dynamics to simulate pump probe signal of HBT(2-(2’-Hydroxyphenyl)benzothiazole) and compare with experiment. Our method will make a brige between experiment and ab-intial calculation, and also provide a framework to describe a chemical reaction in a wave function(density matrix) perspective. Furthermore, because of the quantum mechanical nature of excited state proton transfer, it’s possible to realize a superposition of two pathways for a dimer molecule with two proton transfer sites, which brings a new mechanism for general chemical reaction. Using similar model Hamiltonian, we found for isolated dynamics, a superposition reaction shows interference pattern of nuclear density while single proton transfer does not.

*Thank Kech’s grant for funding.
L70.00372: Dynamic scaling in stochastic chemical kinetics*  JONAH GREENBERG (Presenter), JASON R. GREEN, University of Massachusetts Boston — Universality classes are often comprised of seemingly dissimilar physical systems. Here, we draw a formal analogy between surface-roughening processes and the stochastic kinetics of fundamental chemical reactions. We simulate the chemical kinetics of several classes of reactions with Gillespie’s exact stochastic simulation algorithm and analyze the dynamic scaling of a quantity analogous to the surface roughness, \(w\). For kinetics at chemical equilibrium considered thus far, the growth exponent is \(\beta=1/2\). The dynamic exponent \(z\), however, depends on the molecularity of the reaction. For simple cases these computational results can be verified analytically through the associated master equations. We observe a richer collection of exponents and scaling relations for nonequilibrium kinetics. Overall, these results suggest, just as in surface-roughening phenomena, that seemingly dissimilar chemical systems may also be partitioned into universality classes, some known and others new.

*This material is also based upon work supported by the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-14-1-0359.

L70.00373: Effect of surface morphology on kinetic compensation effect: interactions vs. energetic heterogeneity  NAYELI ZUNIGA-HANSEN (Presenter), Louisiana State University, LEONARDO SILBERT, Central New Mexico Community College, M. MERCEDES CALBI, University of Denver — The kinetic compensation effect, observed in many fields of science, is the systematic variation in the apparent magnitudes of the Arrhenius parameters, the activation energy \(E_a\) and the preexponential factor \(\nu\), as a response to perturbations. In principle, a change in \(E_a\) results in a change in the configurational entropy of the system, which appears as variations in \(\nu\) throughout an activated process. As part of a systematic study, we compare the effects of interactions on these parameters during the thermal desorption of quasi spherical molecules from a 2D glassy surface to the effects of surface energetic heterogeneity. The results of this study show that the decrease in configurational entropy is more pronounced in the presence of interactions. We also explore the role that diffusion plays in the extent to which the parameters offset each other. These results provide a deeper insight into the microscopic events from which compensation effects and isokinetic relations originate in this system, suggesting similar mechanisms may be at play in other systems where compensation effects have been reported, and which can improve our understanding of the mechanisms which control the rates of many activated processes.

L70.00374: Molecular Dynamics Simulations of the Elastic and Structural Properties of Calcium Aluminate Glass: Effects of Low Silica Contents  HICHAM JABRAOUI (Presenter), MICHAEL BADAWI, University of Lorraine, ABDELLATIF HASNIAOUI, Université Hassan 1er, SAID OUASKIT, Université Hassan II de Casablanca, YANN VAILLS, University of Orleans — We have used classical molecular dynamics to investigate the elastic constant behaviors of low silica calcium aluminosilicate glasses where \(\text{SiO}_2=5-25\text{ mol}\%\) and \([\text{CaO}]/[\text{SiO}_2]=2\). To compute the elastic constants, we have used two methods; the minimization energy at zero temperature (Zero-T) and a second one that allows calculating the elastic constants at finite temperature (FT)[1]. To evaluate the reliability of these methods, the obtained results are compared with those already measured by Brillouin light scattering spectroscopy (BLS). To this end, we show that elastic constants decrease with increasing silica content, which can be correlated with some structural features such as oxygen types and short-range order parameters. However, these properties are not easily accessible from experiment [2]. Therefore, our simulations complement well the current knowledge on the influence of low silica contents on the physicochemical properties of calcium aluminate glasses.


L70.00375: Like dissolves like: how like need they be? A statistical field theory for polar liquids and their mixtures*

BILIN ZHUANG (Presenter), Institute of High Performance Computing, ZHEN-GANG WANG, California Institute of Technology — We have been taught the empirical “like-dissolves-like” rule in secondary school chemistry classes, but how like must the solvents be? This question does not yet have a good quantitative answer because of the difficulty in finding a general description for mixture interactions. Here, we present a theory for polar liquids and their mixtures, developed using a statistical field approach. This approach allows us to avoid the use of ad hoc mixing rules, and thus provides a more holistic description of liquid mixtures. The resulting theory consists of simple algebraic expressions for the free energy and the dielectric constant of the liquid, based on just the dipole moments and the sizes of the constituent liquid molecules. Without the use of any adjustable parameters, the theory very well predicts the miscibility for a variety of liquids, thus providing a quantification for the well-known empirical “like-dissolves-like” rule.

*B.Z. gratefully acknowledges the support by an A-STAR fellowship. Acknowledgement is also made to the donors of the American Chemical Society Petroleum Research Fund for partial support of this research.

L70.00376: Determining the role of morphology in the acoustic absorption of materials*

SUMAN KUMARI (Presenter), Department of Chemical Engineering, Indian Institute of Technology Gandhinagar, VINOD NARAYANAN, Department of Mechanical Engineering, Indian Institute of Technology Gandhinagar, PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Development of soundproofing technology that utilizes real-time noise cancellation over a broad range of frequencies has been a challenge in the field of acoustics. In a typical scenario, noise control can be achieved by two approaches, active and passive. In active noise cancellation, the low-frequency sound is sampled and a canceling signal is generated using an external power source. In passive noise cancellation, however, sound absorbing materials, like foams, are used to filter out the unwanted sound mostly at high frequencies. Here, we show that by optimizing the internal structure, or morphology, of the sound absorbing material, the efficiency can be increased. In other words, we demonstrate that the absorption coefficient of polymeric foams, used for passive noise cancellation, increases significantly if the internal morphology of the foam is modified. Using our approach, therefore, it is possible to design thin, lightweight soundproof materials that can absorb noise at a wide range of frequencies and thus, can facilitate the design of miniaturized noise canceling devices.

*DST-SERB (EMR/2016/007778)

L70.00377: Modeling of One-Dimensional Diatomic Molecules through Density Functional Theory

KYLE JONES (Presenter), ANTONIO C CANCIO, Ball State University — We have developed a code to solve the Schrodinger equation of one-dimensional systems of electrons numerically in a plane wave basis. We have tested the accuracy of the code by performing convergence tests versus cell size and plane wave number, for the square-well and the Poschl-Teller well. We use this to calculate numerically accurate electron and kinetic energy densities and compare to simple density functional models for these quantities. We plan to use this code to investigate the results when two potential wells are pulled apart. Density functional theory (the use of only the density to calculate energies) is known to fail in three dimensions as electric bonds are broken and we expect this to be a problem in one dimension as well. Our one-dimensional code will allow for quick testing of new models and theories to see if they are viable avenues for better describing electronic bonding.

L70.00378: WITHDRAWN ABSTRACT

L70.00379: Self-interaction effects in molecular dissociation curves*

KOBLAR JACKSON, ALEXANDER JOHNSON (Presenter), JUAN PERALTA, KAMAL SHARKAS, Central Michigan University — The Fermi-Löwdin Orbital Self Interaction Correction (FLO-SIC) removes unphysical electron self-interaction from Density Functional Theory (DFT), the most widely used first-principles method in condensed matter and chemical physics. Self-interaction errors can be particularly pronounced in situations where bonds are stretched, such as when an atom is dissociated from a molecule. To study the effectiveness of FLO-SIC in this context, we calculated dissociation curves corresponding to removing one H atom from each of the molecules LiH, BeH₂, BH₃, ..., HF, and one F atom from each of LiF, F₂ and FCl. To get a statistical measure of performance, we compare FLO-SIC-DFT and DFT dissociation energies to accurate reference energies at four points along each curve. We find that FLO-SIC improves the performance of the local density approximation (LDA) at all separations, while for the generalized gradient approximation in the Perdew-Burke-Ernzerhof (PBE) form the performance is improved only for large separations. FLO-SIC corrects the tendency of both LDA and PBE to predict charged fragments in the large separation limit.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0018331.
L70.00380: MD Simulation of Ligand Migration and Substrate Binding in Lipoxygenases*  VIPIN KUMAR MISHRA
(Presenter), SABYASHACHI MISHRA, Indian Institute of Technology Kharagpur —
Lipoxygenases are an important class of enzymes with non-haem, non-sulphur iron-containing protein, whose catalytic action has severe consequences in a range of inflammatory diseases and its associated disease. The lipoxygenases are responsible for catalyzing the activation of poly-unsaturated fatty acids by inserting molecular oxygen at a specific position of the substrate, in a highly stereo-specific and regio-specific manner to yield hydro-peroxide [1]. We are currently investigating the pathways of migration of oxygen molecule into the active site of the enzyme and trying to determine the binding modes of the substrate. We have identified the side chains, such as, Arg185, Tyr181, Phe178, Ala592, Ala623, and Leu434 to play an important role in substrate binding. We are investigating the substrate binding propensity for different mutant systems and their roles towards hydroperoxidation. Further, we are investigating the global dynamic of the protein at atomic level. We are interested in providing a detailed description of the reaction pathway with structural and energetic details of the reactants, products, and intermediates along with the transition states separating them.


*LIT Kharagpur and UGC

L70.00381: Nano-Species Release System Activated by Enzyme-Based XOR Logic Gate*  YAROSLAV FILIPOV (Presenter), MARIA GAMELLA, EVGENY KATZ, Clarkson University — An enzyme-based XOR logic gate was realized at interface of an alginate-modified electrode. The biocatalytic production of H2O2 inside the alginate film was controlled by logically processed input signals. The in situ generated H2O2 was decomposed to yield free radicals in a Fenton-type reaction catalyzed by iron cations, which were present in the alginate film as cross-linkers stabilizing the hydrogel. The produced free radicals (*OH, *OOH) resulted in decomposition/dissolution of the alginate film removing it from the electrode surface and stimulating release process of magnetic nanoparticles (MNPs) functionalized with a fluorescent dye and entrapped in the alginate film. The release of the MNPs was analyzed by following fluorescence appearing in the solution. The release process followed the logic features of the XOR gate. The present system is the first realization of the enzyme-based XOR gate functionally integrated with the downstream actuation process in the form of the signal-stimulated release.

*This work was supported by National Science Foundation (award CBET-1403208).

L70.00382: Molecular Modeling of 1-Benzazepine Analogues that bind to the ACh Protein (2PH9) Using Hyperchem and AutoDock  PAOLA COLON, ASTRID SANTIAGO (Presenter), Chemistry, University of Puerto Rico in Humacao — Ligand interactions of the designed analogs to neuronal nicotinic Acetylcholinesterase receptor (nAChR) are being studied to see which one fit into the binding site of an ACh binding protein PDB code (2PH9).1-Benzazepine analogs improve allosteric positive modulation of the nicotinic α-7 acetylcholine receptors.The Heat of Formation, obtained using Schrödinger equations, of 8 benzazepines analogues that were designed in the Hyperchem program were calculated on the PM3 Hyperchem quantum levels. They were pre-optimized using MM + and the PM3 semi-empirical method with the Polak-Ribière conjugate gradient. The protein-ligand binding of these benzazepine analogs to ACh binding protein PDB code is being determined using the Auto Dock Tools and AutoDock Vina programs. The Affinity of the analogues under studies could be calculated using the Command Prompt of the computer, assigning specific x, y and z coordinates with a specific grid box size. It’s obtained that the ligand with the best interaction with the protein was 7-8 dimethoxy-1 BNZ-cinnamic acid with an affinity of -8.6kcal / mol and a Heat of Formation equal to -126.06 kcal / mol. These results, of the 8 ligands, were compared to Galantamine which is the commercial drug used to treat neurodegenerative diseases.

L70.00383: Modeling Circular Current Resonances in a 6-Quantum Dot Ring  YONG JOE (Presenter), Ball State University, ERIC HEDIN, Biola University — A nanoscale ring configuration, modeled as a 6-quantum dot ring, is investigated computationally to study the behavior of circular current resonances. The computational method utilizes the tight-binding approximation to the Schrödinger Equation to solve for the transmission and circular transmission as a function of electron energy, external magnetic flux, and other system parameters. Large amplitude resonances of the circular transmission are found to occur when two poles of the transmission are separated along the imaginary axis. These resonances demonstrate a high degree of flux-sensitivity at specific energy values and flux ranges. Flux-dependent interference between the transmission poles and zeros in the complex energy plane affects the magnitude of the circular transmission resonance amplitudes. The circular transmission and its corresponding current-vs.-voltage characteristics may serve as a nano-sensor, providing a higher degree of correlation with the external flux than is observable with the normal transmission alone.
**L70.00384: Method for the Growth and Stabilization of Rare Earth Nano-Particles**

PATRICK TALBOT (Presenter), PEI-CHUN HO, California State University, Fresno — We are developing a process to create rare-earth metal (REM) nanoparticles (NPs), to the end of studying their magnetic and electrical properties. The large redox potential of REMs hinders the formation and stabilization of these NPs, requiring a strong reducing agent to form the NPs, and their protection from ambient conditions.

Firstly, the ease and efficacy of several organo-metallic reduction compounds, with sodium as an electron source, were compared: 15-crown-5, Benzophenone (anion and dianion), and naphthalene; with naphthalene showing to be the most consistent and convenient due to its: relatively high reduction potential, stability, and singly reduced state.

Secondly, we then compared methods of passivating the NPs; this consisted of looking at the relative stability of NPs using combinations of: ligation with 1-octylamine. Preliminary observations indicate ligation alone provides little protection from oxidation for the pure REM NPs, and is only able to prevent agglomeration.

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**L70.00385: Steering of microwave absorption in MxCo(1-x)Fe2O4 (M: Ni2+, Mn2+, Zn2+) based ferrite-Carbon black/PVA composites by engineering the magnetic microstructures**

GOPAL DUTT (Presenter), Department of Metallurgical and Materials Engineering, Defence Institute of Advanced Technology, Pune, India, CHETAN KOTABAGE, Department of Physics, KLS Gogte Institute of Technology, Belagavi, India, ASHUTOSH C. ABHYANKAR, Department of Metallurgical and Materials Engineering, Defence Institute of Advanced Technology, Pune, India — Microwave mitigation property of ferrite nanoparticles (NFs)-Carbon black/PVA composites by tuning magnetic microstructure and spin arrangement of NFs is studied. The annealing of NiCoFe2O4 at 1000°C reveals significant changes in cationic distribution. The NFs were then used to fabricate the NF-CB hybrids and flexible NF-CB/PVA composite films. A comparative study of Ni-NFs composite prepared from non-annealed and annealed NFs indicates better shielding effectiveness for non-annealed NFs due to increase in cationic disorder, smaller particle size and large interfacial polarization.

The magnetic microstructures and coordination of Fe3+ ions in these NFs were investigated by MFM and Mossbauer spectroscopy, respectively. Zn-NFs have *unique single axis oriented* domains and highly distorted coordination of Fe3+ cations. Multi-domain magnetic microstructure and canted spins in sub-lattice were observed for Mn-NFs and Ni-NFs. Over bandwidth of 8 to 18 GHz, Zn-NF-CB/PVA has the largest shielding effectiveness (SAE = 25dB). It is caused by enhancement in interfacial polarization due to motion of polarons across multiple heterogeneous interfaces. \( \mu'' \) is almost twice in Zn-NF based composites compared to other due to distorted co-ordination of Fe3+ and *unique single axis oriented* domains.

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**L70.00386: Biosensors Protected by Biomimetic Membrane with Carbon Nanotube Porins**

XI CHEN (Presenter), University of California, Merced; Lawrence Livermore National Laboratory, HUANAN ZHANG, RAMYA H TUNUGUNTLA, Lawrence Livermore National Laboratory, ALEKSANDR NOY, University of California, Merced; Lawrence Livermore National Laboratory — Limited biocompatibility and fouling propensity can restrict real-world applications of a large variety of biosensors. Biological systems are adept at protecting and separating vital components of biological machinery with semipermeable membranes that often contain defined pores and gates to restrict transmembrane transport only to specific species. Here we use a fouling-resistant membrane, which mimic the architecture of cellular membranes in nature to protect biosensors. We integrate silicon nanoribbon transistor sensors with an antifouling lipid bilayer coating that contains carbon nanotube porin (CNTP) channels and demonstrate robust detection of proton and cations in a variety of complex biological fluids. Preliminary results of CNTP as a conduit bridging through cell membranes are also discussed.
Iron Oxide Nanoparticles with Controlled Size and Shape

SHIRIN POURMIRI (Presenter), University of Delaware, VASILEIOS TZITZIOS, chemical engineering, Khalifa University of Science and Technology, GEORGE C HADJIPANAYIS, University of Delaware — Controlling the shape of Fe₃O₄ particles is still a big challenge. It has been shown that the SAR value for hyperthermia measurements, has been related to the magnetic anisotropy of the nanoparticles which depends on their size and shape [1]. Therefore, it’s very important to control the shape and the size of Fe₃O₄ nanoparticles precisely.

Here, a simple approach for synthesizing Fe₃O₄ nanoparticles is studied. The synthesis takes place in an oleylamine/dodecylamine solution, using Fe(acac)₃ as the Iron precursor. The XRD measurements, show a pure Fe₃O₄ phase. It is observed that the nanoparticles made with Oleylamine-Oleic acid mixture, are completely spherical; however, the shape of nanoparticles synthesized with Dodecylamine-Octadecene mixture, could be easily changed from spherical to facet. It is shown that by decreasing the amount of dodecylamine from 10 to 2.5 mmol, the nanoparticles start having a more facet shape than spherical shape. Also, the size of particles in both cases was controlled by changing the temperature and time. Our data show that by changing the reaction temperature from 220 to 250 °C, the average diameter of nanoparticles can be increased from 1-3 nm to 8-10 nm.


Resonance Energy Transfer in Arbitrary Media: Two Entangled Photons*

KOBRA NASIRI AVANAKI (Presenter), Northwestern University — We report the resonance energy transfer between two uncoupled two-level atoms jointly excited by temporally entangled field. The virtual photons arising from three-level cascade decay are inherently ordered in time of emission. Since the induced joint resonance in two-atom excitation probability comes from the field correlation and the suppression of one of the time-ordered excitation pathways, we see the rate in two-photon energy transfer increases with the time-frequency entanglement. This is justifying the enhancement of energy transfer through the entangled two-photon by a large factor as compared to uncorrelated photons. Based on the new formulation derived here and due to the permanent entangled field interacting with the system over the time scale of energy transfer, the rate depends on the emitter’s properties dominantly. The situation would be more complicated if the process mediated by inhomogeneous, dispersive media.

*This work was supported by the U.S. National Science Foundation under Grant No. CHE-1465045.

Electrochemical Hydrogen Evolution Reaction of Supported Pt Nanoclusters on MoS₂: Cluster Expansion Investigation

TIMOTHY YANG, University of Pittsburgh, TECK TAN, Institute of High Performance Computing Singapore, WISSAM SAIDI (Presenter), University of Pittsburgh — Supported metal nanoclusters on MoS₂ have shown catalytic activity towards hydrogen evolution reaction (HER) that is comparable or better than bulk Pt. We use density functional theory calculations in conjunction with cluster expansion and ab initio thermodynamics to investigate the activity of supported Ptnanoclusters on MoS₂. We determine the hydrogen adsorption configurations under HER conditions by including multiple adsorption sites. Our results show that both Volmer-Heyrovsky and Volmer-Tafel reactions are facile on the cluster while as only the Volmer-Tafel reaction is observed for Pt (111) surfaces. This results in enhanced catalytic activity of the nano cluster. The underpinning of this behavior is discussed.

Ab-initio investigation of water adsorption and hydrogen evolution on Co₉S₈ and Co₃S₄ low index surfaces*

MARCO FRONZI (Presenter), International Research Centre for Renewable Energy, Xi'an Jiaotong University, HUSSEIN ASSADI, Center for Computational Sciences, University of Tsukuba, MICHAEL J. FORD, School of Mathematical and Physical Sciences, University of Technology, Sydney — We used density functional theory approach, with the inclusion of a semi-empirical dispersion potential to take into account van der Waals interactions, to investigate the water adsorption and dissociation on cobalt sulphides Co₉S₈ and Co₃S₄ (100) surfaces. We first determined the nanocrystal shape and selected representative surfaces to analyse. We then calculated water adsorption and dissociation energies, as well as hydrogen and oxygen adsorption energies, and we found that sulphur vacancies on Co₉S₈ (100) surface enhance the catalytic activity toward water dissociation by raising the energy level of un-hybridized Co3d states closer to the Fermi level. Sulphur vacancies, however, do not have a significant impact on the energetics of Co₃S₄ (100) surface.

*The authors gratefully acknowledge the financial support of the National Natural Science Foundation of China (No. 51323011), and the Australian Government through the Australian Research Council (ARC DP160101301).
L70.00391: Modifying H2 adsorption and desorption on palladium using polymers – a first-principles study  LUCY CUSINATO, ANDERS HELLMAN (Presenter), Chalmers University of Technology — In a future hydrogen-based energy system it will be crucial to have sensors that are able to detect hydrogen leaks immediately. DOE has proposed very demanding performance targets, and in an effort to meet these, optical nanoplasmonic hydrogen sensors based on hydride-forming palladium nanoparticles have been introduced. Experimentally, the presence of metal-organic frameworks or polymers has been shown to lower the apparent activation energy of hydrogen adsorption/desorption. Here, we study this phenomenon from a theoretical (using DFT) point of view. The behavior of palladium and palladium hydride nanoparticles towards H2 adsorption and desorption, with and without polymer (PTFE, PVDF and PMMA) coating, is studied. A particular focus is set on how to model this kind of nanoparticle/polymers systems for the case of bare and hydride palladium. Stability of palladium hydride nanoparticles is studied, as well as different types of interaction at the Pd-polymer interface. These results are then used to shed light on how the presence of polymers, and the existence of a palladium/polymer interface, can affect the kinetics and thermodynamics of the system in order to facilitate H2 adsorption and desorption processes.

L70.00392: The role of potassium on CO oxidation  BIN DI (Presenter), College of Chemistry and Molecular Engineering, Peking University — Alkali metals are regarded as promoters in many catalysts which can promote the reaction rate of various chemical processes including ammonia synthesis, CO oxidation, the water-gas shift reaction and so on. However, an unambiguous picture of how alkali metals impact catalytic activity have not been drawn. In order to uncover alkali-metals promotion effect, we focus on the chemical and physical properties of atomically dispersed alkali metal, such as atomic potassium, supported on ultrathin metal oxide film and the interaction of alkali metals with noble metals which possess promotion effect, we focus on the chemical and physical properties of atomically dispersed alkali metal, such as atomic potassium, supported on ultrathin metal oxide film and the interaction of alkali metals with noble metals which possess promotion effect. Au/CuO can catalyze CO oxidation in a relative low temperature. Using K/CuO/Cu(110) model system, we investigate the potassium atoms in low coverage on one monolayer CuO and K-Au interaction.

L70.00393: Alkali Metals on Ultrathin Oxide Surface: A Low-Temperatruce STM research  ZHANTAO PENG (Presenter), CCME, Peking University — Alkali metal plays an important role in heterogeneous catalysis, semiconductor physics, superconducting physics and has received extensive attention in its adsorption behavior and electronic properties on both single crystal surface and oxide surface. In this report, a low-temperature scanning tunneling microscopy (LT-STM) is employed to investigate the behavior of alkali metal on ultrathin CuO surfaces. While the electronic properties of some transitional metals atoms on such an oxide surface can be dramatically affected by the co-adsorption alkali metals.

L70.00394: Structure, magnetic properties, and thermal stability of chemically prepared nickel carbide nanoparticles*  GRANT LU, Charter High School, JEROME R TROY, GERALD R POIRIER, RODDEL REMY, KARL UNRUH (Presenter), University of Delaware — Single phase nickel carbide nanoparticles and phase separated nickel carbide/elemental nickel nanocomposites have been prepared by the reduction of nickel acetate in triethylene glycol at reduction temperatures between 250 and 290 °C. The structure, magnetic properties, and thermal stability of these samples have been studied by x-ray diffraction (XRD), vibrating sample magnetometry (VSM), and differential scanning calorimetry (DSC) measurements. The XRD measurements indicate that the nickel carbide phase is hexagonal (S.G. 167) with lattice parameters of a=0.45908(1) and c=1.30080(3) nm; somewhat larger values than previously reported. The hexagonal phase has a room temperature magnetization of about 0.2 emu/g and a Curie temperature of about 330 °C. At a heating rate of 10 °C/min the hexagonal phase irreversible transforms to face-center-cubic elemental nickel starting at a temperature of about 380 °C.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR140076.

L70.00395: Collective cell migration induced by the interplay of contractile force and adhesion with delay under ERK signal propagation.  TATSUYA FUKUYAMA (Presenter), HIROYUKI EBATA, Kyushu University, YOHEI KONDO, National Institute for Basic Biology, SATORU KIDOAKI, Kyushu University, KAZUHIRO AOKI, National Institute for Basic Biology, YUSUKE T. MAEDA, Kyushu University — Collective migration is ubiquitously observed in epithelial cell sheets during wound healing and morphogenesis. For epithelial MDCK cells, ERK MAP kinase forms solitary wave and propagate across migrating cells. Cells orient their directions of migration oppose to the ERK wave, however, their guidance is distinct from tactic behavior. To understand the underlying mechanism of ERK directed collective migration, we propose simple theoretical model where interplay of focal adhesion and contractile force is regulated by ERK signal. Given that ERK signal locally increases both contractile force and focal adhesion onto substrate, we construct the equation of force-balance between viscous cellular fluid and dissipative friction. When ERK signal moves in two-dimensional space, local gradients of enhanced contractile force and reduced friction make viscous cell body easily streamed. Then, the net motion of fluids occurs and its velocity is given by an analytical solution. We test theoretical result by using optogenetic control of cell migration and find that cells are steered opposite to synthetic ERK signal. Our finding, including optimal velocity of cell migration against ERK wave, suggests the guidance of collective migration is driven by dissipative mechanics of cells.
The Heusler System And How You Can Use It As A Lego Box To Build The States You Are Interested In

CLAUDIA FELSER (Presenter), Max Planck Institute for Chemical Physics of Solids — The periodic table becomes one hundred years old just this year. The family of Heusler compounds uses nearly all the elements in the Periodic Table to allow for the design of materials with all sorts of properties. These include: hard and soft magnets, shape memory and magnetocaloric metals, thermoelectric semiconductors, topological insulators, and Weyl semimetals. These are just a few examples of more than 1000 known members of this remarkable class of materials that can display such a wide range of extraordinary multifunctional and tunable properties. Many more remain to be discovered! Just like a box of Lego bricks we can put together certain atoms (valence electrons), arranged in a particular symmetry, to achieve a desired electronic energy band structure. A necessary precondition for such a straightforward approach is a single particle picture: this allows for the prediction of many properties in this versatile class of materials, and equally enables “inverse design”. In my talk I will discuss the simple rules that we have learned to date and what the future might portend for further additions to the large and ever-growing Heusler family.


Stacking atomic layers one by one: quest for new materials and physics

PHILIP KIM (Presenter), Harvard University — Modern electronics has been heavily relied on the technology to confine electrons in the interface layers of semiconductors. In recent years, scientists discovered that various atomically thin materials including graphene, a single atomic carbon layer, can be isolated. In these atomically thin materials, quantum physics allows electrons to move only in an effective 2-dimensional (2D) space. By stacking these 2D quantum materials, one can also create atomic-scale heterostructures with a wide variety of electronic and optical properties. I will discuss the creation of new heterostructures based on atomically thin materials and emerging new physics with technological implications therein.

The Design And Growth Of Ultra-Stable Glasses

MARK EDIGER (Presenter), University of Wisconsin - Madison — Glasses are generally regarded as highly disordered and the idea of “controlling” molecular packing in glasses is reasonably met with skepticism. However, as glasses are non-equilibrium materials, a vast array of amorphous structures are possible in principle. Physical vapor deposition (PVD) allows a surprising amount of control over molecular packing in glasses and can be used to test the limits of amorphous packing in two ways. PVD can prepare glasses that approach the limits of the most dense and lowest energy amorphous packings that are possible. The activation barriers for rearrangements in these materials are very high, giving rise to high thermal and chemical stability. In addition, PVD allows control over anisotropic packing in glasses. For rod-shaped molecules, for example, glasses can be prepared in which the molecules have a substantial tendency to stand-up or lie-down relative to the substrate. As these materials have applications in organic electronics, an important question is: How much anisotropic order can be added to a glass without destroying key technological advantages such as macroscopic homogeneity? The high density and anisotropic packing of PVD glasses can be explained by a mechanism that is “anti-epitaxial” as structure is templated by the top surface rather than by the underlying substrate.

*Support from DOE (DE-SC0002161) and the UW-Madison MRSEC (NSF DMR-1720415) is gratefully acknowledged.
Colloidal Crystals, Quasicrystals and the Entropic Bond [Invited] SHARON GLOTZER (Presenter), University of Michigan — Entropy, information, and order are important concepts in many fields, relevant for materials to machines, for biology to economics. Entropy is typically associated with disorder; yet, the counterintuitive notion that particles with no interactions other than excluded volume might self-assemble from a fluid phase into an ordered crystal has been known since the mid-20th century. First predicted for rods, and then spheres, the ordering of hard shapes by nothing more than crowding is now well established. In recent years, surprising discoveries of entropically ordered colloidal crystals of extraordinary structural complexity have been predicted by computer simulation and observed in the laboratory. Colloidal quasicrystals, clathrate structures, and structures with large and complex unit cells typically associated with metal alloys, can all self-assemble from a disordered phase of identical particles due solely to entropy maximization. These findings demonstrate that entropy alone can produce order and complexity beyond that previously imagined. They also suggest that, in situations where other interactions are present, the role of entropy in producing order may be underestimated. We present the latest discoveries for entropic systems of identical particles, including a Bergman-like phase with a 432-particle unit cell, and fluid-fluid transitions preceding crystallization that are reminiscent of liquid-liquid phase separation in water, proteins, and even within cells. To understand these phenomena, and in loose analogy with traditional chemical bonds that produce order in atomic and molecular substances, we introduce the notion of the entropic bond.

Intracellular Liquid Condensates: New approaches to understand and control biomolecular phase transitions in living cells [Invited] CLIFF BRANGWYNNE (Presenter), Princeton University — In this talk I will discuss our work to understand and engineer intracellular phase transitions, which play an important role in organizing the contents of living cells. Membrane-less RNA and protein rich condensates are found throughout the cell, and regulate the flow of genetic information. We’ve shown that liquid-liquid phase separation (LLPS) underlies the assembly of these structures. LLPS driven by intrinsically disordered protein regions (IDRs) explains many condensate features, for example the internal subcompartments of the nucleolus, which has important consequences for sequential ribosomal RNA processing. Our lab has developed a suite of new approaches, which use light to enable spatiotemporal control of intracellular phase transitions, allowing us to engineer the assembly and disassembly of these structures within defined subregions of the cytoplasm and nucleus. We are now using these tools to quantitatively map intracellular phase diagrams for the first time, providing unprecedented access to the biophysical principles underlying RNP condensate self-assembly. This approach has also begun to yield rich insights into the link between intracellular liquids, gels, and the onset of pathological protein aggregation, and still largely unexplored mechanical interactions between these structures and the genome.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P01 DCMP: Fractional Quantum Hall Effect: New Systems BCEC 106 - Robert Willett, Bell Labs

Single photon Chern insulator in superconducting microwave lattices* CLAI OWENS (Presenter), BRENDAN SAXBERG, RUICHAO MA, JONATHAN SIMON, DAVID SCHUSTER, Physics, University of Chicago — We present the latest progress in developing a novel architecture for exploration of topological quantum matter. We construct microwave photonic lattices from tunnel-coupled, time-reversal-broken microwave cavities that are both low loss and compatible with Josephson junction-mediated photon-photon interactions, allowing us access to topological phenomena such as the fractional quantum Hall effect. We employ seamless 3D microwave cavities all machined from a single block of niobium, so our meta-material is scalable and directly compatible with the cQED toolbox, as it is composed only of niobium for the cavities, plus Yttrium-Iron-Garnet (YIG) spheres and Neodymium magnets to produce the synthetic magnetic field. After observing topologically protected chiral edge states with microsecond lifetimes circling the superconducting lattice, we now push to couple tunable qubits to the lattice in order to make lattice sites nonlinear and create particle interactions.

*Support was provided by the Chicago MRSEC, which is funded by NSF through grant DMR-1420709. This work was also supported by ARO Grant No. W911NF-15-1-0397. This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1746045.
**2:42PM P01.00002: Cu[Li$_{1/3}$Sn$_{2/3}$]O$_2$ and Cu[Na$_{1/3}$Sn$_{2/3}$]O$_2$: Crystal Structure and Phonon Dispersion in Quaternary Honeycomb Delafossites**

FARANAK BAHRAMI (Presenter), MYKOLA ABRAMCHUK, Physics, Boston College, OLEG I. LEBEDEV, Laboratorie CRISMAT, ENSICAEN-CNRS, OLLE HELLMAN, Division of Engineering and Applied Science, California Institute of Technology, NATALIA E. MORDVINova, Laboratorie CRISMAT, ENSICAEN-CNRS, JASON W. KRIZAN, Physics, Boston College, KENNETH METZ, Chemistry, Boston College, DAVID A BROIDO, FAZEL FALLAH TAFTI, Physics, Boston College — Magnetic materials with spin-1/2 ions on a two dimensional honeycomb lattice are candidates for a Kitaev spin liquid phase. The study of non-magnetic honeycomb delafossites provides a basis to model the physical properties of magnetic honeycomb materials. Here, we report two new quaternary non-magnetic delafossites, Cu[Li$_{1/3}$Sn$_{2/3}$]O$_2$ and Cu[Na$_{1/3}$Sn$_{2/3}$]O$_2$, with honeycomb ordering synthesized via a topotactic cation-exchange reaction. The monoclinic C2/c space group and twinned stacking faults are determined from the Rietveld refinement and TEM analysis. Additionally, the phonon heat capacity for these non-magnetic layered oxides is captured accurately by first principles calculations. These results are an important step toward having a reliable model to calculate phonon contribution to the heat capacity in magnetic delafossites\(^1\).

\[1\] Inorganic Chemistry 57, 12709 (2018).

*NSF-1708929

**2:54PM P01.00003: Observation of Chiral Surface Excitons in a Topological Insulator Bi$_2$Se$_3$*  

HSIANG-HSI KUNG (Presenter), Quantum Matter Institute, University of British Columbia, ADAMYA P GOYAL, DMITRII MASLOV, Department of Physics, University of Florida, XUEYUEN WANG, ALEXANDER LEE, Department of Physics, Rutgers University, ALEXANDER KEMPER, Department of Physics, North Carolina State University, SANG-WOOK CHEONG, GIRSH E BLUMBERG, Department of Physics, Rutgers University — Photoluminescence (PL) emission arising due to recombination of excitons in conventional semiconductors is usually unpolarized because of scattering by collective modes during exciton thermalization. Here on the contrary, we observe almost perfectly polarization-preserving PL peak centered at 2.3 eV from the surface of an archetypical three-dimensional topological insulator (TI), Bi$_2$Se$_3$. Based on the dependences of the PL spectra on the energy and polarization of incident photons, we propose that the observed PL can be semi-quantitatively explained by composite particles – chiral excitons – formed by the Coulomb attraction between massless (Dirac) electrons and massive holes, both subject to strong spin-orbit coupling which locks their spins and momenta into chiral textures. We experimentally demonstrate that the chiral excitons can be optically oriented with circularly polarized light in a broad range of excitation energies between 2.5 to 2.8 eV, and that the orientation remains preserved even at room temperature.

*HHK, AL and GB acknowledge support from NSF DMR-1104884. DLM acknowledges support from NSF DMR-1720816. XW and SWC acknowledge support from NSF DMREF-DMR-1629059.

**3:06PM P01.00004: Spin wave transport through electron solids and fractional quantum Hall liquids in graphene**

HAOXIN ZHOU (Presenter), HRYHORIY POLSHYN, Department of Physics, University of California, Santa Barbara, CA 93106, USA, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan, ANDREA YOUNG, Department of Physics, University of California, Santa Barbara, CA 93106, USA — In monolayer graphene, the interplay of electronic correlations with the internal spin- and valley- degrees of freedom leads to a complex phase diagram of isospin symmetry breaking at high magnetic fields. Recently, Wei et al. (Science (2018)) demonstrated that spin waves can be electrically generated and detected in graphene heterojunctions, allowing direct experiment access to the spin degree of freedom. Here, we apply this technique to high quality graphite-gated graphene devices showing robust fractional quantum Hall phases and isospin phase transitions. We use an edgeless Corbino geometry to eliminate the contributions of edge states to the spin-wave mediated nonlocal voltage, allowing unambiguous identification of spin wave transport signatures. Our data reveal two phases within the $v = 1$ plateau. For exactly $v=1$, charge is localized but spin waves propagate freely while small carrier doping completely quenches the low-energy spin-wave transport, even as those charges remain localized. We identify this new phase as a spin textured electron solid. We also find that spin-wave transport is modulated by phase transitions in the valley order that preserve spin polarization, suggesting that this technique is sensitive to both spin and valley order.
separating kernel and non-kernel states becomes more interesting because certain of these models (e.g., the "Gaffnian") are related to a non-unitary cft which is now believed to mean that they have gapless bulk excitations in the thermodynamic limit, and perhaps represent critical states at continuous transitions between topologically-distinct FQH states. I will discuss these fundamental questions, and review strategies and progress towards answering them.

conformal field theories (cft). These model Hamiltonians have a non-trivial kernel spanned by a basis of quasi-hole states (quasiparticle) eigenstates of these models, and the persistence of the energy gap in the thermodynamic limit. They have analogies to the AKLT spin-chain model, for which such questions have been answered. The question of proving (or disproving) a lower bound to the spectral gap separating kernel and non-kernel states becomes more interesting because certain of these models (e.g., the "Gaffnian") are related to a non-unitary cft which is now believed to mean that they have gapless bulk excitations in the thermodynamic limit, and perhaps represent critical states at continuous transitions between topologically-distinct FQH states. I will discuss these fundamental questions, and review strategies and progress towards answering them.

*Supported by Department of Energy BES Grant DE-SC0002140.

realization of high-order non-Abelian excitations* TAILUNG WU, ZHONG WAN, ALEKSANDR KAZAKOV, YING WANG (Presenter), LEONID ROKHINSON, Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA, purdue university — It has been proposed that parafermion excitations can emerge in the fractional quantum Hall effect (FQHE) regime if two counter-propagating chiral edge states with fractionally charged excitations and opposite polarization are brought into close proximity in the presence of superconducting coupling. In this work we present formation of conducting channels at boundaries between incompressible polarized and unpolarized states in FQHE regime. We demonstrate that in a triangular quantum well polarizations of a 2DEG can be locally controlled by electrostatic gating at a filling factor ; Conductance of channels formed at a boundary of polarized and unpolarized phases does not depend significantly on the magnetic field direction, indicating formation of helical domain walls. Such local control of polarization allows formation of a reconfigurable network of domain walls and can provide a platform for parafermion manipulation and braiding when superconductivity is proximity-induced into these domain walls.

*Supported by Department of Defense Office of Naval Research Award No. N000141410339, and Z.W. and Y.W.by National Science Foundation Grant No. DMR-1610139.

Particle-Hole Symmetric Pfaffian* KIRYL PAKROUSKI (Presenter), FREDERICK D HALDANE, Princeton University, EDWARD H REZAYI, Physics, California State University, Los Angeles, JIE WANG, Princeton University, KUN YANG, National High Magnetic Field Laboratory and Department of Physics, Florida State University — A recent experiment of Banerjee et al. [Nature 559, 205 (2018)] measured the thermal Hall conductance to be 5/2 for the ν=5/2 fractional quantum Hall effect. This observation is compatible with the particle-hole symmetric Pfaffian topological order where the chirality of the Majorana edge mode is reversed with respect to that of the Pfaffian. The particle-hole symmetric Pfaffian has not appeared as a viable candidate for the stable gapped phase at ν=5/2 in any numerical calculations for a disorder free system. We construct the particle-hole symmetric Pfaffian wavefunction in sphere and torus geometries for a number of system sizes and study its properties and further investigate the prospect of a particle-hole symmetric Pfaffian topological phase in clean systems.

*Supported by Department of Energy, BES Grant de-sc0002140.
Study of the inelastic length under microwave photo-excitation in the GaAs/AlGaAs 2D electron system

RASANGA SAMARAWEERA (Presenter), BINUKA GUNAWARDANA, THARANGA NANAYAKKARA, C. RASADI MUNASINGHE, U. KUSHAN WIJEWARDENA, SAIJITH WITHANAGE, ANNIKA KRIISA, Department of Physics and Astronomy, Georgia State University, CHRISTIAN REICHL, WERNER WEGSCHEIDER, Laboratorium für Festkörperphysik, ETH-Zürich, RAMESH MANI, Department of Physics and Astronomy, Georgia State University — Magnetotransport measurements in ultra-high mobility GaAs/AlGaAs 2D electron systems (2DES) exhibit a narrow negative magnetoresistance (MR) effect around the null magnetic field, which is similar in appearance to the well-known weak localization (WL) effect in metals, semiconductors, etc. However, the origin of WL-like effect in high mobility GaAs/AlGaAs 2DES specimens is still under debate. In this experimental work, the results exhibit that the incident microwave (MW) significantly modifies the observed narrow negative-MR feature, such that the WL-like peaks disappear at high power regime. This study aims to examine the influence of MW power on the WL-like effect. Thus, the observed negative-MR data were fit using 2D WL model by Hikami et al., to extract the characteristic inelastic length ($l_i$) as a function of MW power [1]. Results suggest that the fit extracted $l_i$ is reduced by 50% upon increasing the MW power up to 2 mW. Further analysis of the data suggest that MW induced electron heating is partly responsible for the observed reduction in the $l_i$ under photo-excitation.


Interacting topological phases in Fibonacci quasicrystals

POUYAN GHAEMI MOHAMMADI (Presenter), MOSHE FINK, City College of New York, AREG GHAZARYAN, Physics, Austrian IST — Recently it was realized that quasicrystals could exhibit non-trivial topological properties and topological equivalence between different types of quasicrystals (such as the Harper model and the Fibonacci quasicrystal). Exciton-polaritons have been recently employed to experimentally verify both band structure and the topological character of the Fibonacci quasicrystal. Given these recent advancements, it is essential to understand the effects of interactions, such as exciton-exciton interactions, on the topological nature of the states corresponding to topological quasicrystals. In this work, we have studied the interacting topological phases in Fibonacci quasicrystals and examined the possible experimental signatures for the effect of interactions in exciton-polariton systems formed in quasicrystal structures.

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PSC-CUNY Award, jointly funded by The Professional Staff Congress and The City University of New York

Evolution of the line shape of radiation-induced magnetoresistance oscillations under bi-chromatic microwave excitation

BINUKA GUNAWARDANA (Presenter), C.RASADI MUNASINGHE, RASANGA SAMARWEERA, THARANGA NANAYAKKARA, ANNIKA KRIISA, U. KUSHAN WIJEWARDENA, SAIJITH WITHANAGE, Physics and Astronomy, Georgia State University, CHRISTIAN REICHL, WERNER WEGSCHEIDER, Laboratorium für Festkörperphysik, ETH Zürich, RAMESH MANI, Physics and Astronomy, Georgia State University — We examine the evolution of the line shape of radiation-induced magnetoresistance oscillations under bi-chromatic microwave excitation as the microwave power level at one frequency is held fixed and the power level at the other frequency is varied. In order to overcome signal to noise issues in the limit of small oscillations at very low magnetic fields, we applied a double modulation, double lock-in technique where the magnetic field was modulated sinusoidally while applying a small ac-current to the sample. With this approach, it became possible to measure the magnetic field derivative, $dR_{xx}/dB$, of the diagonal resistance, and realize more oscillations, especially in the low $B$-field limit. Thus, while using this double lock in measurement technique, the sample was bi-chromatically excited at various bi-chromatic microwave frequency combinations. Half cycle plots of $dR_{xx}/dB$ reveal that the bi-chromatic response magneto-transport response follows mostly low frequency response at low magnetic field region and starts following the high frequency response at high magnetic field regions. Here we present the results to address the question of whether or not superposition is followed in the bi-chromatic microwave magnetoresistance response.
4:42PM P01.00012: Interferometer parameters that allow observation of non-Abelian e/4 properties.*

ROBERT WILLETT (Presenter), physical sciences, Nokia Bell Labs, KIRILL SHTENGEL, Dept. of Physics, U.C. Riverside, MICHAEL MANFRA, Dept. of Physics, Purdue University, LOREN PFEIFFER, PRISM, Princeton University, SAeed FALLahi, GEOFFREY GARDNER, Dept. of Physics, Purdue University, KENNETH WEST, KIRK BALDWIN, PRISM, Princeton University — Fabry-Perot interferometers have been used to examine 5/2 filling factor, and have shown interference consistent with Abelian e/2 charges and non-Abelian e/4 charges. Simple magnetic field sweeps and independently side gate sweeps can each expose even-odd effects indicating non-Abelian e/4. These results have been compiled using a series of different heterostructure types, different illumination procedures, and different interferometer geometries, sizes, and gate charging procedures. In this talk summary results will be presented, but the focus will be these device parameters and procedures employed to reveal the non-Abelian properties. Central to this effort is the use of heterostructures that require illumination to produce high mobilities. The illumination and charging protocols exercised on different fundamental heterostructure types will be described, including the consequences, both good and bad, on 5/2 interference. Given these advantages and constraints on the 2D electron material systems, means to mitigate problems in the measurements by adjusting the interference devices themselves will be discussed.

*work at Princeton University funded by Gordon and Betty Moore Foundation, EPIQS initiative Grant GBMF4420, & National Science Foundation MRSEC Grant DMR-1420541

4:54PM P01.00013: A Particle-Hole-Symmetric Model for Paired Fractional Quantum Hall States In a Half-filled Landau Level*

MICHAEL PETERSON (Presenter), WILLIAM HUTZEL, JOHN MCCORD, California State University, Long Beach, PETER RAUM, BEN STERN, Virginia Tech, HAO WANG, Southern University of Science and Technology, VITO SCAROLA, Virginia Tech — The fractional quantum Hall effect (FQHE) observed at half filling of the second Landau level is believed to be caused by a BCS-type pairing of composite fermions captured by the Moore-Read Pfaffian wave function. The generating Hamiltonian for the Moore-Read Pfaffian is a purely three-body model that breaks particle-hole symmetry and lacks properties expected from a physical model. We use exact diagonalization to study the low energy states of a more physical two-body generator model derived from the three-body model. We find that the two-body model exhibits the essential features expected from the Moore-Read Pfaffian: pairing, non-Abelian anyon excitations, and a neutral fermion mode. The model also satisfies constraints expected for a physical model of the FQHE at half-filling because it is: short range, spatially decaying, particle-hole symmetric, and has a roton mode with a robust spectral gap in the thermodynamic limit. Hence, this two-body model offers a bridge between exact generator models of paired states and the physical Coulomb interaction and can be used to further explore properties of non-Abelian physics in the FQHE.

*Supported by the NSF (DMR-1508290, NSF PHY11-25915), ORSP at CSULB, Keck Foundation, AFOSR (FA9550-18-1-0505), ARO (W911NF-16-1-0182).

5:06PM P01.00014: Spin-resolved tunneling in the fractional quantum Hall effect regime*

HEUN MO YOO (Presenter), Massachusetts Institute of Technology, LOREN PFEIFFER, KIRK BALDWIN, KENNETH WEST, Electrical Engineering, Princeton University, RAYMOND ASHOORI, Massachusetts Institute of Technology — Strong Coulomb interactions and internal spin degrees of freedom lead to a plethora of correlated electronic phases in quantum Hall (QH) systems. Despite the successes of nuclear magnetic resonance and optical techniques, spin-sensitive measurements have remained challenging, particularly at low carrier density or in higher Landau levels (LLs). Here we introduce a new method, spin-resolved tunneling, that can probe the spin texture of both the ground and excited states of QH systems. We establish a complete phase diagram of the ground-state spin in a wide range of filling factors $\nu$ and magnetic fields. Our phase diagrams show the detailed structure of the composite fermion (CF) phases in the lowest LL, in which the changes in the Zeeman energy and $\nu$ drive phase transitions between the spin-unpolarized, the spin-polarized, and the topological spin skymion states. On the other hand, the non-Laughlin correlated behavior, such as the absence of spin transitions at $\nu = 2 + 1/2$ and $2 + 2/3$ states, is observed in the first excited LL, where the conventional CF picture is no longer valid due to the softened pair interactions.

*Funded by BES Program of the Office of Science of the US DOE, contract no. FG02-08ER46514, and the Gordon and Betty Moore Foundation, through grant GBMF2931
5:18PM P01.00015: Symmetry protected Luttinger liquids in Quantum Hall Ferromagnets on the surface of Bi(111).*

KARTIEK AGARWAL (Presenter), McGill University, MALLIKA RANDERIA, SHIVAJI SONDHI, ALI YAZDANI, Princeton University, SIDDHARTH PARAMESWARAN, University of Oxford — Quantum Hall Ferromagnets are a unique platform to study the confluence of symmetry-broken order parameter and topology. Recent experiments by Feldman et al.[1] observe clear signatures of valley-polarized Quantum Hall Ferromagnets on the surface of Bi(111) in the presence of strong magnetic fields. The tunneling conductance shows a discrete spectrum indicating the formation of Landau levels while individual nematic Landau level orbits pinned to impurities indicate selective occupation of certain valleys. Further recent experiments[2] observe domain wall states between such nematic domains. Most curiously, domain walls between these domains appear to host low energy excitations that appear to be gapped/gapless depending upon the filling fraction of the nematic quantum Hall states. We explain[3] these observations both qualitatively and quantitatively by highlighting the role of interactions and symmetries in engendering such exotic Luttinger liquids.


*UK Foundation
DOE-BES Grant No. DE-SC0002140
Startup funds from McGill University

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P02 DMP: Topological Materials -- New Theoretical Approaches BCEC 107A - Ying Ran, Boston
Coll - Tag(s): Focus

2:30PM P02.00001: Topological band structures in electric circuits* TOBIAS HELBIG (Presenter), TOBIAS HOFMANN, Institute for Theoretical Physics and Astrophysics, University Wuerzburg, CHING HUA LEE, Department of Physics, National University of Singapore, MARTIN GREITER, RONNY THOMALE, Institute for Theoretical Physics and Astrophysics, University Wuerzburg — Topolectrical circuits [C.H. Lee at al., Comm. Phys. 1,39] present themselves as a platform to investigate fundamental topological states of matter realized in classical synthetic crystals. The manifold degrees of freedom unfolding as lattice connectivity and parameter choice in electric networks enable the implementation of arbitrary tight-binding models. We report on the design, measurement and engineering of admittance band structures in periodic circuits [T. Helbig, T. Hofmann et al., arXiv:1807.09555v1] providing an extensive symmetry classification. Furthermore, we review the effect of individual constituents on the presence of global symmetries. We employ our approach on explicating several examples reaching from the Su-Schrieffer-Heeger and the graphene model over the implementation of a Chern state [T. Hofmann, T. Helbig et al., arXiv:1809.08687v2] up to the realization of non-Hermitian physics in this classical environment.

*This work is supported by ERC-StG-TOPOLECTRICS-336012 and DFG-SFB 1170 (Project B04).

2:42PM P02.00002: Topological Superconductivity in Honeycomb Dirac Systems* TAMAGHNA HAZRA (Presenter), KYUNGMIN LEE, MOHIT RANDERIA, NANDINI TRIVEDI, Ohio State University — There has been a surge of recent interest in superconductivity (SC) in 2D Dirac materials ranging from transition metal dichalcogenides to twisted bilayer graphene. It is important to understand the precise conditions under which one obtains a topological SC state in such systems. We address this question in the simplest honeycomb lattice models that hosts both topological and trivial insulating states in 2D: the Kane-Mele (KM) model for spin-1/2 fermions and the Haldane model for spinless fermions. We describe the results of our extensive self-consistent Bogoliubov-deGennes calculations [1] for these models with a variety of pairing interactions, and show that topological SC states arise only for nearest-neighbor attraction. In the KM model, we find four distinct SC phases, all with finite center-of-mass momentum pairing. Two of these are topological SCs: one a helical spin-triplet SC which is time-reversal invariant and another a chiral spin-triplet SC with Chern number ±1 with equal-spin pairing in one valley and opposite-spin triplet pairing in the other valley. We also discuss possible experimental signatures of these phases.


*Work supported by NSF DMR-1410364 (TH and MR) and NSF DMR-1629382 (KL and NT).
2:54PM P02.00003: Haldane Circuit*  TOBIAS HOFMANN (Presenter), TOBIAS HELBIG, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, CHING HUA LEE, Department of Physics, National University of Singapure, MARTIN GREITER, RONNY THOMALE, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg — We propose an implementation of the Chern state in a topological circuit network, featuring topologically protected, unidirectional propagation of voltage packages at its boundary [T. Hofmann, T. Helbig, et al., arxiv:1809.08687]. Recently, electric circuit arrays have been established as an easily accessible and tunable environment to host synthetic topological states of matter [C. H. Lee, et al., Comm. Phys. 1, 39; T. Helbig, T. Hofmann, et al., arxiv:1807.09555]. The breaking of reciprocity and time-reversal symmetry as well as minimizing dissipation effects constitute the central challenges arising in a circuit realization of the Chern state. In this talk, we present operational amplifiers in a negative-impedance converter configuration as the key component to master these challenges. We report on our results of a dissipation-corrected circuit implementation of the Haldane model.

*This work is supported by ERC-StG-TOPOLECTRICS-336012 and DFG-SFB 1170 (Project B04).

3:06PM P02.00004: Theory of Topological Phases and Topological Band Engineering of Graphene Nanoribbons* TING CAO (Presenter), Physics Department, UC Berkeley and Geballe Laboratory for Advanced Materials, Stanford University, FANGZHOU ZHAO, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Using first-principles and model Hamiltonian calculations, we show that 1D symmetry-protected topological phases exist in graphene nanoribbons (GNRs). Semiconducting GNRs of different width, edge shape, and terminating unit cells can belong to electronic topological classes characterized by different values of a $Z_2$ invariant. Interfaces between topologically distinct GNRs characterized by different $Z_2$ are predicted to support robust in-gap topological interface states which can be utilized as a tool for material engineering. The experimental realizations of these predictions and rational design of topologically-engineered GNR superlattices synthesized from molecular precursors have been achieved. We present here the theoretical basis and calculations for these states, showing novel robust electronic bands with desirable properties. We discuss how this manifestation of 1D topological phases may be used in future studies of 1D quantum spin physics.

*This work is supported by the National Science Foundation (NSF), the NSF Center for Energy Efficient Electronics Science, the Department of Energy, and the Office of Naval Research under the Muri Program. Computational resources have been provided by DOE at NERSC and the NSF through XSEDE resources at NICS.

3:18PM P02.00005: Spin-orbit torques in topological superconducting hybrid structures  CECILIA HOLMQVIST (Presenter), ADAM SZEWCZYK, CARLO CANALI, Linnaeus University — Dirac materials with strong spin-orbit interaction have been shown to generate large surface spin accumulations in response to applied currents. Such materials have, in addition, been demonstrated to exert spin-orbit torques on adjacent ferromagnetic structures. This magnetoelectric effect in these materials is strong due to the efficient spin-momentum locking. In heterostructures consisting of superconductors and three-dimensional superconductors, this spin-momentum locking leads to an induced unconventional superconductivity that may be useful for superconducting spintronics. Here, we investigate theoretically the quantum transport properties of a ballistic junction consisting of two topological superconductors coupled over a quantum dot that is coupled to a ferromagnet. The spin-orbit torques acting on the ferromagnet are examined and are shown to depend strongly on the magnetization direction relative to the current direction.

3:30PM P02.00006: Topological Mechanics from Supersymmetry* MICHAEL LAWLER (Presenter), Department of Physics, Cornell University, USA, JAN ATTIG, Institute for Theoretical Physics, University of Cologne, Germany, KRISHANU ROYCHOWDHURY, Department of Physics, Cornell University, USA, SIMON TREBST, Institute for Theoretical Physics, University of Cologne, Germany — In topological mechanics, the identification of a mechanical system's rigidity matrix with an electronic tight-binding model allows inferring topological properties of the mechanical system, such as the occurrence of 'floppy' boundary modes, from the associated electronic band structure. Here we introduce an approach to systematically construct topological mechanical systems by an exact supersymmetry (SUSY) that relates the bosonic (mechanical) and fermionic (e.g. electronic) degrees of freedom. As examples, we discuss mechanical analogs of the Kitaev honeycomb model and of a second-order topological insulator with floppy corner modes. Our SUSY construction naturally defines hitherto unexplored topological invariants for bosonic (mechanical) systems, such as bosonic Wilson loop operators that are formulated in terms of a SUSY-related fermionic Berry curvature.

*We gratefully acknowledge the hospitality of the Kavli Institute for Theoretical Physics, supported by NSF PHY-1125915, where this work was initiated during the “Intertwined orders” program. The Cologne group acknowledges partial funding from the DFG within CRC 1238 (project C02) and CRC/TR 183 (project B01).
3:42PM P02.00007: Effects of electric field on topological phases in graphene nanoribbons

FANGZHOU ZHAO (Presenter), TING CAO, STEVEN G. LOUIE, University of California, Berkeley — We have recently shown that graphene nanoribbons (GNRs) host distinct topological phases. By first-principles calculations and tight-binding methods, we demonstrated that GNRs of different width, edge shape and end terminations can belong to different topological classes characterized by a $Z_2$ invariant. Electric field, on the other hand, is also an essential external element that can be used to tune the electronic properties of nanomaterials such as their band gaps. We thus carry out studies on the effects of electric field on the topological phases in various graphene nanoribbons by first-principles calculations.

*This work is supported by the National Science Foundation (NSF), the NSF Center for Energy Efficient Electronics Science, the Department of Energy, and the Office of Naval Research under the MURI Program. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

3:54PM P02.00008: Engineering of Chern insulators through defects

EMMA MINARELLI, School of Physics, University College Dublin, KIM PÖYHÖNEN, Department of Applied Physics, Aalto University, GERWIN VAN DALUM (Presenter), Institute for Theoretical Physics, Utrecht University, TEEMU OJANEN, Department of Applied Physics, Aalto University, LARS FRITZ, Institute for Theoretical Physics, Utrecht University — Impurities embedded in electronic systems induce bound states which can hybridize and lead to impurity bands. Recently, doping of insulators with impurities has been identified as a promising route towards engineering electronic topological states of matter. We illustrate how to engineer Chern insulators starting from a three-dimensional topological insulator with a gapped surface that is intentionally doped with magnetic impurities. The main advantage of the protocol is that it is robust and independent of details, always leading to a Chern insulator supporting a topological phase with Chern number one.

4:06PM P02.00009: Symmetry Indicators of Band Topology

[Invited] HOI CHUN PO (Presenter), Massachusetts Institute of Technology — Topological invariants of band structures are generally defined using the Bloch wave functions, which make them challenging to compute in realistic first-principles calculations. Spatial symmetries, however, can provide very powerful shortcuts for diagnosing certain classes of topological materials, as is epitomized by the Fu-Kane criterion for inversion-symmetric topological insulators. I will describe our theory of symmetry indicators\(^1\), which utilizes symmetry data in a maximal manner to diagnose band topology in any symmetry setting, including magnetic materials\(^2\). Aside from serving as an anchor for a more unified theoretical treatment of topological crystalline insulators\(^3\), the simplicity of the theory allows us to perform a comprehensive database search and uncovers thousands of topological materials\(^4\).


4:42PM P02.00010: Anomalous Hall Effect in Symmetry Protected Topological Metals

XUZHE YING (Presenter), ALEX KAMENEV, University of Minnesota — Anomalous Hall effect is known to have several major contributions, including the intrinsic contribution from the Berry phase of Bloch electrons and skew scattering from impurities. Previously we showed that there exists a class of materials dubbed as symmetry protected topological (SPT) metals. In SPT metals, the intrinsic part of the Hall conductivity shows a discontinuity over the topological phase transition. Such a discontinuity is protected by a certain symmetry, like the particle-hole symmetry.

In this work, we studied the skew scattering contribution to the thermal Hall conductivity in such a system. Our model is based on a two dimensional $p+ip$ superconductor with a supercurrent applied in a particular direction. This system breaks time reversal symmetry which is necessary for skew scattering processes. The disorder potential is modeled by a delta potential. The scattering matrix is calculated self-consistently with the Lippman-Schwinger equation. With the help of the Boltzmann transport equation, we were able to show that skew scattering does not smear out the sharp feature from the intrinsic contribution of the thermal Hall conductivity at the topological phase transition.
4:54PM P02.00011: Classification of flat bands from irremovable discontinuities of Bloch wave functions*
JUN-WON RHIM (Presenter), BOHM-JUNG YANG, Seoul National University — We show that flat bands can be categorized into two distinct classes, that is, singular and nonsingular flat bands. In the case of a singular flat band, its Bloch wave function possesses irremovable discontinuities generated by the band crossing with other bands. This singularity precludes the compact localized states from forming a complete set spanning the flat band. Once the degeneracy at the band crossing point is lifted, the singular flat band becomes dispersive and can acquire a finite Chern number in general, suggesting a new route for obtaining a nearly flat Chern band. On the other hand, the Bloch wave function of a non-singular flat band has no singularity, and thus it can be completely isolated from other bands while preserving the perfect flatness. We show that a singular flat band displays a novel bulk-boundary correspondence such that the presence of the robust boundary mode is guaranteed by the singularity of the Bloch wave function. Moreover, we develop a general scheme to construct a flat band model Hamiltonian in which one can freely design its singular or non-singular nature. Finally, we propose a general formula for the compact localized state spanning the flat band.

*J.-W. Rhim acknowledges the support from Institute for Basic Science (IBS-R009-D1)

5:06PM P02.00012: A membrane-network model for (3+1)D topological phases
AKIN MORRISON (Presenter), MENG HUA, ALEXANDER K SIROTA, CHI YAN JEFFREY TEO, University of Virginia — Non-chiral topological phases in 2D can be understood using the Levin-Wen string-net model. Here, we construct a membrane-network model in 3D. The model has as input a generalized tensor category, which consists of a collection of modular tensor categories and equipped with a non-associative product structure, such as anyon pair condensation, that respects locality. The construction outputs an exactly soluble Hamiltonian in 3D. We speculate this model describes topological phases in 3D that dynamically generate (1+1)D stringy excitations that host low-energy conformal field theories.

5:18PM P02.00013: Hierarchical Majoranas in a Programmable Nanowire Network*
ZHICHENG YANG (Presenter), Boston University, THOMAS IADECOLA, Joint Quantum Institute, CLAUDIO CHAMON, Boston University, CHRISTOPHER M MUDRY, Paul Scherrer Institute — We propose a hierarchical architecture for building “logical” Majorana zero modes using “physical” Majorana zero modes at the Y-junctions of a hexagonal network of semiconductor nanowires. Each Y-junction contains three “physical” Majoranas, which hybridize when placed in close proximity, yielding a single effective Majorana mode near zero energy. The hybridization of effective Majorana modes on neighboring Y-junctions is controlled by applied gate voltages on the links of the honeycomb network. This gives rise to a tunable tight-binding model of effective Majorana modes. We show that selecting the gate voltages that generate a Kekule vortex pattern in the set of hybridization amplitudes yields an emergent “logical” Majorana zero mode bound to the vortex core. The position of a logical Majorana can be tuned adiabatically, without moving any of the “physical” Majoranas or closing any energy gaps, by programming the values of the gate voltages to change as functions of time. A nanowire network supporting multiple such “logical” Majorana zero modes provides a physical platform for performing adiabatic non-Abelian braiding operations in a fully controllable manner.

*DOE Grant No. DEFG02-06ER46316

Wednesday, March 6, 2019 2:30 PM - 5:30 PM
Session P03 DCMP: Surfaces of Topological Systems BCEC 107B
Interaction of the Topological Surface States with Spin Excitons in SmB$_6$ - Dependency on the Crystallinity


Preparation of High-Quality Junctions on SmB$_6$ for Planar Tunneling Spectroscopy

JENNIFER SITTLER (Presenter), LAURA H GREENE, Physics, Florida State University, DAE-JEONG KIM, ZACHARY FISK, Department of Physics and Astronomy, University of California- Irvine, WESLEY T FUHRMAN, JUAN CHAMORRO, SEYED KOOPHAYEH, WILLIAM PHELAN, TYREL MCQUEEN, Institute for Quantum Matter, Johns Hopkins University — Previous works have utilized planar tunneling spectroscopy to investigate the possible topological surface states in SmB$_6$ [1,2]. When superconducting Pb is used as a counter-electrode, the tunneling conductance spectra revealed, coherence peaks with an asymmetrical temperature evolution as well as an additional peak at ~ 5 mV. These features were attributed to inelastic tunneling processes involving the emission and absorption of spin excitons [3,4]. The tunnel barrier in these reproducible junctions was formed by oxidizing the top layer of the SmB$_6$ [1,2]. Improving the junction quality even further, would allow for measurements of the second harmonic, which may reveal additional details about the spin excitons. The preparation of high-quality junctions on SmB$_6$ single crystals and thin films will be discussed. [1] W. K. Park et al., PNAS, 113, 6599 (2016). [2] L. Sun et al., Phys. Rev. B. 95, 195129 (2017). [3] W. T. Fuhrman et al., PRL 114, 036401 (2015). [4] G. A. Kapilevich et al., PRB 92, 085113 (2015).

Magnetize Topological Surface States of Bi$_2$Se$_3$ with a CrI$_3$ Monolayer

YUSHENG HOU, University of California, Irvine, JEONGWOO KIM, Department of Physics, Ulsan National Institute of Science and Technology, RUQIAN WU (Presenter), University of California, Irvine — To magnetize surfaces of topological insulators without damaging their topological feature is a crucial step for the realization of the quantum anomalous Hall effect (QAHE), and still remains as a challenging task. Through density functional calculations, we found that adsorption of a semiconducting two-dimensional van der Waals (2D-vdW) ferromagnetic CrI$_3$ monolayer can create a sizable spin splitting at the Dirac point of the topological surface states of Bi$_2$Se$_3$ films. Furthermore, general rules that connect different quantum and topological parameters are established through model analyses. This work provides a useful guideline for the realization of QAHE at high temperature in heterostructures of 2D-vdW magnetic monolayers and topological insulators.

Topological invariant of S4 protected high-order topological insulator

ZHIDA SONG (Presenter), Department of Physics, Princeton University — The point group symmetry S4 protects a high-order topological state that is gapped on all its 2D surfaces but gapless on a 1D hinge. In this talk, I present a bulk topological invariant of this S4 topology in terms of Wilson loop of Wilson loop. The nonlocal Wilson loop operator provides an effective Hamiltonian on the surface, the Wilson loop of which provides an intuitive understanding of the hinge state. Based on this picture, the breaking of Kirchhoff's law on surfaces are discussed.
3:18PM P03.00005: Bound State Signatures in a Mesoscopic TI Josephson Junction* KONSTANTIN YAVILBERG (Presenter), Physics, Ben-Gurion University of the Negev, ERAN GINOSSAR, Advanced Technology Institute and Department of Physics, University of Surrey, EYTAN GROSFELD, Physics, Ben-Gurion University of the Negev — The engineering of hybrid Josephson junctions has increasingly become a key source in the experimental access to topological superconductivity, as these allow a high degree of robustness and control of their characteristic excitations. Here we consider a device where a topological insulator nanowire of type Bi2Se3 is proximitized to an isolated mesoscopic Josephson junction. Threaded with magnetic flux, the nanowire nucleates two pairs of topologically protected Majorana fermions as well as Andreev bound states in the weak-link. We investigate processes of coherent charge transfer mediated by these low-energy bound states in a mesoscopic setting, and show that they have a notable effect on the fermionic parity of the superconductors, as is evident in the response of the system to electromagnetic radiation.

*This project has received funding from the European Unions Horizon 2020 research and innovation programme under grant agreement No. 766714

3:30PM P03.00006: Topological States in Restrictive Geometries* LIAM O’BRIEN (Presenter), Department of Physics, University of Massachusetts Amherst, KARUNYA SHIRALI, DANIEL E SHEEHY, ILYA VEKHTER, Department of Physics & Astronomy, Louisiana State University — Topological Insulators (TIs) are a novel class of materials possessing symmetry-protected surface states that have promising applications in spintronics and quantum computing. The properties and robustness of TI surface states are well understood for macroscopic samples with flat boundaries, but it is not clearly established what features are retained for curved boundaries - especially when the radius of curvature and/or the sample size are decreased and become comparable to the decay length of the surface states. Consequently, here we investigate the nature of the topological surface states for finite samples with curved interfaces. In particular, we study a model of a 2-dimensional TI with circular boundary of radius R, described by a 4 × 4 Dirac-like Hamiltonian. We present exact solutions for the surface states of this system, derive the effective surface Hamiltonian, and discuss the deviations of the dispersion and spin texture from the flat surface case.

*We thank the National Science Foundation for supporting this work through the REU Site in Physics & Astronomy (NSF grant #1560212) at Louisiana State University; we also acknowledge support though NSF grants DMR-1410741 and DMR-1151717.

3:42PM P03.00007: Observation of quadrupole topological insulators MARC SERRA GARCIA (Presenter), VALERIO PERI, SEBASTIAN D HUBER, ETH Zurich — Many topological phenomena can be understood as a symmetry-induced quantization of the Berry phase, which describes the charge polarization inside the unit cell. This theory relating topology and polarization has been recently extended to higher-order multipolar moments. In this talk, we will discuss experimental observations of a multipolar (quadrupole) topological insulator and quadrupole transitions in phononic and LC-circuit platforms. Our measurements confirm the theoretical predictions and provide a route towards protected wave guides in three dimensional materials.

3:54PM P03.00008: Characterization of Electron Beam Damage to (BixSb1-x)2Te3-Based Topological Insulators* LINSEY RODENBACH (Presenter), ILAN ROSEN, ELI J FOX, Stanford University, LEI PAN, PENG ZHANG, KANG L. WANG, University of California Los Angeles, DAVID GOLDHABER-GORDON, Stanford University — Models for topological superconductivity based on proximitized superconductivity in quantum Hall systems have proven difficult to realize, in part, because high magnetic fields destroy Cooper pairing. The discovery of the quantum anomalous Hall (QAH) effect in Cr- and V-doped (BixSb1-x)2Te3 has attracted attention because it provides a platform to demonstrate the same models of topological superconductivity without high magnetic fields. A remaining barrier is fabrication of the desired structures. Photolithographic patterning has been employed with QAH materials to great effect but lacks the spatial resolution needed to define, for example, Josephson junctions and quantum point contacts. Electron beam lithography has largely been avoided for fear of damaging or doping the QAH material, whose Fermi level must be very precisely positioned to observe the QAH effect. We discuss our efforts to characterize electron beam damage to (BixSb1-x)2Te3-based topological insulators. We also propose possible approaches for submicron patterning involving no electrons hitting the substrate.

*This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.
Quantum-Hall to insulator transition in ultraclean topological insulator films

MARYAM SALEHI (Presenter), Materials Sci. & Eng., Rutgers University, HASSAN SHAPOURIAN, Physics, University of Chicago, ILAN ROSEN, Applied Physics, Stanford University, MYUNG-GEUN HAN, Condensed Matter Physics and Materials Science, Brookhaven National Lab, JISOO MOON, Materials Sci. & Eng., Rutgers University, PAVELE SHIBAYEV, DEEPTI JAIN, Physics, Rutgers University, DAVID GOLDHABER-GORDON, Physics, Stanford University, SEONGSHIK OH, Physics, Rutgers University — Under a magnetic field, many two-dimensional electronic systems including semiconductor 2DEGs, graphene, and topological insulators (TIs) exhibit quantum Hall effect (QHE), where $R_{xy}$ is quantized at $h/(\nu e^2)$ while $R_{xx} \to 0$. In the high field limit, the QH state gives way to an insulating state in semiconductor 2DEGs as the Fermi level falls into localized states at the tail of the lowest Landau level. However, for a Dirac system such as TIs, the presence of the zeroth Landau level makes it questionable whether such a QH-to-insulator-transition (QIT) should occur at all. Here, in newly-developed ultraclean TI films, we report the first observation of QIT in TIs, with a well-defined scaling behavior. Surprisingly, the scaling analysis revealed the first example of an unconventional QIT behavior distinct from those in 2DEGs. This observation raises new questions on the origin of the insulating phase near the center of the zeroth Landau level in TIs and other Dirac materials as well.

ONR (N000141210456), NSF (DMR-1308142) and GBMF’s EPIQS Initiative (GBMF4418).

Electronic Properties of Bismuth Iodide (Bi$_4$I$_4$)

YULU LIU (Presenter), RUOYU CHEN, Ohio State University, SHENG LI, XIAOYUAN LIU, University of Texas at Dallas, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, BING LV, FAN ZHANG, University of Texas at Dallas, CHUN NING LAU, Ohio State University — In recent years, topological insulator materials have been attractive to many scientists because of their gapless conductive surface states that are protected against perturbations. Bi$_4$I$_4$ is a quasi-one-dimensional van der Waals material, and its $\beta$-phase is predicted to be a topological insulator, thus offering a new platform for exploring the physics of topological phases. Here we report fabrication and measurement of Bi$_4$I$_4$ devices. Its electrical transport properties are investigated as a function of channel length, electrode materials, mobility and magnetic field.

Local tuning of edge states in a 2D-Topological Insulator quantum well

M. REYES CALVO (Presenter), CIC nanoGUNE, TINEKE VAN DEN BERG, Materials Physics Center (CFM), San Sebastian, Spain, DARIO BERCIOUX, Donostia International Physics Center, San Sebastian, Spain, CHRISTOPH BRÜNE, LAURENS MOLENKAMP, University of Wurzburg, DAVID GOLDHABER-GORDON, Stanford University — We study the conductance of a 2D-Topological Insulator HgTe quantum well device as a function of both the overall density of carriers and the local electric field created by a movable metallic tip. Conductance maps as a function of tip position confirm on the one hand the existence of scattering at the edges due to charge puddles and, on the other hand, show remarkably different behavior for different values of overall carrier density when the tip is positioned above the bulk or the edge areas of the sample respectively. When the bulk is fully depleted, changes in conductance occur only in the case the tip is positioned above the edge - accounting for about a 10% of the unperturbed conductance of the device. The edge areas where the tip has a clear effect in conductance shift towards inner positions of the device bulk with increasing the overall electron doping. These results suggest a scenario where current at the edge is mostly carried by topologically protected Quantum Spin Hall states, in addition to tunable, diffusive extra channels.

Commuting-projector Hamiltonians for 2D time-reversal-invariant fermionic topological phases and many-body topological invariants

JUN HO SON (Presenter), Stanford University, JASON ALICEA, Caltech — Inspired by a recently constructed commuting-projector Hamiltonian for a 2D time-reversal-invariant topological superconductor [Wang et al., Phys. Rev. B 98, 094502 (2018)], we introduce a commuting-projector model that describes an interacting yet exactly solvable 2D time-reversal-invariant topological insulator. We explicitly show that the edge properties of our model, both gapped and gapless, are consistent with those of band-theoretic or weakly interacting quantum spin Hall systems. Additionally, the models for both topological insulators and superconductors can be defined on non-orientable spatial manifolds while retaining the commuting-projector Hamiltonian structure. Ground-state wavefunctions of these models on non-orientable manifolds provide intuitive pictures of many-body topological invariants of time-reversal-invariant fermionic topological phases.
**4:54PM P03.00013: Ferromagnetism in Cr-doped Bi₂Se₃ thin films via surface-state engineering and carrier-selective anomalous Hall effect**  
JISOO MOON (Presenter), NIKESH KOIRALA, Physics and Astronomy, Rutgers, The State University of New Jersey, MARYAM SALEHI, Materials Science and Engineering, Rutgers, The State University of New Jersey, SEONGSHIK OH, Physics and Astronomy, Rutgers, The State University of New Jersey — Anomalous Hall effect (AHE) is a non-linear Hall effect appearing on magnetic conductors, boosted by internal magnetism beyond what is expected from ordinary Hall effect. With the recent discovery of quantized version of the AHE, the quantum anomalous Hall effect (QAHE), in Cr- or V-doped topological insulator (TI) (Sb,Bi)₂Te₃ thin films, AHE in magnetic TIs has been attracting significant interest. However, one of the puzzles in this system has been that while Cr- or V-doped (Sb,Bi)₂Te₃ and V-doped Bi₂Se₃ exhibit ferromagnetic (hysteric) AHE, Cr-doped Bi₂Se₃ has failed to exhibit even ferromagnetic AHE, the necessary predecessor to QAHE, though it is the first material predicted to exhibit QAHE. Here, we have successfully implemented ferromagnetic AHE in Cr-doped Bi₂Se₃ thin films by utilizing a surface state engineering scheme. Surprisingly, all the observed ferromagnetic AHE, as in other Cr- or V-doped TIs, are always p-type even if the majority carrier type remains n-type. This can be well explained by a carrier-selective anomalous-Hall-effect model in which the local magnetic moments interact only through p-type carriers.

*This work is supported by Gordon and Betty Moore Foundation's EPIQS Initiative (GBMF4418) and National Science Foundation (NSF) (EFMA-1542798).

**5:06PM P03.00014: Topological States at Interfaces and in Heterostructures**  
KARUNYA SHAILESH SHIRALI (Presenter), WILLIAM A. SHELTON, ILYA VEKHTER, Louisiana State University — Engineering topological insulator (TI) devices involves making heterostructures which combine these materials with other compounds. For a model Hamiltonian, it was shown [1] that properties of the topological interface states may differ from those of the surface states. Motivated by this observation we use a combination of ab initio and model calculations to investigate the consequences of interface potentials breaking spatial symmetries (with and without time reversal symmetry breaking) on the spectral and spin properties of the interface states. We use first principles density functional theory calculations to investigate the topological states at the boundaries between Bi₂Se₃ and binary semiconductors and magnetic insulators, obtain the form of the spin-momentum locking and anisotropy of energy dispersion, and compare these features with the outcomes of model analytical calculations. We also make connections with recent experiments on topological heterostructures, and discuss the importance of our results for tuning topological materials for potential device applications.


*NSF grant DMR-1410741

**5:18PM P03.00015: Dice Lattice in Ribbons and their Topological Properties**  
RAHUL SONI (Presenter), NITIN KAUSHAL, Physics, University of Tennessee-Knoxville, SATOSHI OKAMOTO, Oak Ridge National Laboratory, ELBIO R DAGOTTO, Physics, University of Tennessee-Knoxville — The existence of nearly flat bands with non-zero Chern numbers in a two-dimensional dice lattice has been studied [1] in the presence of Rashba spin-orbit coupling and a magnetic field. In this work, we studied the topological properties of the dice lattice defined using ribbons both with open and periodic boundary conditions. We found that the Chern numbers [2] are finite even for narrow systems such as Nx3 [3]. We also observed spin currents moving along the edges at half filling, when ribbons are in a cylindrical geometry with open conditions in the long direction. Understanding these topological properties in ribbon-like geometry is important because of computationally exact techniques like DMRG can be used to investigate the effect of Hubbard interactions on dice lattices.


**Wednesday, March 6, 2019 2:30 PM - 5:18 PM**

**Session P04 DMP: Dirac/Weyl Semimetals -- Optical and Spectroscopy**  
BCEC 107C - Guang Bian, University of Missouri - Tag(s): Focus
Optical Control of Chiral Charge Pumping in a Topological Weyl Semimetal

MEHDI JADIDI (Presenter), Columbia University, MEHDI KARGARIAN, Sharif University of Technology, MARTIN MITTENDORFF, YIGIT AYTAC, University of Maryland College Park, BING SHEN, University of California, Los Angeles, JACOB KÖNIG-OTTO, STEPHAN WINNERL, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), NI NI, University of California, Los Angeles, THOMAS E. MURPHY, H. DENNIS DREW, University of Maryland College Park — Solids with topologically robust electronic states exhibit unusual electronic and optical transport properties not seen in other materials. A peculiar example is chiral charge pumping (also called chiral anomaly) in recently discovered topological Weyl semimetals, where simultaneous application of parallel static electric and magnetic fields causes an imbalance in the number of topological chiral carriers. Here, using time-resolved terahertz measurements on the Weyl semimetal tantalum arsenide (TaAs) in a magnetic field, we uncover the optical control of chiral anomaly by dynamically pumping the chiral charges and monitor their relaxation. Rigorous theory based on Boltzmann transport shows that the observed optically-induced control of chiral anomaly is governed by the optical nonlinearity in the chiral charge pumping process. Our measurements reveal that the chiral pumping relaxation is much longer than 1 ns. The optically-controlled long-lived chiral carriers observed here in a Weyl semimetal exhibit similar behavior to the valley-polarized carriers in 2D semiconductors, but with the extra feature of topological protection, suggesting possible valleytronic applications of Weyl semimetals.

Circular photogalvanic effect of layered type-II Weyl semimetal MoTe2 in mid-infrared band

JUNCHAO MA (Presenter), QIANGQIANG GU, YINAN LIU, Peking University, PENG YU, Nanyang Technological University, JIAWEI LAI, XIAO ZHUO, Peking University, ZHENG LIU, Nanyang Technological University, JIANHAO CHEN, JI FENG, DONG SUN, Peking University — Td-Phase Molybdenum ditelluride (MoTe2) has attracted enormous research interests as a Type-II Weyl semimetallic state and the fascinating properties it exhibits. By applying circularly polarized 4.0-μm and 10.6-μm excitation at normal incidence, circular photogalvanic effect (CPGE) has been observed in topological Td-phase MoTe2. The CPGE signal is not allowed by the C2v symmetry by second order nonlinear effect under our experimental geometry. This work is one of the first experimental realizations of this effect in type-II Weyl semimetals with the MIR spectral regime, which is suitable to unveil the physics related to Weyl cones. The occurrence of CPGE in MoTe2 is attributed to a built-in electric field, which can remove full C2v symmetry, resulting in nonzero injection current via an third order nonlinear optical effect. The field is produced by the work function difference between samples and electrodes or photothermoelectric effect after photo-excitation. Additionally, the existence of CPGE in our experiments is an unique signature of the Td phase, which is in consistence with the recently-reported Barkhausen effect during phase transition of MoTe2.

Anisotropic Broadband Photo Response of Layered Type-II Weyl Semimetals

JIAWEI LAI (Presenter), XIN LIU, JUNCHAO MA, QINSHENG WANG, Peking University, KENAN ZHANG, Tsinghua University, XIAO REN, YINAN LIU, QIANGQIANG GU, XIAO ZHUO, WEI LU, Peking University, YU PENG, ZHENG LIU, NTU, YUAN LI, JI FENG, Peking University, SHUYUN ZHOU, Tsinghua University, JIANHAO CHEN, DONG SUN, Peking University — Td-MoTe2 and TaIrTe4, two-dimensional layered Type-II Weyl semimetal, are expected to share several unique advantages with Dirac semimetals for photodetection. The extremely high mobility and the chiral Fermions near the Weyl node lead to several advantages over traditional semiconductor-based photodetectors. Here, we report the realization of broadband self-powered photodetectors based on Td-MoTe2 and TaIrTe4, two-dimensional layered Type-II Weyl semimetal, are expected to share several unique advantages with Dirac semimetals for photodetection. The extremely high mobility and the chiral Fermions near the Weyl node lead to several advantages over traditional semiconductor-based photodetectors. Here, we report the realization of broadband self-powered photodetectors based on Td-MoTe2 and TaIrTe4. Broadband responses from visible to mid-infrared are experimentally tested. The PC generation mechanisms are investigated and it is found that PTE effect plays critical role in PC generation. Furthermore, we found that the anisotropy is wavelength dependent, and the degree of anisotropy increases as the excitation wavelength gets closer to the Weyl nodes which can be used for polarization-sensitive photo detection. Thus Td-MoTe2 and TaIrTe4 provide a new class of material platform for high performance photodetection applications.

This project was supported by the National Natural Science Foundation of China (NSFC Grant Nos. 91750109, 11674013).
Contributions from the bulk and surface states of the studied materials are also distinguished. The relation of the different components of the optical conductivity tensor are determined and studied as a function of frequency. Based on a Wannier interpolation scheme, which takes into account the realistic electronic structure of these materials.

Nöthnitzer Straße-40, 01187 Dresden, Germany, DARIUS TORCHINSKY, Department of Physics, Temple University, JOSEPH ORENSTEIN, University of California, Berkeley — Topological materials, and in particular Weyl semimetals, offer a playground for diverse optical properties. When inversion symmetry is broken, such materials additionally allow second-order bulk nonlinear effects. We present a spectroscopic second harmonic generation study of a Weyl semimetal, and discuss data taken as a function of incident and emitted polarization angle over a range of incident frequencies from the visible to the infrared.

Quantum Materials program supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02- 05CH11231

3:18PM P04.00005: Optical Response Characteristics of the Weyl Semimetals WTe₂ and MoTe₂* 

ADRIAN POPESCU (Presenter), LILIA M WOODS, Department of Physics, University of South Florida — Weyl semimetals are 3D systems exhibiting linear dispersion band crossings which act as Berry curvature monopoles in the reciprocal space. A key signature for Weyl semimetals is the appearance of surface Fermi arcs as a result of the projection of the bulk Weyl points on the surface of the material. Here we report first-principles calculations for the dynamical conductivity tensor, a basic quantity for the light-matter interactions, of the Weyl semimetals MoTe₂ and WTe₂. The calculations rely on the Kubo formula, computed based on a Wannier interpolation scheme, which takes into account the realistic electronic structure of these materials. The different components of the optical conductivity tensor are determined and studied as a function of frequency. Contributions from the bulk and surface states of the studied materials are also distinguished. The relation of the calculated results with the experimental ones, as well as the temperature effects, are also discussed.

*Financial support from the US Department of Energy under Grant No. DE-FG02-06ER46297 is acknowledged.

3:30PM P04.00006: Optical evidence of chiral Landau level in Weyl semimetal 

XIANG YUAN (Presenter), FAXIAN XIU, Fudan University — Weyl semimetal has been extensively studied with exotic phenomena such as chiral anomaly. Despite the numerous experimental efforts to explore the chiral anomaly in different materials, electrical transport is the main approach where negative magneto-resistivity works as a criterion. More evidence of chiral anomaly, such as the existence of chiral Landau level, is desired for further study. Here we report a magneto-optical study in Weyl semimetal. Allowed optical transition under magnetic field can reveal the Landau level structure. The Chiral Landau levels are experimentally found in typical Weyl semimetals NbAs while the system is driven close to the quantum limit. The related optical transition exhibits distinct difference from other normal Landau levels. The z momentum can be finite with unique magnetic field evolution. Meanwhile, multiple carriers with different topological origins are found, indicate complex band structure of the crystal. Our results demonstrate an effective tool for studying complex topological systems. Further evidence of chiral magnetic effect will also be discussed.

3:42PM P04.00007: Second harmonic generation studies on the Weyl semimetal WTe₂ 

EDBERT JARVIS SIE (Presenter), CLARA M NYBY, AARON LINDENBERG, Stanford University — Tungsten ditelluride (WTe₂) is a layered material that is both a ferroelectric and a Weyl semimetal. The coexistence of these two properties stems from inversion symmetry breaking, a condition that is sensitive to the atomic-scale lattice distortions in this material. Here, we performed second harmonic generation (SHG) studies on tungsten ditelluride. We will report on unusual and large-amplitude temperature dependent responses of the SHG as a probe of the inversion-breaking phase in WTe₂.

3:54PM P04.00008: Terahertz Generation Measurements in Inversion-Symmetry Breaking Weyl Semimetals with Spectrally Resolved Excitation Fields* 

DYLAN REES (Presenter), University of California, Berkeley, BAOZHU LU, MANITA RAI, Department of Physics, Temple University, KAUSTUV MANNA, CLAUDIA FELSER, Max-Planck-Institute for Chemical Physics of Solids, Joseph TORCHINSKY, Department of Physics, University of California, Berkeley — Topological materials, and in particular Weyl semimetals, offer a playground for diverse optical properties. When inversion symmetry is broken, such materials additionally allow second-order bulk nonlinear effects. We present terahertz generation data with excitation fields ranging across the near infrared spectrum. Measurements were taken with both linear- and circular-polarized light in a variety of geometries.

*Gordon and Betty Moore Foundation’s EPIQs Initiative, Grant No. GBMF4537.

Quantum Materials program supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02- 05CH11231.

*Gordon and Betty Moore Foundation's EPIQs Initiative, Grant No. GBMF4537.
Recently, Weyl semimetals have been experimentally discovered in both inversion-symmetry-breaking and time-reversal-symmetry-breaking crystals. The non-trivial topology in Weyl semimetals can manifest itself with exotic phenomena which have been extensively investigated by photoemission and transport measurements. Despite the numerous experimental efforts on Fermi arcs and chiral anomaly, the existence of unconventional zeroth Landau levels, as a unique hallmark of Weyl fermions which is highly related to chiral anomaly, remains elusive owing to the stringent experimental requirements. Here, we report the magneto-optical study of Landau quantization in Weyl semimetal NbAs. High magnetic fields drive the system towards the quantum limit which leads to the observation of zeroth chiral Landau levels in two inequivalent Weyl nodes. As compared to other Landau levels, the zeroth chiral Landau level exhibits a distinct linear dispersion in z momentum direction and allows the optical transitions without the limitation of zero z momentum or $\sqrt{B}$ magnetic field evolution. The magnetic field dependence of the zeroth Landau levels further verifies the predicted particle-hole asymmetry of the Weyl cones. Meanwhile, the optical transitions from the normal Landau levels exhibit the coexistence of multiple carriers including an unexpected massive Dirac fermion, pointing to a more complex topological nature in inversion-symmetry-breaking Weyl semimetals. Our results provide insights into the Landau quantization of Weyl fermions and demonstrate an effective tool for studying complex topological systems.

This work was supported by the National Natural Science Foundation of China (Grant No. 11474058, 61674040, 11674189) and the National Key Research and Development Program of China (Grant No. 2017YFA0303302, 2016YFA0203900, 2017YFA0303504).

The chiral anomaly is a phenomenon characteristic of Weyl fermions, which has condensed matter realizations in Weyl semimetals. Efforts to observe a smoking gun signatures of the chiral anomaly in electronic transport has proven non-trivial. Recent works have proposed an alternative approach of probing phonon dynamics for signatures of the chiral anomaly in non-mirror-symmetric crystals. Here, we show that such phononic signatures can be extended to mirror symmetric crystals, broadening the pool of candidate materials. We show that the background magnetic field can break mirror symmetry strongly enough to yield observable signatures of chiral anomaly even in mirror-symmetric materials. Specifically for mirror-symmetric Weyl semimetals such as TaAs and NbAs, including the Zeeman interaction at $B\sim10T$, we predict an IR reflectance peak will develop with an $E_{\text{IR}}B$ dependence.

A.H. was supported by the NSF Fellowship under Grant No. DGE-1650441. Y.Z. was supported by NSF DMR-1308089 and Bethe fellowship at Cornell University. E.-A.K. acknowledges support by the NSF (PARADIM) under Cooperative Agreement No. DMR-1539918.

Weyl semimetals (WSM) are a recently realized class of topological materials with low energy electronic excitations characterized by a three-dimensional, linear dispersion. While much focus has been directed at characterizing and understanding the electronic properties of various WSMs, little attention has been paid to the vibrational properties. In the WSMs NbAs and TaAs such considerations are crucial for understanding the anomalously high mobility and thermal response. We present temperature and polarization dependent Raman spectra which reveal anomalous lineshapes, as well as deviations from standard anharmonic behavior.

U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Award No. DE-SC0018675
US. Department of Energy, Photonics at Thermodynamic Limits Energy Frontier Research Center, Grant No. DE-SC0019140
Optical Evidence of Chiral Magnetic Anomaly in Weyl Semimetal TaAs

ANTONIO LEVY (Presenter), ANDREI B SUSHKOV, Department of Physics, Center for Nanophysics and Advanced Materials, University of Maryland, FENGGUANG LIU, Anhui Agricultural University, BING SHEN, NI NI, Department of Physics and Astronomy, University of California, Los Angeles, HOWARD DREW, Department of Physics, Center for Nanophysics and Advanced Materials, University of Maryland, GREGORY S JENKINS, Laboratory for Physical Sciences — Chiral pumping from optical electric fields oscillating at THz frequencies is observed in the Weyl material TaAs with electric and magnetic fields aligned along both the a- and c-axes. Free carrier spectral weight enhancement is measured directly for the first time, confirming theoretical expectations of chiral pumping. A departure from linear field-dependence of the Drude weight is observed at the highest fields in the quantum limit, providing direct evidence of field-dependent Fermi velocity of the chiral Landau level. Implications for the chiral magnetic effect in Weyl semimetals from the optical f-sum rule are discussed.

*Work at UCLA was supported by the U.S. Department of Energy (DOE) under Award Number de-sc0011978. A.B. Sushkov and H.D.Drew were supported by DOE desc0005436 grant, A.L. Levy, G.S. Jenkins and H.D.Drew were supported by NSF DMR-1610554. F. Liu was supported by China Scholarship Council No. 201508340005.

Wednesday, March 6, 2019 2:30 PM - 5:06 PM

Session P05 DCMP: Nanostructures, Heterostructures and other Artificially Structured Materials BCEC 108 - Parveen Kumar, University of California, Merced - Tag(s): Focus

2:30PM P05.00001: The Electronic Transport Properties of Silicon Meta-lattice Made by High Pressure CVD
ZHAOHUI HUANG (Presenter), VINCENT H. CRESPI, Pennsylvania State University — A nanoscale 3D superlattice, called meta-lattice, can be synthesized by infiltrating a template of close-packed nanometer-scale silica spheres with Si by high pressure chemical vapor deposition. Their structures can be controlled by using different size spheres; accordingly, their electronic transport properties are geometry-dependent, and both localized and extended electronic states in three dimensions may exist, hence both band conduction and variable range hoping (VRH) may occur simultaneously. Metalattices offer a platform to continuously change properties of electronic transport by changing their geometries. We employ a tight-binding method to quantitatively look into the impact of geometry. The resultant electronic band structure is also used in the case of VRH conductance.

2:42PM P05.00002: Observation of Exposed and Hidden Au Quantum Well States in Au/Ag Heterostructures
QIANGSHENG LU (Presenter), GUANG BIAN, University of Missouri — In this work, atomically uniform Au films are grown on a Ag(111) thin film. The Au quantum well states (QWS) are clearly observed by using Angle-resolved photoemission spectroscopy (ARPES). The Au QWSs hybridize with the Ag states and thus, show an energy dependence on the thickness of the supporting Ag film. Furthermore, a sandwich structure of Ag/Au/Ag is fabricated with various thicknesses of each constituent layer. The Au QWSs, though buried under the Ag overlayer, are still observable through hybridization with the Ag states. Interestingly, the hybrid quantum well states with Au d orbitals states possess a large effective mass as a result of hybridization with partially localized d states. Detailed first-principles simulations are performed to illustrate the orbital components of hybrid QWSs and provide an insight into the band dispersion of hybrid states.

* This work is supported by the US National Science Foundation (Grant No. NSF-DMR-0054904).

2:54PM P05.00003: On the formation of suspended double-stranded atomic chains
CARLOS SABATER (Presenter), Departamento de Física Aplicada, Universidad de Alicante, Campus de San Vicente del Raspeig, E-03690 Alicante, Spain, University of Alicante, JUAN JOSE PALACIOS, Departamento de Física de la Materia Condensada, Cantoblanco, 28049 Madrid, Spain, Universidad Autónoma de Madrid., MARÍA JOSÉ CATURLA, CARLOS UNTIEDT, Departamento de Física Aplicada, Universidad de Alicante, Campus de San Vicente del Raspeig, E-03690 Alicante, Spain, University of Alicante — The smallest structures with higher stability connecting two metallic electrodes can be identified by the evolution of the conductance in the process of the controlled breakage of the contact between two metals. Here we report on the identification of double-stranded atomic chains formed on Au using a Scanning Tunneling Microscope. Molecular dynamics simulations and density functional theory electron transport calculations help to unveil the richness of geometric structures possible with double-stranded chains, their stability and how these can evolve to form monoatomic chains.
Universal Conductance Fluctuation in Sierpinski Carpet

Yulei Han (Presenter), University of Science and Technology of China, Fumng Xu, Shenzhen University, Zhenhua Qiao, University of Science and Technology of China

We report a theoretical investigation on conductance fluctuation of disordered two-terminal device in Sierpinski carpet. We find that the conductance fluctuation does not display a universal feature in circular orthogonal ensemble. But in the presence of magnetic field or spin-orbit coupling, a universal conductance fluctuation (UCF) appears. More specify, in the presence of magnetic field, the UCF value is about 0.74 ± 0.01 (e²/h), while when applied spin-orbit coupling the UCF value exists also around 0.74 ± 0.01 (e²/h). By further investigating the conductance distribution in the critical disorder strength, we find that both of the symmetries share the same distribution function. Our work provide a better understanding of the transport properties of regular fractal structure and shed light on more transport studies of fractals.

3:18PM P05.00005: Experimental demonstration of nanoelectronics below 1 mK electron temperature

Nikolai Yurttagül (Presenter), Matthew Sarsby, Attila Geresdi, Delft University of Technology

Extending the experimental temperature domain of nanoelectronic devices into the microkelvin regime would make novel quantum states of matter accessible with great potential for quantum technologies. Cooling bulk metals to microkelvin temperatures by adiabatic demagnetization of nuclear spins has been an established technique for decades, however reaching electron temperatures below 1 mK in nanofabricated devices remained an unsolved challenge up until now. This is due to the thermal decoupling of electrons in micro- and nanostructures from the cold substrate in combination with high frequency electronic noise directly heating the electron system. We demonstrate the first successful nuclear magnetic cooling of electrons in a nanofabricated device to microkelvin temperatures, achieved by integrating indium as nuclear refrigerant onto the metallic islands of a Coulomb blockade thermometer with the device leads attached to bulk indium nuclear cooling stages. By performing the nuclear demagnetization process, we demonstrate electron temperatures below 500 μK by primary electron thermometry, and show that the device stays below 1 mK for several days.

Trapped Ion Heating from Correlated Motion of Electrode Adsorbates

Vincenzo Lordi (Presenter), Keith Ray, Changueun Kim, Lawrence Livermore Nat Lab, Benjamin Foulon, Brenda Rubenstein, Brown University

Trapped ion qubits are plagued by a phenomenon called “anomalous heating,” where motional modes of the ion are excited by the environment causing decoherence of the encoded quantum information. Evidence suggests the origin of this heating is associated with the surface of the trapping electrodes. In this work, we combine first-principles electronic structure calculations, molecular dynamics simulations, and master equations to explore the role of high densities of adsorbed molecules on the electrode surface as a potential source of trapped ion heating. Weakly adsorbed molecules interact with the metallic surface and acquire an induced dipole, which can couple to the ion, causing electric field noise. When a large density of adsorbates are present, on the order of a monolayer, their collective vibrational motion can create non-trivial frequency-dependent electric field noise and thus ion heating. We analyze the coverage dependence of this effect for different possible electrode adsorbates.

2D Fermi-Hubbard Quantum Simulation with and Oxide Nanoelectronic Platform

Shan Hao (Presenter), Jianan Li, Yuhe Tang, Aditi Nethwewala, Yang Hu, Department of Physics & Astronomy, University of Pittsburgh, Hyungwoo Lee, Jungwoo Lee, Chang-beom Eom, Department of Materials Science and Engineering, University of Wisconsin—Madison, Patrick Irvin, Jeremy Levy, Department of Physics & Astronomy, University of Pittsburgh

The interface of LaAlO₃/SrTiO₃ supports a 2D electron gas [1] that can be further reconfigured into nanostructures, using conductive AFM lithography [2]. The density of nanostructures (~2 nm) is comparable to the mean electron separation, giving rise to the idea that this platform could be used for quantum simulation of 2D Fermi-Hubbard problems. Here we describe efforts to create various 2D lattice structures, and investigate their properties at low temperatures and high magnetic fields.


*Prepared by LLNL under Contract DE-AC52-07NA27344.
4:06PM P05.00009: Doping dependence of phonon anomalies in (Bi,Pb)2(Sr,La)2CuO6 revealed by inelastic X-ray scattering* 

YINGYING PENG (Presenter), ALI HUSAIN, SANGJUN LEE, University of Illinois at Urbana-Champaign, AHMET ALATAS, Argonne National Laboratory, KITTIHAT KRONGCHON, XIAOLAN SUN, University of Illinois at Urbana-Champaign, AYMAN SAID, Argonne National Laboratory, YING DING, XINGJIANG ZHOU, Institute of Physics, Chinese Academy of Sciences, LUCAS WAGNER, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — While charge modulations are ubiquitous in high-temperature superconducting cuprates, understanding their coupling to phonons can provide crucial insight into the role of electron-phonon interactions in high-temperature superconductivity. Here, we have used high-resolution inelastic X-ray scattering to study the doping dependence of the low-energy phonons in the monolayer cuprate (Bi,Pb)2(Sr,La)2CuO6+d, from heavily underdoped (p=0.03) to overdoped (p=0.21) samples. We observe that the longitudinal acoustic phonon along the Cu-O bond direction exhibits a line-shape broadening near the wave vector ~ 0.25 rlu in underdoped samples even when charge order is suppressed, while no broadening occurs in the overdoped samples. Surprisingly, an additional low energy mode around 4 meV is observed in the underdoped samples and is absent in overdoped materials. The origin of the longitudinal phonon broadening and the new low energy mode will be discussed especially in relation to charge order.

*This work was supported by DOE grant DE-FG02-06ER46285.

4:18PM P05.00010: High Tc Superconductor-Half metallic ferromagnet planar devices* 

SOPHIE D’AMBROSIO (Presenter), SALVATORE MESORACA, XAVIER PALERMO, ADRIAN BALAN, Unité Mixte de Physique, CNRS/Thales, Université Paris Sud, Université Paris-Saclay, Palaiseau, France, DAVID SÁNCHEZ-MANZANO, FABIAN CUELLAR, GFMC, Dpto. Física de Materiales, Universidad Complutense de Madrid, Spain, CHRISTIAN ULYSSE, Centre de Nanosciences et de Nanotechnologies, CNRS, Université Paris-Saclay, Palaiseau, France, LAURENT VILA, SPINTEC, CEA-INAC/CNRS/Univ. Grenoble Alpes, Grenoble, France, NICOLAS BERGEAL, JÉRÔME LESUEUR, Laboratoire de Physique et d’Etude des Matériaux, ESPCI Paris, PSL Research University, CNRS, Paris, France, ANKE SANDER, Unité Mixte de Physique, CNRS/Thales, Université Paris Sud, Université Paris-Saclay, Palaiseau, France, JACOBO SANTAMARIA, GFMC, Dpto. Física de Materiales, Universidad Complutense de Madrid, Spain, JAVIER VILLEGAS, Unité Mixte de Physique, CNRS/Thales, Université Paris Sud, Université Paris-Saclay, Palaiseau, France — Superconducting spintronics is an emergent field where the interfacial interactions between superconductors (S) and ferromagnets (F) are crucial. These interactions can give rise to equal-spin triplet Cooper pairs, thereby opening the door to coherent, dissipationless spin transport. In this scenario, the case of high-temperature d-wave superconductors (e.g. YBa2Cu3O7) combined with half-metal ferromagnets (e.g. La0.7Sr0.3MnO3) is especially interesting. One of the challenges specific to those materials is the fabrication of nanoscale planar devices in which multiple S/F interfaces can be concatenated and electrically sensed individually. The difficulty comes from the fact that complex-oxides are often incompatible with many of the bottom-up nanofabrication approaches that are standard with metals. We will describe here various top-bottom approaches we have developed ad hoc to fabricate oxide planar S/F nanodevices, which are a combination of Pulsed Laser Deposition, Electron Beam Lithography and Ion Beam Etching. We will also present temperature-dependent magnetotransport measurements performed to characterize their superconducting and magnetic properties.

*Work supported by the ERC grant N 647100 “SUSPINTRONICS” and French ANR grant ANR-15-CE24-0008-01 “SUPERTRONICS”
4:30PM P05.00011: The Formation of Wannier Mott-Frenkel Hybrid Excitonic Polariton In Different Heterostructures  DAVID FACEMYER (Presenter), QUE HUONG NGUYEN, Marshall University — It has been suggested theoretically and realized experimentally that combining organic material and inorganic semiconductors in one heterostructure would result in resonant interactions between the Frenkel excitons in the organic material and the Wannier-Mott excitons in the semiconductors, leading to the formation of an exciton hybridization state. The new materials, possessing the complimentary characteristics of both exciton types, such as large exciton radius, enormous oscillator strength and room-temperature operation properties, would enhance optical nonlinearities and promise to have useful applications in both the field of Bose-Einstein condensation of polaritons and polariton lasers. In this work, we consider a strong coupling of the hybrid excitons and photons near excitonic resonance analytically with the purpose of determining the electronic structure, energy, and dispersion relation of the hybrid exciton-polariton. We study different confinement parameters for various nano-scale heterostructures, and in doing so, we discuss the conditions necessary for their formation. Our ab initio approach moves us a step closer to realizing new, novel optoelectrical materials that exhibit the strengths of each constituent.

4:42PM P05.00012: X-ray Optics Fabrication Using Unorthodox Approaches  Umut Tunca Sanli, Margarita Baluktsian, Modern Magnetic Systems, MPI for Intelligent Systems, Hakkan Ceylan, Metin Sitti, Physical Intelligence, MPI for Intelligent Systems, Markus Weigand, Gisela Schuetz, Kahraman Keskinbora (Presenter), Modern Magnetic Systems, MPI for Intelligent Systems — X-ray microscopes are unique tools for studying buried features of biological and magnetic systems with high spatiotemporal resolution. The limitations of the standard e-beam lithography method for fabricating these delicate nano-photonic devices can be overcome by using unconventional lithography methods such as direct-write and gray-scale ion beam lithography, ion beam implantation lithography, a combination of atomic layer deposition and focused ion beam micromachining and last but not least by using two-photon photopolymerization (2PP). For instance, bottom-up growth of atomic layer deposition allows atomic scale control over the zone width while top-down micromachining using focused ion beams allow freely selectable aspect ratios and tilt angles. In another approach, we took advantage of 2PP and fabricated high aspect ratio diffractive/refractive kinoforms out of low-loss polymeric materials for the first time. We will discuss the benefits of these methods over the conventional fabrication routes based on theoretical coupled wave theory calculations, direct imaging experiments as well as ptychographic coherent diffractive imaging.

4:54PM P05.00013: Observation of Bulk Polarization Transitions and Second-Order Acoustic Corner States Protected by Generalized Chiral Symmetry  Xiang NI (Presenter), Matthew Weiner, The City College of New York, Andrea Alu, Graduate Center of the City University of New York, Alexander Khanikaev, The City College of New York — A new class of topological lattice characterized by bulk polarization has been introduced recently, such system has been shown to host Wannier-type higher order states. Here, we introduce and measure topological bulk polarization in 3D printed two-dimensional acoustic meta-structures, and observe topological transitions as the design parameters are tuned. We also demonstrate that our topological meta-structure hosts both 1D edge and Wannier-type second-order corner states with unique acoustic properties. The edge states have the angular momentum that reverses for opposite propagation direction, thus supporting directional excitation. We observe the second order topological states protected by the generalized chiral symmetry of the meta-structure, which are localized at the corners and are pinned to ‘zero energy’. Interestingly, unlike the corner states protected by the conventional chiral symmetry, the generalized chiral symmetry of our three-atom sublattice enables their spectral overlap with the continuum of bulk states without leakage. The confinement and inherent robustness of the corner states is theoretically analyzed and experimentally confirmed by deliberately introducing disorder. Our findings open new directions for advanced sound propagation and manipulation.

Wednesday, March 6, 2019 2:30 PM - 5:06 PM

Session P06 DCMP: Strongly Correlated Ce- and Yb-based Materials  BCEC 109A - Sheng Ran - Tag(s): Focus
Magnetic Ordering Competition Leading to Disorder Between CeIn₃ and NdIn₃

JACKSON BADGER (Presenter), Department of Chemistry, University of California, Davis, RUMIKA MIYAWAKI, Department of Physics, Tokyo Metropolitan University, PETER KLAVINS, ZACHARY BRUBAKER, RENA ZIEVE, Department of Physics, University of California, Davis, TATSUMA D. MATSUDA, Department of Physics, Tokyo Metropolitan University, VALENTIN TAUFOUR, Department of Physics, University of California, Davis — Both CeIn₃ and NdIn₃ crystallize in the same cubic structure (Pm-3m) and show antiferromagnetic ordering below 10.1 K and 5.9 K, respectively. We investigate the magnetic ordering of single crystals of Ce₁₋ₓNdₓIn₃ and discover a region of frustrated magnetism near x ~ 0.45 where the magnetic order is suppressed to below 1.8 K. In this region, the two antiferromagnetic orderings appear to be in competition with one another despite the fact that antiferromagnetic interactions are still observed. We present the sample synthesis and characterizations, as well as a discussion of the observed magnetic properties in the context of heavy-fermion behavior, Kondo interactions, and magnetic anisotropy.

Electronic structure study of the heavy-fermion superconductor CeIrIn₅ by ARPES

QIUYUN CHEN (Presenter), China Academy of Engineering Physics, KEVIN HUANG, LEI SHU, Fudan University, STEFAN KIRCHNER, Zhejiang University, DONGLAI FENG, Fudan University — Crystal electric field states in rare earth intermetallics show an intricate entanglement with the many-body physics that occurs in these systems and that is known to lead to a plethora of electronic phases. Here we attempt to trace different contributions to the crystal electric field (CEF) splittings in CeIrIn₅, a heavy-fermion compound and member of the CeMIn₅ (M = Co, Rh, Ir) family. To this end, we utilize high-resolution resonant angle-resolved photoemission spectroscopy (ARPES) and present a spectroscopic study of the electronic structure of this unconventional superconductor over a wide temperature range. As a result, we show how ARPES can be used in combination with thermodynamic measurements or neutron scattering to disentangle different contributions to the CEF splitting in rare earth intermetallics. We also find that the hybridization is stronger in CeIrIn₅ than CeCoIn₅ and the effects of the hybridization on the Fermi volume increase is much smaller than predicted.

Weak hybridization effects revealed by ARPES in heavy-fermion Ce₂IrIn₈

HAJJANG LIU (Presenter), HONG DING, YUANJI XU, Institute of physics, Chinese academy of sciences — We utilize high resolution on-resonant (hv~120eV) angle-resolved photoemission spectroscopy (ARPES) to study the band structure and hybridization effect of heavy-fermion compound Ce₂IrIn₈. Hybridization between 4f electron and conduction electron plays a significant role on the behavior of heavy-fermion compounds. Band structure experiments fit well with the results of DFT calculation. We observe obvious flat band below coherent temperature Tcoh~40 K which characterize electrical resistance maxima indicate the onset temperature of hybridization. But the Fermi surface (FS) volume and Fermi vector k_F don't change largely, which challenge the widely believed evolution from high temperature small FS to low temperature big FS.

Critical charge fluctuations and ω/T scaling at the Kondo breakdown of Heavy-fermion systems

YASHAR KOMIJANI (Presenter), PIERS COLEMAN, Rutgers University, New Brunswick — A number of recent experiments on quantum critical materials CeRuIn₄, YbRh₂Si₂, CeCu₂Si₂, and YbAlB₄ have observed critical charge fluctuations coinciding with magnetic transition, a phenomena that goes beyond the Landau-Ginzburg paradigm. We will argue that such soft charge fluctuations are natural consequences of an abrupt change in the Fermi surface volume that accompanies Kondo breakdown (KBD) in heavy-fermion systems.

Using a model 1D Kondo lattice in which each moment is connected to a separate conduction bath, we show that a KBD transition develops between a heavy Fermi liquid and a gapped spin liquid via a QCP with \omega/T scaling, which features residual entropy and a critical charge mode directly associated with the break-up of Kondo singlets.

Furthermore, We contrast the cases of ferromagnetic (FM) and antiferromagnetic (AFM) couplings. While with a purely Ising magnetic coupling, both models map to the dissipative transverse-field Ising model, the Heisenberg limit is quite different: The charge mode is incoherently broadened in the FM system, while it remains sharp, protected by the spin liquid gap, in frustrated AFM system. We discuss the implications of these effects on the experiments.

The suppression of ferromagnetism in metallic systems may result in the appearance of modulated magnetic phases. Recent studies have shown that the application of pressure in the CeTiGe$_3$ system is a possible example of such phenomenon. By combining magnetic field and pressure, a wing-structure phase diagram with a quantum tricritical point is observed. Here we show that substituting vanadium in place of titanium will suppress ferromagnetism, and an antiferromagnetic state is observed near the V-rich end. We discuss the evolution of the ordering temperature and of the magnetic anisotropy as Ti is progressively substituted by V in single crystals of the CeTi$_{1-x}$V$_x$Ge$_3$ series.


3:30PM P06.00006: Evolution of Charge Density Wave Order in CeTe$_2$  
BISHNU SHARMA (Presenter), MANOJ SINGH, BURHAN AHMED, BONING YU, Clark University, PHILIP WALMSLEY, IAN R FISHER, Stanford University, MICHAEL C BOYER, Clark University — The rare-earth tellurides are a family of low-dimensional compounds which host charge density wave (CDW) states. While CDW states in the rare-earth tri-tellurides (RTe$_3$) are relatively well-studied, less is known about CDW states in the rare-earth di-tellurides (RTe$_2$). The RTe$_2$ compounds are quasi two dimensional materials with a crystal structure which consists of alternating insulating rare-earth block layers and single-layer conducting Te sheets. Here we present our scanning tunneling microscopy measurements on CeTe$_2$. Our measurements detect two unidirectional, perpendicular, spatially separated CDW states which smoothly evolve from one to the other. Our measurements shed light on the connection between CDW states and local strain.

3:42PM P06.00007: Thermal expansion measurements of heavy-fermion CeAuSb$_2$*  
SOONBOM SEO (Presenter), SEAN THOMAS, FILIP RONNING, ERIC BAUER, JOE D THOMPSON, PRISCILA ROSA, Los Alamos National Laboratory — CeAuSb$_2$ is a heavy-fermion antiferromagnet hosting two field-induced transitions at $H_{c1} \sim 2.8$ T and $H_{c2} \sim 5.6$ T when field is applied along the c-axis. At $H_{c1}$, the magnetic structure changes from a single-\textit{q} to a multi-\textit{q} spin density wave [3]. Here we report the temperature dependence of the resistivity ($\rho$) and thermal expansion ($\Delta L/L$) of CeAuSb$_2$ when $H \parallel c$-axis. Our results show that $\rho$ and $\Delta L/L$ display signatures of the different magnetic structures, and are susceptible to the critical end point. We will discuss both pressure and field effects on the multiple phase transitions in the three-dimensional phase diagram of CeAuSb$_2$.


*Work at Los Alamos was performed under the auspices of the US DOE, Division of Materials Sciences and Engineering. S. S. acknowledges support of the LANL LDRD program through a Director’s Postdoctoral Fellowship.

3:54PM P06.00008: Competing incommensurate orders in a heavy fermion antiferromagnet CeNiGe$_2$  
LEKH POUDDEL (Presenter), YANG ZHAO, ZHIJUN XU, WILLIAM RATCLIFF, NIST Center for neutron research, National Institute of Standard and Technology, Gaithersburg, MD, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advance Materials, University of Maryland, College Park, MD, JEFFREY W LYNN, NIST Center for neutron research, National Institute of Standard and Technology, Gaithersburg, MD — We have determined the magnetic structure and phase diagram of a heavy fermion compound CeNiGe$_2$ as a function of magnetic field and temperature using single crystal neutron diffraction. At zero field and the base temperature of 0.4 K, CeNiGe$_2$ shows a complex magnetic structure comprising two propagation vectors $k_1 = (0.23, 0, 0)$ and $k_2 = (0.18, 0, 0)$. The intensities observed at several magnetic satellites indicate that the moments are predominantly along the c-axis. At higher temperatures the order parameter corresponding to $k_1$ (OP1) decreases until it is suppressed at $T_{N1} = 3$ K. The order parameter for $k_2$ (OP2) initially increases with increasing temperature and only begins to decrease above $T_{N1}$ until it vanishes at $T_{N2} = 4.2$ K. A similar but opposite trend in order parameters is observed when a magnetic field is applied along the c-axis. OP2 is suppressed at a lower critical field of $B_{c2} = 0.75$ T, whereas OP1 first increases until it reaches maximum at $B_{c2}$ and begins to decrease and vanishes at the critical field of $B_{c1} = 2.75$ T. Taken together, CeNiGe$_2$ provides an interesting platform where competition between two nearby incommensurate orders can be systematically tuned by temperature and magnetic field.
**4:06 PM P06.00009: Thermodynamic and transport properties of R Cd₃P₃ (R = La and Ce) single crystals**  
ANJA RABUS, JEONGHUN LEE, EUDEOK MUN (Presenter), Department of Physics, Simon Fraser University — R Cd₃P₃ (R = La and Ce) compounds crystallize into a hexagonal ScAl₃C₃-type structure. The magnetic Ce atoms form the triangular lattice of the two dimensional layer. Thermodynamic and transport properties of R Cd₃P₃ were investigated by measuring the magnetization, electrical resistivity, and specific heat. The magnetic susceptibility of CeCd₃P₃ follows the Curie-Weiss law at high temperatures with very large negative Weiss temperature. The specific heat measurement of CeCd₃P₃ clearly indicates a magnetic ordering below 0.41 K with large electronic specific heat coefficient. In this talk, anomalous physical properties due to the geometrical frustration of Ce atoms will be discussed.

*This work was supported by the Canada Research Chairs program, the Natural Science and Engineering Research Council of Canada, and the Canadian Foundation for Innovation.

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**4:18 PM P06.00010: Field-induced Pseudogap in the Heavy-fermion Superconductor CeCoIn₅**  
KESHAV SHRESTHA (Presenter), LAURA H GREENE, Florida State University, ERIC BAUER, JOE D THOMPSON, Los Alamos National Laboratory, YOU LAI, RYAN BAUMBACH, Florida State University, KALYAN SASMAL, M BRIAN MAPLE, Department of Physics, University of California, San Diego, WAN KYU PARK, Florida State University — The heavy-fermion superconductor CeCoIn₅, whose order parameter is known to have dx²-y² symmetry [1], manifests an interesting spin density wave-like Q-phase [2]. Despite several recent scanning tunneling spectroscopic measurements [3], there are no phase-sensitive measurements in the Q-phase. Our planer tunneling spectroscopy data at 20 mK show sharp coherence peaks and the estimated gap size is 0.65 meV. Quite intriguingly, the superconducting gap-like features evolve into a pseudogap as superconductivity is destroyed with temperature and magnetic fields. The field-induced pseudogap is enhanced further with increasing fields up to the highest measurements field of 18 T. The possible origin of the pseudogap and implications of our results will be discussed.


*This work was supported by NSF/DMR-1704712 (FSU), NSF/DMR-1157490 (FSU) NSF/DMR-1644779 and the State of Florida (NHMFL), DOE, Office of BES, and Division of MSE (LANL), and NSF/DMR-1810310 (UC-San Diego).

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**4:30 PM P06.00011: Thermal expansion near the bicritical point in YbAgGe**  
GEORGE SCHMIEDESHOFF (Presenter), Physics, Occidental College, J.-H. PARK, D. GRAF, National High Magnetic Field Laboratory, S.L. BUD’KO, P.C. CANFIELD, Physics and Astronomy, Ames Laboratory and Iowa State University — A flexible-plate capacitive dilatometer, designed to operate while immersed in the liquid helium "mash" of a top-loading dilution refrigerator, was used to measure the thermal expansion of the heavy-fermion antiferromagnet YbAgGe near the bicritical point reported near 0.3 K in a magnetic field of 4.5 T applied parallel to the ab-axis [1]. We will discuss the phase diagram and quantum bicriticality of YbAgGe and the new dilatometer.


*Work at Occidental College was supported by the National Science Foundation under DMR-1408598. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation Cooperative Agreement No. DMR-1157490 and the State of Florida. Work at Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.
4:42PM P06.00012: Pressure-temperature phase diagram of YbNi2B2C* LI XIANG (Presenter), YUJI FURUKAWA, Department of Physics, Iowa State University, Ames Laboratory, Ames, Iowa 50011, USA, VIKTOR V. STRUZHKIN, Carnegie Institution of Washington, Geophysical Laboratory, Washington, DC 20015, USA, ALEXANDER GAVRILIUK, FSRC Crystallography and Photonics of Russian Academy of Sciences, Moscow 119333, Russia, SERGEY BUDKO, PAUL CANFIELD, Department of Physics, Iowa State University, Ames Laboratory, Ames, Iowa 50011, USA — The RNi2B2C (R = Gd - Lu, Y) series have attracted much attention due to the interplay between superconductivity and local-magnetism. For the Lu, Tm - Dy, superconducting transition temperature $T_c$ decrease and the AFM transition temperature $T_N$ increases and scales with de Gennes scaling at ambient pressure. However, YbNi2B2C displays neither superconductivity nor magnetism down to low temperature at ambient pressure but rather is a heavy fermion compound with $\gamma \sim 530$ mJ/mol K$^2$. Studies suggest YbNi2B2C might be close to a quantum critical point (QCP) on the nonmagnetic side in the Doniach phase diagram. Resistance of single-crystalline YbNi2B2C is measured under pressure up to 16 GPa down to 50 mK as an attempt to reach QCP. Temperature-pressure phase diagram will be presented and discussed.

*This work is supported by DOE/BES, Materials Science and Engineering Division under contract No. DE-AC02-07CH11358. L. X. was supported, in part, by the W. M. Keck Foundation V.S. acknowledges support by DOE/BES under contract No. DE-FG02-99ER45775. A. G. acknowledges support of RSF 16-12-10464 grant.

4:54PM P06.00013: THz Spectroscopy of the Heavy Fermion Metal YbAl3 DAVID BARBALAS (Presenter), Johns Hopkins University, SHOUVIK CHATTERJEE, UCSB, KYLE M SHEN, DARRELL G. SCHLOM, Cornell University, NORMAN ARMITAGE, Johns Hopkins University — Due to the interaction of local moment physics and mixed-valence behavior in Yb compounds, Yb heavy fermion compounds have not demonstrated the same range of phenomena seen in other f-orbital materials. Up to this point it has been difficult to measure the low energy electrodynamic response of these materials. However, high quality films of YbAl3 have been successfully grown and demonstrate significant changes in the electronic structure of the material mediated by the valence change in Yb. We have investigated the THz range electrodynamic response of these materials and discuss the results from the optical conductivity in the context of prevailing theories.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P07 DCMP: Topological Electronic States in Kondo insulators and other f-electron materials

2:30PM P07.00001: Neutral Fermi surfaces in Mixed Valent Kondo Insulators: Majorana Hubbard Operators* PIERS COLEMAN (Presenter), Rutgers University, New Brunswick — The development of slave particle approaches provides a way to explore different patterns of operator fractionalization in strongly correlated systems. The recent observation of quantum oscillations in mixed valent SmB$_2$ has raised the possibility of neutral Fermi surfaces in this material[1-4]. This motivates a search for a representation of the Hubbard operator in terms of Majorana, rather than Dirac fermions. In this talk I will describe how this can be achieved and using the method, discuss the prospects for a two-phase description of SmB$_6$, in terms of a competition between a fully gapped strong topological insulator and a strange dielectric.


*Work supported by Department of Energy Basic Energy Sciences grant DE-FG02-99ER45790.
The role of $f-p$ hybridization in the bulk $f$-electronic structure of SmB$_6$

Jonathan Denlinger (Presenter), Lawrence Berkeley National Laboratory, Dae-Jeong Kim, Seoul National University, Zachary Fisk, UC Irvine — The topological origin of in-gap surface states of mixed-valent SmB$_6$, a candidate topological Kondo insulator, is currently being debated. In addition, there exist distinct discrepancies in the bulk electronic structure between DFT-based theory, ARPES, recent NIXS determination of the unoccupied $f$-hole symmetry [1], and the existence of low temperature dHvA oscillations [2,3]. Here we explore the role of $f-p$ hybridization in assisting $f-d$ hybridization in the formation of an insulating gap in its $f$-electronic structure. In a five-band model, the relative phase of $f-d$ and $f-p$ hybridizations allows tuning of the $f$-band structure between DFT-like and ARPES-like solutions, and hybridization amplitude tuning allows selection of the unoccupied X-point $f$-hole character. Also theoretically enabled is prediction of a distinct ARPES-measured 3D bulk $f$-hole-like dispersion at the "H"-point between adjacent X-point $d$-electron pockets. The $H$-point $f$-dispersion then naturally leads to exploration of the Landau level sharp DOS-discontinuity model [4] to quantitatively explain the size and shape of the dominant dHvA orbits.


Effect of reduced sample dimensions on the insulating state of SmB$_6$ *

Joonbum Park (Presenter), Mun Chan, Priscila Rosa, Neil Harrison, Los Alamos National Laboratory — The putative topological Kondo insulator SmB$_6$ has shown compelling evidence of robust conductive surface states, however less attention has been paid to the insulating bulk states which lies beneath. Here, we present the electrical transport measurements of the insulating state of SmB$_6$ down to $T \sim 250$ mK. We observed that the temperature dependence of resistivity shows additional power law-like dependence with temperature. These features develop below $T < 1.5$ K with reduction of sample dimensions, typically below 150 μm. We discuss whether the origin of these features are from dominant surface conduction over bulk conduction or due to impurities.

*Authors acknowledge UU DOE BES Support for "Science of 100 Tesla"

Search for charge neutral majorana fermions in SmB$_6$ under uniaxial strain

Brian Casas (Presenter), Laisi Chen, Zachary Fisk, Jing Xia, University of California, Irvine — The existence of a charge neutral fermi surface as evidenced from measurements of a large three dimensional fermi surface has motivated renewed interest in the bulk of samarium hexaboride. Thermal transport measurements have been performed using both flux and floating zone crystals, each resulting in different conclusions regarding a fermionic contribution suggestive of these charge neutral majorana fermions. Uniaxial strain has been shown to tune the mixed valence physics in the bulk and as such may be critical in understanding the underlying behavior of SmB$_6$. Here we report our progress on thermal transport on SmB$_6$ under uniaxial strain.

Ionic liquid gating on Al-flux grown SmB$_6$ using Hall bar geometry*

Alexa Rakoski (Presenter), Dmitri Mihaliov, Cagliyan Kurda, Department of Physics, University of Michigan, Priscila Rosa, Los Alamos National Laboratory, Zachary Fisk, Department of Physics and Astronomy, University of California Irvine — Samarium hexaboride (SmB$_6$) is a correlated material in which strong f-d interactions lead to the opening of a small hybridization gap below 100 K at the Fermi energy. Below 4 K, the plateau in resistivity which was a long standing mystery in SmB$_6$ has been proposed to arise from a crossover to surface conduction due to topological effects. We investigate how this plateau, as well as the corresponding plateau in the Hall coefficient, can be tuned by gating with the ionic liquid DEME-TFSI. Results are obtained on an Al-flux grown sample in Hall bar geometry prepared by finely polishing on all sides. The sample is suspended in the ionic liquid to ensure that all surfaces contributing to transport are gated. We find that resistivity can be changed by over 15% in the range of accessible voltages in the liquid, and that the Hall coefficient demonstrates a much larger effect of up to 33% change over the same range. We also present a model based on measured parameters of the 2D Fermi surface in SmB$_6$ to explore these changes.

*Funding for this work was provided by NSF Grant No. DGE-1256260.
3:30PM P07.00006: Itinerate states in rare-earth hexaborides observed via resonant inelastic x-ray scattering
DONAL SHEETS (Presenter), University of Connecticut, JIAN-XIN ZHU, Los Alamos National Laboratory, MAXIM DZERO, Kent State, DIEGO M CASA, JUNGHOO KIM, Argonne National Lab, PRISCILA ROSA, Los Alamos National Laboratory, ZACHARY FISK, University of California - Irvine, IGNACE JARRIGE, Brookhaven National Lab, JASON HANCOCK, University of Connecticut — We present X-ray resonant inelastic x-ray scattering (RIXS) data collected at the L edges of divalent hexaborides YbB₆ and EuB₆. At an incident energy corresponding to the divalent resonance, we observe strong RIXS signal which appears to be well-described by the unoccupied 5d density of states calculated from density functional theory. In addition, we observe a second set of RIXS excitations at higher incident energy which does not correspond to any observable feature in absorption. This anomalous scattering persists to low incident energy and therefore induces excited states which are relevant to material behavior. The two classes of excitation show distinct polarizationdependence and we propose a process which describes the origin of this RIXS intensity. Our results suggest far-reaching utility of L-edge RIXS in characterizing itinerate states of f-filling materials at a microscopic level.

3:42PM P07.00007: Charge neutral fermions and quantum oscillations in a topological Kondo insulator YbB₁₂
YUKI SATO (Presenter), Physics, Kyoto University, ZHI XU, Physics, University of Michigan, YUICHI KASAHARA, TOMOYA TANIGUCHI, SHIGERU KASAHARA, Physics, Kyoto University, LU CHEN, TOMOYA ASABA, COLIN TINSMAN, Physics, University of Michigan, HINAKO MURAYAMA, Physics, Kyoto University, OHEI TANAKA, YUTA MIZUKAMI, TAKASADA SHIBAUCHI, Advanced Materials Science, University of Tokyo, FUMITOSHI IGA, Science, Ibaraki University, JOHN SINGLETON, Los Alamos National Laboratory, LU LI, Physics, University of Michigan, YUJI MATSUDA, Physics, Kyoto University — Recent observations of quantum oscillations (QOs) in transport and thermodynamic parameters at high magnetic fields in a Kondo insulator YbB₁₂ have been a big surprise since it seems to host a Fermi surface, which is a defining character of a metal. In this talk, I will present low-temperature heat-transport measurements to discuss low energy excitations in the ground state of YbB₁₂. At zero field, despite the conductivity in the zero-temperature limit, κ₀xx/℃ is clearly resolved, leading to a spectacular violation of the Wiedemann-Franz law: the Lorenz ratio L = κ₀xx/ρxx/℃ T is 10⁴-10⁵ times larger than that expected in conventional metals. These data indicate that YbB₁₂ is a charge insulator but a thermal metal, suggesting the presence of itinerant neutral fermions. Remarkably, more insulating crystals with larger activation energies exhibit larger amplitudes of the resistive QOs as well as a larger κ₀xx/℃, in stark contrast to conventional metals. Moreover, we find that these fermions couple to magnetic field, despite their charge neutrality. Our findings expose novel gapless and highly itinerant, charge-neutral quasi-particles in this unconventional quantum state.

3:54PM P07.00008: Enhanced quantum oscillations in Kondo Insulators*
YEN-WEN LU (Presenter), Deparmeny of Physics, National Tsing Hua University, Hsinchu, Taiwan, CHUNG-HOU CHUNG, Electrophysics Department, National Chiao-Tung University, Hsinchu, Taiwan, CHUNG-YU MOU, Deparmeny of Physics, National Tsing Hua University, Hsinchu, Taiwan — We investigate quantum oscillations resulting from the Kondo screening due to Landau levels in Kondo insulators. It is shown that even for large Kondo insulating gap, appreciable amplitudes of oscillations for Kondo insulators in moderate magnetic fields are present in magnetization even at zero temperature. Specifically, based on the Anderson Lattice Hamiltonian, we analyze the magnetization of Kondo insulators by resorting to the slave-boson method. By including Landau levels, mean-field solutions are determined self-consistently. We find that mean-field parameters oscillate in response to the change of the magnetic field. As an outcome, instead of being rigid electronic structure, the energy band of Kondo insulators is non-rigid and oscillate with respect to the change of the magnetic field. Our results indicate that the nonrigidity of the electronic structure in Kondo insulators results in enhanced and observable quantum oscillations in magnetization.

*We acknowledge support from the Ministry of Science and Technology (MoST),Taiwan. We also acknowledge support from Ministry of Education (Taiwan) through Center for Quantum Technology.

4:06PM P07.00009: Anomalous symmetry-breaking response in proposed type-II Weyl semimetal
HALYNA HODOVANETS (Presenter), CHRIS ECKBERG, DANIEL CAMPBELL, DANIEL J KRAFT, SEAN A WINTERS, HYUNSOO KIM, JOHNPIERRE PAGLIONE, University of Michigan, College Park — We present details of flux growth and physical properties of noncentrosymmetric magnetic RAiGe (where R = Rare Earth) single crystals. The RAiGe family has been proposed, based on systematic first-principles band structure calculations, to host key elements of Weyl semimetals and as such offers a playground for new and exciting physics. We will discuss the effects of different rare earth species on the ground state magnetic order, magnetic anisotropy and correlation of the magnetotransport and crystal symmetry in the ordered state.
4:18PM P07.00010: Many-body dynamics and Kondo coherence collapse in an ultrafast driven Kondo insulator

WEI ZHU (Presenter), ALEXIS CHACON, JIAN-XIN ZHU, Los Alamos National Laboratory — Intense ultrafast pulse-driven electronics have provided systematic insights into the dynamics of electrons in condensed matter systems, which opens up prospects for quantum control of solids and all-optical band structure reconstruction. So far the studies have been carried out in solids where ‘bare’ electronic excitations dominate quantum dynamics. However, the underlying many-body dynamics due to correlations and couplings with other degrees of freedom such as lattice, spin or orbitals, has remained out of reach. Here, we introduce an ultrafast laser to optically pump and probe a Kondo lattice, in which conducting electrons strongly couple with magnetically local moments. The laser field excites collective doublon-hole pairs and drives a transient Kondo insulator melting, which are documented through the time-, frequency-, and momentum-dependent influence on the electronic structure. After photo-excitation, doublon-hole re-collision results in high-frequency photon emission. The information that we demonstrate as being accessible with time- and angle-resolved photo-electron spectroscopy and high-harmonic generation spectra, will stimulates the investigation of non-equilibrium dynamics and non-linear phenomenon in heavy-fermion systems.

4:30PM P07.00011: Exploring the valence transition in CeOs4Sb12 in high magnetic fields*

KATHRIN GOETZE (Presenter), MATTHEW J. PEARCE, PAUL GODDARD, Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom, ALIX MCCOLLAM, THOMAS KHOURI, High Field Magnet Laboratory (HFML-EMFL), Radboud University, Toernooiveld 7, 6525 ED, Nijmegen, The Netherlands, MARCELO JAIME, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM 87545, M BRIAN MAPLE, KALYAN SASMAL, Department of Physics, University of California, San Diego, La Jolla, CA 92093, TATSUYA YANAGISAWA, Department of Physics, Hokkaido University, Sapporo 060-0810, Japan, JOHN SINGLETON, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM 87545, PEI-CHUN HO, Department of Physics, California State University, Fresno, Fresno, CA 93740 — We present measurements of resistivity, magnetostriction, and PDO conductivity on the skutterudite CeOs4Sb12 in static and pulsed magnetic fields up to 30/60 T, respectively. The temperature and field dependencies allow us to map out the boundaries of the low temperature phase (L phase) in the H-T-phase diagram which - contrary to previous results - shows an unusual dome-like appearance extending to 45 T. The L phase is characterized by semiconducting behaviour with a small Fermi surface whereas the metallic high-temperature, high-field H phase exhibits a large Fermi surface. Magnetostriction results suggest that the L to H transition is accompanied by a valence transition. Additional features in transport and PDO within the L phase point towards further alteration of the band structure with applied field. We discuss the phase diagram of CeOs4Sb12 in the context of hybridization of 4f electrons and compare it to other skutterudites.

*Research at CSU-Fresno is supported by the NSF; at UCSD by NSF and US DOE; at Hokkaido U. by JSPS KAKENHI; at Univ. of Warwick by EPSRC and ERC. Work performed at NHMFL is supported by NSF, the State of Florida, US DOE, and through DOE Basic Energy Science Field Work Project Science in 100 T. We acknowledge support of HFML-RU/FOM, member of the EMFL.

4:42PM P07.00012: Transport and magnetic properties of correlated Ce3Bi4Pd3 at high magnetic fields*

SATYA K. KUSHWAHA (Presenter), MUN KEAT CHAN, MPA-MAG, Los Alamos National Laboratory, Los Alamos, USA, PRISCILA ROSA, ERIC BAUER, JOE D THOMPSON, MPA-CMMS, Los Alamos National Laboratory, Los Alamos, USA, JIAN-XIN ZHU, T4-PHYS OF CONDENSED MATTER & COMPLEX SYS, Los Alamos National Laboratory, Los Alamos, USA, CHAO CAO, MPA-CMMS, Los Alamos National Laboratory, Los Alamos, USA, NEIL HARRISON, MPA-MAG, Los Alamos National Laboratory, Los Alamos, USA — High magnetic fields are capable of destroying the Kondo effect, hence pro- viding an experimental tool to tune the ground state of f-electron systems.1 Ce3Bi4Pd3 is a narrow gap Kondo insulator recently predicted to be a strongly correlated Weyl semimetal.2 Here we present transport and magnetization measurements in Ce3Bi4Pd3 under pulsed magnetic fields to 60 Tesla, the results are significantly different from Ce3Bi4Pt3.

References:

*Supported by a Laboratory Directed Research and Development Director's Funded Postdoctoral Fellowship and DOE BESMSE Science of 100 Tesla programs.
4:54PM P07.00013: Bulk topological Fermi arcs in heavy fermion systems*  

YUKI NAGAI (Presenter), Japan Atomic Energy Agency, YANG QI, Fudan University, HIROKI ISOBE, VLADYSLAV KOZII, LIANG FU, Massachusetts Institute of Technology — We find that heavy fermion systems can have bulk Fermi arcs. In an interacting electron system, we can define the effective Hamiltonian \( H_{\text{eff}} = H + \Sigma \), where the many-body Hamiltonian is Hermitian, but the one-body quasiparticle Hamiltonian is non-Hermitian due to the finite quasiparticle lifetime. By introducing a topological theory of finite-lifetime quasiparticles, we can find that the low-energy dispersion of the Dirac material is reshaped and a topologically protected bulk Fermi arc appears[1,2]. Finite quasiparticle lifetime is a generic property of quantum many-body systems, resulting from scatterings. The exceptional points of the non-Hermitian quasiparticle Hamiltonian matrix play a crucial role. With the use of the dynamical mean field theory (DMFT) calculation, we confirm our statement in Kondo insulators with a momentum-dependent hybridization in two-dimensions. We show that the concept of the exceptional points in the non-Hermitian quasiparticle Hamiltonian is one of powerful tools to predict new phenomena in strongly correlated electron systems.


*This work was supported by the "Topological Materials Science" (No. 18H04228) JSPS--KAKENHI on Innovative Areas.

5:06PM P07.00014: Exploration of large anomalous Hall effect and topological Berry curvature in strongly correlated d- and f-electron magnets  

ERIC BAUER (Presenter), T. ASABA, NAKHEON SUNG, M. M. PIVA, M. CURTIS, SEAN THOMAS, PRISCILA ROSA, JOE D THOMPSON, FILIP RONNING, Los Alamos National Laboratory — The discovery of new topological states of matter and the effects of topology on the bulk properties of materials has attracted widespread attention [1], as these states are promising candidates for future technological applications such as quantum computing, memory storage, and sensors. While much of the research has focused on the exploration of topological states in materials without strong electronic correlations, these correlations open up new routes to generating novel topological states. For example, competing interactions among the magnetic moments of d- or f-electrons lead to magnetic frustration and often give rise to non-collinear or non-coplanar spin structures. Mobile conduction electrons feel the effects of a large (fictitious) magnetic field when they move in the topological spin texture of these non-collinear and non-coplanar magnets, which gives rise to a large anomalous Hall effect in compounds such as Mn3Sn [2,3]. In this talk, I discuss our recent work on the exploration of the anomalous Hall effect and topological Berry curvature in a variety of strongly correlated d- and f-electron magnets.


5:18PM P07.00015: Possible observation of topological surface states in a d-electron Kondo Insulator with angle-resolved photoemission spectroscopy*  

KEJUN XU (Presenter), YU HE, SUDI CHEN, Stanford University, MAKOTO HASHIMOTO, DONGHUI LU, SLAC national accelerator laboratory, SUNG-KWAN MO, Lawrence Berkeley National Laboratory, ZHIXUN SHEN, Stanford University — We use angle-resolved photoemission to probe the low energy bands of a d-electron Kondo Insulator exhibiting many similar properties as the prototypical f-electron topological kondo insulator candidate SmB6. We find a set of fermi surface features that disperse across \( E_F \), despite the bulk being insulating. Photon energy dependence shows the 2D nature of these bands. We discuss similarity and differences to SmB6 and open questions that challenges the current understanding of strongly correlated insulators.

*We acknowledge support from DOE/BES, Moore foundation, and NSF

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P08 DCMP: Superconductivity: Copper Oxide - Fermiology and Phase Diagram BCEC
150 - Makariy Tanatar, Ames Laboratory
Fermi-surface morphology and signatures of quantum critical points in the high-Tc cuprate HgBa2CuO4+δ revealed by high-magnetic fields* MUN CHAN (Presenter), NEIL HARRISON, ROSS MCDONALD, ERIC BAUER, Los Alamos National Laboratory — A paradigm of unconventional superconductivity invoked for the cuprates is that the unusually high superconducting temperatures is caused by strong electronic interactions near a zero temperature phase transition termed a quantum critical point (QCP). We report measurements of the low temperature electronic structure of the single-layer cuprate featuring the highest superconducting temperatures, HgBa2CuO4+δ (Hg1201). Quantum oscillations indicate that the Fermi surface is comprised of only a single quasi-two dimensional pocket that likely results from Fermi-surface reconstruction by a charge density wave order. High magnetic field measurements up to 90 T allow us to determine the boundaries of this order and identify two putative quantum critical points. Measurements of the doping dependent effective mass and upper critical fields provide additional support for strong-correlations around these QCPs.

*US Department of Energy BES ‘Science at 100T’ grant. The National High Magnetic Field Laboratory is funded by the National Science Foundation Cooperative Agreement Number DMR-1157490, the State of Florida and the U.S. Department of Energy.

Probing the Fermi surface of Nd-LSCO with angle-dependent magnetoresistance measurements YAWEN FANG (Presenter), Physics, Cornell University, ANAELLE LEGROS, GAELE GRISONNANCHE, FRANCIS LALIBERTE, Physics, Université de Sherbrooke, PAUL GODDARD, Physics, University of Warwick, LOUIS TAILLEFER, Physics, Université de Sherbrooke, BRAD RAMSHAW, Physics, Cornell University — Characterizing the Fermi surface of high-temperature superconductors in the pseudogap phase is one of the major challenges in understanding the origin of this mysterious partial gap in the electronic density of states. The Fermi surface between p=0.08 and p=0.15, the same doping range where charge order is observed, has been determined via quantum oscillations to be a small electron pocket. Above the critical doping p*, in the Fermi-liquid phase, a single large hole surface has been reported. However, in the pseudogap phase, the topology of the Fermi surface at low temperature in the absence of superconductivity or charge-density-wave order is still unknown. To study the topology of this Fermi surface, we performed an angle-dependent magneto-resistance (ADMR) study of Nd-LSCO. We measured the ADMR of single crystal La1.6-xNd0.4SrxCuO4 (Nd-LSCO) with x=p=0.2,0.21,0.22,0.23,0.25, up to 45 tesla and down to 6 kelvin. At p=0.25, above p*, we find a large Fermi surface whose geometry is consistent with that observed by ARPES, but with a strongly anisotropic quasiparticle lifetime. Below p*, in the pseudogap state, we observe a dramatic change in the ADMR, and preliminary analysis suggests that strong anti-nodal scattering is responsible.

Superconducting Higgs mode in cuprate thin films HAO CHU (Presenter), MIN-JAE KIM, Max Planck Institute for Solid State Research, KOTA KATSUMI, Department of Physics, University of Tokyo, SERGEY KOVALEV, Helmholtz Centre Dresden-Rossendorf, ROBERT DAWSON, LUKAS SCHWARZ, Max Planck Institute for Solid State Research, NAOHAKA YOSHIKAWA, Department of Physics, University of Tokyo, GIDEON KIM, Max Planck Institute for Solid State Research, SEMYON GERMANSKIY, JAN-CHRISTOPH DEINERT, NILESH AWARI, BERTRAM W GREEN, MIN CHEN, MOHAMMED BAWATNA, Helmholtz Centre Dresden-Rossendorf, GEORG CRISTIANI, GENNADY LOGVENOV, Max Planck Institute for Solid State Research, YANN GALLAIS, Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Diderot, ALEXANDER BORIS, BERNHARD KEIMER, ANDREAS P SCHNYDER, DIRK MANSKE, Max Planck Institute for Solid State Research, MICHAEL GENSH, ZHE WANG, Helmholtz Centre Dresden-Rossendorf, RYO SHIMANO, Department of Physics, University of Tokyo, STEFAN KAISER, Max Planck Institute for Solid State Research — Cuprate high-Tc superconductor hosts multiple competing orders such as the pseudogap, incommensurate magnetism, charge order, etc. These diverse phases were discovered via spectroscopy tools that probe the charge-/spin-excitations of an ordered state. Yet, despite the immense knowledge about cuprates learnt from these experiments, a coherent understanding of the microscopic mechanism behind high-Tc superconductivity is still lacking. A potential answer to this question may come from investigating the collective excitation of the superconducting order parameter itself, which is charge- and spin-neutral and difficult to access by conventional techniques. We accomplish this goal by using an undulator-based high-field THz pulse, which nonlinearly couples to the superconducting condensate and leads to characteristic third harmonic generation. Using this technique, we unveil the collective amplitude oscillation of the superconducting order parameter, the superconducting Higgs mode, in three archetypal families of cuprates for the first time. In addition, we show evidence for a hitherto unreported collective mode universally exhibited by optimally doped samples. A finite Higgs-like response above Tc is also observed in our experiment, suggesting a finite pairing amplitude above Tc.
3:06PM P08.00004: Breaking the universal Tc-P relation to higher Tc of cuprate HTS* CHING-WU CHU (Presenter), LIANGZI DENG, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204, YONGPING ZHENG, Materials Science & Engineering, University of Texas at Dallas, Richardson, TX 75080, ZHENG WU, SHUYUAN HU, CHUN YUAN, HUNG-CHENG WU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204, KYEONGJAE CHO, Materials Science & Engineering, University of Texas at Dallas, Richardson, TX 75080 — By investigating the bulk superconducting state via dc magnetization measurements, we have discovered the resurgence of the superconductive transition temperature Tcs of the monolayer Bi2Sr2CuO6+δ and bilayer Bi2Sr2CaCu2O8+δ to beyond the maximum Tc-maxs predicted by the universal Tc-P relation at higher pressures. We have attributed the resurgence to a possible pressure-induced electronic transition in the compounds, associated with a charge transfer between the Cu 3dx2-y2 and the O 2p bands, leading to an increase of the density of states at the Fermi level, in agreement with our density functional theory calculations. Similar Tc-P behavior has also been reported in the trilayer Br2Sr2Ca2Cu3O10+δ. The observations suggest that higher Tcs in the layered cuprate high temperature superconductors than those previously reported can be achieved by breaking away from the universal Tc-P by the application of higher pressures.

*The work performed at the Texas Center for Superconductivity at the University of Houston is supported by US Air Force Office of Scientific Research Grant FA9550-15-1-0236, the T. L. L. Temple Foundation, the John J. and Rebecca Moores Endowment, and the State of Texas through the Texas Center for Superconductivity at the University of Houston.

3:18PM P08.00005: Thermoelectric evidence of anomalous quantum criticality in the electron-doped cuprates* PAMPA MANDAL SARKAR (Presenter), TARAPADA SARKAR, RICHARD L. GREENE, University of Maryland, College Park — In electron-doped cuprates, the low upper critical field allows one to study the putative quantum critical phenomena at low temperature and to understand its connection to the long standing problem of the origin of high-Tc superconductivity. We have measured the low temperature normal state thermopower (S) of the electron-doped cuprate superconductor La2-xCexCuO4 (LCCO) from x=0.11 to 0.19. We observe quantum critical S/T versus ln(1/T) behavior over an unexpectedly wide doping range x = 0.15 - 0.17 above the putative QCP (x=0.14) with a slope that scales monotonically with the superconducting transition temperature. We find similar behaviour in another n-type cuprate, PCCO, strongly indicating that this is a universal behaviour in electron-doped cuprates. The presence of quantum criticality over a wide doping range provides a new window on the criticality. The thermopower behavior also suggests that the critical fluctuations are linked with Tc. For x = 0.11 and 0.13, S/T has a completely different behavior, an indication of a Fermi surface reconstruction. Above the superconductivity dome, at x=0.19, a conventional Fermi-liquid S-T behavior is found for Ts≤40 K.

*This work is supported by NSF under Grant No.DMR-1708334 and the Maryland Center for Nanophysics and Advanced Materials.

3:30PM P08.00006: Josephson interferometry measurements of the superconducting pairing symmetry in the overdoped cuprate La1.75Sr0.25CuO4 --- search for disorder-induced deviations from d-wave symmetry* DAVID HAMILTON (Presenter), University of Illinois at Urbana-Champaign, MASAKI FUJITA, Tohoku University, DALE J VAN HARLINGEN, University of Illinois at Urbana-Champaign — Extensive measurements have shown that cuprate superconductors exhibit a robust d x2-y2 global superconductor pairing symmetry. It has been proposed that in a disordered d-wave superconductor near criticality, the superconductivity will nucleate in spatially-separated puddles with orthogonal phase alignment of the d-wave order parameter. When these puddles are dilute, such as in highly overdoped samples, Josephson coupling between puddles can favor global s-wave superconductivity. To explore this regime, we perfromed Josephson interferometry measurements of LSCO-Au-Nb Josephson junctions formed on edges and corners of an overdoped single crystal of La1.75Sr0.25CuO4 with a Tc of ~18K. In preliminary measurements of l.c vs. magnetic field, we observe deviations from Fraunhofer patterns expected for uniform edge junctions and from the characteristic corner junction pattern expected for dx2-y2 symmetry. We see rapid modulations in the critical current indicating the presence of discrete order parameter domains with opposite sign. At temperatures near where the junction supercurrent vanishes, we observe diffraction patterns with a maximum centered on zero field in the corner junctions, as we would expect to see in an s-wave superconductor.

*This work was supported by NSF DMR-1710437
3:42PM P08.00007: The New NMR Shift and Relaxation Scenario of the Cuprates  JUERGEN HAASE (Presenter), Leipzig University — Based on experiments and a comprehensive literature analysis of cuprate NMR shift and relaxation data we present the new scenario for the cuprates. It has almost ubiquitous fermionic excitations that govern the nuclear relaxation above Tc and begin to disappear below Tc, i.e., for all materials from slightly underdoped to heavily overdoped. For the highest doping levels, this nuclear relaxation is related to the sample’s spin shift via the Korringa relation for a simple Fermi liquid to which the nuclei couple isotropically. Therefore, it is argued that the spin shifts of the cuprates are typically suppressed, already in the overdoped region, and that there is no enhanced nuclear relaxation compared to that of a Fermi liquid. This means, no spin fluctuations have to be invoked to explain the difference between shift and relaxation. This suppression of the shift above Tc must be related to the pseudogap, which enters nuclear relaxation only through a temperature independent change in the anisotropy of the coupling of the nuclei to the electronic bath. It is argued that two antiferromagnetically coupled spin components that have different orbital origin can explain all the data, even the NMR orbital shift conundrum.

3:54PM P08.00008: Apical charge flux-modulated in-plane transport properties of cuprate superconductors*  XIN LI (Presenter), SOORAN KIM, XI CHEN, WILLIAM FITZHUGH, Harvard University — For copper-based superconductors, the maximum superconducting transition temperature, $T_{c,max}$, of different families measured from experiments can vary by an order of magnitude from 38 K in La$_2$CuO$_4$ to 135 K in HgBa$_2$Ca$_2$Cu$_3$O$_8$ at optimal hole doping concentration. We demonstrate herein, using ab initio computations, a new trend suggesting that the cuprates with stronger out-of-CuO$_2$-plane chemical bonding between the apical anion (O, Cl) and apical cation (e.g. La, Hg, Bi, Tl) are generally correlated with higher $T_{c,max}$ in experiments. We then show the underlying fundamental phenomena of coupled apical charge flux and lattice dynamics when the apical oxygen oscillates vertically. This triggers the charge flux among the apical cation, apical anion and the in-plane CuO$_4$ unit. The effect not only dynamically modulates the site energy of the hole at a given Cu site to control the in-plane charge transfer energy, but also can modulate the in-plane hole hopping integral in a dynamic way by the cooperative apical charge fluxes.


*This work is supported by the computational resources from XSEDE and the Odyssey cluster at Harvard University.

4:06PM P08.00009: Non-equilibrium study of the phase diagram of cuprates  FABIO BOSCHINI (Presenter), ELIA RAZZOLI, MARTA ZONNO, RYAN P DAY, MATTEO MICHIARDI, QMI, University of British Columbia, EDUARDO H DA SILVA NETO, Physics, Univ of California - Davis, GENDA GU, Cond. Matt. Physics and Material Science, Brookhaven Natl Lab, SERGEY ZHDANOVICH, ARTHUR K MILLS, GIORGIO LEVY, DAVID J JONES, QMI, University of British Columbia, CLAUDIO GIANNELLI, Mathematics and Physics, Univ. Cattolica Brescia, ANDREA DAMASCELLI, QMI, University of British Columbia — The phase diagram of cuprates hosts numerous intertwined phases, such as high-temperature superconductivity, charge order and the pseudogap phenomenon. This makes the precise description of each separate phase challenging. In particular, thermal excitations govern the appearance of different phases and thermodynamic phase transitions. We recently demonstrated the capability to study the superconductor-to-normal state transition in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ cuprate superconductor in an ultrafast fashion. In particular, we demonstrated that time-resolved photoemission spectroscopy can disentangle the dynamics of phase fluctuations and charge excitation, establishing the dominant role of phase coherence in the emergence of high-temperature superconductivity [1]. In the same line of thought, we applied this non-equilibrium approach to (i) reveal the transient competition between charge-order and superconducting phases and (ii) explain the enhanced electron-boson band renormalization (kink) in terms of the opening of the superconducting gap and pseudogap.


4:18PM P08.00010: Fluctuating superconductivity and absence of charge order in heavily overdoped cuprate Bi-2212*  YU HE (Presenter), SUDI CHEN, Stanford University, MAKOTO HASHIMOTO, SLAC, ALEX FRANCO, Physics, University of California, San Diego, MING YI, Physics, Rice University, YU SONG, SHAN WU, Physics, University of California, Berkeley, DONGJOON SONG, Physics, Yonsei University, HIROSHI EISAKI, AIST, ROBERT J BIRGENCEAU, Physics, University of California, Berkeley, ZHIXUN SHEN, Stanford University — We identify significant superconducting fluctuations on a single coherent, hole-like Fermi surface in heavily overdoped cuprate superconductor Bi-2212. No evidence of pseudogap or valence electron charge order are found in the meantime. Both amplitude and phase fluctuations are quantitatively estimated via measurements of resistivity anisotropy, specific heat jump, and superconducting coherent length. The important role of the quasi-two-dimensional flat band and the van Hove singularity are discussed in the end.

*US Department of Energy, Basic Energy Sciences
4:30PM P08.00011: Phase fluctuation in overdoped cuprates? Superconducting dome due to Mott-ness of the tightly bound preformed pairs  
ZIJIAN LANG (Presenter), School of Physics and Astronomy, Shanghai jiaoTong University, FAN YANG, School of Physics, Beijing Institute of Technology, WEI KU, School of Physics and Astronomy, Shanghai jiaoTong University — In contrast to the current lore, we demonstrate that even the overdoped cuprates suffer from superconducting phase fluctuation in the strong binding limit. Specifically, the Mott-ness of the underlying doped holes dictates naturally a generic optimal doping around 15% and nearly complete loss of phase coherence around 25%, giving rise to a dome shape of superconducting transition temperature in excellent agreement with experimental observations of the cuprates. We verify this effect with a simple estimation using Gutzwiller approximation of the preformed pairs, obtained through variational Monte Carlo calculation. This mechanism also provides a natural explanation for the observed relation between superconducting temperature and superfluid density near the overdoped end of the dome. This realization suggests strongly the interesting possibility that the high-temperature superconductivity in the cuprates might be mostly described by Bose-Einstein condensation, without crossing over to amplitude fluctuating Cooper pairs.

4:42PM P08.00012: Angular Magnetoresistance Measurements as a Probe of the Fermi Surface in Hg1201*  
KATHERINE SCHREIBER (Presenter), MUN CHAN, NEIL HARRISON, ERIC BAUER, Los Alamos National Laboratory — The Fermi surface of underdoped cuprates is reconstructed by charge density wave order. An elucidation of the exact morphology of the reconstructed Fermi-surface is expected to provide insight into the relationship between charge order and superconductivity. We present measurements of the Fermi surface of underdoped HgBa2CuO4+d (Hg1201), obtained through angular magnetoresistance. Transport along the c-axis was measured in pulsed magnetic fields of up to 65 T, applied along many polar and azimuthal angles in order to map out the Fermi surface. We discuss the implication of our measurements for the shape of the Fermi surface, including the interlayer warping, and comment on its dependence on temperature and doping.

*This work is funded by the US DOE-BES "Science at 100T" LANL F100 grant. Work was done at the National High Magnetic Field Laboratory which is supported by the National Science Foundation through NSF/DMR-1644779 and the State of Florida.

4:54PM P08.00013: Universal $T$-linear resistivity and Planckian dissipation in cuprates  
LOUIS TAILLEFER (Presenter), ANAELLE LEGROS, Université de Sherbrooke, Canada, SIHAM BENHABIB, WOJCIECH TABIS, LNCMI Toulouse, France, FRANCIS LALIBERTE, MAXIME DION, MAUDE LIZAIRE, Université de Sherbrooke, Canada, BAPTISTE VIGNOLLE, DAVID VIGNOLLES, LNCMI Toulouse, France, HÉLÈNE RAFFY, ZZ LI, PASCALE AUBAN-SENZIER, Université Paris-Sud, France, NICOLAS DOIRON-LEYRAUD, PATRICK FOURNIER, Université de Sherbrooke, Canada, DOROTHÉE COLSON, CEA Saclay, France, CYRIL PROUST, LNCMI Toulouse, France — The perfectly linear temperature dependence of the electrical resistivity observed as $T\to 0$ in a variety of metals close to a quantum critical point is a major puzzle of condensed matter physics. Here we show that $T$-linear resistivity as $T\to 0$ is a generic property of cuprates, associated with a universal scattering rate [1]. We measured the low-temperature resistivity of the bi-layer cuprate Bi2212 and found that it exhibits a $T$-linear dependence with the same slope as in the single-layer cuprates Bi2201, Nd-LSCO and LSCO, despite their very different Fermi surfaces and structural, superconducting and magnetic properties. We then show that the $T$-linear coefficient (per CuO$_2$ plane), $A$, is given by the universal relation $A T_F = \hbar / 2 e^2$, where $e$ is the electron charge, $\hbar$ is the Planck constant and $T_F$ is the Fermi temperature. This relation, obtained by assuming that the scattering rate $1 / \tau$ of charge carriers reaches the Planckian limit [2], whereby $h / \tau = 2 \pi k_B T_F$ works not only for hole-doped cuprates but also for electron-doped cuprates, despite the different nature of their quantum critical point and strength of their electron correlations.

Here, we use the d-form factor density wave (DW), imaged via scanning tunneling microscopy, to probe the ground state evolution in superconducting (Pb,Bi)$_2$(Sr,La)$_2$CuO$_{6+\delta}$ (Bi-2201). We employ the disorder caused by local dopant inhomogeneity to gain continuous access to the doping axis of the phase diagram, both via standard Fourier techniques and machine learning. We find a transition in the DW from commensurate to incommensurate, which occurs simultaneously with the Fermi surface transition, where open arcs are replaced by a conventional large Fermi surface. The coincidence of these transitions indicates an intimate link between the commensurate instability and the mechanism underlying the Fermi arcs.

*TW and MHH were funded by the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant GBMF4536.

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**5:18PM P08.00015: Nodeless high-Tc superconductivity in highly-overdoped monolayer CuO$_2$**

KUN JIANG (Presenter), Boston College, XIANXIN WU, Physics, University of Wurzburg, JIANGPING HU, Chinese Academy of Sciences, ZIQIANG WANG, Boston College — We study the electronic structure and superconductivity in CuO$_2$ monolayer grown recently on d-wave cuprate superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Density functional theory calculations indicate significant charge transfer across the interface such that the CuO$_2$ monolayer is heavily overdoped into the hole-rich regime. We show that both the Cu d$_{x^2-y^2}$ and d$_{3z^2-r^2}$ orbitals become important and the Fermi surface contains one electron and one hole pocket associated with the two orbitals respectively. The liberated low-energy d$_{3z^2-r^2}$ band and the hole FS pocket around M enable an analogy to the multiorbital Fe-pnictides superconductors. Constructing a minimal strongly correlated two-orbital model for the e$_g$ complex, we show that the spin-orbital exchange interactions produce an intrinsic nodeless superconductor with extended s-wave pairing symmetry and a pairing energy gap comparable to the bulk d-wave gap, in agreement with recent experiments. The findings point to a direction of realizing new high-Tc superconductors over-extended doping regimes with liberated orbitals in ozone grown transition-metal-oxide heterostructures.

*The work is supported by the U.S. Department of Energy, Basic Energy Sciences Grant No. DE-FG02-99ER45747.

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**Wednesday, March 6, 2019 2:30 PM - 5:30 PM**

**Session P09 DCMP: Superconductivity in Dichalcogenides and Similar Materials**

Patrick Vora, George Mason Univ
Superconductors of monolayered transition metal dichalcogenides such as MoS$_2$ and NbSe$_2$ give rise to TSC. However, as of date, few-layer NbSe$_2$ is produced mainly through mechanical exfoliation. There is a demand to construct large scale NbSe$_2$ thin films to further enable fabrication of scalable heterostructures. In contrast, in this talk, we report our progress on few-layer NbSe$_2$ grown on insulating substrates by MBE. The layers are characterized by in-situ reflection high energy electron diffraction (RHEED) and ex-situ Raman spectroscopy. A clear superconducting transition has been observed with the transition temperature (Tc) above 2K. We will discuss correlations between layer quality and the Tc. We will also present our studies regarding the critical field in thin film NbSe$_2$.

The ability to fit this transition using activated scaling shows that this transition is well described by an infinite-randomness critical point and quantum Griffiths singularities.

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Superconductivity in few-layer NbSe$_2$ grown by molecular beam epitaxy

PENG WEI, University of California, Riverside — Superconductors with strong spin-orbit coupling (SOC) are attractive for generating triplet Cooper pairs and topological superconductivity (TSC). In few-layer NbSe$_2$, strong SOC is reported to give rise to TSC. However, as of date, few-layer NbSe$_2$ is produced mainly through mechanical exfoliation. There is a demand to construct large scale NbSe$_2$ thin films to further enable fabrication of scalable heterostructures that can exhibit the unique properties of TSC. Recent reports show that NbSe$_2$ can be grown on graphene by molecular beam epitaxy (MBE). In contrast, in this talk, we report our progress on few-layer NbSe$_2$ grown on insulating substrates by MBE. The layers are characterized by in-situ reflection high energy electron diffraction (RHEED) and ex-situ Raman spectroscopy. A clear superconducting transition has been observed with the transition temperature (Tc) above 2K. We will discuss correlations between layer quality and the Tc. We will also present our studies regarding the critical field in thin film NbSe$_2$.

This work is supported by the Startup fund from University of California, Riverside.

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Ising superconductivity in NbSe$_2$-Te$_x$ with tunable spin-orbit coupling

ZHENYU ZHANG (Presenter), LEIQIANG LI, WEI QIN, PING CUI, CHANGGAN ZENG, University of Science and Technology of China — The Ising superconductors of monolayered transition metal dichalcogenides such as MoS$_2$ and NbSe$_2$ have been shown to possess strongly enhanced upper critical fields. In these systems, the spin-orbit coupling (SOC) pins the electron spins to the out-of-plane direction because of in-plane mirror symmetry breaking, thereby becoming insensitive to the lateral external magnetic fields. Here, using first-principles density functional theory calculations, we demonstrate that the Te substitution of Se in NbSe$_2$ will enhance the strength of the SOC, as characterized by the increased spin splitting in the electronic structures of NbSe$_2$-Te$_x$. As a consequence, the upper critical fields of these systems will be further enhanced. Moreover, as x approaches to 2, the enhanced SOC leads to a band inversion around the high symmetry M point in the Brillouin zone, indicating a quantum phase transition towards a topological superconducting state.

*Supported by NSF of China

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The enhancement of in-plane Hc$_2$ in monolayer centrosymmetric superconductor 1T'-WTe$_2$ via strong spin-orbital coupling

YINGMING XIE (Presenter), WENYU HE, KAM TUEN LAW, Hong Kong University of Science and Technology — Recently, it was reported that the two-dimensional quantum spin Hall insulator 1T'-WTe$_2$ can be gated into the superconducting phase. The in-plane Hc$_2$ in this centrosymmetric superconductor is enhanced up to 2-4 times Pauli limit. However, unlike the typical enhancement of Hc$_2$ in a non-centrosymmetric superconductor, the mechanism here is not clear. In this work, we find due to the strong spin-orbital coupling (SOC), the spin susceptibility is reduced in the low gating region. In other words, the magnetic field felt by electrons near the Fermi energy is renormalized, which in turn enhances the Hc$_2$. The amplitude of enhancement is comparable to the experiments. Moreover, in this mechanism, the anisotropic SOC will lead to obvious anisotropy in Hc$_2$, which can be tested in experiments by rotating the magnetic field.
3:30PM P09.00006: Superconductivity in Br-doped misfit compounds \((\text{PbSe})_{1.12}(\text{TaSe}_2)\)^* ZHUAN XU (Presenter), Physics Department, Zhejiang University — We report the discovery of superconductivity with a maximum \(T_c\) of 1.28 K in Br-doped \((\text{PbSe})_{1.12}(\text{TaSe}_2)\), which is a new misfit compound consisting of alternating layers of distorted rocksalt PbSe and dichalcogenide TaSe_2. The Br-doping is required for the formation of this misfit compound and superconductivity can be tuned by changing Br content. The large anisotropic parameters in both resistivity and upper critical field \(H_{c2}\) are found. The estimated c-axis coherence length of 6.3 nm is larger than the c-axis lattice constant, which implies that this compound is an anisotropic three-dimensional superconductor. The Hall coefficient measurements suggest that the charge transport is dominated by the hole-type charge carrier and there is a charge transfer from the PbSe layer to the conducting TaSe_2 layer. The small normalized specific heat jump and electron-phonon coupling constant of 0.61 indicate that Br-doped \((\text{PbSe})_{1.12}(\text{TaSe}_2)\) should be a weak-coupling BCS superconductor. The point-contact Andreev reflection spectroscopy is also studied.

*This work is supported by National Key R & D Program of China (2016YFA0300402) and the National Natural Science Foundation of China (Grant No. 11774305).

3:42PM P09.00007: Superconductivity and Charge Density Wave in SnSe\textsubscript{2}-based Heterostructures* YIMIN ZHANG (Presenter), JIA-QI FAN, CANLI SONG, XUCUN MA, QIKUN XUE, Department of Physics, Tsinghua University — We report the direct observation of interface superconductivity and interface-induced charge density wave on monolayer SnSe\textsubscript{2}-based heterostructures. Tunneling spectrums on epitaxial monolayer SnSe\textsubscript{2} grown on graphited SiC(0001) substrate showed a fully-gapped superconducting state with rather conventional character. Occurrence of vortices under external magnetic field further confirmed the superconductivity. We attribute the superconductivity to the two-dimensional gas formed at the interface of SnSe\textsubscript{2} and graphene. Besides, charge density waves (CDW) with \(2 \times 2\) periodicity were observed in SnSe\textsubscript{2} thin films grown on SrTiO\textsubscript{3}(001) and Si(111), which disappear as the film thickness increases. Our finding opens new perspectives to understand not only interface superconductivity but also possible relationship between superconductivity and CDW.

*We acknowledge the financial support from Ministry of Science and Technology of China (Grants No. 2017YFA0304600, 2015CB921001, 2016YFA0301004) and the National Natural Science Foundation of China (Grants No. 11427903, 11504196, 11634007, 11774192).

3:54PM P09.00008: Superconductivity in electron-doped layered 1T-SnSe\textsubscript{2} HANLIN WU (Presenter), SHENG LI, Physics, University of Texas at Dallas, TIMOTHY HAUGAN, MICHAEL SUSNER, Air Force Research Laboratory, Wright-Patterson Air Force Base, BING LV, Physics, University of Texas at Dallas — Layered metal chalcogenide 2D materials have attracted great attention in the recent years due to their emergent new physics phenomena such as surface states, magnetism, giant magnetoresistance, quantum spin Hall effects, and superconductivity. Chemical intercalation, or physical electron-gating, has been found out to be very effective to tune the electronic structures and the associated physical properties. In this presentation, we will focus on our experimental intercalation studies of the CdI\textsubscript{2}-type 1T-SnSe\textsubscript{2} phase. Both electron doping by alkaline metal intercalation and polar organic solvent cointercaltion have been carried out through soft chemical methods. The associated structural characteristics, magnetic, electrical resistivity changes upon doping, and the unconventional superconductivity will be presented. The possible competing orders of charge density wave and superconductivity upon intercalation will be discussed as well.

4:06PM P09.00009: Theory of unconventional superconductivity in gated monolayer WTe\textsubscript{2} YI-TING HSU (Presenter), WILLIAM COLE, RUI-XING ZHANG, JAY SAU, Physics, University of Maryland, College Park — Recent observation of superconductivity in monolayer WTe\textsubscript{2} upon gating has attracted much interest since the undoped WTe\textsubscript{2} has been experimentally established as a quantum spin Hall insulator. Although the nature of the superconductivity remains elusive, the prevailing expectation is that inducing superconductivity in already topological materials is a promising route to identifying new exotic superconductors. Here we investigate the dominant pairing instabilities under different microscopic interactions by solving the linearized gap equation. We find equal-spin paired state that is consistent with the experimentally found high critical field, and we discuss the possibility of topological paired state. Finally, we consider the effects of a single impurity, as the first step towards determining how disorder impacts the phase diagram.
4:18PM P09.00010: Nodeless superconductivity in the type-II Dirac semimetal PdTe2: London penetration depth and pairing-symmetry analysis*  

PETER ORTH (Presenter), SERAFIM TEKNOWJOYO, NA HYUN JO, Iowa State University, MATHIAS SCHEURER, Harvard University, MAKARIV A TANATAR, Iowa State University, KYUIL CHO, Ames Laboratory, SERGEY BUDKO, P.C. CANFIELD, RUSLAN PROZOROV, Iowa State University — London penetration depth and normal-state resistivity were measured in single crystals of type-II Dirac semimetal PdTe2. Superfluid density is exponential at low temperatures and follows single-gap BCS model with weak-coupling \( \Delta(0)/T_c = 1.76 \) in the whole temperature range. Electrical resistivity is compatible with a classical metal with dominant electron-phonon scattering obtained from the fit to Bloch-Grüneisen formula with a Debye temperature of 207 K from specific heat data. We compare these experimental results with expectations from a detailed theoretical symmetry analysis and reduce the number of possible superconducting pairing states in PdTe2 to only three nodeless candidates: a regular, topologically trivial s-wave pairing, and two distinct odd-parity triplet states that both can be topologically nontrivial depending on the microscopic interactions driving the superconducting instability. Finally, we theoretically discuss the effect of disorder on the different pairing states.

*Work done at Ames Laboratory was supported by the U.S. DOE Office of Basic Energy Sciences, DMSE. Ames Laboratory is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358. NHJ by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4411.

4:30PM P09.00011: Robust parity-mixed superconductivity in disordered 2D transition metal dichalcogenides*  

DAVID MÖCKLI, MAXIM KHODAS (Presenter), Hebrew University of Jerusalem — Monolayer NbSe2 is a nodal topological Ising superconductor at magnetic in-plane fields exceeding the Pauli limit, with nodal points strictly on high symmetry lines in the Brillouin zone. Here, we use a combined numerical and group-theoretical approach in real-space to characterize the unconventional superconducting state in monolayer transition metal dichalcogenides. Even with a conventional pairing interaction, the superconducting state is intrinsically parity-mixed and robust against on-site disorder. The interplay between the Zeeman magnetic field, strong spin-orbit interaction, and electronic orbital content confer the unique superconducting and topological properties. The discussion also extends to strongly hole-doped MoS2 and its relatives.

*Israel Science Foundation, Grant No. 1287/15

4:42PM P09.00012: Ising superconductors in in-plane magnetic fields  

STEFAN ILIC (Presenter), JULIA MEYER, MANUEL HOUZET, Univ. Grenoble Alpes, CEA, INAC-Pheliqs, Grenoble, France — Transition metal dichalcogenide monolayers are a new class of two-dimensional superconductors. They host a strong intrinsic spin-orbit coupling (SOC), that acts as an effective Zeeman field with opposite, out-of-plane, orientations in the +K and –K corners of the Brillouin zone (valleys). This SOC causes unconventional “Ising pairing” of the Cooper pairs, formed of electrons from opposite valleys with strongly pinned out-of-plane spins. In-plane fields are thus not efficient in breaking the Cooper pairs by the paramagnetic effect, which results in a large enhancement of the in-plane upper critical field – the main signature of Ising superconductivity.

Using a quasiclassical formalism for disordered Ising superconductors, we calculate the in-plane upper critical field, as well as the density of states in the superconducting phase. We show that these quantities are not affected by intravalley scattering, and are determined by the interplay of the SOC and intervalley scattering. The smearing of the density of states with the applied field cannot be captured with the standard Abrikosov-Gor’kov theory. We compare our results with recent experiments.

4:54PM P09.00013: Superconductivity in Re6Se8Cl2, a Superatomic Two Dimensional Semiconductor  

EVAN TELFORD (Presenter), JAKE RUSSELL, JOSH SWANN, KIHONG LEE, XIAOYANG ZHU, XAVIER ROY, CORY R DEAN, Columbia University — We report on low temperature transport measurements of Re6Se8Cl2 - a synthesized van der Waal cluster solid with a hierarchical structure composed of covalently linked Re6Se8 clusters. Samples are prepared by mechanical exfoliation onto a PDMS stamp, then transferred to metallic leads pre-patterned on a SiO2 substrate. As grown, this material is a weakly-doped semiconductor, with strongly insulating behavior observed at cryogenic temperatures. Using a current annealing technique we demonstrate the ability to induce an insulator to superconductor transition, in situ. This transition is accompanied by an increase in the carrier density by 3-4 orders of magnitude. The chemical (EDX) and structural (Raman) analysis after current annealing show no change in chemical composition or lattice structure. We conjecture that the transition results from a small loss of interplanar chlorine atoms through the application of large currents. Details of the superconducting state and its possible nature will be discussed.
YUN-YI PAI (Presenter), MEGAN BRIGGEMAN, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNG-WOO LEE, Department of Materials Science and Engineering, University of Wisconsin-Madison, MENGCHEN HUANG, JIANAN LI, Department of Physics and Astronomy, University of Pittsburgh, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — We investigate the effects of the geometrical shapes of the 1D nanowires created at LaAlO3/SrTiO3 in order to study the origin of superconductivity of SrTiO3, which has puzzled researchers for more than 50 years. It was recently suggested that electron pairing in SrTiO3 may be related to ferroelastic domain walls [1]. By using conductive-AFM lithography [2] to create 1D superconducting nanowires at the LaAlO3/SrTiO3 interface, we can investigate the influence of nanowire shape, and in particular the effect of sharp turns in the nanowire, on superconducting behavior in the nanowires. We find a significant stabilization of the superconducting state in “zigzag” wires compared with straight control wires, both created at the same time and located only a few micrometers apart. We discuss possible origins for this behavior within the context of ferroelastic domain structure that surrounds the nanowires.


*This work is supported by the NSF (DMR-1609519). C-BE acknowledges DOE Office of Science, Office of Basic Energy Sciences (DE-FG02-06ER46327).

MATTHIAS HECKER (Presenter), TKM, Karlsruhe Institute of Technology (KIT), EREZ BERG, Weizmann Institute of Science, JOERG SCHMALIAN, TKM, Karlsruhe Institute of Technology (KIT) — Under Cu or Nb doping, the topological insulator Bi2Se3 becomes superconducting with a maximal Tc~3-4 K. The pairing symmetry has been intensely studied and in recent years, experiments have consistently pointed towards an unconventional, odd-parity triplet pairing in the two-dimensional irreducible representation Eu of the crystal point group D3d. Due to a low carrier density and a small ratio of the superconducting coherence length and the Fermi wavelength, fluctuations are increasingly important, even to the extent that they allow for a preformed nematic state with T_n> T_c. Inside this performed phase, we study resistivity, elastic constants, and fluctuating diamagnetism. Furthermore, we investigate how the superconducting ground state in a constant magnetic field is affected by the preformed phase.
3:06 PM P11.00002: Design of Two-Level Quantum state in 2D Materials for Single Photon Emission  SUNNY GUPTA (Presenter), JI-HUI YANG, BORIS YAKOBSON, Rice University — Due to reduced dimensionality, defect levels in two-dimensional (2D) semiconductors are often far away from band edges, making 2D semiconductors ideal systems for single photon emission (SPE), if they can host defects forming a two-level quantum state. Recently, SPE was experimentally observed in different 2D materials. However, the defect centers serving as sources for SPE are yet to be identified and the possible mechanism for the formation of the ideal two-level quantum state is yet to be uncovered. Here, using first-principles calculations and group theory analysis we highlight the advantages of 2D materials as host systems and also identify and design defects in various 2D materials for SPE. A generalized strategy is proposed to design defect complex by adding a paramagnetic impurity next to a vacancy defect, which forms an ideal two-level quantum system. The electronic states of the designed defect complex are well isolated from the host band edges, belong to a majority spin eigenstate, and can be controllably excited by $x$-polarized light, thereby satisfying all the criteria required for an ideal SPE. The defect complex is thermodynamically stable, and appears feasible for experimental realization, to serve as an SPE-source, essential for quantum computing.

3:18 PM P11.00003: The Effects of Disorder on 2D Material Properties*  BLAKE DUSCHATKO (Presenter), CHRISTOPHER CICCARINO, PRINEHA NARANG, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Two dimensional materials, such as hexagonal boron nitride and transition metal dichalcogenides, are emerging platforms for quantum information science, where the controlled introduction of atom-like defects can be utilized for numerous applications. While the excitement surrounding these systems has grown, a great deal of work remains to be done in order to realize the full integration of 2D materials into quantum devices. In this talk, I present how recent advances in high precision atomic imaging can be leveraged with ab initio calculations to advance our ability to characterize material properties. Working with atomic coordinates of monolayer MoS$_2$, we find that it possesses out of plane ripples on the order of 50 picometers, effectively hindering equilibration. The general disorder present in such nonzero temperature samples has substantial effects on the dynamics of the material and optical properties of engineered defects. I will show calculations that capture the effects of disorder and discuss how this presents a significant step forward in 2D material theory.

*This work was supported by the DOE Photonics at Thermodynamic Limits Energy Frontier Research Center under grant #DE-SC0019140

3:30 PM P11.00004: Theoretical Investigation of Color Centers in Diamond for Quantum Information Science*  CHRISTOPHER CICCARINO (Presenter), JOHANNES FLICK, Harvard University, MATTHEW TRUSHEIM, Massachusetts Institute of Technology, PRINEHA NARANG, Harvard University — Color centers in diamond have emerged as leading solid-state “artificial atoms” for a range of promising technologies from quantum sensing to quantum networks. While properties and limitations of canonical color centers NV$^-$ and SiV$^+$ have been well documented, exploration and a fundamental understanding of novel color centers presents an exciting opportunity to improve upon the current state of the art. We leverage our unique first-principles methods to detail crucial defect properties in the SnV$^-$, PbV$^+$[1] and SiV$^0$, in addition to novel diamond color centers. We capture the zero phonon line energies and phonon sideband profile and in particular investigate the potential for Jahn-Teller distortion effects in each of these systems, where electron-spin-phonon coupling phenomena are capable of drastically altering predicted spin-orbit splitting and ZPL energies. We detail our unique theoretical approach to the study of these defects, and through our results offer a comprehensive perspective of diamond defects for applications in quantum devices.


*All authors acknowledge support from the Army Research Office MURI (Ab-Initio Solid-State Quantum Materials) grant number W911NF-18-1-0431.
Color centers in hexagonal boron nitride have shown enormous promise as single-photon sources, but a clear understanding of electron-phonon interaction dynamics is critical to their development for quantum communications or quantum simulations. We demonstrate photon antibunching in the zero phonon line. We will discuss the feasibility of quantum phononics via further exploration of the density of states for single photon purity of 80% in a phonon replica and cross-spectral correlations of 82% between a phonon replica and the zero phonon line. We will discuss the feasibility of quantum phononics via further exploration of the density of states for phononic cavities coupled to single quantum emitters in 2D materials.

This research was sponsored by the Laboratory-Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the U.S. Department of Energy (DOE). Rapid thermal processing and spectroscopy experiments were carried out at the Center for Nanophase Materials Sciences, which is sponsored at ORNL by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE. MAF was supported by the Department of Defense through the NDSEG fellowship and the NSF award DMR-1747426.

Microwave dielectric loss of hexagonal Boron Nitride in the low-temperature, single-photon regime* MEGAN YAMOAH (Presenter), Physics, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, JOEL WANG, Research Laboratory of Electronics, Massachusetts Institute of Technology, CHARLOTTE BOETTCHER, Physics, Harvard University, BHARATH KANNAN, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, DAVID K KIM, Massachusetts Institute of Technology Lincoln Laboratory, PHILIP KRANTZ, Research Laboratory of Electronics, Massachusetts Institute of Technology, DANIEL RODAN LEGRAIN, ORIOL RUBIES-BIGORDA, Physics, Massachusetts Institute of Technology, JONILYN L YODER, Massachusetts Institute of Technology Lincoln Laboratory, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Japan, TERRY PHILIP ORLANDO, Research Laboratory of Electronics, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, PABLO JARILLO-HERRERO, Physics, Massachusetts Institute of Technology, WILLIAM D OLIVER, Research Laboratory of Electronics, Physics, Lincoln Laboratory, Massachusetts Institute of Technology — The use of 2D van der Waals (vdW) heterostructures in quantum computing devices, due in part to the potential of combining different materials with epitaxial precision, has begun to merge the superconducting and 2D material platforms. Hexagonal boron nitride (hBN), a vdW material widely used as an ultra-clean substrate, gate dielectric, and protection layer in vdW heterostructures, may be used in building high-quality Josephson elements and qubit capacitors. VdW materials have been extensively studied in the DC and optical regimes, but understanding their response to microwave excitations is vital to introducing them into superconducting circuits. We study hBN in the microwave regime by integrating the material in a superconducting LC resonator to extract its loss tangent. Our scheme can be used for characterizing not only the electromagnetic properties of hBN, but also other 2D materials.

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Towards coherent control of single nuclear spins of $^{171}\text{Yb}$ in YVO* JONATHAN KINDEM (Presenter), ANDREI RUSKUC, JOHN BARTHOLOMEW, JAKE ROCHMAN, ANDREI FARAON, California Institute of Technology — Optically addressable solid-state spins are a promising platform for the development of scalable quantum technologies. Rare-earth ions in crystals are an attractive candidate for such systems due to their long optical and spin coherence lifetimes. By interfacing these ions with nanophotonic cavities, we can significantly enhance the photon-ion interaction to overcome their intrinsically weak optical transition strengths and enable detection and manipulation of single ions.

Here we describe work towards coherent control of long-lived nuclear spins of individual $^{171}\text{Yb}$ ions coupled to a nanoscale photonic crystal cavity fabricated in the YVO host crystal. We first present results on detection and coherent optical manipulation of single ions in such a cavity. We then show that the cavity enhanced emission rate enables efficient optical pumping and spin initialization. Finally, we present initial results towards coherent microwave control of the electron and nuclear spin of single ions.

*The authors gratefully acknowledge funding from the National Science Foundation and the Institute for Quantum Information and Matter.
**4:18PM P11.00008: Characterization of epitaxially grown Er doped Y2O3 for quantum optics applications**

KUMAR SINGH (Presenter), University of Chicago, KHAN ALAM, TJANA RAJH, Argonne National Laboratory, TIAN ZHONG, University of Chicago, SUPRATIK GUHA, Argonne National Laboratory — Rare earth ions (REI) are strong candidates for optical quantum memory applications. Erbium, with optical transition in the 1.5 μm band is of particular interest. Recent studies have shown coherence times exceeding 1 sec in 167Er. The coherence properties of REI are critically dependent on the host crystals, and methods of incorporating REI into the host structures play an important role as structural defects and impurities determine the local environment of the ions, which is an important factor contributing to line-broadening mechanisms.

Rare-earth oxides with low or no nuclear spin, such as CeO2 and Y2O3 are preferred host material for REI defects. The ability to tailor the properties of these systems on demand will be a powerful tool for quantum information applications. Molecular beam epitaxy (MBE) allows us to grow single crystal thin epitaxial films of certain RE oxides, and also enables precise control over the doping concentrations. We have investigated Er-doped Y2O3 thin films, grown epitaxially on Si(111) MBE. A range of concentration is explored. Characterization results using EPR, XRD and photoluminescence are reported. The influence of oxygen vacancies on EPR lines is also discussed.

*The authors acknowledge funding support form the CNM at Argonne and EFRC.

**4:30PM P11.00009: Precisely Located Si Vacancies in 4H-SiC Generated via Focused Li-ion Beam for Quantum Information Science Applications**

SHOJAN PAVUNNY (Presenter), ASEE Research Fellow at U.S. Naval Research Laboratory, 4555 Overlook Ave SW, Washington DC 20375, USA, EDWARD S BIELEJEC, Sandia National Laboratories, Albuquerque, New Mexico 87185, USA, SAMUEl CARTER, Electronics Science & Technology Division, U.S. Naval Research Laboratory, 4555 Overlook Ave SW, Washington DC 20375, USA, HUNTER BANKS, NRC Research Fellow at U.S. Naval Research Laboratory, 4555 Overlook Ave SW, Washington DC 20375, USA, RACHAEL MYERS-WARD, Electronics Science & Technology Division, U.S. Naval Research Laboratory, 4555 Overlook Ave SW, Washington DC 20375, USA, PAUL BARRY KLEIN, KeyW Corp., Arlington, VA 22203, MATTHEW T DEJARLD, ASEE Research Fellow at U.S. Naval Research Laboratory, 4555 Overlook Ave SW, Washington DC 20375, USA, ALLAN S BRACKER, EVAN RICHARD GLASER, DAVID KURT GASKILL, Electronics Science & Technology Division, U.S. Naval Research Laboratory, 4555 Overlook Ave SW, Washington DC 20375, USA — Photo-stable and spin (S = 3/2) coherent silicon vacancies (VSi) in the CMOS compatible semiconductor SiC are of interest for future applications in scalable quantum information and sensing. The ability to precisely create the desired density at the optimal location in a three-dimensional solid-state matrix with nanometer accuracy and excellent optical properties is indispensable for the above applications. Here we demonstrate the precise generation of single and ensemble emitter arrays in defect-free epitaxial 4H-SiC layer through Li-ions, implanted with an energy of 100 keV and doses ranging from $10^{12}-10^{15}$ Li/cm$^2$ using a maskless focused ion beam technique (~25 nm diameter spot positioned with ~25 nm accuracy and having anion travel depth of ~400 nm). High-resolution photoluminescence (E.LC) studies revealed the scalable and reproducible defect generation with a mean efficiency of ~17% and intensity (~8 kC/s), yield (~28%), statistical distribution, average number of single VSi/spot, fluorescence saturation, and photostability of single emitters. Given the encouraging results, we will discuss utilizing this approach to implant single VSi into the mode maximum of SiC photonic crystal cavities with Purcell enhancement of zero-phonon line and increased photon indistinguishability.

**4:42PM P11.00010: Radiationless Creation and Patterning of Color Centers in Diamond**

PATRICK J MCQUADE (Presenter), ANDREW ELIAS-GONZALEZ, MATTHEW A GEBBIE, NICHOLAS A MELOSH, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory — Spatially patterned and scalable creation of optical color centers remains a key bottleneck in fabrication for quantum computing and quantum sensing applications. Host lattice vacancies are necessary to form electronic defect states with transition energies in the visible light range. Current fabrication methods use high-energy ion irradiation to create these vacancies, leading to significant lattice damage and limited spatial control. I will present a new approach for creation and patterning of color centers in diamond without the use of irradiation. We demonstrate vacancy doping into diamond through the use of “vacancy injection” films. We also show the ability to pattern color centers on the nanoscale by using conventional photolithography to pattern film deposition. These methods enable a higher level of control for color center creation and decreased host lattice damage, as compared to methods that rely on high-energy irradiation. Additionally, this method provides a general strategy for controllably doping vacancies into a wide range of materials using conventional CMOS processing techniques, with potential applications in microelectronics and 2-D magnetic materials.

*This work was supported by the Department of Energy, BES, MSE Division.
Strongly Extended Superradiance in Optical Dirac Cone Metamaterials

OLIVIA MELLO (Presenter), Harvard University, YANG LI, Tsingua University, PHILIP CAMAYD-MUNOZ, Physics, California Institute of Technology, LINBO SHAO, CLEAVEN CHIA, ERIC MAZUR, MARKO LONCAR, Harvard University — Zero index metamaterials (ZIM) experience near-perfect spatial coherence and infinite spatial wavelength.[1] We design and simulate a diamond metamaterial with zero refractive index at 737 nm. This occurs due to a Dirac cone within the dispersion of our metamaterial. With this property we analytically and numerically demonstrate the hallmarks of superradiance: an N^2 scaling of enhancement of power within our structure over a spatial extent much greater than a wavelength, where N is the number of emitters, as well as cooperative decay rate enhancement relative to the single emitter decay rate. Additionally, we demonstrate preliminary fabrication results with the intention to experimentally implement this concept using silicon vacancy centers (SiV) in diamond.


Electron-electron interactions in highly degenerately doped embedded Si:P delta layers in silicon produced by variable PH3 dosing

JOSEPH HAGMANN (Presenter), XIQIAO WANG, RANJIT KASHID, PRADEEP NAMBOODIRI, JONATHAN WYRICK, SCOTT W SCHMUCKER, NEIL ZIMMERMAN, M. D. STEWART, RICHARD M. SILVER, CURT A RICHTER, National Institute of Standards and Technology — Key to producing quantum computing devices based on the atomistic placement of dopants in Si by STM lithography is the formation of embedded highly doped Si:P delta layers (δ-layers). This study investigates the transport behavior and the electron-electron interaction (EEI) physics in the highly doped regions of embedded Si:P-based devices by means of self-consistent magnetotransport (MT) measurements. In earlier work, we demonstrated that a careful MT study at low T, along with analysis of the weak localization (WL) signal, allows us to extract parameters associated with the electronic transport that offer a meaningful quantitative characterization of δ-layer quality and dopant diffusion. We build on this work by examining EEI behaviors in a set of samples with embedded Si:P delta layers produced with different PH3 exposure procedures prior to Si encapsulation. We show that the charge carriers behave as 2DEGs in embedded Si:P δ-layers in samples grown with a locking layer (LL) to bolster confinement of the dopants, while samples grown without a LL demonstrate several signatures of transport and EEI in a 3D system. The impact between δ-layer confinement and EEI on screening lengths affects both electrostatic gating of and tunneling transport through Si:P single atom transistors.

Atomic Scale Patterned Arsenic in Silicon

TAYLOR STOCK (Presenter), MARCEL VAN LOON, University College London, OLIVER WARSCHKOW, The University of Sydney, EMILY HOFMANN, ELEANOR CRANE, STEVEN SCHOFIELD, NEIL J CURSON, University College London — Over the past two decades, scanning tunnelling microscopy - hydrogen desorption lithography (STM-HDL) has been developed and utilized to great effect. Atomic scale devices can now be fabricated by positioning phosphorus (P) atoms in a silicon (Si) surface with near atomic precision. Expanding STM-HDL fabrication to include multiple species of dopant impurity atoms could provide new possibilities for device structure and function. Working towards expanding the materials palette of STM lithography, we have examined the compatibility of arsenic (As) with STM-HDL. We have studied AsH3 adsorption on Si(001) and Si(001)-H, and compared this to the well-studied Si(001)-PH3 system (used in 2D patterning of P in Si). We observe a number of subtle, but important differences between these two systems and discuss possible implications for advanced device fabrication strategies. In addition to the adsorption behaviour of the AsH3 molecules on the Si surface, we also discuss the incorporation and encapsulation of patterned 2D As within the Si lattice, and the optimization of electrical transport properties of As delta-layers in Si. Finally, we demonstrate nanoscale device structure patterning in Si using the two unique donor species (P and As) within a single 2D plane.

*Funded by the EPSRC.
2:30PM P12.00001: Scanning Probe Microscopy of Inhomogeneous States in 2D Materials† LAVISH PABBI (Presenter), RIJU BANERJEE, TOMOTAROH GRANZIER-NAKAJIMA, ANNA BINION, MAURICIO TERRONES, ERIC HUDSON, Pennsylvania State University — The ability of the Scanning Tunneling Microscope (STM) to study material surfaces with atomic resolution makes it a perfect tool for measuring local structural and electronic properties and their relationships. This ability is especially beneficial in the investigation of 2D materials, whereby their very nature there are frequently large variations in local structure, for example due to strain or changing substrate interactions, leading to concomitant variations in local electronic properties. As one example, I will here present results of recent STM measurements of single-layer graphene on copper, and on the graphene nano-ribbons that form when draped over copper step edges. In particular, I will focus on the interesting measurement challenge presented by the topological nature of the states that arise at the edges of these and other systems.

*This material is based upon work supported by the National Science Foundation under Grant No. 1229138

2:42PM P12.00002: Isotropic charge screening of the anisotropic black phosphorus revealed by potassium adatoms ZHEN TIAN (Presenter), JIAMIN XUE, ShanghaiTech University — Recent angle-resolved photoemission spectroscopy and transport experiments have shown that at the macroscopic level the electronic structure of black phosphorus can be greatly modified by potassium adatoms. Understanding the effects of individual potassium adatoms at the microscopic level is of great importance. To this end, we use scanning tunneling microscopy to study black phosphorus with potassium adatoms. We find that the potassium atoms are almost fully ionized even at 4.5 K. The Fermi level of black phosphorus is shifted due to electron doping while the band gap shows no significant change. Due to the puckered anisotropic lattice structure, we find that potassium ions can easily migrate along the zigzag direction but not along the armchair direction. Using tip as a moving gate, we can control the ionization of potassium ions. With this technique, we probe the screening effect of charged impurities in black phosphorus at the atomic scale. Remarkably, we find that it shows in-plane isotropic screening behavior even though the underlying electronic dispersion and lattice structure has distinct anisotropy. We also construct two potassium-adatom clusters as a coupled system to study the interaction of them. These results reveal the rich anisotropic physics in black phosphorus.

2:54PM P12.00003: Substrate screening effects on the quasiparticle band gap and defect charge transition levels in MoS2. MIT NAIK (Presenter), MANISH JAIN, Department of Physics, Indian Institute of Science, Bangalore — Monolayer MoS2 has emerged as an interesting material for nanoelectronic and optoelectronic devices. The effect of substrate screening and defects on the electronic structure of MoS2 are important considerations in the design of such devices. We find a giant renormalization to the free-standing quasiparticle band gap in the presence of metallic substrates, in agreement with recent scanning tunneling spectroscopy and photoluminescence experiments. Our sulfur vacancy defect calculations using the DFT+GW formalism, reveal two CTLs in the pristine band gap of MoS2. The (0/-1) CTL is significantly renormalized with the choice of substrate, with respect to the pristine valence band maximum. The (+1/0) level, on the other hand, is pinned 100 meV above the pristine VBM for the different substrates. This opens up a pathway to effectively engineer defect charge transition levels in 2D materials through choice of substrate.

3:06PM P12.00004: Scanning Tunneling Microscopy Study of Epitaxial Growth of Wafer Scale, Single Atomic Sheet Honeycomb BeO Two-dimensional Insulator† MADISEN HOLBROOK (Presenter), University of Texas at Austin, HUI ZHANG, Physics, University of Science and Technology of China, FEI CHENG, HYOUNGDO NAM, MENGKE LIU, University of Texas at Austin, CHI-RUEI PAN, Physics, Georgia Institute of Technology, DAMIEN WEST, SHENGBAI ZHANG, Physics, Rensselaer Polytechnic Institute, MEI-YIN CHOU, Physics, Georgia Institute of Technology, CHIH-KANG SHIH, University of Texas at Austin — We report the discovery of a novel 2D insulator comprised of a single atomic sheet honeycomb structure BeO, though its bulk counterpart has a wurtzite structure. Such a single sheet of BeO is grown epitaxially on Ag(111) thin films, also epitaxially grown on Si(111) wafers. Using scanning tunneling microscopy and spectroscopy (STM/S) we observe this novel BeO atomic sheet has a lattice constant of 2.65 Å and a band gap of 6 eV. We also found the BeO has a weak van der Waals (vdW) interaction with the Ag(111) substrate, which agrees well with predictions of our density functional theory calculations. Moiré pattern analysis shows the BeO honeycomb structure maintains long range phase coherence in atomic registry even across Ag steps. This novel material provides a scalable platform for 2D electronics, as an attractive 2D insulator due to its potentially much higher thermal conductivity than that of hBN. More significantly, the ability to create a single crystalline atomic sheet with no bulk counterpart of similar structure opens a new avenue toward tailoring novel 2D electronic materials.

*Our research was funded by grants from the Welch Foundation (F-1672), the US National Science Foundation (MRSEC DMR-1720595, EFMA-1542747, DMR-1808751) and the US Airforce (FA2386-18-1-4097).
3:18PM P12.00005: The Band Structure and Contact Issues of Quasi One Dimensional TiS₃  SIMEON GILBERT
(Presenter), Physics, University of Nebraska - Lincoln, HEMIAN YI, Synchrotron SOLEIL, TAKASHI KOMESU, Physics, University of Nebraska - Lincoln, ALEXEY LIPATOV, Chemistry, University of Nebraska - Lincoln, GUANHUA HAO, ANDREW J YOST, Physics, University of Nebraska - Lincoln, ALEXANDER SINITSKII, Chemistry, University of Nebraska - Lincoln, JOSE AVILA, CHAOYU CHEN, MARIA ASENSIO, Synchrotron SOLEIL, PETER A DOWBEN, Physics, University of Nebraska - Lincoln — Titanium trisulfide (TiS₃) is a transition metal trichalcogenide whose atoms form chains of trigonal prisms creating a quasi-one-dimensional structure. This 1D structure results in an anisotropic band structure and edge perfection that can reduce the edge scattering effects experienced in sub 10 nm field-effect transistors. Furthermore, a recent theoretical study indicates that monolayer TiS₃ is a direct-gap semiconductor with a bandgap of ~1 eV and an electron mobility near 10,000 cm²V⁻¹s⁻¹ making TiS₃ an ideal candidate for high mobility transistors. Our recent work directly measured the in-plane anisotropy of few layer TiS₃ flakes using nanospot angle resolved photoemission spectroscopy. The effective hole mass at the top of the valence band was found to be -0.95 ± 0.09 mₑ along the chain direction and -0.37 ± 0.1 mₑ perpendicular to the chain direction. The measured mobility for TiS₃ transistors has remained well below the predicted value, but it is common for contact issues to lower the measured mobility. The interactions between TiS₃ and Au or Pt contacts have been investigated using x-ray photoemission spectroscopy which shows that strong bonding with sulfur is the key to prevent Schottky barrier formation.

3:30PM P12.00006: Bulk compressibility measurements of WSe₂ heterostructures  QIANHUI SHI (Presenter), EN-MIN SHIH, Physics, Columbia University, DANIEL A RHODES, BUMHO KIM, Mechanical Engineering, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, JAMES HONE, Mechanical Engineering, Columbia University, CORY R DEAN, Physics, Columbia University — 2D semiconductors have attracted a great deal of attention due to their unique properties including strong spin-orbit coupling, large effective mass and high tunability. However, quantum transport studies have been complicated by the difficulties in making Ohmic contacts. Non-ideal contacts also limit studies in more complex structures such as twisted bilayers and double-layers which may host interesting correlated phases. Here we report on magneto-capacitance measurements on WSe₂ heterostructures which probe the bulk electronic compressibility. This approach has a much lower requirement on the contact quality and allows improved resolution of both zero-field and finite field features, and over a wider range of density than previously accessible.

3:42PM P12.00007: Flavor Symmetry and Ferroelectric Nematics in Transition Metal Dichalcogenides*  PATRICK CHEUNG (Presenter), ZHI-QIAN BAO, FAN ZHANG, University of Texas at Dallas — Recent magneto-transport experiments have provided compelling evidence for the presence of an energetically isolated threefold Q-valley degeneracy in few-layer transition metal dichalcogenides. We study the flavor SU(3) symmetry breaking when each Landau level triplet is one-third filled or empty and predict that a pure flavor nematic phase and a flavorless charge-density-wave phase will occur respectively below and above a critical magnetic field. Surprisingly, electrons carry flavor-dependent electric dipole moments even at zero magnetic field, rendering the nematics ferroelectric, allowing electric-field manipulation of the flavors, and leading to the concept of flavortronics.

*Research was sponsored by the Army Research Office and was accomplished under Grant Number W911NF-18-1-0416.

3:54PM P12.00008: ARPES microscopy of hBN flakes*  ROLAND KOCH (Presenter), Advanced Light Source, Lawrence Berkeley National Laboratory, JYOTI KATOC, Department of Physics, Carnegie Mellon University, SIMON K MOSER, DANIEL SCHWARZ, Advanced Light Source, Lawrence Berkeley National Laboratory, ROLAND KAWAKAMI, Department of Physics, The Ohio State University, AARON BOSTWICK, ELI ROTENBERG, CHRIOS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Laboratory, SOREN ULSTRUP, Department of Physics and Astronomy, Aarhus University — Hexagonal boron nitride (hBN) is an essential component in van der Waals heterostructures. It provides high-quality and weakly interacting interfaces that preserve the electronic properties of adjacent materials. We will present the full valence-band (VB) electronic structure of micrometer-sized exfoliated flakes of hBN using angle-resolved photoemission spectroscopy with micrometer and nanometer spatial resolution. We identify the π - and σ -band dispersions, the hBN stacking order, and determine a total VB bandwidth of 19.4 eV. We compare these results with electronic structure data for epitaxial hBN on graphene on silicon carbide grown in situ using a borazine precursor. The epitaxial growth and electronic properties are investigated using photoemission electron microscopy. Our measurements show that the fundamental electronic properties of hBN are highly dependent on the fabrication strategy.

*We acknowledge funding support by the DAAD, the Danish Council for Independent Research (DFF-4090-00125), the VIL-LUM FONDEN (15375), the Swiss National Science Foundation (P300P2-171221) and the NSF-MRSEC (DMR-1420451). The Advanced Light Source is supported by the Director, Office of Science, BES, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
4:06PM P12.00009: Large-Area Epitaxial Growth of Curvature-Stabilized ABC Trilayer Graphene with Tunable Band Gap* ZHAOLI GAO (Presenter), University of Pennsylvania, SHENG WANG, University of California at Berkeley, JOEL M BERRY, QICHENG ZHANG, JULIAN GEBHARDT, WILLIAM PARKIN, University of Pennsylvania, JOSE AVILA, HEMIAN YI, CHAOYU CHEN, Synchrotron-SOLEIL, SEBASTIAN HURTADO PARRA, MARIJA DRNDIĆ, ANDREW RAPPE, DAVID SROLOVITZ, J. M. KIKKAWA, University of Pennsylvania, ZHENGTANG LUO, Hong Kong University of Science and Technology, MARIA C. ASENSIO, Synchrotron-SOLEIL, FENG WANG, University of California at Berkeley, ALAN T JOHNSON, University of Pennsylvania — The physical properties of epitaxially-grown layered van der Waals (vdW) materials can be engineered to an extraordinary degree by manipulating the number of atomic layers, their compositions, and their relative stacking configurations and twist angles. vdW trilayer graphene (TLG) can stack in either a semi-metallic ABA configuration or a semi-conducting ABC configuration with a gate-tunable band gap but to this point has only been produced via exfoliation, which greatly limits its scientific and technological development. Here we present a scalable approach to epitaxial TLG growth via chemical vapor deposition that reliably enhances the fraction and size of ABC stacked TLG domains compared to other methods. The key insight is that nanoscale substrate curvature can locally stabilize ABC domains, typically leading to alternating regions of ABC and ABA on topographically corrugated growth substrates. Unambiguous electronic signatures of ABC-TLG were revealed by nano angle-resolved photoemission spectroscopy and infrared scanning near-field microscopy. The ABC fraction remains high after transfer onto a device substrate, as confirmed by transport measurements showing a sizable and tunable ABC-TLG band gap.

*This work was supported by the NSF EFRI 2-DARE 1542879.

4:18PM P12.00010: Spin and valley degree of freedom in a bulk massless-Dirac electron system, α-(BEDT-TTF)$_2$I$_3$ under magnetic fields KAZUYA MIYAGAWA (Presenter), MATSUNO MANABU, Applied Physics, University of Tokyo, MICHIHIRO HIRATA, IMR, Tohoku University, TAMURA MASAFUMI, Physics, Tokyo University of Science, KAZUSHI KANODA, Applied Physics, University of Tokyo — Since the discovery of massless-Dirac Fermions (MDF) in graphene, MDF states have found in a range of materials. A quasi-2D organic conductor, α-(BEDT-TTF)$_2$I$_3$, in which a MDF phase appears under pressure. The bulk nature of α-(BEDT-TTF)$_2$I$_3$ enables one to investigate the properties by experimental probes that require sample volume, such as NMR. When the magnetic field is applied normal to the 2D planes of MDFs, the orbital-quantized Landau levels (LLs) contains the n=0 state (zero mode LL). The MDF system has two degrees of freedom, spin and valley. In case of non-zero fields, there are two possible states, depending on which of spin- or valley-splitting dominates over the other in energy, that is, spin polarized (QHF) and a non-magnetic state (QHI).

We measured $^{13}$C NMR with a magnetic field applied perpendicular to the 2D layers. With decreasing temperature, the shift of spectra decreases, since the thermal-averaged density of state characteristic of Dirac cones decreased. At low T, the NMR shift increases because of the formation of the zero-mode LL. Upon further cooling, a large NMR shift is observed, which indicates the generation of local fields. The value of the shift agrees with the value estimated from the Zeeman spin splitting of the zero-mode LL, indicating the QHF state.

4:30PM P12.00011: Strain-dependent ab-initio tight binding Hamiltonians for T-type transition metal dichalcogenides* DANIEL LARSON (Presenter), SHIANG FANG, WEI CHEN, JENNIFER COULTER, STEVEN TORRISI, STEPHEN CARR, EFTHIMIOS KAXIRAS, Harvard University — Many transition metal dichalcogenides (TMDs) adopt a T-structure in which the metal atom is octahedrally coordinated by the chalcogens. In particular, MX$_2$ with M=(Nb, Ta, Ti) and X=(S, Se) all exhibit fascinating electronic properties including various charge density wave phases. Using Density Functional Theory followed by a Wannier transformation we extract the strain-dependent tight binding parameters for single-layer TMDs. The resulting tight binding Hamiltonian respects the crystal symmetry and gives a very accurate yet simple description of the electronic band structure which is easily augmented to include spin-orbit effects and interlayer couplings. The knowledge of the strain dependence of the electronic properties is critical in order to correct for the effects of relaxation in realistic simulations of twisted nanostructures.

*This work was supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319 and by ARO MURI Award W911NF-14-0247. We used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by NSF Grant No. ACI-1053575 and the Odyssey cluster supported by the FAS Division of Science, Research Computing Group at Harvard University.
Interplay between p- and d- orbitals yields multiple Dirac states in two-dimensional ZrB2 and CrB4

ALEJANDRO LOPEZ BEZANILLA (Presenter), Los Alamos National Laboratory — Theoretical evidence of the existence of 12 Dirac cones in the low-spectrum diagram of transition metal-rich monolayered hexagonal networks is provided. Both Zr and Cr are efficient in creating six additional cones with respect to graphene when combined with boron honeycomb lattices. The four d-electrons of Cr, and similarly the two d-electrons of Zr, are yielded to the B sublattices creating an isoelectronic structure to graphene where the interplay between p- and d-orbitals leads to the appearance of Dirac states on both one- and two-dimensional geometries. Ab initio calculations show that, although spin–orbit interaction splits the cone-shaped valence and conduction bands, monolayered ZrB2 and CrB4 are semimetals with compensated electron–hole pockets.

The effect of the adsorption of the toxic hydrazine on the electronic structure of the WS2 monolayer: the first principle calculations

MD RAJIB KHAN MUSA (Presenter), CONGYAN ZHANG, ADEL ALRUQI, GAMINI SUMANASEKERA, MING YU, Physics and Astronomy, University of Louisville — Two-dimensional layered WS2 possesses novel electronic properties and has various promised applications. Its sensitivity to various molecules [1] makes it possible as sensor. Our recent experiment results show that its resistance changes dramatically with the response to the toxic hydrazine vapor. Our first-principle calculations also found the effect of the adsorption of the hydrazine on the electronic structure of WS2 monolayer. In particular, the impurity state associated with the toxic hydrazine just pin at the middle of the band gap, resulting to an n-type like behavior. A detail discussion will be presented. References: [1] Changjie Zhou, Weihuang Yang, and Huili Zhu, J. Chem. Phys. 142, 214704 (2015).

Symmetry controlled adsorption of di-iodobenzene on MoS2

ZAHRA HOOSHMAND

GHAREHBAGH (Presenter), Physics, University of Central Florida, PRESCOTT E EVANS, Physics and Astronomy, University of Nebraska-Lincoln, DUY LE, Physics, University of Central Florida, PETER A DOWBEN, Physics and Astronomy, University of Nebraska-Lincoln, TALAT S. RAHMAN, Physics, University of Central Florida — In a joint experimental and theoretical study, we have uncovered evidence of the importance of symmetry in the adsorption of the isomers of di-iodobenzene on MoS2(0001). The intensity ratio of iodine to molybdenum measured, as a function of exposure for different isomers of the diiodobenzene, show that while for ortho (1,2-) and para (1,4-) di-iodobenzene the rate of adsorption at 100 K is very low, that for meta (1,3-)di-iodobenzene is considerably more facile. We have applied van der Waals corrected density functional theory based calculations to understand the subtleties in the electronic structure and geometry of adsorption of these three di-iodobenzene isomers on MoS2(0001). All three are found to weakly chemisorb onto MoS2(0001) with the same binding strength as well as adopt similar configurations. The calculated electron affinity of the three molecules also do not show a specific trend that would verify experimental data. However analysis of the frontier orbitals indicate that those of 1,3-di-iodobenzene is strongly affected by interactions with MoS2, while that of the other two isomers remain unchanged. Our results show that symmetry is the identifying factor in the adsorption characteristics of di-iodobenzene on MoS2.

Portable Surface-Enhanced Raman Spectroscopy of Pyridine and Diazines on MoS2

ROBERT HART (Presenter), SHARAD AMBARDAR, PRASANA SAHOO, DMITRI VORONINE, University of South Florida — Raman spectroscopy is a widely used analytical technique for biosensing applications. It has been commonly applied to bulk samples. However, the applications to small amounts of chemical substances is challenging due to weak signals. Surface-enhanced Raman scattering (SERS) can be used to improve sensitivity by the electromagnetic enhancement mechanism using plasmonic nanoparticles or by the chemical mechanism using atomically-thin semiconducting 2D materials. Also, portable Raman spectroscopy instrumentation is needed for medical and industrial point-of-care applications. We investigate the effects of the addition of few-layer molybdenum disulfide (MoS2) nanocrystals on the enhancement of Raman signals of pyridine and its diazine derivatives. The introduction of MoS2 leads to the shifts of the Raman peak positions and changes in the relative peak intensities and overall signal strength of respective ν1 mode for each of the diazines and pyridine, as well as affecting a range of other modes for each compound, observed using a handheld Raman spectrometer, an effect most apparent in the pyrimidine ν1 mode. This information can be valuable to a number of potential fields including studies in biophotonics, which could have numerous industrial, medical and public safety applications.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM
2:30PM P13.00001: Effect of MoS₂ thickness on properties of adsorbed Au nanoparticles*  
DUY LE (Presenter), TALAT S. RAHMAN, Department of Physics, University of Central Florida — Transition metal nanoparticles supported by MoS₂ is a system of interest in catalytic applications. The question whether the thickness of MoS₂ plays any critical role in determining the chemical activity of the supported nanoparticle is still debated. In this work, using density functional theory based calculations, we study the electronic density of states of Au nanoparticles of varying size supported by single layer, bilayer, and trilayer MoS₂. We find that thickness of MoS₂ support has only a minor effect on the d states (frontier orbitals) of Au nanoparticles. This effect is most notable on Au atoms located at the perimeter of the nanoparticles, which are in contact with the MoS₂ basal plane. Using CO oxidation as a prototype, we comment on the implication of these findings on catalytic properties of MoS₂-supported Au nanoparticles and compare with available experimental data.

*This work is supported in part by DOE grant DEFG02-07ER15842

2:42PM P13.00002: A complete picture for the band topology in twisted bilayer graphene  
JIANPENG LIU (Presenter), JUNWEI LIU, XI DAI, Department of Physics, Hong Kong University of Science and Technology — We provide a complete picture for the band topology of twisted bilayer graphene. We propose that the electronic structure of twisted bilayer graphene can be understood as Dirac fermions under pseudo magnetic fields generated by the moiré pattern. The two low-energy flat bands from each valley originate from the two zeroth Landau levels of Dirac fermions under such opposite effective magnetic fields. They possess opposite sublattice polarizations and are decoupled from each other as a result of an emergent chiral symmetry in the low-energy subspace. They carry opposite Chern numbers ±1 and give rise to the odd windings of the Wilson loops.

Besides, we show that all the high-energy bands below or above the flat bands are also topologically nontrivial in the sense that the sum of their Berry phases is quantized as ±π. Such quantized Berry phases give rise to two nearly flat edge states, which are robust regardless of the orientation of the edge but depend on truncations on the moiré scale. In addition, we also find the atomic corrugations would significantly enlarge the topological gaps, and may drive transitions between topological insulating and semimetallic phases.

2:54PM P13.00003: Functionalization of hexagonal boron nitride – effect on chemical, morphological, electrical and thermal properties*  
EVGENIYA LOCK (Presenter), Materials Science and Technology Division, Naval Research Laboratory, KARTHIK SRIDHARA, Electronics Science and Technology Division, Naval Research Laboratory, ZARIANA MOBLEY, Materials Science and Technology Division, Naval Research Laboratory, LUKE NYAKITI, Materials Science and Engineering, Texas A&M, BORIS FEIGELSON, Electronics Science and Technology Division, Naval Research Laboratory, DAVID OLSON, JOHN GASKINS, PATRICK HOPKINS, Mechanical and Aerospace Engineering, University of Virginia — Hexagonal boron nitride (h-BN) has gained significant importance in plasmonics and quantum electronics applications. In addition, there is a plethora of theoretical, yet relatively few experimental studies, showing modification of h-BN properties via functionalization, namely through induction of magnetism and band gap engineering. In this effort we show h-BN films functionalization with three different compounds. Chemical, morphological and structural characterization is performed using X-ray photoelectron spectroscopy, Fourier transform infrared reflection absorption spectroscopy, as well as scanning and transmission electron microscopies. This characterization quantifies the elemental composition changes and shows preferential molecular binding towards the edges of the grains after functionalization. In addition, we perform conductive atomic force microscopy studies and thermal boundary conductance mapping to assess the changes in interfacial thermal properties. All of these characterization methods contribute toward the overarching goal of evaluating the potential of functionalized h-BN for practical applications.

*This work was partially supported by the Office of Naval Research through Naval Research Laboratory Base Program.
3:06PM P13.00004: Density of States of Graphene Doped with Transition Metals*  SHOHAM SEN (Presenter), KAUSHIK DAYAL, Civil and Environmental Engineering, Carnegie Mellon University, YANG WANG, Pittsburgh Super Computing, Carnegie Mellon University — We perform electronic structure calculations for Graphene using density functional theory based ab initio method with linear scaling Greens function approach, known as Locally Self Consistent Multiple Scattering Method (LSMS). The Greens function for the Kohn-Sham (KS) equation is solved in the framework of Multiple Scattering Theory (MST), in which the Greens function of the KS equations are calculated in terms of multiple scattering path matrices and single site solutions. The multiple scattering path matrix represents the electron scattering off the atoms in a crystal. By making an assumption of "near-sightedness" or "local interaction zone" of the electronic multiple scattering processes around each atom, the computational cost for calculating the Green function is reduced from O(N^3) to O(N), where N is the number of atoms in the unit cell. We apply the LSMS method to the study of density of states and magnetic structure of Graphene doped with Cobalt.

*We would like to thank the DOD MURI program for financial support.

3:18PM P13.00005: Electronic transport in graphene decorated with adatoms or nanoparticles*  JAMIE ELIAS (Presenter), JOSHUA COHEN, Physics, Washington University, St. Louis, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Material Science, FUDONG WANG, WILLIAM BUHRO, Chemistry, Washington University in St. Louis, ARASHDEEP S THIND, ROHAN MISHRA, Mechanical Engineering and Material Science, Washington University in St. Louis, ERIK HENRIKSEN, Physics, Washington University, St. Louis — There is much interest in inducing a spin-orbit coupling into monolayer graphene in order to engineer the Kane-Mele Hamiltonian and thereby enable observation of the quantum spin Hall effect in graphene. Numerous adatoms have been studied toward this end. Here, we present measurements of monolayer graphene Hall bars with dilute coatings of either osmium adatoms or Bi₂Te₃ nanoparticles (NPs). With osmium adatoms, we find an unusual hole doping to occur, whereas most metals show electron doping. Nanoparticles of Bi₂Te₃ have recently been reported to yield possibly quantized transport [1]. We use high quality NPs, monodispersed with diameters of ~15 nm. Transport is studied after depositing the nanoparticles, and again after an argon anneal to remove the polyvinylidene fluoride coating on the NPs. In this case a small electron doping response is observed. Further measurements on higher density coatings of both osmium adatoms and Bi₂Te₃ nanoparticles will be discussed.


*Sigma Xi Grant-in-Aid of Research
Sandia National Labs

3:30PM P13.00006: Nearly Flat Unoccupied State in Intercalated Graphene: Observation and Interpretation*  YI LIN (Presenter), GE CHEN, Columbia University, JERZY T. SADOWSKI, Brookhaven National Lab, YUNZHE LI, Columbia University, SAMUEL TENNEY, Brookhaven National Lab, JERRY DADAP, Columbia University, MARK HYBERTSEN, Brookhaven National Lab, RICHARD M OSGOOD, Columbia University — By using two-photon-photoemission, we observe a near-zero-dispersion empty state in oxygen-intercalated graphene-Ir interface, approximately 2.6 eV above the Fermi energy and near the Brillouin zone center. DFT method and band-unfolding technique are used to calculate the spectral weights for the graphene-Ir supercells with and without the intercalants. The calculations reproduce the measurements. Our analysis reveals the nature of the observed nearly flat band to be the replicates states from near the Dirac cone that have little dispersion due to trigonal warping. This interpretation is further supported by the results from angle-resolved photoemission. Our work explicitly demonstrates the persisting perturbation on the graphene even for the intercalated quasi-freestanding graphene. Our work demonstrates a pathway for tailoring the graphene electronic structure and generating nearly flat bands by using intercalation.

*We acknowledge support from the US DOE, Office of Basic Energy Sciences, under Contract Number DE-FG02-90ER14104. Our research used resources of the CFN and the NSLS-II, which are U.S. DOE Office of Science Facilities, and the Scientific Data and Computing Center, a component of the Computational Science Initiative, at BNL, under Contract No. DE-SC0012704.
3:42PM P13.00008: Photo-oxidation: Finding the Ambient Air Oxidation Mechanism of WS$_2$*  
JIMMY KOTSAKIDIS (Presenter), Physics and Astronomy, Monash Univ, QUANHUI ZHANG, Civil Engineering, Monash University, AMADEO LOPEZ VAZQUEZ DE PARGA, Condensed Matter Physics, Autonoma de Madrid, SHAUN JOHNSTONE, CHANGXI ZHENG, Physics and Astronomy, Monash Univ, MARC CURRIE, U.S. Naval Research Laboratory, KRISTIAN HELMERSON, Physics and Astronomy, Monash Univ, DAVID KURT GASKILL, U.S. Naval Research Laboratory, MICHAEL FUHRER, Physics and Astronomy, Monash Univ — Monolayer WS$_2$ exhibits exceptional optical and electronic properties, however, it also oxidizes in ambient conditions leading to the degradation of its optical and electrical performance over time.

In this work, we reveal that the oxidation of WS$_2$ in ambient conditions is driven by bandgap photo-excitation (i.e. a photo-oxidation effect) and we describe a possible oxidation chemical reaction pathway. Through a series of controlled experiments, WS$_2$ monolayers grown via chemical vapor deposition were exposed to low power light ($10^3$ to $10^4$ mW/m$^2$) with wavelengths of 532nm, 650nm and 760nm for 7 days. Our findings suggest that WS$_2$ is only oxidised in ambient conditions when exposed to light with enough energy to excite an optical bandgap transition.

Furthermore, we find that even limited exposure to above-bandgap illumination in ambient – at levels routine for photoluminescence or Raman spectroscopy characterization – causes significant oxidation. We predict that this photo-oxidation effect may be universal across all monolayer semiconducting transition metal dichalcogenides, and thus, these results could have far reaching consequences to past, present and future studies.

*We acknowledge support from the Australian Research Council grant DP150103837 and the U. S. Office of Naval Research
ZHIMING WANG, Institute of Fundamental and Frontier Sciences, University of Electro-dissociated oxygen from the SiO2 substrate. Oxygen is released from underneath the substrate and etches the graphene

JIMING BAO, Department of Electrical and Computer Engineering, University of Houston, USA — Planar alignment of disc-like multilayer on 300nm thick SiO2/Si substrates. A recent mechanism was proposed in which the etching was due to transitions as the system goes through a series of local free-energy minima.

First-order transition. In particular, our results show that the transition can be viewed as a sequence of 2D structural transitions as the system goes through a series of local free-energy minima. We performed large-scale MD simulations based on reactive force field potentials to investigate the kinetics of this intriguing first-order transition. In particular, our results show that the transition can be viewed as a sequence of 2D structural transitions as the system goes through a series of local free-energy minima.

4:30PM P13.00011: Planar alignment of graphene sheets by a rotating magnetic field for full exploitation of graphene as a two dimension material* FENG LIN (Presenter), Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, China, GUANG YANG, Department of Materials Science and Engineering, University of Houston, USA, CHAO NIU, Department of Electrical and Computer Engineering, Baylor University, USA, YANAN WANG, ZHUAN ZHU, Department of Electrical and Computer Engineering, University of Houston, USA, HAOKUN LUO, School of Optical and Electronic Information, Huazhong University of Science and Technology, China, CHONG DAI, YANDI HU, Department of Civil and Environmental Engineering, University of Houston, USA, JONATHAN HU, Department of Electrical and Computer Engineering, Baylor University, USA, XUFENG ZHOU, ZHAOPING LIU, Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, China, ZHIMING WANG, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, China, JIMING BAO, Department of Electrical and Computer Engineering, University of Houston, USA — Planar alignment of disc-like nanomaterials is required to transfer their superior anisotropic properties from microscopic individual structures to macroscopic collective assemblies. However, such alignment by electrical or magnetic field is challenging due to their additional degrees of orientational freedom compared to that of rod-like nanostructures. Here, the realization of planar alignment of suspended graphene sheets using a rotating magnetic field produced by a pair of small NdFeB magnets and subsequent demonstration of high optical anisotropy and potential novel device applications is reported. Compared to partially aligned sheets with a static magnetic field, planar aligned graphene suspensions exhibit a near-perfect order parameter, much higher birefringence and anisotropic absorption/transmission. By immobilizing and patterning aligned graphene in a UV-curable polymer resin, we further demonstrated an all-graphene permanent display, which exhibits wide-angle, high dark-bright contrast in either transmission or reflection mode without any polarizing optics. The ability to control and pattern graphene orientation in all three dimensions opens up new exploration and broad device applications of graphene.

*China Scholarship Council, Welch Foundation, National Science Foundation

4:42PM P13.00012: Chemical enhancement of Raman scattering on graphene oxide in the quantum plasmonic regime SHARAD AMBARDAR (Presenter), DMITRI VORONINE, University of South Florida — Optoelectronic and mechanical properties of graphene oxide have been widely investigated. We observed two chemical enhancement mechanisms, one from the gold plasmonic tip via the tip-enhanced Raman spectroscopy (TERS) and the other from graphene oxide via the surface-enhanced Raman spectroscopy (SERS). We observed strong chemical enhancement from the gold plasmonic tip in the quantum plasmonic regime when the tip-sample distance is less than 1 nm. We improve the efficiency of the chemical enhancement by varying the tip-sample distance which allows us to clearly observe the effect of graphene oxide using nanoscale TERS imaging. Strong chemical enhancement can be used to improve the quality of sensors and nanophotonic devices on non-metallic substrates.

4:54PM P13.00013: Large-scale reactive molecular dynamics simulations of structural transitions in transition metal dichalcogenides COLE MILES (Presenter), CHUNRUO DUAN, DESPINNA LOUCA, GIA-WEI CHERN, University of Virginia — We present extensive molecular dynamics (MD) simulations of structural phase transitions in transition metal dichalcogenides (TMD). These quasi-two-dimensional materials are described by the general formula MX2 with M a transition metal atom (Mo, W, etc) and X a chalcogen atom (S, Se, Te). The crystal structure of a TMD consists of Van der Waals bonded layers, resembling that of graphene. TMDs are hosts of exotic quantum states with potential technological applications. Our work is motivated by recent experiments on MoTe2, showing diffuse scattering in the vicinity of the 1T'-Td structural transition which is indicative of stacking disorders resulting from layer misalignments along the c-axis. We performed large-scale MD simulations based on reactive force field potentials to investigate the kinetics of this intriguing first-order transition. In particular, our results show that the transition can be viewed as a sequence of 2D structural transitions as the system goes through a series of local free-energy minima.
5:06PM P13.00014: Angle-resolved photoemission spectroscopy on wet-transferred highly oriented MoS2 monolayers on HOPG substrates*  
WOOJOO LEE (Presenter), Physics, University of Texas at Austin, LI-SHUAN LU, WEI-CHEN CHUEH, WEN-HAO Chang, Electrophysics, National Chiao Tung University, CHIH-KANG SHIH, Physics, University of Texas at Austin — The ability to create a large area of monolayer 2D electronic materials with the same orientation on different substrates will play a very critical role for scalable flatland electronics. It has been shown that highly-oriented monolayer (ML) MoS2 can be grown on a carefully prepared sapphire substrate with nearly full coverage and transferred to different substrates [1]. However, it is still unclear whether such a transfer process will introduce unwanted defects that will affect the electronic structure. Here, we report successful preparation of high quality ML MoS2 transferred to HOPG substrates by using a wet transfer method. With a proper treatment, we reveal detailed electronic band structure using high resolution angle-resolved photoemission spectroscopy. Due to the fact that these MoS2 monolayers are highly oriented and interaction with a substrate is very weak [2], we are able to resolve the electronic band structure clearly including K point band splitting.


*Supported by Welch foundation F-1672, NSF MRSEC DMR-1720595, NSF EFMA-1542747, NSF DMR-1808751 and US AIRFORCE FA2386-18-1-4097

5:18PM P13.00015: Multifunctional nanoporous graphene  
ARAN GARCIA-LEKUE (Presenter), Donostia International Physics Center (DIPC), San Sebastian, Spain, CESAR MORENO, Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain, MANUEL VILAS-VARELA, Centro de Investigación en Química Biológica e Materiales Moleculares (CIQUS), Santiago de Compostela, Spain, BERNHARD KRETZ, Donostia International Physics Center (DIPC), San Sebastian, Spain, MARIUS V. COSTACHE, MARCOS PARADINAS, MIRKO PANIGHEL, GUSTAVO CEBALLOS, SERGIO O. VALENZUELA, Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain, DIEGO PEÑA, Centro de Investigación en Química Biológica e Materiales Moleculares (CIQUS), Santiago de Compostela, Spain, AITOR MUGARZA, Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain — Nanoporous graphene shows a great potential as an active component of field effect transistors and as an atom-thick selective molecular nanosieve. Recently, we have reported the bottom-up formation and electronic characterization of atomically precise nanoporous graphene comprising an ordered array of pores separated by ribbons, which can be tuned down to the one nanometer range [1]. Our combined Density Functional Theory (DFT) and Scanning Tunneling Spectroscopy (STS) study reveals a highly anisotropic electronic structure, where orthogonal one-dimensional electronic bands with an energy gap of ~1 eV coexist with a novel family of confined pore states. These properties can be tuned by changing, e.g. the size and morphology of the pore, making this 2D mesh a highly versatile semiconductor for simultaneous sieving and electrical sensing of molecular species. [1] C. Moreno et al., Science 360, 199 (2018)

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P14 DCMP: 2D Materials: Stack and Twist Theory  
BCEC 153C - Liujun Zou, Harvard University

2:30PM P14.00001: First-Principles Electronic Structure Investigation of 2D Twisted Bilayers  
ISHAAN KUMAR (Presenter), XUAN LUO, National Graphene Research and Development Center — Since the recent experimental observation of unconventional superconductivity in Twisted Bilayer Graphene (TBG) has brought 2D twisted materials to the front lines of research, there is a need to cover the underlying physics accurately and efficiently. We utilize the first-principles method to calculate both band structures and density of states (DOS) for various sized 2D twisted bilayers of Graphene, BN and MoS2. Our results reveal that introducing a twist opens a band gap, and Van Hove Singularities are seen symmetric to the dirac point in the DOS. The introduction of a twist angle in graphene also creates a parabolic band dispersion of the dirac cones, normally seen only in Bernal stacked graphene on account of strong stability and interlayer correlation. We evaluate the contribution of cell size to band structure by enlarging the unit cell from 2x2 to 12x12. The electronic properties of the smaller cell remains constant as the cell size increases. Furthermore, we treat a non-periodic 2D twisted bilayer by introducing a vacuum, from which we can draw parallels between the electronic structures and reveal the deep underlying physics.
2:42PM P14.00002: A multi-scale numerical approach to model two-dimensional layered materials* SHIANG FANG (Presenter), STEPHEN CARR, ZIYAN ZHU, EFTHIMIOS KAXIRAS, Harvard University — Since the discovery of single-layer graphene crystal, more different types of two-dimensional layered materials are exfoliated or synthesized. The theoretical modeling would guide the further design and understanding with these materials. We develop a multi-scale numerical approach to model these layers and their heterostructures. The microscopic modeling is based on the density functional theory (DFT) calculations followed by Wannier transformation to derive localized orbitals. These allow us to capture the effects from coupling with adjacent layers and the deformation within each layer from crystal relaxations. The faithful representation of the wavefunction characters also enables the computation of Berry curvatures and responses to external electric and magnetic fields.

*This work was supported by STC CIQM, NSF Grant No. DMR-1231319, and by ARO MURI Award No. W911NF-14-0247.

2:54PM P14.00003: Gate-Tunable Topological Flat Bands in Trilayer Graphene-Boron Nitride Moiré Superlattices* BHEEMA LINGAM CHITTARI (Presenter), Department of Physics, University of Seoul, Seoul 02504, Korea, GUORUI CHEN, Department of Physics, University of California at Berkeley, Berkeley, CA 94709, USA, YUANBO ZHANG, Institute for Nanoelectronic Devices and Quantum Computing, Fudan University, Shanghai 200433, China, FENG WANG, Department of Physics, University of California at Berkeley, Berkeley, CA 94709, USA, JEIL JUNG, Department of Physics, University of Seoul, Seoul 02504, Korea — We investigate the electronic structure of the flat bands induced by moiré superlattices and electric fields in nearly aligned ABC trilayer graphene-boron nitride interfaces where Coulomb effects can lead to correlated gapped phases. Our calculations indicate that valley-spin resolved isolated superlattice flat bands that carry a finite Chern number \( C = 3 \) proportional to layer number can appear near charge neutrality for appropriate perpendicular electric fields and twist angles. When the degeneracy of the bands is lifted by Coulomb interactions these topological bands can lead to anomalous quantum Hall phases that embody orbital and spin magnetism. Narrow bandwidths of \( \sim 10 \) meV achievable for a continuous range of twist angles \( \theta \leq 0.6^\circ \) with moderate interlayer potential differences of \( \sim 50 \) meV make the TLG/BN systems a promising platform for the study of electric-field tunable Coulomb interaction driven spontaneous Hall phases.


*We acknowledge support from Samsung through SSTF-BA1802-06, and the Korean NRF through NRF-2017R1D1A1B03035932 for B.L.C. and NRF-2016R1A2B4010105 for JJ. We also acknowledge ARO MURI award (W911NF-15-1-0447). and support from National Key Research Program of China (2016YFA0300703) for Y.Z.

3:06PM P14.00004: Composition and Stacking Dependent Topology in Bilayers from the Graphene Family* LILIA M WOODS (Presenter), ADRIAN POPESCU, Department of Physics, University of South Florida, PABLO RODRIGUEZ LOPEZ, Consejo Superior de Investigaciones Cienticas (CSIC), Instituto de Ciencia de Materiales de Madrid (ICMM) — We investigate from first-principles the electronic and structural properties of silicene, germanene, and stanene bilayers. Due to the staggering of the individual layers, several stacking patterns are possible, most of which are not available to the bilayer graphene. Our results reveal the appearance of distinct band features, including orbital hybridization and band inversion, and they are attributed to the combined effects of the composition, stacking, and to the presence of the spin-orbit coupling. It is found that particular arrangements give rise to topological features in the Hall response, offering new directions for exploring Dirac features in 2D systems.

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3:18PM P14.00005: Ultraflat bands and shear solitons in Moiré patterns of twisted bilayer transition metal dichalcogenides MIT NAIK, MANISH JAIN (Presenter), Department of Physics, Indian Institute of Science — Ultraflat bands in twisted bilayers of two-dimensional materials have potential to host strong correlations, including the Mott-insulating phase at half-filling of the band. Using first-principles density functional theory calculations, we show the emergence of ultraflat bands at the valence band edge in twisted bilayer MoS2, a prototypical transition metal dichalcogenide. The computed band widths are comparable to that of twisted bilayer graphene near ‘magic’ angles. Large structural transformations in the Moiré patterns lead to the formation of shear solitons at stacking boundaries and strongly influence the electronic structure. We extend our analysis for twisted bilayer MoS2 to show that flat bands can occur at the valence band edge of twisted bilayer WS2, MoSe2 and WSe2 as well.
3:30PM P14.00006: Topological phases and twisting of graphene on a dichalcogenide monolayer  
ABDULRHMAN ALSHARARI (Presenter), Physics Department, Tabuk University, MAHMOUD ASMAR, Department of Physics and Astronomy, Louisiana State University, SERGIO E ULLOA, Ohio University — Graphene placed in proximity to a transition metal dichalcogenide semiconductor monolayer has been shown to exhibit interesting modifications of its electronic properties. The role of incommensurability and a possible relative twist between layers require implementing a continuum model approach to fully investigate this multilayered system. Results of this model are in agreement with simplified approaches, such as the tight-binding model, that assumes commensurate supercells. We show that the misaligned system can also exhibit multiple different topological phases depending on the relative twist angle and applied gate voltages between the layers[1]. An interesting topological phase exhibits inverted bands which is robust to incommensurate structure effects. Using an effective Hamiltonian to fully describe the continuum model of graphene-TMD heterostructure reveals that a staggered potential and effective SOC are induced onto the graphene, which controls the appearance of the non-trivial topological phase. Our estimates suggest that the intrinsic SOC induced onto graphene deposited on typical TMDs is somewhat weak and must be enhanced by additional means, such as heavy metal intercalation, to achieve a tunable quantum spin Hall phase.


3:42PM P14.00007: Band nesting and valley exciton in monolayer MoS₂  
MACIEJ BIENIEK (Presenter), Department of Theoretical Physics, Wroclaw University of Science and Technology, LUDMILA SZULAKOWSKA, PAWEL HAWRYLAK, Department of Physics, University of Ottawa — We report the effect of band nesting on single valley excitons in monolayer MoS₂. We start with ab-initio based electronic structure obtained within tight binding model of MoS₂ [1]. We next turn on electron-electron interactions, form a Hartree-Fock ground state and construct electron-hole excitations. We compute e.-e. interactions, self-energy in the screened exchange and Coulomb hole approximation and direct and exchange electron-hole interaction. We solve Bethe-Salpeter equation to obtain exciton states and absorption spectrum. We disentangle effects of electron-hole dispersion, details of band structure on Coulomb intra/inter-valley interactions, topology, screening and dielectric environment. In particular, we discuss the effect of Q-points and band nesting on ground and excited states of excitons in MoS₂.


3:54PM P14.00008: A metal-insulator transition by hole doping in boron triangular Kagome lattice  
WOO HYUN HAN (Presenter), Department of Physics, KAIST, SUNGHYUN KIM, Department of Materials, Imperial College London, IN-HO LEE, Korea Research Institute of Standards and Science, KEE JOO CHANG, Department of Physics, KAIST — A flat band is the hallmark of a variety of exotic phases because electrons are confined in a narrow energy window with a very high density of states. Recently, much attention has been paid to magic-angle twisted bilayer graphene which possesses a flat band feature and exhibits strongly correlated and unconventional superconducting phases. This experiment indicates that partially-filled flat bands are the birthplace of many interesting phenomena and motivate further studies for the hidden physics of partially-filled flat bands in other systems. In this work, through first-principles calculations, we investigate the electronic structure and structural stability of a partially-filled flat band in boron triangular Kagome lattice which has been recently predicted. We find that a large Fermi surface nesting in the partially-filled flat band enhances electron-phonon interactions and induces dynamical instability. For hole doping levels above a 2/3-filling of the spin-polarized flat band, a metal-insulator transition occurs. Our results suggest that the boron triangular Kagome lattice is a suitable material to study the effect of partially-filled flat bands on exotic phases.

4:06PM P14.00009: Landau levels in bilayer transition metal dichalcogenides*  
PENG PENG ZHENG (Presenter), FAN ZHANG, University of Texas at Dallas — The quantum binary system at low temperature is not limited to only spin, but that of valley and layer degrees of freedom as well. A prime example is bilayer transition metal dichalcogenide (TMD). Here we examine the Landau level structure of bilayer TMD. We show how the interlayer electric field and the magnetic Zeeman field couple and control the layer and valley pseudospins, respectively, thereby tuning the Landau levels. To understand the underlying mechanics, we develop an effective model accurate within the experimental range to model and analyze the results. Our work sheds a new light on the quantum Hall effects of atomically thin TMD’s.

*Research was sponsored by the Army Research Office and was accomplished under Grant Number W911NF-18-1-0416.
4:18PM P14.00010: Tunable spin-polarized edge currents in proximitized transition metal dichalcogenides*  
NATALIA CORTES, Departamento de Fisica, Universidad Tecnica Federico Santa Maria, OSCAR AVALOS OVANDO (Presenter), Department of Physics and Astronomy, Ohio University, LUIS ROSALES, PEDRO ORELLANA, Departamento de Fisica, Universidad Tecnica Federico Santa Maria, SERGIO E ULLOA, Department of Physics and Astronomy, Ohio University — We explore proximity-induced ferromagnetism on transition metal dichalcogenide (TMD), focusing on molybdenum ditelluride (MoTe2) ribbons with zigzag edges, deposited on ferromagnetic europium oxide (EuO). A three-orbital tight-binding model allows modeling MoTe2 monolayer structures in real space, incorporating the exchange and Rashba fields induced by proximity to the EuO substrate. For in-gap Fermi levels, electronic modes in the nanoribbon are strongly spin-polarized and localized along the edges, acting as 1D conducting channels with tunable spin-polarized currents. We also study the effect of atomic defects on the 1D conducting channels and on the spin-polarized currents, finding a nonvanishing spin-polarized current even in the presence of either Te and/or Mo vacancies. Hybrid structures such as the MoTe2/EuO configuration can serve as building blocks for spintronic devices and provide versatile platforms to further understand proximity effects in diverse materials systems.


*N.C. acknowledges support from Conicyt grant 21160844, and DGIIP. L.R. and P.A.O. acknowledge FONDECYT grant 1180914 and DGIIP USM internal grant. S. E. U. and O. A.-O. acknowledge support from NSF DMR-1508325.

4:30PM P14.00011: Tight-binding modeling of bilayer TMDCs with lithium intercalation  
ZHEYU LU (Presenter), STEPHEN CARR, DANIEL LARSON, EFTHIMIOS KAXIRAS, Harvard University — We present an ab-initio tight-binding modeling of bilayer TMDCs with lithium intercalation based on the wannier transformation of first-principles calculations. Specifically, we take MoS2 as an example. As a starting point, we investigate the energetics of different intercalation sites for Li between layers of MoS2. We find that the intercalation energetics is related to the local coordination type and the number of vertically aligned molybdenum atoms. In addition, we verify that Li intercalation tunes the Fermi level to the conduction bands and make the system metallic. Further, we use three variables to characterize the relative configuration between the sulfur pair and the Li and describe the interlayer sulfur-sulfur interactions. As expected, Li brings extra influence and dramatically tunes the interlayer interactions. Our results pave the way for further modeling of twisted bilayer TMDCs with Li intercalation.

4:42PM P14.00012: Properties of doubly-aligned graphene/boron nitride heterostructures*  
NATHAN FINNEY (Presenter), MATTHEW YANKOWITZ, LITHURSHANAA MURALEETHARAN, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, CORY DEAN, JAMES HONE, Columbia University — A long-wavelength superlattice moiré potential emerges in heterostructures of graphene and boron nitride (BN) with small interlayer twist. The bandstructure of graphene is substantially modified by this superlattice potential, with secondary Dirac cones emerging at finite energy and band gaps opening at both the original and secondary Dirac points. We investigate the behavior of BN-encapsulated graphene in which the bottom BN is aligned to the graphene and the top BN can be rotated freely. We observe a significant enhancement of the band gap at the Dirac point in the case where both the top and bottom BN layers are perfectly aligned to the graphene. Additionally, while rotations of 60° are equivalent in typical graphene on BN heterostructures, we observe symmetry under 120° rotations of the top BN in our doubly-aligned devices, owing to the inequivalence of the boron and nitrogen potentials in the BN unit cell. In particular, we find the resistance of the Dirac point at room temperature is enhanced with the top BN at 0° but suppressed at 60°.

*N.F. acknowledges the Stewardship Science Graduate Fellowship program's support, provided under cooperative agreement number DE-NA0002135.
4:54PM P14.00013: Modifying the Band Structure of Hexagonal Boron Nitride with Metal Electrodes* MEHMET DOGAN (Presenter), MARVIN L COHEN, Physics, UC Berkeley — Tuning the large band gap of BN to make it functional in a given device configuration has been challenging. Theoretical attempts via an external electric field, strain, and changing the interlayer distance have produced promising results, however, at unrealistically high electric field and strain values. In this DFT-based study, we propose an alternate scheme for tuning the electronic states in BN. We investigate systems in which a few layers of BN are sandwiched between two metals with different work functions, such as Cu/BN/K, creating a large electric field through the BN slab. We find that the energy gap among the BN states can be significantly decreased in such configurations. We also report on the dependence of this effect on the different metals used and the number of BN layers, as well as the BN stacking order, as the controlled growth of an alternative (Bernal) stacking order was recently reported (S. M. Gilbert et al., arXiv:1810.04814) and thus became available for such applications.

*This work was supported by the Department of Energy under Contract No. DE-AC02-05-CH11231, and the National Science Foundation under Grant #DMR 1508412.

5:06PM P14.00014: Exchange driven dimerization, band gap, and magnetism of diamond(111) surface from first principles* BETUL PAMUK (Presenter), Cornell University, MATTEO CALANDRA, Sorbonne Université — Strong electron-electron interaction in ultraflat edge states can be responsible for correlated phases of matter, such as magnetism, charge density wave or superconductivity. The diamond(111) surface, after Pandey reconstruction, presents zig-zag carbon chains, generating a very flat surface band. More than 100 years after Bragg determined the structure of bulk diamond, the structure of the (111) surface of diamond is still controversial. Full structural optimization using hybrid density functionals with exact exchange shows that a substantial dimerization occurs on the Pandey π-chains — that is the primary mechanism for the opening of an insulating gap. This effect is absent in standard functionals. The exchange interaction further stabilizes a ferrimagnetic order along the Pandey π-chains with magnetic moments of 0.27 μB, opening a direct band gap of ~1.4 eV, in agreement with experiments. Our work is relevant for systems with flat bands in general and wherever the interplay between structural and electronic degrees of freedom is crucial, as in twisted bilayer graphene, IVB atoms on IVB(111) surfaces such as Pb/Si(111) or molecular crystals.

*We thank the Graphene Flagship, RhomboG grant (ANR-17-CE24-0030) from ANR, PRACE, and NSF (PARADIM) Cooperative Agreement No. DMR-1539918.

5:18PM P14.00015: Nano-Makis: Two-Dimensional Carbon derived from One-Dimensional Carbon LEI ZHAO (Presenter), California State University Northridge, WEI LIU, TAO HU, Beijing Computational Science Research Center, DALAR KHODAGHOLIAN, California State University Northridge, FENGLONG GU, South China Normal University, HAI-QING LIN, Beijing Computational Science Research Center, YONGHAO ZHENG, University of Electronic Science and Technology of China, MAOSHENG MIAO, California State University Northridge — The synthesis of carbon nanotubes and the rediscovery of graphene has sparked experimental and theoretical studies on new allotropes of carbon. Herein, we report first-principles calculations on novel two-dimensional carbon allotropes that are formed from embedding single-walled carbon nanotubes (SWNTs) within graphene sheets. The SWNTs are joined to the sheet via hexagonal or tetragon-octagon rings. We call this predicted allotrope of carbon nano-makisu. Results of phonon and molecular dynamics calculations demonstrate that these new carbon allotropes are dynamically and thermally stable, and they are energetically more favorable than pure SWNTs. Electronic structure calculations indicate that these two-dimensional carbon allotropes are metallic. Moreover, anisotropic Dirac-cone like features are found in nano-makisu. Because of its intriguing electronic transport properties nano-makisu are potential materials for nanoelectronics.
DHAVALA SURI (Presenter), Francis Bitter Magnet Laboratory and Plasma Science and Fusion Center, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, GREGORY STEPHEN, Department of Physics, Northeastern University, WEI KONG, Department of Material Science and Engineering, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, MIRKO ROCCI, Francis Bitter Magnet Laboratory and Plasma Science and Fusion Center, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, NARENDRA KUMAR, YIPING WANG, KENNETH BURCH, Department of Physics, Boston College, JEEHWAN KIM, Department of Material Science and Engineering, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, DON HEIMAN, Department of Physics, Northeastern University, JAGADEESH MOODERA, Francis Bitter Magnet Laboratory and Plasma Science and Fusion Center, MASSACHUSETTS INSTITUTE OF TECHNOLOGY — Ferromagnet (FM)/2D material interface with broken symmetry is a potential avenue for new physics and to realize exchange field controllable future spintronics devices. Proximity-induced effects of a FM on TI and graphene (G) have been explored previously with EuS as the ferromagnet, inducing magnetic correlations in the adjacent layer [1]. Magnetic semiconductor GdN would enable higher temperature operation. We report successful sputter growth of ultrathin excellent GdN films on high-quality G synthesized on SiC substrate to form G/FM heterostructures. The properties of G are unperturbed with 15 nm thick GdN film grown over it, having a magnetic moment ≈ 7 μB and Curie temperature ≈ 33 K. Temperature-dependent Raman spectrum of electric field tunable GdN/G system shows a clear signature of graphene G peak near 1580 cm⁻¹ and G' peak near 2700 cm⁻¹ confirming its quality. The induced magnetic correlations in G creating exchange gap in the Dirac surface states by GdN is investigated. Furthermore, patterning a superconductor over this bilayer for Josephson pair tunnelling studies in G will be presented.


*Funding Acknowledgement: NSF (DMR 1700137) and CIQM (DMR-1231319).

AHMET AVSAR (Presenter), ALBERTO CIARROCCHI, MICHELE PIZZOCHERO, DMITRII UNUCHEK, OLEG YAZYEV, ANDRAS KIS, Ecole polytechnique federale de Lausanne — While intrinsic magnets rarely occur in nature, long range magnetism in nonmagnetic materials can be introduced in a variety of forms, e.g., adatom intercalation, proximity coupling and defect engineering. The latter has been predicted for several two-dimensional (2D) materials including transition metal dichalcogenides (TMDCs), but such magnetic ordering of spins in the atomically thin limit has not been experimentally realized yet. Here, we will present defect-induced magnetism for an environmentally stable 2D TMDC crystal. By utilizing magneto-transport and polar refractive magnetic circular dichroism techniques, we demonstrate ferromagnetic or anti-ferromagnetic ground state orderings depending on the number of layers, similarly to recently discovered CrI₃. Attempts on further manipulation of magnetism within a layer by precise defect engineering will be also shown. Our findings broaden the horizon of 2D magnets to include normally nonmagnetic stable materials by introducing defects.

CHING-HAO CHANG (Presenter), SHENG-CHIN HO, TSE-MING CHEN, National Cheng Kung University, Taiwan, CARMINE ORTIX, Utrecht University — Local deformation in graphene are gathering great interest because it introduces huge pseudo-magnetic field to modify the electronic states nearby to host novel transport properties [1]. The graphene nanobubble, for instance, is predicted to strongly polarize the valley of an injecting current [2]. In this respect, the nontrivial valley-dependent band structure can be introduced when a local deformation turns into periodic. In this talk, we will show that the Rashba-like valley bands form in corrugated graphene systems. Moreover, the low-energy bands refer to magnetic snake states moving along the corrugations and thus can provide one-dimensional-like ballistic valley transport.

**3:06PM P15.00004: Triangular antiferromagnetism on the honeycomb lattice of twisted bilayer graphene***

ALEXANDRA THOMSON (Presenter), Caltech, SUBIR SACHDEV, Harvard University, SHUBHAYU CHATTERJEE, UC Berkeley, MATHIAS SCHEURER, Harvard University — We present the electronic band structures of states with the same symmetry as the three-sublattice planar antiferromagnetic order of the triangular lattice. Such states can also be defined on the honeycomb lattice provided the spin density waves lie on the bonds. We identify cases which are consistent with observations on twisted bilayer graphene: a correlated insulator with an energy gap, yielding a single doubly-degenerate Fermi surface upon hole doping. We also discuss extensions to metallic states which preserve spin rotation invariance, with fluctuating spin density waves and bulk $\mathbb{Z}_2$ topological order.

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**3:18PM P15.00005: Interplay Between Ferromagnetism and Superconductivity in van der Waals Devices***

ROBERT POLSKI (Presenter), HARPREET SINGH ARORA, JEANNETTE KEMMER, Watson Laboratory of Applied Physics, California Institute of Technology, YOUNGJOON CHOI, Department of Physics, California Institute of Technology, HECHEN REN, Watson Laboratory of Applied Physics, California Institute of Technology, YIRAN ZHANG, Department of Physics, California Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, STEVAN NADJ-PERGE, Watson Laboratory of Applied Physics, California Institute of Technology — Two-dimensional van der Waals materials have unlocked the ability to stack electronically dissimilar materials into heterostructures that are highly tunable using proximity effects, gate modulation, and varying layer numbers. Interest in superconducting proximity effects, such as Andreev reflection in superconductor-normal (S-N) junctions and Josephson junctions, have thus provoked numerous studies in these systems, but the combination of spin-singlet superconductors (S) and spin-polarized ferromagnets (F) into S-F interfaces has been largely unexplored in van der Waals materials. Proper understanding and control of these interfaces could lead to advances in spintronics and novel realizations of unconventional superconductivity. We used superconducting and ferromagnetic van der Waals materials to study the electrical properties of S-F interfaces through transport measurements as we vary both the temperature and the magnetic field.

*This work was supported by NSF (Partly through grant DMR 1753306) and by Gist-Caltech collaboration program memorandum of understanding.

**3:30PM P15.00006: Voltage Control of a van der Waals Spin-Filter Magnetic Tunnel Junction***

TIANCHENG SONG (Presenter), University of Washington, MATISSE WEI-YUAN TU, University of Hong Kong, CAITLIN CARNAHAN, Carnegie Mellon University, XINGHAN CAI, University of Washington, TAKASHI TANIGUCHI, KENJI WATANABE, NATIONAL INSTITUTE FOR MATERIALS SCIENCE, STEPHEN MCGUIRE, Oak Ridge National Laboratory, DI XIAO, Carnegie Mellon University, WANG YAO, University of Hong Kong, XIAODONG XU, University of Washington — Atomically thin chromium triiodide ($\text{CrI}_3$) has recently been identified as a layered antiferromagnetic insulator, in which adjacent ferromagnetic monolayers are antiferromagnetically coupled. This unusual magnetic structure naturally comprises a series of anti-aligned spin filters which can be utilized to make spin-filter magnetic tunnel junctions with very large tunneling magnetoresistance (TMR). Here we report voltage control of TMR formed by four-layer $\text{CrI}_3$ sandwiched by monolayer graphene contacts in a dual-gated structure. By varying the gate voltages at fixed magnetic field, the device can be switched reversibly between bistable magnetic states with the same net magnetization but drastically different resistance (by a factor of ten or more). Our work demonstrates new kinds of magnetically moderated transistor action and opens up possibilities for voltage-controlled van der Waals spintronic devices.

**3:42PM P15.00007: Controlling magnetism in layered metal halides by doping***

ZHONG LIN (Presenter), QIANNI JIANG, ZAIYAO FEI, BEVIN HUANG, Physics, University of Washington, Seattle, YUE SHI, Materials Science and Engineering, University of Washington, Seattle, JUN-HAW CHU, XIAODONG XU, Physics, University of Washington, Seattle — van der Waals magnets such as chromium triiodide show thickness dependent magnetic properties which can be further controlled by electrostatic gating. Engineering their intrinsic magnetism via compositional and structural modification remains largely unexplored. I will present our recent efforts on doping layered metal halides, including the characterization of bulk crystals and exfoliated flakes down to their 2D limit.

*This work is supported by DOE BES Pro-QM EFRC (DE-SC0019443).
Spin and charge conversion in two dimensional magnets*  
ABHISHEK SOLANKI (Presenter), AVINASH RUSTAGI, PRAMEY UPADHYAYA, Purdue University — Interconversion between spin and charge degrees of freedom is one of the central goals of spintronics. In recent years, a host of quantum materials—Rashba interfaces, topological insulators, superconductors and non-collinear antiferromagnets—have emerged as promising candidate material systems, where various novel spin-dependent phenomena allow for efficient spin and charge interconversion [npj Quantum Materials **3**, 27 (2018)]. More recently, van der Waal magnets (such as CrI3) [**Nature** **546**, 270 (2017)] have emerged as a unique two-dimensional platform, where electron-electron interactions can be significantly altered—from being ferromagnetic to antiferromagnetic—by charge doping [**Nature Mat.** **17**, 406 (2018)]. In this work, we develop a phenomenological theory of spin-charge interconversion enabled by electrically controlled spin-spin interactions in these two-dimensional magnets, predicting new efficient schemes for converting between spin and charge. In combination with the unique toolkit of heterostructure engineering offered by the van der Waal materials [**Science** **353**, aac9439 (2016)], the predicted spin charge interconversion could give rise to a new set of nonvolatile spintronics devices.

*We acknowledge NSF grant DMR-1838513.

Current-induced torques in heterostructures of 2D van der Waals magnets  
VISHAKHA GUPTA (Presenter), GREGORY STIEHL, ARNAB BOSE, KAIFEI KANG, SHENGWEI JIANG, KIN FAI MAK, JIE SHAN, ROBERT BUHRMAN, DANIEL RALPH, Cornell University — The recent discovery of magnetic order in layered 2D van der Waals materials has opened a new platform for spintronic devices, allowing studies of current-induced torques in high-quality heterostructures of single-crystal 2D magnets and large spin-orbit coupling (SOC) materials. Here, we integrate mechanically exfoliated thin flakes of the insulating 2D ferromagnet Cr2Ge2Te6 into a heterostructure with heavy metal Tantalum as the large SOC material. We report initial results of current induced deflections of the out-of-plane magnetic moment of Cr2Ge2Te6 and characterize the spin-orbit torque generated. This work represents a first step towards improved strategies for magnetic memory and logic using heterostructures of van der Waals 2D magnets.

Ion Implantation Leading to Magnetism in Many-Layer Graphene*  
ALESSANDRO MAZZA (Presenter), Physics, University of Missouri, ANNA L MIETTINEN, Physics, Georgia Institute of Technology, TIMOTHY CHARLTON, Spallation Neutron Source, Oak Ridge National Lab, THOMAS WARD, Materials Science and Technology, Oak Ridge National Lab, XIAOQING HE, Department of Mechanical and Aerospace Engineering and Electron Microscopy Core, University of Missouri, ALEX A DAYKIN, SUCHISMITA GUHA, GUANG BIAN, Physics, University of Missouri, EDWARD H. CONRAD, Physics, Georgia Institute of Technology, PAUL F MICELI, Physics, University of Missouri — P-orbital magnetism observed in graphene is of interest both to fundamental physics and for its potential application in new classes of spintronic devices. In this talk, we will demonstrate how low energy ion bombardment of graphene with hydrogen can be used to manipulate defect type and concentration to induce room temperature ferromagnetism in layered graphene. SQUID magnetometry measurements show that it is possible to control the magnetic properties by varying the H energy and dose. In-situ x-ray diffraction shows that ion distribution leads to layer expansion and an increase in RMS height variations of the graphene layers. Neutron reflectivity reveals that implanted H ions remain in the sample after dosing via chemisorption. The relationship between these results and magnetometry measurements, which show that ion implantation leads to a ferromagnetic moment at room temperature, will be discussed.

*NSF grant no. DGE-1069091, DOE SCGSR, ORNL GO! Programs
4:30PM P15.00011: Kondo Effect in Graphene Nanoribbons with Magnetic Impurities* GINETOM DINIZ (Presenter), Unidade Acadêmica Especial de Ciências Exatas, Universidade Federal de Goiás, Jataí, Goiás 75801-615, Brazil, GISELE IORIO LUIZ, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Minas Gerais 38400-902, Brazil, ANDREA LATGE, Instituto de Física, Universidade Federal Fluminense, Niterói, Rio de Janeiro 24210-340, Brazil, EDSON VERNEK, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Minas Gerais 38400-902, Brazil — In this work we have performed a detailed analysis of the Kondo effect of a magnetic impurity in graphene nanoribbons with zigzag edge termination [1]. We have considered an adatom coupled to the graphene nanoribbon via a hybridization amplitude in two different configurations: hollow or top site. In addition, the adatom is also weakly coupled to a metallic STM tip by a hybridization function that provides a Kondo screening of its magnetic moment. We have described the entire system by the well-known Anderson-like Hamiltonian [2] whose low-temperature physics is accessed by employing the numerical renormalization group approach [3], which allows us to obtain the thermodynamic properties used to compute the Kondo temperature of the system. In our numerical calculation, two screening regimes were observed: local singlet and Kondo singlet, which strongly depends on the impurity adatom location and on the coupling strength of the carbon sites of the graphene nanoribbon with the adatom impurity.


*We acknowledge financial support received from FAPEG, FAPEMIG, FAPERJ, CAPES and CNPq.

4:42PM P15.00012: Analysis of Magnetoresistance in CrI3-graphene Heterostructures via First-principles Calculations JONATHAN HEATH (Presenter), MARCELO KURODA, Auburn University — Recently, spin transport was demonstrated in heterostructures based on two-dimensional (2D) materials. Here we characterize electronic transport through multilayer CrI3 systems (bilayer, trilayer, and tetralayer) using the density functional theory (DFT) and the Landauer formalism for ballistic transport. Electronic structure of these tunneling junctions reveal that the interplay of quantum confinement and metamagnetic configurations defines the different tunneling rates. Hence, atomistic calculations capturing coupling between layers are key to these descriptions. Our ballistic transport calculations are in agreement with recent experimental measurements of magnetoresistance in graphene/CrI3/graphene [Klein et al., Science 360, 1218 (2018)]. We apply our transport studies for this type of tunneling junction to other metallic leads with Fermi level density of states larger than that of graphene and compare to other Cr halides junctions. While tunneling resistivity is significantly reduced, magnetoresistance ratios do not necessarily increase due to the intricate complex band structure of these systems. The atomistic details provided by this work may prove valuable towards the use of these 2D material-based spintronic devices.

4:54PM P15.00013: Assembly, X-ray diffraction and electronic transport measurement of atomically thin Bi2Sr2CaCu2O8+y high temperature superconducting van der Waals cuprate heterostructures. NICOLA POCCIA (Presenter), SHU YANG FRANK ZHAO, YUVAL RONEN, HYOBIN YOO, Department of Physics, Harvard University, Cambridge, MA 02138, USA., RUIDAN ZHONG, GENDA GU, XIAOJING HUANG, HANFEI YAN, YONG S. CHU, Department of Condensed Matter Physics and Materials Science, Brookhaven, Brookhaven National Laboratory, Upton, New York 11973-5000, USA., KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan., SVETLANA POSTOLOVA, Rzhanov Institute of Semiconductor Physics, Siberian Branch, Russian Academy of Sciences, Novosibirsk 630090, Russia., GAETANO CAMPI, Institute of Crystallography, CNR, via Salaria Km 29.300, Monterotondo Stazione, Roma 00016, Italy., VALERII VINOKUR, Materials Science Division, Argonne National Laboratory, 9700 S. Cass Ave, Argonne, IL 60439, USA., PHILIP KIM, Department of Physics, Harvard University, Cambridge, MA 02138, USA. — Unique physical properties of low-dimensional electronic systems arise from the fine balance and interplay of often competing phenomena in the reduced dimensionality. We fabricated van der Waals heterostructure based on atomically thin Bi2Sr2CaCu2O8+y (BSCCO) high temperature superconductor. Unlike conventional superconductors, atomically thin BSCCO film exhibits an intrinsic multi-scale heterogeneity and a complete new set of imaging and nanofabrication tools are required to tame this complexity. In this talk, we will show the structural nanoscale heterogeneity using advanced X-ray nanoprobes of an assembled few-unit cells van der Waals cuprate high temperature superconducting heterostructure. Towards the end, I will demonstrate our recent realization of Josephson junctions made of assembled van der Waals cuprate heterostructures.
Ultrafast photoemission momentum microscopy* CHRISTOPHER CORDER (Presenter), PENG ZHAO, JIN BAKALIS, MICHAEL G WHITE, THOMAS ALLISON, Stony Brook University, Stony Brook, NY 11794 — Understanding the electronic properties in material systems is key to unlocking new technologies. To probe the carrier dynamics on their natural timescale, ultrafast spectroscopies are employed, typically with femtosecond optical lasers. However, the observed features in these measurements are often ambiguous when attempting to identify the carriers involved and their location in the material band structure. Recent advances in ultrafast extreme-ultraviolet sources [1,2] now allow direct observation of carrier energy and momentum using angle-resolved photoelectron spectroscopy with the high data rates and low space-charge required for observing band structures. We demonstrate the capabilities when one of these XUV sources is paired with a time-of-flight momentum microscope [3] enabling time-resolved multidimensional measurements simultaneously spanning energy and two dimensions of momentum space.


*Supported by AFOSR under Award No. FA9550-16-1-0164, DOE Office of Basic Energy Sciences, under Award No. DE-SC0016017, and the Stony Brook Foundation Discovery Prize.

Wednesday, March 6, 2019 2:30 PM - 5:18 PM

Session P16 DCOMP DCP: Aqueous Solutions, Solvated Interfaces, and Ionic Polarization

II BICE 155 - Marivi Fernandez Serra, Stony Brook University - Tag(s): Focus

The Role of Interfaces for Chemical Transformations and Transport under Confinement* [Invited] TERESA HEAD-GORDON (Presenter), University of California, Berkeley — Chemical transformations, selectivity, and transport rarely occur in a single homogeneous aqueous phase, but instead occur in niches, crevices, and impurity sites at confining interfaces between two or more phases of gases, liquids or solids. The effects of confinement are ubiquitously present across diverse fields spanning nanochemistry and chemical catalysis, environmental and energy sciences, geosciences, and functional materials. Fundamentally, confinement at interfaces alters water and solution compositions and phases to reformulate the thermodynamics of selectivity, transition states and pathways of chemical reactions, nucleation events, and kinetic barriers for transport. I will provide three different examples of theoretical studies of confinement around anhydrous clays, synthetic enzymes, and a general non-equilibrium phenomena of confinement which we refer to as dynamical inversion of the energy landscape.

*The catalysis application supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division under Contract No. DE-AC02-05CH11231. The material on theory and methods is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Scientific Discovery through Advanced Computing (SciDAC) program. This research received a 2017 ASCR Leadership Computing Challenge (ALCC) allocation at the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
3:06PM P16.00002: Water/mineral interfaces: Structure and Dynamics from Nonlinear Vibrational Spectroscopy and Ab Initio Molecular Dynamics* [Invited] LUANA PEDROZA (Presenter), Universidade Federal do ABC, Brazil, FABIO R. NEGREIROS, Departamento de Quimica Teorica y Computacional, Facultad de Ciencias Quimicas, Universidad Nacional de Cordoba, Argentina, GUSTAVO DALPIAN, Universidade Federal do ABC, Brazil, JACIARA DE CARVALHO SANTOS, PAULO B MIRANDA, Instituto de Fisica de Sao Carlos, USP, Brazil — Water–mineral interfaces are important for several environmental, industrial, biological, and geological processes. In particular, gypsum is a widespread mineral of high technological, medical, and environmental relevance, but little is known about its surface structure and its interaction with water. A molecular-level understanding of gypsum/water interface is given here by a combined experimental/theoretical study. We investigate the structure and dynamics of water adsorbed from vapor on the gypsum (010) single-crystal surface at room temperature, combining sum-frequency generation (SFG) vibrational spectroscopy experiments and ab initio molecular dynamics (AIMD) simulations. The theoretical results corroborate the experimental ones and provide an accurate atomic characterization of the surface structure.

*We thank the Brazilian agencies FAPESP (grants 11/19924-2, 14/01595-0, 14/14271-9, 18/13753-0, 17/10292-0) and CNPq for financial support. Computer simulations were performed at CENAPAD-SP and on the Santos Dumont supercomputer at LNCC.

3:42PM P16.00003: Efficient calculation of level alignment at weakly coupled molecule-metal interfaces using substrate screening within the GW approach ZHENFEI LIU (Presenter), Department of Chemistry, Wayne State University, FELIPE DA JORNADA, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley, JEFFREY B NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — The physics of level alignment at molecule-metal interfaces can often be accurately captured by the ab initio GW approach. However, the computational cost for such GW calculations for typical interfaces is significant, given their large system size and chemical complexity. In the past, approximate self-energy corrections constructed from image-charge models have been used to compute level alignment with good accuracy. However, this approach neglects dynamical effects of the polarizability and requires the definition of an image plane. In this work, we propose a new approximation for GW calculations of molecule-metal interfaces, where we greatly simplify the evaluation of the polarizability of the combined system. This is done by first computing the polarizability of each individual system in smaller cells, followed by unfolding and interpolation techniques to efficiently combine these quantities. Overall, this approach greatly reduces the computational cost for GW calculations of level alignment without sacrificing the accuracy. Moreover, this approach captures both dynamical and nonlocal polarization effects without the need to invoke a classical image charge expression. We benchmark our approximation for the case of a benzene molecule physisorbed on Al(111) surface.

3:54PM P16.00004: Dielectric dependent hybrid functionals for surfaces and interfaces* HUIHUO ZHENG (Presenter), Leadership Computing Facility, Argonne National Laboratory, MARCO GOVONI, Materials Science Division, Argonne National Laboratory, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — We present a dielectric dependent hybrid density functional which accurately describes the electronic properties of heterogeneous interfaces, as well as those of three- and two-dimensional bulk solids. The functional is constructed by generalizing the dielectric hybrid functional for solids proposed in Ref. [1] to include a spatially varying, local dielectric function. The latter is determined self-consistently using a finite field approach. We present results for the band gap and dielectric constants of bulk materials (2D and 3D), and band offsets for interfaces (Si/Si3N4, Si/H2O) and surfaces (H-Si), as obtained with the Qbox code [2].


*This work was supported by MICCoM, as part of Comp. Mats. Sci. Program funded by the U.S. DOE, Office of Sci., BES, MSE Division. This research used resources of the ALCF, which is a DOE Office of Sci. User Facility under Contract DE-AC02-06CH11357.
**4:06PM P16.00005: Direct Z-Scheme Water Splitting Photocatalyst Based on Two-Dimensional Van Der Waals Heterostructures**

**RUIQI ZHANG** (Presenter), Tulane University, LILI ZHANG, QIJING ZHENG, PENGFEI GAO, JIN ZHAO, JINLONG YANG, University of Science & Technology of China — Mimicking the natural photosynthesis in plants, Z-scheme water splitting is a promising strategy to improve photocatalytic activity. Searching for the direct Z-scheme photocatalysts is urgent and the crucial factor for the photocatalytic efficiency is the photogenerated electron–hole (e–h) recombination rate at the interface of two photosystems. In this report, based on time-dependent ab initio nonadiabatic molecular dynamics (NAMD) investigation, we first report a two-dimensional (2D) metal-free van der Waals (vdW) heterostructure consisting of monolayer BCN and C2N as a promising candidate for direct Z-scheme photocatalysts for water splitting. It is shown that the time scale of e–h recombination of BCN/C2N is within 2 ps. NAMD simulations based on frozen phonon method prove that such an ultrafast interlayer e–h recombination is assisted by intralayer optical phonon modes and the interlayer shear phonon mode induced by vdW interaction. In these crucial phonon modes, the interlayer relative movements which are lacking in traditional heterostructures with strong interactions, yet exist generally in various 2D vdW heterostructures, are significant. Our results prove that the 2D vdW heterostructure family is convincing for a new type of direct Z-scheme photocatalysts searching.

**4:18PM P16.00006: Volume-Dependent Atomic Polarizabilities for Vibrational Spectroscopy**

**MARK DELLOSTRITTO** (Presenter), RUIYU WANG, MICHAEL L KLEIN, ERIC U BORGUET, Temple University — Vibrational spectroscopy methods, such as Raman and SFG, are valuable tools for characterizing the structure and dynamics of a wide range of systems. Computing spectra from MD simulations remains a significant challenge, as accurate polarizabilities (α) are required for a large range of molecular configurations, and ab-initio α can be prohibitively expensive to compute for even small molecules. We extend the Thole model by making the initial atomic α functions of the interatomic distances, scaling them by the radius of the atom as defined by the volume the atom occupies in the molecule. This allows us to compute accurate α for molecules far from their equilibrium configuration. We then compute accurate Raman spectra of water and urea, and SFG spectra at the alumina-water interface.

*This work was supported by the Center for Complex Materials, an Energy Frontier Research Center funded by the U.S. Dept. of Energy, Office of Science, Basic Energy Sciences, (Grant DE-SC0012575), and includes calculations carried out on Temple University's HPC resources and thus was supported in part by the National Science Foundation through major research instrumentation grant number 1625061 and by the US Army Research Lab. under contract W911NF-16-2-0189.

**4:30PM P16.00007: Transferability of local density assisted implicit solvation models for homogeneous fluid mixtures**

**DAVID ROSENBERGER** (Presenter), Technische Universität Darmstadt, TANMOY SANYAL, M. SCOTT SHELL, Chemical Engineering, University of California Santa Barbara, NICO VAN DER VEGT, Technische Universität Darmstadt — Dependency on density or concentration of the state chosen during parametrization leads to low transferability in density/concentration space in bottom-up coarse graining. For fluid phase equilibria the application of local density potentials appears a promising approach to overcome this shortcoming, as shown in previous work by Sanyal and Shell (J. Phys. Chem. B, 2018, 122, 5678). Here, we want to further explore this method and test its ability to model solutions of methanol and water. We find that a water-water LD potential improves the transferability of an implicit-methanol CG model towards high water concentration. Conversely, a methanol-methanol LD potential does not significantly improve the transferability of an implicit-water CG model towards high methanol concentration. These differences appear due to the presence of cooperative interactions in water at high concentrations that the LD potentials can capture. In addition, we formally demonstrate the analytical and numerical assumptions under these relative entropy optimization and the Inverse Monte Carlo method yield equivalent results.

*Funding by the German Research Foundation (DFG) within the SFB-TRR 146 grant and from the National Science Foundation through grant no. CHEM-1300770*
The reconstruction of molecular force fields for small molecules using the recently developed symmetric gradient-domain machine learning (sGDML) approach. The sGDML approach faithfully reproduces complex high-dimensional potential-energy surfaces from just a few 100s of molecular conformations generated by ab-initio MD simulations. The data efficiency of the model allows employing high-level wavefunction-based atomic forces and energies for training, such as the "gold standard" CCSD(T) method. We demonstrate that the flexible nature of this fully data-driven model recovers any local and non-local quantum interaction coming from \(-F=\phi^* \frac{\partial H}{\partial \phi} \phi\) (e.g. H-bonding, proton transfer, lone pairs, changes in hybridization states, steric repulsion and n->pi* transitions) without relying on prior knowledge of the phenomena. The analysis of MD@sGDML trajectories yields new qualitative insights into dynamics, chemistry, and spectroscopy of small molecules close to spectroscopic accuracy.

Nanosecond-scale ab initio molecular dynamics of fully solvated biomolecules with periodic boundary conditions using the Oak Ridge Leadership Computing Facility (OLCF) supercomputers

We present nanosecond-scale molecular dynamics simulations of small ribonucleic acids with full solvation shells of explicit water and ions at the density functional theory (DFT) level, using high performance ab initio molecular dynamics programs and the Oak Ridge Leadership Computing Facility (OLCF) supercomputers. Comparison of the trajectories to classical molecular dynamics is performed, including effects of polarization, changes in molecular conformations, and dynamics of the system in metastable states and with respect to barrier crossing. We find important differences in the conformational dynamics and analyze the effects of dynamic changes in charge density and polarization that are available from the first-principles description and which may be essential to correct simulation of conformational ensembles of these difficult-to-model molecules.

*This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725

Advances in machine learned potentials for molecular dynamics simulation

Recent machine learning techniques allow emulation of quantum chemistry with stunning fidelity. For example, deep neural networks can now predict molecular properties with accuracy approaching that of coupled cluster theory, at a tiny fraction of the computational cost. We present methods for building machine learned potentials based on the following key ideas: (1) encoding physical symmetries, (2) active learning to dynamically grow the training dataset, and (3) transfer learning to incorporate data from varying sources. The aim is to enable large-scale and highly accurate molecular dynamics simulations, e.g., for chemistry, materials science, and biophysics applications.

*LDRD and ASC/PEM programs at Los Alamos National Laboratory.
2:30PM P17.00001: Equation of State Calculations With First-Principles Computer Simulations of Matter at Extreme Conditions* [Invited] BURKHARD MILITZER (Presenter), FELIPE J GONZALEZ, University of California, Berkeley, SHUAI ZHANG, Lawrence Livermore National Laboratory, HENRY PETERSON, University of California, Berkeley, KEVIN P DRIVER, Lawrence Livermore National Laboratory, FRANCOIS SOUBIRAN, University of California, Berkeley — The properties of materials at extreme pressure and temperature conditions are important in astrophysics and fusion science. When models for the interiors of Saturn and Jupiter are constructed to match gravity data from the NASA missions Cassini and Juno, an accurate knowledge of the equation of state of hydrogen-helium mixtures is essential. Modern dynamic compression experiments typically probe megabar and gigabar pressures. In order to provide a comprehensive theoretical description of materials at such extreme conditions, we combine results from path integral Monte Carlo (PIMC) and density functional molecular dynamics simulations. We present equation of state results for first-row elements and compounds such as boron, CH plastic, and oxygen. The shock Hugoniot curves are derived and compared with experimental data. Then we discuss how bound states can be incorporated efficiently into the nodal structure in the PIMC simulations, which enables us to simulate second row elements. We present results from equation of state computations for sodium, aluminum, silicon, and magnesiosilicates.

*This research was supported by the U.S. Department of Energy under Grants No. DE-SC0016248.

3:06PM P17.00002: The Challenge of Assessing Uncertainty in Equation of State (EOS) Generation* CHRISTINE J WU (Presenter), CARRIE PRISBREY, MIGUEL MORALES, Lawrence Livermore Natl Lab — We have recently developed multiphase EOSs for a number of materials including Beryllium and Gallium, based not only on experiments, but also on theoretical calculations for regions where experiments are not available or in conflict. Building EOSs unavoidably involves multiple sources of uncertainties, including experimental error bars, and uncertainties due to theoretical approximations and different choices of the free energy model. We will discuss our baseline EOS models and preliminary attempt to address and bound EOS uncertainties.

*This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344

3:18PM P17.00003: Determining temperature-pressure-density relations of shock-compressed post-transition metals using optimal functionals SHUAI ZHANG (Presenter), MIGUEL MORALES, RICHARD BRIGGS, MARTIN G GORMAN, DAYNE FRATANDUONO, Lawrence Livermore National Laboratory — Dynamic compression techniques offer very useful ways of measuring the equation of state (EOS) of materials at extreme conditions. Many properties, in particular the pressure-density relation along the shock Hugoniot curve, can usually be determined with high accuracy. However, there lacks a generic way to measure temperature. This is problematic when studying phase transformation boundaries of non-transparent materials, which can have large uncertainties depending on the EOS model being used. We propose a method for determining the temperature-pressure-density relation of materials under shock compression using quantum simulations based on optimal functionals. The choice of the functional is constrained by well-established experimental data, such as pressure-density Hugoniot and static compression results. These constraints are from multiple regions of the phase space, therefore making our predictions widely reliable. We apply this method to studying post-transition metals, of which the phase and structural property changes are of great interest to the high-pressure and materials physics communities.

Work prepared under the auspices of LLNL under contract DE-AC52-07NA27344.

3:30PM P17.00004: First-principles calculation of third-order elastic constants via numerical differentiation of the second Piola-Kirchhoff stress tensor DAVID CUFFARI (Presenter), ANGELO BONGIORNO, College of Staten Island — Third-order elastic constants (TOECs) of materials are difficult to measure experimentally and produce large errors. Computational methods are needed for overcoming these difficulties. Previous methods to calculate TOECs are based on fitting energy-strain and/or stress-strain curves calculated from density functional theory (DFT). These methods rely on symmetry relationships, and for this reason, so far they have been applied mainly to cubic and hexagonal crystals. In this paper, we present a novel method to calculate TOECs that is applicable to any system, regardless of its symmetry and dimensionality. This method relies on second-order numerical differentiation of the second Piola-Kirchhoff stress tensor. In this work, we combine this method to a plane-wave DFT approach to calculate the TOECs of aluminum, diamond, silicon, magnesium, graphene, and graphane. A comparison to experimental results shows that our new method is valid and accurate.
3:42PM P17.00005: Analysis of heating curves and optical properties for the liquid-liquid transition to metallic hydrogen

JACQUES TEMPERE (Presenter), MATTHEW HOUTTURE, Theory of Quantum and Complex Systems, Universiteit Antwerpen, ISAAC SILVERA, Lyman Laboratory of Physics, Harvard University — Hydrogen at high temperatures and pressures undergoes a phase transition from liquid molecular to liquid atomic metallic hydrogen. This transition takes place on the planet Jupiter and has been studied in the laboratory. Experiments in a diamond anvil cell for temperatures up to 2000 K and pressures of 100-170 GPa determine heating curves and optical properties. Heating curves (the temperature of the sample as a function of heating power) have a positive slope with increasing power with a plateau in temperature, most likely associated with the latent heat of transformation. Plateaus are associated with an abrupt rise in reflectance and absorption of visible light as expected for a metal. We carry out a realistic finite element analysis of heating curves and optical properties. The simulation shows that the plateaus and onset of absorption are related to the phase transition. However much larger values of latent heat are required than have been predicted by theory. The transition may be more complex than considered in current models.

*NSF Grant DMR-1308641, DoE SSAA DE-NA0003346

3:54PM P17.00006: Free energies of reaction for aqueous glycine condensation chemistry at extreme temperatures

NIR GOLDMAN (Presenter), MATTHEW KROONBLAWD, Lawrence Livermore Natl Lab — We have performed high throughput quantum molecular dynamics simulations to determine the free energy surface for aqueous glycine condensation reactions from moderate to extreme temperatures similar to oceanic hydrothermal vents (1g/cm³ and temperatures ranging from 300 K to 1000 K). Our simulations identify significant changes in the free energy surface topology and subsequent chemical reactivity with increasing temperature. We predict that temperatures at 400 K and below glycine favor dipeptide formation whereas higher temperatures facilitate the reverse hydrolysis reaction, with solvated glycine molecules showing greater stability. This change in favorability is correlated with a shift in the location and characteristics of specific reaction bottlenecks or barriers. Simultaneously, we observe that relative free energy barriers (total energy plus entropic contributions) for both condensation and hydrolysis reactions generally decrease with increasing temperature. Our results indicate that relatively modest temperatures near 400 K may best facilitate formation of oligoglycine molecules in oceanic systems related to the synthesis of life-building compounds. Prepared by LLNL under Contract DE-AC52-07NA27344.

4:06PM P17.00007: First principles simulation of the non-linear Peltier effect

XAVIER ANDRADE (Presenter), ALICIA R. WELDEN, ALFREDO A. CORREA, Lawrence Livermore Natl Lab — When matter is subject to large electric fields or temperature gradients, the usual linear approximations for the transportation of charge and heat, Ohm’s and Fourier’s law, break down. This gives rise to non-linear transport phenomena like negative-differential conduction.

We have developed a method based on real-time electron dynamics to simulate non-linear conduction from first principles. Our approach was first implemented for electrical conduction. We now extend the method to account for non-linear thermal conduction, using a quantum theory of heat based on real-time time dependent density functional theory (TDDFT).

In this talk we present our initial results for the simulation of the non-linear heat transport effects for hydrogen at a high-pressure metallic phase. By applying a strong electric field to the material and following in real time the induced heat current, we can predict the non-linear Peltier coefficient for the material.

The results of these simulations will help us understand when non-linear conduction effects appear and when they are important to understand the behavior of matter under extreme conditions.

*This work was performed under DOE Contract No. DE-AC52-07NA27344. Computing support for this work came from the LLNL Institutional Computing Grand Challenge.
4:18PM P17.00008: Optical absorption properties of laser-dressed matter* BING GU (Presenter), IGNACIO FRANCO, University of Rochester — We develop a theory for the optical absorption of electronic materials driven far from equilibrium by resonant and non-resonant lasers. In it, the interaction between matter and the driving light is treated exactly through a Floquet analysis, while the effects of the probing light are captured to first order in perturbation theory. The formalism is employed to characterize the optical properties of a nanoscale semiconductor dressed by non-resonant light of intermediate intensity (non-perturbative, but non-ionizing). As shown, non-resonant light can reversibly turn this transparent semiconductor into a broadband absorber and open strong absorption/stimulated emission bands at very low frequencies (~meV). These developments offers a platform to understand and predict the emergent optical properties of materials dressed by the electric field of light, and catalyze the design of laser-dressed materials with desired optical properties.

*This material is based upon work supported by the National Science Foundation under CHE-1553939.

4:30PM P17.00009: Radiation Induced Dissociation Pathways and Charge Redistribution in X-ray Free-Electron Laser Imaging* OSCAR GRÅNÄS (Presenter), Department of Physics and Astronomy, Uppsala University — Historically, structure determination of nano-crystals, proteins and macromolecules required the growth of high-quality crystals sufficiently large to diffract x-rays efficiently while withstanding radiation damage. The development of the x-ray free-electron laser (XFEL) has opened the door for high resolution single particle imaging using x-rays, as the extreme intensity ensures that enough diffraction statistics is collected before the sample is destroyed by radiation damage. Still, recovery of the structure is a challenge, in part due to the partial fragmentation of the sample during the diffraction event.

In this study, we use first-principles based methods to study the effect of radiation induced ionization of seven amino-acids. We benchmark a hierarchy of methods, considering theory on the level of Born-Oppenheimer molecular dynamics as well as non-adiabatic molecular dynamics. In addition, we study the impact on our results of how the ionization process is approximated. In order to estimate the effects of radiation damage on structural recovery, we study dissociation pathways, fragmentation statistics and charge redistribution.

*The Strategic Research Foundation (SSF), grant ICA16-0037
The Swedish Science Council (VR), grant 637-2013-7303

4:42PM P17.00010: Matter in Extreme Environments: Theoretical Studies of Light Elements Under Pressure* [Invited] MIGUEL MORALES (Presenter), Lawrence Livermore Natl Lab — Despite their apparent simplicity, light elements at extreme conditions of pressure and temperature display remarkable properties that have fascinated theoreticians and experimentalists for over a century. Recent advances in first-principles simulation methods have allowed us to elucidate ever more properties of these materials giving us predictive capabilities which, when combined with continuously improving experimental platforms, allow us to obtain new insight into the behavior of matter at extreme conditions. In this talk I will present an overview of the current state of the art in first-principles simulation capabilities for light elements at extreme environments. I will pay particular attention to simulation methods that operate directly in the physical picture of electrons and ions, including density functional theory and quantum Monte Carlo. As a demonstrative example of the predictive capabilities of these methods, I will present recent predictions in the phase diagram of hydrogen during metallization and molecular dissociation in connection with recent experimental observations of metallization. I will present the most recent predictions for the location of the metal-insulator transition in the compressed liquid along with predictions of the optical properties near the dissociation regime. We show how state-of-the-art simulations are able to provide a comprehensive picture of molecular dissociation and metallization in the liquid which explains the conflicting experimental results obtained for several different platforms.

*This work was performed in part under the auspices of the US DOE by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P18 DCOMP: Materials Theory and Computation BCEC 156B - Silvina Gatica, Howard University

2:30PM P18.00001: Are most jammed packings of dry, frictionless grains similar? PAPPU ACHARYA (Presenter), Physics, TIFR, Hyderabad — We study disordered jammed packings of frictionless disks interacting by either (one-sided) harmonic or Hertzian contact forces. We show that ensembles of such packings, in mechanical equilibrium, exhibit a very simple structure. In each case, we find that non-trivial fluctuations of the contact force network may be parameterised by a single dimensionless quantity for a large range of densities and disorder strengths. Surprisingly, a harmonic theory for displacement fluctuations in a crystal at thermal equilibrium is able to account for the statistics of these fluctuations.
2:42PM P18.00002: Percolation Around Structurally Disordered Sand Grains: A Dynamical Infiltration Study
DONALD PRIOR (Presenter), Youngstown State University — Percolation transitions, marking the boundary between configurations which admit the fluid or charge flow and those which are impermeable on large scales are salient phenomena for transport through porous materials where flow is through irregular spaces around impenetrable grains instead of well-defined linear channels. Using dynamical infiltration simulations involving virtual tracers moving in void regions, we calculate critical grain densities per unit volume where the inclusions are positionally and orientationally disordered. In addition, as a novel element, we also consider varying degrees of structural disorder, in which the shapes of grains are subject to random variation. In the case of ellipsoids, tetrahedrons, and rectangular solids we find that if expressed in units of the mean grain volume, the critical concentration is remarkably robust, with little variation for light to moderate disorder in the inclusion shapes. We also discuss scenarios in which in random variations in facet plane distances for solids such as dodecahedrons eventually yield non-dodecahedral fragments; with large scale dynamical infiltration simulations we seek to determine if percolation thresholds remain robust with increasing diversity in types of grain shapes or instead undergo a shift.

2:54PM P18.00003: From Birefringent Electrons to a Marginal or Non-Fermi Liquid of Relativistic Spin-1/2 Fermions: An Emergent Superuniversality*
BITAN ROY (Presenter), Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany, MALCOLM KENNETT, Department of Physics, Simon Fraser University, Canada, KUN YANG, Florida State University, Tallahassee, Florida, USA, VLADIMIR JURICIC, NORDITA, the Nordic Institute for Theoretical Physics, Stockholm University and KTH, Stockholm, Sweden — In this talk, we present the quantum critical theory of an interacting nodal Fermi liquid of quasirelativistic pseudospin-3/2 fermions that have a noninteracting birefringent spectrum with two distinct Fermi velocities [1]. As we show, when such quasiparticles interact with gapless bosonic degrees of freedom that mediate either the long-range Coulomb interaction or its short range component (responsible for spontaneous symmetry breaking), in the deep infrared or quantum critical regime in two dimensions, the system is, respectively, described by a marginal- or a non-Fermi liquid of relativistic spin-1/2 fermions (possessing a unique velocity), and is always a marginal Fermi liquid in three dimensions. We consider a possible generalization of these scenarios to fermions with an arbitrary half-odd-integer spin, and conjecture that critical spin-1/2 excitations represent a superuniversal description of the entire family of interacting quasirelativistic fermions.


* M. K. was supported by NSERC of Canada. K. Y. is supported by National Science Foundation Grants No. DMR-1644779 and No. DMR 1442366.

3:06PM P18.00004: Spatially-correlated Site Occupancy in the Nonstoichiometric Meta-stable ε-Al60Sm11 Phase during Devitrification of Al-10.2 at.% Sm Glasses*
LIN YANG, Iowa State University, FENG ZHANG, FAN-QIANG MENG, LIN ZHOU, YANG SUN, XIN ZHAO, ZHUO YE, MATTHEW J. KRAMER, CAI-ZHUANG WANG, Ames Laboratory, KAI-MING HO (Presenter), Iowa State University — We examine a metastable ε-Al60Sm11 phase that appears during the initial devitrification of as-quenched Al-10.2 at.% Sm glasses. The phase is nonstoichiometric in nature since Al occupation is observed on the 16f Sm lattice sites. STEM images reveal profound spatial correlation of Sm content on these sites, which cannot be explained by the “average crystal” description from Rietveld analysis. Monte Carlo simulations based on a cluster-expansion model also give qualitatively different correlation functions from experiments. On the other hand, molecular dynamics simulations of the growth of ε-Al60Sm11 show that when the diffusion range of Sm is limited to ~ 4 Å, the correlation function of the as-grown structure agrees well with that of the STEM images. Our results show that kinetic effects, especially the limited diffusivity of Sm atoms plays the fundamental role in determining the nonstoichiometric site occupancies of the ε phase during the crystallization process.

*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Science and Engineering Division including a grant of computer time at NERSC in Berkeley, under contract # DE-AC02-07CH11358. The GPU-accelerated MD calculations were supported by LDRD of Ames Laboratory.
The interaction of carbon and boron nitride nanotubes as well as graphene with metals*  
CHRISTOPH ROHMANN (Presenter), University of Maryland, College Park, MICHAEL P ZWOLAK, PML, National Institute of Standards and Technology — The interaction of carbon nanotubes with metals is significant for a wide variety of applications. For example, the binding of tubes to transition metal nanoparticles plays a role in their catalytic growth, as well as in their nucleation observed by ETEM, HRTEM, STM or Raman measurement. We performed quantum chemical calculations to investigate (i) the binding strength and geometry of a variety of metals with carbon nanotubes and graphene (ii) the curvature dependence of the binding energy and lastly (iii) we offer an explanation as to why the reported metal-CNT/graphene binding strength varies widely in the literature.

*C. R. acknowledges the support under the Cooperative Research Agreement between the University of Maryland and the National Institute of Standards and Technology Center for Nanoscale Science and Technology, Award 70NANB14H209, through the University of Maryland

WITHDRAWN ABSTRACT —

Ab Initio Calculations of Partial Basal Dislocations in Bilayer Graphene*  
PAVLOS MOURATIDIS (Presenter), KENNY JOLLEY, JAMES MCHUGH, MALCOLM HEGGIE, Chemistry, Loughborough University, PATRICK BRIDDON, School of Engineering, Newcastle University — Graphite has been the material of choice in construction of nuclear reactors for many years due to its low neutron absorption cross-section and high scattering cross-section. The physical properties of a graphite moderator can greatly influence the cost, safety and lifespan of a reactor. Neutron collision damage in graphite results in the formation of basal dislocations. The subsequent interaction of basal dislocations with each other and the surrounding lattice causes severe dimensional changes along the basal direction. There has been a lot of interest recently in AB and AC stacking grain boundaries in bilayer graphene. Transition from AB to AC stacking can be described by the glide of basal dislocations resulting in expansion of dislocation cores and buckling of the bilayer. Herein we present a new model for the dimensional change of nuclear graphite which considers buckling and folding of graphene sheets due to the basal dislocations glide. Full ab initio and molecular dynamics calculations of oppositely sign on basal dislocations in bilayer graphene have been carried out. Analysis of dislocation cores and buckled sinusoidal harmonics has revealed absorbing results compared to previous theoretical works.

*EDF Energy Generation Ltd, United Kingdom.

Plasmonic capacitance and profiling the energy distribution of plasmonic hot electrons in planar metal-dielectric structures  
ABBAS GOUDARZI (Presenter), SAHAR BEHPOUR, YURI ROSTOVTSEV, OSCAR GARCIA, University of North Texas — Propagation of plasmonic excitations in metal-dielectric structures is always accompanied by the loss which includes the generation of hot electrons in the vicinity of the metal surface. This results in the formation of a 2-D hot electron gas in the metal slab. Here, we theoretically show that in a metal-insulator-metal (MIM) capacitor, which is under an applied AC bias, the plasmonic-hot electrons are trapped by the interface states existing in the interfacial region of the dielectric slab leading to the creation of “plasmonic-capacitance”; an increase in the capacitance of the MIM configuration due to the charge of interface that reveals dependence on the frequency of the AC bias. This dependency is used to profile the energy distribution of the plasmonic-hot electrons. Importantly, the obtained energy distribution can be employed as the signature of the plasmonic excitation. The approach we introduce in this work suggests a new way to study all types of plasmonic phenomena occurring in planar hyperbolic metamaterials including high-k hyperbolic plasmons and epsilon near zero modes.

The effect of Ni impurities on the nucleation rates of undercooled Sn droplets  
SITARAM PANTA (Presenter), ERIC J COTTS, Binghamton University — Although high purity Sn can undercool more than forty percent of its melting temperature, small amount of Ni in Sn decrease undercooling to 10 K. We report on measurements of the nucleation rate of undercooled Sn droplets as a function of temperature and Ni content, within the context of classical nucleation theory. The undercooling of these Sn-Ni alloys was found to decrease linearly up to 0.5at% of Ni. Analysis of the dependence of nucleation rates of Sn-Ni alloy on temperature revealed that the barrier height to nucleation systematically decreased with Ni concentration, by more than three orders of magnitude upon the addition of Ni. Such a huge increase in nucleation rate is difficult to explain with a simple picture of heterogeneous nucleation of Sn on Ni3Sn4 which eventually forms during solidification process. Previous work has revealed that Ni3Sn4 is a poor inoculant for Sn nucleation. In contrast, the huge increase in nucleation rate observed in this work would require very low wetting angles to explain with such a heterogeneous nucleation picture. The increase in nucleation rate and hence the decrease in energy barrier can be explained by a decrease in surface energy between liquid and nucleating solid.
4:18PM P18.00010: Generating amorphous structures by combining Reverse Monte Carlo and molecular dynamics and analyzing with graph theory algorithm* ALEC MISHKIN (Presenter), JUN JIANG, MAHER YAZBACK, Department of Physics and Quantum Theory Project, University of Florida, KIRAN PRASAI, RICCARDO BASSIRI, MARTIN FEJER, Ginztom Laboratory, Stanford University, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — We present results from atomistic modeling of amorphous zirconia-doped tantala with an aim to understand the sources of mechanical loss in its structure. This material is a candidate for future LIGO gravitational wave detector mirror coatings, where lower mechanical loss coatings are essential to reduce thermal noise. We use Reverse Monte Carlo (RMC) modeling, which is a common technique used to generate atomic models based on experimental data. Here we use pair distribution functions (PDFs) as the reference experimental data set for the RMC. However, the structural solutions from RMC based on PDFs are not unique, and other constraints are needed to rule out unphysical solutions. In this work, we use molecular dynamics as the additional constraint, and show that allowing the structure to perform ionic and volume relaxation in between RMC runs can generate models that are in good agreement with the PDF data and energetically favorable. We also present an analysis of the intermediate range order from these models. This analysis is achieved by converting amorphous structures into graphs, where atoms are vertices and bonds are edges, and analyzing the structures that are responsible for short and intermediate range segments of the PDF.

*NSF/PHY 170870 NSF/PHY 1707964 NSF/PHY 1404110

4:30PM P18.00011: Scaling of emergent symmetry at a first-order transition in the simplest classical model* JUN TAKAHASHI (Presenter), Institute of Physics, Chinese Academy of Sciences, Beijing, China, ANDERS W SANDVIK, Boston University / IOP-CAS, Beijing — Emergent symmetry has attracted attention due to its possible connections with deconfined quantum criticality, where the phase boundary between a dimerized and a Neel phase is generically continuous, contrary to the standard Ginzburg-Landau picture where a first-order phase transition is predicted.

While emergent symmetries of multicritical points have been studied in various ways [1], less is known about how the emergent symmetry remains at the first-order transition line starting from such multicritical points [2].

In this study, we analyze a simple model with two competing orders, by extensive Monte Carlo simulation. The model has three phases (one paramagnetic and two Z2 symmetry-breaking phases) when varying the temperature and a parameter in the Hamiltonian. We observe that the bicritical point where the three phases meet has emergent O(2) symmetry, as predicted by field-theory [1]. Furthermore, we find that the first-order transition line separating two ordered phases has a remainder of the emergent symmetry up to a certain length scale. We quantitatively discuss how this length scale diverges.


*This work was supported by NSF DMR-1710170 and Simons Foundation.

4:42PM P18.00012: Magnetic Cooling for Nanoelectronics below 1 mK* YEMLIHA BILAL KALYONCU, CHRISTIAN SCHELLER, MARIO PALMA, DARIO MARADAN, University of Basel, Department of Physics, ANNA V FESHCHENKO, MATTHIAS MESCHKE, Aalto University, Low Temperature Laboratory, DOMINIK ZUMBUHL (Presenter), University of Basel, Department of Physics — Temperatures below 1 mK in quantum transport experiments could open the door for new physics such as novel nuclear spin phases, fragile fractional QH states, topological phases and unprecedented coherence. However, this is a formidable challenge since the thermal coupling becomes weak, making devices susceptible to heat leaks, microwaves and electronic noise. Our approach is to provide a separate nuclear refrigerator in each sample wire, cooling the device through the electronic degree of freedom.

Combining on-and-off chip demagnetization provides cooling of the islands of a Coulomb blockade thermometer as well as the electrical leads connecting to the sample, thus reducing external heat leaks [1]. The device comprises a linear array of Al/AlOx/Al tunnel junctions with huge copper islands in between, serving as spin reservoirs for demagnetization, thus enabling on-chip cooling. This scheme results in a lowest electronic temperature of 1.8 ± 0.1 mK. We also present a model which gives a good match and suggests how to overcome the main limitations to cool below 1 mK, thus opening the door for future microkelvin nanoelectronics.


*Supported by Swiss NSF, NCCR QSIT, SNI, and the European Microkelvin Platform
**4:54PM P18.00013: Compressive photoacoustic imaging in scattering media**  
YUNING GUO (Presenter), XIAOBO YIN, BAO Wen LI, Department of Mechanical Engineering, University of Colorado Boulder — Nowadays optical imaging in highly scattering media is still challenging to meet the requirement for wide-field visualization with a high resolution across the physical and biomedical science. Photoacoustic imaging, which relies on the ultrasonic waves emitted by absorbing structures under pulsed light illumination via thermoelastic stress generation, provides an efficient way to overcome the optical diffusion limitation. Compressive sensing, an efficient signal processing technique by finding solutions to underdetermined linear systems, is adapted to reduce the burden posed by traditional imaging requirements. It can be used to improve the trade-off between spatial resolution and acquisition time of sequential measurements, which can overcome the limiting of real-time applications to relative low resolutions. Based on compressive sensing, we design a photoacoustic imaging system that can achieve effective 3D imaging in scattering media with just a few sensors. It has the capability to image structured objects hidden in diffused media with a high resolution at a faster pace and works in the fields where the signal reduction is beneficial such as invasive bioimaging.

*Y. Guo acknowledges the financial support from the Acoustical Society of America.

**5:06PM P18.00014: Manipulating thin film properties by search for substrates over databases**  
PEDRAM TAVADZE (Presenter), LIAN LI, CHENG CEN, ALDO H ROMERO, Physics Department, West Virginia University — Substrates can have major effects on the growth direction, orientation, nucleation, morphology, field emission in carbon nanotubes, superconductivity, and etc. The influence of substrate on the thin film can be mechanical, electronic, or both. Specific applications require different substrates. In order to tune the characteristics of the thin film to ones needs, one has to explore a large set of possible substrates. As experimentally this work is almost impossible, one has to use computational methods to evaluate possible substrates. In this work we report a flowchart on how to search for optimal substrates and complement the selection by specific electronic structure characterization. We apply our methodology to FeSe, where the superconductor properties are very sensitive to the substrate. We employ the available algebraic algorithm provided by MPInterfaces package to search for geometrical matches in the OQMD database and calculate the work-function of the matched substrates as the criteria to select a good substrate. The results from the geometrical matches are input to a machine learning algorithm to increase the search speed in the databases.

*Bridges and Stampede XSEDE-NSF supercomputers and DMREF-NSF 1434897, NSF OAC-1740111 and DOE DE-SC0016176 projects.

**5:18PM P18.00015: A novel semi-metallic allotrope of carbon**  
JOEL THERRIEN, MICHAEL MASAKI (Presenter), ECE, University of Massachusetts Lowell, PURUSOTTAM JENA, Physics, Virginia Commonwealth University — A previously unknown allotrope of 3-dimensional crystalline carbon has been synthesized via CVD. Formation occurs when specific hydrocarbons react with certain metal or metal-oxide catalysts such as copper or aluminum oxide at temperatures above 800°C. The material has been characterized by XRD, Raman, FTIR and XPS. Raman spectra indicate the material consists of a mixture of sp² and sp³ bonded carbon. X-ray diffraction shows distinct peaks which do not correlate with graphite or diamond. Upon annealing at 1,100°C the diffraction peaks show considerable sharpening indicating the formation of larger domains. This is also reflected in the Raman spectrum which also shows a sharpening of the D and G carbon peaks. XPS analysis did not indicate the presence of any element beside carbon. The material has a high reflectivity from far UV to mid IR and visually appears mirror-like when deposited on smooth substrates. The temperature dependent conductivity has a negative temperature coefficient suggesting the material is most likely a semi-metal as opposed to a true metal; something not unexpected with carbon.

**Wednesday, March 6, 2019 2:30 PM - 5:30 PM**

Session P20 DCOMP DMP GMAG: First-principles Modeling of Excited-state Phenomena in Materials IX: Applications of First Principles Methods to Magnetic and Catalytic Materials BCEC 157A - David Strubbe, University of California, Merced - Tag(s): Focus
Charge separation and band alignment at photo-electrochemical interfaces* [Invited] ISMAILA DABO (Presenter), Pennsylvania State University — Solar energy is the most abundant energy source available to humankind, but this energy cannot be harnessed on demand due to the variability of sunlight. Artificial photosynthesis overcomes that variability through the direct photocatalytic storage of solar power into chemical fuels. Nevertheless, most of the stable photocatalysts in use today rely on metal oxide semiconductors whose bandgap does not match the solar spectrum. This presentation will discuss the development and experimental validation of computational protocols to understand, predict, and optimize visible-light-active materials that can split water into hydrogen and oxygen with a focus on answering the critical questions that surround (1) solar compatibility using electronic-structure methods beyond density-functional theory, (2) electrochemical stability by exploiting quantum-continuum embedding methods, and (3) band-edge alignment by means of machine-learning statistical techniques.

*This work is supported by the National Science Foundation under grant number DMR-1729338.

Ground and excited states of iron-phthalocyanine: a DFT+DMFT analysis* VOLODYMYR TURKOWSKI (Presenter), SHREE RAM ACHARYA, Physics, University of Central Florida, Orlando, 32816 FL, CARLOS GARCIA-FERNANDEZ, NICOLAS LORENTE, Donostia International Physics Center, 20018 San Sebastian, Spain, TALAT S. RAHMAN, Physics, University of Central Florida, Orlando, 32816 FL — Although the iron-phthalocyanine (FePc) molecule has been the subject of numerous experimental and theoretical studies, questions still remain about its ground and excited states. We have performed a Density Functional Theory+Dynamical Mean-Field Theory (DFT+DMFT) analysis of the spin resolved density of states of this interesting molecule to show that local dynamical effects (time-resolved on-site electron-electron interactions), which are inherently taken into account within DMFT, modify the DFT and DFT+U electronic spectrum of the molecule in the following way: they shift energy of a number of levels (most notably in the HOMO-LUMO energy range) and lead to new peaks. Such a modification may help resolve the issue of the ground state of FePc (complicated by the competing close-in-energy configurations) and can dramatically affect the transport, electronic and other properties of the molecule. Though further experimental test of the results are needed to quantify the accuracy of the DMFT approach for nanoscale systems, our results suggest that similar to extended systems time-resolved on-site electron-electron interactions play an important role in molecules that contain transition-metal atoms.

*Work supported in part by DOE grant DE-FG02-07ER46354

Electron-phonon coupling in photoexcited Bi$_2$Te$_3$* JOSE QUERALES-FLORES (Presenter), IVANA SAVIC, Tyndall National Institute, ÉAMONN MURRAY, Department of Physics and Department of Materials, Imperial College London, STEPHEN B FAHY, Department of Physics, University College Cork, JONATHAN SOBOTA, Department of Applied Physics, Stanford University, SAMUEL W TEITELBAUM, SLAC National Accelerator Laboratory, Stanford Institute for Materials and Energy Sciences, TAKAHIRO SATO, MATTHIEU CHOLLET, Stanford PULSE Institute, SLAC National Accelerator Laboratory, JAMES M GLOWNIA, SLAC National Accelerator Laboratory, MARIANO TRIGO, SLAC National Accelerator Laboratory, Stanford Institute for Materials and Energy Sciences, TREVOR P BAILEY, CTIRAD UHER, Department of Physics, University of Michigan, PATRICK S KIRCHMANN, SLAC National Accelerator Laboratory, Stanford Institute for Materials and Energy Sciences, ZHI-XUN SHEN, Stanford University, COSTEL R. ROTUNDU, Department of Applied Physics, Stanford University, THOMAS HENIGHAN, DAVID A REIS, Stanford University — Bi$_2$Te$_3$ is a topological insulator and thermoelectric material with a high figure-of-merit at room temperature. Strong spin-orbit coupling leads to the inversion of its bulk valence and conduction bands, which results in the formation of topologically-protected surface states [1]. Despite this protection, the surface states may be scattered by lattice vibrations [2]. Here we study the electron-phonon interaction of the surface states in Bi$_2$Te$_3$ using density functional theory and density functional perturbation theory. We calculate the deformation potentials of the surface states due to coupling to the coherent A$_{1g}$ modes driven by photoexcitation. Our computed deformation potential values agree well with those obtained from time-resolved ARPES measurements and time-resolved Bragg diffraction. Our calculations also quantitatively reproduce the experimentally observed magnitude of the surface phonon softening. These findings open opportunities for reliable first principles predictions of the topological transport properties of Bi$_2$Te$_3$ and related V$_2$-VI$_3$ materials.


*This work was supported by Science Foundation Ireland under Investigators Programme No. 15/IA/3160.
3:30PM P20.00004: Calculation of excitation energies using locally-projected real-space geminal screened electron-hole interaction kernel* PETER MCLAUGHLIN, ARINDAM CHAKRABORTY (Presenter), Syracuse University — The geminal-screened electron-hole interaction kernel (GSIK) is a real-space representation for describing electron-hole correlation in charge-neutral excitations. Unlike MBPT and EOM methods, the GSIK method avoids using virtual or unoccupied orbitals for constructing electron-hole interaction kernel. This feature allows GSIK method to be used for chemical systems where inclusion of a large number of unoccupied orbitals will be computationally prohibitive. This talk will present the locally-projected formulation of the GSIK method where the electron-hole interaction kernel is calculated using an atom-in-cluster approach. It will be demonstrated that the local-projection allows the evaluation of the kernel to be performed at a linear-scaling cost. The locally-projected GISK method was applied to large metallic (Au300) and semiconductor (Pb150S150) nanocluster for calculation of optical gap and electron-hole binding energies. The results from these calculations demonstrate the efficacy of the GSIK method for capturing electron-hole correlation in large clusters and nanoparticles.

*This research was supported by the National Science Foundation under Grant No. CHE-1349892.

3:42PM P20.00005: Structural parameters governing excited-state properties of self-assembling π-conjugated peptides: a classical and quantum study* BRYCE THURSTON (Presenter), Center for Integrated Nanotechnologies, Sandia National Laboratories, ETHAN SHAPERA, Physics, University of Illinois at Urbana-Champaign, ANDRE SCHLEIFE, Materials Science and Engineering, University of Illinois at Urbana-Champaign, ANDREW L FERGUSON, Institute for Molecular Engineering, University of Chicago — Peptides that self-assemble are of significant interest for use in the fabrication of biocompatible nano-aggregates. Non-natural π-conjugated subunits may be embedded into the peptide backbone, leading resulting β-sheet-like ribbons formed from self-assembly to have electronic and photophysical properties. Alteration of the amino acid composition of the peptides can have a significant impact on the measured absorption spectra of aggregates, but the exact geometric origin of these changes is unknown. In order to probe these composition-induced alterations, we utilize time-dependent density functional theory calculations to study the excited state properties of peptide configurations extracted from molecular dynamics simulations. We identify geometric variables describing π-conjugated core geometries that appear to be determinative of the wavelength at which the absorption spectrum reaches its peak. When applied to MD simulations, the resulting regression model is shown to be in qualitative agreement with experiment, laying the foundation for in silico prediction of absorption properties of peptide aggregates.

*National Science Foundation Grant No. DMR-1729011

3:54PM P20.00006: Understanding battery and catalytic reactions via core-level spectroscopies [invited] LIANG LI, Argonne National Laboratory, JOHN VINSON, ERIC SHIRLEY, National Institute of Standards and Technology, MARIA CHAN (Presenter), Argonne National Laboratory — Materials often undergo local changes in structure and electronic properties during operations. For example, transition metal oxide battery materials and catalysts often undergo coordination and oxidation state changes. In order to probe these changes, core-level spectroscopy including x-ray absorption, emission, non-resonant and resonant inelastic x-ray scattering, as well as electron energy loss spectroscopy, is often informative. Because of the integrated nature of these signals, the interpretation of these experiments can be at times ambiguous, but can be significantly aided by the use of first principles modeling of core-level spectra. In this talk, we discuss the use of OCEAN [1], a code based on the Bethe-Salpeter Equation, for accurate prediction of core-level spectra, and how the results have helped informed oxygen redox accompanying battery reactions [2,3,4] and detection of CO adsorption during catalytic CO2 reduction reaction [5] in transition metal oxides.

4:30PM P20.00007: Quantum Nonlinear Ferroic Optical Hall Effect*  HUA WANG (Presenter), XIAOFENG QIAN, Department of Materials Science and Engineering, Texas A&M University — Nonlinear optical responses provide basis for ultrafast probing of material's intrinsic symmetry [1]. Here we present first-principles theory of quantum nonlinear ferroic optical Hall effect (QNFOHE)[2], a Hall-like photocurrent originated from the second order current response in (multi)ferroics. The interplay of crystalline, permutation, gauge, time reversal symmetries and inherent causality governs the symmetry of QNFOHE. We elucidate QNFOHE in a class of 2D multiferroics [3] using first-principles calculations and group theoretical analysis. Our results suggest QNFOHE-based optical technique as a route for ultrafast characterization of multiferroic orders and domain evolution in multiferroic materials. These microscopic understandings of QNFOHE from first-principles theory, together with very recent discoveries of 2D ferroics/multiferroics, will open up a variety of new avenues for nonlinear optoelectronics.


*This research was supported by NSF under award number DMR-1753054 and Texas A&M High Performance Research Computing.

4:42PM P20.00008: Polar magneto-optical Kerr effect from antiferromagnetic M2As (M=Cr, Mn, and Fe) under external magnetic field*  KISUNG KANG (Presenter), KRITHIK PUTHALATH, DAVID G CAHILL, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Polar magneto-optical Kerr effect (PMOKE) is a great tool to detect ferromagnetic domains and their magnetization but is of no use for antiferromagnets without external magnetic field. To understand PMOKE from antiferromagnets under external magnetic field, we use first-principles density functional theory. Due to the lack of net magnetization in the ground state, spin tilting is only induced by an external field, leading symmetry breaking and thus PMOKE signal arises. Based on band structure analysis, exchange splitting and spin-orbit coupling effects are confirmed, similar to ferromagnetic materials. While the spin-orbit coupling is affected little by the external field, exchange splitting arises due to spin tilting. Majority and minority spin states are increasingly separated as external magnetic field increases. Furthermore, in antiferromagnets magnetic susceptibility is related to spin tilting. We compute the magnetic susceptibility of Cr2As, Mn2As, and Fe2As and find that Fe2As presents largest PMOKE signal at a given external magnetic field as well as the largest susceptibility. Large susceptibility leads to larger spin tilting and, hence, more exchange splitting and stronger PMOKE signal.

*Illinois MRSEC NSF DMR-1720633

4:54PM P20.00009: Study of LaScO3 by electronic structure quantum Monte Carlo methods  CODY MELTON (Presenter), LUBOS MITAS, North Carolina State University — Transition Metal Oxide perovskites (ABO3) are a set of materials that have been widely studied due to the coupling of their charge, spin, orbital, and lattice degrees of freedom, leading to a variety of interesting properties. These materials are typically studied with DFT+U, hybrids, or GW methods to correct for the self-interaction errors within DFT, typically due to the localized nature of the occupied d-orbitals and are often further complicated by various magnetic states. However, even in cases where there is no d-occupancy and the material is a non-magnetic insulator, such as LaScO3, there can be significant errors from these methods due to inaccuracies in the description of electron correlation. For example, the GW methods underestimate the bandgap by roughly 1.5 eV, and hybrid DFT must be tuned in order to reproduce the bandgap. Here, we present a study of LaScO3 using the highly accurate Fixed-Node Diffusion Monte Carlo (FNDMC) method. We show that by carrying out the standard FNDMC methodology, we are able to accurately reproduce the experimental bandgap of LaScO3 without any parameter tuning as is required by DFT and related methods. Additionally, we present calculations of the cohesive energy, equation of state, and other properties using FNDMC.
Photoactive metal-organic frameworks for gas separation

ROBERTA POLONI (Presenter), Univ. Grenoble Alpes, CNRS, Grenoble, CLAUDIO ATTACCALITE, CINAM, CNRS, Marseille, JING LI, Institut Neel, CNRS, Grenoble, ASEEM RAJAN KSHIRAGAR, Univ. Grenoble Alpes, CNRS, Grenoble — Metal-organic frameworks (MOFs) are attracting much attention in recent years for their potential use in CO2 capture technologies. Recently, it has been shown that an efficient capture-and-release process can be obtained upon light treatment in photoactive MOFs [1,2]. We demonstrated that in these MOFs the notable change in gas uptake, upon light irradiation, is due to the blocking of the strongly adsorbing metal sites upon isomerization of the azo groups from trans to cis [3]. Interestingly, our study suggests a large fraction of cis at the photostationary state. A large S1/S2 absorption band separation between trans and cis within the MOF could support this hypothesis. In order to address this, we have computed the optical absorption spectra of these MOFs and their ligands using embedded GW/BSE calculations as implemented in FIESTA. Embedding is considered first at the DFT level (COSMO solvation model and ESP charges) and then, in the calculation of the modified screened Coulomb potential. CASSCF/CASPT2 and periodic GW/BSE are performed to benchmark, respectively, the DFT starting point and the choice of the fragment. Work supported by ANR-15-CE06-0003-01. [1] Park et al, JACS 134, 99 (2012); [2] Wang et al, Nature Commun. 7, 13872 (2016);

Electronic and Magnetic Properties of KTa\textsubscript{1-x}Mn\textsubscript{x}O\textsubscript{3}; (x = 0, 0.50, 0.67)

GOPI CHANDRA KAPHLE (Presenter), NIRMALA ADHIKARI, Central Department of Physics, Tribhuvan University — KTa\textsubscript{1-x}Mn\textsubscript{x}O\textsubscript{3} (x = 0, 0.50, 0.67) are perovskites used for fuel cells, memories devices, and spintronic applications. In the present work, we performed the first-principles calculations to study the structural, electronic and magnetic properties of pristine KTaO\textsubscript{3} perovskite and Manganese doped perovskites KTa\textsubscript{1-x}Mn\textsubscript{x}O\textsubscript{3} system along Ta site of super-cell. Our study based on super-cell calculations. Our finding shows that the pure perovskite KTaO\textsubscript{3} is indirect type band gap semiconductor having band gap 2.13 eV which is close agreement with experimental reported value 2.15 eV within 1% deviation. In the study of Mn doped system, we observed that there is indirect band gap decrease from 2.13 eV to 0.84 eV at 50% Mn doped on perovskite KTa\textsubscript{0.5}Mn\textsubscript{0.5}O\textsubscript{3} along Ta site and 0.81eV at 67% Mn doped on perovskite KTa\textsubscript{0.33}Mn\textsubscript{0.67}O\textsubscript{3} along Ta site. Further investigations shows antisymmetric distribution of DOS for spin-up and spin-down electronic states for Mn doped states. The contribution to total DOS is due to 2p-orbital of oxygen and 3d-orbital of manganese around the Fermi level. Whole doped system behaves as half metallic.

G.C.K. thanks Dr. M. P. Ghimire, CDP, TU for fruitful discussions.

*G.C.K acknowledges the computational support from CMPRC-Butwal and Prof. Regmi, CDP, TU.
AIDAN THOMPSON (Presenter), Sandia National Laboratories — Molecular dynamics (MD) is a powerful materials simulation method whose accuracy is limited by the interatomic potential (IAP). In many materials science applications suitably accurate potentials simply do not exist. SNAP is an automated methodology for generating application-specific IAPs using large and diverse datasets of quantum electronic structure calculations. The SNAP IAP is formulated in terms of a set of general four-body geometric invariants that characterize the local neighborhood of each atom. This approach has been used to develop potentials for diverse applications, including metal plasticity (Ta), defects in III-V semiconductors (InP), and fusion energy materials (W/Be/He/H). In each case, the SNAP IAP is fit to density functional theory calculations of energy, force, and stress for many small configurations of atoms. Cross-validation analysis and evaluation on test problems are used to further improve IAP fidelity and robustness. Varying the number of geometric descriptors allows a continuous tradeoff between computational cost and accuracy. The resultant potentials enable high-fidelity MD simulations of these materials, providing insight into their behavior on lengthscales and timescales unreachable by other methods. The relatively large per-atom computational cost of SNAP is offset by combining LAMMPS' spatial parallel algorithms with Kokkos-based hierarchical multithreading, enabling the efficient use of large CPU and GPU clusters, allocating only a few atoms to each node. Recent extensions of the SNAP approach include multi-element geometric descriptors and the use of higher-order terms.


ARAVIND KRISHNAMOORTHY (Presenter), University of Southern California, PANKAJ RAJAK, Argonne Leadership Computing Facility, Argonne National Laboratory, AIJIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, University of Southern California — Scalable synthesis of two-dimensional (2D) materials is a major bottleneck to more widespread adoption of layered material-based devices. Chemical vapor deposition (CVD) has emerged as a viable method for large-scale synthesis of 2D materials. However, neither experiment nor theory has been able to decipher mechanisms and selection rules, or make predictions of optimized growth parameters. Experimental challenges stem from the use of probes like TEM to characterize CVD growth reactions in situ under elevated temperatures and pressures. Computational synthesis, which simulates CVD processes using reactive molecular dynamics methods provides the atomistic resolution necessary for the deduction of reaction mechanisms. Here we use neural networks trained on trajectories from several hundred simulations of computational synthesis of MoS2 monolayers to uncover the dependence of product stoichiometry, crystallinity and phase distribution on reaction parameters like temperature, sulfur and hydrogen partial pressures, thus paving the way for rational design of CVD synthesis techniques.

This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607.

TALAT S. RAHMAN (Presenter), DUY LE, Department of Physics, University of Central Florida — Recently, defects in hexagonal boron nitride (h-BN) have been shown to play an important role in determining its novel chemical and optical properties, which may have a variety of possible technological applications. Characterization of the structure and dynamics of these defects would be most facilitated by the availability of accurate interatomic potentials that enable large length and time scale simulations. In this work, we will summarize our development of an artificial neural network (ANN) potential for h-BN with and without defects. The ANN potential was trained by using about 70000 data points obtained from ab initio molecular dynamic simulations of point defect on a (6x6) h-BN layer. The trained ANN potential is capable of producing system energetics in agreement with that obtained from density functional theory (within few meV per atom for both training and validation). The structure and dynamics of defects and grain boundaries in h-BN using the ANN potential will be presented and results compared with available experimental data.

This work is supported in part by DOE grant DE-FG02-07ER15842
**Active-learning strategy for the development of application-specific machine-learning force fields**

HUAN TRAN (Presenter), ROHIT BATRA, JAMES CHAPMAN, CHIHO KIM, ANAND CHANDRASHEKARAN, RAMAMURTHY RAMPRASAD, Georgia Institute of Technology — Emerging data-driven approaches in materials science have triggered the development of a plethora of machine-learning (ML) force fields (FFs). In practice, they are constructed by training a statistical model on a reference database to predict potential energy or atomic forces. While most of the FFs can accurately recover the reference data, some of them are becoming useful for actual molecular dynamics simulations. In this work, we develop a simple active-learning strategy for the development of ML FFs targeted at specific simulations (applications). The strategy involves (1) preparing and fingerprinting a diverse reference database of atomic configurations and forces, (2) generating a pool of ML FFs by learning the reference data, (3) validating the FFs against a series of targeted applications, and (4) selectively and recursively improving the FFs that remain unsuitable for a given application while keeping their performance on other applications uncompromised. We demonstrate this strategy by developing a series Al and Cu ML FFs that can simultaneously be used for various applications, including (elastic) stress/strain analysis, stacking-fault energy calculations, and melting simulations. This strategy is generalizable, i.e., it may be used for other materials as well.

**Deep Generative Model of Interfacial Structures in Phase Transformation of an MoWSe2 Monolayer**

PANKAJ RAJAK (Presenter), Argonne national laboratory, ARAVIND KRISHNAMOORTHY, AIICHIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, University of Southern California — Optical and electrical properties of two-dimensional layered materials can be tuned by mechanical straining, which induces transformations from semiconducting to metallic phases. We use deep generative variational autoencoder (VAE) model, trained by molecular dynamics simulation data of dynamic fracture in an MoWSe2 monolayer, to predict transition pathways consisting of novel intermediate structures (a and b) between the semiconducting (2H) and metallic (1T) phases. In addition, a conditional variational autoencoder (CVAE) is used to generate intermediate structures such as a or b, and defects. Structures synthesized from VAE and CVAE are validated by quantum simulations based on density functional theory. Quantum simulations show that structures generated by VAE and CVAE are stable and can be used for nanoelectronics applications.

*The work was supported by the grant DE-SC0018195 funded by the U.S. Department of Energy, Office of Science. Simulations were performed at the Argonne Leadership Computing Facility under the DOE INCITE program and at the Center for High Performance Computing of the University of Southern California.

**Magnetism and superconductivity in amorphous carbon**

YUKI SAKAI (Presenter), Institute for Computational Engineering and Sciences, University of Texas at Austin, JAMES CHELIKOWSKY, Department of Physics, University of Texas at Austin, MARVIN L COHEN, Department of Physics, University of California at Berkeley — We study magnetic and superconducting properties of amorphous carbon based on molecular dynamics simulations. First we use spin constrained first-principles simulations to obtain amorphous carbon structures with a desired magnetization. We show that the existence of sp2-like threefold coordinated carbon atoms plays an important role in causing magnetism in amorphous carbon. We predict detailed geometries of threefold carbon atoms that induce the magnetic order in amorphous carbon. We also consider the effect of boron doping on superconducting properties of amorphous carbon. By considering amorphous structures with various sp2:sp3 ratios, we find that sp3-hybridized atoms are necessary for high superconducting transition temperature in contrast to the magnetism.

*YS and JRC acknowledge DOE grant DEFG02-06ER46286. Computational resources are provided in part by NERSC and TACC. MLC acknowledges NSF Grant DMR-1508412 and Theory of Materials, LBNL, DoE Contract No. DE-AC02-05CH11231.
Magnetostriction and Long-Range Interactions in Coupled Spin and Lattice Dynamics*

JULIEN TRANCHIDA (Presenter), MITCHELL A WOOD, ATTILA CANGI, STAN G. MOORE, Sandia National Laboratories, PASCAL THIBAudeau, Le Ripault, CEA-DAM, STEVEN JAMES PLIMPTON, AIDAN THOMPSON, Sandia National Laboratories — A scalable and symplectic algorithm for coupled spin dynamics and molecular dynamics was recently released in the molecular dynamics code LAMMPS. Our presentation will focus on two of its recent improvements: (1) incorporating magnetostrictive effects in and (2) implementing scalable techniques to compute long-range magnetic interactions.

A methodology accounting for magnetostriction in hexagonal crystals based on Néel's work on pair anisotropy models was developed and applied to HCP-cobalt. We parametrized our model using ab-initio calculations within the Spin-Dependent Density Functional Theory framework including the Spin-Orbit coupling. We will show how typical magnetostrictive results were recovered. Although negligible for most small magnetic simulations, the magnetic dipolar energy becomes fundamental for larger configurations, where magnetic domains can nucleate and be stabilized. In order to account for it (and for the associated magneto-mechanical interactions), two methodologies, Ewald sums and Particle-Particle Particle-Mesh, were coupled to the spin-lattice symplectic algorithms developed in LAMMPS. Scaling and energy preservation results will be presented.

*JT acknowledges financial support through a joint CEA-NNSA grant.

Employing autoencoders for configuration space sampling: Application to small molecules.

IGOR POLTAVSKYI (Presenter), ALEXANDRE TKATCHENKO, FSTC, University of Luxembourg — The behavior of molecular systems in different equilibrium physical processes or chemical reactions is governed by the free energy (FE). Calculations of FE require a thorough sampling of configuration space for given external conditions. State-of-the-art sampling techniques, based on molecular dynamics, are formally applicable to systems of arbitrary size. However, in practice, they suffer from the curse of dimensionality and the limitation of the time step by the fastest process present in the system. These make FE calculations for complex molecules, where the entropy effects are of utmost importance, extremely challenging and computationally demanding. Here we propose to use a machine-learning approach based on autoencoders to generate new sampling configurations. By transition to the feature space, we effectively decrease the dimensionality of the problem and resolve the time step limitation. Training autoencoders cost only a small fraction of statistically converged molecular dynamics simulations, paving the way to efficient calculations of thermodynamic properties for complex molecular systems.

Atomistic mechanisms of phase transitions from Machine Learning*

RODRIGO FREITAS (Presenter), EVAN REED, Department of Materials Science and Engineering, Stanford University — Identifying and characterizing atomic mechanisms of phase changes is of fundamental importance in the study of the kinetics of the nucleation and growth process. This talk will describe a new approach in extracting information from atomistic simulations of phase transitions using Machine Learning (ML) methods. In this approach the local neighborhood of atoms is characterized in terms of symmetry functions that are used as input to a ML algorithm trained to identify atomic rearrangements leading to structural transformations. The application of the method is illustrated using Molecular Dynamics simulations of crystallization from the liquid or amorphous phase. We also discuss how meaningful physical properties can be extracted from the output of the ML algorithm.

*This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0002007.

Efficient Training of Neural-Network Interatomic Potentials with Atomic Forces*

SIMON BATZNER (Presenter), BORIS KOZINSKY, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Neural-Network Interatomic Potentials have emerged as a promising method to accelerate time and length scales in Molecular Dynamics simulations of condensed systems. In the learning process, models are usually trained to a set of reference energies from electronic-structure calculations. In addition to total energies, local atomic forces are often also available by the Hellmann–Feynman theorem. Including atomic forces of quantum-mechanical accuracy in the training process can greatly enhance fidelity of the learned potential energy surface as it provides a wealth of additional information about its shape. However, this training scheme often comes at a much greater computational expense. In this talk, we address the speed and fidelity of integrating forces into the training process and examine strategies for rapid training of neural-network potentials for complex systems involving large training sets.

*S.B. acknowledges support from the Skoltech-MIT Center for Electrochemical Energy Storage.
2:30PM P22.00001: Electrons modified by phonons: Adiabatic versus non-adiabatic, and the persistence of electron quasiparticles* [invited] PHILIP B. ALLEN (Presenter), Stony Brook University — This talk will briefly review various types of renormalization of electron quasiparticles by phonons, including the question of when quasiparticle properties persist. Several new concerns will be discussed. In summary, band structure energies of order eV's are affected by phonons of energy 100 times smaller. Semiconductor band gaps are altered by shifts of order 0.1 eV, and are temperature (T)-dependent. The component from thermal expansion is typically smaller than the renormalization from phonons. In metallic bands, an additional low T "mass renormalization", m*/m > 1 is observed. The ratio can range between 1.1 and 3.0. This is a non-adiabatic effect. At low T, metallic electrons notice the time-dependence of the vibrational displacements. The Eliashberg reformulation of conventional BCS superconductivity is closely related. The spectral functions of metallic electrons are often so broad that no recognizable quasiparticle peak is seen. Yet the quasiparticle picture functions nicely for understanding resistivity. Developments in computation have enabled good calculations of semiconductor band renormalization by phonons, which is mostly an adiabatic effect. Recently it has been realized that Froehlich polaron effects (and also piezo-polaron effects) need special treatment when computing energies of electrons close to the band gap. The (non-adiabatic) Froehlich polaron has a clear quasiparticle peak, plus phonon "satellites" in its spectral function. Surprisingly, the peak and satellites are badly misplaced in a conventional perturbative treatment. A "cumulant" version of the spectral function appears to solve the problem nicely. There are still aspects of phonon interactions with electrons that need reformulation, and remain challenges for theory and computation.

*This work was supported in part by DOE grant No. DE-FG02-08ER46550.

3:06PM P22.00002: The electron-phonon problem reconsidered ILYA ESTERLIS (Presenter), STEVEN KIVELSON, Stanford University, DOUGLAS J SCALAPINO, Physics, University of California Santa Barbara — The phase diagram of the electron-phonon (e-p) problem, as a function of e-p coupling and temperature, is presented. We work with the Holstein model and present determinant quantum Monte Carlo results for both large and infinite ion mass. In weak-coupling the system is a Fermi-liquid (and ultimately a "low temperature" superconductor), while beyond a critical coupling strength there is a transition to a (π,π) charge-density wave state. At elevated temperatures we find a cross-over to a pseudo-gap regime, corresponding to the formation of bound pairs of electrons with large effective mass (bipolarons). We compare MC results both with predictions from Migdal theory and strong-coupling expansions. For sufficiently weak coupling the Migdal approximation works extremely well but breaks down catastrophically upon entering the pseudo-gap regime, where the physics is accurately described by an Ising lattice gas model, as expected from the strong-coupling expansion.

3:18PM P22.00003: Temperature effects on the electronic band structure of PbTe from first principles* STEPHEN B FAHY (Presenter), University College Cork, JOSE QUERALES-FLORES, JIANG CAO, IVANA SAVIC, Tyndall National Institute — We present a fully ab-initio calculation of the temperature dependence of the electronic band structure of PbTe [1]. We address two main features relevant for its thermoelectric figure of merit: the temperature variations of the direct gap and the difference in energies of the two topmost valence band maxima located at L and Σ [2]. We account for the energy shift of the electronic states due to thermal expansion, as well as electron-phonon interaction computed using the Allen-Heine-Cardona formalism within density functional perturbation theory [3]. We capture the increase of the direct gap with temperature in very good agreement with experiment. We also predict that the valence band maxima at L and Σ become aligned at ~ 620 K. We find that both thermal expansion and electron-phonon interaction have a considerable effect on these temperature variations. The electron-phonon induced renormalization of the direct gap and the two topmost valence band maxima is produced mostly by high-frequency optical phonons.

*This work was supported by Science Foundation Ireland under Investigators Programme No. 15/IA/3160.

3:30PM P22.00004: First-principles electronic lifetimes and phonon-limited mobility in Si, Diamond, GaP, GaN and SnO$_2$*  
GUILLAUME BRUNIN (Presenter), HENRIQUE MIRANDA, MATTEO GIantomassi, GIAN-MARCO RignaneSE, GEOFFROY HAUTIER, Universite catholique de Louvain — Correctly understanding and computing the electronic transport quantities is crucial for the discovery and developments of new functional materials. Within the Boltzmann transport formalism, the computation of the electrical conductivity of a material is usually performed using the constant relaxation time approximation. In this framework, the electronic lifetime is a parameter extracted either from experimental data or from various semi-empirical models. Only recently, \textit{ab initio} computations of the electronic lifetimes due to electron-phonon interactions have been reported for various semiconductors and metals, making the full \textit{ab initio} computation of the phonon-limited (intrinsic) conductivity of materials possible [1-2].

In this work, we compute the electronic lifetimes for Si, Diamond, GaP, GaN and SnO$_2$, and explain how they are used to compute the intrinsic conductivity within the semi-classical Boltzmann transport equation. We compare the lifetimes obtained with EPW [3] and ABINIT [4] and explore ways to reduce the computational load while keeping a similar accuracy for the electronic lifetimes.


*GB acknowledges the FRS-F.N.R.S.

3:42PM P22.00005: Anharmonic suppression of charge-density-wave instability in bulk and monolayer NbS$_2$  
RAFFAELLO BIANCO (Presenter), Caltech, ION ERREA, University of the Basque Country, LORENZO MONACELLI, Università di Roma, La Sapienza, MATTEO CALANDRA, CNRS, FRANCESCO MAURI, Università di Roma, La Sapienza — The superconducting transition-metal dichalcogenide 2H-NbS$_2$, in sharp contrast to the isoelectronic compound 2H-NbSe$_2$, at low temperature does not show any charge-density-wave (CDW) ordering co-existing with the superconductive phase. That is in strong disagreement with \textit{ab initio} harmonic phonon calculations, which predict that 2H-NbS$_2$ is dynamically unstable. In this talk we will show that anharmonicty is the key factor to reconcile numerical results with experiments. With the stochastic-self-consistent-harmonic technique [1], we go beyond the harmonic approximation including quantum anharmonic effects in the \textit{ab initio} calculations and we obtain temperature-dependent phonon frequencies in quantitative agreement with experiment. In particular, the instability observed at harmonic level is removed. Furthermore, we analyze the effect of anharmonicity at low dimensions. Despite in the trigonal single layer form the CDW instability is even more incipient than in the bulk, the system still remains stable at low temperatures. Finally, we verify that the striking difference between 2H-NbS$_2$ and 2H-NbSe$_2$ is not simply ascribable to a mass effect, but it is dominated by the different electron screening felt by the ions in the two cases.


3:54PM P22.00006: Ab Initio Approach for Exciton-Phonon Interactions  
HSIAO-YI CHEN (Presenter), Department of Physics, Caltech, DAVIDE SANGALLI, CNR-ISM, Division of Ultrafast Processes in Materials (FLASHit), ANDREA MARINI, Istituto di Struttura della Materia of the National Research Council, MARCO BERNARDI, Department of Applied Physics and Materials Science, Caltech — We derive a formalism to compute exciton-phonon (ex-ph) interactions in crystals within the \textit{ab initio} GW-Bethe Salpeter equation (BSE) approach. Using first order perturbation theory and the Tamm-Dancoff approximation, we express the ex-ph coupling constant as a superposition of electron- and hole-phonon coupling processes. We discuss numerical calculations of such ex-ph coupling and the related scattering rates, which are challenging as they combine electron-phonon and finite-momentum BSE calculations; we carry them out by using the YAMBO code to obtain exciton dispersions and the PERTURBO code to compute electron-phonon coupling and the ex-ph scattering rates. We apply this framework to investigate ex-ph interactions in bulk hexagonal boron nitride (h-BN), for which we compute the exciton relaxation time due to ex-ph interactions and map it onto the exciton dispersions. We also employ an exciton Boltzmann transport equation to simulate the out-of-equilibrium dynamics of excitons and their equilibration with phonons in h-BN. Our work is a first step toward understanding electron-phonon interactions in composite electronic quasiparticles. It sheds light on correlated electron-phonon processes and provides new computational tools to investigate excited state dynamics.

4:06PM P22.00007: WITHDRAWN ABSTRACT
are solved, a computation of e-ph interactions reliably by using a pseudopotential method remains as an open question for further research. Before the problems are solved, a full-potential method for the calculation of e-ph interactions can be used to circumvent the problems.

*The work was funded in part by NSF (Award # HRD 1736136) and ARO (Award # W911NF-15-1-0483).


FENG GAO (Presenter), GUANG-LIN ZHAO, Southern University — The calculations of electron-phonon (e-ph) interactions in solid materials from first-principles remain as an important fundamental and applied problem in condensed matter physics. The pseudopotential method has been successfully used to study the valence electronic structure and related physical properties of solid materials. However, when atoms move, they will carry their true electronic potentials with them, not pseudopotentials. The derivatives of true electronic potentials with respect to atomic shifts in a solid will be quite different from the derivatives of pseudopotentials with respect to the same atomic shifts because of the smooth and non-local nature of the pseudopotentials. The essential part of the calculations of e-ph interactions is a reliable computation of the derivatives of electronic potential with respect to atomic position shifts. Consequently, determining how to calculate e-ph interactions reliably by using a pseudopotential method remains as an open question for further research. Before the problems are solved, a full-potential method for the calculation of e-ph interactions can be used to circumvent the problems.

Work at the University of Missouri is supported by the Department of Energy, Basic Energy Sciences, Award DESC0019114.

**4:42PM P22.00010: Plasmonic hot carriers in transition metal nitrides**

ADELA HABIB (Presenter), FRED FLORIO, RAVISHANKAR SUNDARARAMAN, Rensselaer Polytechnic Institute — Transition metal nitrides (TMNs) are well established as hard protective coatings on account of their excellent mechanical properties and chemical stability. With recent advances in synthesis, they are becoming increasingly competitive for their opto-electronic properties as refractory plasmonic materials. However, their potential for plasmonic hot carrier harvesting remains largely unknown. In this talk, we show that certain TMNs have a unique wide-band plasmonic behavior that extends deep into the ultraviolet regime. From first-principles calculations, we predict plasmonic response, hot carrier generation and subsequent thermalization of all group IV, V and VI transition metal nitrides, fully accounting for direct and phonon-assisted transitions as well as electron-electron and electron-phonon scattering mechanisms. We find hot carrier lifetimes and mean free paths in these TMNs comparable to those of gold and silver. Finally, we explore mechanisms responsible for the negative real permittivity extending to high frequencies in TMNs, an exciting prospect for stable ultraviolet plasmonics.

**4:54PM P22.00011: Electron-phonon coupling within Quasiparticle Self-consistent GW**

SAVIO LARICCHIA (Presenter), NICOLA BONINI, MARK VAN SCHILFGAARDE, Department of Physics, King’s College London — There is clear evidence that standard Density Functional Theory (DFT) underestimates electron-phonon coupling interaction in many materials, including even simple sp-bonded compounds. Hybrid functionals and quasiparticle GW corrections suggest that nonlocal exchange-correlation enhances the electron-phonon interaction as a consequence of an improved description of the electronic screening. This has highlighted the need to move beyond local exchange-correlation functionals within DFT, but complete field-theoretic investigations are still missing. In this talk I will introduce the development of a field-theoretic methodology which is able to predict on an equal footing electronic quasiparticles and phonons as well as their interaction. Such an approach has been implemented within the Quasiparticle Self-consistent GW (QSGW) formalism which describes well the electronic properties for a wide range of materials, including many where standard DFT fails.
5:06PM P22.00012: Ab Initio Next-to-Leading Order Electron-Phonon Interactions: Two-Phonon Electron Scattering Processes and their Temperature and Energy Dependence  NIEN-EN LEE (Presenter), JIN-JIAN ZHOU, HSIAO-YI CHEN, MARCO BERNARDI, Caltech — Electron-phonon (e-ph) interactions are a current focus of first-principles calculations. The lowest-order e-ph self-energy is computed in most works, and only recently there were attempts to include higher-order e-ph interactions using the cumulant method. However, diagrammatic approaches beyond the lowest order have not been attempted for computing e-ph interactions ab initio.

Here, we compute the scattering rates of e-ph processes involving two external phonons. Their expression is derived using many-body perturbation theory and the Matsubara technique on the two skeletonically nontrivial second-order diagrams. The numerical calculations are challenging since they involve Brillouin zone integrals over two crystal momenta and the intermediate state lifetime plays a critical role. Using random grids and Monte Carlo integration, we are able to compute and systematically converge such next-to-leading order e-ph scattering rates. Results are discussed for GaAs and SrTiO3, in which we analyze the two-phonon contributions to e-ph scattering as a function of temperature and carrier energy, and compare them with the lowest-order results. We discuss how our formalism can be extended to detect strong e-ph coupling and polaron formation.

5:18PM P22.00013: Simulation of time-resolved electron-phonon scattering on a Dirac cone  BENJAMIN NOSARZEWSKI (Presenter), Stanford University, ARTHUR K MILLS, MENGXING NA, FABIO BOSCHINI, MATTEO MICHIARDI, RYAN P DAY, ELIA RAZZOLI, ALEXANDER SHEYERMAN, MICHAEL SCHNEIDER, GIORGIO LEVY, SERGEY ZHDANOVICH, University of British Colombia, ALEXANDER KEMPER, North Carolina State University, THOMAS DEVHEREUX, Stanford University — Ultrafast spectroscopy is a powerful tool for studying the dynamical properties of quantum materials driven out of equilibrium. The relaxation dynamics of the non-equilibrium state can provide insights into the properties of the elementary scattering process and many-body interactions present in equilibrium. Using the Keldysh formalism we simulate time- and angle-resolved photoemission spectroscopy on a Dirac cone to capture the quantized relaxation processes of electrons coupled to optical phonons. Including retarded electron-phonon interactions, the simulation naturally captures the appearance of a direct excitation peak at an energy set by the frequency of the pump pulse and the delayed appearance of a secondary non-thermal peak above the Fermi level due to electron-phonon scattering as observed in an experiment performed on graphite.

Wednesday, March 6, 2019 2:30 PM - 4:54 PM

Session P23 GMED: Physics in Medicine: Computational Modeling  BCEC 158 - Robert Austin, Princeton University

2:30PM P23.00001: Synergistic Effect of Immunotherapy and Radiotherapy: a Computational Model  DAMIJAN VALENTINUZZI (Presenter), Jozef Stefan Institute, KATJA URSIC, Department of Experimental Oncology, Institute of Oncology Ljubljana, URBAN SIMONČIČ, Faculty of Mathematics and Physics, University of Ljubljana, MATEA MARUNA, Department of Experimental Oncology, Institute of Oncology Ljubljana, SIMON BUCEK, Department of Cytopathology, Institute of Oncology Ljubljana, MARUŠA TURK, Faculty of Mathematics and Physics, University of Ljubljana, MARTINA VRANKAR, Division of Radiotherapy, Institute of Oncology Ljubljana, MAJA CEMAZAR, GREGOR SERSA, Department of Experimental Oncology, Institute of Oncology Ljubljana, ROBERT JERAJ, Department of Medical Physics, University of Wisconsin – Madison — The Nobel Prize in Medicine 2018 was awarded for discovery of cancer immunotherapy (IT). Treatment effects are impressive, however, only a minority of patients respond. Because of favourable effects of radiotherapy (RT) on the immune system, combinations of IT and RT have been widely studied to improve the response rates. To identify possible biomarkers of response, we built a physical model capable of simulating tumour response to IT + RT. Interplay between a tumour, the immune system and the therapeutic effects is described with an experimentally verifiable population model, because the underlying biology is described with a minimum number of parameters. The model was able to reproduce experimental results from literature. To analyse possible biomarkers of response, sensitivity study of key parameters was performed. The most sensitive parameter was major histocompatibility complex class I expression, i.e. a receptor responsible for presentation of foreign proteins. Model predictions will be benchmarked against experiments on 3 different murine tumours, which will receive a single dose of RT with different IT schedules. Such models show promise to support, guide and accelerate immunotherapy research.
2:42PM P23.00002: Computational model of treatment resistance heterogeneity  MARUŠA TURK (Presenter), URBAN SIMONČIČ, Faculty of Mathematics and Physics, University of Ljubljana, ALISON ROTH, Department of Medical Physics, University of Wisconsin, Madison, DAMIJAN VALENTINUZZI, F8, Jozef Stefan Institute, ROBERT JERAJ, Department of Medical Physics, University of Wisconsin, Madison — In metastatic cancer patients, diverse levels of resistance, which are the result of genetic heterogeneity, lead to treatment response (TR) heterogeneity. To evaluate the role of resistance on TR, we constructed a population model, simulating cellular dynamics in individual metastasis. The model was benchmarked with imaging metrics extracted from the 18F-NaF PET/CT scans of 39 metastatic prostate cancer patients, received at baseline and after 3 cycles of therapy. Patients were treated with chemotherapy or hormonal therapy. Two model settings were evaluated: one considering only inter-patient and one considering both inter- and intra-patient heterogeneity in the proportion of intrinsically resistant cells (IR). Model performance, considering both settings, was evaluated using the Akaike information criterion (AIC). TR after 6, 9, and 12 months was predicted and compared using the Wilcoxon rank sum test. Considering both inter- and intra-patient heterogeneity in IR resulted in significantly better model performance (AIC=-250) than considering only inter-patient heterogeneity (AIC=6). Differences in predicted TR were not significant between treatment groups (p>0.15). The model has identified IR as an important factor influencing on inter- and intra-patient TR heterogeneity.

2:54PM P23.00003: Dynamics of Tumor Subpopulations in Response to Targeted Therapies*  DAVID MCCLATCHY (Presenter), CHANGRAN GENG, SOPHIA KAMRAN, HENNING WILLERS, HARALD PAGANETTI, AARON HATA, CLEMENS GRASSBERGER, Massachusetts General Hospital — Drugs targeting the specific genetic expression of a patient’s tumor have revolutionized the treatment of metastatic cancer. However, these tumors commonly recur due to the somatic evolution of drug persistent and resistant subpopulations during treatment. To better understand and combat acquired drug resistance, we developed a coupled, non-linear, differential system to model the dynamics of resistant and persistent tumor subpopulations. A Gompertz growth model is used to simulate bounded cell growth, while a general stochastic evolutionary pathway leading to drug resistance is implemented, based on in-vitro observations. Work will be presented on model development, and its parameterization based on measured tumor responses in lung cancer patients treated with targeted therapy. We further performed a comprehensive sensitivity analysis of model behavior in response to varying degrees of genomic instability, and derive estimates of initial pre-existing/persisting drug resistance that hold independent of parameter choice.

*National Cancer Institute Grant U19CA21239 (PI: Harald Paganetti) and American Lung Association Grant LCD-400286 (PI: Henning Willers)

3:06PM P23.00004: Understand the role of chemotherapeutic gradient in the emergence of polyploid giant cancer cells using mean field model*  KE-CHIH LIN (Presenter), Princeton University, GONZALO TORGA, Johns Hopkins University, YUSHA SUN, Princeton University, ROBERT AXELROD, University of Michigan, KENNETH J. PIENTA, Johns Hopkins University, JAMES STURM, ROBERT AUSTIN, Princeton University — Polyploid giant cancer cells (PGCCs) have been shown to correlate with poor response to chemotherapy and contribute to tumor heterogeneity regulation through asymmetric cell division [1][2]. However, most in vitro cancer studies do not replicate the complexity of in vivo tumors, while animal models are difficult to study in a comprehensive manner. The dynamics of PGCC emergence remain unclear in the context of the complex heterogeneity of the tumor ecosystem. In a recent paper, we presented the Evolution Accelerator (EA) [3], which allowed the quantitative study of the interactions of multiple cell types on a chemotherapy gradient. Utilizing the EA technology, we discovered that a docetaxel gradient greatly elevated the emergence of PGCCs and increased survival of the cancer population. With population analysis and careful experimental control, we demonstrated with a simple mean field model that the coexistence of the emerging drug-resistance PGCCs and proliferative diploid cells may serve as a survival strategy for the cancer population.


*This work was supported by NSF PHY-1659940.
TOPAS-nBio: Modeling effects of radiation with nanometer-scale Monte Carlo simulations

JAN SCHUEMANN (Presenter), AIMEE L MCNAMARA, Radiation Oncology, Massachusetts General Hospital & Harvard Medical School, Boston, MA, JOSE RAMOS-MENDEZ, Radiation Oncology, University of California San Francisco, San Francisco, CA, JOSEPH PERL, SLAC National Accelerator Laboratory, Menlo Park, CA, KATHRYN D HELD, HARALD PAGANETTI, Radiation Oncology, Massachusetts General Hospital & Harvard Medical School, Boston, MA, SEBASTIEN INCERTI, CNRS, IN2P3, CENBG, UMR 5797, F-33170 Gradignan, France, BRUCE FADDEGON, Radiation Oncology, University of California San Francisco, San Francisco, CA — The Monte Carlo (MC) method has been successfully employed to simulate radiotherapy down to the cellular scale. In order to understand how energy deposition within irradiated cells (physics) connects via molecular reactions (chemistry) to cell kill/repair (biology), one has to understand how damage and repair of cellular components is linked to frequencies of energy depositions in sub-cellular targets such as DNA.

MC simulation offers a unique tool to explore these effects. To make this method more accessible we developed TOPAS-nBio, a nanometer scale extension for radiobiology to the TOPAS MC system layered on top of the Geant4/Geant4-DNA MC toolkit. TOPAS-nBio includes detailed cell geometries, such as various DNA models, mitochondria and cells (e.g. fibroblasts or neurons). Two implementations of chemistry can be used with up to 72 reactions classified into 6 types between neutral and charged species. We reproduced time-dependent G-values within 7% for $^\cdot$OH and $e^-_{aq}$ and 50% for $H_2O_2$ as well as DNA damage in plasmids within 50%. The physical and chemical simulations depict direct and indirect damages to cells which are propagated using mechanistic models of DNA repair kinetics.

*Supported by the National Institutes of Health (NIH)/National Cancer Institute (NCI) grant R01 CA187003.

Computational Assessment of Radiation Dose Enhancement and Secondary Electron Production for Variable Sizes and Concentrations of Gold Nanospheres in a Tumor using MCNP6.2

TARA GRAY (Presenter), KATHRYN MAYER, Physics, University of Texas at San Antonio, NEIL KIRBY, Medical Physics, UT Health San Antonio MD Anderson Cancer Center — The purpose of this study is to computationally quantify dose enhancement effects of using different concentrations and sizes of gold nanospheres in high dose rate (HDR) brachytherapy and external beam radiotherapy. A MicroSelectron HDR Ir-192 brachytherapy source and a Varian 600C gantry head with a 6MV photon energy were modeled using Monte Carlo N-Particle radiation transport software (MCNP 6.2, Los Alamos National Laboratory). The repeating structures capability of MCNP6.2 was utilized to simulate nanospheres of sizes 4.5 nm, 30 nm and 60 nm at varying nanosphere concentrations of 5 nM, 10 nM and 20 nM, inside a tumor, with a diameter of 1 x 1 x 1 cm$^3$. Dose enhancement factors (DEFs) were computed as the ratio of dose to the tumor containing gold nanospheres relative to that without. The highest DEF of 1.7 was observed with the Ir-192 source for a total nanosphere concentration of 20 nM and diameters of 4.5 nm. It was observed that increasing concentration and decreasing the size of the nanospheres produced the greatest dose enhancement for both HDR brachytherapy and external beam radiotherapy cases. This work indicates the potential for significant dose enhancement and more effective tumor cell killing in radiation oncology practice.

*Funded by San Antonio Medical Foundation

Physical dose enhancement of gold nanoparticles and their impact on water radiolysis in radiotherapy

BENEDIKT RUDEK (Presenter), Radiation Oncology, Massachusetts General Hospital and Physikalisch-Technische Bundesanstalt, AIMEE L MCNAMARA, Radiation Oncology, Massachusetts General Hospital, HILARY BYRNE, ZDENKA KUNCIC, University of Sydney, JAN SCHUEMANN, Radiation Oncology, Massachusetts General Hospital and Harvard Medical School — Gold nanoparticle (GNP) radio-sensitization is a promising technique to increase the dose deposition in the tumor while sparing neighboring healthy tissue. The sensitization is most pronounced for keV x-rays, where the mass energy-absorption coefficient of gold is up to 150 times larger than that of soft tissue. Measurements in vitro and in vivo also showed an effect on cell survival and tumor control for other modalities such as MV photons and proton beams, where the physical dose enhancement by GNPs is expected to be negligible.

Most simulation studies have, thus, focused on photon irradiation of isolated GNPs in water neglecting experimental evidence of GNP clustering within cells. In a systematic study, we use the Monte Carlo simulation tool TOPAS-nBio to model the GNP radio-sensitization within a cell as a function of GNP concentration, size and clustering for a wide range of energies for photons, protons and carbon ions. Moreover, we include water radiolysis and subsequent chemistry as implemented in Geant4-DNA.

While the physical dose enhancement for 10MeV protons at 1% GNP concentration was only 0.07% compared to 62% for 50keV photons, we find the yield of reactive oxygen species change by up to 15% which could partly explain the experimental dose enhancement for protons.
3:54PM P23.00008: Compensatory enlargement of atherosclerotic vessels — An analysis through morphoelasticity*

PAK-WING FOK (Presenter), University of Delaware — In 1987 Seymour Glagov published a key result on how atherosclerotic arteries remodel. His post-mortem data on human coronary arteries suggested that over the course of atherosclerotic disease, the vessel wall expands, keeping the lumen area approximately constant before before luminal encroachment occurs. This “compensatory” enlargement has been confirmed in-vivo and in other organisms. However, this behavior has never been explained physically.

We propose a three-layer morphoelastic model to describe arterial remodeling. Each layer is described as a collagen-fiber reinforced anisotropic composite. Growth occurs in the intima only. This simple biomechanics model is able to reproduce the main features of the data. We discuss a methodology using finite elements and provide a physically appealing explanation of Glagovian remodeling.

*Simons Foundation
Delaware CTR SHoRe pilot grant (NIGMS IDeA US4-GM104941)

4:06PM P23.00009: Computational Modeling Helps Tissue Engineered Heart Repair*

MORITZ KALHÖFER-KÖCHLING (Presenter), Fluid Physics, Pattern Formation, and Biocomplexity, Max-Planck-Institute for Dynamics and Self-Organization, MARTIN UECKER, WOLFRAM ZIMMERMANN, Universitätsmedizin Göttingen, EBERHARD BODENSCHATZ, YONG WANG, Fluid Physics, Pattern Formation, and Biocomplexity, Max-Planck-Institute for Dynamics and Self-Organization — Understanding the mechanical influence of scarred tissue is key to understand how ischemia affects the efficacy of the heart and consequently how supportive devices can help restoring the same. With medical images and nonlinear mechanics, we are developing a patient-specific heart model for tissue engineering. Employing the Holzapfel-Ogden rule we analyse how different types of infarcts impair the contractile function of the left ventricle using end diastolic and end systolic pressure volume relations as key markers. The patient specific tissue properties and hence model parameters play a crucial role on how much heart function will be compromised after an infarct, demanding an in-depth study of said parameter space, in order to develop patient-specific solutions. As such, we also investigate how engineered heart muscle tissue can restore healthy capacity targeting at clinical applications.

*This work was supported by the Max Planck Society and the German Center for Cardiovascular Research.

4:18PM P23.00010: Improving influenza vaccine development with the pEpitope model: application to the 2018-19 season*

MELIA BONOMO (Presenter), Department of Physics & Astronomy, Rice University, RACHEL KIM, Weiss School of Natural Sciences, Rice University, MICHAEL DEEM, Department of Bioengineering, Department of Physics & Astronomy, Rice University — The annual influenza vaccine has been shown to reduce flu-related hospitalizations and severe illness outcomes. Minimizing the antigenic differences between the vaccine strain and circulating strains ensures the vaccine will adequately prime the immune system against infection. We developed a theory of antibody response to infection following vaccination that produced a novel measure of antigenic distance. The model, called pEpitope, considers the modularity and hierarchy of antibody binding to the epitope regions of the viral hemagglutinin protein. The pEpitope model is able to explain over 90% of the variance in human vaccine epidemiological data from recent studies conducted by the US Centers for Disease Control and Prevention. Analysis of A(H3N2) strains circulating during the 2017-18 season identified the emergence of a new quasispecies cluster that is sufficiently distant from the 2018-19 vaccine and is therefore predicted to dominate. The pEpitope model is a valuable tool that predicts vaccine effectiveness to enhance vaccine strain selection and development.

*This work was supported by the Center for Theoretical Biological Physics at Rice University and The Welch Foundation.

4:30PM P23.00011: Network physiology reveals relations between network topology and physiological function*

XIYUN ZHANG (Presenter), FABRIZIO LOMBARDI, Physics Department, Boston University, RONNY BARTSCH, Department of Physics, Bar-Ilan University, PLAMEN CH IVANOV, Physics Department, Boston University — The human organism is an integrated network where complex physiological systems, each with its own regulatory mechanisms, continuously interact, and where failure of one system can trigger a breakdown of the entire network. Identifying and quantifying dynamical networks of diverse systems with different types of interactions is a challenge. Here we develop a framework to probe interactions among diverse systems, and we identify organ interaction networks. We find that each physiological state is characterized by a specific network structure, demonstrating a robust interplay between network topology and function. Across physiological states, the organ interaction network undergoes specific reorganization process that is preserved across subject with different ages, indicating the existence of a robust relation between organ interaction networks and physiological states.

*We acknowledge support from the W M Keck Foundation.
CHRISTINA POSPISIL (Presenter), Mathematics and Physics Department, University of Massachusetts Boston, TONG SHU, Physics Department, Yale University — In this first part we present a theoretical mathematical model for the information flow from teeth to organs, which is a part of a study modelling illness (e.g. catching a cold, etc.) and health conditions from the physics point of view and leads to the question of interaction/ reciprocal action of information as a phenomenon (as we understood it, physics is the science of phenomena) in general (getting ill is a certain kind of interaction with the environment). Moreover, we will give an overview about how this model can be tested experimentally.

Wednesday, March 6, 2019 2:30 PM - 5:18 PM

Session P24 DAMOP DCMP: Non-Equilibrium Physics in AMO Systems III

BCEC 159 - Michael Buchhold, Caltech

2:30PM P24.00001: Observation of the Higgs mode in the superfluid BEC-BCS crossover in Fermi gases* JOHANNES KOMBE (Presenter), ALEXANDRA BEHRLE, TIMOTHY HARRISON, KUIYI GAO, MARTIN LINK, JEAN-SEBASTIEN BERNIER, CORINNA KOLLATH, MICHAEL KOEHL, University of Bonn — Thanks to recent advances, investigating the non-equilibrium dynamics of interacting systems is now possible. Using time-dependent perturbations, one can probe from a different angle the mechanisms responsible for the collective phenomena present in correlated systems. Taking advantage of this progress, we investigate both theoretically and experimentally the evolution of a three-dimensional Fermi gas while the interaction strength is effectively modified. Our study, carried out on the BCS side, reveals various collective excitations. Interestingly, this approach highlights the presence of the Higgs mode.

*European Research Council grant no: 648166
Deutsche Forschungsgemeinschaft: SFB/TR 185 project B4

2:42PM P24.00002: Constrained Hilbert Spaces and Many-body Scars in a Landau Level SANJAY MOUDGALYA (Presenter), Physics, Princeton University, NICOLAS REGNAULT, Laboratoire Pierre Aigrain, B ANDREI BERNEVIG, Physics, Princeton University — We study a "pair-hopping" model that arises within a Landau level in the thin-torus limit of the quantum Hall effect. At filling \( \nu = 1/3 \), we show that the model maps on to the "PXP model", a constrained model for the Rydberg atom chain known to exhibit quantum many-body scars (ETH-violating states in the middle of the spectrum). Further, for general fillings factors \( \nu = p/(2p+1) \), we show the mapping onto spin-chains with constrained Hilbert spaces that share several features with the PXP model, including the presence of many-body scars and slow thermalization of particular product states. Finally, we investigate the stability of scars in the presence of electrostatic and long-range hopping terms that are always present in the quantum Hall setup.

2:54PM P24.00003: Computing thermalization times and hydrodynamic modes from microscopic quantum dynamics* EHUD ALTMAN (Presenter), XIANGYU CAO, DANIEL PARKER, University of California, Berkeley, DAVID HUSE, Physics, Princeton University — Computing quantum dynamics of an interacting system presents a fundamental challenge. The Heisenberg time evolution of a local operator generates superpositions with an exponentially growing number of terms, each representing increasingly non local operators. To address this problem, we construct the graph of basis operators (Pauli string in spin-half systems) spanned by applying the Liouvillian \( n \) times; \( n \) serves as a truncation cutoff. Integrating out the outward flow of operators across the truncation boundary toward "large operators" gives rise to an imaginary self energy term that acts as an absorbing boundary condition. The resulting non-unitary dynamics respects all conservation laws related to local operators, e.g. energy, charge and spin. The approximation scheme depends on a single free rate parameter, which we determine numerically by requiring the results to become cutoff independent asymptotically. For a broad class of ergodic models this scheme allows to identify slowly decaying operators, and compute the diffusion constant of hydrodynamic modes. Furthermore this scheme captures the non diffusive dynamics in certain integrable models.

*EA and XC acknowledge support from ERC synergy grant UQUAM
TIBOR RAKOVSZKY (Presenter), FRANK POLLMANN, Physics Department, Technical University of Munich, CURT W VON KEYSERLINGK, School of Physics and Astronomy, University of Birmingham — We investigate how the incoherent (diffusive) transport of conserved quantities affects the growth of entanglement in generic non-integrable systems. We develop a general picture by considering random unitary circuit dynamics with a U(1) symmetry which allows for an efficient numerical treatment and, in a certain coarse-grained limit, leads to a simple equation of motion for the entanglement entropy, which takes the form of a random, space-time dependent surface growth model. Based on this we argue that an initial state with large-scale inhomogeneities in the conserved densities gives rise to an uneven entanglement profile across the system, with features whose "height" and "width" both grow as $t^{1/2}$. We confirm this prediction by numerically investigating a variety of different initial states, both in the random circuit model away from the coarse-grained limit, and in a deterministic spin chain. Moreover, we investigate the effects of charge-fluctuation and find that these can lead to a slow-down in entanglement growth even for spatially homogenous states.

*RT and FP are supported by Research Unit FOR 1807 through grants no. PO 1370/2-1 and the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement no. 771537).

JOHANNES FELDMEIER (Presenter), MICHAEL KNAP, FRANK POLLMANN, Technical University of Munich — The study of dynamical properties in systems with local constraints has attracted a lot of interest, spurred by experiments with Rydberg blockaded atoms, that naturally implement constrained many-body models. We study the quench dynamics in a 2D quantum dimer model to identify dynamical phase transitions in constrained models by means of exact diagonalization on systems of sizes up to 8x8 sites. We find that the quenched quantum system thermalizes efficiently by determining the relaxation dynamics of both the order parameter (OP) and local correlation functions. The observed fast relaxation to thermal expectation values allows us to study the underlying thermal BKT-transition between a columnar ordered valence bond solid (VBS) and a symmetric liquid (VBL) phase in the form of a dynamical phase transition. The existence of this finite-temperature transition in the dynamics is confirmed by the long-time averaged values of the OP. Moreover, upon quenching across the VBS-VBL phase boundary, the dynamical transition can be shown to be manifest in the Loschmidt-echo, whose rate-function displays kinks at the zero-crossings of the columnar OP.

*We acknowledge support from the DFG grant No. KN 1254/1-1 and DFG TRR80 (Project F8).

KRISTOF HARMS (Presenter), LORENZO CEVOLANI, STEFAN KEHREIN, SALVATORE MANMANA, Institute for Theoretical Physics, University of Göttingen — We investigate the dynamics of a one-dimensional system of spinless fermions, which is initially prepared in a highly correlated groundstate of an interacting Hamiltonian. In particular, for a global quench that turns off the interaction, we evolve the initial state obtained via density matrix renormalisation group (DMRG) using analytical solutions of the equations of motion. This allows us to reach arbitrary times. We examine features of the dynamics of density-density correlations and susceptibilities on several time scales. Shortly after the quench, we identify, in addition to the typical lightcone-behavior, periodic recurrences of the initial correlations outside the lightcone. At very long times, we use our approach to investigate the Fluctuation-Dissipation theorem in this strong nonequilibrium situation.

*Funding by the SFB/CRC 1073 (project B03) of the Deutsche Forschungsgemeinschaft (DFG) is gratefully acknowledged.

VALENTIN KASPER (Presenter), JAMIR MARINO, Department of Physics, Harvard University, SI CONG, JOERG SCHMIEDMAYER, Institute of Atomic and Subatomic Physics, TU Vienna, EUGENE DEMLER, Department of Physics, Harvard University — The high flexibility of ultracold atoms allows for the design, control and investigation of quantum matter. In this work we consider two one-dimensional Ramsey tunnel-coupled Bose gases and show that the low-energy effective theory of this system is described by the quantum Prokrovsky-Talapov model. We study the ground state with variational wave-functions and elaborate on the modification of the quantum phase transition due to a finite system size. Finally, we consider the non-equilibrium evolution determined by quench from an uncoupled Bose gases to the Ramsey tunnel coupled case and predict the experimental relevant evolution of phase correlations.
Dynamics of fractional Chern insulators under global quantum quenches  

JOHANNES MOTRUK (Presenter), JOEL MOORE, University of California, Berkeley and Lawrence Berkeley National Laboratory — Recent progress in the control of synthetic gauge fields in optical lattices has brought the realization of strongly correlated topological phases in cold atom experiments within reach. Due to longer time scales compared to solid state systems, the quantum dynamics in such setups are experimentally more amenable and may encode information about the topological properties of the state.

In this work, we investigate quantum quenches between Hamiltonians with a fractional Chern insulator (FCI) ground state and topologically trivial Hamiltonians. Focusing on the experimentally realized Hofstadter model, we study the post-quench behavior of various quantities such as edge currents, Hall response and Loschmidt echo and determine how they display signatures of the topologically ordered initial state. Furthermore, we comment on implications for dynamically detecting FCI states in cold atom experiments.

Loschmidt Amplitude and Work Distribution in Quenches of the Sine-Gordon Model*  

COLIN RYLANDS (Presenter), University of Maryland, College Park, NATAN ANDREI, Physics, Rutgers University — The Sine-Gordon model is ubiquitous in low-dimensional physics, with applications that range from cold atom and strongly correlated systems to quantum impurities. In this talk we present a study of its non-equilibrium dynamics using the quantum quench protocol. By means of the Bethe Ansatz we calculate exactly the Loschmidt amplitude, the fidelity and work distribution characterizing the quench for different values of the interaction strength. Some universal features are noted as well as an interesting duality relating quenches in different parameter regimes of the model.

*Supported by NSF grant DMR 1410583

Quench dynamics across topological quantum phase transitions*  

SHIUAN-FAN LIOU (Presenter), KUN YANG, Physics, National High Magnetic Field Laboratory and Florida State University — We study the dynamics of systems quenched through topological quantum phase transitions and investigate the behavior of the bulk and edge excitations with various quench rates. Specifically, we consider the Haldane model and checkerboard model in slow quench processes with distinct band-touching structures leading to topology changes. The generation of bulk excitations is found to obey the power-law relation Kibble-Zurek and Landau-Zener theories predict. However, an anti-Kibble-Zurek behavior is observed in the edge excitations. The mechanism of excitation generation on edge states is revealed, which explains the anti-Kibble-Zurek behavior.

Reference: PRB 97, 235144 (2018)

*This work was supported by National Science Foundation Grant No. DMR-1442366 and was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1644779 and the state of Florida.

Phonon Coupling’s Role in the Non-Equilibrium Dynamics of a Quasicondensate*  

RYAN PLESTID (Presenter), DUNCAN O’DELL, McMaster University — Cold atoms loaded into cigar shaped traps can realize the Lieb Liniger model where the effective 1-D coupling constant depends both on the three-dimensional scattering length of the atomic species, and on the trap’s transverse frequency. By performing a quantum quench of the transverse trapping frequency, non-equilibrium density and phase dynamics can be induced. In the low temperature regime, these dynamics are well characterized by Bogoliubov theory, however at higher temperatures intermode (i.e. phonon-phonon) coupling can become important. In this work we report on classical field simulations of a quasi condensate undergoing the quench protocol outlined above, and comment on the consequences of intermode coupling both for damping, and energy transfer.

*This research is supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada.
to argue that our results are generally applicable to other problems with multifractal wavefunctions.

long time limit. Despite focusing on the Aubry-Andre model, we invoke the universality of the single particle wavefunctions

also focus on the core-hole Green function, which effectively translates this phenomena to the time domain and find a

overlaps, where the overlap distribution becomes significantly broad at the critical point of the Aubry-Andre model. We

from the plane wave limit, with a much slower decay. This behavior is also manifested in the distribution of wavefunction

wavefunction overlap vanishes in a power law fashion as a function of the system size. This power law is markedly distinct

find that the orthogonality catastrophe remains between the pre and post quench wavefunctions where the average

We focus on the case where the many-body wavefunction is composed of single particle eigenstates that are generated

qubit-mirror distances.

particular, both the relaxation rates and the Lamb shifts of the qubits are modified as a function of the inter-qubit and

1D transmission line terminated by a mirror. By tuning the qubits into resonance, we observe collective effects. In

many interesting phenomena. In this work, we embedded two transmon qubits, separated by wavelength distances, in a

demonstrated strong interaction between resonant propagating microwave photons and superconducting qubits in such a

achieve nearly ideal spatial mode-matching for a microwave field. Taking advantage of this, experiments have

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Session P25 DAMOP: Quantum Information Science in Atomic, Molecular, and Optical Physics

BCEC 160A - Monika Schleier-Smith, Stanford University

2:30PM P25.00001: Cooperative effects for qubits in a semi-infinite one-dimensional transmission line  PING YI WEN

Presenter), Department of Physics, National Tsing Hua University — In a one-dimensional (1D) transmission line, it is possible to

achieve nearly ideal spatial mode-matching for a microwave field. Taking advantage of this, experiments have

demonstrated strong interaction between resonant propagating microwave photons and superconducting qubits in such a

system. When the system contains more than one qubit, photon-mediated interactions between the qubits gives rise to

many interesting phenomena. In this work, we embedded two transmon qubits, separated by wavelength distances, in a

1D transmission line terminated by a mirror. By tuning the qubits into resonance, we observe collective effects. In

particular, both the relaxation rates and the Lamb shifts of the qubits are modified as a function of the inter-qubit and

qubit-mirror distances.
2:42PM P25.00002: Quantum Zeno effect and the many-body entanglement transition* YAODONG LI (Presenter), University of California, Santa Barbara, XIAO CHEN, Kavli Institute for Theoretical Physics, MATTHEW P A FISHER, University of California, Santa Barbara — We introduce and explore a one-dimensional "hybrid" quantum circuit model consisting of both unitary gates and projective measurements. While the unitary gates are drawn from a random distribution and act uniformly in the circuit, the measurements are made at random positions and times throughout the system. By varying the measurement rate we can tune between the volume law entangled phase for the random unitary circuit model (no measurements) and a "quantum Zeno phase" where strong measurements suppress the entanglement growth to saturate in an area-law. Extensive numerical simulations of the quantum trajectories of the many-particle wavefunctions (exploiting Clifford circuitry to access systems up to 512 qubits) provide evidence for a stable "weak measurement phase" that exhibits volume-law entanglement entropy, with a coefficient decreasing with increasing measurement rate. We also present evidence for a novel continuous quantum dynamical phase transition between the "weak measurement phase" and the "quantum Zeno phase", driven by a competition between the entangling tendencies of unitary evolution and the disentangling tendencies of projective measurements.

*Gordon and Betty Moore Foundation
Heising-Simons Foundation
Caltech IQIM
NSF DMR-1404230, DMR-1720256, CNS-1725797

2:54PM P25.00003: Tomography of the temporal-spectral state of subnatural-linewidth single photons from atomic ensembles* CE YANG (Presenter), ZHENJIE GU, PENG CHEN, Department of Physics, East China Normal University, Shanghai 200241, China, Quantum Institute for Light and Atoms, ZHONGZHONG QIN, Shandong University, Taiyuan, Shanxi 030006, China, Collaborative Innovation Center of Extreme Optics, JIEFEI CHEN, Department of Physics, East China Normal University, Shanghai 200241, China, Quantum Institute for Light and Atoms, WEIPING ZHANG, Department of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China, Tsung-Dao Lee Institute — The temporal mode of a single photon is considered more and more important in quantum information processing. On one hand, qubits or multi-dimension qudits can be constructed in photonic temporal mode, which are advantageous in long-distance transportation compared to other degrees of freedom, and thus have important applications in photonic quantum processing. On the other hand, to achieve a maximum efficiency in quantum memory, the temporal mode of a single photon is important in the matter-light coupling. Here we utilize cavity-free homodyne detection scheme for reconstructing the temporal density matrix of the subnatural-linewidth single photons generated from a cold atomic cloud. The characterization of the pure temporal-spectral state of narrowband single photons paves the way for exploiting the temporal-spectral degree of freedom to develop photonic quantum information processing.

*This work is supported by the National Key Research and Development Program of China under Grant number 2016YFA0302001, and the National Natural Science Foundation of China through Grant No. 11674100, 11654005, 11234003, and also it is supported the ECNU Fund for International Conferences.

3:06PM P25.00004: Floquet-engineered quantum state preparation in a noisy qubit MOHIT PANDEY (Presenter), ERIC BOYERS, DRIES SELS, DAVID K CAMPBELL, ANATOLI POLKOVNIKOV, ALEX SUSHKOV, Boston University — Noise and decoherence caused by the environment are two major challenges in applying adiabatic protocols to quantum technologies. Counter-diabatic (CD) and fast-forward (FF) driving protocols, which are also known as "shortcuts-to-adiabaticity," provide powerful alternatives by allowing one to change Hamiltonian parameters rapidly while still mimicking adiabatic dynamics. However, implementing exact CD or FF driving in complex systems is hard in general. In this work, we propose a new efficient and generic method of Floquet engineered FF protocols, which effectively realize CD driving. We report on its experimental realization in a single nitrogen-vacancy center in diamond. Our protocol achieves near unit fidelity with our target state for fast protocols when our system is driven periodically at high frequency. Moreover, we find experimentally that our Floquet-engineered protocols are less susceptible to decoherence than standard fast forward protocols and allow us to reach near perfect fidelity even in the presence of a strong external noise.
3:18PM P25.00005: Amplification without Population Inversion from a Strongly Driven Superconducting Qubit
PING YI WEN, Department of Physics, National Tsing Hua University, Taiwan, ANTON FRISK KOCKUM, Department of Microtechnology and Nanoscience, Chalmers University of Technology, Sweden, HOU IAN, Institute of Applied Physics and Materials Engineering, University of Macau, Macau, JENG-CHUNG CHEN, Department of Physics, National Tsing Hua University, Taiwan, FRANCO NORI, Center for Emergent Matter Science, RIKEN, Japan, IO CHUN HOI (Presenter), Department of Physics, National Tsing Hua University, Taiwan — Amplification of EM fields is often achieved by strongly driving a medium to induce population inversion such that a weak probe can be amplified through stimulated emission. Here we strongly couple a superconducting qubit to the field in a semi-infinite waveguide. When driving the qubit strongly on resonance such that a Mollow profile appears, we observe a few percent amplitude gain for a weak probe at frequencies in between the Mollow profile. This amplification is not due to population inversion, but instead results from a four-photon process that converts energy from the strong drive to the weak probe. We find excellent agreement between the experimental results and numerical simulations without any free fitting parameters.

3:30PM P25.00006: Multiphoton pumping between two microwaves mediated by transmon qubit
HOSSEIN JOOYA (Presenter), ITAMP, Harvard-Smithsonian Center for Astrophysics, GUOZHU SUN, JIAZHENG PAN, PEIHENG WU, Research Institute of Superconductor Electronics, Nanjing University, SIYUAN HAN, Department of Physics and Astronomy, University of Kansas, HOSSEIN R. SADEGHPOUR, ITAMP, Harvard-Smithsonian Center for Astrophysics — In this work, we analyze the interference patterns, observed in the multiphoton absorption spectrum of a transmon qubit, when it is driven by a pair of microwaves, tuned near and far off the qubit resonance. The appearance of such structures in the spectrum is explained as various photon contributions from the two microwave drives. We show that each of these manifolds demonstrates single or multiphoton pumping from one microwave to another. A many-mode Floquet formalism, with longitudinal coupling, is used to simulate the observed quantum interference. An intuitive graph theoretic approach is introduced to derive the effective Hamiltonian that elucidate main features of the Floquet results. The analytical solutions also illustrate how controllability is achievable for desired single- or multiphoton pumping processes in a wide frequency range. The proposed experimental design and the theoretical approach can be extended to tunable qubit circuits or solid state semiconductors, in general, which offer full controllability of the energy gaps.

3:42PM P25.00007: Periodically Pulsed Quantum Light from a Superconducting Qubit Ensemble
ELENA REDCHENKO (Presenter), FARID HASSANI, MATILDA PERUZZO, Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria, MATTHIAS ZENS, HIMADRI SHEKHAR DHAR, DMITRY O. KRIMER, STEFAN ROTTER, Institute for Theoretical Physics, Vienna University of Technology (TU Wien), Wiedner Hauptstraße 8-10/136, 1040, Vienna, Austria, European Union, JOHANNES FINK, Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria — Nonclassical light sources are extremely important in the fields of quantum information, quantum communication, and photonic quantum technologies. We study a driven inhomogeneous ensemble of superconducting qubits coupled to a microwave resonator. The constructive rephasing of spins in the frequency comb is predicted to result in a periodic pulse train of quantum light ($g_2(t,0)<1$) which corresponds to the collective transfer of excitations from the qubit ensemble to the resonator [1]. Such periodic nonclassical pulses are interesting for a temporal synchronization in quantum memory protocols. We will present results of our ongoing experiments on periodic quantum light generation in the system of five transmon qubits capacitively coupled to a coplanar waveguide resonator.


*This work was supported by the European Research Council under the grant agreement No 758053 (ERC StG QUNNECT).
In nano-electromechanics, quantum mechanical phenomena can be studied in the literal sense. For example, the coupling of a nanomechanical element to a superconducting resonator allows to cool the mechanical mode to its ground state and to squeeze its motion. Replacing the linear microwave resonator with a nonlinear one enables the preparation of more complex non-classical mechanical states.

In this presentation, we discuss various opto-mechanical coupling schemes in nano-electromechanical circuits employing nonlinear elements. In this context, Josephson junctions in superconducting circuit environments are the obvious choice. In particular, we envisage the scenario of a mechanically compliant tensile string embedded in a resonator including Josephson junctions, e.g. a transmon qubit or a flux-tunable resonator. We discuss realistically achievable opto-mechanical coupling strengths for these circuit layouts. In addition, we set this in context with the limitations imposed by such circuits, in particular in view of the photon numbers. Such hybrid systems open new perspectives in the field of optomechanics ranging from sensing applications to the preparation of quantum states.

*We acknowledge funding via the Nanosystems Initiative Munich and EU project MaqSens (Proj. No:736943)

**Engineered Reservoirs for Thermalization of Many-Body Quantum Systems**

**MEKENA METCALF** (Presenter), **MOHAN SAROVAR**, Sandia National Laboratories California, **JONATHAN MOUSSA**, Molecular Sciences Software Institute — Engineering genuine thermal states in quantum analog simulation platforms are addressed by a technique based on a many-body spin Hamiltonians coupled to driven, dissipative ancilla spins. A Born-Markov master equation describing the dynamics of a many-body system coupled to fast-relaxing, driven ancilla qubits is developed, and if the ancilla energies are periodically modulated and swept across the system energy spectrum, with a carefully chosen hierarchy of timescales, one can effectively thermalize a many-body system. Analytical proofs and numerical investigations are used to validate the requirements of thermalization and demonstrate the true thermal state is an approximate dynamical fixed point.

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**A phononic network of spin qubits for quantum computing**

**MARK KUZYK** (Presenter), **HAILIN WANG**, University of Oregon — We describe a general architecture for networking solid-state qubits through vibrational motion. The architecture makes use of alternating phononic crystal waveguides to facilitate communication between distant qubits in a scalable manner. We discuss a specific realization of the architecture using Nitrogen vacancy centers in diamond, and show that state-of-the-art devices operating at 500 mK can implement two-qubit universal quantum gates with a fidelity exceeding 0.99.

*This work is supported by AFOSR and by NSF under grants No. 1606227 and No. 1641084
4:30PM P25.00011: Quantum phase investigation of a single nuclear spin in a magnetic molecule  
CLÉMENT GODFRIN (Presenter), Physique, Université de Sherbrooke, RAFIK BALLOU, EDGAR BONET, Institut Néel, Université Grenoble Alpes, MARIO RUBEN, SVETLANA KLYATSKAYA, WOLFGANG WERNSDORFER, Karlsruhe institute of technology, FRANCK BALESTRO, Institut Néel, Université Grenoble Alpes — More than a hundred years ago, physicists used thought experiments to debate the controversial point of quantum theory while undoing the experimental constraints. Since then, advances in experimental techniques offer physicists the opportunity to study systems worthy of those imagined by the founders of the quantum theory. During the presentation, we will investigate the quantum dynamic of one of these toy model systems, namely a single 3/2 nuclear spin.

We will first see how to measure a single electronic [1] and nuclear spin using a molecular magnet transistor. Then we will couple the nuclear spin to a microwave electric field [2] and measure the coherent manipulation of the 3 nuclear spin transitions, thus demonstrating a full controlled of a 4-level quantum system, a qudit [3]. With their state space of dimension d>2, Qudits open fascinating experimental prospects. In this presentation I will show implementation of protocols based on a generalization of the Ramsey interferometry to a multi-level system to measure the accumulation of geometric phases and of quantum gate phase [4].


4:42PM P25.00012: Practical Implementations of Photonic Quantum Walks on Graphs*  
SHUTO OSAWA (Presenter), DAVID SIMON, ALEXANDER SERGIENKO, Boston University — Discrete-time quantum walks have become a subject of great interest because of their potential applications for quantum information processing tasks. Quantum walk-based algorithms provide significant speedup over classical algorithms in a range of tasks including search algorithms, solving the element distinctness problem, and evaluating NAND trees. Up to this point, work on quantum walk-based algorithms has been largely theoretical, as discrete-time quantum walk systems are difficult to implement beyond a few time steps. Here we demonstrate a step forward in producing practical experimental realization of optical quantum walks by means of directionally-unbiased linear optical multiports, which have recently been experimentally demonstrated in the form of tabletop setups. These multiports or other related devices, such as reversible optical tritters, can be considered as additional fundamental blocks for quantum walk applications, and can serve as scattering vertices for practical implementations of optical graph systems.

*This research was supported by the National Science Foundation EFRI-ACQUIRE Grant No. ECCS-1640968, AFOSR Grant No. FA9550-18-1-0056, and by the Northrop Grumman NG Next.

4:54PM P25.00013: Double-slit Interference as a Lossy Beam-splitter  
SIMANRAJ SADANA (Presenter), Raman Research Institute, BARRY SANDERS, University of Calgary, URBASI SINHA, Raman Research Institute — A post-selected unitary description of optical interferometers makes them a good machine for quantum information processing and computation. However, slit diffraction/interference lacks a unitary description. We present a classical post-selected unitary description of slit diffraction, bringing it at par with other interferometers.

The solution of Helmholtz equation in three dimensions with N sources are projected on two-dimensional surfaces called slices, all parallel to each other. A post-selected unitary description of slit diffraction is achieved by representing diffraction as a map between slices as they pass through slits and projecting the slices on N detectors to obtain an N × N transfer matrix.

Using such a formalism, we show that a double-slit with post-selection taking into account the losses in the diffraction process, is a beam-splitter. With the use of FDTD simulations, the application of this formalism is demonstrated for near-field and far-field cases. We also show that such a framework can be used to get a post-selected unitary description of a diffraction grating.

The classical treatment sets the stage for future research on diffraction-based quantum interferometry which involves quantizing the fields and the construction of sophisticated interferometers.
Nearly optimal quantum control: an analytical approach*  
CHEN SUN (Presenter), Brown University, AVADH SAXENA, NIKOLAI SINITSYN, Los Alamos National Laboratory — We propose nearly optimal control strategies for changing the states of a quantum system. We argue that quantum control optimization can be studied analytically within some protocol families that depend on a small set of parameters for optimization. This optimization strategy can be preferred in practice because it is physically transparent and does not lead to combinatorial complexity in multistate problems. As a demonstration, we design optimized control protocols that achieve switching between orthogonal states of a naturally biased quantum two-level system.

*The work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396. Authors also thank the support from the LDRD program at LANL.

Limitations on the Use of the Heisenberg Picture in Quantum Optics  
JAMES FRANSON (Presenter), RICHARD A BREWSTER, University of Maryland, Baltimore County — The Heisenberg picture is often used to analyze the performance of optical components, such as a beam splitter or an optical parametric amplifier. We consider a sequence of two or more unitary transformations and show that the Heisenberg operator produced by the first transformation cannot be used as the input to the second transformation [1]. As a result, an inappropriate use of the Heisenberg picture can give misleading or incorrect conclusions. The experimental consequences of this will be illustrated using several examples from quantum optics.


Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P26 DQI: Superconducting Circuits: New Qubit Components and Packaging BCEC
160B - Sami Rosenblatt, IBM Thomas J. Watson Research Center

Scaling up package I/O for superconducting qubits*  
STEVEN WEBER (Presenter), DANNA ROSENBERG, JOVI MILOSHI, JOHN CUMMINGS, JAMES KRIEGER, SAM ALTERMAN, DAVID CONWAY, RABINDRA DAS, CYRUS F. HIRJIBEHEDIN, DAVID K KIM, ELIZABETH KOWALSKI, MIT Lincoln Laboratory, BENJAMIN LIENHARD, Massachusetts Institute of Technology, ALEXANDER MELVILLE, BETHANY M. NIEDZIELSKI, JOHN ROKOSZ, WAYNE WOODS, JONILYN L YODER, ANDREW JAMES KERMAN, WILLIAM D OLIVER, MIT Lincoln Laboratory — Device packages, which house qubit chips and make connections to control and readout wiring, are an essential component of any superconducting qubit architecture. In this presentation, we discuss our efforts to design packages with an increasing number of signal connections, for applications in quantum annealing and gate-based quantum computing. We present strategies for achieving high-density wiring while avoiding package modes and reducing crosstalk. We characterize package performance using electromagnetic simulations, room-temperature measurements, and cryogenic qubit measurements.

*This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.
2:42PM P26.00002: Simulation and Analysis of Packaging of Superconducting Qubits*

Benjamin Lienshard (Presenter), Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Wayne Woods, Danana Rozenberg, MIT Lincoln Laboratory, Kevin P O'Brien, Electrical Engineering and Computer Science, Research Laboratory of Electronics, Massachusetts Institute of Technology, Greg Calusine, Steven J. Weber, MIT Lincoln Laboratory, Terry Philip Orlando, Electrical Engineering and Computer Science, Research Laboratory of Electronics, Massachusetts Institute of Technology, Simon Gustavsson, Research Laboratory of Electronics, Massachusetts Institute of Technology, William D Oliver, Department of Physics, Research Laboratory of Electronics, Lincoln Laboratory, Massachusetts Institute of Technology — Precise and accurate coherent control of qubits is critical to the success of superconducting quantum computing. Microwave crosstalk is a ubiquitous problem for large scale superconducting quantum processors and poses a challenge to scaling up few-qubit coherent control results. Although crosstalk is classical, deterministic, and can be mitigated to some degree with electromagnetic nulling, the frequency dependence of crosstalk and significant calibration overhead for compensation schemes motivate hardware solutions. 3D integration techniques such as through silicon vias and bump bonds offer a solution at the cost of fabrication complexity. We propose and present initial experiments on a crosstalk mitigation scheme using commercial multilayer printed circuit boards (PCBs) to enable rapid turnaround and widespread adoption.

2:54PM P26.00003: Engineering the environment of superconducting quantum processors with multilayer PCBs

Kaidong Peng, Kevin O'Brien (Presenter), Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology — Arrays of superconducting lumped circuit elements can be used to make metamaterial resonant structures, which can exhibit novel spectra with a high density of modes in the same frequency range where superconducting qubits are typically operated. We study the dynamics of a flux-tunable transmon qubit when coupled to such a metamaterial. We measure the coupling strength of the qubit to several modes by tuning the flux bias and compare the resulting vacuum Rabi splittings with numerical and analytical models. Using a separate conventional resonator to read out the qubit state, we are able to track the qubit as we tune it through many of the metamaterial resonances. With this capability, we are able to measure the qubit T1 time as a function of frequency. We observe that T1 correlates with the metamaterial spectrum and is consistent with Purcell loss into the various modes, as described by a circuit model. In addition, we present measurements of Stark shifts of the qubit transition while driving a separate microwave tone in the vicinity of the various metamaterial modes.

3:06PM P26.00004: Qubit Dynamics in a Multi-mode Environment with a Superconducting Metamaterial Resonator

Sagar Indraneet (Presenter), Haozhi Wang, Matthew D Hutchings, Matthew Lahaye, Syracuse University, Bruno G. Taketani, Frank K Wilhelm, Saarland University, Britton L Plourde, Syracuse University — Precise and accurate coherent control of qubits is critical to the success of superconducting quantum computing. Microwave crosstalk is a ubiquitous problem for large scale superconducting quantum processors and poses a challenge to scaling up few-qubit coherent control results. Although crosstalk is classical, deterministic, and can be mitigated to some degree with electromagnetic nulling, the frequency dependence of crosstalk and significant calibration overhead for compensation schemes motivate hardware solutions. 3D integration techniques such as through silicon vias and bump bonds offer a solution at the cost of fabrication complexity. We propose and present initial experiments on a crosstalk mitigation scheme using commercial multilayer printed circuit boards (PCBs) to enable rapid turnaround and widespread adoption.

3:18PM P26.00005: Kerr- and cross-Kerr-free Josephson four-wave mixing device*

Shantanu O. Mundhada (Presenter), Nicholas E. Frattini, Shruti Puri, Akshay Koottandavid, Shyam Shankar, Steven Girvin, Michel H. Devoret, Department of Applied Physics, Yale University — Parametrically pumped four-wave mixing is a key building block for many developments in the field of superconducting quantum information processing. However, undesired frequency shifts such as Kerr, cross-Kerr and Stark shifts, inherent with four-wave mixing, lead to difficulties in tuning up the desired parametric processes and, for certain applications, severely limit the fidelities of the resulting operations. In this talk, we explore a Josephson four-wave mixing device consisting of a SQUID transmon coupled to a half-flux biased SNAIL transmon, a.k.a. capacitively shunted flux qubit. When the two transmons have matching frequencies, an interference effect cancels the negative Kerr of the SQUID transmon with the positive Kerr of the SNAIL transmon while preserving parametric four-wave mixing capabilities. We present the design and experimental characterization of such a device.

*ARO, ONR, NSF, AFOSR, and YINQE
3:30PM P26.00006: Quickly tunable refrigerator for superconducting qubits* JAN GOETZ (Presenter), ANDRAS GUNYHO, QCD Labs, Aalto University, MATTI SILVERI, Research Unit of Nano and Molecular Systems, University of Oulu, HAO HSU, GIANLUIGI CATELANI, JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, MIKKO MÖTTÖNEN, QCD Labs, Aalto University — The emerging quantum technological devices call for fast and accurate initialization of functional quantum degrees of freedom to a low-entropy state. Here, we theoretically study a recently demonstrated quantum-circuit refrigerator \[1\] in the case of superconducting qubits. We find that for typical parameters, the refrigerator is suitable for quickly cooling both transmon and flux qubits close to their ground states. The maximum refrigeration rate of transmon qubits is roughly an order of magnitude stronger than that of resonators \[2\], providing additional flexibility in the design criteria. The on/off ratio of the refrigerator assumes values above \(10^4\) with typical experimental parameters. Thus the refrigerator is a promising tool for quantum technology and for studies of open quantum systems. Finally, we present an experimental realization based on transmon qubits and coupled qubit-resonator systems, which are the workhorses of quantum processors based on superconducting circuits.


*This research was supported by European Research Council under Grant No. 681311 and Marie Sklodowska-Curie Grant No. 795159; by Academy of Finland under its Centres of Excellence Program grants.

3:42PM P26.00007: Quickly Tunable Electromagnetic Environment for Superconducting Quantum Circuits* VASILI SEVRIUK (Presenter), KUAN YEN TAN, MATTI SILVERI, SHUMPEI MASUDA, JAN GOETZ, MATTI PARTANEN, DIBYENDU HAZRA, QCD Labs, Aalto University, JOONAS GOVENIUS, Aalto University, RUSSELL LAKE, Boulder, NIST, VISA I VESTERINEN, LEIF GRÖNBERG, JUHA HASSEL, SLAWOMIR SIMBIEROWICZ, Technical Research Centre of Finland Ltd, VTT, MARTON GUNYHO, AARNE KERÄNEN, JANI TUORILA, Aalto University, TAPIO ALA-NISSILA, Departments of Mathematical Sciences and Physics, Loughborough University, HERMANN GRABERT, Department of Physics, University of Freiburg, MIKKO MÖTTÖNEN, QCD Labs, Aalto University — In the qubits operation it is of utmost importance to be able to quickly remove any unwanted excitations on demand for fast and accurate initialization. We recently introduced a device referred to as a quantum-circuit refrigerator (QCR) \[1\]. It is a stand-alone component that can readily be integrated into superconducting quantum electric devices, with negligible perturbation to the device operation. In our experiments, we demonstrate the ability to tune the dissipation of a superconducting resonator by orders of magnitude by the convenient application of a bias voltage on the QCR. The switching time of the tunable dissipation can be as low as a few nanoseconds. We also observe a tunable Lamb shift owing to the dissipation induced by the QCR. 1 K. Y. Tan \textit{et al.}, \textit{Nat. Commun.} \textbf{8}, 15189 (2017)

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3:54PM P26.00008: Optimal Impedance Taper in the Presence of Nonlinear Voltage Reflections* ROBERT ERICKSON (Presenter), MUSTAFA BAL, DAVID PAPPAS, Quantum Devices, NIST-Boulder — A signal introduced into a load-bearing transmission line will partially reflect back along the input line if an impedance mismatch exists at the injection interface. Placement of a tapered impedance transformer at the interface can reduce these reflections. \[1\] In earlier work we showed how to determine the optimal shape of a continuous lossless taper of wide frequency bandpass. \[2\] Our theory assumed impedance mismatch sufficiently small that large voltage reflections within the taper could be considered negligible. Here we extend our earlier theory, allowing for arbitrarily sized impedance mismatches and large voltage reflections, reporting results for a lossless taper. Our extended theory has important application to the design of tapered transformers for electronic devices with unavoidably large impedance mismatches, and can be leveraged to construct on-chip Purcell filters used in the fast readout of superconducting transmon and Xmon qubits.


*This work was supported by the NIST Quantum Initiative. RPE acknowledges grant 70NANB17H033 from the US Department of Commerce, NIST.
be presented.

the thermal noise coming from the resonator at 1 K through the photon-induced qubit dephasing. Preliminary results will

the refrigerator. To verify this cooling mechanism, we use a transmon qubit as a quantum spectrum analyzer and measure

the 1 K stage of a dilution refrigerator is overcoupled to a 20 mK environment anchored to the mixing chamber stage of

lower temperature. In this talk, we will introduce an experiment in which a 10 GHz superconducting resonator anchored to

non-negligible thermal photon populations at microwave frequencies. To resolve this conflict, the electrical resonator at a

higher temperature can predominantly be coupled to, and thus radiatively cooled by the black-body radiation at a much

lower temperature. In this talk, we will introduce an experiment in which a 10 GHz superconducting resonator anchored to

the 1 K stage of a dilution refrigerator is overcoupled to a 20 mK environment anchored to the mixing chamber stage of

the refrigerator. To verify this cooling mechanism, we use a transmon qubit as a quantum spectrum analyzer and measure

the thermal noise coming from the resonator at 1 K through the photon-induced qubit dephasing. Preliminary results will be

presented.

*Work supported by: ARO, AFOSR and YINQE

4:18PM P26.00010: Fast flux control of 3D transmon qubits using a magnetic hose  STEFAN OLENSCHKO (Presenter),

OSCAR GARGIULO, University of Innsbruck, JORDI PRAT-CAMPS, University of Sussex, MAXIMILIAN ZANNER, GERHARD

KIRCHMAIR, University of Innsbruck — An important feature in analog quantum simulation experiments with

superconducting qubits [1] is the possibility to change the frequency of SQUID-based transmon qubits by applying

magnetic flux. Implementing fast flux control on a transmon remains challenging in the 3D cavity architectures due to the

presence of a massive metallic cavity. Here we introduce a new approach for fast flux control on 3D transmon qubits. We

use a magnetic hose similar to the one proposed by C. Navau et al. [2] to guide a fast flux pulse from the outside to the inside of a microwave cavity. This hose enables us to locally circumvent any magnetic shielding effects such as the appearance of eddy currents in cavities made out of copper or the Meissner effect in superconducting cavities made out of aluminum. First experiments show that the transition frequency of a transmon can be tuned in less than 100 nanoseconds. Besides the high speed, the frequency shift is precise, without showing any ringing or hysteresis. Using a magnetic hose with an aluminum cavity preserves the benefits of a superconducting cavity, like providing magnetic field shielding and a high internal quality factor, along with the possibility to fast-tune individual qubits.


4:30PM P26.00011: Kinetic Inductance Microwave Resonators for Quantum Simulation of Nonequilibrium Bose-Hubbard Models*  MATTIAS FITZPATRICK (Presenter), ALICIA KOLLAR, ANDREW HOUCK, Princeton University — The field of circuit-QED (cQED) provides a rich toolbox for doing both quantum computation and quantum simulation with superconducting circuits. Here we will discuss the use of kinetic inductance nonlinearities in microwave resonators as a new tool for quantum and classical-nonlinear simulation of Bose-Hubbard models. We explore the interplay between nonlinearities, dissipation, and disorder in large-scale circuits consisting of cavity arrays or multimode cavities. In contrast to other quantum simulation platforms, the particles in cQED (photons) are inherently dissipative, allowing the study of Bose-Hubbard models from a driven-dissipative and open system context.

*We acknowledge funding from the NSF MURI W911NF-15-1-0397.

4:42PM P26.00012: Josephson Junctions with Two-Dimensional van der Waals Tunnel Barrier  KAN-HENG LEE (Presenter), SRIVATSAN CHAKRAM, FAUZIA MUJID, CHIBEOM PARK, HUI GAO, DAVID SCHUSTER, JIWOONG PARK, The University of Chicago — Better device structure and materials control have contributed to the performance improvement of the Al/AIO_{x}/Al-based superconducting qubits, allowing the technology to initiate practical applications in quantum computing. However, one current limitation of such qubits is the use of amorphous alumina as the tunnel barrier, which is known to have defects that may compromise the qubit coherent time and performance stability. Here, we report novel Josephson Junctions with 2D van der Waals tunnel barriers made with stacked N-layer MoS_{2} that has minimal number of defects. We first generate a MoS_{2} membrane with controlled layer number N by vacuum stacking monolayer MoS_{2} as the tunneling barrier, and then depositing Al superconductor on either side to form the Josephson junctions. We show that we can reliably fabricate large numbers of Josephson junction devices on a single chip, and they show critical supercurrent that can be directly tuned by changing the N. We also characterize the microwave properties of Al/MoS_{2}/Al junctions in a bulk superconducting cavity. Our work offers a new, powerful platform for generating and studying novel qubits with diverse 2D materials, and thus may provide an additional route to further improve the qubit performance for advancing the quantum technology.
4:54PM P26.00013: Observation of a broadband Lamb shift in a superconducting resonator* MATTI SILVERI, Department of Physics, University of Oulu, SHUMPEI MASUDA, BASILII SEVRIUK, KUAN YEN TAN, ERIC HYYPÄ, MATTI PARTANEN, JAN GOETZ, QCD Labs, Aalto University, RUSSELL LAKE, Boulder, NIST, LEIF GRÖNBERG, QTF Centre of Excellence, VTT Technical Research Centre of Finland, MIKKO MÖTTÖNEN (Presenter), QCD Labs, Aalto University — The shift of energy levels owing to broadband electromagnetic vacuum fluctuations—the Lamb shift—has been pivotal in the development of quantum electrodynamics and in understanding atomic spectra. Currently, small energy shifts in engineered quantum systems are of paramount importance owing to the extreme precision requirements in applications such as quantum computing. However, without a tunable environment it is challenging to resolve the Lamb shift in its original broadband case. Consequently, the observations in other than atomic systems are limited to environments comprised of narrowband modes. Here, we experimentally observe in high-quality superconducting resonators a Lamb shift of several megahertz, by externally tuning the coupling strength of an engineered broadband environment based on hybrid normal-metal–superconductor tunnel junctions. Our results may lead to improved control of dissipation in high-quality engineered quantum systems such as superconducting qubits.

*We acknowledge European Research Council Grant No. 681311 (QUESS); Academy of Finland grants Nos. 312300, 312059, 265675, 305237, 305306, 308161, 312300, 314302, 316551; the Jane and Aatos Erkko Foundation, and the Technology Industries of Finland Centennial Foundation.

5:06PM P26.00014: Quantum Dynamics of a few-photon Microwave Parametric Oscillator ZHAOYOU WANG (Presenter), MAREK PECHAL, AMIR SAFAVI-NAEINI, Stanford University — We experimentally investigate quantum dynamics of a non-linear superconducting RF resonator in the intermediate (n ~ 5) photon number regime. In particular, we study parametric processes induced by modulation of the resonator’s inductance to prepare non-classical photon states, which may be useful in future continuous-variable quantum error correction schemes. The system can be described as a Kerr parametric oscillator (KPO) with linewidth significantly smaller than the single photon Kerr shift. We observe narrowing of the linewidth when approaching the parametric stability threshold as well as non-classical signatures in the resonator state’s free evolution caused by the Kerr non-linearity. To read out the quantum state of the resonator, we developed a tomography method which utilizes its nonlinear character to estimate the system’s density matrix from the power spectrum of the field emitted by it.

5:18PM P26.00015: Packaging Large-scale Superconducting Quantum Computer with Airbridge* HIROTO MUKAI (Presenter), KEICHI SAKATA, Physics, Tokyo University of Science, DEVITT J SIMON, Faculty of Engineering and Information Technology, University of Technology Sydney, RUI WANG, YUKITO NAKAJIMA, JAW-SHEN TSAI, Physics, Tokyo University of Science — For superconducting circuits with quantum error correction, a two-dimensional array of qubits is required. Recently it is challenged to build a practical large-scale superconducting circuit with the array on a chip by using this three-dimensional wiring technique to control the qubits, while maintaining high fidelity operations. In this talk, we present the novel arrangement of the array of qubits without non-monolithic special technology of three-dimensional wiring. In this architecture, standard two-dimensional external lines are adopted and local crossovers of interqubit connections are required. The crossovers are realized by airbridge technology. We show this novel architecture and the result of quality factor of resonator with airbridge at center line.

*This research is supported by NEDO IoT project, JST CREST project and ImPACT project in Japan.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P27 DQI: General Quantum Information and Quantum Computation BCEC 160C - Todd Brun, University of Southern California
2:30PM P27.00001: Fundamental limits to quantum channel discrimination* STEFANO PIRANDOLA (Presenter), RICCARDO LAURENZI, COSMO LUPO, University of York — What is the ultimate performance for discriminating two arbitrary quantum channels acting on a finite-dimensional Hilbert space? Here we address this basic question by deriving a general and fundamental lower bound. More precisely, we investigate the symmetric discrimination of two arbitrary qudit channels by means of the most general protocols based on adaptive (feedback-assisted) quantum operations. In this general scenario, we first show how port-based teleportation can be used to completely simplify these adaptive protocols into a much simpler non-adaptive form, designing a new form of teleportation stretching. Then, we prove that the minimum error probability affecting the channel discrimination cannot beat a bound determined by the Choi matrices of the channels, establishing an ultimate and elegant formula for quantum hypothesis testing. As a consequence of this bound, we derive the ultimate limits for adaptive quantum illumination and single-photon quantum optical resolution. Finally, we show how the methodology can also be applied to other tasks, such as quantum metrology, quantum communication and secret key generation.

*This work is supported by the EPSRC via the `UK Quantum Communications Hub' (EP/M013472/1) and by the Innovation Fund Denmark (Qubiz project).

2:42PM P27.00002: Quantum Dimension Witness and Assisted Quantum State Discrimination* UMAN KHALID (Presenter), YOUNGMIN JEONG, HYUNDONG SHIN, Department of Electronic Engineering, KyungHee University, Korea — The relevance between quantum information processing tasks such as witnessing the dimension of an unknown quantum system and quantum state discrimination is indebted to the statistics obtained from the quantum measurement. A quantum dimension witness (QDW) provides a lower bound on the minimum dimensions that are necessary to describe the quantum correlation originated from the measurements on an unknown quantum system. Such measurement-based quantum correlations (MbQCs) are not only observer dependent but also depend on how strongly an observer perturbs the unobserved system. Based on the aforementioned measurement scenario, we present a quantitative measure that is both the QDW and MbQC measure for arbitrary dimensional bipartite quantum systems. The quantitative measure serves well for bipartite mixed quantum systems and vanishes only for a non-quantum system. We also show that MbQCs are more general than traditional quantum correlations in an optimal assisted quantum state discrimination task.

* This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2016R1A2B2014462), and by the Basic Science Research Program through the NRF funded by the Ministry of Education (No. 2018R1D1A1B07050584).

2:54PM P27.00003: Fidelity estimation via local measurements in the presence of arbitrarily correlated noise LIANGZHONG RUAN (Presenter), STEPHANIE WEHNER, QuTech, Delft University of Technology — Fidelity estimation for entangled states shared by remote nodes is an essential building block for the quality control in quantum networks. In the literature, the issue of minimizing the efficiency loss in fidelity estimation due to the limitation of local operations and the issue of characterizing the accuracy of fidelity estimation protocols in the presence of arbitrary noise remain interesting challenges. This work addresses these two challenges, designs a protocol for estimating the average fidelity of qubit pairs shared by remote agents, whose efficiency reaches the fundamental upper bound achievable with local operations, and characterizes the performance of the proposed protocol in the presence of arbitrary noise. Analysis has been performed to characterize which factors affect the estimation accuracy and how. Numerical tests have been performed to check the preciseness and robustness of the proposed protocol, as well as to characterize the proper parameter setting. The analysis and numerical tests have identified the distinctive factors that affect the estimation accuracy in the presence of arbitrary noise, and have given clear instructions on how to properly address these factors.

3:06PM P27.00004: Effective Hamiltonian theory of the geometric evolution of quantum systems* VLADYSLAV SHKOLNYKOV (Presenter), GUIDO BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — We present an effective Hamiltonian description of the quantum dynamics of a generalized Lambda system undergoing adiabatic evolution [1]. We assume the system to be initialized in the dark subspace and show that its holonomic evolution can be viewed as a conventional Hamiltonian dynamics in an appropriately chosen extended Hilbert space. In contrast to the existing approaches, our method does not require the calculation of the non-Abelian Berry connection and can be applied without any parametrization of the dark subspace, which becomes a challenging problem with increasing system size.


*We acknowledge funding from DFG through SFB767.
3:18PM P27.00005: Dense Measurements for Gate-Model Quantum Computers* LASZLO GYONGYOSI (Presenter), University of Southampton, SANDOR IMRE, Budapest Univ. of Tech — The measurement procedure is a fundamental cornerstone of gate-model quantum computers. The main issues in current quantum measurement strategies are the high number of measurement rounds to determine a global optimal measurement output and the low success probability of finding a global optimal measurement output. Each measurement round requires preparing the quantum system and applying quantum operations and measurements with high-precision control in the physical layer. These issues result in high-cost measurements with a low probability of success. Here, we define a novel measurement for gate-model quantum computers called dense quantum measurement. The dense measurement strategy aims at fixing the main drawbacks of standard quantum measurements by achieving a significant reduction in the number of necessary measurement rounds and by radically improving the success probabilities of finding global optimal outputs. We provide application scenarios for quantum circuits with arbitrary unitary sequences. The dense measurement also provides an experimentally implementable solution for practical quantum computations.

*This work was partially supported by Project No. 2017-1.2.1-NKP-2017-00001, by OTKA K-112125 and in part by the FIKP grant of EMMI (BME FIKP-MI/SC).

3:30PM P27.00006: Why the Quantum WILLIAM STUCKEY (Presenter), Physics, Elizabethtown College — To answer Wheeler’s question `Why the quantum?` via quantum information theory per Bub, one must explain why the world is quantum rather than classical and why the world is quantum rather than superquantum, i.e., `Why the Tsirelson bound?` We show that the quantum correlations resulting from two Bell basis states, which uniquely produce the Tsirelson bound for the Clauser-Horne-Shimony-Holt quantity, can be derived from the conservation of angular momentum (on average) for the quantum exchange of momentum. This explanation of the Tsirelson bound does not require hidden variables or `causal influences`. Since superquantum correlations exceed quantum correlations, we know that they would violate conservation of angular momentum and we show how this happens using the Popescu-Rohrlich correlations. Thus, quantum correlations responsible for the Tsirelson bound satisfy conservation of angular momentum for the quantum exchange of momentum while both classical and superquantum correlations can fail to satisfy this constraint. We generalize the result to conservation per any measurement associated with a Bell basis state. While this constraint is not surprising per se, the details on how it obtains evidence a deeper principle at work in Nature, i.e., no preferred reference frame.

3:42PM P27.00007: Wavefunction; The Guided Energy of Wave DESMOND AGBOLADE ADEMOLA (Presenter), Physics, Olabisi Onabanjo University — This paper expound the true nature of wavefunction and answered questions that arise from quantum foundation such as what is nature of wavefunction? Is mathematical formalism of wavefunction correct? Does wavefunction collapse during measurement? Do quantum physical entanglement and many world interpretations really exist? In addition, is there uncertainty in the physical reality of our nature as being concluded in the quantum foundation? The fundamental analysis presented in this work show that mathematical formalism of wavefunction was wrongly formulated. Because, we discovered that, wavefunction is the guided energy of wave by the reason that the universe and everything in it from large particle to the smallest tiny particle, physical and imaginary, visible and invisible, existing and non-existing has guided energy which is wavefunction. We further show that wavefunction is not collapse, only disengaged and engaged gradually. The gradual process of wavefunction disengagement display how the particle-like behavior return to wave-like behavior and the gradual process of wavefunction engagement also display how wave-like behavior return to the particle-like behavior. Convergence and divergence of wavefunction exhibit precise position of a particle and wave amplitude respectively.

3:54PM P27.00008: Quaternion Series Spin DOUGLAS SWEETSER (Presenter), Quaternions.com of Acton, MA — Abstract

Quantum mechanics today uses a complex-valued Hilbert vector space for its mathematical substructure. Quaternion series quantum mechanics is an effort to replace every complex number with a quaternion. Each quaternion can represent physical quantitat such as events in space-time, 4-potentials, energy-momentum, 4-currents, etc.. A series of quaternions is a vector. One can multiply quaternion series together because the quaternion series are a semigroup with inverses. This may of limited utility given the key role of unitarity to quantum mechanics.

The intrinsic spin of a particle can be described by a quaternion series with two state dimensions. The spin operator is often characterized as one quaternion. With quaternion series quantum mechanics, spin operators are 2x2 matrices of quaternions, so four simple quaternions in all (zero, plus one, and negative one, normalized is one possible representation). Much effort is devoted to understanding the operators. If one instead examines what a spin operator does to a spin state, there is a simple message: spin operators can mix information found in a spin state in every possible way.
4:18PM P27.00010: Entropic Energy-Time Uncertainty Relation† PATRICK J COLES, Theoretical Division, Los Alamos National Laboratory, VISHAL KATARIYA (Presenter), Department of Physics and Astronomy and Center for Computation and Technology, Louisiana State University, SETH LLOYD, Dept. of Mechanical Engineering and Research Laboratory of Electronics, Massachusetts Institute of Technology, IMAN MARVIAN, Departments of Physics & Electrical and Computer Engineering, Duke University, MARK M WILDE, Department of Physics and Astronomy and Center for Computation and Technology, Louisiana State University — Energy-time uncertainty plays an important role in quantum foundations and technologies, and it was even discussed by the founders of quantum mechanics. However, standard approaches (e.g., Robertson’s uncertainty relation) do not apply to energy-time uncertainty because, in general, there is no Hermitian operator associated with time. Following previous approaches, we quantify time uncertainty by how well one can read off the time from a quantum clock. We then use entropy to quantify the information-theoretic distinguishability of the various time states of the clock. Our main result is an entropic energy-time uncertainty relation for general time-independent Hamiltonians, stated for both the discrete-time and continuous-time cases. Our uncertainty relation is strong, in the sense that it allows for a quantum memory to help reduce the uncertainty, and this formulation leads us to reinterpret it as a bound on the relative entropy of asymmetry. Due to the operational relevance of entropy, we anticipate that our uncertainty relation will have information-processing applications.

*The authors would like to thank the following funding agencies: LANL ASC Beyond Moore's Law Project, Dept. of P&A, LSU, IARPA QEO Program, NSF, ARO Blue Sky Initiative, and NSF grant no. 1714215 respectively.

4:30PM P27.00011: Duality and free energy analyticity bounds for few-body Ising models with extensive homology rank† YI JIANG (Presenter), Department of Physics & Astronomy, University of California, Riverside, ILYA DUMER, Department of Electrical Engineering, University of California, Riverside, ALEXEY KOVALEV, Department of Physics & Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, LEONID PRYADKO, Department of Physics & Astronomy, University of California, Riverside — We consider pairs of few-body Ising models such that each model can be obtained from the dual of the other after freezing \( k \) spins on large-degree sites. Such a pair of Ising models can be interpreted as a two-chain complex with \( k \) being the rank of the first homology group. Our focus is on the case where \( k \) is extensive. In the presence of bond disorder, we prove the existence of a low-\( T \) weak-disorder region where additional summation over the defects has no effect on the free energy density \( f(T) \) in the thermodynamical limit, and of a high-\( T \) region where in the ferromagnetic case an extensive homological defect does not affect \( f(T) \). We also discuss the convergence of the high- and low-temperature series for the free energy density, prove the analyticity of \( f(T) \) at high and low temperatures, and construct inequalities for the critical point(s) where analyticity is lost. As an application, we prove multiplicity of the conventionally defined critical points for Ising models on all \( \{ f, d \} \) tilings of the infinite hyperbolic plane. For these infinite graphs, we show that critical temperatures with free and wired boundary conditions differ, \( T_c^{(f)} < T_c^{(w)} \).

*This work was supported in part by the NSF under Grants No. PHY-1415600 (AAK), ECCS-1102074 (ID), and PHY-1416578 (LPP)

4:42PM P27.00012: Complexity phase transition in interacting and long-range bosonic Hamiltonians NISHAD MASKARA, Department of Physics, Caltech, ABHINAV DESHPANDE (Presenter), CONG MINH TRAN, BILL FEFFERMAN, Joint Center for Quantum Information and Computer Science, MICHAEL FOSS-FEIG, Army Research Laboratory, ALEXEY V GORSHKOV, Joint Center for Quantum Information and Computer Science — We investigate the complexity of sampling from time-evolved states due to bosonic Hamiltonians. We obtain timescales for which approximate sampling is easy and hard, generalising the results in Ref. [1] to systems with interacting bosons and to systems with long-range couplings. The easiness results rely on recent developments in the simulation of spatially local Hamiltonians [2,3]. For free bosons with long-range hops, where the strength of the hopping term decays with distance as a power law, we observe the hardness setting in earlier than the nearest-neighbor case. We also obtain hardness results for interacting bosons. Along the way, we develop methods and tools that are of independent interest. Our work maps out the timescale between easiness and hardness of sampling on a “complexity phase diagram”, giving a testbed for exploring physical manifestations of the computational complexity of simulating interacting quantum systems.

4:54PM P27.00013: Unitary designs for continuous variable systems* THOMAS SCHUSTER (Presenter), QUNTAO ZHUANG, University of California, Berkeley, BENI YOSHIDA, Perimeter Institute for Theoretical Physics, NORMAN YAO, University of California, Berkeley — The study of information scrambling in many-body systems has sharpened our understanding of quantum chaos. In discrete variable (DV) systems (finite-dimensional, e.g. spins), the scrambling ‘strength’ of a unitary is often measured by its closeness to a Haar random unitary. This leads to a hierarchy of increasingly fine-grained measures of scrambling known as ‘unitary k-designs’. Here, we extend the notion of unitary designs to continuous variable (CV) systems (infinite-dimensional, e.g. photons). Although there is no generalization of Haar randomness to CV systems, we show that averages of physical quantities over Haar random unitaries remain well-defined in the CV limit, and use this to define CV unitary designs. Surprisingly, Gaussian unitaries, despite being non-interacting, form a CV 2-design and can therefore `quasi-scramble' information. Extending further, we show that unitary 4-designs maximize the phase space volume of generic time-evolved operators.

*DOE, NSF, Government of Canada.

5:06PM P27.00014: Scrambling and complexity in phase space* QUNTAO ZHUANG (Presenter), THOMAS SCHUSTER, Department of Physics, University of California, Berkeley, California 94720, USA, BENI YOSHIDA, Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada, NORMAN YAO, Department of Physics, University of California, Berkeley, California 94720, USA — In this talk, we will describe extensions of the study of scrambling and complexity to infinite-dimensional continuous variable (CV) systems. Unlike their discrete variable (DV) cousins, continuous variable systems exhibit two complementary domains of information scrambling: 1) scrambling in the phase space of a single mode and 2) scrambling across multiple modes. Moreover, for each of these domains, we identify two distinct "types" of scrambling: strict scrambling, where an initial operator localized in phase space spreads out and quasi-scrambling, where a local ensemble of operators distorts but the overall phase space volume remains fixed. To characterize these behaviors, we introduce a CV out-of-time-order correlator (OTOC) based upon displacement operators, which can be experimentally measured. By studying operator spreading and entanglement formation in a random local Gaussian circuit ensemble, we infer the dynamics of generic, chaotic, locally-interacting systems. Our work opens the door to experimentally probing phase space scrambling in CV systems, including cavity QED and quantum optics architectures.

*DOE, NSF, and Govt. of Canada.

5:18PM P27.00015: Characterizing the performance of continuous-variable Gaussian quantum gates KUNAL SHARMA (Presenter), MARK M WILDE, Louisiana State University — The required set of operations for universal continuous-variable quantum computation can be primarily be divided into two categories: Gaussian and non-Gaussian operations. Furthermore, any Gaussian operation can be decomposed as a sequence of phase-space displacements and symplectic transformations. Although Gaussian operations are ubiquitous in quantum optics, their experimental realizations are generally approximations of the ideal Gaussian unitaries. In this work, we study different performance metrics to analyze how well these experimental approximations simulate the ideal Gaussian operations. In particular, we find that none of these experimental approximations converge uniformly to the ideal Gaussian processes. However, convergence occurs in the strong sense, or if the discrimination strategy is energy bounded, then the convergence is uniform. We indicate how these energy-constrained bounds could be used for experimental implementations of these Gaussian operations in order to achieve any desired accuracy.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P28 DQI: Quantum Measurement and Sensing II BCEC 161 - Bradley Moores, University of Colorado, Boulder
2:30PM P28.00001: Imaging Vortex Dynamics in High-Tc Superconductors using Ensemble Nitrogen Vacancy (NV) Centers in Diamond* ADITYA MALUSARE (Presenter), SUMIRAN PUJARI, Department of Physics, Indian Institute of Technology Bombay, SHAMASHIS SENGUPTA, Centre de Sciences Nucléaires et de Sciences de la Matière (CSNSM), KASTURI SAHA, Department of Electrical Engineering, Indian Institute of Technology Bombay — Nitrogen-Vacancy (NV) centers are excellent quantum sensors due to their long spin-coherence time and ultrahigh magnetic field sensitivity. An ensemble of NVs can be used for vector magnetometry of high-Tc superconductors to investigate several processes of interest with nanometer resolution over a wide field. We study the feasibility of measuring vortex dynamics, which plays a pivotal role in understanding the mechanisms underlying superconductivity. In this work, we make a fully functional simulation of a thin-film type-II superconductor with properties similar to materials like BSCCO or YBCO and theoretically demonstrate a scheme for mapping vortices in real time. Utilizing the capabilities of the NV center as a high-speed imaging sensor, we can probe the dynamics of vortex pinning and nucleation. Effects of impurities, thermal fluctuations, varying thickness and other defects can be examined through NVs with nanometer resolution as shown in our simulations as well.

*This work was supported by the IIT-SEED grant

2:42PM P28.00002: Zappe Photon Upconverters for Quantum Measurements of Low-Frequency Electrical Resonators, Part I: Theory* SAPTARSHI CHAUDHURI (Presenter), Stanford University, HSIAO-MEI CHO, SLAC National Accelerator Laboratory, CARL DAWSON, Stanford University, PETER W. GRAHAM, Stanford Institute for Theoretical Physics, RACHEL GRUENKE, STEPHEN KUENSTNER, Stanford University, DALE LI, SLAC National Accelerator Laboratory, ARRAN TJ PHIPPS, CHARLES TITUS, Stanford University, BETTY YOUNG, Santa Clara University, CYNDIA YU, KENT DAVID IRWIN, Stanford University — We present the Zappe Photon Upconverter (ZPU), a Josephson-junction-based readout amplifier for performing quantum measurements on lumped-element LC resonators (100 Hz-300 MHz). The ZPU exploits the symmetries of a three-junction Zappe interferometer embedded inside a microwave resonator. The Zappe element acts as a flux-variable inductor, cleanly implementing a three-wave-mixing interaction between the low-frequency resonator at the flux input and the high-frequency (~6 GHz) microwave resonator. The interaction is analogous to the interaction between resonators in electromechanical and optomechanical systems. We establish protocols for flux sensing at the Standard Quantum Limit (SQL), as well as backaction evasion techniques that permit measurements below the SQL. We discuss applications of ZPUs, in particular axion dark matter searches, where these devices can enable scan rate enhancements of orders of magnitude.

*The authors would like to acknowledge the support of the Department of Energy's Quantum Information Science Enabled Discovery (QuantISED) program.

2:54PM P28.00003: Zappe Photon Upconverters for Quantum Measurements of Low-Frequency Electrical Resonators, Part II: Implementation of the Prototype* STEPHEN KUENSTNER (Presenter), SAPTARSHI CHAUDHURI, Stanford University, HSIAO-MEI CHO, SLAC National Accelerator Laboratory, CARL DAWSON, Stanford University, PETER W. GRAHAM, Stanford Institute for Theoretical Physics, RACHEL GRUENKE, Stanford University, DALE LI, SLAC National Accelerator Laboratory, ARRAN TJ PHIPPS, CHARLES TITUS, Stanford University, BETTY YOUNG, Santa Clara University, CYNDIA YU, KENT DAVID IRWIN, Stanford University — We describe progress towards the first Zappe Photon Upconverter (ZPU), a Josephson-junction-based device capable of performing quantum mechanical readout protocols on low-frequency, lumped-element electromagnetic resonators. The prototype ZPU is being constructed using techniques similar to those used in superconducting transmon qubits, where the Josephson device is connected to a lithographed antenna immersed in the electromagnetic field of a three-dimensional microwave cavity. We describe the constraints on the circuit design and propose targets for the component values. We also present measurements of the quality factor of the superconducting microwave cavity designed for use with the first-generation ZPU, numerical modeling of the circuit parameters, and projections of the sensitivity enhancement available from backaction evading measurements using a prototype ZPU.

*The authors would like to acknowledge the support of the Department of Energy's Quantum Information Science Enabled Discovery (QuantISED) program.
3:06PM P28.00004: Optical sensing of biological processes with nitrogen-vacancy centers in nanodiamonds

CHANGHAO LI (Presenter), Research Laboratory of Electronics and Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, DOMINIKA LYZWA, Research Laboratory of Electronics, Massachusetts Institute of Technology, MOHAMMAD KOHANDEL, Department of Applied Mathematics, University of Waterloo, PAOLA CAPPELLARO, Research Laboratory of Electronics and Department of Nuclear Science and Engineering, Massachusetts Institute of Technology — Nitrogen-vacancy (NV) centers in nanodiamonds are very attractive probes for sensing chemical reactions and biological processes. Their relaxation times are especially sensitive to the surrounding environment and can be probed with an all-optical protocol. To induce strong variations in the relaxation, the nanodiamonds can be brought in proximity to Gadolinium (Gd) ions which are strongly paramagnetic and can effectively quench the NV relaxation time. By optically monitoring the relaxation, it is possible to observe chemical and biological processes that affect the distance between Gd and nanodiamond. Here we first directly cover the nanodiamonds with chelated Gd and characterize the quenching effect for different Gd concentrations on an ensemble of nanodiamonds with an average diameter of around 20 nm. We will further show how the nanodiamonds can be connected with Gd via a cleavable peptide sequence. Specific enzymes, released during apoptosis, can cut the connection thus separating NVs from Gd and decreasing the relaxation rate. The nanodiamond sensors have the potential to be used simultaneously as drug delivery probes in addition to optical sensing, hence they might allow for monitoring chemotherapy.


RAJESH PATEL (Presenter), ANGELO FRANGESKOU, GUY STIMPSON, ELEANOR NICHOLS, WILLIAM THORNLEY, BEN G BREEZE, BEN GREEN, Department of Physics, University of Warwick, Coventry, CV4 7AL, UK, SHINOBU ONODA, Takasaki Advanced Radiation Research Institute, National Institutes for Quantum and Radiological Science and Technology, Takasaki, Gunma 370-1292, Japan, JUNICHI ISOYA, Research Center for Knowledge Communities, University of Tsukuba, 1-2 Kasuga, Tsukuba, Ibaraki 305-8550, Japan., GAVIN MORLEY, Department of Physics, University of Warwick, Coventry, CV4 7AL, UK — The negatively charged nitrogen-vacancy (NV) centre in diamond is one of the most studied solid-state defects because it has spin states that can be initialised and detected optically at room temperature [1]. A key technological development is the use of an ensemble of these defects for applications in high sensitivity magnetometry [2] which may lead to the development of medical devices for techniques such as magnetocardiography [3]. We present a fiber-coupled system which aims to detect the magnetic fields produced by electrical currents in the heart.


*We gratefully acknowledge the funding provided by the Engineering and Physical Sciences Research Council and the Royal Society of the United Kingdom.

3:30PM P28.00006: Dopant-Free Single Electron Pumps for Quantum Metrology

FRANCOIS SFIGAKIS (Presenter), BRANDON BUONACORSI, ARJUN SHETTY, Institute for Quantum Computing, University of Waterloo, Waterloo, Canada, CHRIS DEIMERT, ALAN TAM, HOSUNG KIM, ZBIG WASILEWSKI, Department of Electrical and Computer Engineering, University of Waterloo, Waterloo, Canada, NIELS UBBELOHDE, FRANK HOHLS, Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany, JONATHAN D BAUGH, Institute for Quantum Computing, University of Waterloo, Waterloo, Canada — At low temperature, we have observed low-disorder quantized conductance in quantum wires fabricated in dopant-free GaAs/AlGaAs two-dimensional electron gases (2DEG) with mobilities up to $7 \times 10^5$ cm$^2$/Vs (at $2.9 \times 10^{11}$ /cm$^2$), with a 1D subband energy level spacing that can be tuned from 1 meV to more than 5 meV on individual devices. The absence of (intentional) dopants produces an environment with ultra low disorder [1] and very little charge noise [2]. Single electron pumps [3,4] were fabricated and measured at 1 MHz, with up to 3 quantized current plateaus observed. Thus, dopant-free quantum wires provide a unique platform to investigate electron-electron interactions, and could offer a path towards single electron pumps suitable for a quantum current standard [5].


*This research was undertaken thanks in part to funding from NSERC, Defence Research and Development Canada (DRDC), the Canada First Research Excellence Fund, and the University of Waterloo's Quantum NanoFab facility.
MARK KU (Presenter), Harvard - Smithsonian Center for Astrophysics & Department of Physics, Harvard University, TONY ZHOU, Department of Physics, Harvard University & School of Engineering and Applied Sciences, Harvard University, QING LI, YOUNG JAE SHIN, JING SHI, CLAIRE BURCH, Department of Physics, Harvard University, HUILIANG ZHANG, FRANCESCO CASOLA, Harvard - Smithsonian Center for Astrophysics & Department of Physics, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, PHILIP KIM, AMIR YACOBY, Department of Physics, Harvard University & School of Engineering and Applied Sciences, Harvard University, RONALD L WALSWORTH, Harvard-Smithsonian Center for Astrophysics & Department of Physics, Harvard University & Center for Brain Science, Harvard University — Collective behavior due to strong electron-electron interactions can lead to transport resembling that of a hydrodynamic fluid. Novel flow patterns, for example parabolic velocity profile known as the Poiseuille flow, arise due to viscosity in such electron fluids. In this work, we directly observe viscous Poiseuille flow in hBN-encapsulated graphene channels via imaging the associated stray magnetic field with nitrogen-vacancy (NV) centers in diamond. With wide-field magnetic imaging, we obtain diffraction-limited 2D image of the stray field generated by current flow in a graphene device on a diamond surface. The measured current density across the channel strongly deviates from the profile of a uniform flow and instead matches that of a viscous fluid. We then employ scanning NV microscopy to image the stray field with ~50 nm resolution. As a benchmark, we demonstrate the ability to image the uniform Ohmic flow in a thin metallic wire. In the case of a graphene channel, we observe a parabolic current profile corresponding to viscous Poiseuille flow. Our measurement establishes the viscous flow of a hydrodynamic electron fluid in graphene at room temperature.

3:54PM P28.00008: Imaging the local charge environment of nitrogen-vacancy centers in diamond*  
THOMAS MITTIGA (Presenter), SATCHER HSIEH, CHONG ZU, BRYCE H KOBRIN, FRANCISCO MACHADO, PRABUDHYA BHATTACHARYYA, NICHOLAS Z RUI, ANDREY JARMOLA, SOONWON CHOI, DMITRY BUDKER, NORMAN YAO, University of California, Berkeley — Characterizing the local internal environment surrounding solid-state spin defects is crucial to harnessing them as nanoscale sensors of external fields. This is especially germane to the case of defect ensembles which can exhibit a complex interplay between interactions, internal fields and lattice strain. In this talk, we demonstrate that local electric fields dominate the magnetic resonance behavior of ensembles of nitrogen-vacancy (NV) centers in diamond at low magnetic field. We introduce a microscopic model that quantitatively captures the observed spectra for samples with NV concentrations spanning over two orders of magnitude. Motivated by this understanding, we present the implementation of a novel method for the nanoscale localization of individual charges within the diamond lattice.

*This work was supported as part of the Center for Novel Pathways to Quantum Coherence in Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-AC02-05CH11231. SH acknowledges support by the National Science Foundation Graduate Research Fellowship under Grant No. DGE 1752814.

4:06PM P28.00009: Spatial noise filtering through new error-correcting codes for quantum sensing  
DAVID LAYDEN (Presenter), Research Laboratory of Electronics, Massachusetts Institute of Technology, SISI ZHOU, LIANG JIANG, Department of Physics, Yale University, PAOLA CAPPELLARO, Research Laboratory of Electronics, Massachusetts Institute of Technology — Quantum systems can be used to measure various quantities in their environment with high precision. Often, however, their sensitivity is limited by the decohering effects of this same environment. Dynamical decoupling schemes are widely used to filter environmental noise from signals, but their performance is limited by the spectral properties of the signal and noise at hand. Quantum error correction schemes have therefore emerged as a complementary technique without the same limitations. To date, however, they have failed to correct the dominant noise type in many quantum sensors, which couples to each qubit in a sensor in the same way as the signal. We show how quantum error correction can correct for such noise, which dynamical decoupling can only partially address. Whereas dynamical decoupling exploits temporal noise correlations in signal and noise, our scheme exploits spatial correlations. To this end, we introduce a new family of quantum error-correcting codes for sensing, which are both application- and hardware- adapted.

4:18PM P28.00010: Continuous error correction for quantum metrology  
SHENGLI PANG (Presenter), Fermilab, YI-CONG ZHENG, Tencent Quantum Lab, Tencent, TODD BRUN, University of Southern California, ANDREW N JORDAN, University of Rochester — Protecting the information in quantum metrology by quantum error correction has been studied intensively in recent years. The usual assumption in quantum error correction is that the syndrome measurements and correction operations are done frequently enough so that errors generated by the noise are correctable with high probability. Here, we analyze how the rate of continuous-time quantum error correction affects quantum metrology. We show that if the rate of error correction is finite, the Heisenberg limit in quantum metrology can only be sustained for a finite period. Moreover, in contrast to quantum metrology without noise (or with sufficiently fast quantum error correction), a longer evolution time does not always produce more information. There exists an optimal time at which the Fisher information reaches the maximum. We use the simple three-qubit bit-flip code to illustrate this result.
4:30PM P28.00011: Optical hyperpolarization in nanodiamonds: towards quantum-enhanced NMR/MRI

ASHOK AJJOY (Presenter), RAFFI NAZARYAN, XUDONG LV, KRISTINA LIU, EMANUEL DRUGA, JEFFREY A REIMER, University of California, Berkeley, CARLOS A. MERILES, Physics, CUNY, ALEXANDER PINES, University of California, Berkeley — Atom-like defect center spins in wide bandgap materials, such as Nitrogen Vacancy (NV) center spins in diamond, are compelling platforms for the optical dynamic nuclear polarization (DNP) of nuclear spins. NV electronic spins can be optically polarized at room temperature, and this polarization potentially transferred to external nuclei to hyperpolarize them to levels far in excess of Boltzmann levels. Nanodiamond powder is particularly attractive in this quest: they have large surface areas (>7m²/g for 100nm particles), and one could arrange for a close physical contact between the polarized NVs and external nuclear spins.

In this work, we produce "optically hyperpolarized nanodiamonds", obtaining high bulk $^{13}$C polarization (~1%) [1]. We develop a remarkably simple, low-field optical DNP technique that proves to be fully orientation independent [2]. Our technique also allows simple control of the hyperpolarization direction, that only depends on the direction of microwave sweeps across the electron spectrum. This paves for quantum-assisted classical NMR and MRI, allowing for vastly accelerated spectroscopy and imaging with chemical specificity.


4:42PM P28.00012: Optically hyperpolarized Nano-Diamond MRI at Room Temperature

XUDONG LV (Presenter), EMANUEL DRUGA, RAFFI NAZARYAN, TOMMY MCKNELLY, ALEXANDER PINES, ASHOK AJJOY, University of California, Berkeley, JEFFREY WALTON, University of California, Davis — Diamond nano-particles with surface functionalization nanoparticles for biomedical applications such as targeting, sub-cellular tracking, and non-toxic therapy [1]. The versatility of nano-diamond has motivated the development of new diamond-based imaging agents that will 'light up' under MRI to produce a bright field contrast image. Conventional Dynamic Nuclear Polarization mechanism which has been successfully demonstrated in diamond to hyperpolarize $^{13}$C nuclei, has to rely on high fields and cryogenic temperatures. Here we demonstrate a room temperature hyperpolarized nano-diamond $^{13}$C imaging with an enhancement of ~600 against 7T thermal polarization[2]. We were also able to achieve back ground suppression in magnetic resonance imaging with the ability of on demand controlling the sign of the hyperpolarization signal. Furthermore, combing both MRI and optical imaging of powder diamond, we present a new dual-modality nano-diamond imaging approach with orders of magnitude SNR enhancement.


4:54PM P28.00013: Environment-assisted quantum sensing with entangled electronic spins in diamond

WON KYU CALVIN SUN (Presenter), Massachusetts Institute of Technology, ALEXANDRE COOPER, California Institute of Technology, JEAN-CHRISTOPHE JASKULA, PAOLA CAPPELLARO, Massachusetts Institute of Technology — Intuitively, enlarging a quantum system by the addition of controllable qubits should only enhance—not decrease—its performance: in other words, any extra qubit should prove a resource. For quantum metrology, the transition from N=1 to N=2 qubits seems especially good for both promised improvement in sensitivity—via N-fold faster phase accumulation—and in readout—via quantum non-demolition measurements. This transition is further motivated in solid-state spin systems that inevitably host a decohering spin bath: its partial conversion into resources simultaneously reduces its size. Thus, utilizing a single nitrogen-vacancy (NV) center and a nearby electron spin (X) in diamond, we explore this question by comparing the performance of N=1 (NV) and N=2 (NV + X) register in ac magnetometry. We find experimentally the ostensible benefits of the resource can be overshadowed by its very cost: namely the increased complexity to perform the same task—resulting in decreased control fidelity and duty cycle—and sensitivity to noise—resulting in decreased dynamic range. We analytically confirm these results and find a parameter space in which the bath qubit will prove a resource. Extending this work for few-qubit algorithms should aid designs of small-scale registers with a quantum advantage.
5:06PM P28.00014: Nanoscale mechanical sensing at ambient conditions*  CHUFENG LIU (Presenter), KANGWEI XIA, WENG HANG LEONG, ZHIYUAN YANG, QUAN LI, REN-BAO LIU, Physics, The Chinese University of Hong Kong — Negative charge nitrogen vacancy center in diamond (NV center) has attracted huge interest due to its unique spin properties even at room temperature. Its spin state could be optically addressed, manipulated and readout with excellent photo stability. Meanwhile, NV center is sensitive to many parameters, such as magnetic field, strain, and temperature, which opens up many applications ranging from magnetometry, temperature sensing to nanoscale NMR spectroscopy. In this talk we will discuss the application of diamond NV centers in nanoscale mechanical sensing at ambient conditions.

*This work was supported by RGC/CRF C4006-17G and CUHK group research scheme

5:18PM P28.00015: Nanoscale mechanical sensing in aqueous solutions* KANGWEI XIA (Presenter), CHUFENG LIU, WENG HANG LEONG, MAN-HIN KWOK, REN-BAO LIU, QUAN LI, Department of Physics, The Chinese University of Hong Kong — Negatively charged NV- center is optically active, and photo-stable. It shows unique properties that the electron and nuclear spins of NV centers can be optically initialized, coherently manipulated and optically readout in ambient conditions. Meanwhile NV centers are also sensitivity to the surrounding environments. The varying of the local magnetic field, electric field, temperature and strain will affect the performance of the NV centers. Thus, they can be explored as magnetic, electric, temperature and strain sensor in extreme precision with nanometer spatial resolution, with many applications ranging from magnetometry, temperature sensing to nanoscale NMR spectroscopy. In this talk we will discuss the application of diamond NV centers in nanoscale mechanical sensing in aqueous solutions.

*This work was supported by RGC/CRF C4006-17G and CUHK group research scheme.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P29 DQI: Semiconducting QC Architectures and Quantum Photonics BCEC 162A - Samuel Carter, United States Naval Research Laboratory - Tag(s): Focus

2:30PM P29.00001: Full 300mm fin based QD device characterization HUBERT C GEORGE (Presenter), NICOLE THOMAS, RAVI PILLARISETTY, LESTER LAMPERT, THOMAS WATSON, JEANETTE MARIE ROBERTS, STEPHANIE BOJARSKI, PAYAM AMIN, JESSICA TORRES, MATTHEW METZ, Components Research, Intel Corporation, GUOJI ZHENG, ANNE-MARIJE ZWERVER, JELMER BOTER, JUAN PABLO DEHOLLAIN, GERTJAN EENINK, LEONARDO MASSA, DIEGO SABBAGH, NODAR SAMKHARADZE, CHRISTIAN VOLK, BRIAN PAQUELET WÜTZ, MENNO VELDHORST, GIORDANO SCAPPUCI, LIEVEN VANDERSYPEN, QuTech and Kavli Institute of Nanoscience, TU Delft, JIM CLARKE, Components Research, Intel Corporation — Intel's efforts towards the fabrication of spin qubit devices have required a comprehensive device characterization, from transistors and quantum dots, to qubits, which have been co-fabricated in the same die/wafer. In this talk, we will present an in-depth device characterization, and the results from quantum dot devices manufactured in a full 300mm line. We will give details of the fin based process flow which yields high charging energy devices. The extraction of QD related figures of merit from room and low temperature testing (1.6K) are part of the method to rapidly screen 300mm wafers with thousands of devices which are used to determine the spin qubit devices that will be taken to the milli-kelvin measurements; keeping up with the pace of the 300mm fab output.

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2:42PM P29.00002: Simulating Nagaoka Ferromagnetism in a 2×2 Quantum Dot Array
UDITENDU MUKHOPADHYAY (Presenter), JUAN PABLO DEHOLLAIN, VINCENT P. MICHAL, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, CHRISTIAN REICHL, WERNER WEGSCHEIDER, Solid State Physics Laboratory, ETH Zurich, BERNHARD WUNSCH, Department of Physics, Harvard University, MARK RUDNER, Niels Bohr International Academy, University of Copenhagen, EUGENE DEMLER, Department of Physics, Harvard University, LIEVEN VANDERSYPEN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — The Fermi-Hubbard model provides a description of interacting electrons in a lattice. The interaction between electrons in arrays of electrostatically defined quantum dots is naturally described by a Fermi-Hubbard Hamiltonian; moreover, the high-degree of tunability in these systems make them a perfect platform to explore different regimes of the Hubbard model through analogue quantum simulations1.

Last year we established a 2x2 gate-defined quantum dot array as a promising solid-state analogue quantum simulator2. Here we present results on simulation of Nagaoka Ferromagnetism in this system. We experimentally observe a ferromagnetic ground state in an almost-half-filled lattice, as predicted3. We use the high-levels of control in our system to manipulate the Hamiltonian parameters and perform measurements that test the validity of our observations. For example, breaking the periodic boundary condition gets rid of the ferromagnetic ground state altogether. To our knowledge, this is the first experimental verification of Nagaoka's prediction as well as the first simulation of magnetism using quantum dot arrays.


2:54PM P29.00003: Coherent control of individual electron spins in a two-dimensional array of tunnel coupled quantum dots* 
[Invited] TRISTAN MEUNIER (Presenter), CNRS Institut Néel — Controlling nanocircuits at the single electron spin level in quantum dot arrays is at the heart of any scalable spin-based quantum information platform. The cumulated efforts to finely control individual electron spins in linear arrays of tunnel coupled quantum dots have permitted the recent coherent control of multi-electron spins and the realization of quantum simulators. However, the two-dimensional scaling of such control is a crucial requirement for simulating complex quantum matter and for efficient quantum information processing, and remains up to now a challenge.

Here we demonstrate such two-dimensional coherent control using individual electron spins in arrays up to 9 tunnel-coupled lateral quantum dots. Two-electron spin initialization, spin readout and spin transfer enable exploration of the spin dynamics in the QDs array. We demonstrate a procedure that permits local enhancement of the tunnel coupling between two dots of the array up to a range where coherent exchange oscillations, the basis of the two-qubit gates for electron spin qubits, are observed. Taking advantage of the tunability of the structure, we finally realize complex and multi-directional displacements of one and two electrons through quantum dot arrays. This work demonstrates key quantum functionalities, crucial for using two-dimensional quantum dot arrays for quantum simulation and computation.


*We acknowledge funding support from the National Science Foundation and the Army Research Laboratory Center for Distributed Quantum Information.

3:30PM P29.00004: A large-scale single-photon source and spin qubit arrays in a photonic integrated chip* NOEL WAN (Presenter), TSUNG-JU LU, KEVIN CHEN, MATTHEW TRUSHEIM, LORENZO DE SANTIS, MICHAEL WALSH, ERIC BERSIN, SARA MOURADIAN, Massachusetts Institute of Technology, EDWARD S BIELEJEC, Sandia National Laboratories, DIRK R. ENGLUND, Massachusetts Institute of Technology — Single-photon sources are essential components in a variety of optical quantum technologies. We demonstrate a large array of single-photon sources and spin qubits on a single photonic chip. Our single-photon source array is composed of color centers in a monolithic diamond nanophotonic structure that is efficiently coupled to a photonic integrated circuit. Additionally, the long-lived spin states of color centers in diamond may serve as quantum memories in a repeater network.

*We acknowledge funding support from the National Science Foundation and the Army Research Laboratory Center for Distributed Quantum Information.
3:42PM P29.00005: On-chip Integrable Spectrally Uniform Ordered Quantum Dot Single Photon Source Array with High Emission Purity (>98.99%) for Scalable Quantum Optical Networks* JIEFEI ZHANG (Presenter), SWARNABHA CHATTARAJ, University of Southern California, SIYUAN LU, IBM Thomas J. Watson Research Center, ANUPAM MADHUKAR, University of Southern California — Towards the goal of building scalable on-chip optical networks we have proposed a new paradigm that integrates an array of mesa top single quantum dot (MTSQD) single photon sources (SPSs) with dielectric light manipulating units (LMUs) [1]. We demonstrated InGaAs/GaAs MTSQDs in 5x8 array [1] showing remarkably improved spectral uniformity than the typically studied self-assembled island QDs but, more importantly, several pairs of MTSQDs exhibit emission wavelengths within 300μeV, the instrument resolution [2]. The measured single photon emission purity was thus limited to 90% at 9K. In this talk we report studies with improved high resolution of ~10μeV demonstrating single photon emission purity > 98.99% (g(2)(0)<0.02) in these MTSQDs at 9.4K. The MTSQD neutral exciton's intrinsic linewidth and fine structure splitting are found to be ~10µeV and <10µeV, respectively. The results highlight the potential of the spatially-ordered MTSQDs-LMU integrated system for realizing quantum optical circuits[3]. Work on examining photon indistinguishability and coherence is underway.


*This work is funded by AFOSR(FA9550-17-01-0353) and ARO(W911NF-15-1-0298).

3:54PM P29.00006: Tuning Photonic Crystal Cavity Resonances with Phase Change Material GeTe* JEROME THOMAS MLACK (Presenter), NRC Research Associate at the Naval Research Laboratory, ALLAN S BRACKER, JOEL Q GRIM, SAMUEL CARTER, U. S. Naval Research Laboratory, MIJIN KIM, KeyW Corporation, CHUL SOO KIM, MICHAEL K YAKES, U. S. Naval Research Laboratory, BUMSU LEE, NRC Research Associate at the Naval Research Laboratory, DANIEL G GAMMON, U. S. Naval Research Laboratory — Photonic crystal slabs are a promising architecture for a variety of computational and sensor architectures including quantum computers and neuromorphic networks. Such devices consist of a 2-D membrane of cavities and waveguides with embedded quantum dots (QDs). While many advances such as demonstrations of indistinguishable single photon sources and quantum entanglement have been shown, such devices are still difficult to scale as a network. The primary limitations are from natural variations during material growth and device fabrication, which cause resonances of the QDs and cavities to span energies much larger than their linewidths. One solution is to use capping layers which can tune the underlying device, changing properties such as strain and effective index of refraction, and whose structural phase can be locally altered using laser annealing, potentially allowing for local tuning of QDs or cavities. We show results of using thin films of such a phase change material, GeTe, to tune cavity resonances independent of local QDs in such devices. This tuning is dependent on the original resonance energy of the cavity and the amount of material deposited.

*JTM and BL are funded via the NRC Research Associate program. This project was funded via the Office of Naval Research.

4:06PM P29.00007: Integrated Quantum Networks of Mie-resonance based All-Dielectric Optical Circuits with Single Photon Sources for Quantum Entanglement* SWARNABHA CHATTARAJ (Presenter), Ming Hsieh Department of Electrical Engineering, University of Southern California, JIEFEI ZHANG, Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, SIYUAN LU, IBM Thomas J. Watson Research Center, Yorktown Heights, ANUPAM MADHUKAR, Mork Family Department of Chemical Engineering and Materials Science, University of Southern California — Recently we introduced [1] a new approach to on-chip optical circuits based on subwavelength scale dielectric building blocks (DBBs) metastructures integrated with single photon sources (SPSs) such as the mesa-top single quantum dot (MTSQD) ordered array [1] in which a single collective Mie resonance of the DBB metastructure provides all needed five light manipulating functions [2]: (1) SPS emission rate enhancement, (2) emission directionality, (3) wave-guiding (4) beam-splitting and (4) beam-combining. The simulations reported were for spherical DBBs as it enables analytical calculations [1]. The lithographic fabrication of such structures will have rectangular DBBs and thus in this talk we present the design and simulation of networks of rectangular DBBs, co-designed for monolithic integration with GaAs/InGaAs MTSQD SPS arrays such that every MTSQD is coupled to the same single collective mode of the network. Finite element based simulation results for such networks with coupled SPSs will be presented that suggest quantum effects such as path-entanglement and super-radiance- constituting a step towards quantum information processing.


*This work is funded by ARO, Grant#W911NF-15-1-0298.
4:18PM P29.00008: Optical locking of a quantum dot electron spin qubit  JONATHAN BODEY (Presenter), CLAIRE LE GALL, ROBERT STOCKILL, DORIAN GANLOFF, GABRIEL ETHERI-MAJCHER, METE ATATURE, University of Cambridge — InGaAs quantum dots (QDs) can function as solid state quantum network nodes, offering a field-leading interface between a single spin and an optical mode [1]. Exploiting this interface requires complete control of a QD spin, to tailor spin-photon entanglement in such a network. Whilst the rotations offered by the current state of the art are highly coherent [2], full SU(2) control relies on varying delays between sequential pulses, limiting the scheme to simple few-gate sequences. Spectral splitting of a laser into two sidebands through modulation allows us to resonantly address a Raman transition between the two ground states of a spin in our QD. This all-optical scheme gives direct access to the phase and frequency of the field linking our states, releasing us from the need for well-defined sequence delays. We use Rabi oscillations and Ramsey interferometry to demonstrate complete control of our Rabi vector. This enables us to perform spin-locking, protecting our qubit state for longer than the homogeneous dephasing time and allowing high-fidelity gates on this timescale. Our work represents versatile spin control and provides a way towards on-chip all-optical spin manipulation.


4:30PM P29.00009: 4H-SiC-on-Insulator Platform for Quantum Photonics with Color Centers*  DANIIL LUKIN (Presenter), CONSTANTIN DORY, MARINA RADULASKI, SHUO SUN, DRIES VERCRUYSSE, JELENA VUCKOVIC, Stanford University — Defects in Silicon Carbide (SiC) are considered for quantum photonics applications because of their favorable spin coherence properties and optical emission wavelengths. To aid integration of these defects into nanophotonic structures, we develop a 4H-SiC-on-insulator platform based on bonding and thinning techniques. The process results in 4H-SiC films of pristine crystal quality with no radiative defects in the 800 - 1000 nm wavelength range. Color centers are readily introduced via irradiation. We demonstrate 4H-SiC ring resonators and photonic crystal cavities with Q ~ 10^4

*Air Force Office of Scientific Research (AFOSR) MURI Center for Attojoule Nano-Optoelectronics (FA9550-17-1-0002); DARPA EXTREME Program, Grant number HR0011171007

4:42PM P29.00010: Scalable frequency locking of single photon sources for quantum photonic technologies*  JACQUES CAROLAN (Presenter), UTTARA CHAKRABORTY, Research Laboratory of Electronics, Massachusetts Institute of Technology, NICHOLAS C HARRIS, Lightmatter, MIHIR PANT, Research Laboratory of Electronics, Massachusetts Institute of Technology, TOM BAEHR-JONES, MICHAEL HOCHBERG, Elenion Technologies, DIRK R. ENGLUND, Research Laboratory of Electronics, Massachusetts Institute of Technology — Large-scale quantum technologies require exquisite control over many individual quantum systems. Typically, such systems are very sensitive to environmental fluctuations, and diagnosing errors via measurements causes unavoidable perturbations. Here we present an in situ frequency locking technique that monitors and corrects frequency variations in single photon sources based on microring resonators. By using the same classical laser fields required for photon generation as a probe to diagnose variations in the resonator frequency, our protocol applies feedback control to correct photon frequency errors in parallel to the optical quantum computation without disturbing the physical qubit. We implement our technique on a silicon photonic device and demonstrate feedback controlled quantum state engineering. Our approach enables frequency locking of many single photon sources for large-scale photonic quantum technologies.

*Supported by the AFOSR MURI for Optimal Measurements for Scalable Quantum Technologies (FA9550-14-1-0052) and by the AFOSR program FA9550-16-1-0391, supervised by Gernot Pomrenke. J.C. is supported by EU H2020 Marie Sklodowska-Curie grant number 751016. U.C. is supported by the National Defense Science and Engineering Graduate Fellowship.
Event-ready entangled photons from a solid-state single-photon source. MARCELO DE ALMEIDA (Presenter), NOR AZWA ZAKARIA, ARC Centre of Excellence for Engineered Quantum Systems, The University of Queensland, Brisbane, Australia., JUAN CARLOS LOREDO, Centre de Nanosciences et de Nanotechnologies, CNRS, Univ. Paris-Sud, Univ. Paris-Saclay, Marcoussis, France., LEONARDO ASSIS, JIHUN CHA, ARC Centre of Excellence for Engineered Quantum Systems, The University of Queensland, Brisbane, Australia. — Solid-state emitters, such as semiconductor quantum dots, are a promising platform to develop single-photon sources. Recent breakthroughs in material syntheses and fabrication processes led to a new generation of devices, combining high emission brightness with near unity indistinguishable pure single-photon output [1]. These new generation single-photos sources are staring to enable experiments with multiple indistinguishable photons [2], a key step towards large-scale optical quantum technologies.

Here we employ a quantum dot source to demonstrate a 4-qubit Type-II Fusion Entangling Gate [4]. The Type-II Fusion Gate relies on the conditional detection of two ancillary qubits to generate entanglement between the two remaining qubits. We study the performance of this entangling gate as a function of the single-photon indistinguishability. We also discuss potential applications for the Type-II fusion gate as an event-ready source entangled photons.


Lithium Niobate as a Wide Bandgap Quantum Photonics Platform* IAN CHRISTEN (Presenter), Electrical Engineering and Computer Science, Massachusetts Institute of Technology, MICHAEL MILLER, KENNETH DOUGLAS, MATT EICHENFIELD, Sandia National Laboratories, DIRK R. ENGLUND, Electrical Engineering and Computer Science, Massachusetts Institute of Technology — A robust and active photonics platform is essential for scalably-engineered photon-mediated quantum interactions. Such a platform must have sufficiently wide bandgap, as atom-like quantum systems emit dominantly into the visible spectrum. Lithium niobate is a compelling material platform satisfying these requirements: being transparent down to the UV and having a strong electrooptic nonlinearity. We examine the performance—in particular, the achievable propagation loss and the effect of photo refractive damage—of x-cut and magnesium-doped lithium niobate nanophotonic waveguides across and beyond the visible spectrum. We explore the modulation of light at wavelengths of relevance for a wide range of leading quantum memories including, in particular, diamond color centers, cold atoms, and quantum dots.

*Work funded by NSF awards EFMA-1641064, DMR-1231319, and DMR-1747426.

Optimized Quantum Photonics in Diamond* CONSTANTIN DORY (Presenter), DRIES VERCRUYSSE, KYOUL YANG, NEIL V. SAPRA, ALISON RUGAR, SHUO SUN, DANIIL LUKIN, ALEXANDER Y. PIGGOTT, JINGYUAN LINDA ZHANG, MARINA RADULASKI, KONSTANTINOS LAGOUTHAKIS, JELENA VUCKOVIC, Stanford University — Diamond hosts a variety of quantum emitters and is thus a promising material platform for applications in quantum information processing and quantum sensing. Such quantum technologies will likely operate at the level of single or few photons. Therefore, they require highly efficient integrated photonic circuits to harness the full potential of the excellent optical properties of color centers in diamond. However, state-of-the-art design and fabrication techniques for diamond devices in quantum optics strongly limit the geometry and variety of the device components. We utilize inverse design optimization and fabrication methods based on quasi-isotropic etching to significantly improve on efficiency, scalability, and functionality of diamond photonics. To showcase the significance of these advances, we solve outstanding design challenges, such as optical free space interfaces and improve on efficiency and scalability of diamond photonics.

*Army Research Office (ARO) (W911NF1310309); Air Force Office of Scientific Research (AFOSR) MURI Center for Attojoule Nano-Optoelectronics (FA9550-17-1-0002); Gordon and Betty Moore Foundation; Andreas Bechtolsheim Stanford Graduate Fellowship

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P30 DPOLY: Polymer Networks, Gels, and Elastomers III: Architecture BCEC 162B - Ross Behling, 3M Corp. - Tag(s): Focus
2:30PM P30.00001: Relationship between optical properties and network topology in gels crosslinked using controlled radical polymerization*  MAHATI CHINTAPALLI (Presenter), STEPHEN MECKLER, GABRIEL IFTIME, JESSY B. RIVEST, PARC — Controlled radical polymerization can be used to prepare crosslinked polymer gels and aerogels with a variety of unique features: tunable optical transparency, high specific surface area, controlled pore size, and narrow pore size distribution. Such materials enable a range of applications in size- and interaction-selective separations, catalysis and photocatalysis, and thermally insulating materials. We demonstrate that controlled radical polymerization can be used to control network topology, which directly impacts the optical properties and pore structure of crosslinked polymer gels. Two novel methods to control the degree of “livingness” in the gelation reaction are reported. The degree of livingness in the gelation was used to tune the visible light transmittance of a 3 mm gel from 0 % to >70 %. Porous aerogels can be produced from the solvated gels by solvent evaporation at ambient pressure and temperature. Controlled radical gelation led to aerogels with porosities over 60 % and Brunauer Emmett Teller surface areas over 1000 m²/g.

*This work is funded by the ARPA-E SHIELD program, award # DE-AR0000734.

2:42PM P30.00002: Mechanical and Thermal Performance of Interpenetrating versus Single Networks of Dynamically Crosslinked Polymers*  MEHDI ZANJANI (Presenter), BALLAL AHAMMED, Mechanical and Manufacturing Engineering, Miami University, BORUI ZHANG, DOMINIK KONKOLEWICZ, Chemistry and Biochemistry, Miami University, ZHIJIANG YE, Mechanical and Manufacturing Engineering, Miami University — Dynamically crosslinked polymer composites have received great attention in the past decade due to their unique properties such as self-healing, malleability, and shape memory. Dynamic crosslinkers of two main types, i.e. non-covalently bound crosslinkers and dynamic covalently bound crosslinkers, provide a versatile platform to engineer various types of crosslinked networks with desired properties.

Here, we report a combined computational and experimental study of two main categories of self-healing polymer composites: Interpenetrating Networks (IPNs) and Single Networks (SNs). We establish detailed models of the polymer networks by implementing a coarse-grained scheme: IPNs are modeled based on allowing one type of crosslinker per polymer chain, while SNs are modeled through random positioning of both types of crosslinkers along polymer chains. We then perform Non-equilibrium Molecular Dynamics simulations to evaluate mechanical and thermal properties of various IPN and SN systems. Our predictive models and experiments show that, in general, IPNs outperform SNs in terms of their mechanical and thermal properties provided that the overall crosslinker densities are the same within the two network types.

*We acknowledge support from NSF (DMR 1749730) and the OSC (Award PMIU0139).

2:54PM P30.00003: Influence of weak ionic associations on the mechanical properties of hydrogels crosslinked by hydrophobic associations*  BRYAN VOGT (Presenter), CHAO WANG, ROBERT A WEISS, KATHERINE DEITRICK, The University of Akron — Since the initial reports of double network hydrogels, a variety of routes to provide energy dissipation in hydrogels have been reported such as the inclusion of physical crosslinks to provide reversible crosslinks. These hydrogels based on physical crosslinks tend to creep due to the reversibility. Inclusion of a second stronger network generally has been used to reduce creep and improve the elastic recovery. Here we take the opposite approach and include weak ionic associations (zinc diacrylate) to manipulate the mechanical behavior of hydrogels formed by hydration of copolymers of hydroxyethyl acrylate (HEA) and 2-(N-ethylperfluorooctane-sulfonamido)ethyl methacrylate (FOSM). The terpolymer-based hydrogel contained >85% of the water of a HEA-FOSM copolymer hydrogel with the same FOSM content, but the storage modulus was nearly an order of magnitude larger for the terpolymer hydrogel. To obtain the same storage modulus, the FOSM content would need to be more than doubled, but this HEA-FOSM copolymer-based hydrogel has almost 40 % less water than the terpolymer hydrogel. These results illustrate the ability to tune the mechanical response of hydrogels through weak ionic associations.

*This work was supported by NSF-DMR 1659531 and NSF-CBET 1606685
This talk will highlight two distinct reversible covalent crosslinking mechanisms, namely the reversible addition and reversible exchange mechanisms, leading to distinctly different mechanical responses. The incorporation of reversible addition crosslinks into the network, such as a Diels–Alder (DA) reaction, enables one to explore the properties related to conversion, such percolation near the gel point. Furthermore, external triggering of reversible gelation in a DA–ferromagnetic nanoparticle polymer composite is demonstrated using an AC field. The incorporation of reversible exchange moieties, such as an allyl sulfide, enables light-triggered network connectivity shuffling. Additional functionality within the network provides a mechanism for photo-directed materials strengthening, exhibiting a local increase in the modulus and also enabling simultaneous healing in fractured materials. Finally, the shape of the elastomer can be manipulated and locked into place via irradiation, providing a route to engineer wrinkled topography for lens and sensors to surface functionalization for coatings.

This gel consists of collapsed PS endblock aggregates acting as crosslinks, while PI midblocks bridge those aggregates. The gel architecture, as captured by the small angle x-ray scattering, is tuned by varying the polymer volume fraction and midblock length. Tensile experiments reveal a rate dependent mechanical properties, particularly for the samples with entangled midblocks. Energy release rate (G) for fracture scales linearly with the crack-tip velocity (v) indicating a velocity toughening effect in these gels. The G-v relationship strongly depends on the polymer concentration and chain length. These gels fail as a result of endblocks pullout from aggregates. The pullout process involves an entropic penalty associated with the midblock stretching, friction with other endblocks in aggregates, and an enthalpic penalty associated with pulling the endblocks in the non-favorable solvent. We attempt to incorporate all these factors in estimating G and compare that with the experimental values.

*NSF-CAREER (DMR-1352572)

### 3:54PM P30.00006: Modelling of chemo-mechanical coupling in polymer gels via nonlinear finite element method

PRIYANKA NEMANI (Presenter), Department of Chemical Engineering, Indian Institute of Technology Gandhinagar, RAVI SASTRI AYYAGARI, Department of Mechanical Engineering, Indian Institute of Technology Gandhinagar, PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Design of multifunctional biomimetic materials that exhibit large amplitude actuation through chemical triggers has been a challenge in the field of smart materials. Polymer gels that utilize self-oscillating Belousov Zhabotinsky (BZ) reactions are pioneers among smart materials due to their biomimetic characteristic of chemo-mechanical transductions. Here, we present a computational framework to simulate the dynamics of self-oscillating polymer gels that undergo large deformations under isothermal conditions. Unlike earlier approaches, we harness a complete nonlinear finite element framework that combines the reaction-diffusion phenomena occurring in BZ reaction, with elastic deformations of the polymer gel. Specifically, we use three variable Oregonator model to incorporate reaction kinetics, non-Gaussian mechanical theory for elastic deformations and Flory-Huggins theory to couple the chemical kinetics with the deformation. We demonstrate that actuation capacity of self-oscillating polymer gels can be amplified and controlled by manipulating the reaction kinetics under specific conditions. We believe that our approach brings in a new perspective to design complex bio-inspired systems and provides the necessary framework to control their behaviour.

*DST-SERB (EMR/2016/007778)
4:06PM P30.00007: Expanding Gelation Conditions in Dynamically Crosslinked Networks* SETH CAZZELL (Presenter), NIELS HOLten-ANDerSEN, Massachusetts Institute of Technology — Polymer networks with dynamic physical crosslinks have generate widespread interest as tunable and responsive viscoelastic materials. A subclass of these materials containing multi-component, or complimentary, crosslinks, such as host-guest interactions and metal-coordination, are limited by their ability to percolate under stoichiometric imbalances of their crosslink components. Here we present a method to relax this stoichiometric requirement through the use of a third component, a dynamic, free competitor. This approach to expand the conditions that result in gelation is demonstrated experimentally with metal-coordinated hydrogels, and simulations are used to show the thermodynamic criteria that are necessary to expand the previously understood tight stoichiometric tolerance for gelation. This work can then be generally applied to advance engineering of the broadening class of polymer materials with dynamic crosslinks.

*This work was supported primarily by the MRSEC Program of the National Science Foundation under award number DMR 14-19807.

4:18PM P30.00008: Melt Blown Cross-linked Fibers from Thermally Reversible Diels-Alder Polymer Networks* KAILONG JIN (Presenter), SUNG-SOO KIM, JUN XU, FRANK BATES, CHRISTOPHER ELLISON, Chemical Engineering and Materials Science, University of Minnesota — Melt blowing is a process in which liquid polymer is extruded through orifices and then drawn by hot air jets to produce nonwoven fibers. Melt blown nonwovens constitute more than 10% of the $50 billion global nonwovens market. Thermoplastic feedstock, such as polyethylene, polypropylene, and poly(butylene terephthalate), have dominated melt blown nonwovens because of their combined cost, good chemical resistance and high-temperature performance. Cross-linked nonwovens from other commodity polymers (e.g., (meth)acrylates, styrenics, silicones, etc.) could be attractive alternatives; however, no commercial cross-linked nonwovens currently exist. Here, cross-linked fibers were produced via one-step melt blowing of thermoreversible Diels-Alder polymer networks comprised of furan- and maleimide-functional methacrylate-based polymer backbones. These dynamic networks decross-link and flow like viscous liquids under melt blowing conditions, then revert to a network via cooling-induced cross-linking during/after melt blowing. Finally, the resulting cross-linked fibers can be recycled because of their reversible dynamic nature, which may help address the microfiber pollution problem.

*The authors thank Cummins Filtration for financial support.

4:30PM P30.00009: Carefully Controlled Photo-catalyzed Thiol-ene Networks of Poly(lactic acid)* NICHOLAS BAKSH (Presenter), Mechanical Engineering, University of South Florida, RYAN TOOMEY, Chemical Engineering, University of South Florida, NATHAN GALLANT, Mechanical Engineering, University of South Florida — PLA is researched for TE scaffolds, drug delivery, implants, and environmentally safe plastics. Bulk PLA has a tensile and flexural modulus of 3.5 and 6 GPa respectively and a Rockwell hardness of 88; thus despite bioabsorbable advantages, it is weak compared to metal implants. Additionally, a uniform degradation rate, which needs to be tuned to match tissue growth and regulate drug delivery, requires minimal molecular variability. Crosslinkable PLA would not only improve mechanical properties, but offer tunability via crosslink density. Further, catalysis by cell safe light and orthogonality of crosslinkable groups allow in-vivo crosslinking, minimizing implant procedures. Bis alpha, omega –ene functionalized PLA oligomers for use with thiolene chemistry were synthesized with polydispersities around 1.3 using organic catalysts. Ordered networks were photo-catalyzed with a multi-arm thiol. End functionalities allow crosslink density to be controlled by oligomer length, and the ordered network minimizes molecular variability. Crosslinked samples prepared with the same oligomer consistently show identical characterizations as analyzed by DSC, NMR, FTIR, and nano-indentation. Lastly, stress-strain curves exhibited a singular linear elastic regime.

*NSF CMMI - 1538727

4:42PM P30.00010: Characterizing Network Structure and Protein Separation in Lignin-Based Hydrogel Composites NICHOLAS GREGORICH (Presenter), JUNHUAN DING, MARK C THIES, ERIC DAVIS, Clemson University — Lignin-based hydrogels have recently garnered attention for use in a variety of biological applications involving proteins such as protein separation and delivery as lignin is a sustainable, naturally abundant biopolymer. However, to date, the use of these materials in protein related applications has been hindered by our limited understanding of how the addition of lignin, both as a crosslinker and ‘passive’ filler, affects the network (pore) structure of the crosslinked hydrogel. In this study, lignin-poly(vinyl alcohol) composites were synthesized using lignin of controlled, narrow molecular weights (MWs), allowing for the fabrication of membranes with more homogeneous network structures. The permeability of different proteins through the hydrated composites was measured via ultraviolet-visible spectroscopy, where protein permeability was found to depend on the MW and end group functionality of the lignin. In addition, poroelastic relaxation indentation was used to characterize both the mechanical (elastic modulus) and transport properties (diffusivity, effective pore size) of the composites. Results from this study illustrate how the incorporation of well-defined lignin into hydrogel composites can be used to directly tune the properties of the resultant membrane.
Modeling reconstituted silk fibroin gels during deformation

PETER OLMSTED, PEIRAN JIN (Presenter), Georgetown University — Silk from silkworms has been used in the textile industry for thousands of years. It consists of β-sheet structures formed from hydrophobic domains in the protein fibroin. Recently, a physical electrogel (e-gel) was made by reconstituting Bombyx mori silk into stable aqueous solutions and then applying small DC electric field [Tabatabai et al, Soft Matter 11 (2015) 756]. The e-gels exhibit distinctive strain hardening and are partially recoverable from strain.

We build a coarse-grained model of fibroin protein polymers, which comprise crystallizable domains and amorphous domains. To study the structural changes and nonlinear behavior of the gel during deformation, gels are tested by shearing, oscillating and stretching. We find that the kinetics of unfolding and refolding of crystallizable domains changes the number and functionality of crosslinks in the physical network, and thus causes the strain hardening of the gel and the non-recoverable strain. This model can also be useful in other associating polymer systems.

Overcoming the Achilles' Heel of Dynamic Vitrimer Networks: Modification and Application of Flory-Stockmayer Theory to Minimize Creep

LINGQIAO LI (Presenter), JOHN TORKELSON, Northwestern University — Vitrimers are a promising class of dynamic polymer networks, but they have an Achilles' heel: above Tg, vitrimers exhibit significant creep under conditions where permanently cross-linked networks exhibit little or no creep. Vitrimers can be designed with strongly suppressed creep and excellent reprocessability by incorporating a subcritical fraction of permanent cross-links. This fraction of permanent cross-links, which has little or no effect on reprocessability, is defined by the gelation point of only permanent cross-links leading to a percolated permanent network. Modifying Flory–Stockmayer theory, we developed a simple theory that predicts an approximate limiting fraction. To test our theory, we designed vitrimers with controlled fractions of permanent cross-links. Our experiments support our theoretical prediction: when the fraction of permanent cross-links is subcritical, the vitrimer can be reprocessed with full recovery of cross-link density. In particular, with a predicted limiting fraction of 50 mol %, a vitrimer system designed with 40 mol % permanent cross-links achieved full property recovery associated with cross-link density after reprocessing and ~70% creep reduction relative to a similar vitrimer without permanent cross-links.

Defects as a Highway to Stress Relaxation of Vitrimers

SIMONE CIARELLA (Presenter), Eindhoven University of Technology, FRANCESCO SCIORTINO, Sapienza Universita’ di Roma, WOUTER ELLENBROEK, Eindhoven University of Technology — Vitrimers are a promising class of plastics made by disordered networks of polymers. They are an ideal recyclable material being both strong and malleable, because unlike common plastics, vitrimers can swap their bonds without breaking. The swap mechanism also grants them exceptionally versatile properties ranging from self-healing to responsiveness to chemical and physical stimuli. Understanding how the mechanics of vitrimers follow from such bond-swap dynamics is a key physical question that we address using a new coarse-grained MD model which captures the essence of the bond dynamics while being insensitive to other chemical details. Our results reveal a dramatic dependence of their malleability on the number of polymer chains that loop back onto themselves. This highlights the importance of choosing the right building blocks for these new materials, as choices concerning polymer architecture have immediate implications for the number of such loops. Our work thus provides new guidelines for designing and developing these remarkable plastics. [1] Ciarella et al., PRL 2018.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P31 DCP: Advances in Hierarchical Systems: Theory and Experiments II BCEC 203 -
Neeraj Rai, Mississippi State University; Dongxia Liu, University of Maryland - Tag(s): Invited
2:30PM P31.00001: Nanosized zeolites: targets and challenges* [Invited] SVETLANA MINTOVA (Presenter), CNRS, ENSICAEN, Normandy University, Laboratory of Catalysis and Spectrochemistry — This presentation will highlight recent developments in the synthesis and unconventional applications of nanosized zeolites. The factors controlling the formation of nanosized zeolites underlining the most promising approaches from the viewpoint of large-scale production will be discussed. The strategies available for the preparation of nanosized zeolites including organic-template assisted, organic-template free, and seed approach will be presented. A special attention will be paid to zeolite formation in conventional organic-template-free zeolite yielding systems. Additionally the preparation of defect free zeolites using a “soft” chemistry approach will be discussed.

Finally, the advantages and limitations of the synthesis methods for nanosized zeolites and their utilization in existing and advanced applications will be addressed. The newest developments in the preparation of nanosized zeolites (either free of organic template or free of defects), supported zeolite films/layers, and self-assembled structures for optical and medical applications will be revealed.

*The Region of Normandy, France and the Thousand-talent program, CUP-Qingdao, China for the financial support are gratefully acknowledged.

3:06PM P31.00002: Characterization of silanol defect sites on amorphous versus crystalline 2-D silicate surfaces* [Invited] NICOLAS GROSSO GROSSO-GIORDANO, Chem and Biomol Eng, UC Berkeley, CHRISTIAN SCHROEDER, Institut für Physikalische Chemie, Universität Münster, ALEXANDER OKRUT, Chem and Biomol Eng, UC Berkeley, HUBERT KOLLER, Institut für Physikalische Chemie, Universität Münster, STACEY I. ZONES, Chevron Energy Technology Company, ALEXANDER KATZ (Presenter), Chem and Biomol Eng, UC Berkeley — We compare and contrast the nature of silanols on open, two-dimensional surfaces comprising amorphous and crystalline siliceous materials. We compare the thermal treatment of silanols in both sets of materials, using several forms of spectroscopy for characterization. The ramifications of the observed differences on applications will be highlighted.


3:42PM P31.00003: Synthesis and Catalytic Performance of Hierarchical Materials Derived from Metal-Organic Frameworks* [Invited] JASON HICKS (Presenter), Chemical & Biomolecular Engineering, University of Notre Dame — Hierarchical materials have many benefits in catalytic applications. We have been specifically interested in the synthesis of hierarchical materials for a variety of energy-related applications including biomass fast pyrolysis, coupling of aldehydes and/or ketones from biomass feed streams, and sulfur removal from petroleum feed sources.1-4 This presentation will provide our current progress in the following areas: 1) synthesis and characterization of hierarchical metal-organic framework (MOF) materials, and 2) metal nanoparticles supported on hierarchical carbon supports derived from MOFs. I will discuss a vapor-assisted crystallization method developed in our lab using zeolite synthesis literature as inspiration, where a dry gel is initially formed that promotes MOF crystallization and the formation of hierarchical materials. The detailed characterization of these novel materials will be discussed, as well as their catalytic performance.


*Acknowledgement is made to the donors of the American Chemical Society Petroleum Research Fund for support of this research (PRF# 53874-DNI10). We also thank the ND Energy Materials Characterization Facility and the Notre Dame Integrated Imaging Facility.
Hierarchical zeolites are advanced materials possessing the catalytic and adsorption properties of conventional zeolites while potentially eliminating their transport limitations through the introduction of mesopores. Recent experiments comparing the adsorption and transport in hierarchical self-pillared pentasil (SPP) zeolites (SPP) to microporous silicalite-1 (MFI) revealed an interesting crossover in sorbate loading and significantly slower than expected diffusion for alkanes, but explanation for these observations are not readily available through experimental probes due to the complications arising from the presence of multiple adsorption sites and blocked pore entrances. In this talk, we will present results from Gibbs ensemble Monte Carlo and canonical ensemble molecular dynamics simulations to unravel the peculiar properties of SPP zeolites. Computed isotherms for argon, hydrogen, alkanes, ethanol, and water demonstrate striking differences in the adsorption behavior for these adsorbates. Depending on the loading, diffusion can proceed via the micropores, on the mesopore walls, or through the mesopore interior.

*This work was primarily supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences through the Nanoporous Materials Genome Center under award numbers DE-FG02-12ER16362 and DE-FG02-17ER16362. The work used computational resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357. Additional computer resources were provided by the Minnesota Supercomputing Institute.

Hierarchical zeolites and zeolite nanocrystals with micropore lengths on the order of nanometers have been synthesized with the aim of reducing mass transfer limitation. However, due to the large external surface to volume ratios, the mass transport in these materials can be hindered by a secondary rate limitation step imposed on the external surface of the zeolites. In this talk, I will present our recent study on the mass transport in hierarchical zeolites and zeolite nanoparticles. We show that surface barrier is related to the presence of pore re-entry caused by strong sorbate/sorbent interaction at the zeolite surface. In order to understand the nature of the surface barrier, a set of silica nanoparticle (SNP)/Silicalite-1 composites with different external surface to micropore surface ratios was synthesized. It was found that the strong sorbate/sorbent interaction at the external surface of Silicalite-1 nanoparticles can cause diffusing molecules to re-enter into micropores and repeat the micropore diffusion process. This pore re-entry step can lead to an unusually long micropore diffusion length. We also demonstrate that this repeated micropore diffusion process can be effectively reduced by mixing the zeolite nanoparticles with secondary, nonporous nanoparticles. It was concluded that the surface barrier in hierarchical zeolites and zeolite nanoparticles is likely due to a combination of pore re-entry of adsorbates and pore blockage.

*This work was supported by the Catalysis Center for Energy Innovation, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, and Office of Basic Energy Sciences under award number DE-SC0001004

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P32 DCP: Gas Phase Clusters - Experiment and Theory in Concert (C): Other Clusters (GPC3) BCEC 204A - Knut Asmis, Leipzig University - Tag(s): Focus
2:30PM P32.00001: Finite temperature anharmonic gas phase vibrational spectroscopy with DFT-based MD simulations* [Invited] MARIE-PIERRE GAIGEOT (Presenter), Physics, LAMBE UMR8587, Universite d'Evry val d'Essonne, Universite Paris-Saclay — We will review our works on gas phase vibrational spectroscopy of gas phase molecules and clusters by finite temperature DFT-based molecular dynamics simulations. The anharmonic dynamical spectra have been used in order to make systematic links to the most advanced action spectroscopy experiments.

Our combined theoretical-experimental works on the IR-MPD (Infra Red Multi Photon Dissociation) and IR-PD (Infra Red Pre-Dissociation) action spectroscopies of gas phase molecular ions will be shown, where the importance of conformational dynamics, proton transfers, temperature, potential energy surface and dipolar anharmonicities, entropic effects, high energy conformers, will be emphasized. Our more recent works on the far-IR/THz spectroscopy of gas phase peptides will also be presented in relation with the most advanced IR-UV ion dip experiments probing the 100-800 cm\(^{-1}\) spectral domain. In this spectral range, DFT-MD anharmonic spectroscopy has proved essential into assigning spectral features to 3D structures, with a robustness not reached by other anharmonic theoretical methods. We will emphasize the importance of large amplitude motions and highly flexible H-Bonds into the 100-800 cm\(^{-1}\) signatures, and will show which modes are intrinsically anharmonic vs harmonic. This calls for the development of mixed harmonic/anharmonic methods. Our recent innovative theoretical developments into the calculation of gas phase anharmonic spectra from DFT-MD simulations, going beyond the time-correlation function of dipole moments, will also be presented.

*Collaborative works with Prof. J.M. Lisy USA ; Dr A.M. Rijs The Netherlands ; group of the late Prof J.P. Schermann France ; Works achieved with PhD/Post-Doc students J. Mahé, S. Jaeqx, D. Bakker, D.R. Galimberti, V. Brites, A. Cimas. S. Bougueroua
Works funded by ANR PROBIO, ANR-NSF SPIONCLUS, Excellence Lab LABEX CHAR3MAT, Fédération CPPS Paris Saclay, PICS CNRS France-The Netherlands. GENCI-France for computational time.

3:06PM P32.00002: Deconstructing the curious behavior of carboxylate at the air-water interface with cluster ion spectroscopy* [Invited] MARK JOHNSON (Presenter), Yale Univ — The transport of divalent metal ions (e.g., Mg\(^{2+}\) and Ca\(^{2+}\)) into the troposphere is thought to arise from preferential complexation with the anionic head groups of fatty acids at the surfaces of sea-spray aerosols. Attempts to quantify the formation of these ionic complexes by monitoring the vibrational frequencies of the CO stretching vibrations has proven to be difficult, however, because the ion-driven spectral response is surprisingly similar to that of the hydrated anion. We trace the origin of this effect by studying the stepwise hydration behavior of the isolated carboxylate and contact ion pair in the gas-phase. The results reveal the critical importance of solvent coordination in the structural interpretation of surface-sensitive spectral signatures of ion complexation at the interface. Surprisingly, not only does stepwise hydration of the RCO\(^{-}\) anion and the [Ca\(^{2+}\)-RCO\(^{-}\)]\(^+\) contact ion pair yield solvatochromic responses in opposite directions, but in both cases, the responses of the two (symmetric and asymmetric stretching) CO bands to hydration are opposite to each other. The result is that the two CO bands evolve toward their interfacial asymptotes from opposite directions. Theoretical simulations of the [Ca\(^{2+}\)-RCO\(^{-}\)]\(^+\)\(-(H_{2}O)_{n}\) clusters indicate that the metal ion remains directly bound to the head group in a contact ion pair motif as the asymmetric CO stretch converges at the interfacial value by \(n = 12\). This establishes that direct metal complexation can account for the interfacial behavior.

We discuss these effects in the context of a model that invokes the water network-dependent local electric field along the C-C bond that connects the head group to the tail as the key parameter driving the observed trends.

*NSF CCI CAICE
3:42PM P32.00003: Accurate spectroscopic characterization of molecular complexes as a first step toward the understanding of intermolecular interactions [Invited] CRISTINA PUZARINI (Presenter), Dpt. Chemistry “Giacomo Ciamician”, University of Bologna — Noncovalent interactions play a key role in several biological and technological processes, yet their characterization and interpretation are still far from being satisfactory. Integrated experimental and computational investigations of molecular complexes can play an invaluable role to understand the properties of intermolecular interactions.

In the past decade, many gas-phase spectroscopic investigations have focused on the understanding of the nature of weak interactions in model systems, and a great effort has been devoted – for example – to studies dealing with complexes formed by small biomolecules with either water or other solvents. In this connection, molecular complexes involving hydrogen bonding between nitrogen-containing systems can be considered as prototypes for studying the (N-H...N) interaction in biological systems [1].

Along with the well-established hydrogen bonds, emerging classes of noncovalent interactions are attracting increasing attention, such as those involving a pnictogen or chalcogen atom [2,3] because of the fundamental role they play in different fields such as catalysis, drug design, self-assembly processes, and crystal packing. Understanding the mechanisms at the basis of these technological processes requires the characterization of the directionality, strength, and nature of such interactions as well as a comprehensive analysis of their competition with other noncovalent bonds, also taking into account the tuning of these properties by different environments.


4:18PM P32.00004: A cluster approach to solvation effects in flexible peptides* [Invited] ETIENNE GARAND (Presenter), University of Wisconsin - Madison — Utilizing a method based upon a unique combination of mass spectrometry and laser spectroscopy, our research focuses on capturing and characterizing complexes of interest to provide a molecular-level detailed examination of their structures and interactions. To access microsolvated charged complexes, we have developed new capabilities to perform controlled gas-phase clustering in cryogenic ion trap. This versatile approach enables us to form clusters with >30 solvent molecules surrounding any bare ion obtained by electrospray ionization. The structures of these carefully isolated and prepared complexes are then directly probed in the mass spectrometer using infrared predissociation spectroscopy, yielding well-resolved spectra that contain a wealth of information. Recent studies on the solvation-dependent structures of flexible model peptidic systems, (Gly)nH+ and (Ala)nH+ will be presented. In addition, this talk will highlight two methodologies necessary for deconvoluting the complex vibrational spectra of these species: IR-IR conformer-specific spectroscopy and solvent-specific isotope labeling. This combination of spectroscopic characterizations yields unambiguous spectral assignments and clearly reveals the structural evolution of the flexible peptides in response to increasing solvation. The results also provide insights on the isomerization pathways and energetics involved in these structural changes.

*This research is funded by the Department of Energy under grant DE-SC0018902

4:54PM P32.00005: Observation of H2O and D2O water dimers in CCl4 at room temperature via Matrix Isolation Spectroscopy DOSEOK KIM (Presenter), ADAM H TURNER, SUNG HYUN HUH, SOO RYEON RYU, Sogang University — The vibrational spectrum of a single molecule is typically investigated in the gas phase, however, the spectrum is crowded by combination bands with rotational transitions and not all molecules can be prepared in the gas phase. Room-temperature matrix isolation spectroscopy (MIS) is a tool that utilizes a low solubility of the solute molecule as well as weak interactions between solute and solvent molecules to obtain a spectrum of isolated solute molecules. Water (H2O and D2O) was loaded on top of the nonpolar solvent CCl4, and the in situ inclusion process was monitored in the CCl4 phase by infrared absorption spectroscopy. These in situ spectra showed non-linear deviations from the monomer spectrum over time attributed to formation of water dimers. The water dimer spectrum was extracted from the time-series of the spectra using 2D correlation spectroscopy and principal component analysis (PCA). These dimer peaks from the 2D correlation and PCA analysis compared to those obtained from DFT calculations using the CC-VSCF approximation showed good agreement and allowed the assignment of the dimer modes. Changes from the monomer to the dimer spectra as well as the difference between H2O and D2O dimer spectra were discussed in terms of hydrogen bonding.
5:06PM P32.00006: Exploring molecular formation and growth upon ionization of van der Waals clusters using ab-initio molecular dynamics  TAMAR STEIN (Presenter), Chemistry, Hebrew University of Jerusalem Israel, PARTHA BERA, TIMOTHY J LEE, NASA, MARTIN HEAD-GORDON, University of California, Berkeley — Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in the interstellar medium (ISM)\(^1\). The mechanism for their formation in the low temperature environment of the ISM is, as of yet, nonetheless a mystery. Understanding the mechanism of formation of complex molecules such as PAHs and nitrogen-based PAHs (PAHN) is a long-standing challenge which has been drawing much attention for the past several decades.

Formation of the building blocks of PAHs and PAHNs upon ionization of van der Waals clusters will be presented. Results on small (up to 6 acetylene/HCN units) van der Waals clusters, indicate that, due to the fact that the clusters possess a large amount of extra energy after ionization, a rich chemistry can occur\(^2\). For example, after ionization, structures on the \(\text{C}_6\text{H}_6^+\) potential energy surface (PES) are accessible without barriers. Moreover, the formation of the basic building block of PAHs, namely the benzene cation, has been demonstrated by means of ab-initio molecular dynamic. The presence of spectator molecules has been proven to change the PES as well as to partake a catalytic role in the formation of the benzene cation\(^2\).


5:18PM P32.00007: Investigation of effect of temperature and size on the ionization potential of semiconductor clusters using effective stochastic potential method*  SHAFI ALI (Presenter), JEREMY SCHER, ARINDAM CHAKRABORTY, Syracuse University —

Knowledge of the ionization potential (IP) give important chemical insights into electron-attachment and electron-detachment processes. For semiconductor cluster and nanoparticles, the effect of structure on IP is extremely important because of the quantum confinement effect. However, traditional methods for calculating IPs become computationally expensive for the determination of non-zero temperature ensemble-averaged properties which require the calculation of a large number of structures. This presentation will present the ESP-GF method which combines the effective-stochastic potential (ESP) method with 1-particle Green's function theory for efficient calculation of the ionization potential to obtain ensemble-averaged properties at non-zero temperatures. The ESP method uses random-matrix theory to describe the distribution of structures present in the NVT ensemble which allows an efficient calculation of IPs. The ESP-GF method has been applied to a series of colloidal ZnSe clusters at \(T=300\text{K}\) and the distributions of IPs will be presented. The results from this project highlight the importance of performing ensemble-averaged calculations for predicting quasiparticle properties in semiconductor clusters.

*NSF

Wednesday, March 6, 2019 2:30 PM - 5:18 PM

Session P33 FIAP: Spectroscopy and Oxides  BCEC 204B - Harishankar Jayakumar, City College of New York
2:30PM P33.00001: Time-Domain Spectroscopy of Mesoscopic Conductors Using Voltage Pulses* PABLO BURSET (Presenter), JANNE KOTILAHTI, Department of Applied Physics, Aalto University, MICHAEL MOSKALETS, Department of Metal and Semiconductor Physics, NTU Kharkiv Polytechnic Institute, CHRISTIAN FLINDT, Department of Applied Physics, Aalto University — The development of single-electron sources are paving the way for a novel type of experiments in which individual electrons are emitted into a quantum-coherent circuit. However, to facilitate further progress towards fully coherent on-chip experiments with electrons, a detailed understanding of the quantum circuits is needed. We propose to perform time-domain spectroscopy of mesoscopic conductors by applying Lorentzian-shaped voltage pulses to an input contact. We show how characteristic timescales of a quantum-coherent conductor can be extracted from the distribution of waiting times between charge pulses propagating through the circuit. To illustrate our idea, we employ Floquet scattering theory to evaluate the electron waiting times for an electronic Fabry-Pérot cavity and a Mach-Zehnder interferometer. Our spectroscopic method benefits from the particle-like behavior of the charge pulses, while still being sensitive to their quantum statistics. This unique combination makes our scheme promising for the characterization of quantum-coherent circuits.


*EU Horizon 2020 research and innovation program, Marie Sklodowska-Curie Grant No. 743884. Academy of Finland project No. 308515 and 312299.

2:42PM P33.00002: Dynamics of strongly coupled singlet fission molecules in optical microcavity BIN LIU (Presenter), City College of New York, CUNY, MATTHEW Y SFEIR, Brookhaven National Laboratory, VINOD M MENON, City College of New York, CUNY — We have experimentally studied the dynamics of a singlet-fission molecule-metal microcavity system under strong coupling by using pump-probe transient absorption technique. Under one-photon pump, where the system is selectively pumped by wavelengths which are resonant with exciton, upper, and lower polariton, the dynamics of polariton states is found to be determined by that of the exciton, which has long-time character. Moreover, comparing to the neat film without cavity, the kinetics of the molecular triplet state is not significantly modified by strong singlet molecular exciton-photon coupling within the cavity. Under two-photon pump, short-time (sub-picosecond) dynamics is observed from both the polariton cavity system and solid-state neat film, indicating this results from the ultrafast optical response of the nonlinear organic molecules.

2:54PM P33.00003: Measurement of Quadratic Terahertz Optical Nonlinearities Using Second-Harmonic Lock-in Detection* SHUAI LIN (Presenter), SHUKAI YU, DIYAR TALBAYEV, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA, United States. — We present a method to measure quadratic terahertz optical nonlinearities in terahertz time-domain spectroscopy. We use a rotating linear polarizer (a polarizing chopper) to modulate the amplitude of the incident terahertz pulse train. We use phase-sensitive lock-in detection at the fundamental and the second harmonic of the modulation frequency to separate the materials' responses that are linear and quadratic in a terahertz electric field. We demonstrate this method by measuring the quadratic terahertz Kerr effect in the presence of the much stronger linear electro-optic effect in the (110) GaP crystal. We propose that the method can be used to detect terahertz second-harmonic generation in noncentrosymmetric media in time-domain spectroscopy, with broad potential applications in nonlinear terahertz photonics and related technology.

*NSF (Grant No. DMR-1554866); the Carol Lavin Bernick Faculty Grant Program
3:06PM P33.00004: Optical spectroscopy of emission from GeSn waveguides on Si

JAY MATHEWS (Presenter), Department of Physics, University of Dayton, ZAIRUI LI, ELAHEH GHANATI, Department of Electro-Optics and Photonics, University of Dayton, JOHN KOUVETAKIS, School of Molecular Sciences, Arizona State University, JOSE MENENDEZ, Department of Physics, Arizona State University, IMAD AGHA, Department of Physics, University of Dayton — GeSn alloys are attractive for infrared emission due to the tunable band gap in the infrared and the quasi-direct or direct nature of the gap. Epitaxial growth of GeSn on Si has been demonstrated using multiple growth techniques and is now being incorporated into commercial device fabrication. Recently, laser emission from GeSn waveguides on Si has been demonstrated at temperatures up to 240 K, but the search for room temperature Si-based laser continues. In this work, we investigate the optical emission from optically-pumped GeSn waveguides at room temperature using optical spectroscopy. The results show that there is a highly nonlinear dependence on the total emission output power with respect to the input pump power. However, measurements of the emission spectrum do not show any narrowing of the emission peak, and Fabry-Perot measurements do not show any observable modes. Modeling of spontaneous emission from these materials indicates that the experimental power dependence can only be the result of optical gain in the GeSn. This result shows that optical gain at room temperature is possible.

*Funding for this project was provided by an Air Force Office of Scientific Research Young Investigator Award, Grant No. FA95501710146.

3:18PM P33.00005: The Physics of Optical Dispersion Equations

WILLIAM KARSTENS (Presenter), Saint Michael’s College, DAVID SMITH, University of Vermont and Argonne National Laboratory — We explore the disparate optical dispersion equations used to interpolate the refractive index from measurements at a limited number of spectral lines. Initial 19th-century formulations were based on elastic and electromagnetic theories. Subsequent developments were primarily empirical fits to optical-glass data and are misleading when applied to non-polar semiconductors. We show that the theoretical results of Cauchy, Sellmeier, etc., either classical or quantum-mechanical, follow from linear-response theory via the Kramers-Kronig relations regardless of the mechanism assumed. Their use is limited by the number of parameters required. In contrast, most empirical relations were chosen for simplicity and compatibility with classical ray-tracing. Their reliance on measurements in the visible blurs the roles of electronic and ionic polarization. Moreover, most empirical equations predict indices of odd parity in photon energy, in conflict with time-reversal invariance. A reformulation of the empirical dispersion equations consistent with linear-response theory corrects the parity error and clarifies their application to polar and non-polar materials.

*Supported in part by the US Department of Energy, Office of Science, Office of Nuclear Physics under contract DE-AC02-06CH11357.

3:30PM P33.00006: Calculating form-dependent optical scattering at vacuum- and extreme-ultraviolet wavelengths off nanoelectronic structures

BRYAN BARNES (Presenter), MARK-ALEXANDER HENN, HUI ZHOU, MARTIN SOHN, RICK SILVER, Nanoscale Device Characterization Division, National Institute of Standards and Technology — Form birefringence, where the orientation of periodic structures yields effective refractive index differences between orthogonal polarizations, is the basis for several applications including the successful detection of aperiodic imperfections (e.g., defects in nanoelectronics) at visible and ultraviolet wavelengths. As shorter wavelengths are employed by industry, the key assumption behind form birefringence - that the wavelength is larger than the periodicity - is challenged even with decreasing device dimensions. Here, the form dependence of high spatial-frequency scattering off periodic structures is numerically assessed among deep-, vacuum-, and extreme-ultraviolet illumination wavelengths (DUV, VUV, EUV). Form-dependent scattering intensity ratios of the scattering off ideal periodic arrays decrease with wavelength into the VUV, but dramatically increase for the 47 nm EUV wavelength due primarily to the wavelength-dependent optical properties of the dielectrics involved. After adding a bridging defect to this array, the 47 nm wavelength remains most sensitive to these patterning faults. These results should be extensible, not only to structures in nanoelectronics, but also to emerging engineered optical materials for DUV and shorter wavelengths.
Exceptional points (EPs) are generic degeneracies of non-hermitian systems, where two eigenvalues and eigenvectors of a linear operator coalesce, e.g. degenerate resonances of an open system. We identify a new kind of physically realizable exceptional point (EP) corresponding to degenerate coherent perfect absorption, in which two purely incoming solutions of the wave operator for electromagnetic or acoustic waves coalesce to a single state. Such non-hermitian degeneracies can occur at a real-valued frequency without any associated noise or non-linearity, in contrast to EPs in lasers. The absorption lineshape for the eigenchannel near the EP is quartically flat in frequency around its maximum in any dimension. In general, for the parameters at which an operator EP occurs, the associated scattering matrix does not have an EP. However, in one dimension, when the S-matrix does have a perfectly absorbing EP, it takes on a universal one-parameter form with degenerate values for all scattering coefficients. For absorbing disk resonators, these EPs give rise to chiral absorption: perfect absorption for only one sense of rotation of the input wave.

*This work was done under NSF Grant No. DMR-1743235

Hydrothermal Growth of zinc oxide nano-rods doped with manganese*

RAJNI BAGGA (Presenter), VO-VAN TRUONG, PABLO BIANUCCI, Concordia University — We synthesised ZnO Nanorods arrays doped with and without Mn doping (at a 1% concentration of the precursor salts) by a hydrothermal method at low temperature. They were characterised by scanning electron microscopy (SEM), Photoluminescence (PL) and electron paramagnetic (EPR) spectroscopy. All samples produced broad band Photoluminescence (PL) emissions in the yellow-orange-red range, typically attributed to defects in the crystalline structure. The PL spectra does not seem to show significant changes in the ratio of the near band edge emission and the defect emission with the Mn doping. From this, we infer that the crystal quality of the ZnO nanorods does not change with Mn doping. The EPR spectrum from the ZnO nanoparticles formed in the growth solution confirms the presence of Mn in them. We use Micro-Raman spectroscopy to investigate the local crystal structure of the nanomaterials. Room temperature micro-Raman spectra confirms the wurtzite structure.

*National Science and Engineering Research Council (NSERC) of Canada, through the Discovery Grant program (grant 435875-2013).
4:30PM P33.00011: Hysteresis response of 2D electron nematics in the presence of material disorder* SAYAN BASAK (Presenter), ERICA CARLSON, Purdue University, KARIN ANDREA DAHMEN, University of Illinois at Urbana-Champaign — Electron nematic phases, which break the rotational symmetry of the host crystal while retaining liquidity, have been observed in a variety of systems, including strontium ruthenates, iron superconductors, cuprate superconductors, the (111) surface of bismuth, and high fractional Landau levels. Depending upon interactions with the lattice, the nematic may either be in the XY or the Ising universality class.

Previously, we proposed new experimental tests [1] that can reveal the universality class, based on hysteresis: Upon cycling an applied orienting field, a clean 2D XY electron nematic will show no hysteresis, whereas a clean Ising nematic will show robust hysteresis.

However, no material system is defect-free, and no spontaneous symmetry breaking can occur in the 2D Ising model in the presence of random fields. In this talk, we discuss the hysteresis characteristics of XY and Ising nematics in the presence of material disorder.


*We acknowledge support from NSF Grant No.DMR-1508236 and Department of Education Grant No. P116F140459. This research is also supported by computation resources through XSEDE startup allocation (TG-DMR180098). SB will be supported through Bilsland Dissertation Fellowship in Spring 2019.

4:42PM P33.00012: Supersonic propagation of atomic motion by phasons in fresnoite* MICHAEL MANLEY (Presenter), Oak Ridge National Laboratory, PAUL J STONAHA, Physics, Idaho State University, DOUGLAS L ABERNATHY, SONGXUE CHI, Oak Ridge National Laboratory, RAFFI SAHUL, Meggitt Sensors, RAPHAEL HERMANN, JOHN D BUDAI, Oak Ridge National Laboratory — Our recent inelastic neutron scattering measurements reveal that waves of atomic motion propagate at surprisingly high speeds of up to 4.3 times the speed of sound in the form of phasons in the piezoelectric mineral fresnoite (Ba$_2$TiSi$_2$O$_8$). Phasons are quasiparticles that exist because of an incommensurate modulation (or ‘wrinkles’) in the flexible framework structure of fresnoite. They are associated with atomic rearrangements that change the phase of waves describing the incommensurate modulation. Phasons are usually overdamped and move diffusively, and are thus much slower than phonons (vibrations involving the translation of atoms, rather than rearrangements). However, the phasons in fresnoite are found not to be overdamped owing to a characteristic rotation of the phasons away from the driving soft phonon, yielding the supersonic propagation. These supersonic phasons enhance thermal conductivity and channel lattice energy at speeds well beyond the limits of phonons.

*This work was sponsored by the Office of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy.

4:54PM P33.00013: Effects of substitutional defects on the thermal-physical properties of Gd$_2$Zr$_2$O$_7$ pyrochlores* FENGAI ZHAO (Presenter), XIAN-MING BAI, Department of Materials Science and Engineering, Virginia Tech, HAIYAN XIAO, XIAOTAO ZU, University of Electronic Science and Technology of China — Rare-earth pyrochlores, particularly Gd$_2$Zr$_2$O$_7$, have been proposed as promising candidates for the next-generation thermal barrier coatings (TBCs) due to their good structural stability, low thermal conductivities at high temperatures. In this work, systematic studies of the incorporation of Yb$^{3+}$, Nd$^{3+}$, La$^{3+}$, Ti$^{4+}$, Hf$^{4+}$, Ce$^{4+}$ into cation sites in Gd$_2$Zr$_2$O$_7$ has been investigated by density functional theory (DFT) calculations to explore the underlying mechanisms for modifying its thermal-physical properties. Among these doped cations, incorporation of oversized Ce$^{4+}$ at the Zr-site leads to significantly smaller Young’s modulus, better ductility, smaller Debye temperature, and lower thermal conductivity. In particular, the thermal conductivity of Ce-doped Gd$_2$Zr$_2$O$_7$ decreases as large as 21 % with the complete Ce substitution based on the Clarke’s model. The incorporation of oversized Ce cations weakens the interatomic bonds, which is the main factor for the improved thermal-physical properties of Gd$_2$Zr$_2$yCe$_y$O$_7$ pyrochlores. The results provide theoretical predictions of the behavior and performance of pyrochlores at high temperatures and may promote experimental investigation in the future.

*X.T. Zu and F.A. Zhao were supported by the NSAF Joint Foundation of China (Grant No. U1630126).
**5:06PM P33.00014: Investigations on the Electronic and Optical Properties of Double Perovskites Ba$_2$BiSbO$_6$**

BISHNU PRASAD BELBASE (Presenter), SHALIKA RAM BHANDARI, GOPI CHANDRA KAPHLE, MADHAV PRASAD GHIMIRE, Central Department of Physics, Tribhuvan University, DINESH KUMAR YADAV, Advanced Materials Laboratory, Condensed Matter Physics Research Center — Recent research on double perovskites with large spin-orbit coupling (SOC) assisted materials are of great interest due to their novel properties. Materials with band gap in the visible range are found suitable for optoelectronic devices. Depending on the types of gaps (indirect or direct), materials can be used for photo detectors or optoelectronic emitters. Using first principle density functional (DF) approach, we study the electronic and optical properties of newly synthesized Ba$_2$BiSbO$_6$. Within generalized gradient approximation without SOC, an indirect band gap of 1.85 eV was observed which reduces to 1.72 eV when SOC is taken into account. Significant changes due to SOC has been found at Gamma point in the band structure where band splitting of ~1.3 eV has been observed just above the fermi level with possible indication from indirect to direct band gap semiconductor. Strong hybridization between Bi-6p, Sb-5p and O-2p states observed on the electronic density of states. Optical study shows interband electron transition with energy larger than the bandgap of the material. This suggests Ba$_2$BiSbO$_6$ as a candidate material for photodetectors (absorbers).

*B.P.B and G.C.K acknowledges the technical support provided by CMPRC-Butwal, Nepal.

**Wednesday, March 6, 2019 2:30 PM - 5:30 PM**

**Session P34 FIAP: Recent Advances on Spintronics-based Computing: from Deterministic to Probabilistic**

**2:30PM P34.00001: Recent progress in reducing the current and time for magnetization switching in magnetic tunnel devices for memory applications**

JONATHAN SUN (Presenter), IBM Thomas J. Watson Research Center — In spin-transfer-torque switched magnetic random access memory (STT-MRAM) using magnetic tunnel junctions (MTJ), the STT switching current directly affects selection transistor size and circuit density. This is a critical attribute for cost competitiveness in commercial applications. Recent developments in STT-MRAM have been focusing on reducing switching current well below 100 uA, increasing speed beyond 50 ns, and improving switching reliability to better than $10^{-9}$, while simultaneously aiming for data retention of 10 years at operating temperatures ranging between -40 and + 85°C or beyond. In this talk, I will review the fundamental device and materials physics that govern the STT-switching dynamics. While the switching threshold current is more directly related to data-retention, the actual operating switching current for ensuring a certain speed and reliability (switching error) for fast, below 10ns switching can also exceed macrospin expectations. Experiments show the switching current required to achieve deep error floor can be less than estimated from macrospin. For further improvements it is important to understand the dynamics involving a nanomagnet's internal degrees of magnetic freedoms during STT switching, a potentially complex subject rich in nonlinear dynamics. These complex nonlinear mechanisms can speed-up the intended switching of the MTJ, but can also affect the reference-layer stability, requiring special care. Longer term, for even faster manipulation of nanomagnets approaching or below 1 ns, new sources of spin-current with better charge-to-spin current conversion needs to be considered, such as thermal magnonic or spin-orbit-derived spin-currents. I will briefly discuss recent advances with these new sources of spin currents, and the likely common challenges they will give rise to, in terms of materials and device design and development.

*With the MRAM group at IBM Research, supported in part by partnership with Samsung Electronics.
3:06 PM P34.00002: Spintronic Devices for Neural Networks* [Invited] SHUNSUKE FUKAMI (Presenter), Research Institute of Electrical Communication, Tohoku University — Representing the human brain in computers, so-called neuromorphic computing, is one of the focuses of interest in recent electronics as the brain is a model system that can readily accomplish complex tasks at small power consumption level, in contrast to conventional von Neumann computers. An artificial neural network offers a promising approach for low-power and intelligent neuromorphic computing. A key ingredient for the network is an artificial synapse that has analog and nonvolatile memory functionalities and frequent learning capability as in the real synapse in the brain. Here we show an artificial neural network with spintronic artificial synapses, which meet these requirements [1]. We will first describe an analog spin-orbit torque (SOT) switching device consisting of an antiferromagnet/ferromagnet bilayer structure [2], which can serve as the artificial synapse. The mechanism of analog and nonvolatile property [3] will be described. Secondly, a proof-of-concept demonstration of an artificial neural network with 36 SOT devices will be shown. An associative memory operation is performed based on the Hopfield model and learning ability of the spintronic artificial synapse is confirmed [4].

This work is jointly carried out with H. Ohno, W. A. Borders, A. Kurenkov, S. Sato, Y. Horio, and H. Akima of Tohoku University and P. Gambardella of ETH Zurich.


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3:42 PM P34.00003: Supervised learning of an artificial opto-magnetic neural network with picosecond laser pulses [Invited] THEO RASING (Presenter), Radboud University, Nijmegen, Netherlands — The explosive growth of data and its related energy consumption is pushing the need to develop novel, brain inspired and energy efficient schemes and materials for data processing and storage. The prospect of continuous magnetization state manipulation of a Co/Pt thin film via picosecond optical laser pulses offers the possibility of exploiting this material for neuromorphic computing. Here, we demonstrate that such material can be used as an artificial adaptive synapse by controlling its internal magnetization state using circularly polarized picosecond laser pulses. We also show experimentally an efficient implementation of perceptron learning on a supervised opto-magnetic neural network, consisting out of such magnetic synapses. Importantly, we show that optimization of synaptic weights is achieved by a global feedback mechanism, such that learning does not rely on external storage or additional optimization schemes.

4:18 PM P34.00004: p-Bits for Probabilistic Spin Logic* [Invited] SUPRIYO DATTA (Presenter), Purdue University — The growing field of quantum computing is based on the concept of a q-bit which is a delicate superposition of 0 and 1, along with coherent coupling techniques for entangling them. By contrast a probabilistic bit or a p-bit is a robust classical entity that fluctuates between 0 and 1, and can be correlated using techniques borrowed from the field of neural networks. Correlated p-bits are of course no substitute for entangled q-bits, but we will argue that they can be used as a poor man’s q-bits that address a broad class of important problems including inference, “invertible” logic and optimization, using the same quantum algorithms but with added versatility. Further we will show that existing embedded MRAM technology with minor modifications can be used to implement room temperature p-bits and build large scale p-circuits [1].


*This work was supported in part by ASCENT, one of six centers in JUMP, a Semiconductor Research Corporation (SRC) program sponsored by DARPA and in part by the Center for Probabilistic Spin Logic for Low-Energy Boolean and Non-Boolean Computing (CAPSL), one of the Nanoelectronic Computing Research (nCORE) Centers, a Semiconductor Research Corporation (SRC) program sponsored by the NSF.
Brains display many features typical of non-linear dynamical networks, such as synchronization or chaotic behavior. These observations have inspired a whole class of models that harness the power of complex non-linear dynamical networks for computing. In this framework, neurons are modeled as non-linear oscillators, and synapses as the coupling between oscillators. However, there are few hardware implementations of these systems, because large numbers of interacting non-linear oscillators are necessary. In this talk, we will see why coupled magnetic nano-oscillators are very promising for realizing cognitive computing at the nanometer scale. Then, we will present our experimental and theoretical results. We will show how speech recognition can be performed using the transient dynamics and the synchronization of a few harmonic spin torque oscillators [1]. These results highlight key opportunities and requirements for harnessing spintronics for bioinspired computing. We will also show how superparamagnetic oscillators can code and transform information in a robust population-type scheme [2]. These results highlight that some apparently undesirable phenomena like superparamagnetism can become compelling for bioinspired schemes. We will finally discuss how this line of research can take inspiration from both neuroscience and machine learning, and finish by open questions raised by our research.


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Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P35 DQI: Theory and Scaling of Benchmarking and Tomography 8CEC 205B - Matthew Ware, BBN Technologies - Tag(s): Focus

2:30PM P35.00001: A new class of randomized benchmarking protocols: theory and experiment* [invited] JONAS HELSEN (Presenter), XIAO XUE, LIEVEN VANDERSYPEN, STEPHANIE WEHNER, Delft University of Technology — In this talk I will discuss a new class of randomized benchmarking protocols called character randomized benchmarking. Character randomized benchmarking allows one to extend standard randomized benchmarking in a principled manner to groups beyond the Clifford group. I will discuss the theory of character randomized benchmarking, some example protocols such as benchmarking a T gate and performing two qubit interleaved randomized benchmarking using only single qubit gates as reference, and I will also present some recent experimental implementations of character randomized benchmarking.

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3:06PM P35.00002: Randomized Benchmarking as Convolution SETH MERKEL (Presenter), HRL Laboratories — We show that the standard randomized benchmarking protocol can be described as a convolution, and is thus amenable to Fourier analysis. We utilize a form of Fourier transform that maps matrix-valued functions on group elements to matrix-valued functions of the group’s irreducible representations in order to map the average over sequences of Clifford operations to the power of a single matrix. We can then demonstrate that as long as our faulty gate-set is close to some representation of the Clifford group, an RB sequence is described by the exponential decay of a process that has exactly two eigenvalues close to one and the rest close to zero, even though the bounds with respect to any particular representation of the Clifford group may not tightly describe the rate of decay.
3:18PM P35.00003: Randomized Benchmarking under Different Gatesets  KRISTINE BOONE (Presenter), ARNAUD CARIGNAN-DUGAS, JOEL WALLMAN, JOSEPH EMERSON, University of Waterloo — We provide a comprehensive analysis of the differences between two important standards for randomized benchmarking (RB): the Clifford-group RB protocol proposed originally in [1] and [2], and a variant of that RB protocol proposed later by the NIST group in [3]. While these two protocols are frequently conflated or presumed equivalent, we prove that they produce distinct exponential fidelity decays leading to differences of up to a factor of 3 in the estimated error rates under experimentally realistic conditions. These differences arise because the NIST RB protocol does not satisfy the unitary two-design condition for the twirl in the Clifford-group protocol and thus the decay rate depends on non-invariant features of the error model. Our analysis provides an important first step towards developing definitive standards for benchmarking quantum gates and a more rigorous theoretical underpinning for the NIST protocol and other RB protocols lacking a group-structure. We conclude by discussing the potential impact of these differences for estimating fault-tolerant overheads.


3:30PM P35.00004: On the freedom in representing quantum operations*  JUNAN LIN (Presenter), BRANDON BUONACORSI, RAYMOND LAFLAMME, JOEL WALLMAN, University of Waterloo — We discuss the effects of a gauge freedom in representing quantum information processing devices, and its implications for characterizing these devices. We demonstrate with experimentally relevant examples that there exists equally valid descriptions of the same experiment which distribute errors differently among objects in a gate-set, leading to different error rates. Consequently, it can be misleading to attach a concrete operational meaning to figures of merit for individual gate-set elements. We propose an alternative operational figure of merit for a gate-set, the mean variation error, and a protocol for measuring this figure.

*This research was supported by the U.S. Army Research Office through grant W911NF-14-1-0103, the Government of Ontario, and the Government of Canada through CFREF, NSERC and Industry Canada.

3:42PM P35.00005: Using Fourier Analysis and Maximum Likelihood Estimation to Identify and Model Non-Markovian Noise in Quantum Operations  GARRETT SIMON (Presenter), Massachusetts Institute of Technology, COLIN BRUZEWICZ, KEVIN OBENLAND, Lincoln Laboratory, ISAAC CHUANG, RICHARD RINES, JULES STUART, Massachusetts Institute of Technology, ROBERT NIFFENEGGER, JOHN CHIAVERINI, JEREMY SAGE, Lincoln Laboratory — The most well-studied error models for quantum operations or gates are Markovian, which assume that the error is “memoryless.” Generically, most error sources can lead to gate errors which violate this assumption. One such source includes periodic noise, which causes the amplitude of gate errors to fluctuate at a characteristic frequency, requiring a non-Markovian error model. Characterizing periodic errors, rather than just identifying them, requires data processing and error modeling beyond the standard procedures used to identify Markovian errors. Using an open-source Fourier transform implementation for qubit measurement data (pyGSTi), we were able to identify the presence of periodic error in quantum operations on trapped-ion qubits. This information allowed us to hypothesize the sources of periodic noise, and create a time-dependent error model, or waveform, whose parameters we optimized to fit the measured data via maximum likelihood estimation. This procedure allows us to quantitatively characterize and predict error sources in an experimental set up, as well as provide a basis for building more generalized non-Markovian error models.

3:54PM P35.00006: Idle tomography: Efficient gate characterization for N-qubit processors*  ROBIN BLUME-KOHOUT (Presenter), ERIK NIELSEN, KENNETH RUDINGER, KEVIN YOUNG, MOHAN SAROVAR, TIMOTHY PROCTOR, Sandia National Laboratories — Quantum process tomography is famously unscalable to many qubits. But the problem is actually the size of the model — arbitrary $N$-qubit process matrices — rather than the number of qubits. The vast majority of possible $N$-qubit errors will not occur in real processors. Here, we introduce a concrete reduced model of low-weight (few-qubit) errors on $N$ qubits. It has $O(N^2)$ parameters, and captures all the commonly conceived failure modes. Then, we introduce a simple and transparent tomography protocol for measuring the error rates, whose complexity scales very efficiently with $N$. We demonstrate it with simulations and experimental results.

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Randomized benchmarking of many-qubit devices

TIMOTHY PROCTOR (Presenter), KENNETH RUDINGER, ROBIN BLUME-KOHOUT, Sandia National Laboratories, ARNAUD CARIGNAN-DUGAS, Institute for Quantum Computing and the Department of Applied Mathematics, University of Waterloo, ERIK NIELSEN, KEVIN YOUNG, Sandia National Laboratories — Quantum information processors incorporating 5 - 10s of qubits are now commonplace, but the standard method for benchmarking quantum gates - Clifford randomized benchmarking - is infeasible to implement on more than a few qubits in any near-term devices. In this talk, we present a series of modifications to Clifford randomized benchmarking that enable truly holistic benchmarking of entire devices. Importantly, these new techniques are adaptable based on experimental goals. They can be made highly robust or more scalable as needed, and they can be used to estimate, e.g., two-qubit gate error rates or the magnitude of crosstalk errors. Moreover, our methods allow for the benchmarking of universal gates, and continuously parameterized gates. We demonstrate our techniques on current systems, with experimental results on up to 16 qubits.

*Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525. This research was funded by IARPA. The views expressed in the article do not necessarily represent the views of the DOE, IARPA, the ODNI, or the U.S. Government.

Perturbative density matrix propagation in Gate Set Tomography

ERIK NIELSEN (Presenter), Sandia National Laboratories, ROBIN BLUME-KOHOUT, Center for Computing Research, Sandia National Laboratories, TIMOTHY PROCTOR, Sandia National Laboratories, KENNETH RUDINGER, Center for Computing Research, Sandia National Laboratories, MOHAN SAROVAR, KEVIN YOUNG, Sandia National Laboratories — Model-based quantum tomography protocols like Gate Set Tomography optimize a noise model with some number of parameters in order to fit experimental data. As the number of qubits increases, two issues emerge: 1) the number of model parameters grows, and 2) the cost of propagating quantum states (density matrices) increases exponentially. The first issue can be addressed by considering reduced models that limit errors to being low-weight and geometrically local. In this talk, we focus on the second issue and present a method for performing approximate density matrix propagation based on perturbative expansions of error generators. The method is tailored to the likelihood optimization problem faced by model-based tomography protocols. We will discuss the advantages and drawbacks of using this method when characterizing the errors in up to 8-qubit systems.

*Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525. This research was funded in part by IARPA. The views expressed in the article do not necessarily represent the views of the DOE, IARPA, the ODNI, or the U.S. Government.

Benchmarking the quantum processing power of large-scale quantum processors to execute specific programs

JOSEPH EMERSON (Presenter), JOEL WALLMAN, Institute for Quantum Computing, University of Waterloo — We propose an experimentally measurable quantity, the circuit quality Q of any hardware implementation of a quantum circuit, which can be efficiently estimated via clock cycle benchmarking, and discuss how this quantity can be applied to two key applications of circuit benchmarking: (i) determining the size of a quantum program that can be run on specific quantum hardware to within a specified tolerance; and (ii) establishing a family of cross-platform benchmarks for overall hardware performance. The first application provides an efficient means of assessing the overall error probability with which hardware can implement a quantum program beyond the horizon of classical computability, which will be tremendously important once quantum processors can outperform their classical counterparts. The second application is to define a practical, even-handed, and robust cross-platform benchmark of hardware performance for standardized quantum circuits. Our proposal for circuit benchmarking overcomes several problematic limitations of the `quantum volume' figure of merit and the implicit recipe for measuring it. These circuit quality benchmarks will be essential to assessing and improving hardware performance on the road to practical quantum computation that can solve real-world problems.

*Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525. This research was funded in part by IARPA. The views expressed in the article do not necessarily represent the views of the DOE, IARPA, the ODNI, or the U.S. Government.
4:42PM P35.00010: Efficient learning of Pauli channels: learning tensor network models. STEVEN FLAMMIA (Presenter), University of Sydney; Yale University; Quantum Benchmark Inc.; JOEL WALLMAN, University of Waterloo; Quantum Benchmark Inc. — Noise is the central obstacle to building large-scale quantum computers. Of crucial importance is the ability to reliably and efficiently characterize quantum noise afflicting a large scale quantum device with high precision. Here we show that where we have a Pauli channel whose errors are have only k-local correlations we can learn the entire n-qubit Pauli channel to relative precision ε with only O(ε^{-2} n^2 log(n)) measurements. This is efficient in the number of qubits and represents a major breakthrough in the characterization of multi-qubit devices. These results have proven recovery guarantees for quantum channels to relative precision, representing a qualitative shift in the ability to characterize quantum devices. These results are practical, relevant and immediately applicable to characterizing error rates in current intermediate scale and future large-scale quantum devices on hundreds to thousands of qubits.

4:54PM P35.00011: Efficient learning of Pauli channels: learning sparse models JOEL WALLMAN (Presenter), University of Waterloo, STEVEN FLAMMIA, School of Physics, University of Sydney — The recent development of randomized compiling ensures that the general noise channel afflicting a universal quantum device can be reduced to stochastic Pauli noise. To characterize and optimize the remaining errors, methods are needed to characterize Pauli noise channels in intermediate and large-scale quantum devices. Here we introduce estimation protocols with relative error guarantees that enable efficient reconstructions of both complete and sparse Pauli channels. The protocol developed and analyzed is a variant of randomized benchmarking and the recently introduced cycle benchmarking. Like those protocols, the estimate is robust to state preparation and measurement error (SPAM). This robustness to SPAM together with the relative precision guarantees make the protocol appropriate for applications involving the characterization of high-accuracy gates. These results enable a host of applications beyond just characterizing noise in large-scale quantum systems: they pave the way to tailoring quantum codes, optimizing decoders, and customizing fault tolerance protocols to suit a particular device.

5:06PM P35.00012: Experimental reconstruction of all correlated error rates on a 16 qubit device. ROBIN HARPER (Presenter), University of Sydney, Quantum Benchmark, STEVEN FLAMMIA, University of Sydney, Yale University, Quantum Benchmark, JOEL WALLMAN, JOSEPH EMERSON, University of Waterloo, Quantum Benchmark — Recent results by Flammia and Wallman have shown how to reliably and efficiently characterize Pauli channels on intermediate and large-scale quantum devices. Here we leverage those results to give a complete, efficient, and high-precision, characterization of IBM's online 16 qubit device. Using experimental results from the device we obtain and present complete information about the correlated error rates across the device, comparing device characteristics when qubits are operated in single qubit mode and with qubit-to-qubit interactions enabled. The protocol we use obtains multiplicative precision and robustness to SPAM errors by using techniques originating from randomized benchmarking, and it can be executed on all current NISQ devices. The protocol is easy to implement, involving just computational basis state preparation and measurement together with only one-qubit Clifford gates. We show how this protocol can be scaled up to even larger devices of 100 or even 1000 qubits.

5:18PM P35.00013: Efficient Unitarity Randomized Benchmarking of Few-qubit Clifford Gates BAS DIRKSE (Presenter), JONAS HElsen, STEPHANIE WEHNER, QuTech, Delft University of Technology — Unitarity randomized benchmarking (URB) is an experimental procedure for estimating the unitarity of implemented quantum gates independently of state preparation and measurement (SPAM) errors. The unitarity is a measure of coherence of a quantum gate that provides information independent of average fidelity. A central problem in the URB experiment is relating the number of data points to rigorous confidence intervals around the unitarity. In this work we analyze the statistics of Clifford URB. We provide a bound on the required number of data points as a function of confidence and experimental parameters. The main ingredient for this result is a sharp bound on the variance of the data points due to the random sampling. Our result shows that estimating the unitarity of gates requires fewer data points as the gates become closer to being unitary, up to constant contribution due to SPAM errors. The bound is sufficiently sharp to benchmark small-dimensional systems in realistic parameter regimes using a modest number of data points. For example, we show that the unitarity of single-qubit Clifford gates can be rigorously estimated using few hundred data points under the assumption of gate-independent noise. This is a reduction of orders of magnitude compared to previously known bounds.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P37 GMAG DCMP DMP: Honeycomb Lattice and Other Low-D Models BCEC 206A -
Matthias Gohlke, Max-Planck-Institut fur Physik komplexer System - Tag(s): Focus
ZHENG-XIN LIU (Presenter), Department of Physics, Renmin University of China, BRUCE NORMAND, Neutrons and Muons Research Division, Paul Scherrer Institute — Kitaev materials have attracted great attention thanks to their potential for realizing the Kitaev model, an exactly solvable spin model that hosts topological quantum spin liquids. However, most Kitaev materials undergo phase transition into a magnetically ordered phase at low temperatures, indicating that non-Kitaev interactions are non-negligible. Recent experiments on the Kitaev material α-RuCl3 showed that, under very low temperature an intermediate in-plane magnetic field can suppress the static zigzag magnetic order and induce a liquid-like disordered phase. The nature of the field-induced disordered phase was not fully understood. Motivated by this issue, we studied the K-Γ model (K = 6.8 meV and Γ = 9.5 meV) which was the minimal model proposed to describe the low-energy physics of α-RuCl3. From variational Monte Carlo calculations, we found that in-plane magnetic field can indeed cause a phase transition from a zigzag ordered phase into a gapless U(1) Dirac spin liquid phase [1]. Our results semi-quantitatively explain the observed temperature dependence of spin-lattice relaxation rate $1/T_1 \sim T^3$ in a recent nuclear magnetic resonance experiment [2]. It was also shown that an out-of-plane magnetic field can induce a Kalmeyer-Laughlin-type abelian chiral spin liquid phase, which would show an integer-quantized thermal Hall effect. Our theory hopefully captures the low energy physics of α-RuCl3 and provides a clue to understand the experiments in related materials.


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DAVID RONQUILLO (Presenter), ADU VENGAL, NANDINI TRIVEDI, Ohio State University — The main question we address is how to probe the fractionalized excitations of a quantum spin-liquid (QSL), for example, in the Kitaev honeycomb model. From analyzing the energy spectrum and entanglement entropy, for antiferromagnetic couplings and a field along either [111], or [-110], we find a new gapless QSL phase, sandwiched between the non-Abelian Kitaev QSL and polarized phases. Rotating the field towards [001] destroys this intermediate QSL phase and results in a considerable reduction in the number of frequency modes. In certain parameter regimes, we observe a beating pattern in the local dynamical correlations, possibly observable in pump-probe experiments. Finally, we explore the field strength and orientation dependence of the longitudinal and transverse thermal conductivities of this model as a function of temperature.

*We acknowledge the support of DOE-BES grant DE-FG0207ER46423

JACOB GORDON (Presenter), ANDREI CATUNEANU, University of Toronto, ERIK SORENSEN, McMaster University, HAE-YOUNG KEE, University of Toronto — The Kitaev model is a rare example of an exactly solvable model which exhibits a spin liquid ground state, and hosts non-Abelian anyon excitations. Recent research has focused on material realization of Kitaev physics, with α-RuCl3 emerging as a leading candidate. Compelling evidence for a chiral spin liquid (CSL) is a half-quantized thermal Hall conductivity in α-RuCl3, a signature of Majorana edge currents. However, it remains a non-trivial task to explain the existence of a CSL in α-RuCl3 from a microscopic model, due to dominant ferromagnetic (FM) Kitaev interactions. This is because the FM Kitaev phase almost immediately transitions to the polarized phase in an applied field, with no intervening phase. Here we present a microscopic theory describing the existence of a CSL near the FM Kitaev regime under a magnetic field. Further implications related to the quantized thermal Hall conductivity are also discussed.

*This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC), the Canadian Institute for Advanced Research (CIFAR), and Compute Canada.
3:30PM P37.00004: Classical Kitaev model in a magnetic field  JEFFREY G. RAU (Presenter), PAUL A. MCCLARTY, Max Planck Institute for the Physics of Complex Systems, KARLO PENC, Hungarian Academy of Sciences, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems — We study the classical version of Kitaev's honeycomb model in the presence of a magnetic field. For an anti-ferromagnetic Kitaev coupling a classical spin liquid phase persists over a large window of field strength, independent of field direction. We characterize this phase using analytic arguments, a coarse-grained theory and via Monte Carlo simulations, finding the Coulomb correlations present at zero-field are immediately destroyed when the field is applied. We further probe the nature of this phase via the introduction of vacancies. Over a wide field range we find removing a site leaves the magnetization unchanged, the liquid exactly compensating the missing spin. Finally, we speculate on implications for the quantum model in the semi-classical limit.

3:42PM P37.00005: Plaquette order in classical spin liquid stabilized by strong off-diagonal exchange  ZHIJIE FAN (Presenter), PREETHA SAHA, DEPEI ZHANG, GIA-WEI CHERN, University of Virginia — We report a new classical spin liquid in which the collective flux degrees of freedom break the translation symmetry of the honeycomb lattice. This exotic phase exists in frustrated spin-orbit magnets where a dominant off-diagonal exchange, the so-called $\Gamma$ term, results in a macroscopic ground-state degeneracy at the classical level [1]. We demonstrate that the system undergoes a phase transition driven by thermal order-by-disorder at a critical temperature $T_c \approx 0.04 |\Gamma|$. Interestingly, while the cubic symmetry is broken at $T < T_c$, spins in the low temperature phase remain disordered. We show that this phase transition actually corresponds to plaquette ordering of hexagonal fluxes. By introducing a proper order parameter to describe this translational symmetry breaking, we performed extensive Monte Carlo simulations and finite-size analysis to investigate the nature of the plaquette-ordering transition. We also study the dynamical behavior of fluxes and the influence of other types of interactions on the phase transition.[1] I. Rousochatzakis and N. B. Perkins Phys. Rev. Lett. 118, 147204 (2017).

3:54PM P37.00006: Designing $S = 1$ Kitaev materials*  ANDREI CATUNEANU (Presenter), PANAGIOTIS PETER STAVROPOULOS, DARREN PEREIRA, HAE-YOUNG KEE, University of Toronto — As the spin $S = 1/2$ Kitaev model is gaining increasing attention, there have been theoretical efforts to understand if $S = 1/2$ Kitaev features appear in generalized Kitaev models with higher spins. In particular, numerical studies on the $S = 1$ Kitaev model show interesting results, but there is no microscopic understanding on how to generate such a bond-dependent $S = 1$ interaction in solid state materials. Here we present a microscopic mechanism and necessary ingredients to design the $S = 1$ Kitaev interaction. Candidate materials are also discussed.

*Supported by the NSERC of Canada, CIFAR and Compute Canada.

4:06PM P37.00007: Dynamical and finite temperature properties of Kitaev magnet beta-Li2IrO3 in magnetic field*  MENGQUN LI (Presenter), University of Minnesota, IOANNIS ROUSOCHATZAKIS, Department of Physics, Loughborough University, NATALIA PERKINS, University of Minnesota — We present theoretical study of the field-induced magnetic phases in the three-dimensional, hyperhoneycomb Kitaev compound beta-Li2IrO3. We show that a relatively weak magnetic field along the crystallographic b-axis drives the system from its incommensurate counter-rotating order to a correlated paramagnet, with a significant uniform ‘zigzag’ component superimposing the magnetization along the field. We compute the magnon excitation spectra, the dynamical spin structure factors and their polarization dependence and argue that our results provide additional distinctive fingerprint that can be checked experimentally. Finally, using extensive Monte Carlo simulations, we study the evolution of the magnetic orders with temperature and provide the finite temperature phase diagram of field-induced magnetic phases.

*NSF DMR-1511768

4:18PM P37.00008: Using light to tune magnetism on the honeycomb lattice  VICTOR QUITO (Presenter), REBECCA FLINT, Department of Physics and Astronomy, Iowa State University — The search for spin liquid phases in condensed matter systems has generated a lot of interest in recent years. In practice, however, such phases are usually restricted to small regions of phase diagrams, which makes them challenging to access in experiments. Concerning this issue, circularly polarized Floquet potentials have been shown to generate chiral fields on the kagome lattice, making it possible to tune between Z2 and chiral spin liquids [1]. Given the potential deconfined criticality and chiral spin liquid phases on honeycomb lattices, here we address the effects of different Floquet potentials in these lattices. We discuss, in particular, how periodic optical drives can be used to manipulate different spin exchange couplings. We also comment on how our results can be relevant to experiments.

Classification of spin liquids on the stuffed honeycomb lattice

JYOTISMAN SAHOO (Presenter), Iowa State University, DMITRII KOCHKOV, BRYAN CLARK, Physics, University of Illinois at Urbana Champaign, REBECCA FLINT, Iowa State University — We introduce the stuffed honeycomb lattice (a honeycomb lattice coupled to its dual - a triangular lattice) that interpolates between the triangular and the honeycomb lattices. We consider $S = 1/2$ Heisenberg spins. Our classical phase diagram reveals a multi-critical point on the triangular lattice axis, with two new neighboring noncollinear phases appearing only off axis. Our quantum phase diagram found via exact diagonalization hosts a large spin liquid (SL) region that eats up most of the phase space of the new classical phases around the multi-critical point. We present a projective symmetry group analysis of all possible symmetric SLs on the stuffed honeycomb lattice and attempt to probe the possible nature (gapless, nematic, etc) to compare to the SL region found in exact diagonalization. Among these SLs, we focus on characterizing the competitive ones found in a variational Monte Carlo analysis.

Field-induced Spin Liquid-like State in a Magnetic Honeycomb Lattice

RUIDAN ZHONG (Presenter), ROBERT CAVA, Department of Chemistry, Princeton University — Quantum fluctuations in magnetic lattices can yield a quantum spin liquid (QSL) state, where no long-range order appears even at zero temperature. The variety of mechanisms that can generate the spin liquid state and the more exotic QSL state remain unclear, however. Here, we report a new magnetic honeycomb system, BaCo$_2$(P$_{1-x}$V$_x$)$_2$O$_8$, in which the spin correlations can be tuned by the disorder, leading to different magnetic behaviors. At low $x$, the material has a spin glass ground state that appears to be due to coexisting and competing correlations. We have found that an external magnetic field can introduce spin liquid-like behavior for some members of the solid solution, testified by the magnetic and thermodynamic experiments. Our results suggest that structural geometry, chemical disorder and external field may help enhance quantum fluctuations in magnetic honeycomb materials.

Ripple state in the frustrated honeycomb-lattice antiferromagnet

TOKURO SHIMOKAWA (Presenter), Okinawa Institute of Science and Technology Graduate University, HIKARU KAWAMURA, Osaka University — Rich nontrivial magnetic structures in multiple-$q$ states have attracted much attention these days. One of the most celebrated example might be a skyrmion-lattice state known as a triple-$q$ state with forming periodic vortex-crystal structure. We have found a new type of multiple-$q$ state, a "ripple state" in the $J_1$-$J_2$ classical honeycomb-lattice Heisenberg antiferromagnet by means of extensive Monte Carlo simulations. This honeycomb model has been known to have an infinite ring-like degeneracy in the ground state. In the ripple state, surprisingly, order-by-disorder mechnism does not work and all wavevectors on the degenerate ring equally contribute to its order. The real-space spin texture of the ripple state does not form a crystal in spite of the breaking of the translational symmetry and seems to be like a "water ripple" observed when we throw a stone on the surface of water. We will talk about the detail of the intriguing properties of the ripple state and discuss the possible realization in the honeycomb-lattice spin-liquid material, Bi$_3$Mn$_4$O$_{12}$(NO$_3$).

AKLT-like valence bond solid state in the frustrated ferromagnetic $J_1$-$J_2$ chain

CIÒ EFTHIMIA AGRAPIDIS (Presenter), STEFAN-LÜDWIG DRECHSLER, JEROEN VAN DEN BRINK, S. NISHIMOTO, Institute for Theoretical Solid State Physics, IFW Dresden — Frustrated one-dimensional (1D) magnets are known as ideal playgrounds for new exotic quantum phenomena. We consider an elementary frustrated 1D system: the spin-1/2 ferromagnetic ($J_1$) Heisenberg chain with next-nearest-neighbor antiferromagnetic (AFM) ($J_2$) interactions. On the basis of density-matrix renormalization group calculations we show the existence of a finite spin gap at $J_2/|J_1| > 1/4$ and we find the ground state in this region to be a valence bond solid (VBS) with spin-singlet dimerization between third-neighbor sites. The VBS is the consequence of spontaneous symmetry breaking through order by disorder. Quite interestingly, this VBS state has an Affleck-Kennedy-Lieb-Tasaki-type topological order. We also investigate the possibility of multipolar physics induced by AFM interchain coupling.

*This research is part of the Blue Waters sustained petascale computing project - supported by the NSF (award numbers OCI-0725070 and ACI-1238993) and the State of Illinois. RF and JS - supported by NSF DMR-1555163. BC and DK - supported by SciDAC grant DE-FG02-12ER46875. We also acknowledge the hospitality of the Aspen Center for Physics, supported by NSF Grant No. PHYS-1066293.

*This research was supported by Gordon and Betty Moore Foundation, EPIQS initiative, grant number GBMF-4412.

*This work is supported by SFB 1143 of the Deutsche Forschungsgemeinschaft.
5:18PM P37.00013: Critical properties of six-state clock model on randomly frustrated 2D lattices* TASRIEF
SURUNGAN (Presenter), Physics, Hasanuddin University, INDONESIA — We study the antiferromagnetic six-state clock model on bond-diluted triangular lattice, which is randomly frustrated. The corresponding pure system of the model experiences two separated phase transitions, i.e., the Kosterlitz-Thouless (KT) transition of magnetic ordering and the chiral ordering transition which occurs at slightly higher temperature. Due to discrete symmetry of spins there exists an additional KT transition at lower temperature, separating the true (magnetic) and the quasi-long range order (QLRO). As randomness is important for phase transition, it is desirable to probe the role played by dilution in affecting the existing KT transitions as well as the chiral ordering transition. With the presence of bond dilution in the triangular lattice the system is transformed from the fully frustrated into a randomly frustrated case. As the energy of the model is represented by the multiple of $J/2$, where $J$ is the coupling constant, we use Wang-Landau algorithm of Monte Carlo method. Various concentrations of depleted bonds were simulated. We observed a systematic decrease of critical temperatures, both for the KT transition and chiral transition, as the concentration of dilution increases. We obtained the phase diagram of the system.


Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P38 GMAG DMP: 2D Magnetism III BCEC 206B - Roopali Kukreja, University of California, Davis - Tag(s): Focus

2:30PM P38.00001: Properties of Monolayer Vanadium Dichalcogenides grown by molecular beam epitaxy* [Invited]
MATTIHAS BATZILL (Presenter), University of South Florida — Ferromagnetic ordering in monolayer vanadium dichalcogenides was predicted by DFT, despite the lack of ferromagnetic ordering in its bulk form. Ferromagnetic 2D materials with high Curie temperatures are highly sought to enable spintronic devices based on van der Waals heterostructures. In this talk we present a discussion of VSe$_2$ and VTe$_2$ monolayers grown by molecular beam epitaxy and study the difference of their monolayer properties compared to the bulk. In addition, to charge order states and structural variations of the monolayer and the bulk, we critically assess the origin of the measured ferromagnetic properties [1] in (sub)monolayer VSe$_2$.


*National Science Foundation DMR-1701390

3:06PM P38.00002: Rashba-type Dzyaloshinskii-Moriya interaction in h-BN/Co and graphene/Co heterostructures
JINGHUA LIANG (Presenter), Key Laboratory of Magnetic Materials and Devices, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, China, ALI HALLAL, FATIMA IBRAHIM, Univ. Grenoble Alpes, INAC-SPINTEC, F-38000 Grenoble, France, HONGXIN YANG, Key Laboratory of Magnetic Materials and Devices, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, China, MAIRBEK CHSHIEV, Univ. Grenoble Alpes, INAC-SPINTEC, F-38000 Grenoble, France — With the recently observed chiral domain wall structures at the graphene/ferromagnet interfaces [1,2], the Dzyaloshinskii-Moriya interaction (DMI) in light element/ferromagnet heterostructures has become of great interest for spintronics. Here, we present a comparative study of the Rashba-type DMI in the h-BN/Co and graphene/Co heterostructures using first-principles calculations. Unexpectedly, they show opposite trend as a function of Co thickness. With the increase of Co thickness, the DMI coefficient of h-BN/Co first increases gradually and then saturates at around 1.1 meV for thick Co layers, whereas the DMI at graphene/Co interfaces first decreases and then stabilizes at about 0.1 meV for large Co thickness. For thick Co layers, the DMI strength of h-BN/Co is one order of magnitude larger than that of graphene/Co. The origin of this discrepancy is attributed to the different contribution from the hybridization between dz$^2$ and d$xz$ orbitals of the interfacial Co layer to the DMI energy source. These results give deeper insight into microscopic formation of DMI and should help to optimize the material selection for future spin-orbitronic devices.

**3:18PM P38.00003: Strong and Tunable Spin Lifetime Anisotropy in Dual-Gated Bilayer Graphene**
JINSONG XU (Presenter), TIANCONG ZHU, YUNQIU (KELLY) LUO, YUAN-MING LU, ROLAND KAWAKAMI, Ohio State University — We report the discovery of a strong and tunable spin lifetime anisotropy with excellent out-of-plane spin lifetimes up to 7.8 ns at 100 K in dual-gated bilayer graphene. Remarkably, this realizes the manipulation of spins in graphene by electrically-controlled spin-orbit fields, which is unexpected due to graphene's weak intrinsic spin-orbit coupling (~12 μeV). We utilize both the in-plane magnetic field Hanle precession and oblique Hanle precession measurements to directly compare the lifetimes of out-of-plane vs. in-plane spins. We find that near the charge neutrality point, the application of a perpendicular electric field opens a band gap and generates an out-of-plane spin-orbit field that stabilizes out-of-plane spins against spin relaxation, leading to a large spin lifetime anisotropy (defined as the ratio between out-of-plane and in-plane spin lifetime) up to ~12 at 100 K. This intriguing behavior occurs because of the unique spin-valley coupled band structure of bilayer graphene. Our results demonstrate the potential for highly tunable spintronic devices based on dual-gated 2D materials.

*NSF MRSEC under award number DMR-1420451

**3:30PM P38.00004: Ultrafast Spin and Charge Dynamics in Monolayer WSe₂-Graphene Heterostructures**
MICHAEL NEWBURGER (Presenter), YUNQIU (KELLY) LUO, Ohio State University, KATHLEEN MCCREARY, Naval Research Lab, Iwan MARTIN, ELIZABETH MCCORMICK, Ohio State University, BEREND JONKER, Naval Research Lab, ROLAND KAWAKAMI, Ohio State University — Monolayer transition metal dichalcogenides (TMDs) have garnered much attention due to their long spin/valley lifetimes and ability to optically excite spin/valley polarization. Additionally, one of the great strengths of TMDs is their ability to compliment other materials, such as graphene, by acting as a means of optical spin injection or proximity coupling. Recently proximity mediated charge transfer and optical spin injection has been demonstrated in TMD/graphene heterostructures. However, the spin transfer dynamics across a TMD/graphene interface remain largely unexplored.

Here we use time-resolved Kerr rotation (TRKR) microscopy to image the spatial dependence of spin/valley dynamics in monolayer WSe₂/graphene heterostructures. While the bare WSe₂ demonstrates long-lived spin valley lifetimes, spatial maps reveal a quenching of spin-valley signal at the WSe₂/graphene interfaces. Time delay scans show this quenched lifetime to be up to 3 orders of magnitude lower than in bare WSe₂. These interfaces also exhibit quenched photoluminescence and enhanced photoconductivity, demonstrating efficient charge transfer from WSe₂ to graphene. Consequently, we attribute the ultrafast spin/valley quenching to spin transfer by conducted charge carriers.

**3:42PM P38.00005: Organization and magnetic properties of mass-selected FePt nanoparticles deposited on epitaxially grown graphene on Ir(111)**
FLORENT TOURNUS (Presenter), PIERRE CAPIOD, LAURENT BARDOTTI, ALEXANDRE TAMION, VERONIQUE DUPUIS, Institut Lumière Matière, Université Lyon 1-CNRS, GILLES RENAUD, INAC, Univ. Grenoble Alpes - CEA, PHILIPPE OHRESSER, Synchrotron SOLEIL — The FePt alloy, when chemically ordered in the L1₀ phase, is among the magnetic materials displaying the highest magnetic anisotropy constant. Therefore it is a perfect candidate for ultra-high density magnetic storage applications, provided nanoparticles can be prepared in such a high anisotropy phase and organized in a 2D array. One path of bottom-up elaboration following a physical route consists in using template surfaces with specific sites regularly distributed. Such a 2D lattice can be obtained with the moiré (hexagonal lattice of 2.5 nm cell parameter) displayed by a graphene layer epitaxially grown on a Ir(111) surface [2]. For the first time, we have characterized the organization and the magnetic properties of FePt nanoparticles on such a moiré pattern. FePt/graphene/Ir(111) samples have been prepared using Low Energy Cluster Beam Deposition [3] of preformed size-selected FePt nanoparticles (around 2 nm diameter). We will discuss the organization of such particles on specific sites of the moiré lattice, as determined by grazing incidence x-ray scattering measurements [4]. The deposited nanoparticles are sensitive to the moiré pattern and we find that the resulting organization can be preserved up to temperatures around 700°C. Using X-ray Magnetic Circular Dichroism measurements, we will report a clear evolution of the magnetic properties of the FePt nanoparticles induced by annealing (anisotropy modification, interface effects between FePt and the graphene...), while the particles keep their individuality (no layer formation is observed).

which could be useful to manipulate spins for a long time at room temperature. Our work provides an insight into the physical origin of long-lived spin polarization in Weyl semimetals addition, we find the spin polarization is firmly pinned along the strong internal out-of-plane magnetic field induced by recombination rate and suppression of backscattering required by time-reversal and lattice symmetry operation. In this work, we show a room-temperature spin relaxation time of 1.2 ns (0.4 ns) in CVD-grown WTe2 (MoTe2) thin films using measurements allow us to calculate the momentum relaxation time as a function of carrier concentration and compare it to the spin lifetime [1]. We demonstrate the operation of WS2/graphene/fluorographene non-local spin valves and extract the spin lifetimes for a range of carrier concentrations by Hanle effect measurements. Four-terminal charge transport measurements allow us to calculate the momentum relaxation time as a function of carrier concentration and compare it to the spin lifetime. These data show that the Dyakonov-Perel' mechanism is the dominant spin relaxation mechanism for WS2/graphene/fluorographene devices. Without WS2, linear scaling between the spin and momentum lifetimes points to spin-flip scattering during strong elastic scattering events strongly coupled to the electron spin. We attribute the change in spin relaxation type in part with the inclusion of WS2 as a substrate to proximity induced spin-orbit coupling due to the adjacent WS2 layer, and we compare our data to the literature. [1] A.L. Friedman, et al. Carbon 131, 18-25 (2018).

**4:42PM P38.00008: Oscillated Dzyaloshinskii-Moriya interaction at hydrogenated Graphene/Co interfaces**

BAISHUN YANG (Presenter), QIRUI CUI, JINGHUA LIANG, HONGXIN YANG, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences — Magnetic topological structures such as chiral domain walls and Skyrmions are becoming a hot topic due to its potential application for future information storage. One of the key ingredient for the formation of these spintextures is the Dzyaloshinskii-Moriya interaction (DMI) in symmetry broken systems. Recently, it was reported that DMI can be induced in Co/Gr heterostructure due to the Rashba effect.[1] Considered that hydrogenated graphene (H-graphene) can enhance the spin orbit coupling of carbon atoms. Therefore, here, we propose to use interfaces between Co and H-graphene to tune DMI. Using first principles calculations, we find that the strength of DMI can be largely modulated by the concentration of H coverage on graphene, e.g., the anti-clockwise chiral of Co/Gr could be tuned to clockwise chiral in a Co(2ML)/1/2H-graphene with amplitude up to 1.0 meV/bond. Moreover, there is an obvious oscillation of DMI as a function of Co thickness ranging from 1ML to 7ML. The strength of DMI and this oscillation may origin from the change of SOC energy and electron filling in Co/Gr with different hydrogen concentration.


**4:30PM P38.00007: Examination of the magnetic interactions between divacant Fe dimers in graphene**

RONALD E PUTNAM (Presenter), Department of Physics, University of North Florida, ALEXANDER BALATSKY, Institute for Materials Science, Los Alamos National Laboratory, JASON HARALDSEN, Department of Physics, University of North Florida — In this study, we investigate the isolated magnetic interactions between two identical Fe atoms substituted into graphene. Using density functional theory, we simulated the electronic and magnetic properties for a supercell of graphene with variably-spaced iron atoms in the divacant configuration. Overall, we find that the exchange interaction between the two Fe atoms fluctuates from ferromagnetic to antiferromagnetic as a function of the spatial distance in the armchair direction. Given the induced magnetic moment and increased density of states at the Fermi level by the surrounding carbon atoms, we conclude that the exchange interactions between the Fe atoms can be characterized by an RKKY-like interaction. Furthermore, we examined the same interactions for Fe atoms along the zig-zag direction in graphene and find no evidence for an RKKY interaction as this system shows standard superexchange between the transition-metal impurities. Therefore, we determine that Fe-substituted graphene produces a directional-dependent spin interaction, which may provide stability to spintronic and multifunctional devices and applications for graphene.

*Institute for Materials Science at Los Alamos

**4:42PM P38.00008: Spin relaxation and proximity effect in WS2/graphene/fluorographene non-local spin valves**

ADAM FRIEDMAN (Presenter), Laboratory for Physical Sciences, KATHLEEN MCCREARY, JEREMY T ROBINSON, OLAF M VAN TERVE, BEREND JONKER, US Naval Research Laboratory — Control of the spin relaxation in graphene-based structures is necessary to achieve the envisioned utility of graphene in future spintronic devices beyond Moore's law. Proximity induced spin relaxation caused by contact to a high spin-orbit material, such as WS2, offers a promising avenue to manipulate the spin lifetime [1]. We demonstrate the operation of WS2/graphene/fluorographene non-local spin valves and extract the spin lifetimes for a range of carrier concentrations by Hanle effect measurements. Four-terminal charge transport measurements allow us to calculate the momentum relaxation time as a function of carrier concentration and compare it to the spin lifetime. These data show that the Dyakonov-Perel' mechanism is the dominant spin relaxation mechanism for WS2/graphene/fluorographene devices. Without WS2, linear scaling between the spin and momentum lifetimes points to spin-flip scattering during strong elastic scattering events strongly coupled to the electron spin. We attribute the change in spin relaxation type in part with the inclusion of WS2 as a substrate to proximity induced spin-orbit coupling due to the adjacent WS2 layer, and we compare our data to the literature. [1] A.L. Friedman, et al. Carbon 131, 18-25 (2018).

**4:54PM P38.00009: Room-temperature long-lived spin polarization in Weyl semimetal thin film**

QISHENG WANG (Presenter), HYUNSOO YANG, Department of Electrical and Computer Engineering, and NUSNNI-NanoCore, National University of Singapore — The Weyl semimetals WTe2 and MoTe2 show a great potential in generating large spin currents since they possess topologically-protected spin-polarized states and can carry a very large current density. In addition, the intrinsic noncentrosymmetry of WTe2 and MoTe2 endows with a unique property of crystal symmetry-controlled spin-orbit torques. An important question to be answered for developing spintronic devices is how spins relax in WTe2 and MoTe2. In this work, we show a room-temperature spin relaxation time of 1.2 ns (0.4 ns) in CVD-grown WTe2 (MoTe2) thin films using the time-resolved Kerr rotation (TRKR). Based on ab initio calculation, we identify a mechanism of long-lived spin polarization resulting from a large spin splitting (~40 meV) around the bottom of the conduction band, low electron-hole recombination rate and suppression of backscattering required by time-reversal and lattice symmetry operation. In addition, we find the spin polarization is firmly pinned along the strong internal out-of-plane magnetic field induced by large spin splitting. Our work provides an insight into the physical origin of long-lived spin polarization in Weyl semimetals which could be useful to manipulate spins for a long time at room temperature.
5:06PM P38.00010: Gate-tunable magnetism of C adatoms on graphene* JOHANNES NOKELAINEN (Presenter), Lappeenranta University of Technology, IGOR ROZHANSKY, Ioffe Institute, BERNARDO BARBIELLINI, ERKKI LAHDERANTA, KATARIINA PUSSI, Lappeenranta University of Technology — We have performed density functional theory calculations of graphene decorated with carbon adatoms, which bind at the bridge site of a C–C bond. Earlier studies have shown that the C adatoms have magnetic moments and have suggested the possibility of ferromagnetism with high Curie temperature. Here we propose to use a gate voltage to fine tune the magnetic moments from zero to 1\(\mu_B\) while changing the magnetic coupling from antiferromagnetism to ferromagnetism and again to antiferromagnetism. These results are rationalized within the Stoner and RKKY models. When the SCAN meta-GGA correction is used, the magnetic moments for zero gate voltage are reduced and the Stoner band ferromagnetism is slightly weakened in the ferromagnetic region.

*This work was supported by the Academy of Finland Grants No. 277829, 318500 and benefited from the generously allocated computer time at CSC — Finnish IT Center for Science.

5:18PM P38.00011: Quench dynamics of localized zero energy states in graphene* DEEPAK IYER (Presenter), Physics and Astronomy, Bucknell University, MATTHEW FOSTER, Physics and Astronomy, Rice University — In an external magnetic field, graphene forms Landau levels with an 'anomalous' level spacing due to the low energy linear dispersion. This creates a significant difference between the Landau level splitting and Zeeman splitting, allowing for nontrivial spin dynamics within a Landau level. It is expected that the ground state of the half-filled zeroth Landau level supports Skyrmions as low energy charged excitations, which can in principle exhibit collective dynamics under an external time dependent electromagnetic field via direct coupling to the Skyrmion (topological) charge density. In order to understand the dynamics, we study the related problem of massive Dirac fermions in two dimensions after a quench from an initial state containing localized zero-modes (vortices, in particular) into a homogeneous system with a Haldane mass. The Haldane term gives the leading order effect of a high-frequency drive. The one dimensional version of the problem with mass defects also leads to localized zero modes, and fractional charge. We follow the time evolution of various order parameters in these models and look for dynamical signatures of these zero modes.

*The authors acknowledge funding from the U.S. Army Research Office (Grant W911NF-17-1-0259) and NSF CAREER Grant No. DMR-1552327

Wednesday, March 6, 2019 2:30 PM - 5:06 PM

Session P39 GMAG DCMP DMP: Magnetism and Spins in Semiconductors BCEC 207 - Yu-Sheng Ou, University of Delaware - Tag(s): Focus

2:30PM P39.00001: First-principles investigation of the magnetic transition in Fe-doped GaSb and InSb HIKARI SHINYA (Presenter), Yokohama National University, TETSUYA FUKUSHIMA, AKIRA MASAGO, KAZUNORI SATO, Osaka University, HIROSHI KATAYAMA-YOSHIDA, The University of Tokyo — Recently, Fe-doped semiconductors have been attracting much attention as ferromagnetic semiconductors due to the possibility of high Curie, fascinating functions such as low power consumption and high-speed operation, and fabrication of both n- and p-type. In this study, we have focused on GaSb and InSb as host semiconductors, and performed density functional theory calculations using the Korringa-Kohn-Rostoker Green's function method with the coherent potential approximation (KKR-CPA). Our calculations reveal that, (Ga,Fe)Sb and (In,Fe)Sb show complex magnetic properties, which are determined by the correlation between magnetic exchange coupling constants and chemical pair interactions. Isoelectronic Fe-doped GaSb and InSb show strong antiferromagnetic interactions that originate from the super-exchange mechanism works between the Fe atoms. By modulating the chemical potentials—i.e., by n- or p-type doping—, the magnetic property can be changed drastically from antiferromagnetism to ferromagnetism, because the ferromagnetic double exchange mechanism becomes dominant. This transition can be well understood in terms of the Alexander-Anderson-Moriya mechanism. Our calculations indicate the possibility of manipulating (Ga,Fe)Sb and (In,Fe)Sb to achieve high Curie temperatures.
2:42PM P39.00002: A multi-bands Hubbard model of intrinsic long range magnetic order in diluted magnetic semiconductors* WEIYI GONG (Presenter), CHING-HIM LEUNG, CHUEN-KEUNG SIN, JINGZHAO ZHANG, XIAODONG ZHANG, BIN XI, JUNYI ZHU, Physics, The Chinese University of Hong Kong — Recently, new long range ferromagnetic order has been discovered both experimentally and theoretically in carrier free semiconductor. However, there lacks quantitative model to explain the coupling mechanism that may extend to 7th nearest neighbors. In this work, we derived a multi-bands Hubbard model to explain the long range mechanism mediated by localized d states. Based on this model and combining with DFT calculations, we discovered a long range AFM order in DMS systems. Our model provides fundamental understandings of the new type of magnetic order in DMS.

*We are grateful for the financial support of Chinese University of Hong Kong (CUHK) (Grant No.4053084), University Grants Committee of Hong Kong (ECS Grant No. 24300814, GRF Grant No. 14319716, GRF Grant No. 14307018), and start-up funding of CUHK.

2:54PM P39.00003: Theoretical prediction of maximum Curie temperatures of Fe-based dilute magnetic semiconductors by first-principles calculations HIKARI SHINYA, Yokohama National University, TETSUYA FUKUSHIMA (Presenter), AKIRA MASAGO, KAZUNORI SATO, Osaka University, HIROSHI KATAYAMA-YOSHIDA, The University of Tokyo — Recently, Fe-based dilute magnetic semiconductors (DMSs), such as (In,Fe)As, (In,Fe)Sb and (Ga,Fe)Sb, have strongly attracted scientific and industrial attention, because of their high Curie temperatures and n-type carrier induced ferromagnetism. Several experiments showed that the ferromagnetic properties in Fe-based DMSs are strongly related to the inhomogeneous distribution of the Fe atoms, i.e., the Curie temperatures are modulated by the spinodal nano-decomposition, depending on crystal growth conditions. In this work, we predict the maximum Curie temperatures of the Fe-based DMSs with the spinodal nano-decomposition, on the basis of the Korringa-Kohn-Rostoker (KKR) Green's function method within the density functional theory. The magnetic exchange coupling constants between the Fe atoms are calculated by the Liechtenstein's formula, and then the Curie temperatures are estimated by the mean field approximation. It is found, from our calculations, that one can expect very high Curie temperatures beyond the room temperature in Fe-based DMSs, if the many Fe atoms gather together in the host semiconductor with keeping the zinc-blende structure and additional n- or p-type carriers are introduced.

3:06PM P39.00004: Element- and momentum-resolved electronic structure of the dilute magnetic semiconductor manganese doped gallium arsenide [Invited] SLAVOMIR NEMSAK (Presenter), Advanced Light Source, Lawrence Berkeley National Laboratory, JAN MINÁR, University of West Bohemia, CHARLES S FADLEY, Department of Physics, University of California, Davis — The dilute magnetic semiconductors have shown great promise in spin-based electronics applications due to their potential for ferromagnetic order at room temperature, and various unique switching and spin-dependent conductivity properties. However, the precise mechanism by which the transition-metal doping produces ferromagnetism has been controversial. We have studied a dilute magnetic semiconductor (5% manganese-doped gallium arsenide) with Bragg-reflection standing-wave hard X-ray angle-resolved photoemission spectroscopy (SW-HARPES), and resolved its electronic structure into element- and momentum- resolved components. The measured valence band intensities have been projected into element-resolved components using analogous photon energy scans of Ga 3d, Mn 2p, and As 3d core levels, with results in excellent agreement with element-projected Bloch spectral functions, further clarifying the electronic structure of this prototypical material. We will further discuss the capabilities of the SW-HARPES technique, which should be broadly applicable to other multi-element materials.

Reference
Nemsak, Gehlmann, Kuo, Lin, Schlueter, Mlynczak, Lee, Plucinski, Ebert, Di Marco, Minár, Schneider, Fadley, Nat. Comm. 9, 1-8 (2018)

3:42PM P39.00005: Ferromagnetic Stabilization of Eu-doped GaN Enhanced by Ga-vacancies AKIRA MASAGO (Presenter), CSRN, Osaka University, HIKARI SHINYA, Graduate School of Engineering, Yokohama National University, TETSUYA FUKUSHIMA, INSD, Osaka University, KAZUNORI SATO, Graduate School of Engineering, Osaka University, HIROSHI KATAYAMA-YOSHIDA, CSRN, The University of Tokyo — We report that the ferromagnetic states are stabilized by the double exchange interaction which enhanced by partially occupied N-2p hole band caused by Ga-vacancies in Eu-doped GaN, based on self-interaction-corrected (SIC) local density approximation. Eu-doped GaN is renowned for red light emitting diodes (LEDs), whereas it is interesting as a circular-polarized emission in the magnetic materials. In this study, we used a constant volume assumption and the coherent potential approximation (CPA) in the Korringa-Kohn-Rostoker (KKR) method with SIC. As a result, it indicates that electron-hole doping enhances the ferromagnetic states, because the dominant magnetic interaction is changed from Zener's p-f exchange interaction to Zener's double exchange interaction caused by the partially occupied N-2p band. In the enhancement, a major contribution to the magnetism is derived from the Ga-vacancies more than magnetic impurities Eu, which coupled with N anti-ferromagnetically.
4:06PM P39.00007: Biaxial-stress driven tetragonal symmetry breaking in and high-temperature ferromagnetic semiconductor from half-metallic CrO$_2$ * XIANG-BO XIAO (Presenter), BANG-GUI LIU, Institute of Physics — Here, we find through first-principles investigation that when a biaxial compressive stress is applied on rutile CrO$_2$, the density of states at the Fermi level decreases with the in-plane compressive strain, there is a structural phase transition to an orthorhombic phase at the strain of -5.6%, and then appears an electronic phase transition to a semiconductor phase at -6.1%. Further analysis shows that this structural transition, accompanied by the tetragonal symmetry breaking, is induced by the stress-driven distortion and rotation of the oxygen octahedron of Cr, and the half-metal-semiconductor transition originates from the enhancement of the crystal field splitting due to the structural change. Importantly, our systematic total-energy comparison indicates that the ferromagnetic Curie temperature remains almost independent of the strain, near 400 K. This biaxial stress can be realized by applying biaxial pressure or growing the CrO$_2$ epitaxially on appropriate substrates.

*This work is supported by the Nature Science Foundation of China (Grant No. 11574366), by the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No.XDB07000000), and by the Department of Science and Technology of China (Grant No. 2016YFA0300701).

4:18PM P39.00008: Design of Super-High-T$_C$ high-entropy ferromagnetic semiconductors in Fe-doped III-V compound semiconductors by spinodal nano-decomposition and volume compensated codoping HIKARI SHINYA, Yokohama National University, TETSUYA FUKUSHIMA, AKIRA MASAGO, KAZUNORI SATO, Osaka University, HIROSHI KATAYAMA-YOSHIDA (Presenter), The University of Tokyo — Based on the three general design rules of (1) the volume compensations [VC] by codoping, (2) spinodal nano-decomposition [SND], and (3) high-entropy ferromagnetic semiconductors [HEFS], we design the super-high-T$_C$ (T$_C$ > 1000K) HEFS in Fe-doped III-V compound semiconductors by computational nano-materials design. The substitutional(S) Fe impurity [Fe(S)] reduces the volume, while the interstitial (I = tetrahedral or octahedral site) Fe impurity [Fe(I)] expands the volume in III-V compound semiconductors, which is called volume compensation. The solubilities of the Fe(S) and Fe(I) are low due to the positive formation energy, so that the SND occurs due to the positive mixing energy. Based on the codoping of isoelectric Fe(S) and triple donors of Fe(I) more than 15~20%, we design the HEFS with super-high-T$_C$ based on the strong ferromagnetic double exchange interactions in SND.

4:30PM P39.00009: Interlayer Exchange Coupling Mediated by a Bulk Rashba Semiconductor * MAHMOUD ASMAR (Presenter), WANG KONG TSE, Physics and Astronomy and The Center for Materials for Information Technology, The University of Alabama, Tuscaloosa. — Spin orbit coupling (SOC) in solids is a crucial ingredient in spintronic and magnetoelectronic phenomena. An example of SOC in solids is the 3D Rashba effect that arises in materials with broken inversion symmetry such as BiTeX (X=I,Cl and Br). These bismuth tellurohalides exhibit a giant Rashba coupling and are known as bulk Rashba semiconductors. In this talk, we present a RKKY theory for the interlayer exchange coupling in ferromagnet-BiTeX-ferromagnet trilayers. Due to the helical in-plane spin textures and associated Berry phase of the low-energy electrons, the interlayer exchange coupling as a function of layer thickness is found to exhibit unconventional dependence on the Rashba SOC.

*This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Early Career Award #DE-SC0019326.
4:42PM P39.00010: Bias dependence of spin accumulation voltage in a non-degenerate Si spin valve  
SOOBEOM LEE (Presenter), FABIEN RORTAIS, RYO OHSHIMA, YUICHIRO ANDO, Department of Electronic Science and Engineering, Kyoto University, SHINJI MIWA, YOSHISHIGE SUZUKI, Graduate School of Engineering Science, Osaka University, HAYATO KOIKE, Advanced Products Development Center, TDK Corporation, MASASHI SHIRAISHI, Department of Electronic Science and Engineering, Kyoto University — Si spintronics attracts great attention, and recent achievements in the field, such as the room temperature (RT) operation of spin MOSFET and the output spin voltage of more than 1 mV at RT due to the spin drift effect [1, 2], have been done by using non-degenerate (ND) Si. In the previous research [2], the spin voltages exhibited saturation under a high electric current ($I_{inj}$) injection regime, suggesting a possibility of modification of spin transport properties in the ND Si. Hence, we clarified the origin of the $I_{inj}$ dependence of the spin signals in the ND Si in this study.

The non-local 4-terminal measurement and the Hall measurement revealed that spin lifetime of the ND Si channel were independent of the $I_{inj}$ at RT. Meanwhile, interface resistance of Fe/MgO/Si contact was reduced to the same order of spin resistance of the Si channel. A model calculation considering these results nicely reproduced the experimental $I_{inj}$ dependence [3]. The detail will be discussed in the presentation.


4:54PM P39.00011: Magnetotransport in InSb nanowires with ferromagnetic contacts  
ZEDONG YANG (Presenter), University of Minnesota, YIFAN JIANG, University of Pittsburgh, DIANA CAR, SASA GAZIBEGOVIC, Eindhoven University of Technology, PAUL CROWELL, University of Minnesota, SERGEY M FROLOV, University of Pittsburgh, ERIK P. A. M. BAKkers, Eindhoven University of Technology, VLAD S Pribiag, University of Minnesota — InSb semiconductor nanowires are a promising and intensely-studied platform for investigating Majorana bound states [1]. Their strong spin-orbit coupling also makes them interesting for all-electrical control of single spins [2]. Moreover, owing to their relatively long mean free paths and quasi-one-dimensionality, InSb nanowires also have great potential for novel devices which could allow electrical control of spin currents. Motivated by these intriguing possibilities, we fabricated InSb nanowire devices with ferromagnetic contacts, which show evidence of ballistic transport. We report hysteretic features in the magneto-conductance measured at different back-gate voltages, and discuss the possible physical mechanisms responsible for these observations.


Wednesday, March 6, 2019 2:30 PM - 5:06 PM

Session P40 GMAG DMP DCOMP: Emergent Magnetism in Oxide Films and Heterostructures  
BCEC 208 - Jian Liu, University of Tennessee - Tag(s): Focus

2:30PM P40.00001: Decoupling the Strain and Doping Effects on Magnetic Anisotropy in La$_x$Sr$_{1-x}$MnO$_3$ via ferroelectric Polarization Control*  
YIFEI HAO (Presenter), ANIL K RAJAPITAMAHUNI, LINGLING TAO, XIAOSHAN XU, EVGENY Y TSYMBAL, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln — In this study, we use epitaxial Pb(Zr,Ti)O$_3$ (PZT)/ La$_{0.8}$Sr$_{0.2}$MnO$_3$ (LSMO) heterostructures as a model system to decouple the effects of epitaxial strain and charge doping on the magnetocrystalline anisotropy (MCA) in LSMO. By switching the polarization of PZT, we have achieved nonvolatile modulation of the biaxial in-plane magnetic anisotropy in LSMO, as revealed by planar Hall effect studies. The magnetic anisotropy energy (MAE) in the hole accumulation state is enhanced by about 22% compared to the depletion state, in quantitative agreement with the DFT calculations. In contrast, the MAE extracted in chemically doped LSMO films is significantly lower than the theoretical prediction, clearly illustrating the difference between the electric field effect doping and chemical substitution. The discrepancy has been attributed to the different lattice parameters for bulk LSMO at these compositions, where the higher doping sample is subjected to a larger tensile strain on SrTiO$_3$ substrates, concomitantly lowering the MCA. Our result provides the first combined experimental and theoretical study that unambiguously identifies the role of charge doping in determining the MCA in LSMO.

*This work was supported by NSF through Grant No. DMR-1710461 and MRSEC Grant No. DMR-1420645.
Ultra-low-power magnetization rotation by orbital selection at a La$_{0.67}$Sr$_{0.33}$MnO$_3$/SrTiO$_3$ interface*

LE DUC ANH (Presenter), TAKASHI YAMASHITA, HIROKI YAMASAKI, DAISEI ARAKI, MUNETOSHI SEKI, HITOSHI TABATA, MASAAKI TANAKA, SHINOBU OHYA, University of Tokyo — Reducing the power consumption for magnetization switching is essential for the realization of energy-saving spin devices. Here, using a magnetic tunnel junction consisting of La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO) / SrTiO$_3$ (STO) / LSMO grown on STO (001), we demonstrate a deterministic and magnetic-field-free 90°-magnetization switching solely by applying an extremely small electric field of 0.05 V/nm on the tunnel barrier and an infinitesimal current density of ~ 10$^{-2}$ A/cm$^2$, which is ~8 orders of magnitude smaller than that in the present magnetic random access memory. We reveal that this magnetization rotation is induced by a sharp change in the magnetic anisotropy (MA), which occurs at the bias voltage $V$ of ~ ±0.1 V. By measuring the angular dependence of the density of states on the magnetization direction for the same device, we show that the change of MA occurs when the quasi-Fermi level ($E_F$) moves from $e_g$ to $t_{2g}$ bands at the LSMO/STO interface with increasing $|V|$ [1]. These findings suggest that highly efficient magnetization control can be realized by designing materials so that the $E_F$ lies close to the band edges of different-symmetry orbitals.


*This work was supported by Grants-in-Aid for Scientific Research, CREST of JST, and Spin-RNJ.

Oxygen Vacancies Control Interface Magnetism in La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrTiO$_3$ Heterostructures*

JUAN I. BELTRAN, JAVIER GRANDAL, JAVIER TORNOS, CARLOS LEON, JACOBO SANTAMARÍA, MARIA VARELA (Presenter), Complutense University, M. CARMEN MUÑOZ, ICMM-CSIC, Spain — O vacancies strongly influence the properties of complex oxides and give rise to novel and unexpected phenomena. Here we combine first-principles density-functional theory with high spatial resolution electron energy-loss spectroscopy and energy-loss magnetic chiral dichroism (EMCD) to show that O vacancies control interface magnetism in La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrTiO$_3$ heterostructures grown by high-pressure O$_2$ sputtering. EMCD measurements obtained at low temperature (<100K) are sensitive to the local magnetization with atomic resolution, revealing the formation of Ti and the increase of Mn magnetic moments near the interface. Comparison to the calculated electronic properties unambiguously demonstrates the O vacancy origin of the enhanced interface magnetism. The ideal interface - cleavage of bulk components - shows no charge transfer to the STO, while O vacancies induce finite occupancy of the Ti d-orbitals and hole depletion at the Mn interface planes, enhancing interface magnetism. Our results indicate that the control of O vacancies is a promising approach to improve the magnetic properties of LSMO/STO interfaces.

*We acknowledge financial support by the Spanish Ministerio de Ciencia, Innovación y Universidades through Grants MINECO/FEDER MAT2015-66888-C3-1R and 3R.

Local Control of Magneto-crystalline Anisotropy of La$_{0.7}$Sr$_{0.3}$MnO$_3$ Thin Films through Ion Implantation*

MICHAEL STEVEN LEE, Materials Science and Engineering, University of California, Davis, RAJESH V CHOPDEKAR, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, YAYOI TAKAMURA (Presenter), Materials Science and Engineering, University of California, Davis — Control of the functional properties of thin films, including the magneto-crystalline anisotropy, is critical for the development of future memory and spintronic devices. Perovskite oxides offer stimulus-sensitive properties due to the strong coupling between their spin, orbital, lattice, and charge degrees of freedom. In this work, we found that ion implantation of La$_{0.7}$Sr$_{0.3}$MnO$_3$ films induces changes in the magnetic anisotropy by causing an out-of-plane lattice expansion while the film remains coherently strained to the substrate. However, the ion implantation also leads to a reduction in Curie temperature and saturation magnetization. X-ray absorption spectroscopy shows this degradation in magnetic properties is in part due to the reduced Mn oxidation state, in addition to crystalline damage. With the proper substrate selection and optimization of ion implantation conditions, the easy axis of the film can be tuned from in-plane to out-of-plane while minimizing the reduction in magnetization. These results may enable the design of unique magnetic spin textures such as magnetic skyrmions in a single layer of material containing adjacent regions of in-plane and out-of-plane magnetization.

*This work was supported by the National Science Foundation (DMR 0747896 & 1411250).
Precipitating the unique transition from paramagnet to ferromagnet found in LaCoO₃ films. In essence, spin state order is frozen by epitaxial strain, concurrent order of Co charge and spin states arises, as shown by a combination of resonant x-ray scattering and as observed in the x-ray absorption near edge structure (XANES) and stabilize an ordered arrangement of Co sites. In turn, symmetry from rhombohedral in bulk to monoclinic. These structural distortions reduce the Co-O orbital hybridization strain lengthens the in-plane Co-O bonds, thereby distorting the cobalt containing oxygen octahedra, and lowers the observed magnetic phase transition, from antiferromagnetic at 5 unit cells (uc) of LMO or below to ferromagnetic at 6 ucs or above. Here, we offer an atomic resolution picture of electronic reconstruction by quantifying the charge distribution across this abrupt magnetic transition using STEM-EELS. We find that the electronic reconstruction is confined within the first 2 ucs of LMO from the interface, and more importantly, it is robust against oxygen non-stoichiometry. When restoring stoichiometry, we achieve a ferromagnetic insulating state in LMO films with a thickness as thin as 2 nm, making LMO readily applicable as barriers in spin filters.


*Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. DOE Office of Science by Argonne National Laboratory (ANL), was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357. Use of Blues, a high-performance computing cluster operated by the Laboratory Computing Resource Center at ANL is also acknowledged.

Size restricted magnetotransport in the non-magnetic delafossite metals PdCoO₂ and PtCoO₂

NABHANILA NANDI (Presenter), Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, THOMAS SCAFFIDI, Department of Physics, University of California, Berkeley, California 94720, USA, SEUNGHYUN KHAM, PALLAVI KUSHWAHA, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, JOEL MOORE, Department of Physics, University of California, Berkeley, California 94720, USA, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — Ultra-pure delafossite metals can present bulk mean free paths as long as tens of microns, long enough such that the momentum conservation of the electron fluid might play a role in electrical transport [1]. As the signatures of this are most prominent in the mesoscopic limit, we use focussed ion beam (FIB) techniques to thin bulk samples down to widths as small as submicron, much smaller than the bulk mean free path. In this talk I will present magnetotransport measurements in these highly-conducting delafossites, specifically PdCoO₂ and PdCoO₂, at the mesoscopic limit. Magnetic field introduces a variable length-scale, the cyclotron radius, to the system which can be used to tune through different transport regimes. I will discuss the ballistic and hydrodynamic signatures in the transport that in principle become accessible through magnetic field tuning in such mesoscopic samples.

Emergent Ferromagnetism in (111)-oriented CaRuO3/CaMnO3 superlattices* MARGARET KANE (Presenter), CHARLES FLINT, Material Science and Engineering, Stanford University, ARTURAS VAILIONIS, Geballe Laboratory for Advanced Materials, Stanford University, ALEXANDER GRUTTER, National Institute of Standards and Technology, YURI SUZUKI, Applied Physics, Stanford University — Emergent ferromagnetism has been observed at the interface of CaRuO3 (CRO), a paramagnetic metal, and CaMnO3 (CMO), an antiferromagnetic insulator. The leakage of itinerant CRO electrons into the CMO results in a double exchange interaction among interfacial Mn. Since CMO is a G-type antiferromagnet, films grown in (111) direction should have fully uncompensated surfaces and higher interfacial moments than compensated (001) surfaces. We demonstrate the synthesis and characterization of (111) CRO/CMO superlattices with 3 layers of CRO and 3-19 layers of CMO. To grow smooth (111) superlattices, we developed an interval pulsed laser deposition process. SQUID magnetometry measurements indicate larger interfacial Mn moments in our (111) superlattices compared to (001) superlattices. Coercive fields of the superlattice are similar, regardless of CMO thickness, and with increasing CMO thickness, the exchange bias field in the magnetization loops increases. Since CMO and CRO are isovalent, CRO/CMO systems do not exhibit a polarity mismatch across the interface, providing a model system to explore emergent ferromagnetism.

*Funded by Department of Energy, Director, Office of Science, Office of Basic Energy Sciences, Div. of Mat. Sci. and Eng., under Contract No. DESC0008505 and NSF GRFP.

Strain induced topological Hall effect of SrRuO3 single-layered thin films LUDI MIAO (Presenter), HARI NAIR, NATHANIEL SCHREIBER, JACOB P RUF, YINGFEI LI, CYRUS ZELEDON, SHENGWEI JIANG, BERIT GOODGE, ISMAIL EL BAGGARI, KIN FAI MAK, JIE SHAN, LENA KOURKOUTIS, DARRELL G. SCHLOM, KYLE M SHEN, Cornell University — Topology in condensed matter physics has led to fruitful areas such as topological insulators, Majorana fermions and valleytronics. Among them, the topological Hall effect (THE) of magnetic materials has attracted much attention due to the discovery of magnetic skyrmions, a topologically protected spin texture that is promising for future magnetic/electronic devices. Recently, a THE has been observed at the interface between a ferromagnetic SrRuO3 (SRO) and a heavy metal SrIrO3 (SIO), although the spin texture of both bulk SRO and bulk SIO are topologically trivial. Here, we will demonstrate the discovery of an unexpected THE on perovskite SRO single-layered films stabilized by molecular beam epitaxy. We will show that the epitaxial strain in SRO films stabilizes a non-coplanar spin texture and leads to the topologically non-trivial phenomenon. SRO is a widely-used material in complex oxide heterostructures. Our results can potentially lead to major progresses in novel phenomena in SRO-based heterostructures as well as the applications of next generation all-oxide electronic and magnetic devices.

Anisotropic magnetoresistance in Nb: SrTiO3 thin films under epitaxial strain LUCÍA IGLESIAS (Presenter), FRANCISCO RIVADULLA, CIQUIS, University of Santiago de Compostela — We report the effect of epitaxial strain and cationic vacancies on the anisotropic magnetoresistance (AMR) of SrTiO3 (STO) thin films. Cationic vacancies affect the structural properties of the STO thin films, determining the rotation pattern of the TiO6 octahedra [1], and produce a characteristic minimum at T* in the temperature dependence of the electrical resistivity of this material. Our results show a change of sign of the AMR, from negative above T*, to positive below this temperature. Seebeck coefficient measurements do not support an interpretation based on the Kondo effect. We will discuss the possible existence and the nature of a magnetic phase below T*. As the effect is only observed in thin films <20 nm, and it is lost in thicker films (>35 nm), this suggests a contribution from accumulated defects close to the interface with the substrate.

4:54 PM P40.00011: Magnetic and Electrical Transport Properties of YbFe$_2$O$_4$*  
RAM RAI (Presenter), J HINZ, MICHELLE K PASCOLINI, JAMES PAWLAK, M DEMARCO, Buffalo State College —

We present magnetic properties, Mössbauer, resistivity, magnetoresistance, and dielectric properties of a polycrystalline YbFe$_2$O$_4$ prepared by an electron-beam assisted solid state reaction. The ferrimagnetic transition temperature of YbFe$_2$O$_4$ was measured at 242 K, followed by the two low-temperature transitions at ~200 K and 70 K, respectively. The M-H hysteresis loops exhibit a strong temperature dependence with the strongest coercive field and residual magnetization at ~100 K. The temperature dependence of the magnetic properties suggests that YbFe$_2$O$_4$ has a complex magnetic phase below 100 K. Room temperature Mössbauer measurement indicates the presence of Fe$^{2+}$ and Fe$^{3+}$ ions in the sample. Resistivity of YbFe$_2$O$_4$ has been analyzed based on Mott's variable-range hopping model. The magnetoresistance effects in the ferrimagnetic state were observed and the effects could be attributed to the field-induced changes in the electron hopping processes. We also discuss the temperature and frequency dependence of the dielectric constant of YbFe$_2$O$_4$, which were found to be strongly influenced by the contact effects, indicating no evidence of the intrinsic ferroelectricity.

*National Science Foundation (DMR-1406766)

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P41 GMAG DMP: Thermal Spintronics BCEC 209 - Joseph P Heremans, Ohio State Univ - Columbus - Tag(s): Focus 2:30PM P41.00001: Controlling heat by spin caloritronics*  
[Invited] KEN-ICHI UCHIDA (Presenter), National Institute for Materials Science — Interaction between spin and heat is actively studied in the field of spin caloritronics from the viewpoints of both fundamental physics and applications. Early studies on spin caloritronics mainly focused on phenomena that generate a spin current from a heat current, such as the spin Seebeck effect, toward the development of versatile thermoelectric generators. In contrast, there are many heat-generation phenomena that use spin and charge currents as input, e.g., the spin Peltier effect, which is the reciprocal of the spin Seebeck effect; the anisotropic magneto-Peltier effect, in which the charge-to-heat current conversion efficiency depends on the angle between the charge current and magnetization in a ferromagnet; and the anomalous Ettingshausen effect, in which a heat current is generated in the direction perpendicular to both the applied charge current and magnetization. Recently, we successfully observed the thermal response from these phenomena by means of an active infrared emission microscopy called the lock-in thermography, and demonstrated thermal control functions that cannot be actualized without using spins [1-4]. In this talk, we review our recent experimental results by focusing particularly on the thermal imaging measurements of the spin-caloritronic phenomena.


*This work was partially supported by CREST “Creation of Innovative Core Technologies for Nano-enabled Thermal Management” (JPMJCR1711) from Japan Science and Technology Agency.

3:06PM P41.00002: Spin-Seebeck Effects in Pyrochlore Iridates  
BOWEN MA (Presenter), University of Texas at Austin, BENEDETTA FLEBUS, UCLA Foundation, GREGORY FIETE, University of Texas at Austin — The spin-Seebeck effect (SSE) refers to voltage signals induced by the Inverse Spin Hall Effect (ISHE), with thermally driven spin currents through adjacent magnetic systems. It has been studied before mostly in collinear magnetic systems. Here, we present a general theory of the SSE in the case of a non-collinear antiferromagnetic insulator (AFI)/non-magnetic metal heterostructure. In our model, we apply a periodic boundary condition in the transverse plane and an open boundary condition at the interface. If there is a non-equilibrium temperature difference within the two materials, the exchange coupling between the electrons in the metal and magnons of interfacial spins in the AFI can give rise to a longitudinal spin current across the system. We also numerically compute the spin current using a pyrochlore iridate as the AFI where the spin configuration is the all-in-all-out (AIAO) ground state. We compare the results of different crystal interfaces arising from different crystalline orientations to make a connection with experiments and practical devices.
Spin Seebeck effect induced by antiferromagnetic magnons and spin fluctuations in epitaxial FeF₂ films

JUNXUE LI (Presenter), Department of Physics and Astronomy, University of California, Riverside, CA 92521, USA, ZHONG SHI, School of Physics Science and Engineering, Tongji University, Shanghai 200092, China, VICTOR ORTIZ, MOHAMMED ALDOSARY, CLIFF CHEN, PENG WEI, JING SHI, Department of Physics and Astronomy, University of California, Riverside, CA 92521, USA — Recently, the spin Seebeck effect (SSE) in antiferromagnetic (AFM) Cr₂O₃ and MnF₂ has been reported and the signals were found to rise significantly above the spin-flop (SF) field. However, it is still unclear whether the SSE requires an induced magnetic moment or just the presence of AFM magnons. Here we report a study of the SSE of FeF₂/Pt heterostructures in which FeF₂ is an insulating AFM epitaxial film. The high SF field (42 T) of FeF₂ makes it a perfect candidate for studying the SSE below the SF field. The AFM properties of FeF₂ film are characterized by exchange bias. The SSE signal of FeF₂/Pt under different magnetic fields shows very similar temperature-dependent behaviors. First, there is a peak at around 11.6 K due to AFM-magnons’ contribution. Second, we observe a “bump” at the AFM ordering temperature (70 K), beyond which the SSE signal decays and persists up to 250 K under high magnetic fields, indicating that short-range spin fluctuations also contribute to the SSE signal.

This work was supported as part of the SHINES, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences under Award No. SC0012670. This work was also supported by the Startup Funds from University of California, Riverside.

Spin Seebeck imaging of spin-torque switching in antiferromagnetic Pt/NiO/Pt heterostructures

ISAIAH GRAY (Presenter), Applied and Engineering Physics, Cornell University, TAKAHIRO MORIYAMA, Institute for Chemical Research, Kyoto University, NIKHIL SIVADAS, Applied and Engineering Physics, Cornell University, RYAN NEED, BRIAN KIRBY, NIST Center for Neutron Research, National Institute for Standards and Technology, DAVID LOW, Applied and Engineering Physics, Cornell University, GREGORY STIEHL, Department of Physics, Cornell University, JOHN HERON, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, DANIEL RALPH, KATJA NOWACK, Department of Physics, Cornell University, TERUO ONO, Institute for Chemical Research, Kyoto University, GREGORY FUCHS, Applied and Engineering Physics, Cornell University — We demonstrate spin Seebeck microscopy as a sensitive table-top method for imaging in-plane antiferromagnetic order in thin films. In Pt/NiO(111)/Pt samples, we resolve antiferromagnetic spin domains within crystalline twin domains and image the effects of DC current-induced spin-orbit torque switching. We find a linear correlation between spin-torque-induced changes in the integrated spin Seebeck signal and the spin Hall magnetoresistance, confirming that we image the Néel order. The measurements show that changes driven by spin-orbit torque can occur both by antiferromagnetic domain wall motion and domain flopping, and only a small fraction of the NiO sample is altered.

This research was supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875) and by JSPS KAKENHI Grant Numbers JP15H05702, JP17H04924, and JP17H05181. This work made use of the CCMR Shared Facilities and the Cornell NanoScale Facility, an NNCI member supported by NSF Grant ECCS-1542081.

Characterization of topological band structures by the anomalous Nernst effect

YAN SUN (Presenter), JONATHAN NOKY, JOHANNES GOOTH, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids — Resolving the structure of energy bands in transport experiments is a major challenge in condensed matter physics and material science. Sometimes, traditional electrical conductance or resistance measurements only provide very small signals, and thus limit the ability to obtain direct band structure information. In this case, it has been proven beneficial to employ thermoelectric measurements which are sensitive to the first derivative of the electrical characteristics with respect to energy, rather than to its value itself. The common way to access the Berry curvature in topological materials directly via measurements is the anomalous Hall effect, but the corresponding signal can be too small to be detected when the topological band structures lie far off the Fermi level. In this work we propose to investigate topological band structure features utilizing the anomalous Nernst effect, that are elusive in anomalous hall measurements. This work demonstrates that anomalous Nernst measurements can be an effective tool for characterization of topological band structures away from Fermi level.

This work was financially supported by the ERC Advanced Grant No. 291472 ‘Idea Heusler’ and ERC Advanced Grant No. 742068 ‘TOPMAT’.

This work was supported as part of the SHINES, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences under Award No. SC0012670. This work was also supported by the Startup Funds from University of California, Riverside.

Spin Seebeck imaging of spin-torque switching in antiferromagnetic Pt/NiO/Pt heterostructures

ISAIAH GRAY (Presenter), Applied and Engineering Physics, Cornell University, TAKAHIRO MORIYAMA, Institute for Chemical Research, Kyoto University, NIKHIL SIVADAS, Applied and Engineering Physics, Cornell University, RYAN NEED, BRIAN KIRBY, NIST Center for Neutron Research, National Institute for Standards and Technology, DAVID LOW, Applied and Engineering Physics, Cornell University, GREGORY STIEHL, Department of Physics, Cornell University, JOHN HERON, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, DANIEL RALPH, KATJA NOWACK, Department of Physics, Cornell University, TERUO ONO, Institute for Chemical Research, Kyoto University, GREGORY FUCHS, Applied and Engineering Physics, Cornell University — We demonstrate spin Seebeck microscopy as a sensitive table-top method for imaging in-plane antiferromagnetic order in thin films. In Pt/NiO(111)/Pt samples, we resolve antiferromagnetic spin domains within crystalline twin domains and image the effects of DC current-induced spin-orbit torque switching. We find a linear correlation between spin-torque-induced changes in the integrated spin Seebeck signal and the spin Hall magnetoresistance, confirming that we image the Néel order. The measurements show that changes driven by spin-orbit torque can occur both by antiferromagnetic domain wall motion and domain flopping, and only a small fraction of the NiO sample is altered.

This research was supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875) and by JSPS KAKENHI Grant Numbers JP15H05702, JP17H04924, and JP17H05181. This work made use of the CCMR Shared Facilities and the Cornell NanoScale Facility, an NNCI member supported by NSF Grant ECCS-1542081.

Characterization of topological band structures by the anomalous Nernst effect

YAN SUN (Presenter), JONATHAN NOKY, JOHANNES GOOTH, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids — Resolving the structure of energy bands in transport experiments is a major challenge in condensed matter physics and material science. Sometimes, traditional electrical conductance or resistance measurements only provide very small signals, and thus limit the ability to obtain direct band structure information. In this case, it has been proven beneficial to employ thermoelectric measurements which are sensitive to the first derivative of the electrical characteristics with respect to energy, rather than to its value itself. The common way to access the Berry curvature in topological materials directly via measurements is the anomalous Hall effect, but the corresponding signal can be too small to be detected when the topological band structures lie far off the Fermi level. In this work we propose to investigate topological band structure features utilizing the anomalous Nernst effect, that are elusive in anomalous hall measurements. This work demonstrates that anomalous Nernst measurements can be an effective tool for characterization of topological band structures away from Fermi level.

This work was financially supported by the ERC Advanced Grant No. 291472 ‘Idea Heusler’ and ERC Advanced Grant No. 742068 ‘TOPMAT’.

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A comparative study of spin Seebeck effect and anomalous Nernst effect in a ferromagnetic metal/normal-metal bilayer system.

AVIRUP DE (Presenter), Physics, Indian Institute of Science Education and Research, Pune, ARUP GHOSH, Physics, National University of Singapore (NUS), Singapore, RAJESH MANDAL, SUNIL NAIR, Physics, Indian Institute of Science Education and Research, Pune — In the emerging field of Spin Caloritronics, the central interest is the study of the interactions of spins with heat current. Thus a pure spin current got an enormous importance for such kind of studies. On the other hand, spin seebeck effect (SSE) pertains to the generation of pure spin current under application of a thermal gradient across a magnetic material. Although for magnetic-metals, the SSE signal is contaminated by the anomalous Nernst signals (ANE). In this work, we identify and investigate longitudinal spin seebeck effect (LSSE) phenomenon in La0.7Ca0.3MnO3 /Pt bilayer system over a wide temperature range 20K ≤ T ≤ 295K. We separate out LSSE from the ANE. Further a detailed-analysis on LSSE shows a very good agreement with the current theoretical models.

Avirup De is thankful to UGC, Govt. of India for providing financial support through a Senior Research Fellowship.

Enhancement of Thermal Spin Injection Effects in Nonlocal Spin Valves on Silicon Nitride Membranes

RACHEL K BENNET (Presenter), University of Denver, ALEX HOJEM, University of California - San Diego, DEVIN J WESENBERG, BARRY L ZINK, University of Denver — Nonlocal spin valves (NLSVs) have the unique capability to separate charge and spin currents, and thus are an important tool for both applied and fundamental research in nanomagnetism. [1,2] Previous research shows that changes to the composition of the NLSV substrate can have a marked effect on the background nonlocal resistance by changing the substrate thermal conductance.[3] Our research demonstrates enhancement of non-local spin resistance by the anomalous Nernst effect (ANE) and dramatically lowered thermal conductance in NLSVs fabricated on SiN membranes.[4,5]

We present refined values as low as 0.27 for the Nernst coefficient of permalloy as determined by 2D finite-element analysis of Py/Al NLSVs, where the thermal gradient is confined to two dimensions by the membrane-supported construction. We also present new insight into thermal spin injection effects other than ANE, including thermally-assisted electrical spin injection.


NSF grant ECCS-1610904

Spin-orbit torque and Nernst effects in Bi-Sb/ferromagnet heterostructures

NIKLAS ROSCHEWSKY (Presenter), Physics, University of California, Berkeley, EMILY S WALKER, ECE, University of Texas, Austin, PRAVEEN GOWTHAM, EECs, University of California, Berkeley, SARAH MUSCHINSKE, ECE, University of Texas, Austin, FRANCES HELLMAN, Physics, University of California, Berkeley, SETH R BANK, ECE, University of Texas, Austin, SAYE EL SALAHUDDIN, EECs, University of California, Berkeley — Topological insulators have gained considerable interest recently due to their potential as spin current generators for room temperature memory applications. In this work we show harmonic Hall measurements of spin-orbit torque (SOT) in MBE grown Bi-Sb/Co bilayers [1]. We find that signals in our samples are dominated by the ordinary Nernst effect (ONE). This thermal effect can be a spurious signal in harmonic Hall measurements and has not been taken into account in previous experiments.

We are proposing two control experiments to separate the ONE in Bi-Sb from SOT. First, we compare harmonic measurements in Bi-Sb/Co and Bi-Sb/Al. While SOT is absent in the sample without magnet, we still see large signals in the second harmonic Hall voltage due to the ONE. Second, we investigate the scaling of V2ω with external magnetic field Bext. While it is expected that SOT effects are suppressed at large magnetic fields, we find that the second harmonic voltage in Bi-Sb/Co scales linearly with the external field, as expected from the ONE. These results provide an important contribution to the understanding of the ultra-large SHA that was recently reported in TI/ferromagnets.

The spin-Seebeck effect (SSE) is an advective transport process in a bilayer composed of a ferromagnet (FM) and a nonmagnetic (NM) material with strong spin-orbit coupling. In a temperature gradient, the flux of magnons in the FM transfer spin angular momentum to the electrons in the NM, which, by the ISHE contributes an SSE voltage. In contrast, the intrinsic anomalous Nernst (ANE) conductivity in homogeneous FMs is understood as a non-advective process due to the effect of the temperature gradient on electrons: in MnBi, one can calculate the ANE conductivity from the Berry curvatures using a 32 band tight-binding Hamiltonian with the spin-orbit interaction and magnetization. We show that there can be an additional advective magnonic contribution to the ANE similar to the SSE effect but in uniform metallic FMs. Further, as was done in Ni/Pt, we synthesized composites of aligned MnBi needles in a Bi matrix. In this geometry, we expect an additional SSE contribution from the magnons in MnBi to the Nernst effect in the Bi. In composites with Mn concentration far below the percolation threshold, we observe a large boost in the thermopower and Nernst over the Bi host, which we attribute to advective spin transport.

**5:06PM P41.00001: Pure Spin Current Driven by a Thermally Induced Magnon Chemical Potential**

KEVIN OLSSON (Presenter), University of Texas at Austin, KYONGMO AN, École Polytechnique Fédérale de Lausanne, JIANSHI ZHOU, LI SHI, XIAOQIN (ELAINE) LI, University of Texas at Austin — A major goal of spintronics is to develop devices that rely on spin current, rather than charge current. Of the few methods for generating pure spin current in magnetic insulators (MI), the spin Seebeck effect (SSE) is an attractive method, due to its simplicity. The SSE relies on a thermal gradient to generate a nonequilibrium distribution of magnons, collective spin quasiparticles, which carry spin current. Describing these magnons requires a thermally driven magnon chemical potential, never before measured in such a nonequilibrium system. Here we report the use of Brillouin light scattering for measuring a magnon chemical potential generated by a thermal gradient in the MI yttrium iron garnet (YIG): Y3Fe5O12. Boltzmann transport analysis allows for the quantification of spin currents due to the magnon temperature and chemical potential gradients. Finally, the range of energies and wavevectors of the magnons that contribute to the spin current are identified. Experimental determination of these items will facilitate advancing the theories describing coupled heat and spin transport. Furthermore, this technique allows for the determination intrinsic spin current generating ability of an MI, not possible using previous techniques.

*Work supported by the NSF, DOE, ARO, and EUH 2020.

**5:18PM P41.00003: Effects of thermal spin disorder on the half-metallicity of Co2MnSi with antisite defects and Fe substitution**

GIOVANNI BAEZ FLORES (Presenter), KIRILL BELASHCHENKO, University of Nebraska - Lincoln — Heusler alloys based on Co2MnSi have a high Curie temperature and high spin polarization at the Fermi level, which is promising for applications in spintronics. Band structure calculations show Co2MnSi to be half-metallic at zero temperature. Alloying with Fe on the Mn sublattice is believed to shift the Fermi level closer to the middle of the half-metallic gap. Here, we study the effects of thermal spin fluctuations on the electronic spectrum near the Fermi level, both in pure Co2MnSi and in the presence of crystallographic defects or Fe substitution for Mn. We find that all magnetic antisite defects are strongly exchange-coupled to the host magnetization, and thermal spin fluctuations do not easily destroy the half-metallic gap. In this respect, Co2MnSi differs from NiMnSb, where Mn antisites on the Sb sublattice strongly reduce the spin polarization already at rather low temperatures [1]. We also find that partial substitution of Mn by Fe results in considerable changes in the Bloch spectral function near the Fermi level, which are very different from the rigid-band picture that is usually assumed.


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**Wednesday, March 6, 2019 2:30 PM - 5:30 PM**

**Session P42 DQI: Quantum Annealing: Architectures** BCEC 210A - Richard Harris

**2:30PM P42.00001: A proposed superconducting circuit quantum annealer with fully programmable all-to-all coupling**

PETER MCMAHON (Presenter), TATSUHIRO ONODERA, EDWIN NG, Stanford University — A grand challenge for quantum annealing is the development of annealing hardware that allows fully programmable all-to-all connectivity between logical qubits, with the lowest possible overhead in physical resources. The LHZ [1] scheme achieves fully programmable all-to-all connectivity with a planar architecture that is amenable to implementation with superconducting circuits [2], but does so at a cost of $O(N^2)$ physical qubits to realize $N$ logical qubits. We propose a novel architecture for a superconducting circuit quantum annealer that requires only $N$ physical qubits to realize $N$ logical qubits, and present analytical and numerical evidence that fully connected and programmable quantum annealers with $N=1000$ logical qubits can be constructed with technology that requires only modest improvements over what currently exists.


*This work was partially supported by a Stanford Nano- and Quantum Science and Engineering Postdoctoral Fellowship, and by the Impulsing Paradigm Change through Disruptive Technologies (ImPACT) Program of the Council of Science, Technology and Innovation (Cabinet Office, Government of Japan).
2:42PM P42.00002: Coherent oscillations in the annealing of a flux qubit* MOSTAFA KHEZRI (Presenter), HUO CHEN, HUMBERTO MUNOZ BAUZA, DANIEL A LIDAR, University of Southern California — Annealing of a single qubit under certain schedules can reveal characteristics related to the coherence of a 2-level system in the form of oscillations in the success probability vs anneal time. We study how these characteristics appear in a multi-level superconducting flux qubit by mapping the Ising coefficients to qubit control fluxes. We investigate the effects of higher energy levels on the problem, and analyze the possibility of an experimental implementation using state-of-the-art flux qubits.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.

2:54PM P42.00003: Modeling Coherent Oscillations in the Ground State Probability of Annealed Qubits* HUMBERTO MUNOZ-BAUZA (Presenter), HUO CHEN, MOSTAFA KHEZRI, DANIEL A LIDAR, University of Southern California — The ground state amplitude of an annealed qubit oscillates as a function of the anneal time away from the adiabatic limit. We propose and characterize classes of anneal schedules that exhibit experimentally accessible oscillations as signatures of quantum coherence of a qubit, presenting both time-dependent perturbation theoretic analysis and open system results.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.

3:06PM P42.00004: Coupling annealing-capable high-coherence flux qubits* STEVEN DISSELER (Presenter), JAMES I. BASHAM, JEFFREY GROVER, SERGEY NOVIKOV, DAVID FERGUSON, ZACHARY A STEGEN, ALEXANDER MARAKOV, Northrop Grumman, DAVID K KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, JONILYN L YODER, MIT Lincoln Laboratory, ROBERT HINKEY, Northrop Grumman, DANIEL A LIDAR, University of Southern California, KENNETH M. ZICK, Northrop Grumman — Despite progress in quantum annealing algorithms and hardware development, key questions remain regarding the role of quantum coherence, entanglement, etc., on key figures of merit needed for real world applications. In this talk we will discuss results of small scale annealing experiments with high-coherence superconducting flux qubits as a part of the Quantum Enhanced Optimization program, which seeks to understand and address these issues. Using systems of two and three fully-connected qubits, we demonstrate controllable, scalable couplings between the Z-like fields of individual qubits. We will discuss the impact of coupling on the coherence of the system as it relates to both multi-qubit measurement fidelity as well as the potential importance as a source of error during computation.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) through the Army Research Office (ARO) Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).

3:18PM P42.00005: Development of a Scalable Annealing Machine Dedicated to Integer Factoring* HANPEI KOIKE (Presenter), KENTARO IMAFUKU, SHIRO KAWABATA, National Institute of Advanced Industrial Science and Technology — Commercial annealing machines such as D-Wave and Fujitsu necessarily features general-purpose programmability to cover as wide area of combinatorial optimization problems and thus to obtain as much markets as possible. On the contrary, research annealing machines can enjoy freedom to specialize in a specific problem and to investigate the optimal calculation method to maximum extent. We call this approach Application Specific Annealing Circuit (ASAC). We chose integer factoring as the first target application in our ASAC research. Integer factoring is accomplished by reverse-directional calculation of a digital multiplier circuit by expressing the logic circuit as an energy function and by finding the minimum energy state using annealing method. We have developed a scalable classical ASAC machine using commercial electronic components as a proof of concept. We call our experimental machine AIST Analog Annealer (AAA). We are going to introduce this machine in our presentation.

*This presentation is partly based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO), Japan.
Fluxonium Qubit Systems for Coherent Quantum Annealing

MAXIM VAVILOV (Presenter), ZHENYI QI, Department of Physics, University of Wisconsin - Madison, Madison, WI 53706, MARK DYKMAN, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, VLADIMIR MANUCHARYAN, Department of Physics, University of Maryland, College Park, MD 20742 — Fluxonium systems are perfect candidates for coherent quantum annealing. Individual fluxonium qubits have: (i) substantially long coherence time in excess 5 μs away from sweet spot and 100 μs at the half-flux sweet spot[1], (ii) strong X-X qubit coupling, which can be made to exceed the qubit transition energy[2], and (iii) two low-energy states, well separated from higher-energy states. These characteristics are expected enable long-coherence annealing protocols, while keeping the system in the computational subspace. A potential resource for quantum speed up is multiqubit tunneling in hard optimization problems [3]. In this talk, we describe the multiqubit tunneling in the system of strongly coupled fluxonium qubits during annealing. We discuss the effect of flux noise and dielectric losses on the multiqubit tunneling events.


Flux qubit readout at the degeneracy point*

MARIUS SCHÖNDORF (Presenter), Saarland University, ADRIAN LUPASCU, University of Waterloo, FRANK K WILHELM, Saarland University — The role of measurement is crucial for the realization of a real world quantum computer. A promising candidate to deliver a platform to perform quantum algorithms are superconducting qubits, one of which is the flux qubit. Due to their natural coupling properties, flux qubits are especially interesting for the implementation of quantum annealer. The most robust point of flux qubits against environmental effects that decohere the qubit (e.g. 1/f noise) is the so called degeneracy point. Because of this property one wants to operate at this specific point. However, performing a readout that conserves the measured observable (QND) is difficult here.

In this work we present an indirect measurement scheme for flux qubits which works at arbitrary bias points, most interesting also at the degeneracy point. We show that our protocol is able to reach high fidelities while acting QND on the measured qubit.

*This research is funded by the Intelligence Advanced Research Activity (IARPA). The views and conclusions contained in this presentation are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of IARPA or the U.S. Government.

High coherence annealing, Part 1: fast, high-fidelity readout*

JAMES BASHAM (Presenter), JEFFREY GROVER, STEVEN DISSELER, SERGEY NOVIKOV, DAVID FERGUSON, ZACHARY A STEGEN, ALEXANDER MARAKOV, ROBERT HINKEY, MOE S KHALIL, Northrop Grumman, DAVID KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, JONILYN L YODER, MIT Lincoln Laboratory, ANTHONY J PRZYBYSZ, Northrop Grumman, DANIEL A LIDAR, University of Southern California, KENNETH M. ZICK, Northrop Grumman — Recently developed capacitively-shunted flux qubits offer a promising path toward building a high-coherence quantum annealer. These qubits take advantage of lower persistent currents to achieve lower noise sensitivity. As such, readout of their state at the end of the anneal operation presents unique challenges. We report experimental results of a persistent current readout scheme that provides fast readout while isolating the qubit from the resonator during the anneal.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) through the Army Research Office (ARO) under Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).
High coherence annealing, Part 2: fast annealing experiments

JEFFREY GROVER (Presenter), JAMES I. BASHAM, STEVEN DISSELER, SERGEY NOVIKOV, DAVID FERGUSON, ZACHARY A STEGEN, ALEXANDER MARAKOV, Northrop Grumman, DAVID K KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, JONILYN L YODER, MIT Lincoln Lab, ROBERT HINKEY, MOE S KHALIL, Northrop Grumman, DANIEL A LIDAR, Univ of Southern California, KENNETH M. ZICK, Northrop Grumman — Recently developed capacitively-shunted flux qubits offer a promising path toward building a high-coherence quantum annealer. These qubits take advantage of lower persistent currents to achieve lower noise sensitivity. Using the fast readout scheme and device discussed in Part 1, Part 2 presents single-qubit annealing experiments performed using RF bias lines. We study the behavior of the qubit transition width by changing the annealing time, and we use excited state readout to determine other parameters of the system. This setup also allows for programming highly nonlinear annealing schedules to probe quantum coherence.

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High-order and long-range connectivity for embedding problems in quantum annealing with superconducting flux qubits

DENIS MELANSON (Presenter), ANTONIO MARTINEZ, Physics and Astronomy, Institute for Quantum Computing, Waterloo Institute for Nanotechnology, University of Waterloo, MUHAMMET ALI YURTALAN, Electrical and Computer Engineering, Institute for Quantum Computing, Waterloo Institute for Nanotechnology, University of Waterloo, YONGCHAO TANG, Physics and Astronomy, Institute for Quantum Computing, Waterloo Institute for Nanotechnology, University of Waterloo, DAVID K KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, JONILYN L YODER, MIT Lincoln Laboratory, SERGEY NOVIKOV, Northrop Grumman Corporation - Mission Systems, EVGENY MOZGUNOV, DANIEL A LIDAR, University of Southern California, ADRIAN LUPASCU, Physics and Astronomy, Institute for Quantum Computing, Waterloo Institute for Nanotechnology, University of Waterloo — A high degree of connectivity between qubits is believed to be important in quantum annealing. An approach for implementing high connectivity in superconducting flux qubit annealers was proposed in which the qubits are connected via chains of rf-SQUID couplers. We report an application of this concept in building problem-specific annealing architectures with high-order connectivity. We analyzed the coupling strength between qubits and the coupler network induced qubit decoherence for application-oriented architectures, using both simplified spin models and full quantum circuit models. We designed devices with capacitively shunted flux qubits coupled by coupler trees. We discuss experimental prospects and the relevance for large scale annealing.

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Multi-body flux-qubit couplers for quantum annealing

GIOELE CONSANI (Presenter), PAUL A. WARBURTON, NEDEEN AL SHARIF, University College London — Despite the enormous progress achieved in the field of quantum annealing over the last decade, the demonstration of a computational advantage over classical methods remains elusive. One possible solution is to provide quantum annealers with qualitatively new features, such as higher-order terms in the driver and/or problem Hamiltonians and error-suppression. These capabilities both rely on the physical implementation of multi-body interactions. While interactions between pairs of flux qubits can be achieved rather easily, multi-body interactions require more sophisticated constructions. Some of these use ancillary qubits, while others are based on coupling loops with carefully-engineered flux non-linearities. Here we present a comparative analysis of a few such proposed implementations and propose a quantitative way to compare their performances, with specific focus on their possibility to generate the correct quantum energy spectrum during the annealing process.

*This research was supported in part by Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office Contract No. W911NF-17-C-0050
SERGEY NOVIKOV, STEVEN DISSELER, JAMES BASHAM, JEFFREY GROVER, ALEXANDER MARAKOV, ZACHARY A STEGEN, and spin-boson Hamiltonian are employed respectively. This comparison is done numerically for a small frustrated between qubits. We compare the efficiency of ground state preparation for direct and mediated couplings, for which Ising by the standard Nb superconducting multilayer integration technology.

network. Where qubits can be fabricated by the standard Al angled evaporation, the resonator network can be fabricated actual fabrication of the system, we can conveniently separate the fabrication processes of qubit itself and resonator exceedingly gigantic compound qubit, we can realize a unique network of fully coupled large number of spins. For the arrangement of deep strongly coupled circuit QED system is resulted with an extremely long novel quantum system. With quantum annealers based on flux qubits. This device consists of two RF-SQUIDs coupled to the measured qubits. We simulate the quantum measurement process, including realistic implementation effects. We consider generalizations of this approach to higher-order parity measurements. We also present a different approach based on symmetrical coupling of a flux readout device, designed to measure parity information. Prospects for experimental demonstration are discussed.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).

Quantum annealing with mediated interactions: from a perturbative to a ultrastrong mediated coupling.* MANUEL PINO GARCIA (Presenter), JUAN JOSE GARCIA-RIPOLL, Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas — We present a study of a quantum annealer where bosons mediate the Ising-type interactions between qubits. We compare the efficiency of ground state preparation for direct and mediated couplings, for which Ising and spin-boson Hamiltonian are employed respectively. This comparison is done numerically for a small frustrated antiferromagnet, with a careful choice of the optimal adiabatic passage that reveals the features of the boson-mediated interactions. Those features can be explained by taking into account what we called excited solutions: states with the same spin correlations as the ground-state but with a larger bosonic occupancy. For similar frequencies of the bosons and qubits, the performance of quantum annealing depends on how excited solutions interchange population with local spin errors. We report an enhancement of quantum annealing thanks to this interchange under certain circumstances.

*Financial support by Fundación Gneral CISC (Programa Comfuturo) is acknowledged.

Schrieffer-Wolff Methods for Interacting Superconducting Qubits RUDOLPH J MAGYAR (Presenter), DAVID FERGUSON, Northrop Grumman — There are many possible methods for implementing a low-energy Pauli decomposition of a quantum circuit Hamiltonian as a continuous function of qubit and coupler control fields. Effective low energy models are helpful designs tools to optimize performance in device applications where quantum effects are important. In this talk, we report a method based on the Bravyi et al Schrieffer-Wolff transformation [1] that provides a Pauli decomposition with the following desirable properties: (i) the effective Hamiltonian remains block diagonal so that the computational subspace is completely decoupled from the non-computational states, (ii) the adiabatic connection terms generated by the time dependence of the computational subspace are block off-diagonal and thus do not generate any terms within the computational subspace, and (iii) the computational subspace has a non-trivial holonomy over the control parameter manifold. We report application of these methods to tunable flux qubits comparing results to more explicit models and experimental measurements.


*This material is supported by the Intelligence Advanced Research Projects Activity (IARPA) through the Army Research Office (ARO) Contract No. W911NF-17-C-0050.

Superconducting Quantum Annealing Architecture with LC Resonators* AKIYOSHI TOMONAGA (Presenter), HIROTU MUKAI, Physics, Tokyo University of Science Kagurazaka Campus, JAW-SHEN TSAI, CEMS, Riken,Wako Saitama Japan — We report on the architecture and experimental results of superconducting quantum annealer with LC resonator. In the architecture, qubit and a LC resonator are connected via a Josephson junction to realize deep strong-coupling. Such arrangement of deep strongly coupled circuit QED system is resulted with an extremely long novel quantum system. With the exceedingly gigantic compound qubit, we can realize a unique network of fully coupled large number of spins. For the actual fabrication of the system, we can conveniently separate the fabrication processes of qubit itself and resonator network. Where qubits can be fabricated by the standard Al angled evaporation, the resonator network can be fabricated by the standard Nb superconducting multilayer integration technology.

*This research is supported by NEDO IoT project, JST CREST project and ImPACT project.
2:30PM P45.00001: *Operando* bi-modal studies of complex oxides growth with RHEED and surface x-ray diffraction*

HAWOONG HONG (Presenter), Argonne National Laboratory, XINYUE FANG, MENG-KAI LIN, TAI-CHANG CHIANG, Department of Physics, University of Illinois Urbana-Champaign, FRIEDERIKE WROBEL, ANAND BHATTACHARYA, Argonne National Laboratory — An oxide MBE chamber was developed for simultaneous use of RHEED and surface x-ray diffraction at the same time. It is mounted and coupled to a 6-circle diffractometer. X-ray reflection intensity measurement at one point in reciprocal space is similar to RHEED intensity oscillation measurement. The relationship between two methods has been reported for homo-epitaxial complex oxide growth [1]. With large photon flux at the Advanced Photon Source, the x-ray intensity measurement could be extended to a real-time collection of data on a large swath of a line scan utilizing multi-angle fly scans [2]. Rapid acquisition in the volume around x-ray diffraction rods and RHEED measurements were obtained simultaneously during the growth. This bimodal study was made during La$_2$CuO$_4$ (001) film growth on SrLaAlO$_4$ (001) substrates with MBE techniques. Discussed will be the relation between two different observations and future impacts from utilizing this bimodal method.


*Work performed at Argonne National Laboratory was supported by the U.S. Department of Energy, BES, under Contract No. DE-AC02-06CH11357.

2:42PM P45.00002: Suppression of Bi disproportionation in minimally electron doped BaBiO$_3$ epitaxial thin films*

HUI CAO (Presenter), Department of Chemical Physics, University of Science and Technology of China — BaBiO$_3$ is a semiconductor due to three dimension charge density wave (CDW), and it can become a superconductor, with a maximum $T_C$ of 30K via holes doping. We have studied the three-dimensional charge-density-wave in high quality BaBiO$_3$ and electron doped BaBiO$_3$ single crystal thin films by X-ray photoelectron spectroscopy, X-ray absorption spectroscopy, Raman shift and ellipsometry technique. The electron doping is achieved by very small amount of oxygen vacancies purposely induced by vacuum annealing. Our results have found that the electron doping can remove bismuth disproportionation ($2\text{Bi}^{4+} \rightarrow \text{Bi}^{3+} + \text{Bi}^{5+}$) but has less effect to the insulating gap. Different from the hole-doping side, the amount of electron needed to suppress the bismuth disproportionation is extremely small. Our study provides new insights to the intricate correlation between CDW and the hybridization between oxygen 2p and Bi 6s orbitals.

*National Natural Science Foundation of China (Grants No. 11574287)

2:54PM P45.00003: Polarization switch on h-LuFeO$_3$ multiferroic*

PETRUCIO BARROZO DA SILVA (Presenter), BHAGWATI PRASAD, VISHAL THAKARE, SUJIT DAS, RAMAMOORTHY RAMESH, Physics Department, University of California, Berkeley — The properties of improper ferroelectrics are known to be very different from properties present in the proper ferroelectrics. However, the switching behavior of the electric polarization and the dynamics of the ferroelectric domain walls in the multiferroics with improper ferroelectricity don't have been yet reported. In this work, we study the ferroelectric properties of hexagonal LuFeO$_3$ (h-LFO). This structure was firstly obtained in 2004 [1], but its properties are yet not all understood. The epitaxial thin films of h-LFO on YSZ(111) was produced by pulsed laser deposition. The switch of polarization was studied in the screen of Ishibashi-Orihara model [2]. We have observed that the electrical coercive field in improper ferroelectric (h-LFO) grow very fast with the frequency if compared with proper ferroelectric (e.g. PbTiO$_3$ or BiFeO$_3$). In this presentation, we also will discuss mechanisms to reduce the electrical coercive field as well as how to reduce the dependence of the electrical coercive field with the frequency.


*Thanks to Brazilian fund agencies CNPq and CAPES.
3:06PM P45.00004: Superconductivity in doped SrTiO₃  LUCA GALLETTI (Presenter), KAVEH AHADI, YUNTIAN LI, SUSANNE STEMMER, University of California, Santa Barbara — We report on the transport properties of a series of doped 250-nm-thick SrTiO₃ films, grown by molecular beam epitaxy on undoped (001) SrTiO₃ substrates. In particular, we demonstrate anomalies in the superconducting properties. A systematic study of the critical temperatures and fields as a function of the carrier density and type of doping atom reveal deviations from BCS behavior and points towards the role of the specific doping atom. Moreover, the transport properties of the normal state show peaks in the transverse resistance, which indicates an electron nematic phase above the superconducting transition. We discuss the mechanisms of superconductivity of SrTiO₃ thin films.

3:18PM P45.00005: Comparative Study of Surface Structural and Physical Properties of Sr₃T₂O₇ (T = Mn, Ru)  YIFAN YANG (Presenter), LINGYI XING, MOHAMMAD SAGHAYEZHIAN, RONGYING JIN, E WARD PLUMMER, Louisiana State University — Double-layered Ruddlesden-Popper oxides are known to exhibit a strong correlation between octahedral distortion and physical properties. Using low-energy electron diffraction (LEED) and high-resolution electron energy loss spectroscopy (HREELS), we have investigated the surface structural and physical properties of Sr₃T₂O₇ (T = Mn, Ru). While surface RuO₆ octahedron in Sr₃Ru₂O₇ has both rotation (~ 12°) and tilt (~ 3°), our LEED – IV analysis reveals that MnO₆ octahedron in Sr₃Mn₂O₇ has a similar rotation (~ 11°) but no tilt. HREELS data suggest that both the surface of Sr₃Mn₂O₇ and Sr₃Ru₂O₇ are semiconducting but for different reasons. The implication of these findings will be discussed.

3:30PM P45.00006: Electronic and magnetic properties of double perovskite thin film Sr₂CrReO₆*  JOSE FLORES (Presenter), KENG-YUAN MENG, ADAM AHMED, FENGYUAN YANG, Ohio State University — Chiral magnetic spin textures, such as skyrmions, have been found in systems that have the Dzyaloshinskii-Moriya interaction and ferromagnetic exchange, e.g., heavy metal/ferromagnet bilayers. However, to make skyrmions relevant for modern applications, skyrmions need to operate at room temperature and be sufficiently small for high information densities. Oxides offer an excellent platform to accomplish this owing to their pristine epitaxy and highly tunable properties. We explore this possibility in high magnetic ordering temperature Sr₂CrReO₆ thin films. Sr₂CrReO₆ films were grown by off-axis dc magnetron sputtering on SrTiO₃(001) and Sr₂CrNbO₆/LSAT(001) substrates. Films were characterized by X-ray diffraction and atomic force microscopy showing both a high degree of crystalline quality and smooth surface topography, respectively. We will also discuss how choice of substrate for growth of Sr₂CrReO₆ is crucial as strain can significantly change the magnetic anisotropy—a crucial tuning parameter for skyrmion stability. Lastly, we will show magnetic and electrical characterization of these films and the potential for future skyrmion heterostructures.

*This research was supported by the Defense Advanced Research Projects Agency Grant No. D18AP00008

3:42PM P45.00007: High-k perovskite dielectric BaHf₁₋ₓTiₓO₃  HAHOON LEE (Presenter), DOWON SONG, KOOKRIN CHAR, Seoul National University — Interest in high-k materials continues as the semiconductor devices shrink in size and in its operating voltage. BaTiO₃ is a well-known perovskite ferroelectric material and BaHFO₃ is a perovskite high-k dielectric material with a dielectric value of 38. In this study, we fabricated capacitors with an atomically-mixed BaHf₁₋ₓTiₓO₃ (BHT, with x varying from 0 to 0.8) layer as the dielectric insulator with a perovskite semiconductor La-doped BaSnO₃ (BLSO) layer as the electrode. All the layers were epitaxially grown on SrTiO₃ substrates by pulsed laser deposition. X-Ray diffraction was used to investigate the structural properties, from which we confirmed the epitaxial growth of all the layers and obtained their respective lattice constants. The electrical properties of the capacitors, such as the capacitance and breakdown field, were measured. As the x value increased, the relative permittivity value increased and the dielectric breakdown field decreased. When the x value of BHT was 0.4, the relative permittivity and breakdown field values were 61.7 and 5.85 MV/cm, respectively, yielding the maximum 2D charge density 2x10¹⁴ cm⁻². We will report on the field effect transistor performances with BHT as the gate dielectric and BLSO as the channel layer.
Defect-controlled transport phenomena at complex oxide interfaces

JACQUELINE BOERGERS, MARC ROSE, RWTH Aachen University, REGINA DITTMANN, Forschungszentrum Julich, FELIX GUNKEL (Presenter), RWTH Aachen University — Electric-field control of 2-dimensional electron systems (2DES) in oxide heterostructures is a key tool for tuning properties such as carrier density, magnetism, and superconductivity. There remain open questions however if in all cases gate-tunable properties can be ascribed to electronic phenomena deriving directly from varying the charge accumulated in the interfacial potential well. Here, we discuss that various gate-tunable properties observed in 2DES can also be mimicked by controlling the ionic defect structure and lattice disorder in the vicinity of the interface. As we will show accumulation of scatter centers at the interface can result in diminished charge transfer, while the magnetic response of the electron system is enhanced and quantum interference phenomena (weak-anti-localization) arise. Additionally, we discuss how a controlled and homogenous defect background in thin film SrTiO3 intrinsically yields a transition from positive to negative magnetoresistance, at comparable carrier concentration. Our results yield an ionic-electronic perspective on electrical gating experiments frequently conducted in the oxide electronics community. We provide a comprehensive discussion of the coupling of electronic gating and gradual defect profiles.

Superoxygenation study of cuprate and iridate thin films

HAO ZHANG (Presenter), CHAO ZHANG, Department of Physics, University of Toronto, NICOLAS GAUQUELIN, SHAOBO CHENG, GIANLUIGI BOTTON, Canadian Centre for Electron Microscopy and Brockhouse Institute for Materials Research, McMaster University, CHRISTOPHER MCMAHON, DAVID G HAWTHORN, Department of Physics and Astronomy, University of Waterloo, PATRICK CLANCY, SAE HWAN CHUN, Department of Physics, University of Toronto, AMBROSE SEO, Department of Physics and Astronomy, University of Kentucky, JOHN Y.T. WEI, Department of Physics, University of Toronto — High-pressure O2 has been used to hole-dope and to stabilize high-oxidation phases of cuprates. We extend this superoxygenation technique to YBa2Cu3O7-δ thin films, which are more reactive due to their large surface-to-volume ratio, and to the layered iridate Sr2IrO4, which is difficult to hole-dope by cation substitution. First, YBa2Cu3O7-δ thin films grown by PLD are annealed in up to 700 atm O2 and then characterized by TEM, XRD and XAS. The annealed films show phaseconversion to Y2Ba4Cu7O15-δ and Y2Ba4Cu8O16, as well as regions of YBa2Cu5O9-δ and YBa2Cu6O10-δ. Second, epitaxial thin films of Sr2IrO4 are subjected to extended high-pressure annealing and similarly characterized. The post-annealed films show up to 3 order-of-magnitude drop in room temperature resistivity and an evolution towards semi-metallic behaviour. Furthermore, as film thickness is reduced, the annealed films show a structural transformation towards a quasi-cubic phase. Our results demonstrate the potential of using superoxygenation to stabilize exotic phases of transition metal oxides not achievable in bulk form. [1]


Temperature-induced metal-to-insulator transition in epitaxially grown NbO2 films

TOYANATH JOSHI (Presenter), ELI CIRINO, DAVID LEDERMAN, University of California, Santa Cruz — Transition metal oxides demonstrating metal-to-insulator transitions (MIT), such as VO2 and NbO2, are widely studied materials for use as selector elements in resistive random-access memory (RRAM). The MIT transition temperature (TMIT) of VO2 is close to room temperature (~340 K). NbO2, on the other hand, has a much higher transition temperature (TMIT = 1081 K), which complicates the direct observation of the MIT in thin films and has not been reported in an epitaxial film, so far. In this presentation, we will demonstrate temperature dependent electrical resistivity of epitaxially grown NbO2 thin films revealing the actual mechanism of MIT in NbO2. High-quality epitaxial films were grown using pulsed laser deposition and structural characterization was performed using x-ray diffraction and atomic force microscopy. The resistivity of the as-grown films was measured from room temperature to 1100 K under a controlled environment using the four-probe resistivity measurement technique. Also, we will examine the effect of epitaxial strain to MIT of NbO2 was demonstrated by varying thickness of the films from 12 to 45 nm.
4:30PM P45.00011: Interfacial Mott state in iridate-nickelate superlattices*  XIAORAN LIU (Presenter), MICHELE KOTIUGA, HEUNG SIK KIM, Rutgers University, New Brunswick, ALPHA N’DIAYE, Advanced Light Source, YONGSEONG CHOI, Advanced Photon Source, YANWEI CAO, Chinese Academy of Science, BANABIR PAL, FANGDI WEN, MIKHAIL KAREEV, Rutgers University, New Brunswick, JOHN WILLIAM FREELAND, DANIEL HASKEL, Advanced Photon Source, PADRAIC SHAFER, ELKE ARENHOHLZ, Advanced Light Source, KRISTJAN HAULE, DAVID VANDERBILT, KARIN RABE, JAK CHAKHALIAN, Rutgers University, New Brunswick — In new SrIrO3/LaNiO3 superlattices up to a full electron transfer at the interface from Ir to Ni is experimentally observed, triggering a massive structural and electronic reconstruction. The large crystal eld splitting from the distorted interfacial IrO6 octahedra surprisingly dominates over the spin-orbit coupling, and together with the Hund’s coupling results in the high-spin (S = 1) configurations on both Ir and Ni sites. First-principles calculations agree well with the experimental results, supporting the formation of an intricate Mott state in the superlattices.

*1. Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4534, and by the Department of Energy under grant DE-SC0012375.
2. Oce of Naval Research grant N00014-17-1-2770 and the Department of Defense High Performance Computing Modernization Program for computational resources.
3. NSF DMREF DMR-1629059.

4:42PM P45.00012: Doping study of ultra-wide bandgap spinel semiconductor ZnGa2O4 films  SUNGYUN HONG (Presenter), YEAJU JANG, JIHOON SEO, Seoul National University — ZnGa2O4 is a cubic spinel oxide with a bandgap of about 4.6 eV, almost same as that of monoclinic b-Ga2O3 in which the interest keeps increasing for its potential in high power devices. We will report the effect of various dopants on ZnGa2O4. For this study, we grew ZnGa2O4 films on c-Al2O3 substrates via pulsed laser deposition. XRD analysis conirmed the epitaxial growth of the films. Three elements, Sn, Si, and H were chosen as dopant candidates. The Sn-doped film remained highly insulating, showing no significant decrease in resistivity compared to the undoped film. The resistivity of the Si-doped film decreased to the order of 10^3 Ω*cm, confirming that some carriers were generated by Si dopants. The H-doped films showed a large decrease in resistivity down to the order of 10^1 Ω*cm. Further annealing of the H-doped films under an O2 environment increased the resistivity up to the order of 10^0 Ω*cm while the Hall measurements on the post-annealed H-doped films yielded mobility values of up to ~50 cm^2*V-1*s-1 with a carrier density of ~10^17 cm^-3.

4:54PM P45.00013: AFM Study of Temperature Driven Phase Transitions in Vanadates*  ANNA BINION (Presenter), RIJU BANERJEE, LAVISH PABBI, JASON M LAPANO, ROMAN ENGEL-HERBERT, ERIC HUDSON, Pennsylvania State University — Vanadates have many interesting properties with possible applications ranging from solar energy to transparent electronics. As many applications depend on the variation of structural and electronic properties thru phase transitions, to develop new applications it is important to have a good understanding of these transitions. Here we present results from atomic force microscopy studies of vanadates undergoing temperature driven phase transitions. In particular, we observe changes in a stripe order parameter as the materials pass through their structural transition temperatures. These observations give us insight into the nature of these transitions and how they can be controlled.

**This material is based upon work supported by the National Science Foundation under Grant No. 1229138

5:06PM P45.00014: Inversion symmetry breaking at the heterointerface of SrRuO3 thin films  CHANG JAE ROH (Presenter), Department of Physics and Photon science, Gwangju Institute of Science and Technology, JEONG RAE KIM, Department of physics, Seoul National University, YONG RYUN JO, Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, JEONG GI CHOI, Department of Physics and Photon science, Gwangju Institute of Science and Technology, JIN KWON KIM, YEONGJAE SHIN, BONGJU KIM, Department of physics, Seoul National University, BONG JOONG KIM, Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, TAE WON NOH, Department of physics, Seoul National University, JONGSEOK LEE, Department of Physics and Photon science, Gwangju institute of Science and Technology — We investigate the structural symmetry of SrRuO3 thin films grown on the SrTiO3 substrate by exploiting optical second harmonic generation (SHG) technique. We observe that SHG responses are strongly dependent on the film thickness and temperature; the azimuth-dependence becomes more anisotropic as the film becomes thicker, and the SHG response diminishes as temperature increases above 400 K. We analyze the azimuth dependences by considering the electric dipole and electric quadrupole contributions, and find that the tetragonal and orthorhombic phases are stabilized in fully strained and strain-relaxed regions, respectively. In particular, we demonstrate that the inversion-symmetry-broken state emerges as a stable phase at the interface between centrosymmetric tetragonal and orthorhombic phases.
5:18PM P45.00015: Effect of perovskite dielectric $Ba_xSr_{1-x}HfO_3$ on $BaSnO_3$  

HYEONGMIN CHO (Presenter), YOUNG MO KIM, KOOKRIN CHAR, Seoul National University — La-doped BaSnO$_3$ (BLSO) is a wide bandgap semiconducting perovskite oxide with high electron mobility and excellent oxygen stability at room temperature [1]. In recent reports on the excellent carrier modulation of BLSO channel by field effect on perovskite SrTiO$_3$ (STO) [2] and non-perovskite MgO substrates [3], we found an optimized thickness for undoped BaSnO$_3$ (BSO) buffer layer to be around 150 nm. However, BSO shows persistent and large photoconductivity under the light with wavelength smaller than 400 nm.

To prevent the change of channel conductance by such photoconductivity of the BSO buffer layer, we fabricated an atomically-mixed $Ba_xSr_{1-x}HfO_3$ (BSHO) buffer layer. Both BaHfO$_3$ (BHO) and SrHfO$_3$ (SHO) have wider bandgaps than BSO (5.8 eV and 6.1 eV respectively) and show no measurable photoconductivity. Also, BHO is a high-k dielectric material with a dielectric constant of 38. We reduced BSHO lattice mismatch with BLSO by finding a suitable ratio of BHO to SHO. We will report on the field effect transistor performances with BSHO as a buffer layer on BLSO channel layer as well as a gate dielectric.


Wednesday, March 6, 2019 2:30 PM - 5:18 PM

Session P46 DMP GMAG: Complex Oxide Interfaces & Heterostructures -- Skyrmions & Novel Magnetism

2:30PM P46.00001: Observation of Nanoscale Skyrmions in SrIrO$_3$/SrRuO$_3$ Bilayers and SrRuO$_3$ Single Layers in Two Distinct Regimes*  

[Invited] ADAM AHMED (Presenter), KENG-YUAN MENG, Ohio State University, ANDRADA-OANA MANDRU, MIRKO BACANI, XUE ZHAO, Empa, Swiss Federal Laboratories for Materials Science and Technology, BRYAN D. ESSER, JOSE FLORES, DAVID W. MCCOMB, Ohio State University, HANS-JOSEF HUG, Empa, Swiss Federal Laboratories for Materials Science and Technology, FENGYUAN YANG, Ohio State University — The advent of skyrmion imaging and electrical detection is an exciting avenue of research as skyrmions hold promise for next-generation magnetic storage. Oxide materials are a great platform to study in this regard owing to their highly tunable properties, pristine epitaxy, and stability. In this talk, I will show Hall detection and real-space imaging of nanoscale skyrmions in perovskite oxide heterostructures of SrIrO$_3$/SrRuO$_3$ (SIO/SRO) epitaxial films grown on SrTiO$_3$(100) substrates. We show regions of large topological Hall resistivity at low temperatures which coincide with the field where the magnetization reverses. Additionally, we present a new high-temperature topological Hall effect not seen before in both bilayer SrIrO$_3$/SrRuO$_3$ and single layer SrRuO$_3$ films. This high temperature phase manifests as a “coercive field switching” in the electrical data and, consequently, as a large topological Hall effect signal. To corroborate our topological Hall signals with skyrmions, we have collected real-space images of isolated skyrmions with low-temperature magnetic force microscopy and show nanoscale skyrmions with diameters as small as 10 nm. Remarkably, the region where skyrmion bubbles are present precisely coincides with the topological Hall peaks. Our results open a platform for tunable nanoscale skyrmions in functional oxide materials.

*This research was supported by the Defense Advanced Research Projects Agency Grant No. D18AP00008.
3:06PM P46.00002: Observation of room-temperature polar skyrmions in oxide superlattice  YUNLONG TANG (Presenter), SUJIT DAS, Department of Materials Science and Engineering, University of California, Berkeley, California 94720, USA., ZIJJAN HONG, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, M. A. P. GONCALVES, Luxembourg Institute of Science and Technology (LIST), 5 avenue des Hauts-Fourneaux, L-4362 Esch/Alzette, Luxembourg., MARGARET MCCARTER, Department of Materials Science and Engineering, University of California, Berkeley, California 94720, USA., CHRISTOPH KLEWE, Lawrence Berkeley National Laboratory, F. GOMEZ-ORTIZ, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, E-39005 Santander, Spain., PADRAIC SHAFER, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, VLADIMIR A STOICA, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, SHANG-LIN HSU, Department of Materials Science and Engineering, University of California, Berkeley, California 94720, USA., B. WANG, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, COLIN OPHUS, J. F. LIU, Lawrence Berkeley National Laboratory, CHRIS NELSON, Oak Ridge National Laboratory, Bethel Valley Rd., Tennessee 37831-6071, USA, SAHAR SAREMI, BHAGWATI PRASAD, Department of Materials Science and Engineering, University of California, Berkeley, California 94720, USA., DARRELL G. SCHLOM, A. B. MEI, Cornell University, Ithaca, New York 14853, USA, JORGE INIGUEZ, Luxembourg Institute of Science and Technology (LIST), 5 avenue des Hauts-Fourneaux, L-4362 Esch/Alzette, Luxembourg., PABLO GARCIA-FERNANDEZ, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, E-39005 Santander, Spain., LONG Q. CHEN, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, JAVIER JUNQUERA, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, E-39005 Santander, Spain., LANE MARTIN, R RAMESH, Department of Materials Science and Engineering, University of California, Berkeley, California 94720, USA. — Recent discovery of polarization flux closures, vortices and skyrmions in polar oxide superlattices suggests the presence of a complex, multi-dimensional system capable of exotic physical responses.[i]-[ii],[iii] where the exploration of novel emergent phenomena and exotic phases in condensed-matter physics is greatly facilitated. Here, we have observed a room-temperature polar skyrmions in a PbTiO3/SrTiO3 superlattices grown on SrTiO3 (001) substrate. X-Ray diffraction and large scale scanning transmission electron microscopy imaging confirmed the present of the polar skyrmions phase. In addition, phase-field modeling and second-principles calculations reveal that the polar skyrmions have a skyrmion number of +1. Moreover, special uniform chirality was revealed by resonant soft X-ray diffraction experiments showing obvious circular dichroism. Such nanometer-scale polar skyrmions are the electric analogs of magnetic skyrmions, and could advance ferroelectrics towards new levels of functionality.


3:18PM P46.00003: Electric field Controllable “Negative Capacitance” in Polar Skyrmions: Topological transition?* SUJIT DAS (Presenter), University of California, Berkeley, ZIJJAN HONG, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, SAHAR SAREMI, BHAGWATI PRASAD, University of California, Berkeley, PABLO G. FERNANDEZ, Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, E-39005 Santan, MARGARET MCCARTER, YUN-LONG TANG, University of California, Berkeley, JAVIER JUNQUERA, Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, E-39005 Santan, LONG Q. CHEN, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, LANE MARTIN, SAYEEF SALAHUDDIN, RAMAMOORTHY RAMESH, University of California, Berkeley — Complex topological configurations are a fertile arena to explore novel emergent phenomena and exotic phases in condensed-matter physics. For example, the recent discovery of polar skyrmions, vortices and skyrmions in polar superlattices suggests the presence of a complex, multi-dimensional system capable of exotic physical responses. Here, we demonstrate electric field controlled room-temperature negative capacitance and topological phase transition in polar skyrmions. In epitaxially grown heterostructures of PbTiO3 and SrTiO3 capacitance was found to be larger compared to its individual constituent’s capacitance SrTiO3, PbTiO3. This indicates the indicates the ferroelectric was stabilized in a state of negative capacitance at room temperature. This phenomenon could be controlled by electric field and temperature. The STEM measurement, Phase field and Second principle calculation confirms the stable negative capacitance is due to boundary of polar skyrmions. Such phenomena could advance ferroelectrics towards new levels of functionality.


*Gordon and Betty Moore Foundation’s EPIQS Initiative.
3:30PM P46.00004: Resonant X-ray diffraction study of chiral polar skyrmions in PbTiO3/SrTiO3 superlattices*
MARGARET MCCARTER (Presenter), Department of Physics, University of California, Berkeley, SUJIT DAS, Department of Materials Science & Engineering, University of California, Berkeley, YUN-LONG TANG, Materials Science Division, Lawrence Berkeley National Laboratory, CHRISTOPH KLEWE, PADRAIC SHAFER, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, JAVIER JUNQUERA, Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Universidad de Cantabria, LANE MARTIN, RAMAMOORTHY RAMESH, Department of Materials Science & Engineering, University of California, Berkeley —
Emergent topologies in ferroelectric heterostructures—the polar analogs of magnetic vortices and skyrmions—have become a recent topic of interest for their potential to host exotic functionalities (e.g., emergent chirality and negative capacitance). These topologies can be stabilized in low-dimensional ferroelectrics; namely, superlattices of PbTiO3/SrTiO3. Polar skyrmion structures have been observed in PbTiO3/SrTiO3 superlattices grown on SrTiO3 substrates with a combination of scanning transmission electron microscopy, X-ray diffraction, and second-principles calculations. Using resonant soft X-ray diffraction, we study the chirality of these polar skyrmions and show that the skyrmions have a preferred handedness. The origin of the circular dichroism is shown to be a chiral configuration of the titanium orbitals in the skyrmions.

*Gordon and Betty Moore Foundation's EPiQS Initiative, under grant GBMF5307

3:42PM P46.00005: Living on the edge: multiple phase competition and topological order in pyrochlore oxides*
[Invited] NICHOLAS SHANNON (Presenter), HAN YAN, Okinawa Institute of Science and Technology, OWEN BENTON, Condensed Matter Theory, RIKEN, LUDOVIC JAUBERT, CNRS Bordeaux — Pyrochlore oxides, A2B2O7, are one of nature's best tricks - ubiquitous minerals, capable of incorporating an extremely wide range of metal cations. Over the past decade these materials have risen to prominence in the community studying frustrated magnetism, for their ability to instantiate so many different novel, and topological phases of matter. Best known among these is spin ice, celebrated for its magnetic monopole excitations, but small changes in chemistry can lead to a wide range of other exotic phenomena, including both classical and quantum spin liquids.

In this talk, we explore one particular avenue in this lively field, namely the multiple-phase competition which occurs in magnetic oxides with strong spin-orbit coupling. Considering Yb2Ti2O7, Er2Ti2O7 and Er2Sn2O7 as examples, we show how the seemingly diverse physics of these systems can be understood through a single unifying principle, namely the interplay between different competing forms of order [1]. We also explore how this conceptual framework can be used to "design" new forms of spin liquid, including phases which realise fracton topological order.

Finally, we pose the question, could different modes of growth give us access to pyrochlore oxides with even more exotic, or controlable, properties?


*This work was supported by the Theory of Quantum Matter Unit, of the Okinawa Institute of Science and Technology Graduate University.

4:18PM P46.00006: Anisotropic magnetoresistance in multiorbital systems*
ILIA KHAIT (Presenter), NAZIM BOUDJADA, ARUN PARAMEKANTI, Department of Physics, University of Toronto — Magnetotransport is a useful probe for studying magnetism, electron-electron interactions, as well as the underlying symmetries of a crystal. We study the impact of an in-plane magnetic field on 2D multiorbital electron gases as a function of electron density, scattering length, temperature, and spin-orbit interactions. These parameters affect the shape of the different spin-split Fermi surfaces, which in turn is shown to set the amplitude of the anisotropic magnetoresistance and its dominant symmetry components. We comment on the validity of the relaxation-time approximation and the necessity to resort to the full Boltzmann equation.

*This work was supported by the Natural Sciences and Engineering Research Council of Canada and the Canadian Institute for Advanced Research. NB acknowledges support from the Fonds de Recherche du Québec - Nature et Technologies.
**4:30PM P46.00007: Imaging, controlling and harnessing non-collinear magnetism in perovskite oxides** [Invited]

MANUEL BIBES (Presenter), CNRS/Thales — In magnetic perovskites, first-neighbour antiferromagnetic super-exchange interactions usually dominate, but may coexist with other terms such as ferromagnetic double-exchange or Dzyaloshinskii-Moriya interactions. This often produces non-collinear spin configurations leading to weak ferromagnetism or to spatially modulated spin structures. A prototypical non-collinear magnetic oxide is multiferroic BiFeO₃ that shows a cycloidal order with a 64 nm period in the bulk. In this talk, I will present real-space images of the cycloidal structure and its manipulation by electric field [1]. In a second part, I will report the observation of a very large topological Hall effect (THE) in thin films of a lightly electron-doped manganite. Magnetic force microscopy reveals the presence of small magnetic bubbles, whose density vs. magnetic field peaks near the THE maximum, as is expected to occur in skyrmion systems. The THE critically depends on carrier concentration and diverges at low doping, near the metal-insulator transition, suggesting its amplification by strong correlations, in the vicinity of the Mott transition [2].


*Supported by the ERC CoG MINT (#615759)

**5:06PM P46.00008: High-throughput Design of Interfacial Perpendicular Magnetic Anisotropy at Heusler/MgO Heterostructures**

KESONG YANG (Presenter), SAFDAR NAZIR, University of California, San Diego — Thin magnetic tunnel junctions (MTJs) with a large interfacial perpendicular magnetic anisotropy ($K_I$) have great applications in spin transfer torque magnetoresistance random access memories. A large $K_I$ is required for achieving a high thermal stability of the MTJ, and thus to design an interfacial perpendicular magnetic anisotropy at the interface between ferromagnetic electrodes and oxide barriers is of great interests. Here we show that, by modelling Heusler/MgO heterostructures using high-throughput first-principles electronic structure calculations, we are able to rapidly identify a series of Heusler/MgO heterostructures with a large $K_I$ value. This work shows an effective way to design novel magnetic materials via high-throughput electronic structure calculations.

*The author acknowledges support by Vannevar Bush Faculty Fellowship program sponsored by the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering under the Office of Naval Research grant N00014-16-1-2569.

**Wednesday, March 6, 2019 2:30 PM - 5:18 PM**

**Session P47 GERA: Recent Advances in Energy Conversion Devices** BCEC 213 - Jeffrey Owrutsky, United States Naval Research Laboratory

**2:30PM P47.00001: Battery alternative: Harvesting energy from vibrations** MILLICENT GIKUNDA (Presenter), PAUL THIBADO, University of Arkansas — Development of energy harvesting systems is becoming increasingly important. This is due to an increased need to produce self-charging, portable, implantable and wireless electronics with extended lifespans. Operation of these devices require low power which is normally supplied by batteries that require regular replacement. Emphasis has been placed on scavenging vibrational energy as an alternative to batteries. A notable breakthrough is the discovery that mechanical buckling (change of curvature from concave to convex and vice versa) in freestanding graphene occurs spontaneously at room temperature. This spontaneous mechanical buckling is a source of renewable energy that is to be harvested. Here, I will discuss the relationship between the energy barrier which separates the two lowest energy configurations to strain and height of the ripple and model the ripple curvature inversion dynamic due to thermal energy using Langevin’s equation for freestanding graphene. Mechanical power calculations estimates that a naturally occurring ripple can yield up to and a ripple can yield Thus a quartz wristwatch whose approximate consumption is can be powered by a ripple.
By adjusting the structural properties, we find a minimum thermal conductivity to be reached at ~ 35 mWm\(^{-1}\)K\(^{-1}\) in air, whereas 7 mWm\(^{-1}\)K\(^{-1}\) can be achieved in vacuum. Thus, tailor-made particle ensembles based on hollow silica nanoparticles represent a dispersion processable, breathable, and non-flammable alternative to common polymer foams.

*This project was funded by a Lichtenberg Professorship provided by the Volkswagen Foundation. Additional support was provided by the Bavarian Polymer Institute, BPI, the SFB840, and DFG project RE3550/2-1
3:30PM P47.00006: Reversing Thermal Equilibration by Differential Magneto-Thermal Force  WEILI LUO (Presenter), JUN HUANG, DARIAN SMALLEY, Physics,, University of Central Florida, T. S. LIU, Western Michigan University — A special magnetic body force was proposed to reverse thermal equilibration in a fluid [1]. In this work, we discuss the fulfilment of the requirements for this force and the experiment to verify it. We present experimental [2-3] and analytical [4] results that clearly demonstrate: 1) approaching thermal equilibrium in our magnetic fluid sample was indeed “reversed” as the magnetic body force introduces the localized flows that stop the conventional convective heat transfer; 2) The differential magneto-thermal force density calculated with experimental parameters agrees with the design principle. These results prove the feasibility of the proposed mechanism for a new generation of heat transfer apparatus that has high efficiency and no exhaust, a clean energy source that will improve our environmental protection.

References:

3:42PM P47.00007: Development of Thermoacoustic Arrays for Power.  OREST SYMKO (Presenter), SEO YOUNG AHN, University of Utah — Thermoacoustic heat engines with piezoelectric devices provide a simple approach to converting heat to electricity. Heat generates sound in an acoustic resonator, which is converted to electricity. For high power, arrays of engines are used. The development of such approach deals with the coupling of engines for synchronization, frequency tuning of resonant components, stability, and performance. Standing wave thermoacoustic engines (2 to 6) at ~2.5 kHz were mounted on a cavity housing piezoelectric devices for converting sound to electricity, and the cavity provided coupling. Above a threshold temperature difference, oscillations were initiated, and they appeared synchronized. The engines were tuned to the piezos. Temperature changes led to detuning. This was compensated by using two piezos of different resonant frequencies, and each piezo was coupled to a Helmholtz resonator, making broadband response and maintaining sensitivity. The increase in power density in the above-coupled engines can be eventually applied to large systems, i.e. arrays.

*University of Utah Department of Physics and Astronomy

3:54PM P47.00008: Electronic, Magnetic and Magnetocaloric Properties of Hole-Doped La$_2$MnFeO$_6$ and their Potential for Magnetic Refrigeration*  C. GAUVIN-NDIAYE (Presenter), ANDRE-MARIE TREMBLAY, REZA NOURAFKAN, Institut quantique, RQMP, Université de Sherbrooke — Magnetic refrigeration at room-temperature is a technology that could potentially be more environmentally-friendly, efficient and affordable than traditional refrigeration. Known ferromagnets that satisfy the requirements of near room temperature Curie temperature and large refrigerant capacity are expensive. Double Perovskites La$_2$MnXO$_6$ with X=Ni,Co have refrigerant capacity comparable to the more expensive materials but their Curie temperature $T_C$ is low [1]. Previous theoretical studies have reproduced the trend in $T_C$ of these materials and shown that strong electronic interactions in Fe-d orbitals [2] make the X=Fe compound a ferrimagnet. Based on this insight, we use ab initio, mean-field and Monte-Carlo calculations to propose two materials with promising magnetocaloric properties. They are obtained by hole doping the X=Fe compounds by substituting half of the lanthanum with Sr or Ba, LaBaMnFeO$_6$ and LaSrMnFeO$_6$ [3].


*Canada First Excellence Research Fund, NSERC Grant RGPIN-2014-04584, Research Chair in the Theory of Quantum Materials, Compute Canada, Calcul Québec, CIFAR
4:06PM P47.00009: Photoelectrochemical water splitting systems for the sustainable growth of hydrogenotroph biomass* CAMILLA TOSSI (Presenter), LASSI HÄLLSTRÖM, ERICH SEE, Electronics and Nanoengineering, Aalto University, MICHAEL LIENEMANN, JUHA-PEKKA PITKÄNEN, MARJA NAPPA, PETER BLOMBERG, JUSSI JÄNTTI, MERJA PENTTILÄ, VTT Technical Research Centre of Finland, Ltd., ILKKA TITTONEN, Electronics and Nanoengineering, Aalto University — An important and presently not yet deeply investigated application of photoelectrochemical (PEC) water splitting is the use of the generated hydrogen to feed a population of hydrogenotroph bacteria. Such bacteria exist in a sufficient variety to satisfy different demands, from fuel components to edible and highly proteic biomass. The need for sustainable food production techniques is an urgent matter, as our planet is expected to produce enough nourishment to sustain 9 billion people by 2050, while at the same time reducing the carbon footprint of the population. We developed a PEC cell equipped with a bioreactor, demonstrating the growth of a Rhodococcus Opacus population with forced electrolysis over the span of several days: the present focus is on the engineering progress of the working electrode, a stack of semiconductor thin films with noble metal co-catalyst nanoparticles, to match both the durability and the solar-to-hydrogen efficiency necessary to the self-sustainability of the system.

*The authors acknowledge the financial support from the Academy of Finland project 13285972, from the Vilho, Yrjö ja Kalle Väisälä Fundation grant issued by the Finnish Academy of Arts and Sciences and from the Aalto University ELEC Doctoral School.

4:18PM P47.00010: Density functional theory study of water splitting on ZnO catalyst adsorbed on Graphene Oxide* DUWAGE PERERA (Presenter), JAYENDRAN C RASAIAH, University of Maine — We discuss results from density functional theory (DFT) calculations of water splitting on ZnO surfaces using the hybrid B3LYP exchange functional and the 6-311G basis sets. The production of H2 and O2 occurs through the formation of a Zn-H bond generated from the hydrolyzed product of ZnO. We discuss the Transition state of the reaction using the Synchronous Transit-Guided Quasi-Newton (STQN) method following calculations of the Intrinsic Reaction Coordinate (IRC) using the same level of theory. We discuss an extension of our work using RB3LYP/DGDZVP method for water splitting on ZnO adsorbed on graphene oxide (GO) surface (GO-ZnO) which forms a p-n hetero junction enhancing the rate of H2 evolution as it does for a GO-TiO2. GO sheet can facilitate exciton formation and acts as an electron sink to store the separated electrons. Hydrogen production was observed on the GO-ZnO surface using five different GO models.

*We thank Stephen Cousins of the University of Maine High Performance Computing Group for his technical assistance and significant allotment of computer time.

4:30PM P47.00011: Synthesis of Zn-doped MoS2-graphene heterostructure for efficient water splitting MD DELOWAR HOSSAIN (Presenter), ZHENGTANG LUO, Chemical and Biological Engineering, The Hong Kong University of Science and Technology — The demand of renewable energy increases day by day as we progress towards near future. Here we report new type of 2D heterostructures which show superior electrochemical performance towards both hydrogen and oxygen evolution reaction. We demonstrate the synthesis of heterostructure by mixing graphene oxide, Mo-salt, and thiourea via hydrothermal method at 180 oC for 12 hrs. The heterostructure has lots of defected area which enhanced the active sites for both reactions, was revealed by SEM, TEM characterization. Later on, we have performed density functional theory calculation, which demonstrate that the activity mainly comes from sulfur and zinc sites of this heterostructure represented by Gibbs free energy diagram. The density of states calculation shows that the presence of zinc in MoS2-graphene heterostructure increases the electron density throughout the whole structure. Finally, the band structure calculation reveals that zinc reduces the band gap for heterostructure and increases the water splitting capacity into hydrogen and oxygen.

4:42PM P47.00012: Engineered Photo-electrochemical Properties of Nano-Structured SnO2 ZINEB KERRAMI (Presenter), Physics, Mohammed V University — In the present study, photo-electrochemical properties of SnO2 Thin-film have been examined using first principles calculation. Increasing SnO2 film thickness from 0.3 nm to 2.5 nm results in band gap decrease, which revealed a strong quantum confinement effect. Our results indicate that visible-light absorption and charge carrier's mobility of a chosen SnO2 film (2.5 nm) could be improved by applying tensile strain. Although, large pH value (pH ≥ 10) is needed to enhance band edges positions relative to the water redox (H2O/H2) levels. All these improvements make tensile strained-SnO2 a potential candidate for hydrogen production through water splitting.
4:54PM P47.00013: Close Space Sublimation Synthesis and Photoelectrochemical Efficiency of Vertical Tin Disulfide (SnS$_2$) Nanoflake Photoanodes  BINOD GIRI (Presenter), PRATAP RAO, Worcester Polytechnic Institute — Tin disulfide (SnS$_2$) is a 2-dimensional material similar to MoS$_2$ and WS$_2$, with layers held together by weak Van der Waals forces. It has excellent optical and electronic properties that are suitable for a number of applications. Because of its high optical absorption coefficient, moderate band gap, and conduction and valence band edges that straddle the reduction and oxidation potentials of water, SnS$_2$ is a promising material for photoelectrochemical (PEC) water splitting. Several reports describing fundamental properties and synthesis methods have been published, however very few have successfully realized SnS$_2$-based photoanodes.

In this work, vertically aligned 2D SnS$_2$ nanoflakes were grown directly on FTO-glass substrates using a scalable close space sublimation (CSS) method. Scanning electron microscopy revealed that our nanoflakes contain vertical tapered structures with high aspect ratios and high density of exposed edges. They exhibit an indirect bandgap of 2.28eV and are excellent photoabsorbers. Photoanodes consisting of these nanoflakes were synthesized and measured in aqueous pH7 buffer containing Na$_2$SO$_3$ as hole-scavenger. Photocurrents up to 4.5mAcm$^{-2}$ were obtained at 1.23 V vs. RHE under simulated sunlight.

5:06PM P47.00014: 2D Photocatalysts on GaN Nanowires*  XIANGHUA KONG (Presenter), DAWEI KANG, BAOWEN ZHOU, McGill University, ZETIAN MI, University of Michigan, HONG GUO, McGill University — Hydrogen generation via PEC water splitting is an appealing approach for conversion of solar energy into chemical fuel. PEC requires photocatalysts to function and 2D photocatalysts have received tremendous attention. We report an investigation of solar fuel generation using defect-free GaN nanowires as linker between planar Si wafer and 2D photocatalyst MoS$_2$, focusing on the modeling side [1]. The electronic interaction as well as excellent geometric-matching structure between GaN and MoS$_2$ enable excellent electron-migration channels for high charge extraction efficiency, leading to outstanding photocatalytic performance. Our approach[1] of constructing super-heterostructures offers clear benefits for solar water splitting, including the use of low-cost, large-area Si wafer for light harvesting, earth-abundant MoS$_2$ catalyst for proton reduction, and defect-free GaN nanowires for highly efficient charge carrier extraction and for exposing a high-density of active sites. We further report a general numerical procedure for quantitative estimation of band edge positions and band edge shifts and microscopic origins of these shifts for solid/liquid system[2].


*NSERC
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Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P48 DFD GSOFT GSNP: Thin Films, Surface Flows, Interfaces and Microfluidics II
BCEC 251 - Anand Oza, New Jersey Institute of Technology

2:30PM P48.00001: Characteristic interfacial structure behind a rapidly moving contact line*  MENGFEI HE (Presenter), SIDNEY ROBERT NAGEL, University of Chicago — A solid rapidly pushed into a liquid, of viscosity $\eta$, at velocity $U$ entrains surrounding air along with its moving surface. Using high-speed interferometry we find a robust characteristic structure of the entrained air layer: there is a thin-thick alternation of gap thickness in the transverse direction and this feature occurs both in wetting and de-wetting. In the thin regions we find that the gap thickness scales approximately as $(\eta U)^{0.5}$. We present a model using the assumption that the velocity profile is robust to thickness fluctuations that gives a good quantitative estimate of this gap thickness. This is in contrast to the Landau-Levich analysis which had previously been assumed applicable to this problem.

*This work was primarily supported by the University of Chicago MRSEC, funded by the National Science Foundation under award number DMR-1420709 and by NSF Grand DMR-1404841.
Levitation of fizzy fluids

PHILIPPE BOURRIANNE (Presenter), DIVYA PANCHANATHAN, PHILIPPE NICOLLIER, KRIIPA K VARANASI, GARETH MCKINLEY, Massachusetts Institute of Technology — Liquids generally spread on solids they encounter. However, under particular circumstances, such a wetting can be reduced or even avoided, a situation of obvious practical interest in terms of anti-adhesion or even thermal and mechanical insulations. By using superhydrophobic coating, a water drop can thus limit its contact with the substrate at a low fraction. Liquid levitation can even be achieved using the volatility of the liquid and creating a thin insulating vapor layer as early described by Leidenfrost in 1756. More recently, other strategies have been developed involving external fields such as air flows, Faraday waves or magnetic fields. We here describe a novel approach using active liquids able to sustain levitation in the absence of external forces. We will first discuss the levitation of carbonated water. In this regime, the drop self-generates the gas cushion which provides levitation. We will model the lubrication theory behind this insulation. Finally, we will generalize this new regime to different kinds of substrates and non-volatile liquids.

Dewetting Front Instabilities for Micro-patterning

SAMANTHA MCBRIDE (Presenter), Massachusetts Institute of Technology, SEVERINE ATIS, Harvard University, KRIIPA K VARANASI, Massachusetts Institute of Technology — It has long been known that fluid instabilities can be harnessed for low-effort self-assembly of ordered structures on the nano- and micro- scales. Here, we demonstrate how a known thin film instability resulting from Van der Waals forces in an evaporating film can generate a number of extraordinarily ordered nano- and micro-structures. The patterns that can arise include hexagonal lattices, lines, branches, and triangular sawtooth structures. We find that the patterning mechanism is driven by fluid dynamics and Ostwald ripening of crystallizing salts at the fluid dewetting front. Controllability of these patterns can be further enhanced by application of flow-control strategies. We present a phase diagram of substrate properties that result in patterning, and perform stability analysis to predict the wavelength of the instability. Such patterns may have potential applications in sensor arrays, photonics, dielectric materials, and materials of controlled porosity.

Nanosecond Pulsed Imaging for Ethanole Electrospraying Breakup in a Modified Nozzle

ELAHE JAVADI (Presenter), Mechanical Engineering, Northeastern University, MOHAMMAD REZA MORAD, Department of Aerospace Engineering, Sharif University of Technology — An electrified liquid jet breakup behavior and modes of disintegration indifferent ow rates and applied voltages are investigated. The present phenomenology belongs to a new injector introduced recently by Morad et al. (2016). This injector is shown to highly extend the stability and ow rate of electrospray particularly in the Taylor cone-jet mode. The experimental investigation is performed using a high-power light-emitting diode (LED) illumination as the light source. The light source is developed to operate in the pulsing condition when synchronized with a digital camera, and is particularly designed to function properly in presence of high electromagnetic interference (EMI). Details of the light source development is presented with the captured images from the jet breakup at different modes. The operational map of the new injector is obtained, and the physical mechanisms of different behaviors are explained and discussed.

From droplets to waves: interfacial instabilities of viscosity-stratified flows in microchannels

XIAOYI HU (Presenter), THOMAS CUBAUD, Stony Brook University — Rapid layering of viscous materials in microsystems encompasses a range of hydrodynamic instabilities that facilitate mixing and emulsification processes of fluids having large differences in viscosity. We experimentally study dispersed droplet and separated viscous wave flow regimes arising from viscosity-stratified microflows made of fluid pairs with large viscosity ratios and systematically investigate the effects of control parameters such as flow rate, viscosity ratio, and interfacial tension between model fluid pairs. We demonstrate that key features of periodic droplets and interfacial viscous waves, including emission frequency, propagating celerity, and wavelength, can be readily described by functional relationships, which delineate effects of inertial, capillary and viscous forces. We also shed light on wave crest breaking process, which produces viscous ligaments that continuously transport thick material into the fast co-flowing low-viscosity stream. Finally, we examine the transition from droplet to wave regime to provide a comprehensive scenario of interfacial instabilities in microfluidic viscosity-stratified flows.

*National Science Foundation under Grant No. CBET-1150389
3:54PM P48.00008: High precision characterization of a binary fluid interface using surface light scattering spectroscopy* NABIN K. THAPA (Presenter), Physics, Kent State University, ANTHONY E. SMART, Scattering Solutions, Inc., Costa Mesa, CA, WILLIAM V. MEYER, ALEXANDER BELGOVSKIY, Scattering Solutions, Inc., Cleveland, OH, J. ADIN MANN, Chemical Engineering, Case Western Reserve University, ELIZABETH MANN, Physics, Kent State University — Thermally excited capillary waves (ripplons) with an rms height of ~1 nm perturb any fluid interface. The Doppler spectrum of these ripplons, which can be characterized by Surface Light Scattering Spectroscopy (SLSS), depend upon interfacial properties such as surface tension and surface viscoelasticity, via the capillary wave surface response function, a refinement of the classical dispersion equation. Innovative optical design has increased signal and signal-to-noise ratio. This enhances measurement accuracy over the entire range of wave numbers, while enabling measurements at higher wave numbers above 1500/cm. We demonstrate the validity of the technique with high precision and high accuracy measurements of standard fluids. Subsequent measurements of pentane/2-methyl pentane mixtures anticipate an upcoming NASA microgravity experiment intended to optimize the effectiveness of wickless heat pipes for space flight applications.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1709985.

4:06PM P48.00009: NEMD Simulations Quantifying the Influence of Surfaces Roughness on Conductive Heat Transfer at Liquid/Solid Interfaces HIROKI KAIFU (Presenter), SANDRA TROIAN, MC128-95, CALTECH, Pasadena, CA 91125 — Rapid developments in extreme ultraviolet lithography are soon expected to produce integrated circuit components with feature sizes of about 10 nm. At these small scales, the interfacial or so-called Kapitza resistance, which tends to increase with diminishing system size, progressively hinders the transfer and evacuation of heat, ultimately compromising performance. Although numerous experiments and simulations over the past few decades have elicited trends in the Kapitza resistance which correlate with system size and surface roughness, good quantitative understanding for atomistically rough interfaces is still lacking. In this talk, we discuss some of the effects on Kapitza resistance induced by surface roughness at liquid/solid interfaces as investigated by non-equilibrium molecular dynamics (NEMD) simulations using realistic solid walls modeled by an interacting 12-6 Lennard-Jones potential. Comparison between atomistically smooth and rough interfaces, contrasting such behavior as the vibrational density of states, helps interrelate the phonon spectrum and phonon modes transmitted across the interface with various quantitative measures characterizing interfacial roughness.

4:18PM P48.00010: Oblique water entry of micron particles* BINGQIANG JI (Presenter), QIANG SONG, QIANG YAO, Tsinghua University — Water entry problem has attracted much interest in the past century, but few research focused on the oblique water entry of micron particles, which is very common in nature and industrial processes. The oblique water entry of micron PMMA particles with different impact angles is realized by a self-made impactor and observed with a high speed camera. It was found that the distortion of the liquid surface after impact is non-axisymmetric due to the lateral velocity of the particle, and the wetted part of the particle surface is not axisymmetric along the impact direction, which produces a force perpendicular to the impact direction and makes the particle's motion direction changes during the water entry process. The critical velocity for the particle to sink increases with the decrease in impact angle. A simple model is established to analyze the energy balance during the critical sinking process and the expression of the critical sinking velocity is given, which agrees well with our experimental results.

*This work is supported by the National Natural Science Foundation of China (51576109).

4:30PM P48.00011: Rebound dynamics of a superhydrophobic sphere* ISABELLE BAUMAN (Presenter), DANIEL M HARRIS, School of Engineering, Brown University — Small solid particles impacting a water surface can become trapped, rebound, or pass through the interface [Lee & Kim, Langmuir, 24 (2008)]. In the present work, we focus on the bouncing dynamics of millimetric superhydrophobic spheres impacting the surface of a quiescent water bath. Through experiments, we characterize the dependence of the normal coefficient of restitution and contact time on the impact velocity, radius, and relative density of the sphere. We also highlight a qualitatively new regime identified that occurs near the sinking threshold for many spheres. Ongoing work and future directions will be discussed.

*We would like to acknowledge the financial support of the Brown Seed Award and the Brown Undergraduate Teaching and Research Award (UTRA).
Characterization of Liquid Transport in MicroCapillaries via X-Ray Photon Correlation Spectroscopy

DHIRAJ NANDYALA (Presenter), Stony Brook University, ANDREI FLEURASU, YUGANG ZHANG, Photon Sciences, Brookhaven National Laboratory, CARLOS E COLOSQUI, Stony Brook University — X-ray photon correlation spectroscopy (XPCS), a novel x-ray scattering technique analogous to dynamic light scattering, enables probing the hydrodynamics of liquids on length scales ranging from microns to nanometers and time scales ranging from seconds to microseconds. The National Synchrotron Light Source II (NSLS-II) of Brookhaven National Laboratory (BNL), which started operating in 2015 as one of the world's most advanced synchrotrons can enable XPCS studies with unprecedented spatio-temporal resolution. This presentation will discuss ongoing work at the Coherent Hard X-ray Scattering (CHX) beamline of NSLS-II where XPCS techniques are employed to characterize flow velocity profiles and mass diffusivity in microcapillaries. A genetic algorithm is developed to determine local flow velocities and diffusion coefficients from the intensity autocorrelation function obtained from XPCS experiments. The developed XPCS techniques and analytical methods can provide new insights into the hydrodynamic and rheological behavior of liquids in micro/nanoscale confinement.

*This work is supported by the Environmental Engineering Program of The National Science Foundation (CBET 1605809).

Suppression of the viscous fingering instability by shear

THOMAS ERIK VIDEBÆK (Presenter), SIDNEY ROBERT NAGEL, Physics, University of Chicago — During the viscous fingering instability, the interface between two fluids confined to a thin gap is unstable to finger formation when the less viscous fluid invades the higher viscosity one. Here, we study the instability between pairs of miscible fluids. When experiments are conducted in a radial geometry there is a period of stable growth which persists up to a critical radius that depends on the viscosity ratio of the fluids and the injection rate. The presence of fingers appears to be tied to specific interfacial structure across the small dimension of the gap. In this work we see how actively interfering with this structure formation affects the instability. By applying an oscillatory translational shear to the top plate of our Hele-Shaw cell we observe a dramatic delay in the onset of the instability. We suggest that this delay is tied to changing the curvature of the interface at the leading edge of the pattern. This phenomenon could lead to novel control techniques to suppress this instability.

Experimental Pressure Analysis Techniques in the Viscous Fingering Instability

SAVANNAH GOWEN (Presenter), THOMAS ERIK VIDEBÆK, SIDNEY ROBERT NAGEL, Physics, University of Chicago — When a lower viscosity fluid displaces a higher viscosity one in a confined geometry, the interface between the two fluids is unstable to the formation of fingers. The fluid flow is governed by Darcy's law so that the local velocity is proportional to the pressure gradient. Using thin rings of dyed fluid we visualize the local flow field within a radial Hele-Shaw cell and are able to map pressure gradients throughout the pattern-formation process. In particular, we measure the pressure gradients as a function of distance from the unstable fluid interface. Using various image processing techniques, we examine the role of the fluids' viscosity ratio as a parameter governing pattern formation.

Equilibrium shapes and their stability for liquid films in fast flows

ANAND OZA (Presenter), Department of Mathematical Sciences, New Jersey Institute of Technology, LIKHIT GANEDI, Department of Mathematical Sciences, Carnegie Mellon University, MICHAEL JOHN SHELLEY, Courant Institute / Flatiron Institute, LEIF RISTROPH, Courant Institute — We present the results of a combined experimental and theoretical investigation of a suspended liquid film deformed by an external flow en route to forming a bubble. We identify a family of nonminimal but stable equilibrium shapes for flow speeds up to a critical value, beyond which the film inflates unstably. A model based on free-streamline theory accounts for the observed nonlinear deformations and forces. Our theoretical predictions suggest that bubble formation at low speeds results from the instability of overly-inflated shapes, and at high speeds from the loss of equilibrium solutions.

*We acknowledge support from the grant NSF-CBET-1805506, and from the Lilian and George Lyttle Chair.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P49 DPOLY GSOFT DFD GSNP: Tribology of Polymers and Soft Materials II: Friction and Slip

BCEC 252A - Catheryn Jackson - Tag(s): Focus
ASHLIE MARTINI (Presenter), ARASH KHAJEH, JEJOON YEON, Mechanical Engineering, University of California Merced, XIN HE, SEONG KIM, Chemical Engineering, Penn State University — Shear force is used to drive chemical reactions in many natural and engineering processes. However, despite the important role of these so-called tribochemical reactions, their fundamental mechanisms are still poorly understood due to challenges associated with directly measuring processes that occur inside a moving contact. To address this, we investigate shear-driven polymerization of molecules adsorbed on silica surfaces, a model system that enables identification of shear-driven reaction pathways. This system is studied using reactive molecular dynamics simulations complemented by pre- and post-sliding surface characterization. The results show that interfacial shear not only accelerates polymerization reactions but opens reaction pathways that are not accessible thermally. Specifically, the simulations reveal that chemisorption and shear-induced deformation of the reactants are critical steps in tribochemical processes. In general, these findings may form the basis for design of systems where shear force can be leveraged to tune or lower the energy cost of chemical reactions.

*National Science Foundation Grant No. CMMI-1727356 and 1727571

MARION GRZELKA (Presenter), MARCEAU HÉNOT, Univ of Paris - Sud 11 CNRS, ALEXIS CHENNEVIÈRE, Laboratoire Léon Brillouin CEA Saclay, CNRS, LILIANE LÉGER, FREDERIC RESTAGNO, Univ of Paris - Sud 11 CNRS — The slippage of polymer melts is now well understood. In particular, Hénot et al. have investigated the dependence of the slip length on the viscosity of the sheared polymer melt [1]. They proved that the friction of polymer melt is due to the friction of monomers on the surface.

More recently, we studied the effect of temperature on slippage of polymer melts far above glass transition temperature [2]. We showed that friction is a thermodynamically activated process.

With solutions, the concentration can change the interdigitation between the chains anchored to a surface and the solution. Furthermore, depletion layer may appear. The disentanglement and depletion are competing.

We will present the results of experiments of friction of polystyrene in diethyl phthalate on different substrates. We investigate the dependence of the slip length on concentration of the solutions in the Newtonian and the shear-thinning regimes.


*This work was supported by ANR-ENCORE program (ANR-15-CE06-005).

DAISUKE KAWAGUCHI (Presenter), NOZOMI ITAGAKI, YUKARI ODA, Kyushu University, NORIFUMI L. YAMADA, KEK, KEIJI TANAKA, Kyushu University — Frictional Properties, which are closely related to aggregation states at the outermost surface, of hydrogels are pivotal importance for many applications. Recently, we synthesized poly(2-methoxyethyl vinyl ether) (PMOVE) containing photo-cross-linkable 2-(vinylloxy)ethyl methacrylate (VEM) units by living cationic polymerization. Here, interfacial density profiles and frictional properties of cross-linked PMOVE (c-MrV) thin films in water were examined by neutron reflectivity (NR) and lateral force microscopic (LFM) measurements, respectively. The density profile of the c-MrV films in close proximity to the water interface was well described by a parabolic function, which was generally used for polymer brushes in a liquid. The lateral force ($F_L$) for the hydrogel films swollen in water was a function of normal force ($F_N$) applied on to a probe tip. For all films, $F_L$ first increased with $F_N$ and then remained constant at an $F_N$. The critical depth, in which $F_L$ reached a constant, well corresponded to the thickness of the interfacial swollen layer determined by the NR measurement.
3:30PM P49.00004: Microgel systems containing phospholipid: Role of component interactions on rheology and tribology  
BARBARA FARIAS, SAAD KHAN (Presenter), North Carolina State University — Microgel systems containing phospholipids are often used in personal care products due to their gelling and emulsifying properties. Herein, we investigate how the type of microgel (hydrophobically modified versus hydrophilic) and its interaction with phospholipid manifest itself on the tribology and rheological behavior of the system. We examine two different polymers one forming a microgel with hydrophobic moieties on the surface (Pemulen) and the other being a hydrophilic microgel (Carbopol). While both polymers exhibit gel-like features rheologically, their mode of interaction with phospholipid is different. Phospholipid addition to the Pemulen leads to an increase in elastic modulus because of the interaction of the hydrophobic moieties with the phospholipid tails. Such active participation is verified using heat of interaction measured through isothermal calorimetry. Tribological behavior, measured with a soft model polydimethylsiloxane (PDMS) contact, reveals lower friction coefficients in the boundary regime for the hydrophobic Pemulen with and without phospholipid. Adsorption of phospholipids and Pemulen on the PDMS substrate are attributed to the decreased friction coefficient, which we verify through optical microscopy and with Quartz Crystal Microbalance measurements.

3:42PM P49.00005: Orientation of nanodomains of star-shaped (PMMA-b-PS)$_6$ in thin films with different molecular weights*  
SOYEONG PARK (Presenter), CHUNGRYONG CHOI, KYUSEONG LEE, SEUNGKYOOP KARK, EUNSEOK KIM, JIN KIM, Pohang University of Science and Technology — To apply block copolymer (BCP) to nanolithography, vertically oriented nanodomains in thin film are needed. When the chain architecture of BCPs was changed from linear to star shape, vertically oriented cylinders and lamellae were obtained by using only thermal annealing without any special treatment. This is because the vertical orientation is entropically favored over parallel oriented one. Here, we study the effect of the molecular weight of (PMMA-b-PS)$_6$ star shaped block copolymer on the orientation of nanostructures on a silicon oxide changed. When the molecular weight is small, but still larger than the critical molecular weight corresponding to the order-disorder transition (ODT), parallel orientation is observed. This is because the entropic loss arising from the formation of vertical oriented nanostructures is not large; thus the orientation of nanostructures is greatly affected by surface treatment of a substrate. On the other hand, at large molecular weights, the entropic penalty for parallel orientation becomes huge, resulting in vertical orientation.

*This work was supported by the National Creative Research Initiative Program supported by the National Research Foundation of KOREA(2013R1A3A2042196).

3:54PM P49.00006: Concentration-Dependent Long-Range Repulsive Interactions of Adsorbed Associative Polymers  
TIMOTHY MURDOCH (Presenter), Chemical and Biomolecular Engineering, University of Philadelphia, EUGENE PASHKOVSKI, Lubrizol, ROBERT W CARPICK, Mechanical Engineering and Applied Mechanics, University of Philadelphia, DAEYON LEE, Chemical and Biomolecular Engineering, University of Philadelphia — Colloidal atomic force microscopy is used to study the quasi-static and velocity-dependent normal force-separation response of adsorbed layers of associative and non-associative olefin copolymers (OCP). OCP containing a small fraction of a polar group forms transient bonds, leading to a stronger concentration-dependent viscosity than native OCP. This functional group also imparts a strong surface affinity to OCP, leading to strong adsorption. Quasi-static measurements show that the surfaces with native OCP have minimal interaction on approach, and strong adhesion on retraction due to bridging. In contrast, surfaces with associative OCPs exhibit repulsive interactions on approach with the magnitude and onset increasing with the polymer concentration. The interaction distances are long range, approaching 10x the unperturbed polymer dimension. Adhesion on retraction is greatly reduced and occurs over a range close to the contour length of the polymer. Increasing the approach velocity leads to long range repulsion for both polymers due to hindered solvent drainage. The magnitude of repulsion is highest for the associating OCP, but the onset of interaction is comparable for both. These results correlate well with impact of these polymers on friction in the boundary regime.

4:06PM P49.00007: Beyond the lubrication approximation: capillary levelling of holes in freestanding polymer films  
JOHN NIVEN (Presenter), McMaster University, VINCENT BERTIN, ESPCI, THOMAS SALEZ, University of Bordeaux, ELIE RAPHAEL, ESPCI, KARI DALNOKI-VERESS, McMaster University — Capillary levelling experiments have been used previously to study nano-scale flow in thin viscous films with a variety of hydrodynamic boundary conditions. Theoretical models developed to understand these experiments have primarily used the lubrication approximation, which omits flow normal to the film. In this work, thin bilayer polystyrene films were prepared freestanding in air, with one of the two films containing micrometer scale cylindrical holes. The viscoelastic relaxation of the holes was studied using atomic force microscopy. In order to equilibrate internal Laplace pressure, a hole will undergo a viscous symmetrization process, resulting in identical holes at the two interfaces. A novel 3D axisymmetric hydrodynamic model, which includes vertical flow, was developed to understand the dynamics of this symmetrization process, and is shown to be in excellent agreement with experiments.
4:18PM P49.00008: Understanding Polymerization-Induced Nanostructural Transitions Using in situ Characterization Methods  
ROBERT HICKEY (Presenter), JACOB A LANASA, EVERETT ZOFCHAK, Pennsylvania State University  
Polymerization-induced structural transitions have been used to create nanostructured in a host of applications ranging from energy to separation technologies. Recently, our group has achieved order-order and disorder-order structural transitions by polymer grafting from linear block polymers mixed with monomer. In our approach, we are able to induce either a lamellar-to-hexagonally-packed cylinder (LAM-HEX) or a disordered-to-HEX transition via the polymerization of styrene, which initially acts as a neutral solvent for the lamellar-forming diblock copolymer, poly(styrene)-block-poly(butadiene) (PS-PBD). In situ small-angle X-ray scattering (SAXS) and rheological experiments during the polymerization process reveal a complex phase path in which we initially disorder the lamellar morphology at elevated temperatures. During the progression of the polymerization, the disordered phase transitions first to an ordered state, and then converts into the double gyroid phase. We are able to recover the HEX phase after polymerization when the sample is cooled to room temperature. The work presented here highlights how the chemical process of converting standard linear diblock copolymers to grafted-block polymers drives interesting and controllable morphology transitions.

4:30PM P49.00009: Lubricated friction on microtextured soft substrates*  
YUNHU PENG (Presenter), CHRISTOPHER SERFASS, LILIAN HSIAO, North Carolina State University  
Natural cartilage is durable and elastic, providing a low friction coefficient to moving joints under frequent applications of heavy loads. However, the physical mechanisms contributing to this low friction coefficient is not well understood. We hypothesize that the non-ideal surface geometry of cartilage gives rise to its low friction coefficient in certain directions of motion. We design soft poly(dimethyl siloxane) (PDMS) substrates with controlled dimensions and spacings to study the influence of surface geometry on their frictional and lubrication properties. Tribological tests performed with a thin layer of aqueous glycerol solution between the PDMS substrates show that the frictional behavior does not follow the type of Stribeck curve that is typically observed with flat surfaces. This major difference can be explained by a scaling theory we developed, in which the friction force and the normal force are expressed with a combination of lubricant properties, experimental conditions and surface geometries. Our study establishes a design framework for the friction of elastomers based on their surface microtextures, and paves the way for engineering soft materials in technological applications such as wearable electronics, antifouling coatings, and synthetic implants.

* CBE@NCSU

4:42PM P49.00010: Effective Orientation Control of Block Copolymer Nanostructures in Thin Films by Surface Modification using Self-assembled Copolymer Adsorption Layer  
DONG HYUP KIM (Presenter), SO YOUN Y KIM, Ulsan National Institute of Science and Technology  
Block copolymers (BCPs) have been extensively studied due to their ability to self-assemble into well-defined nanostructures. In particular, self-assembly of BCPs in a two-dimensionally confined state of thin films has been widely exploited for a bottom-up nanofabrication in the use of many applications. In order to achieve meaningful nanopatterns in BCP thin films, a perpendicular orientation of BCP morphology is required. Here, we demonstrate that self-assembled copolymer adsorption layers (SCALs) can effectively control the morphology orientation of BCPs in thin films as modifying a surface energy of substrates. SCALs were derived from an interfacial self-assembly (ISA) of BCPs based on our finding that the self-assembled BCPs at the air/water interface can be transferred and irreversibly adsorbed onto a solid substrate. Precise modification of the surface energy was possible by controlling nanostructures of SCALs as a function of a surface pressure for ISA of BCPs. Moreover, we found irreversible adsorption for ISA of BCPs is universal for any substrates. Therefore, SCALs can be readily prepared on wherever ISA of BCPs is transferred to, thus enabling much more effective surface modification of various substrates, such as metals, ceramics, flexible or curved substrates.
Contact and slip mechanics between crosslinked hydrogel surfaces using in situ microscopy

ALISON DUNN (Presenter), CHRISTOPHER L JOHNSON, JIHO KIM, SHABNAM Z BONYADI, University of Illinois at Urbana-Champaign — The contact mechanics of soft-soft interfaces provide a backdrop for the slip mechanics due to the conformal contact at the interface, in which any surface asperities are fully compressed, and the apparent area of contact is the real area of contact. However, assumptions regarding the nature of the soft material as a thermal, semi-dilute mesh network, poroelastic solid, or other, will control the contact mechanics, especially over time. In this work we show detailed measurements of contact areas with polyacrylamide hydrogels during microindentation and slip which are revealed through particle inclusion and/or exclusion microscopy. The particles are green fluorescent polystyrene spheres of 0.5 or 1 µm in diameter. We identify time-dependent contact mechanics in migrating, stationary, and self-mated “Gemini” contact. Our data suggest that for long times, Gemini contact approaches a constant-pressure contact model, which depends upon the equilibrium osmotic pressure of the sample. Finally, we present for the first time asymmetric contact areas as visualized by in situ particle exclusion which manifests as a flow field around the probe. The results of this work begin to connect hydrogel material properties with surface mechanics.

*This work was support by NSF Award Number 1751945.

Wall slip of complex fluids: Interfacial friction versus slip length

BENJAMIN CROSS, CHLOÉ BARRAUD, LiPhy, Université Grenoble Alpes, CYRIL PICARD, LILIANE LÉGER, FREDERIC RESTAGNO (Presenter), Université Paris-Sud, ELISABETH CHARLAIX, LiPhy, Université Grenoble Alpes — If the slip length is an useful notion to describe the friction of simple fluids, we will show that the slip length is not appropriate for viscoelastic liquids. Rather, the appropriate description lies in the original Navier’s partial slip boundary condition, formulated in terms of an interfacial friction coefficient. We establish an exact analytical expression to extract the interfacial friction coefficient from oscillatory drainage forces between a sphere and a plane, suitable for dynamic SFA or atomic force microscopy noncontact measurements. We use this model to investigate the boundary friction of viscoelastic polymer solutions over 5 decades of film thicknesses and 1 decade in frequency. The proper use of the original Navier’s condition describes accurately the complex hydrodynamic force up to scales of tens of micrometers, with a simple Newtonian-like friction coefficient that is not frequency dependent and does reflect closely the dynamics of an interfacial depletion layer at the solution-solid interface.


*This work was supported by ANR-ENCORE program (ANR-15-CE06-005)

Mechanical and thermodynamic properties of Aβ42, Aβ40 and α-synuclein fibrils from molecular-scale simulation

ADOLFO POMA (Presenter), Biosystems and Soft Matter, Polish Academy of Sciences, HORACIO VARGAS, Polymer Theory, Max Planck Institute for Polymer Research, MAI SUAN LI, PANAGIOTIS THEODORAKIS, Theoretical Physics, Polish Academy of Sciences — Atomic force microscopy (AFM) is a versatile tool to characterise the mechanical properties of biological systems. However, AFM deformations are tiny, which makes impossible the analysis of the mechanical response by experiment. Here, we have employed a simulation protocol to determine the elastic properties of several biopolymers (i.e. biological fibrils). For these systems, the simulation approach is sufficient to provide reliable values for three different types of elastic deformation, i.e. tensile ($Y_t$), shear ($S$), and indentation ($Y_I$). Our results enable the comparison of the mechanical properties of these fibrils. In particular, we find a significant elastic anisotropy between axial and transverse directions for all systems. In addition, our methodology is sensitive to molecular packing of the fibrils. Interestingly, our results suggest a significant correlation between mechanical stability and aggregation propensity (rate) in amyloid systems, that is, the higher the mechanical stability the faster the fibril formation takes place.

*This research has been supported by the National Science Centre, Poland, under grant No. 2017/26/D/NZ1/00466 and the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 665778.

Wednesday, March 6, 2019 2:30 PM - 5:18 PM

Session P50 DPOLY DMP: Organic Electronics II: Structure and Morphology

DeLongchamp, National Institute of Standards and Technology - Tag(s): Focus
3:06PM P50.00004: Exploring the impact of atomistic substitution on thin-film structure in a germanyl-ethynyl functionalized pentacene  JANIS SORLI (Presenter), Department of Chemical and Biological Engineering, Princeton University, QIANXIAI AI, DEVIN GRANGER, CHAD RISKO, JOHN ANTHONY, Department of Chemistry, University of Kentucky, LYNN LOO, Department of Chemical and Biological Engineering, Princeton University — Functionalization of organic semiconductors through the attachment of bulky side groups to the conjugated core has imparted solution processability to this class of otherwise insoluble materials. A consequence of this functionalization is that the bulky side groups impact the solid-state packing of these materials. To examine the importance of side group electronic character on accessing the structural phase space of functionalized materials, germanium was substituted for silicon in trisopropylsilyl-ethynyl-pentacene (TIPS-Pn) to produce trisopropylgermanyl-ethynyl-pentacene (TIPGe-Pn), with the TIPGe side group comparable in size to TIPS, but higher in electron density. We find TIPGe-Pn single crystals to exhibit slip-stack, herringbone and brickwork packing depending on growth conditions, a stark contrast to TIPS-Pn, which only accesses the brickwork packing motif in both single crystals and thin films. Polycrystalline thin films of TIPGe-Pn exhibit two new, unidentified polymorphs from spin-coating and post-deposition annealing. Our experiments suggest that access to the structural phase space is not solely guided by the size of the side group. Its electronic character appears to play a significant role in dictating the accessible solid structures.
3:18PM P50.00005: Investigation on charge transport properties of Cyclopentadithiophene-based D-A type semiconducting copolymers* JIYOU LEE (Presenter), JISANG HONG, Pukyong National University — We have studied the charge transporting properties in Cyclopentadithiophene (CDT)-based donor (D) – acceptor (A) type semiconducting copolymer, which is known to have high performance, as an active layer of a field-effect transistor. In order to investigate the relationship between the charge-carrier mobility and the structural property of each polymer, the CDT-based polymer thin-films were analyzed by ultraviolet-visible spectroscopy, Raman spectroscopy, and density function theory (DFT) simulation. From our experimental results, it was found that the charge transports in the CDT-based polymeric thin-film is more dependent on the efficient intramolecular transport than the intermolecular charge transports. These results suggest that improving the planarity and rigidity of the polymer backbone is essential for efficient intramolecular charge transfer in order to design a high performance D-A type semiconducting copolymer.

*This research was supported by the Basic Science Research Program through NRF funded by the Ministry of Science, ICT & Future Planning of Korea (code no. 2018R1A1A105021060).

3:30PM P50.00006: Printing Conjugated Polymers to Order via Non-Equilibrium Assembly* [Invited] YING DIAO (Presenter), Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign — Controlled morphology evolution via directed assembly has played a central role in the development of modern electronic, optical and clean energy materials. In comparison to conventional ‘hard’ materials, polymer-based functional materials can be easily processed into diverse form factors by low-cost, high-throughput methods such as roll-to-roll printing and 3D printing. The printing conditions intimately couple with the assembly process and sensitively modulate the solid-state properties in the fabricated devices. We are particularly interested in semiconducting polymers which have demonstrated potential uses in a diverse range of applications from transistors, thermoelectrics, sensors, light-emitting diodes to solar cells etc. However, major challenges remain, in controlling the nucleation, growth and aggregation of conjugated polymers during solution printing and coating, which critically impact the printed device performance by orders of magnitude. The rapid printing process creates a complex environment with coupled physics that drive the polymer assembly far from equilibrium.

In our work, we combine printing experiments, morphology and device characterizations with governing-equation-based modeling and simulations to present new insights and strategies for controlling multi-scale assembly of semiconducting polymers. We observe unexpected flow-induced morphology and electronic transition that accompanies change in printing regimes. We elucidate that printing flow in a moving, drying meniscus can drastically alter the polymer assembly pathways by flow-induced conformation change. We further establish tools for investigating design rules for flow-induced conjugated polymer crystallization. High degree of morphology control from molecular to device scale further enables new insights into charge transport properties of semiconducting polymers and realizes advanced electronic device applications.

*NSF DMR grant #16-41854

4:06PM P50.00007: Molecular Orientation in Thin Films of Poly(3-hexylthiophene) And Poly(3-(6-bromohexyl)-thiophene) Crystallized on Graphene OLEKSANDR DOLYNCHUK (Presenter), Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg, PHILIP SCHMODE, PAUL M. REICHSTEIN, Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, MATTHIAS FISCHER, Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg, MUKUNDAN THELAKKAT, Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, THOMAS THURN-ALBRECHT, Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg — Recent findings have shown that crystallization of polymers on a substrate is advantageous for inducing molecular orientation, especially for semicrystalline conjugated polymers due to their anisotropic charge transport properties. Although graphite induces face-one crystal orientation in monolayers of poly(3-hexylthiophene) (P3HT), a full face-one orientation in thicker P3HT films was not realized so far. The latter is assumed to be a result of two competing interfacial orientations due to different interactions of P3HT side chains with vacuum and the graphite substrate. Here we show that modification of the chemical structure of P3HT side chains can alter the interfacial interactions and result in completely face-on oriented crystals. Specifically, we present a comparative study of the substrate induced molecular orientation of poly(3-(6-bromohexyl)-thiophene) (P3BrHT) and P3HT. The crystal orientation in ultrathin films of both polymers crystallized on a single layer graphene was explored by grazing incidence XRD. The results indicated that P3BrHT on graphene had solely face-on oriented crystals, whereas P3HT on graphene showed mixed crystal orientation with edge-on crystals formed at the top surface.
A Study on Intrinsic Mechanical Properties of n-type Conjugated Polymer via Controlling the Molecular Weight: The Importance of Critical Molecular Weight for Stretchable Organic Electronics

JONNYEONG CHOI, Department of Chemical and Biomolecular Engineering, KAIST, WANSUN KIM, TAEK-SOO KIM, Department of Mechanical Engineering, KAIST, BUMJOON KIM (Presenter), Department of Chemical and Biomolecular Engineering, KAIST — The understanding on the mechanical properties of semicrystalline n-type conjugated polymers is very important for developing the stretchable electronics. In this work, we investigated the intrinsic mechanical properties of naphthalene diimide (NDI) based n-type conjugated polymer, P(NDI2OD-T2) via controlling the number-average molecular weight (Mn), ranging from low to very high Mn = 15, 20, 48, 103 and 163 kg mol⁻¹. While we observed the general increasing trend of tensile properties as a function of Mn, a sharp transition in the strain at fracture and toughness values was observed between 48 and 103 kg mol⁻¹ with an increase by a factor of 26 and 160, indicating the presence of the critical molecular weight. This distinct transition from brittle to ductile is mainly attributed to large fraction of amorphous regions including tie molecules and interchain entanglements, which can effectively dissipate a substantial strain energy. The molecular weight dependence of mechanical behavior coincide well with thermal, viscoelastic and microstructural and thin film morphological properties. Therefore, our work suggests design rule for n-type conjugated polymer having good compromise between mechanical reliability and electrical performance for producing stretchable electronics.

Critical Role of Electron-donating Thiophene Group on the Thermomechanical Property of Donor-Acceptor Semiconducting Polymers

SONG ZHANG (Presenter), XIAODAN GU, University of Southern Mississippi — Organic semiconducting polymers are promising candidates for stretchable electronics for their mechanical compliance. Donor-Acceptor type conjugated polymers have been the key drive for recent boost in device performance. Up to date, the effect of the backbone structure on the thermomechanical property of conjugated polymers has not been carefully studied. This paper investigated the structure and thin film mechanical property relationship for donor-acceptor polymers with systematically varied backbone structures. The pseudo-free standing tensile test was used to obtain the full stress-strain curve, the glass transition temperature was measured for both thin and bulk films. In the meantime, detailed morphology was detected using AFM, UV-vis, and GIWAXS for further understanding. A general trend was observed and applied to the design of new stretchable conjugated polymers.

Polymer light-emitting diodes with an emitting layer based on a nano-confined semiconducting polymer blend

ANIELEN RIBEIRO, PAUL BLOM, JASPER MICHELS (Presenter), Max Planck Institute for Polymer Research — Blending a visible light-emitting organic semiconductor with an insulator alleviates the trap-limited nature of the electron current. Organic light emitting diodes (OLEDs) comprising such a blend as emissive layer exhibit a two-fold increase in luminous efficiency with only 10% semiconductor. Due to this low content of semiconductor, polymer-LEDs are more attractive than small molecule-based devices. However, polymers impose the difficulty of an inherently low miscibility. In a plain blend macro-phase separation can be avoided if the molecular weight is kept low, which, in case of the semiconductor, is a disadvantage as it suppresses charge carrier mobility. An alternative strategy is to impose a nano-confinement. We prepare aqueous nanodispersions of red (PPV) and blue (polyfluorene) emitting polymers, blended with polystyrene as insulator. We seem to fully suppress macro-phase separation in both cases. For the latter, the combination of nano-confinement and blending influences the phase morphology of the semiconductor in an unprecedented way. Fabricating OLEDs with an emitting layer consisting of nanoparticles poses a considerable challenge due to high operational current densities. We now succeed in fabricating such devices in a reproducible way at very decent efficiencies.
Complexation of a Conjugated Polyelectrolyte and Impact on Optoelectronic Properties*

SCOTT DANIELSEN (Presenter), THUC-QUYEN NGUYEN, GLENN FREDRICKSON, RACHEL SEGALMAN, University of California, Santa Barbara — Electrostatic assembly of conjugated polyelectrolytes (CPEs), which combine a π-conjugated polymer backbone with pendant ionic groups, offer an opportunity for overcoming the limited solubility of most semiconducting polymers to make concentrated inks with tunable materials properties and device performance. Complex coacervation, a liquid–liquid phase separation upon complexation of oppositely charged polyelectrolytes in solution, is used to form dense suspensions of π-conjugated material. A model system was used to investigate this complexation behavior of conjugated polyelectrolytes in terms of electrostatic strength, solvent quality, and polymer concentration. The balance of electrostatic interaction between the oppositely charged polyelectrolytes together with their charge compensating counter-ions and solvent quality for the hydrophobic π-conjugated backbone leads to a rich phase diagram of soluble complexes, precipitates, and complex coacervates. The CPE in the polyelectrolyte complexes has an increased π-conjugation length and enhanced emissivity, with ideal chain configurations due to the reduction of kink sites and torsional disorder.

*The authors gratefully acknowledge support from the U.S. Department of Energy Office of Basic Energy Sciences under Grant No. DE-SC0016390

Atomistic modeling of conjugated PEDOT:PSS complexes*

WESLEY MICHAELS (Presenter), JIAN QIN, Chemical Engineering, Stanford University — The performance of poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) complexes as conductive or thermoelectric coatings is sensitive to film microstructure and molecular packing details inaccessible to experiment. We combine ab initio calculation, DFT, and atomistic simulation to investigate the effects of ion doping, molecular polarizability, and cosolvent addition on PEDOT-PSS complexation. The results suggest that ionic liquids which bind more strongly to PEDOT are more likely to induce morphological rearrangements. Conformational properties of PEDOT:PSS under varying salinity and processing conditions are characterized, providing the basis for multi-scale morphological modeling of this conjugated polyelectrolyte complex.

*This material is based upon work supported by the National Science Foundation under Grant No. 1656518.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P52 DPOLY: Polymer Nanocomposites III: Polymer Blends and Solutions BCEC 253B - Robert Ferrier, Univ of Pennsylvania - Tag(s): Focus

Chemical and Dynamic Heterogeneities in Interfaces for Adaptive Polymer Nanocomposites*

PINAR AKCORA (Presenter), Stevens Institute of Technology — It is well-known that particle-polymer interactions strongly control the binding and conformations of adsorbed chains on particles. Interfacial layers around nanoparticles consisting of adsorbed and free matrix chains have been extensively studied to reveal their contribution to the overall thermal and mechanical behavior of nanocomposites. Using miscible polymers of different chemistries as adsorbed and matrix layers in composites, the interfacial layer dynamics, hence the mechanical properties can be modulated unusually. We recently showed that when glass transition temperature difference between adsorbed and matrix polymers were large and polymer-polymer interactions were neutral, they reversibly stiffened with temperature. In this talk, I will present the extent of chemical heterogeneity of interfacial layers in adsorbed and polymer-grafted nanoparticles and discuss the role of interfacial layer mixing and chain conformation on the mechanical properties. Low glass-transition temperature composites with different matrix polymers (poly(vinyl acetate), poly(methyl acrylate) and poly(ethylene oxide)) will be discussed with particles of different surface chemistry; and polymers with different architectures. Interfacial layer design strategies in polymer nanocomposites will be outlined. These dynamic and chemical heterogeneities in interfacial layers can be used to design mechanically adaptive polymer nanocomposites.

*This work is funded by NSF-CMMI-MEP, Grant #1538725, 1825250.
3:06 PM P52.00002: Coexistence Curve and Theta Temperature of Polymer Grafted Nanoparticle (PGN) Solutions
SARAH IZOR, TONY Dagher, CHRIS GRABOWSKI, ALI JAWAID, KYOUNGWON PARK, RICHARD VAIA (Presenter), Materials and Manufacturing, Air Force Research Laboratory — PGNs are emerging as an enabling technology, not only for nanocomposite formulation, but also for separations, energy storage, devices and coatings. Their tunability arises from the modularity of the hard-soft architecture, and understanding its impact on phase behavior in small molecules is crucial to fabrication and processing. Unfortunately, minimal data or theoretical insight is available; or how PGNs relate to the role of macromolecular architecture on solution phase behavior. Herein, we discuss the upper critical solution coexistence curve and theta temperature (Θ) of polystyrene (PS)-grafted Au-nanoparticles in cyclohexane. As molecular weight of the PS graft increases (20—50kDa), the coexistence curve shifts to higher temperatures (e.g. $T_c \sim 12$—20°C @ 10nM ($\Phi \sim 3 \times 10^{-5}$)), as determined by spectroscopy, dynamic light scattering, and x-ray scattering. Θ, estimated from extrapolating the low concentration region of the co-existence curve, also increased with graft size (Θ~25–27°C). Overall, these values are less than prior reports of PS stars (Θ~30°C) and linear chains (Θ~33°C). Understanding the macroscopic and mesoscopic solution behavior of these soft colloids in context to structured macromolecules and curved brushes is essential to their future development.

3:18 PM P52.00003: Simulating Nanoparticle Dynamics in Semidilute Polymer Solutions
RENJIE CHEN (Presenter), RYAN POLING-SKUTVIK, Department of Chemical and Biomolecular Engineering, University of Houston, Houston, ARASH NIKOUBASHMAN, Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg, MICHAEL P HOWARD, McKetta Department of Chemical Engineering, University of Texas at Austin, Austin, SERGEI EGOROV, Department of Chemistry, University of Virginia, Charlottesville, JACINTA CONRAD, JEREMY C PALMER, Department of Chemical and Biomolecular Engineering, University of Houston, Houston — The dynamics of polymers and particles in nanocomposites are of great interest in materials processing. Particle mobility is well described by the generalized Stokes-Einstein relation when the particles are much larger than the polymers, but less understood when it comes to smaller or comparable sized particles. We investigate this smaller sized regime using advanced particle-based simulation techniques, with the multi-particle collision dynamics (MPCD) scheme modeling solvent-mediated hydrodynamic interactions. We demonstrate that the translational center-of-mass motions of both particles and polymers are sub-diffusive on short times before transitioning into the diffusive regime, and the highly correlated sub-diffusive exponents suggest that not only local polymer relaxations but also polymer center-of-mass motions play a role in the coupling between the dynamics of polymers and nanoparticles. Finally, we perform simulations tuning flexibility of the polymers, and as the persistence length increases, the particle dynamics become more sub-diffusive and decouple from the dynamics of the polymer chain center-of-mass.

3:30 PM P52.00004: Interphase structures and dynamics near nanofiller surfaces in polymer solutions*
TADANORI KOGA (Presenter), DEBORAH BARKLEY, MAYA ENDOH, Stony Brook University, MICHIHIRO NAGAO, NIST, TAKASHI TANIGUCHI, Kyoto University, JAN-MICHAEL CARRILLO, BOBBY G SUMPTER, ORNL, MAHO KOGA, Cornell University, TOMOMI MASUI, HIROYUKI KISHIMOTO, SRI — We report the structures and dynamics of hydrogenated polybutadiene (PB) chains bound to carbon black nanoparticle surfaces in polymer solutions composed of deuterated PB and deuterated toluene using small-angle neutron scattering and neutron spin echo techniques together with molecular dynamics (MD) simulations. The experimental results showed that the swollen bound chains exhibit the so-called breathing dynamics at polymer concentrations $c$ below and above the overlap polymer concentrations. Interestingly, the collective dynamics slowed down by a factor of 2 compared to that in pure $d$-toluene when the chain lengths of the bound and matrix polymer are equal. However, when the free polymer chains were longer than the bound chains, the decrease in collective dynamics was not as significant. MD simulations showed that the matrix chains, whose length is equal to that of the bound chains, can be accommodated in the bound layer effectively and are “strangulated” by the bound chains, while the longer matrix chains only partly penetrate into the bound chains and the diffusion behavior was hardly affected compared to that in bulk.

*T. K. acknowledges partial financial supports from NSF Grant No. CMMI-1332499.
3:42PM P52.00005: Dynamics of polymer-grafted nanoparticles controlled by soft confinement  ALI SLIM (Presenter), RYAN POLING-SKUTVIK, JACINTA CONRAD, RAMANAN KRISHNAMOORTI, Chemical and Biomolecular Engineering, University of Houston — The efficacy of polymer-grafted nanoparticles (PGNPs) in applications depends on their transport within complex soft matrices featuring heterogeneities similarly sized to the PGNPs. Further, the deformability of the grafted polymers leads to soft interactions that may alter the dynamics, depending on the relative size of the grafted polymer and particle core. When the radius of gyration $R_g$ of grafted polymer is much smaller than NP radius $R_{NP}$, dynamics of PGNPs are expected to be similar to a hard sphere. Conversely, when $R_g$ is much larger than $R_{NP}$, PGNPs behave like a dendritic polymer or a star. In the intermediate regime where $R_g$ and $R_{NP}$ are comparable, the structure and dynamics become complex soft matrices featuring heterogeneities similarly sized to the PGNPs. Further, the deformability of the grafted polymers could be tracked to the resolution of a few nanometers.

4:06PM P52.00007: Solvent-Induced Self-Assembly of Triblock Copolymers for Creating Polymer Nanocomposite Gels  CHAO LANG (Presenter), YIFAN XU, JACOB A LANASA, MANISH KUMAR, ROBERT HICKEY, Pennsylvania State University — The self-assembly of ABA triblock copolymers has been a focus of many studies over the years because of their possible applications in thermoplastic elastomers, solid electrolytes, and drug delivery systems. Triblock copolymers exhibiting ABA-type polymer architectures will self-assemble into either flower-like micelles or physically-crosslinked gel networks when added to B-block selective solvent. Although the two final states, micelles and gels, are well-established, controlling the self-assembly process to design specific nanostructures, while incorporating inorganic nanoparticles has yet to be fully established. Here, we present a recently developed method for creating nanostructured nanocomposite hydrogels by quickly injecting a solution containing ABA amphiphilic triblock copolymers and hydrophobic nanoparticles into water. During the ABA polymer/nanoparticle solution injection process, the nanoparticles aggregate within the physically-crosslinked hydrophobic A-block domains. By adding hydrophobic gold nanoparticles to the initial polymer solution, we are able to incorporate plasmonic properties into the nanostructured gels. The research presented here highlights the great potential in kinetic manipulation of self-assembled structures for making polymer nanocomposite gels.

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YIGE GAO (Presenter), PAUL KIM, SATYAM SRIVASTAVA, ALEXANDER RIBBE, THOMAS RUSSELL, DAVID HOAGLAND, University of Massachusetts Amherst — Functionalized with polymer ligands, nanoparticles can segregate to liquid interfaces, where their two-dimensional organization and dynamics depend on nanoparticle areal fraction. Here, these organization and dynamics were imaged for PEGylated silica nanospheres on ionic liquids, the latter's nonvolatility facilitating high resolution scanning electron microscopy at vacuum. An in situ liquid cell varied surface area and thereby areal fraction, and particle interactions were well approximated as those of hard spheres. A focus was high areal fraction nanoparticle mixtures approaching and/or exceeding the threshold for jamming; such mixtures were prepared for nanospheres of different diameter and nanospheres mixed with nanorods, and in both cases, composition was varied. By image analysis, quality of mixing and nanoparticle organization were assessed through orientational and translational order parameters. For uniform nanospheres, when compressed beyond jamming, surface wrinkling and buckling were observed, and when held jammed for large times before decompression, cracking was noted; throughout the imaging, individual nanospheres could be tracked to the resolution of a few nanometers.

*NSF/DMR-1807255
4:30PM P52.00009: Self-assembly of Janus rods in binary blends of polymers. Part I: phase behavior under equilibrium*  
SHAGHAYEGH KHANI (Presenter), FELIPE LEIS PAIVA, Macromolecular Science and Engineering, Case Western Reserve University, ARMAN BOROMAND, Mechanical Engineering and Material Science, Yale University, VERONICA CALADO, School of Chemistry, Universidade Federal do Rio de Janeiro, ARGIMIRO SECCHI, COPPE Chemical Engineering Graduate Program, Universidade Federal do Rio de Janeiro, JOAO MAIA, Macromolecular Science and Engineering, Case Western Reserve University — Janus rods due to their shape anisotropy and amphiphilic nature result in superior properties when incorporated into multi-phase polymer systems. Self-assembly of these particles at the interface of binary polymer blends can provide a means for fabrication of advanced functional materials. In this presentation we will discuss the interplay between the entropic and enthalpic factors that determine the self-assembled structure of Janus rods at the interface of two immiscible liquids. We have performed molecular simulations to investigate the role of individual parameters. Janus rods orientation is controlled by the entropic factors such as aspect ratio and concentration as well as the interfacial energy which also has consequences on the dynamics. Their interfacial assembly is also shown to be highly influential in altering the phase separation process in binary polymer blends. Janus rods exhibiting hexagonally-packed, liquid crystalline-like structures favor faster phase separation kinetics, while Janus rods of higher aspect ratio that are tilted at the interface aggregate side-by-side; are able to hinder phase separation kinetics.

*The authors thank Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for financial support.

4:42PM P52.00010: Self-assembly of Janus rods in binary blends of polymers. Part II: phase behavior under shear flow and relaxation*  
FELIPE LEIS PAIVA (Presenter), SHAGHAYEGH KHANI, Macromolecular Science and Engineering, Case Western Reserve University, ARMAN BOROMAND, Mechanical Engineering and Materials Science, Yale University, VERONICA CALADO, School of Chemistry, Universidade Federal do Rio de Janeiro, ARGIMIRO SECCHI, COPPE Chemical Engineering Graduate Program, Universidade Federal do Rio de Janeiro, JOAO MAIA, Macromolecular Science and Engineering, Case Western Reserve University — Janus particles are highly active at the interface of immiscible fluids and thus they can self-assemble into different structures when incorporated into multiphase systems. In Part I, we performed mesoscale Dissipative Particle Dynamics simulations to investigate the influence of individual parameters on the structures formed by Janus rods at the interface of two immiscible liquids. In particular, we showed how interfacial orientation and self-assembly of Janus rods are highly influential in controlling the phase separation process when added to a polymer blend. Moreover, we also monitor herein the microstructures formed by these systems under flow conditions and upon relaxation after flow cessation. We verified in our simulations various stabilizing effects provided by Janus rods of higher aspect ratio that present a tilted configuration at the interface. We also studied the Janus aggregate-breakup process during shear and how these interfacial aggregates rebuild upon flow cessation. The results of this study can be used for designing new approaches for directing nano-particles into desired morphologies by applying shear flow.

*The authors thank Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for financial support.

4:54PM P52.00011: Fabrication and Optical Properties of Polymer-Grafted Gold Nanorod Assemblies  
JASON STREIT (Presenter), KYOUNGWEON PARK, Air Force Research Lab, JOON-JAE YI, Wright State University, RICHARD VAIA, Air Force Research Lab — Precise, large-scale assembly of polymer-grafted nanoparticles (PGNs) has shown great promise for the scalable manufacturing of sensors, energy storage devices, and photonic elements. Different than traditional ligand-coated nanoparticles, PGNs are stabilized by high molecular weight polymers at relatively low grafting densities. In this regard, PGNs behave as soft colloids, possessing favorable processing properties typical of polymer systems while still retaining the ability to pack into ordered structures. Herein, we demonstrate that large scale, highly uniform monolayer films of gold-polystyrene nanorods can be fabricated from PGN inks within a few seconds using a simple flow-coating technique. Using a combination of AFM, SEM, and GISAXS, we observe nanorod positional and orientational order dependent on coupling between processing conditions, polymer canopy, and surface energy. Additionally, optical extinction measurements reveal strong plasmonic coupling between the gold nanorods which can systematically be tuned by varying film morphology. With fundamental understanding of structure-processing relationships, we demonstrate optical notch filters using laser-induced reshaping of resonant nanoparticle subpoulations.
Constructing conductive composites by spinodal decomposition of miscible polymer blends with graphene nanoplatelets

YANGMING KOU (Presenter), XUANG CHENG, CHRIS W MACOSKO, Department of Chemical Engineering and Materials Science, University of Minnesota — Conductive polymer composites (CPCs) enjoy broad industrial applications such as electrostatic discharge (ESD) protection. Herein, we construct CPCs by solution-blending graphene nanoplatelets (GNPs) in a miscible blend of poly(methyl methacrylate) (PMMA) and poly(styrene-co-acrylonitrile) (SAN). By inducing PMMA/SAN spinodal decomposition via annealing above the lower critical solution temperature (LCST), we obtain spatially regular, cocontinuous polymer domains where high aspect ratio GNPs preferentially localize within the SAN phase to form a conductive network. Compared to the traditional CPC manufacture approach of blending carbon black into a homopolymer, our approach lowers the percolation threshold required to enhance electrical conductivity. At 1 wt% GNP loading, our blend shows a bulk electrical conductivity of up to ~10^{-8} S/cm upon phase separation, suitable for ESD protection. To understand the structure-property relations of our CPCs, we develop TEM image analysis methods to quantitatively characterize the final PMMA/SAN/GNP blend morphology and GNP localization, allowing us to address important questions such as how the state of GNP dispersion within the blend affects the coarsening length scale and domain size distribution throughout the composite.

*NSF CMMI-1661666

Molecular dynamics simulation of spherical PEO brush: Curvature and Grafting Density Effect

ELENA DORMIDONTOVA, UDAYA R DAHAL (Presenter), Polymer Program, Institute of Materials Science and Physics Department, University of Connecticut, Storrs, CT 06269 — Nanoparticle modification by polyethylene oxide (PEO) is commonly used to ensure nanoparticle solubility, dispersion and protection from undesirable interactions. Using atomistic molecular dynamics simulations, we studied spherical PEO brushes grafted to gold nanoparticles of different radii and with varying grafting densities. We analyzed the scaling behavior of the radial polymer volume fraction, which is found to follow the Daoud-Cotton model, except for low grafting density when PEO adsorption onto gold surface is observed. We also investigated PEO hydration in the spherical brush and determined the existence in the surface vicinity of a dehydrated or low hydration zone, which substantially expands with an increase of grafting density and/or decrease of nanoparticle radius of curvature. The implications for water exchange within the polymer brush and with the surrounding solution will be discussed.

*This work was supported by the National Science Foundation under Grant No.DMR-1410928

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P54 DPOLY DBIO: Tuning Polymer Sequence and Architecture

Polymer chain sequence effects on the glass transition

WILLIAM DRAYER (Presenter), DAVID SIMMONS, Department of Chemical and Biomedical Engineering, University of South Florida — Progress in synthetic chemistry over the last 20 years has opened the door to synthesis of polymers with an increasing spectrum of monomer sequence control, ranging from gradient copolymers to peptoids. In many of these polymers as in sequence non-controlled polymers, the glass transition plays a central role in dynamic, mechanical, and transport properties. However, the effect of sequence on the glass transition remains poorly understood. Here we employ molecular dynamics simulations of sequence controlled glass-forming liquids to quantify the effect of sequence on glass transition behavior. Results indicate that sequence can have a profound impact on Tg. Ultimately, we explore the transition from sequence effects to interface effects on Tg as monomer block size increases to the phase-separating limit.

*This material is based in part on work supported by the National Science Foundation NSF Career Award grant number DMR1554920.
Identical levels of block saturation, indicating a strong enhancement in compatibility. Further work delineating the effect of measured $X$ of 0.30 MPa, which is lower than the measured $X$ (uncorrected) of a PI-hPB diblock copolymer (0.52 MPa) with selectively saturated block-random copolymer with ~10 wt% styrene in the random block (PI-hSBR10) exhibited a $X$ of 0.81 MPa, after correcting the measured value of $X$ for the imperfect selectivity of the hydrogenation catalyst. A selective saturation of the butadiene units. Diblock copolymers with no S (PI-hPBs) exhibited an interaction energy density generally show limited compatibility (high interaction energy density, $X$). We investigate the thermodynamic interactions in symmetric amorphous polydiene-polyolefin block copolymers composed of polyisoprene (PI) and hydrogenated medium-vinyl polybutadiene (hPB). The regular solution model suggests that styrene units (S), given the higher solubility parameter of polystyrene, can boost inter-block miscibility when incorporated in small amounts into the hPB block via random copolymerization (hSBR). Block and “block-random” copolymers were prepared by anionic polymerization, followed by activated bond breakage and local cage reorganization processes, and the correlation between structure and dynamics, are studied as a function of experimentally controllable variables such as polymer volume fraction, fraction of stickers, strength and spatial range of the attractive interaction, and chain length.

*We thank the United States Department of Energy (Basic Energy Sciences, DE-SC0014458), Samsung (17A01588), and Thomas & Kipp Gutshall Professorship for financial support.

**2:54PM P54.00003: Coherent States Field Theory Simulations for Supramolecular Multiblock Copolymers**  DANIEL VIGIL (Presenter), Chemical Engineering, University of California, Santa Barbara, KRIS T DELANEY, Material Research Laboratory, University of California, Santa Barbara, GLENN FREDRICKSON, Chemical Engineering, University of California, Santa Barbara — We present simulation results for a binary mixture of telechelic polymers that can reversibly bond to the opposite species to form multi-block copolymers. Traditional auxiliary-field (AF) polymer field theory can neither accurately nor efficiently simulate the telechelic system because of the challenges of counting an infinite number of possible reaction products. Instead, we extend a “coherent states” framework (CS), originally due to Edwards and Freed, to a form that automatically accounts for all reaction products. A previously reported algorithm for simulating CS theories did not converge in ordered block copolymer microphases, so new algorithms were developed for this work. We verify our methods against the classic diblock copolymer system and present new results for the phase behavior of binary telechelic polymer mixtures.

*The authors acknowledge support from the NSF Graduate Research Fellowship Program under Grant No. 1650114 and the NSF CMMT Program under Grant No. DMR-1822215. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the NSF.

**3:06PM P54.00004: Miscibility Enhancement in Polyisoprene-Polyolefin Block Copolymers**  SRAVYA JANGAREDDY (Presenter), RICHARD ALAN REGISTER, Chemical and Biological Engineering, Princeton University — Polydienes and polyolefins generally show limited compatibility (high interaction energy density, $X$). We investigate the thermodynamic interactions in symmetric amorphous polydiene-polyolefin block copolymers composed of polyisoprene (PI) and hydrogenated medium-vinyl polybutadiene (hPB). The regular solution model suggests that styrene units (S), given the higher solubility parameter of polystyrene, can boost inter-block miscibility when incorporated in small amounts into the hPB block via random copolymerization (hSBR). Block and “block-random” copolymers were prepared by anionic polymerization, followed by selective saturation of the butadiene units. Diblock copolymers with no S (PI-hPBs) exhibited an interaction energy density of 0.81 MPa, after correcting the measured value of $X$ for the imperfect selectivity of the hydrogenation catalyst. A selectively saturated block-random copolymer with ~10 wt% styrene in the random block (PI-hSBR10) exhibited a measured $X$ of 0.30 MPa, which is lower than the measured $X$ (uncorrected) of a PI-hPB diblock copolymer (0.52 MPa) with identical levels of block saturation, indicating a strong enhancement in compatibility. Further work delineating the effect of S content on inter-block miscibility is underway.

**3:18PM P54.00005: Theory of interchain packing and dynamics in associating copolymer liquids**  ASHESH GHOSH (Presenter), KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — We employ liquid state theory to explore the role of attractive groups regularly co-polymerized in a chain backbone on the structure and dynamics of unentangled polymer liquids that can form thermoreversible bonds. Significant progress has been made by others using coarse-grained polymer physics models based on phenomenological input parameters that quantify the sticker association energy and bond dissociation lifetime. However, these approaches are not force-based, and do not include molecular-scale information about packing correlations and its consequences on sticker clustering, dynamic bond formation and dissociation events. Based on the microscopic forces and single chain structure as input, we combine equilibrium integral equation theory and generalized Rouse models that capture local caging and physical bond formation to study the latter aspects and related issues such as emergent elasticity. The timescale for stickers and non-stickers that define the coupled activated bond breakage and local cage reorganization processes, and the correlation between structure and dynamics, are studied as a function of experimentally controllable variables such as polymer volume fraction, fraction of stickers, strength and spatial range of the attractive interaction, and chain length.
WEIHUA LI, Fudan University, JIN KIM, Pohang University of Science and Technology — Block copolymers have been extensively investigated because of their various nanostructures. For a simple diblock copolymer, hexagonally packed cylindrical microdomains have been found with volume fractions of one block (fA) having 0.2~0.35, while gyroid microdomains were observed at fA having ~0.35. So, gyroid and cylindrical microdomain could not prepare pore volume larger than this value (~0.35) in diblock copolymers, because lamellar microdomains are expected. Here, we investigated morphology transitions of linear tetrablock copolymers of polystyrene-block-polyisoprene-block-polystyrene-block-polyisoprene (S1I1S2I2) by varying volume fraction of PI1 block (fPI1), while maintaining the symmetric volume fraction of total PS blocks and PI blocks (fPS1+fPS2 : fPI1+fPI2 = 1:1). An interesting sequence of morphology transitions was observed as fPI1 was increased: lamellae→asymmetric lamellae→hexagonally packed PI-cylinders→double gyroid with PI-network domains→short-period lamellae. It is particularly interesting that cylindrical and gyroid morphologies were observed in linear block copolymers with symmetric overall volume fraction.

*This work was supported by the National Creative Research Initiative Program supported by the National Research Foundation of KOREA(2013R1A3A2042196).

3:42PM P54.00007: Genetically encoded biomaterials that self-assemble across multiple length scales [Invited] ASHUTOSH CHILKOTI (Presenter), Duke University — Elastin like polypeptides (ELPs), composed of repeats of VPGXG pentapeptides that recur in all tropoelastin sequences, are the best studied class of peptide polymers that exhibit lower critical solution temperature (LCST) phase behavior in water, and these polymers have enabled innovative approaches to nanoparticle self-assembly, cancer therapy, regenerative medicine and protein purification. I will discuss how this class of intrinsically disordered polypeptides is an enormously mutable model system that has allowed us to probe the sequence origins of aqueous phase behavior in polypeptides, leading to the identification of sequence heuristics for the de novo design of peptide polymers that exhibit aqueous phase behavior. I will also discuss how we have used ELPs as a template to encode higher order, hierarchical self-assembly into macroscopic biomaterials by modulating the degree of order in these intrinsically disordered polymers, and by genetically encoding a post-translational modification into an ELP.

4:18PM P54.00008: Multicompartment Copolymer Micelles: effects of chain architecture, composition and interaction strength BOYUAN YU (Presenter), Institute for Molecular Engineering, University of Chicago, ABELARDO RAMIREZ-HERNANDEZ, COE BIOMEDICAL ENGINEERING, The University of Texas at San Antonio, JUAN DE PABLO, Institute for Molecular Engineering, University of Chicago — Controlling the self-assembly of block copolymers in solution will enable engineering of multicompartment micelles (MCMs), with target structures for applications including drug delivery, or stimuli-responsive carriers. While extensive research has been carried out on amphiphilic di-block copolymers, little is known about the phase behavior of multiblock polymers in solution. In this work, a mesoscopic approach is used to explore the self-assembly behavior of tetrablock copolymers with varying architectures, block sequences, compositions, and interaction strengths. Our results are summarized in phase diagrams that reveal the influence of different parameters on the morphologies of MCMs. The results presented in this work could provide a useful guide for the synthesis of new MCMs.

4:30PM P54.00009: Interpreting the hierarchical morphology of ABC miktoarm terpolymers using self-consistent field theory* JYOTI MAHALIK (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, HYEYOUNG KIM, Polymer Science and engineering, University of Massachusetts Amherst, MATTHIAS ML ARRAS, Large Scale Structures Group, Neutron Scattering Division, Oak Ridge National Laboratory, WEIYU WANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, SERGEY CHERNYY, Micro- and Nanotechnology, Technical University of Denmark, Productionstorvet, 2800 Lyngby, Denmark, KUNLUN HONG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, GREGORY S SMITH, Large Scale Structures Group, Neutron Scattering Division, Oak Ridge National Laboratory, BOBBY G SUMPTER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, THOMAS RUSSELL, Polymer Science and engineering, University of Massachusetts Amherst, RAJEEV KUMAR, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Miktoarm stars based on poly(cis 1,4-isoprene), poly(styrene) and poly(2-vinylpyridine) (ISV) were studied using small-angle X-ray scattering (SAXS), small-angle neutron scattering (SANS), transmission electron microscopy (TEM) and self-consistent field theory (SCFT). Array of morphologies are observed for different composition of ISV-x (where x is the volume ratio of V:I and I:S are kept fixed at 1:1). Typically, TEM and SANS are sufficient to characterize the bulk morphology of diblock copolymers. But for ABC miktoarms additional characterization tools are necessary. Picking one system from the array of samples, we have demonstrated how self-consistent field theory (SCFT) can guide the interpretation of hierarchical morphology. The SCFT studies also provides guidelines for deuterating the correct arm prior to SANS investigation.

*Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy (DOE).
**4:42PM P54.00010: Miktoarm Stars via Grafting-Through Copolymerization: Self-Assembly and the Star-to-Bottlebrush Transition**

JOSHAU LEQUIEU (Presenter), ADAM E LEVI, CHRISTOPHER M BATES, GLENN FREDRICKSON, University of California, Santa Barbara — The grafting-through copolymerization of two distinct macromonomers via ring-opening metathesis polymerization is typically used to form random or diblock bottlebrush polymers with large total backbone degrees of polymerization ($N_{BB}$) relative to that of the side-chains ($N_{SC}$). Here, we demonstrate that Grubbs-type chemistry in the opposite limit, namely $N_{BB} \ll N_{SC}$, produces well-defined materials with excellent control over ensemble-averaged properties, including molar mass, dispersity, composition, and number of branch points. The dependence of self-assembly on these molecular design parameters was systematically probed using small angle X-ray scattering and self-consistent field theoretic simulations. Our analysis reveals that two-component bottlebrush copolymers with small $N_{BB}$ behave like miktoarm star polymers. The star-to-bottlebrush transition is quantifiable for both random and diblock sequences by unique signatures in the experimental scaling of domain spacing and simulated distribution of backbone/side-chain density within lamellar unit cells. These findings represent a conceptual framework that simplifies the synthesis of miktoarm star polymers when dispersity in molar mass and composition can be tolerated.

**4:54PM P54.00011: Exploring the Phase Behavior of Poly(styrene)-block-Poly(dimethylsiloxane) Brush Block Copolymers**

HUAIFENG FEI (Presenter), BENJAMIN M YAVITT, XIYU HU, GAYATHRI KOPANATI, ALEXANDER RIBBE, JAMES J WATKINS, University of Massachusetts Amherst — We report the experimental phase behavior of a family of poly(styrene)-block-poly(dimethylsiloxane) (PS-b-PDMS) bottlebrush block copolymers (BBCPs). The BBCPs rapidly self-assemble into microphase separated morphologies after mild thermal annealing. By systematically tuning architectural parameters such as volume fraction ($f_{PS}$), side chain length ($N_{SC}$), and overall backbone length ($N_{bb}$), a diverse array of morphologies were resolved and a phase map was constructed. We identify ordered lamellar, cylindrical, and deformed spherical morphologies. The lamellar window spans a wide range of $f_{PS}$ from 0.40 to 0.75 when $N_{bb}$ is short and $N_{SC}$ of PS and PDMS are equal. However, order-order transitions to cylindrical and spherical morphology are observed as $N_{bb}$ increases and $N_{SC}$ becomes asymmetric. The self-assembly and phase transitions are described by a contrast between both the backbone and side chain flexibility of the PDMS and PS blocks. These findings provide an insight into the rich phase behavior of this architecturally complex class of macromolecules and provide direction towards the future fabrication and design of BBCP templated functional materials.

*NSF Center for Hierarchical Manufacturing at the University of Massachusetts, Amherst

**5:06PM P54.00012: Molecular Architecture Driven Self-Assembly of Block Copolymers**

SHIFENG NIAN (Presenter), ZIHAO GONG, Materials Science and Engineering, University of Virginia, LIHENG CAI, Materials Science and Engineering and Chemical Engineering, University of Virginia — Block copolymers composed of immiscible polymeric blocks self-assemble to a rich variety of ordered nanostructures that find applications in many technologically important realms. Among different types of block copolymers, linear-bottlebrush-linear (LBBL) triblock copolymers present an emerging platform for creating multifunctional nanostructures. However, little is known about the fundamental mechanism of their self-assembly. We synthesize a series of LBBL polymers with precisely controlled anisotropy of bottlebrush block and weight fraction of the linear block. Characterizing morphology and microphase separation of the self-assembled nanostructures, we find that the molecular anisotropy of bottlebrush is sufficient to drive LBBL polymers self-assemble to long range ordered nanostructures with exceptionally large domain sizes inaccessible by existing copolymer systems. Our results suggest that the self-assembly of LBBL polymers is driven by their molecular architecture rather than detailed chemistry. Such understanding may enable discovery of polymeric nanostructures with unprecedented properties and multifunction.

**5:18PM P54.00013: Strong Induced Chiroptical Effects in Light Emitting Polymer Blends**

JESSICA WADE (Presenter), LIWAN, Imperial College London — Current OLED displays rely on a circularly polarised (CP) filter to enhance contrast by trapping ambient light inside the display. This means that 50% of the randomly polarised light emitted from each OLED pixel never leaves the screen, halving display efficiency and decreasing operational lifetime. To overcome this, we pair a chiral small molecule with a non-chiral device optimised polymer, which allows for CP-dependent applications while retaining the performance properties of the original polymer. Previously circularly polarised polymer emission has been achieved by the propagation of linearly polarised light through cholesteric stacks, where light becomes circularly polarised as it moves through an entire pitch. For the first time, we demonstrate a system where CP electroluminescence arises due to both intrinsic emission from chiral dipoles and extrinsic propagation through a cholesteric stack. Remarkably, this competition results in an inversion of the handedness of the CP EL emission as a function of film thickness. We compare how the chemical structure of the polymer and post-deposition processing impacts the chiroptical response of the resulting device in an effort to provide a set of design rules for future high performance CP-OLEDs.
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Session P55 DPOLY: Polymer Crystallization I: Structure and Morphology BCEC 254B - T. Miyoshi,
University of Akron Rufina Alamo, Florida A&M and Florida State University - Tag(s): Focus

2:30PM P55.00001: Microscopic Observation of Interface-Induced Crystallization via Prefreezing from Polymers Melts* [Invited]  ANN-KRISTIN FLIEGER, OLEKSANDR DOLYNCHUK, MUHAMMAD TARIQ, THOMAS THURN-ALBRECHT (Presenter), Institute of Physics, Martin-Luther University Halle-Wittenberg —
The microscopic ordering process that a liquid undergoes during crystallization is often initiated at an interface to a solid. Different processes have been suggested by theory to occur at this interface. Of special interest is prefreezing - the formation of a thin crystalline layer at the interface already at temperatures above the melting temperature. Because of the difficult accessibility of the buried interface, experimental proof of crystallization by prefreezing has been elusive in molecular systems. We here present in situ AFM-observations of such a process in two polymeric model systems and show that prefreezing is a first-order prewetting transition. A quantitative description of the phenomena is possible with a phenomenological theory. The results not only contribute to our fundamental understanding of crystallization but might also be useful for the preparation of well-ordered oriented thin films of crystalline organic materials.

References

*We acknowledge funding by the Deutsche Forschungsgemeinschaft SFB TRR 102.

3:06PM P55.00002: Supramolecular Crystals and Crystallization  STEPHEN Z D CHENG (Presenter), Polymer Science, University of Akron — Supramolecular crystal and crystallization is a field that is an extension of polymer crystals and crystallization. This topic associates with non-equilibrium thermodynamic features via analyzing and understanding structures and morphologies of supramolecular crystals. These crystals possess semi-ordered structures which are caused by crystallization and phase transformation kinetics controlled by nucleation processes and growth. We will focus on a few examples of the formation of Frank-Kasper phase and quasicrystal kinetics in the melt and transition between these phases. Specific mechanisms of phase stricture changes will be revealed in these supramolecular crystals.

3:18PM P55.00003: Crystallization of conjugated polymers* LUCIA FERNANDEZ-BALLESTER (Presenter), RAMIN HOSSEINABAD, University of Nebraska — The final semicrystalline morphology of a polymer strongly depends on the processing conditions under which crystallization occurs. Even small variations in the degree of crystallinity, size/orientation of crystallites, and connectivity between crystalline aggregates can lead to significant changes in final properties. For conjugated polymers, the basic interplay between molecular structure, processing parameters and structure development remains particularly elusive because, typically, the crystallization process occurs under ill-defined flow and thermal conditions while a solvent evaporates relatively quickly. Here, we explore the crystallization behavior of poly-3-hexylthiophene of various molecular weights under well-defined conditions. The results suggest that memory and self-nucleation can play an important role in the way crystallization proceeds.

*DMR-1809888
3:30PM P55.00004: Tuning the Phase Behavior of Hydrogenated Polynorbornene via Epimerization  
JARED PHILLIP KLEIN (Presenter), RICHARD ALAN REGISTER, Princeton University — Hydrogenated polynorbornene (hPN) synthesized by ring-opening metathesis polymerization exhibits a thermotropic polymorphic transition at a temperature \( T_{cc} \) below the melting point \( T_m \). Though atactic, hPN is able to crystallize, and the ability of hPN to accommodate defects within the crystal allows the influence of a variety of defects on \( T_{cc} \) to be studied. Polynorbornene (PN) can be saturated via multiple pathways, and the choice of hydrogenation route influences both the crystal structure and \( T_{cc} \). Three hydrogenation routes for complete PN saturation are compared: a homogeneous route that generates a diimide molecule \textit{in situ}, a Ni/Al catalyst complex, and a supported Pd catalyst. The resulting polymer chains show zero, minor (\(< 4 \%\)), and major (\( > 8 \%\)) amounts of epimerization of the cyclopentylene ring (from \textit{cis} to \textit{trans}) for the diimide, Ni/Al, and Pd-hydrogenated hPNs respectively, but all show similar degrees of crystallinity. The window of stability of the rotationally-disordered polymorph (\( T_m - T_{cc} \)) increases with increasing epimerization. The crystal structure of the rotationally-ordered polymorph – observed below \( T_{cc} \) – changes sharply with low levels of epimerized units along the chain, but is weakly influenced by further epimerization.

3:42PM P55.00005: Gap Dependent Percolation of Spherulites during Crystallization: Rheology, Microscopy and Simulation  
DEBJANI ROY, DEBRA AUDUS, KALMAN MIGLER (Presenter), National Institute of Standards and Technology — We employ simultaneous mechanical rheology and optical microscopy, with augmentation by deterministic reconstruction and simple simulations to develop a geometrical model of spherulitic percolation during polymer crystallization. We observe nucleation of surface and bulk spherulites of isotactic polypropylene which are initially isolated and then impinge on each other to form clusters that eventually span the gap, and correlate this with rheology. There is a strong gap dependence to our observations, which is explained by two distinct mechanisms that both work to enhance kinetics at lower gaps. First, the time required for a cluster to span the gap decreases with decreasing gap width, attributable to finite size effects in percolation theory. Second surface nucleation enhances the overall crystallization rate in a fashion which increases in relative importance as the gap width decreases. The modulus-crystallinity relationship can be described through general effective medium theory which indicates a transformation from percolating behavior at large gap towards a linear behavior at small. We describe our results in terms of dimensionless parameters that indicate when gap dependent effects can be anticipated.

3:54PM P55.00006: Miniemulsions as Dynamic Confinement Environments for Polymer Crystallization  
MARK STAUB (Presenter), CHRISTOPHER LI, Drexel University — Introducing interfaces and/or confinement to the polymer crystallization process is unique as the resulting kinetics, structure, and morphology can be vastly different compared to the bulk. Manipulating the confinement size and interfacial energy can provide control over the crystallization process resulting in tunable morphologies and properties. Miniemulsions where polymer/poor solvent is used as the dispersed phase present an intriguing case where the confinement is introduced by the liquid/liquid (L/L) interface and the confinement length scale, droplet size, can be readily tuned. A unique aspect of this system is the (L/L) interface that is dynamic when compared to solid/liquid, solid/solid, or vapor/liquid and that has a tunable interfacial energy by choice of emulsifier, solvent, and polymer. The nanoscale curvature of the interface is also interesting in regard to polymer crystallization where the curvature is incommensurate with the crystal’s translational symmetry. Our group has recently utilized a miniemulsion system to study polymer crystallization at curved (L/L) interface for a variety of polymers and hybrid materials. This talk will focus on our findings of the unique nanoscale morphologies obtained along with the unique thermal and mechanical properties observed.

4:06PM P55.00007: Solvent Vapor Annealing to Control Polymer Crystal Morphology  
SAMUEL E BLIESNER, JULIE ALBERT (Presenter), Chemical and Biomolecular Engineering, Tulane University — Poly(\( \varepsilon \)-caprolactone) (PCL) is a semi-crystalline, hydrophobic, biodegradable polymer that has found uses in the packaging industry and in biomedical engineering as an anti-adhesion biomaterial film and drug delivery medium among other applications. Degree of crystallinity, crystal morphology, and crystal size are known to affect the biodegradation profile of PCL fibers and films by enzymes, so morphological control is important to designing PCL coatings and films for these applications. Inspired by the literature related to solvent vapor annealing (SVA) in block copolymer films and solvent-induced crystallization in semi-crystalline polymers, we are studying how SVA treatments impact crystal morphology. We use in-situ grazing incidence wide-angle X-ray scattering to determine when/if polymer crystals dissolve during solvent uptake and at what solvent concentrations recrystallization occurs during solvent removal. Additionally, we examine polymer morphology across multiple length scales using a combination of optical microscopy, profilometry, and atomic force microscopy.

*1. NSF 1554555 (J. N. L. Albert, NSF CBET CAREER)  
4:18PM P55.00008: Crystallite Dissolution in Poly(ethylene oxide) Polymers Caused by Water  DANIEL HALLINAN (Presenter), ONYEKACHI D OPARAJI, OLUWAGBENGA IYIOLA, Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, MATTEO MINELLI, ANDREA SARDANO, Department of Civil, Chemical, Environmental and Materials Engineering (DICAM), Alma Mater Studiorum; University of Bologna — Poly(styrene)-block-poly(ethylene oxide) (PS-b-PEO) is a semicrystalline block copolymer (BCP) with interesting properties. It is mechanically tough and amphiphilic. The mechanical toughness is due to the crystallinity of PEO and the glassiness of PS, as well as the morphological structure of the BCP. These polymers have high CO₂, water, and salt solubility that derive from the polar PEO component. Potential applications include CO₂ separation, water purification, and lithium air batteries. In all of the aforementioned applications, water transport is an important parameter. The presence of water can also affect thermal and mechanical properties. Water transport and thermal and mechanical properties of a lamellar PS-b-PEO copolymer, as well as PS and PEO homopolymers have been measured as a function of water activity. Water was found to dissolve PEO crystallites and plasticize PS, which in turn affects the transport. Fourier transform infrared-attenuated total reflectance (FTIR-ATR) spectroscopy was employed to examine crystallite dissolution and water diffusion. A model accounting for both processes captured the experimental observations.

4:30PM P55.00009: Epitaxial growth of polyethylene oxide atop muscovite mica  JASON LIU (Presenter), CRAIG ARNOLD, Department of Mechanical and Aerospace Engineering, Princeton University, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — Semi-crystalline polymers confined to nanoscale dimensions often crystallize in unexpected ways vastly different from that of bulk crystallization. The crystallization of ultrathin (< 100 nm) films atop solid surfaces is one example, in which the interaction of polymer chains with the underlying substrate is vital in determining the crystallization kinetics and film morphology. Additionally, geometric matching at the molecular scale between the polymer and substrate may induce epitaxial growth. In this work, we deposit ultrathin films of polyethylene oxide atop muscovite mica by matrix-assisted pulsed laser evaporation. We demonstrate an epitaxial relationship between needle-like polymer crystals and the substrate. Mechanisms of nucleation and growth of the epitaxial crystals are discussed.

4:42PM P55.00010: Effect of zone annealing on anisotropic nanoparticle reordering in polymer nanocomposites*  ALEJANDRO KRAUSKOPF (Presenter), ANDREW JIMENEZ, SANAT KUMAR, Columbia University, ELIZABETH LEWIS, BRYAN VOHT, The University of Akron, JULIA PRIBYL, BRIAN C BENICEWICZ, University of South Carolina — Improving mechanical properties of polymeric systems is a primary research focus within the soft matter community. Isothermal crystallization studies have been performed on systems composed of polymer-grafted nanoparticles dispersed within a polymeric matrix, where the crystallized samples exhibit an increase in the tensile modulus by almost an order of magnitude as compared with the well-dispersed samples. Recently, a technique called zone annealing has been developed in which samples are rotated or translated across a fixed temperature gradient. This technique reduces processing times from days to hours. Initial X-ray scattering experiments have demonstrated that the nanoparticles seem to order in an anisotropic fashion along the crystallizing polymer lamellae after zone annealing.

4:54PM P55.00011: Utilizing Mixed Nanofillers to Control Crystallization Induced Ordering*  ANDREW JIMENEZ (Presenter), SANAT KUMAR, Columbia University, JACQUES JESTIN, CEA/CNRS, Laboratoire Léon Brillouin — The technique of controllably tuning nanoparticle ordering in semicrystalline polymers by crystallizing at very slow growth velocities (i.e. high temperatures) represents a very interesting physical situation. While organized PMMA-g-silica fillers have been shown to further enhance the mechanical properties, the particles' inherent effect on the crystallization process leads to significantly longer processing times and lower degrees of crystallinity than is desirable. To combat this, a mixture of fillers of different sizes (specifically a bimodal distribution) is used to simultaneously increase the rate of crystallization, through nucleation, while allowing smaller fillers to continue to organize. This provides the simultaneous benefit of adding another level to the hierarchically ordered system. By tuning the relative size of either particle or aggregate one can optimize this nucleation effect while benefiting from the structural reinforcement of the secondary filler.

*United States Department of Energy, Office of Science Gates Millennium Scholars Program Columbia University Soft Matter Grant

*DOE
Crystallization behavior in spin-coating film-forming processes has been investigated for Poly(ε-caprolactone) (PCL) having the weight-average molecular weight ($M_w$) of $129 \times 10^3$, $39 \times 10^3$ and $16.8 \times 10^3$ by time-resolved measurements of grazing-incidence small-angle and wide-angle X-ray scattering (GISWAXS) using synchrotron radiation in SPring-8 (RIKEN, Japan). Effect on the rotational speed, the PCL concentration in solutions and the molecular weight of PCL on crystallization kinetics and lamellar orientation during spin-coating will be explained in my presentation.

This research was partly supported by JSPS KAKENHI Grant Number 26410135 and CREST, JST. The synchrotron radiation experiments were performed at BL45XU in SPring-8 with the approval of RIKEN (Proposal No. 20140061, 20150076, 20160041, 20170094).

Regenerated cellulose fibers: Relating mechanical response to semicrystalline microstructure

We compare regenerated cellulose fibers manufactured using Viscose and Lyocell processes. These fibers show qualitatively similar mechanical response in different experiments e.g. stretching, stress relaxation and stress recovery. We show that the linear viscoelastic response of these fibers is accurately captured using a phenomenological model. The model parameters correlate well to the structural features and thus provide a robust structure-property relation for the linear region response. When stretched beyond the linear region, regenerated cellulose fibers show a transition in the slope of stress strain curve at a critical strain. This transition has been attributed in the literature to yielding of fibers. We demonstrate that this is incorrect and that the critical strain corresponds to an apparent yield. When subjected to strains higher than this apparent yield point, the fibers retain a memory of the mechanical deformation, that decays logarithmically with time and is lost over about a day as the fiber structure transitions back to the original as spun fiber.

We acknowledge Aditya Birla Science and Technology Company Pvt. Ltd. For funding.

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Exploring the mechanics of curved creased origami with a discrete bar and hinge model

Simulation approaches from computer graphics were some of the first to study the complex geometries and resultant elastic behaviors of curved crease origami. In this work, we present an extension of these approaches by adapting a simplified, discrete, and physics-based bar and hinge approach to simulate the mechanics of these intriguing origami structures. This model can capture stretching and shearing of the thin sheet, bending of the sheet along principle curvature directions, and bending along the prescribed curved creases. With insight from differential geometry, we use the model to explore the elastic folding sequence, the stiffness, and the global large deformation mechanics of curved crease origami.

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2:42PM P56.00002: Mapping of Fold Path Bifurcations in Origami Structures  ANDREW GILLMAN (Presenter), UES Inc. / Air Force Research Laboratory (WPAFB), PHILIP BUSKOH, Air Force Research Laboratory (WPAFB) — Origami has proven value in numerous technological applications including lightweight composites, soft robotics, metamaterial design, and deployable space structures, where discrete and modular folding motifs are leveraged to form novel tessellations. The material (stiffness mismatch among deformation modes) and geometric (slender elements) contrasts in origami structures can lead to highly nonlinear mechanical behavior with unique macroscopic properties, such as multi-stability. To efficiently navigate this complex nonlinear space, we have recently developed an efficient nonlinear truss finite element model with linear eigenanalysis heuristics for branch switching off the flat state. However, more efficient and robust methods have proven essential when performing topology optimization in this non-convex design space involving energy landscapes with many bifurcations and stable equilibrium points. Our work focuses on the incorporation of robust continuation methods for bifurcation point detection and branch switching to map these multistable energy landscapes and characterize the role of discrete fold stiffness distributions.

2:54PM P56.00003: Pairing global symmetries with folding mechanics to transform all periodically triangulated origami  D. ZEB ROCKLIN (Presenter), JAMES MCINERNEY, Georgia Institute of Technology, BRYAN G CHEN, Physics, University of Pennsylvania, LOUIS THERAN, Math, University of St. Andrews, CHRISTIAN SANTANGELO, Physics, U. Mass. Amherst — Thin sheets restricted to folding at designated creases, as in the traditional Japanese art of origami, have been engineered to deploy devices from the atomic to the macroscopic scale. However, the relation between the crease pattern and the paths to accessible structures is highly nontrivial. We investigate the entire class of periodically triangulated origami, revealing a hidden symmetry between global motions and linear folding mechanisms. Such periodic patterns always admit a two-dimensional manifold of cylindrical configurations as previously shown by Tomohiro Tachi. Adding a single quadrilateral face to the unit cell restricts the system to a single degree of freedom without fine-tuning the geometry. By transforming along these paths, we can change the mechanical response at the boundary. Our analysis can be extended to similar systems with balanced constraints and degrees of freedom such as kirigami, continuum sheets, and magnetic systems.

3:06PM P56.00004: Mechanics-Based Design for Computational Fabrication  [Invited]  EMILY WHITING (Presenter), Boston University — Advancements in rapid prototyping technology are closing the gap between what we can simulate with computers and what we can build, as it is now possible to create shapes of astounding complexity. Despite innovations in hardware, however, costly bottlenecks still exist in the design phase. Today's computational tools for design are largely unaware of the fundamental laws that govern how geometric models will behave in the real world. In this talk I will present recent work combining digital geometry processing, engineering mechanics, and rapid prototyping. The aim is to infuse principles of mechanics into design processes for fabrication. I will highlight specific applications including balance, buoyancy, acoustics, and architectural construction.

3:42PM P56.00005: Geodesy: Self-rising 2.5D Tiles by Printing along 2D Geodesic Closed Path  JIANZHE GU (Presenter), Human-Computer Interaction Institute, Carnegie Mellon University, DAVID E. BREEN, Computer Science, Drexel University, JENNY HU, School of Design, Carnegie Mellon University, LIFENG ZHU, Department of Mechanical Engineering, Carnegie Mellon University, YE TAO, Human-Computer Interaction Institute, Carnegie Mellon University, TY ZANDE, School of Design, Carnegie Mellon University, GUANYUN WANG, Human-Computer Interaction Institute, Carnegie Mellon University, JESSICA YONGJIE ZHANG, Department of Mechanical Engineering, Carnegie Mellon University, LINING YAO, Human-Computer Interaction Institute, Carnegie Mellon University — Thermoplastic and Fused Deposition Modeling (FDM) based 4D printing is rapidly expanding to allow for space- and material-saving 2D printed sheets morphing into 3D shapes when heated. However, to our knowledge, all the known examples are either origami-based models with obvious folding hinges, or beam-based models with holes on the morphing surfaces. Morphing a flat thermoplastic sheet into continuous double-curvature surfaces remains a challenge, both in terms of a tailored toolpath-planning strategy and a computational model that simulates it. In Geodesy, we focus on the morphing of continuous double-curvature surfaces or surface textures. We suggest a unique tool path - printing thermoplastics along 2D closed geodesic paths to form a surface with one raised continuous double-curvature tiles when exposed to heat. The shape space is further extended to more complex geometries composed of a network of rising tiles (i.e., surface textures). Both design components and a mass-spring-model-based computational pipeline are explained in the paper, followed by several printed geometric examples.
3:54PM P56.00006: Estimating friction in cloth, using simulation and machine learning*  ABDULLAH RASHEED (Presenter), VICTOR ROMERO, FLORENCER BERTAILS-DESCOUBES, Univ. Grenoble Alpes, Inria, CNRS, Grenoble INP, LJK, Grenoble, France, ARNAUD LAZARUS, Sorbonne Université, Institut Jean Le Rond d’Alembert, Paris, France, STEFANIE WUHRER, JEAN-SEBASTIEN FRANCO, Univ. Grenoble Alpes, Inria, CNRS, Grenoble INP, LJK, Grenoble, France — We explore the utility of deep neural networks to estimate parameters in cloth motion, specifically the friction coefficient. Our idea is to use realistic cloth motion sequences as video training data for our model and use both spatial and temporal features for parameter estimation. Following recent works, we aim to avoid complex experimental setup for the generation of training data by leveraging cloth simulation as a ground truth model for cloth dynamics. However, this is only meaningful if the simulation is accurate and predictable enough in the range of scenarios envisioned. To ensure realistic simulations, we validate the physical accuracy of Argus, a recent cloth simulator developed in computer graphics which relies on an implicit contact friction solver for capturing exact Coulomb friction. We successfully verify the physical realism of this simulator by conducting physical experiments analogous with simulations, following a protocol previously suggested in literature for measuring Coulomb’s friction coefficient in a Hookean elastic material contacting a rigid surface. We further investigate utilizing a similar protocol for cloth with varying material properties, which is modelled as an orthotropic material in the simulator.

*Supported by the ERC grant GEM (StG-2014-639139)

4:06PM P56.00007: Discrete Kirchhoff Rod Networks for Optimization-Driven Design  BERNHARD THOMASZEWSKI (Presenter), JONAS ZEHNDER, Computer Science and Operations Research, Université de Montréal — Many examples from architecture, mechanical engineering, and material science can be described as networks of elastic rods. Designing rod networks that exhibit desired characteristics is made difficult by the fact that the mapping between design parameters and performance at equilibrium is highly nonlinear. We propose a computational approach to this problem that leverages simulation and optimization algorithms for rapid design exploration. The technical core of our approach is formed by an efficient computational model for networks of discrete elastic Kirchhoff rods, paired with an inverse problem solver based on sensitivity analysis. We validate our model against standard solid finite element simulations and present applications to compliant mechanisms, deployable pretensioned membranes, structural curve networks, and mechanical metamaterials.

4:18PM P56.00008: Inverse design of a suspended Kirchhoff rod: From theory to practice*  VICTOR ROMERO (Presenter), FLORENCER BERTAILS-DESCOUBES, Université Grenoble Alpes, Inria, CNRS, Grenoble INP, LJK, ALEXANDRE DEROUET-JOURDAN, OLM Digital Inc., ARNAUD LAZARUS, University of Paris VI: Pierre-and-Marie-Curie University — Our study focuses on finding the natural shape of a given hanging deformed isotropic rod, made of a known material, the input shape is described as a mere geometric curve that we subsequently frame to compute a material curvature field and feed our inverse problem.

We prove that the natural shape of the rod satisfying equilibrium exists and is unique, regardless of the infinity compatible frames for the input curve. The natural shape is computed efficiently by solving in sequence three linear initial value problems. We illustrate our theoretical results through numerical examples of well known curves to which we apply our inverse procedure. By direct simulation we show that indeed those natural shapes fall, under the effect of gravity, onto the expected equilibrium. We stress on the fact that the obtained rest shapes are complex and far from intuitive.

We complement this study with experimental corroborations. By means of a standard array of cameras, we spatially reconstruct real elastic hanging rods with well-defined geometrical features. We find some good agreements with model prediction despite the experimental limitations on the estimation of the curvature fields of the rod’s center line.

*This work was supported by the European Research Council grant GEM (StG-2014-639139)
**4:30PM P56.00009: Jamming limiting the percolation of square tiles on square lattices**  
**EUGENIO VOGEL (Presenter), JULIO F. VALDES, University of La Frontera, Chile, PAULO M. CENTRES, ANTONIO J. RAMIREZ-PASTOR, Univ. Nac. San Luis, Argentina — Square tiles of $k \times k$ sites ($k^2$-mers) are deposited irreversibly on $L \times L$ square lattices of exactly the same inter-site distance; no overlapping is allowed. Coverage is defined as $q = Nk^2/L^2$, where $N$ represents the number of deposited tiles. Percolation thresholds $q_p(k)$ are reported with high precision for $k=1, 2,$ and $3$. For $k \geq 4$ jamming suppresses percolation. The coverages at which jamming appears $q_j(k)$ are also reported accurately [1]. It is observed that $q_p(2) < q_j(2)$ and $q_p(3) < q_j(3)$ while this inequality is reversed for $k \geq 4$, namely, $q_p(k) > q_j(k)$, which explains the suppression of percolation for $k \geq 4$. Monte Carlo techniques are used to simulate these depositions for $k^2$-mers from $k=2$ to $k=100$, and lattice sizes with sides much larger than $k$. Calculations based on exact enumeration were done for $k \leq 6$ and several $L$ values to show that this property is inherent to these systems. Finite size scaling is used to estimate the thresholds in the thermodynamic limit. The universality class of this deposition corresponds to random percolation; the corresponding critical exponents $\nu$, $\gamma$, and $\beta$ are reported with good accuracy.


*Fondecy 1150019; Conicyt FB0807; CONICET PIP 112-201101-00615

**4:42PM P56.00010: Rotating Matter: The Bearing State**  
**HANS HERRMANN (Presenter), PMMH, ESPCI Paris — Granular materials are characterized by an additional degree of freedom, rotations, which become particularly relevant for spherical particles. A packing of spheres is called bi-chromatic if every loop formed by contacts is even. In three dimensions, bi-chromatic bearings have many different sliding-free configurations, so called bearing states. Packings with bearing states can even be made space-filling. Their bearing states can be viewed as a realization of solid turbulence exhibiting Kolmogorov scaling and anomalous heat conduction. In three dimensions a continuum of such configurations can be obtained as cuts through four-dimensional space-filling bearing states. Bearings states can be perceived as physical realizations of networks of oscillators with asymmetrically weighted couplings. These networks can exhibit optimal synchronization properties through tuning of the local interaction strength as a function of node degree or the inertia of their constituting rotor disks through a power-law mass-radius relation. Under this condition, the average participation per disk is maximized and the energy dissipation rate is homogeneously distributed among elementary rotors. The synchronization of rotations occurs in avalanches following a broad size distribution.

*ERC Advanced Grant 319968-FlowCCS

**4:54PM P56.00011: Non-equilibrium dynamics of isostatic spring networks**  
**FEDERICO GNESOTTO (Presenter), BENEDIKT REMLEIN, CHASE BROEDERSZ, Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München — Mechanical systems exhibit rich critical behavior in the vicinity of the isostatic point. Inspired by living matter such as cytoskeletal networks and tissue, we here consider marginal assemblies driven out of equilibrium by internal activity. To date it remains unclear how the critical nature of such systems affects their non-equilibrium dynamics. We elucidate the role of the isostatic threshold in active diluted spring networks: heterogeneously distributed active noise sources drive the system into a non-equilibrium steady state. The non-equilibrium dynamics between pairs of network nodes are quantified by the characteristic cycling frequency $\omega$—a measure of the circulation of the associated phase space currents. We reveal critical scaling of the cycling frequencies and intuitively understand their local behavior employing a mean-field approach. Overall, our work serves as a bridge connecting the well-established theory of mechanical stability to the novel field of non-equilibrium statistical mechanics.
Contact networks in jammed granular systems, derived from contact forces between dry grains in mechanical equilibrium, can be represented in a dual force space as a network of edges that form a space-filling tiling. This force tiling paradigm has been found to be particularly useful in the characterization of stress-induced transitions in granular materials. As a generic network itself, the force network can be studied with techniques used in the investigation of more conventional networks.

Using jammed granular packings obtained from simulations, we explore the duality between the resultant real-space contact networks and force tilings. We analyze the relationship between zero modes and states of self-stress in these dual networks, and connect it to physical properties of jammed packings and to unjamming. In particular, this can provide improved understanding of the stability of granular systems against the effect of external perturbations.

*This work has been supported by NSF-CBET 1605283.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P57 GSNP DBIO: Noise-driven Dynamics in Far-from-equilibrium Systems I

2:30PM P57.00001: Noise-induced dynamics in far-from-equilibrium electronic transport systems [invited] STEPHEN TEITSWORTH (Presenter), JUAN PABLO GONZALEZ, YURIY BOMZE, Duke University, JOHN NEU, Mathematics, University of California, Berkeley — Bistable systems occur throughout the natural sciences and when such systems are subjected to noise, one observes probabilistic transitions between co-existing metastable states. Such behavior is found in chemical reaction kinetics, driven nonlinear mechanical systems, nonlinear electronic transport systems, climate dynamical models, and pulse propagation dynamics in neurons, to name but a few. In the case of electronic transport systems, experimental studies focus on probabilistic switching transitions between distinct states of electrical current flow in tunneling structures such as semiconductor superlattices and tunnel diodes. In particular, tunnel diode circuits provide an excellent experimental platform for the precision measurement of switching time statistics over a wide dynamic range. Furthermore, the measurement of mean switching times versus system parameters such as applied voltage near bifurcation points allows the determination of scaling behavior with remarkable precision. In related work, we have experimentally and theoretically studied linear electrical networks that are driven by non-thermal noise sources with a focus on the development of novel methods to characterize violations of detailed balance. Three methods of particular interest for experiments are: 1) construction of probability current from data, 2) stochastic area measurement, and 3) construction of statistical fluctuation loops. In this talk, we highlight the advantages and limitations of each of these approaches.

3:06PM P57.00002: Learning force fields from stochastic trajectories PIERRE RONCERAY (Presenter), ANNA FRISHMAN, Princeton University — When monitoring the dynamics of microscopic systems, disentangling deterministic forces from thermal noise is challenging. Indeed, we show that there is an information-theoretic bound on the rate at which information about the force field can be extracted from a trajectory. We propose a practical method, Stochastic Force Inference, that optimally uses this information to approximate force fields. This technique readily permits the evaluation of out-of-equilibrium currents and entropy production with a limited amount of data.

Ref: arXiv:1809.09650

3:18PM P57.00003: Noise-driven ionic currents in a viscosity gradient* DEREK STEIN (Presenter), BENJAMIN WIENER, Physics, Brown University — Gradients of voltage, pressure, temperature, or salinity can transport objects in micro- and nanofluidic systems by well-known mechanisms. I will describe the discovery of an electrokinetic transport effect driven by a viscosity gradient: An imposed liquid viscosity gradient causes an ionic current to flow inside a glass nanofluidic channel. Measurements of the current and numerical simulations reveal that the counterions in the electric double layers near the nanochannel surfaces drift in the direction of decreasing viscosity. The measurements are well described by a simple model in which the counterion drift speed equals the gradient of an ion's local diffusivity. Drift in a viscosity gradient, or viscophoresis, is a consequence of multiplicative (state-dependent) noise, where the magnitude of the thermal fluctuations experienced by a particle depends on its position.

*We acknowledge support from NSF under award 1409577 and from Oxford Nanopore Technologies.
SHAYAN LAME (Presenter), DEREK STEIN, physics, Brown University — We report an experimental technique to increase and control the diffusivity of individual DNA polymers in a nanofluidic environment. We applied white electrical noise with a Gaussian distribution of voltage fluctuations across nanofluidic slits containing fluorescently labeled DNA molecules. The effective diffusivity of the molecules in the direction parallel to the applied fields increased linearly with the noise power, reaching 19 times the thermal diffusivity with an applied noise amplitude of 36 V. This technique, which can subject DNA molecules to noise levels equivalent to 5300 K, enables us to experimentally investigate noise-driven dynamical phenomena in a previously inaccessible regime.

*We acknowledge support from NSF under award 1409577

SAHIL AGARWAL (Presenter), Yale Univ, WOOSOK MOON, Stockholm University and Nordita, JOHN WETTLAUFER, Yale University and Nordita — Understanding multidecadal variability is an essential goal of climate dynamics. For example, the recent phenomenon referred to as the "global warming hiatus" may reflect a coupling to an intrinsic, preindustrial, multidecadal variability process. Here, using a multifractal time-series method, we demonstrate that 42 data sets of 79 proxies with global coverage exhibit pink-noise characteristics on multidecadal timescales [1]. To quantify the persistence of this behavior, we examine high-resolution ice core and speleothem data to find pink noise in both pre- and postindustrial periods. We examine the spatial structure with an empirical orthogonal function analysis of the monthly averaged surface temperature from 1901 to 2012. The first mode clearly shows the distribution of ocean heat flux sinks located in the eastern Pacific and the Southern Ocean and has pink-noise characteristics on a multidecadal timescale. We hypothesize that this pink-noise multidecadal spatial mode may resonate with externally driven greenhouse gas forcing, driving large-scale climate processes.


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NASA NNH13ZDA001N-CRYO

CHLOE GAO (Presenter), DAVID LIMMER, University of California, Berkeley — Nonlinear response occurs naturally when a strong external perturbation takes a system far from equilibrium. While linear response can be directly related to equilibrium fluctuations, nonlinear response is difficult to predict in a general and efficient way. In this talk, we illustrate a method to compute arbitrarily high order transport coefficients of stochastic systems from derivatives of a large deviation function. We explore a selection of examples ranging from a single Brownian ratchet to thermal rectification in a mass-graded Fermi-Pasta-Ulam chain. Our method not only derives transport coefficients with relatively small statistical error, but also can be useful in studying mechanism by which nonlinear behavior arises.

ALEXANDRU BACANU (Presenter), JAMES PELLETIER, JUNANG LI, JORDAN HOROWITZ, TODD GINGRICH, NIKTA FAKHRI, Massachusetts Institute of Technology — Many biological systems act as ATP chemostats, maintaining a constant ATP chemical potential across numerous and variable free energy sources and sinks. It remains unclear how much free energy cells allocate to active mechanical fluctuations of the cytoplasm among other processes. To characterize nonequilibrium cytoskeletal mechanics, we imaged shape fluctuations of single-walled carbon nanotubes (SWNTs) embedded in an actin-intact Xenopus cytoplasmic extract. Normal mode decomposition of SWNT shape fluctuations resolved the spatial structure of myosin-driven forces, which were not only stochastic, but also nonstationary due to dynamic remodeling of the actomyosin network. Based on the normal mode correlation functions, we defined metrics for nonequilibrium mechanical activity. To measure how active cytoskeletal mechanics depended on the ATP chemical potential and flux, we increased the ATP chemical potential via a phosphoenolpyruvate energy mix and decreased it via apyrase-catalyzed ATP hydrolysis. These passive measurements reveal how local nonequilibrium fluctuations of the cytoplasm respond to global thermodynamics and the ATP chemical potential.
4:18PM P57.00008: Mutual information driven colloidal heat engine* GOVIND PANERU, SANDIPAN DUTTA, TSVI TLUSTY, Center for Soft and Living Matter, Institute for basic science, HYUK KYU PAK (Presenter), Ulsan National Institute of Science and Technology — We report on the direct measurement of the mutual information as a function of error size for a Brownian information engine operating in non-equilibrium steady state. Each engine cycle consists of the measurement of the particle position, feedback control, resetting of the particle position and relaxation. The measurement involves a Gaussian noise of controlled width. The performance of the information engine depends on the cycle period τ and the width of the noise N. The mutual information decreases with decrease in τ and increase in N, thereby reducing the amount of work extraction. Our system operates as a cooling or a heating device depending on the noise width. The efficiency of information-to-work conversion increases as the system is allowed to relax more at the end of each cycle. The maximum efficiency is obtained at the finite value of N. The generalized Jarzynski equality was found to be valid either when the initial state of the system is in thermal equilibrium, or when noise and signal width are equal.

*This work was funded by the Korean government through grant IBS-R020-D1.

4:30PM P57.00009: Realization of an artificial active bath with controlled activity* JINTAE PARK (Presenter), Ulsan National Institute of Science and Technology, GOVIND PANERU, Center for Soft and Living Matter, Institute for Basic Science, HYUK KYU PAK, Ulsan National Institute of Science and Technology — We study the motion of a Brownian particle in artificially generated active bath. The particle is confined in a time dependent optical harmonic potential generated by optical tweezers. Therefore, the particle feels an external active noise in the background of a thermal white noise. This system is assumed to mimic the motion of a Brownian particle in active bath such as a bath of swimming bacteria. In comparison to the real bacterial bath experiments in which the activity parameters cannot be controlled easily, in this experiments the activity of the artificially generated active bath can be modulated in more controlled manner. Consequently, it allows us to study the thermodynamics of the Brownian particle in the active bath of various conditions.

*This work was supported by the Korean government under the grant IBS-R020-D1.

4:42PM P57.00010: Deformation of nonequilibrium limit cycle oscillators due to stochasticity JANAKI SHETH (Presenter), Physics, University of California at Los Angeles — Non-equilibrium dynamics are exhibited by numerous biological systems, often modeled as non-linear oscillations driven by an internal energy-consuming process. Thermal processes lead to stochasticity in the measurements of their variables. Thus, experiments can only access the mean limit cycle, which may be different from the underlying zero-temperature one. This can lead to discrepancies between measurements and deterministic numerical models.

One example of an active oscillator is the inner ear hair cell. Its dynamics are here modeled with a set of equations that incorporates the physiological variables and their noise amplitudes. We observe a gradual rounding of the mean limit cycle with increasing noise strength and explore causes for such rounding that makes sharper features of the noiseless oscillator experimentally inaccessible.

To simplify the system, we simulate a generalized Hopf oscillator, with added features in the scalar potential. The oscillation, powered by an internal active mechanism, requires a nonzero vector potential. By varying noise strengths under such general conditions, we observe distortion of the zero-temperature limit cycle. We suggest that this temperature effect imposes inherent limitations on complex models seeking to reproduce experimental dynamics.

4:54PM P57.00011: Numerical study for controlling surface roughening in KPZ growth process* PRIYANKA. (Presenter), UWE CLAUS TAUBER, MICHEL PLEIMLING, Virginia Tech — The Kardar-Parisi-Zhang (KPZ) equation has been used to describe growth processes in a variety of systems, and the corresponding exponents have been shown to prevail in both numerical models and experiments. Our objective in this work is to control the surface roughening for the KPZ growth process in (1+1) dimensions. We aim to saturate the surface roughness to the desired value using feedback control and try to understand the effect of the feedback control on the underlying dynamics. To this end, we apply a numerical integration scheme of the KPZ equation (with and without control) using the pseudo-spectral method. The numerical results show that controlling only a few small wave numbers leaves the system in the KPZ universality class. However, perturbing the wave numbers beyond a certain threshold changes the underlying kinetics, depending on the specific type of implemented (linear or nonlinear) control.

*This research is supported by the Army Research Office under the Grant Number W911NF-17-1-0156.
5:06PM P57.00012: Self-organization in robot swarms and beyond*  PAVEL CHVYKOV (Presenter), Massachusetts Institute of Technology, WILLIAM C SAVOIE, ZACHARY JACKSON, AKASH VARDHAN, KURT A WIESENFELD, Physics, Georgia Tech, JEREMY L ENGLAND, Massachusetts Institute of Technology, DANIEL GOLDMAN, Physics, Georgia Tech — Swarms of interacting simple robots are interesting because of their potential for adapting rapidly to the demands of different group tasks. They also provide a playground for studying the physics of emergent self-organization. We studied a closely packed ensemble of periodically deforming simple robots, and observed the group to spontaneously organize into orderly patterns of collective motion. Viewing the collective as an emergent whole, we characterized its dynamics using an analysis originally developed for understanding fruit-fly behaviors. Our findings point to design principles for the controlled stabilization of ordered behaviors in interacting systems.

*Federal grant W911NF1810101

5:18PM P57.00013: Negative differential response of chemical reaction currents  GIANMARIA FALASCO, TOMMASO COSSETTO (Presenter), EMANUELE PENOCCHIO, MASSIMILIANO ESPOSITO, University of Luxembourg — Reaction currents in chemical networks can decrease when increasing their driving affinities. Such negative differential response (NDR), a hallmark of nonequilibrium physics, is found in reaction schemes of major biological relevance, namely, substrate inhibition and autocatalysis. We display it by deriving the full counting statistics of two minimal representative models by large deviation methods. We explore the consequences of NDR for biochemical networks in terms of precision-dissipation tradeoff and stability against external perturbations. Furthermore, we go beyond the realm of biochemistry and examine the relevance of NDR in artificial applications, showing how it limits the performance of dissipative self-assembly.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P58 GSOFT: Disordered and Glassy Systems II BCEC 257A - Elijah Flenner, Colorado State Univ

2:30PM P58.00001: Measurement and modification of two-level tunneling states in amorphous aluminum oxide*  THOMAS METCALF (Presenter), XIAO LIU, MATTHEW ABERNATHY, United States Naval Research Laboratory, BATTOGTOKH JUGDERSUREN, KeyW Corporations — Low energy excitations modeled as two-level tunneling systems (TLSs)—a significant source of decoherence in qubits built around superconducting Josephson junctions—are found nearly universally in amorphous dielectrics. Although TLS-free amorphous dielectric materials would be a technological boon, to date there is only one such material system: amorphous silicon thin films vapor deposited onto substrates held at elevated temperatures. The question arises whether TLSs can be eliminated in other, technologically pertinent amorphous dielectrics. To this end we have measured the internal friction of 100–300nm sputter-deposited aluminum oxide films, at substrate temperatures up to 500°C. This measurement directly yields the tunneling strength parameter from the TLS model, and we find a factor of five reduction in tunneling strength for films deposited at high temperatures.

*Work supported by the Office of Naval Research

2:42PM P58.00002: Entropy-dominated squeezout force and incipient glass formation in confined ionic liquids*  ROSARIO CAPOZZA (Presenter), Environmental Engineering, Edinburgh University, UK, ERIO TOSATTI, SISSA and ICTP, Trieste, Italy — The squeezout force for an ionic liquid (IL) confined in a nanoscale channel between two approaching plates generally shows just short-range layering steps. Close to freezing temperature and at large squeezout speeds, recent data in a simple IL showed instead that short-range layering is replaced by a smooth intermediate range repulsive force tail. Along with the expected viscosity rise as in experiment, our squeezout simulations in a simple IL model additionally show that the confinement-induced strong and smooth repulsive squeezout force is of entropic origin, whereas the short-range layering steps are only controlled by internal energy. Our interpretation is guided by bulk glass-forming liquids, where the viscosity rise upon cooling is indeed associated with an entropy drop through the Adam-Gibbs mechanism, involving the formation of cooperatively rearranging regions (CRRs). We find that the confined IL the entropy drop and viscosity rise which accompany squeezout are also connected with remnants of a confinement-induced glassy CRRs forming at constant temperature, a mechanism that should be more general than this specific case.

*Supported by ERC MODPHYSFRICIT Contract no. 320796
Topological phases, fragility- and reversibility-widows in GePxSe100-2x ternary

AARON WELTON (Presenter), RALPH CHBEIR, SOUMENDU CHAKRAVARTY, PUNIT BOOLCHAND, University of Cincinnati — The fragility index, \( m \), in homogenized chalcogenide melts, are found to display values of \( m < 20 \) for compositions that reside in the Intermediate Phase (IP) in the Ge-Se, Ge-S binary systems yielding a fragility window. The enthalpy of relaxation of corresponding glasses, \( \Delta H_{nr}(x) \), becomes minuscule in IP displaying a reversibility window[1]. That correlation between \( \Delta H_{nr}(x) \) and \( m(x) \) illustrates a basic principle that melt dynamics encode glass topological phases. Here we examine the titled glasses to investigate if the principle extends to the present ternary. We have synthesized titled glasses over a wide range of compositions, \( 2\% < x < 26\% \) by alloying the pure elements in evacuated quartz tubes. Melts were alloyed till the variance in Ge stoichiometry \( x \) across the 2 gram batch composition nearly vanished using Raman profiling. In such homogenized glasses we are now examining the variation in \( \Delta H_{nr}(x) \) and \( m(x) \) using Modulated DSC, and will present the results of these observations. In a previous study[2] variation of \( \Delta H_{nr}(x) \) was examined but no attempt to measure the fragility index was made.


The Energy Distribution of Two-Level Systems in Various Amorphous Thin Films Measured Using Internal Friction

MATTHEW ABERNATHY (Presenter), XIAO LIU, THOMAS METCALF, Code 7130, Naval Research Laboratory, Washington, DC, BATTOGTOKH JUGDERSUREN, KeyW Corporations, Hanover, MD — Amorphous materials are known to universally possess various low-energy excitations generally modeled as two-level systems (TLS) capable of tunneling between states at low temperatures (~1K) and thermal excitation at higher temperatures (>5 K). The measurement and modeling of these states in bulk materials is well represented in the literature, however, relatively few measurements of amorphous thin films have been similarly analyzed. In this presentation, we fit the model of Rau et al. (Phys. Rev. B, 52, 7179, 1995) to the mechanical loss features attributed to TLS in thin films of a-Se, a-Al2O3, and others.

*This work is supported by the Office of Naval Research

Can you hear the shape of a crumpled sheet?

YOAV LAHINI, Tel Aviv University, SHMUEL RUBINSTEIN, ARIEL AMIR (Presenter), Harvard University — Thin, crumpled sheets show surprisingly intricate dynamics: when subject to a constant load, they exhibit an extremely slow volume relaxation that spans many decades in time – from fractions of a second to weeks. After an abrupt change in the load, they show slow, non-monotonic aging and memory effects reminiscent of glassy systems. We have recently shown that these dynamics and scaling relations can be captured accurately using a phenomenological model in which the relaxation process is assumed to be governed by a linear superposition of many relaxation modes, that have a broad distribution of relaxation times. Here, we study, theoretically and experimentally, the statistics of discrete micro-mechanical relaxation events occurring within the system as it relaxes or exhibits memory. We find that during logarithmic relaxations the waiting time between these micro-mechanical ‘quakes’ displays approximate Poisson-statistics at any point in time, but with an average that grows linearly with the age of the system from preparation. The model is also used to predict the pattern of micro-relaxation events during the non-monotonic aging regime. The model predictions and experimental data of acoustic emission show good agreement.
3:30PM P58.00006: Critical size for dynamic crossover in amorphous nanoparticles*  
SHAN ZHANG (Presenter), PENGFEI GUAN, LIJIN WANG, Beijing Computational Science Research Center — The fragility, defined according to the non-Arrhenius degree of the viscosity-temperature dependence of a system in a supercooled state, is the essential, crucial, and universal dynamic attribute of the glass-forming liquid. It is related to the material-specific properties in liquid and glass state. We found that with the metallic glass nanoparticle's size reduced to critical size $R_c$, a fragile-to-strong transition appeared. This transition is the result of particle size reduction and the fast surface dynamic behavior. The analysis of morphology in PEL suggests that the strong liquids have the large fraction of low-energy excitations, reflecting the systems have a lower density of minima, fewer paths to translate into structural collapse. Meanwhile, this phenomenon is related to the atomic inherent structure energy and the two-body excess entropy in the surface. This fragile-to-strong transition is conducive to understand the micro-mechanism of the metallic glass at nano-scale further.


*MOSF 973 program (Grant No. 2015cb856800) NSAF joint program (Grant No. U1530401)

3:42PM P58.00007: Terahertz Time-Domain Spectroscopy of Alkali Borate Glass: Boson Peak Dynamics*  
TATSUYA MORI (Presenter), YUTA IIJIMA, Division of Materials Science, University of Tsukuba, YASUHIRO FUJII, Department of Physical Sciences, Ritsumeikan University, SUGURU KITANI, Laboratory for Materials and Structures, Tokyo Institute of Technology, JAE-HYON KO, Department of Physics, Hallym University, AKITOSHI KOREEDA, Department of Physical Sciences, Ritsumeikan University, HITOSHI KAWAJI, Laboratory for Materials and Structures, Tokyo Institute of Technology, SEIJI KOJIMA, Division of Materials Science, University of Tsukuba — The boson peak (BP) is a universal feature of amorphous materials and it appears in the spectra of $g(\nu)/\nu^2$ ($g(\nu)$: vibrational density of states), in the terahertz region. The BP can be famously detected by inelastic neutron scattering, low-temperature specific heat, and Raman scattering. Recently, we confirmed that terahertz time-domain spectroscopy (THz-TDS) is suitable to detect the BP. The BP in the infrared (IR) spectra appears in the spectrum of $\alpha(\nu)/\nu^2$ ($\alpha(\nu)$: absorption coefficient). In this study, we investigate the BP dynamics of lithium borate glass by THz-TDS and evaluate IR light-vibration coupling coefficient.

*This work was partially supported by JSPS KAKENHI Grants No. 17K14318, No. 18H04476 and No. 26287067, and the Asahi Glass Foundation.

3:54PM P58.00008: The relation between ridges and crumples*  
ANDREW CROLL (Presenter), TIMOTHY TWOHIG, THERESA M ELDER, North Dakota State University — Crumpling is the name given to the structure created when a thin sheet has been forced to occupy a volume much smaller than the sheet's largest dimension. Crumples strongly resist compression, making them an interesting lightweight material. How a crumple resists compression is a challenging question to answer, though recently we have proposed an empirical relation which applies to both elastic and plastic sheets. Here we examine different 'building block' structures for clues as to the origin of the empirical force law. Specifically, we focus on the stretching ridge which joins two developable-cones and has long been hypothesized to be responsible for the crumple's strength. We show that elastic and plastic ridges, though geometrically identical when formed, behave very differently under compression. The elastic ridge smoothly collapses annihilating one d-cone in the process, whereas the plastic material allows no motion of the d-cone cores, building stress until buckling. Remarkably, before failure the plastic and elastic ridges can be fit by the same empirical model as can the crumple itself. We discuss the curious relationship.

*The authors gratefully acknowledge support from the AFOSR under the Young Investigator Program (FA9550-15-1-0168).
Evidence of a fragility window that correlates with the reversibility window in (Na2O)x(B2O3)100-x glasses

CHARLES SKIPPER (Presenter), RALPH CHBEIR, KANDASAMY VIGNAROOBAN, PUNIT BOOLCHAND,
University of Cincinnati — Evidence for a reversibility window in titled glasses was reported1 recently and permitted fixing the Topological phases. The reversibility window permitted one to identify glasses at x < 20% to be in the Stressed-rigid phase those at x > 40% to be in the flexible phase and those in between with the Intermediate Phase. We now report on melt fragility index using mDSC. The imaginary part of Cp, examined in the cool down mode, shows a Gaussian-like peak that shifts to higher T as the modulation frequency is increased. By tracking the peak shift in Cp^imag with T, we establish how τ , the enthalpic relaxation time with T and deduce the fragility index (m). Our results show that m(x) also displays a square-well like variation with m< 20 in the 20 < x < 40% range of soda, coinciding with the reversibility window. Remarkably if the glasses are not dry the variation of m(x) changes qualitatively2; m(x) increases quadratically in x underscoring that Na^+ ions now diffuse more rapidly. Glass synthesis conditions can qualitatively alter melt dynamics.

1. K. Vignarooban et al 2014 EPL 108 56001

Supported by NSF grant DMR0853957

Melt fragility index, configurational entropy, and topological phases in ternary GexAsxSe100-2x Chalcogenides

RALPH CHBEIR (Presenter), University of Cincinnati, MATTHIEU MICOULAUT, Univ Pierre et Marie Curie, MATHIEU BAUCHY, University of California, Los Angeles, PUNIT BOOLCHAND, University of Cincinnati — The melt fragility index, m, of titled chalcogenides display a global minimum with m < 20, in the narrow connectivity range 2.28(3) < <r> < 2.51(3) defining a fragility window. Separately, the non-reversing enthalpy of relaxation (ΔHnr) at Tg in corresponding glasses shows a square-well like global minimum, with the ΔHnr term nearly vanishing in the same 2.28(3) < <r> < 2.51(3) connectivity range, defining the reversibility window, which represents the isostatically rigid Intermediate Phase (IP). The near vanishing ΔHnr for IP glasses is signature for the change in excess configurational entropy (ΔS_ex) between melt and glass to be minuscule, and leads to super-strong melts as expected. The order of magnitude increases in ΔHnr for non-IP glass compositions as one goes away from the IP glass compositions, lead both ΔS_ex and m to steadily increase for non-IP melts as observed in experiments.

*NSF Grant DMR 0853957

Observation of a sharp reversibility window in rejuvenated homogenized equimolar Ge_xAs_xSe_100-2x bulk glasses

BADRIAH ALMUTAIRI (Presenter), RALPH CHBEIR, SOUMENDU CHAKRAVARTY, L.C.R. WIJEWARDHANA, PUNIT BOOLCHAND, University of Cincinnati — We have synthesized 1.5-gram sized batches of the title glasses over a wide composition range 2% ≤ x ≤ 25%, taking special care to alloy the starting materials for an extended period (several weeks) in evacuated quartz tubes, and recording FT Raman spectra along the length of the melt column till the spectra became identical. Using Modulated DSC, we then examined calorimetric properties, Tg(x), ΔCp , and ΔHnr (x), and find Tg(x) to increase monotonically with x, and the enthalpy of relaxation, ΔHnr (x) to display a sharp square-well like reversibility window with an onset near x =9.0(5)% (rigidity transition) and an endpoint x = 16.0(5)% (stress transition) in rejuvenated glasses. In FT- Raman scattering we observe modes of Ge-centered CS and ES tetrahedra and the As-centered Pyramidal and Quasi-Tetrahedral units besides modes of S8 rings and polymeric Sn chains. The mode near 537 cm^(-1) due to S=As(S_{1/2}) QT units is observed in FT-Raman but not in dispersive Raman using 514 nm excitation. Complex Cp measurements using MDSC are being undertaken to establish variation in melt fragility index.


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Variation in fragility-index, Enthalpy of relaxation at $T_g$ and Molar volumes in especially homogenized bulk As$_x$S$_{100-x}$ glasses*

SOUMENDU CHAKRAVARTY (Presenter), RALPH CHBEIR, PING CHEN, University of Cincinnati, MATHIEU MICOULAUT, Univ Pierre et Marie Curie, MATHIEU BAUCHY, Univ of California - Los Angeles, PUNIT BOOLCHAND, BADRIAH ALMUTAIRI, University of Cincinnati — We have measured the variation of fragility index ($m$), Non-reversing enthalpy of relaxation ($\Delta H_{nr}$) and molar volumes ($V_m$) with $x$ in especially homogenized As$_x$S$_{100-x}$ batches of 1.5 gram in size. FT Raman profiling was used to ascertain homogeneity of glasses. Our results show that $\Delta H_{nr}$ displays a square-well like minimum in the 22.5(5)% < $x$ < 28.5(5)% range defining the reversibility window. Variation of $m$ displays a minimum of $m$ < 20 in the same range of $x$, defining the fragility window. Inverse of the activation energy ($E_a$) for enthalpy relaxation shows a maximum in the IP. Variation in $V_m(x)$ displays a Gaussian-like local minimum in the reversibility window. The fragility-window coinciding with the reversibility window underscores that super-strong (fragile) melts upon cooling give rise to IP (non-IP) glasses. The maximum in $1/E_a$ shows that the excess configurational entropy ($S_{ex}$) peaks for IP glasses. On the other hand, the large build up in $\Delta H_{nr}$ and small increase in $\Delta C_p$ for non-IP compositions (as $x$ > 28.5(5)% and $x$ < 22.5(5)% as one goes away from the IP, accounts for the increased fragility of stressed-rigid and flexible melts.


*Supported by NSF grant DMR-08-53957

New scenario of sound damping in glasses*

LIJIN WANG (Presenter), Beijing Computational Science Research Center, China, LUDOVIC BERTHIER, Laboratoire Charles Coulomb (L2C), University of Montpellier, CNRS, France, ELIJAH FLENNER, Department of Chemistry, Colorado State University, USA, PENGFEI GUAN, Beijing Computational Science Research Center, China, GRZEGORZ SZAMEL, Department of Chemistry, Colorado State University, USA — An understanding of the difference between the universal low-temperature properties of amorphous solids and crystalline solids requires an explanation of the stronger damping of long-wavelength phonons in amorphous solids. A quartic scaling of the sound attenuation coefficient on the wavevector, which was deduced from experiments and later found support in a number of theoretical and simulation investigations, has recently been questioned in a new large scale simulation. Subsequently, quartic scaling was found in another large scale simulational study. These recent conflicting results reopened the problem of the wavevector dependence of sound attenuation. Here, we study simulated glasses with a wide range of stability and demonstrate the existence of a quartic scaling regime of the sound attenuation coefficient on wavevector in very stable glasses but not in poorly annealed glasses. For transverse sound waves in all glasses examined, we observe a long-wavelength quadratic scaling regime whose upper wavevector cutoff increases with increasing stability. Our results demonstrate an intimate connection between stability and sound damping in glasses and a new, unexpected damping scenario.

*NSF of US (DMR-1608086), the Simons Foundation, and NSF of China (51571011)

Topological phases of (Na$_2$O)$_x$(P$_2$O$_5$)$_{100-x}$ glasses and their molecular structure from Raman scattering.

AVIK MANDAL (Presenter), VAMSHI GOGI, CHANDI MOHANTY, RALPH CHBEIR, AARON WELTON, University of Cincinnati, MATHIEU BAUCHY, University of California Los Angeles, MATHIEU MICOULAUT, University Pierre et Marie Curie, PUNIT BOOLCHAND, University of Cincinnati — The observation of both a reversibility window and a fragility window in the 37.5% < $x$ < 46% range of soda in titled glasses from Calorimetric experiments fixes the 3 topological phases. Raman polarization and glass compositional studies show that the feature near 1166 cm$^{-1}$ in glasses at $x$ = 50% consists of a triad of modes, a majority symmetric mode of Q$^2$ species and two minority “defect modes” due to termination of the Q$^2$ bearing long chains by Q$^1$ like local structures, not only at $x$ > 50% but also at $x$ < 50%. These defects are under-constrained and contribute to an increasing baseline in the non-reversing heat flow term with increasing $x$. The fractions of Q$^3$,Q$^2$ and Q$^1$ local structures with composition deduced from respective Raman active modes in the 20% < $x$ < 60% range nicely track the usual mean-field behavior, independently deduced from NMR but with some minor but noticeable differences.

5:18PM P58.00015: Structure of (Na2O)x (P2O5)100-x glasses from Infrared reflectance measurements*  VAMSHI KIRAN GOGI (Presenter), AVIK MANDAL, CHANDI MOHANTY, University of Cincinnati, MATHIEU BAUCHY, University of California, Los Angeles, MATHIEU MICOULAUT, University Pierre and Marie Curie, PUNIT BOOLCHAND, University of Cincinnati — IR reflectance has served as a useful complementary probe to Raman scattering on glasses. One observes a phonon near 1172.2 cm⁻¹, associated with the long chains of Q² species in Raman scattering of c-NaPO₃. On the other hand, in g-NaPO₃, the corresponding vibrational feature consists of a triad of modes¹; a majority mode (1165.6 cm⁻¹) and two minority ones (1151.4 cm⁻¹ and 1105.3 cm⁻¹). These minority modes are weakly excited in Raman but rather strongly in IR TO-response. The minority modes are ascribed to Q¹-like chain terminating topological defects of the long Q² chains and display a global minimum in concentration in the IP composition range¹; 37.5% < x < 46.0%. Additionally, when we examine the variation in the LO-TO splitting of the Q²_asym (near 1282 cm⁻¹) and Q³_asym (near 1316 cm⁻¹) modes with glass composition 'x', one observes a global minimum in the IP range. A similar result is also observed for (Na₂O)x (GeO₂)100-x glasses², suggesting that the reduction of local Electric fields set up in the IP glassy networks could be a general feature.

*Supported by NSF grant DMR 08-53957

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P59 GSOFT DBIO: Driving, Actuating, and Triggering Activity in Biopolymer Networks BCEC 257B - Jennifer Ross, University of Massachusetts Amherst - Tag(s): Focus

2:30PM P59.00001: Closed Loop Mechanical Actuation of Cardiac Microtissue* JOSH JAVOR (Presenter), SUBRAMANIAN SUNDARAM, ANANT CHOPRA, CHRIS CHÉN, DAVID JOHN BISHOP, Boston University — Mechanical forces play a significant role in the maturation and function of stem cell derived cardiac tissue. We present a micromechanical test bed with closed loop actuation to control tissue strain with sub-micron spatial and 10 ms temporal resolution. A hydrogel is self-assembled between two custom elastomer posts, where one post is functionalized with a rare-earth magnet. Opposing it is a spherical pillar top facilitating hydrogel attachment. An anti-Helmholtz coil imposes gradient magnetic fields on the magnet translating to nanoNewton forces and tissue strain. The cardiomyocytes beat spontaneously, imposing another force on the magnet. The magnet position is detected without contact by imbedding a hall sensor. The detected signal is processed by analog filters and phase-sensitive detection. The loop is closed with an Arduino MEGA, which digitizes the signal, performs an algorithm, and drives the coils with an arbitrary analog signal.

*This work was supported primarily by the NSF CELL-MET ERC award no. 1647837. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect those of the National Science Foundation.

2:42PM P59.00002: Microscale Mechanics of triggered bundling and unbundling of actin networks* BEKELE GURMESSA (Presenter), University of San Diego, LEILA FARHADI, Department of Physics, University of Massachusetts, Amherst, MICHAEL RUST, Molecular Genetics and Cell Biology Institute for Genomics and Systems Biology, University of Chicago, JENNIFER ROSS, Department of Physics, University of Massachusetts, Amherst, MOUMITA DAS, Department of Physics, Rochester Institute of Technology, RAE ROBERTSON-ANDERSON, University of San Diego — Networks of semiflexible actin filaments play key roles in many mechanical processes. The functionality of actin networks arises from the ability for actin filaments to dynamically entangle, crosslink, and bundle with one another. For example, simply increasing divalent salt concentration can trigger varying degrees and types of bundling in entangled actin networks. However, how the mechanical properties vary with varying degrees of salt-induced bundling remains unknown. More importantly, how the mechanical properties vary in time as actin networks transition between bundled and unbundled states has yet to be explored. Here, we couple optical tweezers microrheology with microfluidics to measure the viscoelastic response of entangled actin networks during triggered bundling and unbundling. We measure the frequency-dependent viscoelastic moduli in set time intervals as we cyclically vary the salt concentration via microfluidic perfusion chambers. We also use fluorescence confocal microscopy to image labeled filaments and characterize the corresponding time-varying network mobility and structure. Our measurements shed new light into how bundling and unbundling can dynamically tune the mechanical properties of actin networks.

*NSF CAREER #1255446; W.M. Keck Foundation Research Grant
2:54PM P59.00003: Modeling dividing actomyosin droplets as colloids in liquid crystal*  KINJAL DASBISWAS (Presenter), Physics, University of California Merced, ELI ALSTER, Chemical Engineering, Northwestern University, KIMBERLY WEIRICH, THOMAS A WITTEN, MARGARET GARDEL, SURIYANARAYANAN VAIKUNTHANATHAN, University of Chicago — Biopolymer networks are often organized into oriented bundles both in reconstituted in vitro situations and in the cell. Motivated by dividing fluid droplet-like bundles of actomyosin observed in experiments, we propose a theoretical mechanism for division of a droplet of liquid crystal material induced by a colloidal particle. The preferred alignment of actin filaments at the droplet surface and that at the motor cluster, modeled as a colloidal inclusion wet by the droplet, together result in a deformed droplet having minimal free energy. The dynamics of the model are illustrated by continuum simulations which show droplet deformation and pinching off into two equal daughter droplets. While colloidal inclusions are widely known to induce defects in a surrounding bulk liquid crystal, we predict here that the colloid can in principle deform and divide droplets of liquid crystal. Our description of these liquid crystal droplet dynamics, where the active forces of molecular motors is accounted for effectively through aligning interactions, explores the physical aspects of complex fluid phase separation in biology and suggests that self-assembly of motors may occur through interactions mediated by ordered biopolymers.

*NSF and University of California, Merced

3:06PM P59.00004: Light-controlled biomolecular phase transitions in living cells [Invited]  JEFFREY MORRIS (Presenter), City College of New York — In this talk I will discuss recent advances toward understanding and engineering intracellular phase transitions, which play an important role in organizing the contents of living cells. Membrane-less RNA and protein rich condensates are found throughout the cell, and regulate the flow of genetic information. We’ve shown that liquid-liquid phase separation (LLPS) underlies the assembly of these structures. LLPS driven by intrinsically disordered protein regions (IDRs) explains many condensate features, for example the internal subcompartments of the nucleolus, which has important consequences for sequential ribosomal RNA processing. Our lab has developed a suite of new approaches, which use light to enable spatiotemporal control of intracellular phase transitions, allowing us to engineer the assembly and disassembly of these structures within defined subregions of the cytoplasm and nucleus. We are now using these tools to quantitatively map intracellular phase diagrams for the first time, providing unprecedented access to the biophysical principles underlying RNP condensate self-assembly. This approach has also begun to yield rich insights into the link between intracellular liquids, gels, and the onset of pathological protein aggregation.

3:42PM P59.00005: Elucidating the consequences of heterogeneous activity in an actin based liquid crystal  STEVEN REDFORD (Presenter), RUI ZHANG, NITIN KUMAR, University of Chicago, PAUL RUIJGROK, Stanford University, ALI MOZAFFARI, AARON DINNER, VINCENZO VITELLI, University of Chicago, ZEV BRYANT, Stanford University, JUAN DE PABLO, MARGARET GARDEL, University of Chicago — Active matter is generally studied in cases in which activity is spatially uniform. However, many of the biological systems that inspire this line of research, such as forces in a cell, feature activity that is highly spatially inhomogeneous. While generating spatially inhomogeneous stress has historically been difficult, here we present an experimental system in which spatial control of myosin activity in an actin liquid crystal allows for patterning of activity within the sample. Using this system, and comparing with hydrodynamic simulations, we show that patterned activity has the potential to direct the motion of +1/2 defects within a liquid crystal and constrain fluid flow.

3:54PM P59.00006: Driving, Actuating, and Triggering Activity in Biopolymer Networks [Invited]  WEIHONG TAN (Presenter), University of Florida — Active and driven biopolymer networks, such as networks of cytoskeleton proteins, have been intensely investigated over the past decade due to their promise for designing smart materials and understanding cell mechanics. These materials continuously alter their mechanical properties by varying the structural properties and interactions of the comprising biopolymers. Non-equilibrium activity can be driven by external triggers such as light, salt, temperature, or magnetic or electric fields. Activity can also be internally driven via molecular motors. This session will bring together studies on a wide-range of non-equilibrium biopolymer networks to elucidate the functional design principles of driven soft matter, as well as the time-dependent structural and rheological properties of these non-equilibrium networks. Advances in modulating and characterizing driven networks will also be discussed.
Myosin II filament size and activity influences localization in nematic actin droplets

KIMBERLY WEIRICH (Presenter), University of Chicago, KINJAL DASBISWAS, University of California, Merced, THOMAS A WITTEN, SURIYANARAYANAN VAIKUNTANATHAN, MARGARET GARDEL, University of Chicago — Soft, active materials self-organize from macromolecules in cells to form precisely structured assemblies, such as the mitotic spindle, that orchestrate specific biological functions. A central question is how these self-organized assemblies arise from their macromolecular components. We investigate mechanisms of self-organization in structured biopolymer assemblies, using a minimal model system of biopolymer droplets constructed from cross-linked actin filaments. These droplets have nematic structure, which arises from the actin filaments. Myosin II motor proteins, which form filaments that bind to and translocate actin filaments, spatially self-organize in these actin droplets. We find that motors large compared to the characteristic structure of the nematic liquid self-organize to the center of the droplet, evocative of mitotic spindle configurations. In contrast, motors small compared to the liquid are dispersed throughout the droplet. We investigate the influence of motor size and activity on the dynamics and localization within the droplet and capture the spatial localization with a continuum model based on liquid crystal theory. Our results reveal potential physical mechanisms of self-organization in biological assemblies and bio-inspired soft materials design.

The paradoxical material properties of living matter*

GIJSJE KOENDERINK (Presenter), AMOLF — This talk will focus on the mechanics of the polymeric load-bearing structures that support living matter: cells have a fibrous cytoskeleton, whilst tissues are supported by the extracellular matrix. Living matter uses dynamic materials in order to combine mechanical resistance with the ability to adapt and self-heal. Whereas synthetic transient networks readily fracture due to the inherent force sensitivity of dynamic bonds, biological networks are surprisingly strong. How does biological matter achieve the ability to flow without risking mechanical failure? I will discuss our recent findings on the nonlinear time-dependent mechanical properties and rupture of passive and active biopolymer networks reconstituted from purified components, which begin to shed some light on this question.

Nonequilibrium dynamics of semiflexible filaments in an active fluid

JUNANG LI (Presenter), SHREYAS GOKHALE, SAMI KAYA, ALEXANDRE SOLON, JEFFREY GORE, NIKTA FAKHRI, Massachusetts Institute of Technology — Active fluids exhibit a variety of complex dynamical phenomena that are not observed in their passive counterparts, largely due to the breaking of detailed balance at the particle level. This breaking of detailed balance can also be manifested in the dynamics of passive objects immersed in an active fluid. For instance, Nikola et al. have demonstrated numerically that a semiflexible filament exhibits spontaneous buckling and directed motion when immersed in an active bath. Despite considerable progress on the theoretical and numerical front, experimental investigations of the dynamics of passive objects in active media were so far restricted to the simplest cases. Here, we have developed an experimental system to systematically analyze the nonequilibrium dynamics of semiflexible filaments in an active fluid. We perform optical video microscopy on DNA-linked magnetic colloidal chains immersed in a quasi-2D bacterial bath, and quantify the diffusivity and the amplitudes of the bending mode fluctuations of the chains as a function of chain length, stiffness and bacterial density. Using fluorescent bacteria, we compute the active flow fields to uncover the underlying mechanism of the nonequilibrium dynamical phenomena.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P61 GSOFT DBIO GSNP: Active Matter VI BCEC 258B - Benjamin Loewe, Syracuse University - Tag(s): Focus
2:30PM P61.00001: Spontaneous buckling of contractile poroelastic actomyosin sheets [Invited] YARON IDESES, VITALY ERUKHIMOVITCH, RON BRAND, Chemical Engineering and Ilse Kats Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, SAMUEL A SAFRAN, Chemical and Biological Physic, Weizmann Institute of Science, KARSTEN KRUSE, Biochemistry and Theoretical Physics, University of Geneva, ANNE BERNHEIM-GROSWASSER (Presenter), Chemical Engineering and Ilse Kats Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev — Shape transitions in developing organisms can be driven by active stresses, notably, active contractility generated by myosin motors. The mechanisms generating tissue folding are typically studied in epithelia. There, the interaction between cells is also coupled to an elastic substrate, presenting a major difficulty for studying contraction induced folding. Here we study the contraction and buckling of active, initially homogeneous, thin elastic actomyosin networks isolated from bounding surfaces. The network behaves as a poroelastic material, where a flow of fluid is generated during contraction. Contraction starts at the system boundaries, proceeds into the bulk, and eventually leads to spontaneous buckling of the sheet at the periphery. The buckling instability resulted from system self-organization and from the spontaneous emergence of density gradients driven by the active contractility. The buckling wavelength increases linearly with sheet thickness. Our system offers a well-controlled way to study mechanically induced, spontaneous shape transitions in active matter (Ideeses Nat. Comm. 2018).

3:06PM P61.00002: ABSTRACT WITHDRAWN —

3:18PM P61.00003: Collective dynamics of microtubule-based 3D active fluids from gliding assay EDWARD JARVIS (Presenter), TEAGAN E BATE, MEGAN VARNEY, KUN-TA WU, Worcester Polytechnic Institute — Flows in passive fluids require temperature or pressure gradients. The gradients are not required for active fluids due to their capability of consuming local fuel to generate kinetic energy. The energy generated at a microscopic scale cascades up, resulting in macroscopic flows. However, the relation between microscopic and macroscopic dynamics remains unclear. Here we approach the problem with molecular motor-driven, microtubule (MT)-based 3D active fluids. We measure their flow mean speed at a millimeter scale, as a function of temperature, comparing with MT 2D gliding assay at a micron scale. We found that despite both systems differed in scales and dimensionality, they responded to temperature similarly. Moreover, such similarity was invariant under the change of motor processivity. Our work demonstrates collective dynamics of microtubule-based active fluids depends primarily on motor’s energy transducing rates, rather than motor’s dynamic details. Our finding expands flexibility in designing 3D active fluids using miscellaneous types of motors, as well as paves the path to outlining principles of self-organization of active fluids.

3:30PM P61.00004: Active nematic microtubule systems in confined geometries DIMITRIUS KHALADJ (Presenter), AMANDA TAN, LINDA S. HIRST, Physics, University of California, Merced — With the growing interest in active nematic systems, the introduction of restricted geometries is a novel method to investigate flows and mixing in active networks. In this study, we demonstrate active nematic motion of microtubules driven by kinesin clusters in confined and non-confined micro-environments. We use photolithography to fabricate bio-compatible micro-channels with varying widths to confine the active nematic microtubule network. Remarkably, we observe that nanoscale motion leads to continuous large-scale flow dynamics reminiscent of microscopic mixing. Furthermore, we propose that increasing confinement can have a significant effect on these large-scale transport phenomena. To quantify mixing, we directly couple beads to the microtubule network and apply methods from non-linear fluid dynamics to the spontaneous flows in the active nematic. We use fluorescence microscopy to track bead motion and record their trajectories. From this data, we measure Lyapunov exponents and Mean-Square-Displacement (MSD). We are interested in the relationship between flow dynamics and geometrical confinement.

3:42PM P61.00005: Active phase separation of biphasic polymer gels* NICHOLAS DERR (Presenter), Harvard University, CHRISTOPH WEBER, Max Planck PKS, L MAHADEVAN, CHRISTOPHER RYCROFT, Harvard University — Biological systems allow for the generation of active stresses, which can lead to mechanical and chemical instabilities and the formation of patterns. Many relevant systems - e.g. bone, developing tissue, cellular interiors - can be described as multiple immiscible phases of varying rheology, introducing a rich set of couplings between active stress generation and the corresponding passive mechanical responses. One area of particular interest is the generation of contractile forces within the cytoskeleton by the binding of myosin and kinesin motor proteins onto actin and microtubule networks, respectively. In this talk, we present a phenomenological model for active stresses induced by the fuel-dependent binding dynamics of molecular motors in biphasic, incompressible, transiently cross-linked polymer gels. We show that these stresses are analogous to a spatially and temporally varying dis-affinity between polymer and solvent which drives phase separation. The system’s behavior on long time scales is investigated by time-integration of the complete non-linear system of gel equations, and the results are contrasted with the case of a demixing passive gel described by classical Flory-Huggins theory.

*ND acknowledges support by DoD through the NDSEG Fellowship.

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AMANDA TAN (Presenter), KEVIN MITCHELL, LINDA S. HIRST, University of California, Merced — We study an active self-mixing fluid composed of biopolymers (microtubules) and molecular motors (kinesin). The kinesin motors are clustered together and crosslink bundles of microtubules. As the motors hydrolyze ATP, they walk along the microtubule bundles, forcing the bundles to extend away from each other. When confined in 2D at an oil-water interface, the network forms an active nematic with defects that are continuously created and annihilated. We consider these defects to be virtual stirring rods and the microtubule/kinesin system to be the fluid. We use fluid dynamic concepts to characterize this new self-mixing fluid by measuring the mixing efficiency, or topological entropy, by coupling beads directly onto the microtubule bundles and tracking their motion as they are mixed. The separation between beads in the material is exponential. We use these trajectories to measure the rate of separation in the material and thereby to calculate the topological entropy. In addition, we change the local stretching rate by varying the ATP concentration to study how changing the energy input on the microscale changes the global mixing efficiency.

*NSF-DMR 1808926
NSF-CREST: Center for Cellular and Biomolecular Machines at UC Merced (NSF-HRD-1547848)

KEVIN MITCHELL (Presenter), AMANDA TAN, ERIC ROBERTS, University of California, Merced, SPENCER SMITH, Physics, Mount Holyoke, LINDA S. HIRST, University of California, Merced — Recent years have seen a surge of interest in active materials, in which energy injected at the microscale gives rise to larger-scale coherent motion. One prominent example is an active 2D liquid crystal composed of microtubules in the nematic phase. The activity is generated by molecular motors that consume ATP to generate local shearing between the microtubules. The resulting 2D fluid flow exhibits self-generated mesoscale chaotic dynamics with a characteristic folding and stretching pattern. We analyse this dynamics in the context of chaotic advection, in which the fluid can be viewed as "stirred" by the topological defects in the nematic order parameter. We compute the topological entropy from the braiding of these defects and show that all of the entropy arises from the positive one-half defects; the negative one-half defects, which are also present, contribute nothing to the entropy. We also show that the topological entropy generated by this stirring can be understood as a direct consequence of the micro-scale stretching quantified by the Lyapunov exponent, which is computed from PIV data. Our work is based on experimental fluorescence images of the microtubule structure.

*This work is supported in part by NSF grant DMR-1808926.

SHUO GUO (Presenter), University of Minnesota, XINLIANG XU, complex systems, Beijing Computational Science Research Center, XIANG CHENG, University of Minnesota — For an equilibrium system, thermodynamic pressure is considered as a fundamental state variable of the system, which always equals to mechanical pressure, i.e., force per unit area acting on confining walls. In contrast, for an active system out-of-equilibrium such as bacterial suspensions, mechanical pressure is no longer a state variable, which may depend on the stiffness and shape of confining walls. Here, by combining optical tweezers with biochemical engineering technique, we create quasi-two-dimensional bacterial suspensions and systematically study active pressure exerted by swimming E. coli on confining walls of different geometries. In particular, we measure the pressure of bacterial suspensions on V-shaped walls of different angles. We find that the active pressure is a function of the angle of the walls: a sharper angle leads to a stronger pressure. In addition, the fluctuation of pressure increases with decreasing angle. We construct a simple model based on the wall-induced alignment of bacteria to quantitatively explain our observations. Our study provides benchmark experiments for characterizing the mechanical pressure of bacterial suspensions and sheds new light on the nonequilibrium statistical principle of active fluids.

*NSF CBET-1702352, DARPA YFA-D16AP00120
Bacteria Motility in Porous Media: Not a Random Walk

TAPOMY BHATTACHARJEE (Presenter), Andlinger Center for Energy and the Environment, Princeton University, SUJIT DATTA, Chemical and Biological Engineering, Princeton University — While bacterial motility is well-studied for motion on flat surfaces or in unconfined liquid media, most bacteria are found in heterogeneous porous media, such as biological gels and tissues, soils, sediments, and subsurface formations. Understanding how confinement alters bacterial motility is therefore critical to model the progression of infections, apply beneficial bacteria for drug delivery, and bioremediation. Unconfined bacteria move via runs and tumbles, leading to random walk-like motion; in a porous medium, previous research has assumed random walk-like motion for bacteria, with a reduced diffusivity due to collisions with obstacles. However, this assumption has never been directly tested due to the inability to visualize processes in opaque 3D media. Here, we directly visualize the motion of single E. coli cells inside a model 3D porous medium, having controlled pore structure. By analyzing the individual cell trajectories, we find that the bacteria do not move via a random walk process. We will present how bacterial motility depends sensitively on pore-scale confinement. Our findings overturn standard assumptions made in the field and provide guidance for the development of more accurate macroscopic models of bacterial motion.

Shape-directed rotation of homogeneous micromotors via catalytic self-electrophoresis

ALLAN BROOKS (Presenter), Chemical Engineering, Pennsylvania State University, MYKOLA TASINKEVYCH, Centro de Fisica Teorica e Computacional, Departamento de Fisica, Universidade de Lisboa, SYEDA SABRINA, DARRELL VELEGOL, Chemical Engineering, Pennsylvania State University, AYUSMAN SEN, Chemistry, Pennsylvania State University, KYLIE J. M. BISHOP, Chemical Engineering, Columbia University — The purpose of this work is to demonstrate that platinum microparticles with asymmetric geometries move spontaneously in hydrogen peroxide solutions. We can rationally design these motions by controlling particle shape using nanofabrication techniques. We design particles with n-fold rotational symmetry that rotate about their axis at rates specified by their extent of shape asymmetry. Experiments support a self-electrophoretic propulsion mechanism, where anodic oxidation and cathodic reduction of hydrogen peroxide occur at different rates at different locations across the particle surface. We develop a model to explain how the transport-limited electrochemical decomposition of hydrogen peroxide across an asymmetric particle surface leads to electro-osmotic flows that drive particle motion. Our results suggest that geometric control is an effective method to encode micromotor dynamics at the individual particle level. Insights from our proposed mechanism should be useful to design catalytic micromachines with complex dynamics and functions.

Controlling Morphology of Aerotactic Bacterial Bands

HIRAN WIJESINGHE (Presenter), ERIC MUMPER, ZACHARY OESTREICHER, STEVEN LOWER, BRIAN LOWER, RATNASINGHAM SOORYAKUMAR, Ohio State University — Microorganisms have perfected numerous evolutionary adaptations to improve their odds of survival and proliferation. This study exploits some of these adaptations such as flagellated swimming, aerotaxis and magnetotaxis in magnetic bacteria (MTB) to reshape entire swarms of them. These microorganisms have specialized strategies to navigate oxygen landscapes, of which perhaps the most intriguing is the biomineralization of magnetic nanoparticles that are thought to help them align with the geomagnetic field (magnetotaxis) and swim along natural oxygen gradients. Resulting migration to oxic-anoxic transition zones (OATZ) leads to aerotactic band formation. Many bacteria achieve motility through spinning helical flagellar appendages that produce flow fields that are well described in the far field by analytical models. However near-field dynamics remain elusive. We utilize lattice Boltzmann-based numerical models to simulate near field hydrodynamic interactions, metabolism-dependent oxygen diffusion in the medium, aerotactic response of the cells, as well as field controlled magnetotaxis. Strategies to achieve swarm morphologies beyond simple MTB aerotactic bands will be discussed.

Three-body Interactions Drive the Transition to Polar Order in a Simple Flocking Model

PURBA CHATTERJEE (Presenter), NIGEL DAVID GOLDENFELD, Physics, University of Illinois at Urbana-Champaign — Active systems are characterized by a discontinuous flocking transition from a disordered isotropic state to a polar ordered state with increasing density and decreasing noise. A large class of mesoscopic or macroscopic theories for flocking are coarse grained from microscopic models that feature binary interactions as the chief aligning mechanism. However, at the high densities at which the system flocks, binary interactions are too weak to account for the ordering transition. Here we introduce a solvable one-dimensional model of flocking, and derive a series of approximations for the stochastic hydrodynamics. We show that three-body interactions are not only necessary but also sufficient to capture the full phenomenology of flocking.
5:18PM P61.00013: Active reorientation in an active granular system powered by toy vibrobots* KYLE WELCH (Presenter), BO-KAI ZHANG, Complex Systems Division, Beijing Computational Science Research Center, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota, XINLIANG XU, Complex Systems Division, Beijing Computational Science Research Center — While emergent collective motion in systems of self-propelled objects is remarkable, one proclivity of active agents, particularly animals, is often overlooked when building models: collision avoidance. We present here an active granular experiment of disks propelled by toy vibrobots, which integrates an “active reorientation” behavior in analogy to collision avoidance in animals. The system demonstrates local flocking, wherein particle velocities locally align. Inspired by this experiment, we develop a computational model of self-propelled disks with an active reorientation mechanism. This simple numerical model exhibits rich phase behaviors: a disordered state, a flocking state and a clustering state under different parametric conditions. We find a notable suppression of aggregation in regions of parameter space corresponding to strong collective motion. Clusters develop quickly in this region, but are metastable, and collapse once the flocking state is achieved. Our experiment and model demonstrate the importance of active reorientation on emergent behaviors in systems of self-propelled agents, and illustrate the profound interplay between different emergent phases of active matter.

*This research is supported by NSFC funds 11750110409 (KJW), 11575020 (XXL), and U1530401 (XXL).

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P62 DCOMP GSCCM: Physics of Planetary Interiors: Modeling Planets From Atomic to Global Scale BICEC 258C - Philip Armitage, JILA - Tag(s): Invited, Undergraduate

2:30PM P62.00001: What Juno and Cassini have told us about Giant Planet interiors* [Invited] DAVID STEVENSON (Presenter), Caltech — Juno is in orbit about Jupiter and will likely continue collecting data for several more years. Cassini collected data during close encounters within the Saturn ring plane for several months in 2017. The main source of information is the gravity data and magnetic field data, augmented in the case of Juno by microwave radiometry data that inform us about atmospheric composition, a key boundary condition for the interior. Juno gravity indicates that the innermost part of Jupiter is enriched in heavy elements (everything heavier than H and He), perhaps at the extent of around 10 or 15 Earth masses (~5% of the planet mass) but this enrichment is not in the form of a discrete core but is instead diluted by the overlying H and He. This is consistent with current ideas for planet formation, where very high temperatures lead to evaporation and mixing of incoming solids. The distribution of heavier elements in the region where hydrogen begins to metallize is less clear and may be affected by and entangled with the possible rain-out of helium. Saturn, unlike Jupiter, benefits from ring seismology: the existence of ring structure that must be attributed to density anomalies within the planet. In both Jupiter and Saturn, the region of magnetic field generation extends out beyond the metallic hydrogen region in to primarily molecular hydrogen that is sufficiently hot and compressed that it has significant conduction electrons. Coupling of the magnetic field to the zonal flow extends out further still, to a region where the electrical conductivity is of order 1 S/m. Although there has been much improvement in our understanding of H-He, the uncertainties, both in theory and experiment, remain large enough that they limit our ability to make full use of the spacecraft results. We need experiments at relevant temperatures and pressures, since most current experiments are either too hot or too cold at the pressures of importance.

*Work supported by the Juno mission

3:06PM P62.00002: Setting the stage: dynamics of planet formation and water delivery* [Invited] SEAN RAYMOND (Presenter), Laboratoire d’Astrophysique de Bordeaux, CNRS — In addition to our Solar System, exoplanet systems provide a sample of thousands of outcomes of planet formation. Even though Jupiter is the only Solar System planet likely to be detected with present-day technology, the past decade of observations has shown that the Solar System is quantifiably unusual among exoplanet systems at the ~1% level. Instead, at least half of main sequence stars host close-in “super-Earths”, and ~10% have Jupiters on non-Jupiter-like orbits. In this talk I will explore how the Solar System fits in a larger context by addressing key steps in planetary system formation. I will present models to explain the diversity of observed planetary systems and the mechanisms that create that diversity. I will focus on the processes that create a diversity in planetary compositions and formation times, with a particular emphasis on the origin of water. While there is as yet no consensus on exactly how the Solar System formed it is clear that Jupiter played a central role.

*I thank the Agence Nationale pour la Recherche for support via grant ANR-13-BS05-0003-002 (grant MOJO) and acknowledge NASA Astrobiology Institute’s Virtual Planetary Laboratory Lead Team, funded via the NAI under solicitation NNH12ZDA002C and cooperative agreement No. NNA13AA93A.
3:42PM P62.00003: Imaging the Earth's Interior based on Seismic Full Waveform Inversion* [Invited] JEROEN TROMP
(Presenter), Geosciences, Princeton University — Information about Earth’s interior comes from seismograms recorded at its surface. Seismic imaging based on spectral-element and adjoint-state methods has enabled assimilation of this information for the construction of 3D (an)elastic Earth models. These methods account for the physics of wave excitation and propagation by numerically solving the equations of motion, and require the execution of complex computational procedures that challenge the most advanced high-performance computing systems. Current research is petascale; future research will require exascale capabilities. Our research addresses the long-standing challenge of imaging Earth's interior based on full-waveform inversion. What we mean by 'full-waveform inversion' is combining 3D forward simulations with Fréchet derivatives computed in 3D background models to fit complete three-component seismograms both in phase (traveltime) and amplitude.

The inverse problem consists of reconstructing the characteristics of the medium from -often noisy- observations. A nonlinear functional is minimized, which involves both the misfit to the measurements and a Tikhonov-type regularization term to tackle inherent ill-posedness. Achieving scalability for the inversion process on tens of thousands of multicore processors is a task that offers many research challenges.

We are performing global adjoint tomography using a data set of 1,480 events recorded by tens of thousands of seismographic stations. We observe a significant increase in the resolution of plume and slab features throughout the mantle. The level of detail in our current model enables us to answer some of the questions the geosciences community has been asking about the existence of plumes and hotspots. In this presentation I will present our latest model.

*National Science Foundation

4:18PM P62.00004: Spin crossover in iron in lower mantle minerals* [Invited] RENATA WENTZCOVITCH (Presenter), Columbia University — Pressure and temperature induced spin-state change in iron in lower mantle minerals is an unusual phenomenon with previously unknown consequences. High pressure and high temperature experiments have offered a wealth of new information about this class of materials problems, which includes the insulator to metal transition in Mott systems. I will discuss key experimental data, contrast them with our ab initio results and thermodynamic models, show the implications for fundamental phenomena taking place at the atomic scale and their macroscopic manifestations, and discuss potential geophysical consequences of this phenomenon.

*Research Funded by National Science Foundation grant EAR-1503084

4:54PM P62.00005: Numerical Simulations of Mantle Convection and Plate Tectonics in the Earth and Planets: From Magma Oceans to Present Day [Invited] PAUL J TACKLEY (Presenter), CHARITRA JAIN, ANTOINE B ROZEL, PATRICK SANAN, Department of Earth Sciences, ETH Zurich, DIOGO LOURENCO, Department of Earth and Planetary Sciences, University of California, Davis — The coupled system of convection of the Earth's solid mantle and plate tectonics is the driver of geological change on our planet, including continental drift, volcanoes, earthquakes, crustal production, atmospheric degassing the recycling, and cooling of the core, which drives the geodynamo. Modelling of this process is challenging due to the wide range of length scales (from faults to continents) and time scales (seconds to billions of years) and the complex rheology of rocks, which exhibit visco-elasto-plastic behaviour with strongly temperature-dependent viscosity varying by orders of magnitude over short length scales. Nevertheless, it is now routine to perform global-scale 3-D spherical simulations that span the 4.5 billion year age of our planet and contain complex effects such as partial melting and crustal production and solid-solid phase transitions.

StagYY [1] is one of the leading codes for performing such simulations. It uses a finite-volume discretization on a yin-yang spherical grid. Both built-in geometric multigrid, and the range of solvers available through PETSc, can be used. Here, technical details will be discussed, including recent enhancements made with funding from the Swiss Platform for Advanced Scientific Computing (PASC) project. Recent scientific results on contrasting tectonic regimes and the long-term evolution of Earth, solar system planets and exoplanets will be presented [2-4].


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NIKO BEERENWINKEL, Biology, ETH Zurich, ALEX GAVRYUSHKIN, Computer Science, University of Otago, JEAN CARLSON, Physics, UC Santa Barbara, NIKO BEERENWINKEL, Biosystems Science & Engineering, ETH Zurich, VILHELM ANDERSEN WOLTZ (Presenter), CLARE I ABREU, JEFFREY GORE, Massachusetts Institute of Technology — The fly gut serves as an effective combinatorial model to dissect the gut microbiome. Interactions with previous colonizers due both to spatial and metabolic interactions. These interactions also shape host fitness, altering the lifespan and reproduction of flies. We find that colonization ability of new species is strongly influenced by these interactions influence physiology of the fly. To deconstruct this complexity, my lab develops a microbiome model using the fruit fly as the host and its natural set of just five stably colonizing gut bacteria as the microbiome. We reconstruct this system combinatorially, starting with germ-free flies, to ask how bacteria influence each other's ability to colonize the gut and how these interactions influence physiology of the fly. We find that colonization ability of new species is strongly influenced by previous colonizers due both to spatial and metabolic interactions. These interactions also shape host fitness, altering the lifespan and reproduction of flies. We introduce new mathematical tools called epistatic filtrations to calculate microbiome interactions. The fly gut serves as an effective combinatorial model to dissect the gut microbiome.

*WBL acknowledges NIH grant 1DP5OD017851.

3:06PM P63.00002: Predictability in the assembly of microbial communities JEFFREY GORE (Presenter), Massachusetts Institute of Technology — Multispecies microbial communities are essential for the health of the planet as well as the human body. A major challenge is to develop a predictive understanding of which species will be able to coexist in a given environment. This task is potentially made even more difficult if there are strong higher-order interactions between species, in which the presence of a third species changes the nature of the interaction between two other species. In a series of laboratory experiments we have demonstrated that pairwise competitive outcomes are typically sufficient to predict the composition of simple communities containing three species. These results argue that higher-order interactions, while undoubtedly present, are typically not so strong as to make prediction impossible.

3:18PM P63.00003: Alternative stable states in microbial communities induced by environmental fluctuations VILHELM ANDERSEN WOLTZ (Presenter), CLARE I ABREU, JEFFREY GORE, Physics, Massachusetts Institute of Technology — Environmental fluctuations are pervasive in ecosystems, from daily and yearly variations in temperature to gut microbes receiving influxes of resources. In experiments with soil microbes, we have observed that a fluctuating environment causes a two-species community to exhibit alternative stable states that depend on the initial abundances of each species. Environmental disturbances were administered via daily dilutions of bacteria competitions. The magnitude of the daily dilution factor determines the fraction of cells discarded and therefore the depth of disturbance to the environment. We found the outcome of a competition with a fluctuating dilution factor to be the same as that with a constant dilution factor equal to the average of the fluctuating dilution factors. This outcome is in line with a prediction of the Lotka-Volterra competition model with an added global mortality rate: an environment with a fluctuating death rate equilibrates to the same fixed point as one with the time-averaged added mortality rate. We also observed fluctuation-induced alternate stable states in a more complex community with three species. These results suggest that, at least in a simple ecosystem, a fluctuating environment and a constant environment are in fact equivalent.

3:30PM P63.00004: Increasing Temperature Favors Slower-Growing Bacterial Species SIMON LAX (Presenter), CLARE I ABREU, JEFFREY GORE, Massachusetts Institute of Technology — Temperature is among the cardinal environmental variables which affect the growth and survival of microorganisms. Although the effects of temperature on the growth rates and metabolic activities of individual species is a central focus of microbiology, the manner in which temperature regulates competition between species is less well understood. Using a simple adaptation of the Lotka-Voltera competition models, we hypothesize that temperature should have generic effects on microbial competition, such that slower-growing species should consistently be favored by increasing temperature. We demonstrate that this prediction holds true in experimental pairwise competitions between a diverse set of species, and discuss how a community-wide death rate and the growth rates of the individual species interact to shape competitive landscapes. Finally, we show that pairwise dynamics are predictive of competitive outcomes in more complex communities, suggesting it should be possible to make general predictions for how communities might react to warming environments.
3:42PM P63.00005: Decomposition of generalized Lotka-Volterra systems and microbiome recovery*  ERIC JONES (Presenter), JEAN CARLSON, University of California, Santa Barbara — In the gut microbiome the successful administration of fecal microbiota transplantation (FMT) will convert a person's diseased microbial composition into a healthy one. We model these "healthy" and "diseased" microbial states as idealized ecological species, and characterize their behavior by homogenizing the properties of their constitutive microbial populations in a process called "steady state reduction" (SSR). This method decomposes a generalized Lotka-Volterra (gLV) system of many microbial species into two-dimensional (2D) subsystems that each span a pair of steady states of the high dimensional model and obey gLV dynamics. We investigate an experimentally derived model of antibiotic-induced *C. difficile* infection (CDI), and study the clinically relevant transition between CDI-vulnerable (diseased) and CDI-resilient (healthy) states with the 2D subspace generated by SSR. Specifically, we investigate the ability of FMT to convert a diseased state into a healthy state, and observe that a delay in FMT administration following antibiotics may undermine its success.

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

3:54PM P63.00006: What's love got to do with it? Stable marriage in microbial ecosystems limited by two essential nutrients  SERGEI MASLOV (Presenter), VERONIKA DUBINKINA, Bioengineering and Carl R. Woese Institute for Genomic Biology, University of Illinois at Urbana-Champaign, YULIA FRIDMAN, Department of Plasma Technologies, Kurchatov Institute, Moscow, Russia, PARTH PRATIM PANDEY, Carl R. Woese Institute for Genomic Biology and National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign — Microbial communities routinely have several alternative stable states observed for the same environmental parameters. A possibility of sudden and irreversible transitions between these states (regime shifts) complicates external manipulation of these systems. Can we predict which specific perturbations may induce such regime shifts and which would have only a transient effect? To study this topic we introduce and study a model of a microbial ecosystem colonized by a large number of specialist species. Each species can be limited by essential nutrients of two types, e.g. carbon and nitrogen, each represented in the environment by multiple metabolites. We demonstrate that our model has an exponentially large number of potential stable states realized for different nutrient fluxes. Using game theoretical methods adapted from the stable marriage problem, we predict all of these states based only on ranked lists of competitive abilities of species for each of the nutrients. We show that several mutually uninvadable stable states are generally feasible for a given set of environmental conditions, and explore an intricate network of discontinuous transitions between these states upon changes of nutrient fluxes.


4:06PM P63.00007: The Minimum Environmental Perturbation Principle*  ROBERT MARSLAND (Presenter), Physics, Boston University, WENPING CUI, Physics, Boston College, PANKAJ MEHTA, Physics, Boston University — Variational principles have served as powerful conceptual tools throughout all areas of physics, often providing some geometrical intuition for the behavior of an otherwise intractable model. Variational principles have also been found for some of the paradigmatic models of theoretical ecology, but they usually lack a clear physical interpretation, and are therefore of limited use for building intuition. In this talk, I will show that competition among consumers for a common pool of resources leads to steady-state resource concentrations that solve a constrained optimization problem. Specifically, the magnitude of the environmental perturbation induced by resource consumption is minimized, subject to the constraint that the per-capita growth rate of each consumer species in the regional pool is zero or negative. This "Minimum Environmental Perturbation Principle" applies to a wide class of models with arbitrarily large numbers of species and resource types, whether the resources are substitutable or essential. But it is broken by environmental feedbacks, whereby consumers return resources to the environment as metabolic byproducts or decaying biomass.

*This work was supported by NIH NIGMS grant 1R35GM119461 and by a Simons Investigator (MMLS) award to PM
4:18PM P63.00008: Higher order interaction inhibits bacterial invasion of a producer-predator microbial community*  HARRY MICKALIDE (Presenter), SEPP KUEHN, University of Illinois at Urbana-Champaign — Microbial communities must resist invasion in order to maintain biodiversity, stabilize industrial bioreactors, and preserve human microbiome health. It is widely believed that the more diverse a microbial community is, the more resistant to invasion it will be, and that this increased invasion resistance arises from a niche complementarity effect: more diverse communities consume a greater range of resources and thus eliminate niches for would-be invaders. Here we show that in a community of the algae *Chlamydomonas reinhardtii* (producer) and the ciliate *Tetrahymena thermophila* (predator), invasions by the bacteria *Escherichia coli* fail even when there is a niche of resources available to the bacteria. In contrast, bacteria successfully invade communities of algae or ciliates alone. We attribute the invasion resistance of the algae-ciliate community to a higher-order (3-way) interaction: the algae inhibits the bacteria’s ability to aggregate which leaves the bacteria susceptible to the ciliate’s predation. This method of invasion resistance requires both the algae and the ciliate to be present and thus provides an example of diversity leading to invasion resistance due to a higher-order interaction rather than niche complementarity.

*UIUC Physics
C Woese Institute for Genomic Biology

4:30PM P63.00009: Bacterial cohesion predicts spatial distribution in the larval zebrafish intestine*  BRANDON SCHLOMANN (Presenter), TRAVIS WILES, ELENA WALL, KAREN GUILLEMIN, RAGHUVEER PARTHASARATHY, University of Oregon — Are there general biophysical relationships governing the spatial organization of the gut microbiome? Despite growing realization that spatial structure impacts microbial ecological dynamics, it is unclear in any animal gut whether structure is governed by predictive, unifying rules, of if it results from contextual, species-specific behaviors. I'll present work that explores this question through light sheet fluorescence microscopy of live, larval zebrafish that are raised germ-free and then associated with model microbial communities consisting of fluorescently tagged, symbiotic bacteria. Through comparative study of seven different species in isolation, we uncovered an unexpected and striking correlation between bacterial cohesion—the degree to which bacteria auto-aggregate—and position along the length of the intestine. We propose that this relationship emerges from the mechanical response of communities to flows generated by peristaltic contractions, and test this idea with genetic and antibiotic perturbations that modulate bacterial cohesion. The generality of this phenomenon points to bacterial cohesion as an ideal target for precision microbiome engineering.

*Supported by the NIH under T32 GM007759 to BS and by the Kavli Foundation.

4:42PM P63.00010: Spatial dynamics of multispecies mutualism  KIRILL KOROLEV (Presenter), RAJITA MENON, Boston University — Ecosystems function via a network of interactions between the species. Many of these interactions require physical proximity and are therefore affected by the spatial distribution of the species. We explore spatial structure that emerges due to facilitation and mutualism in multispecies communities and investigate its effects on ecosystem dynamics. In addition to one-way and two-way metabolite exchanges, interactions in multispecies community include loops of cyclic cross-feeding and higher order interactions such as collective mutualism. Collective mutualism requires that several species simultaneously contribute to a particular task such as digestion of a complex polysaccharide. We show that collective interactions become increasingly unstable to demographic fluctuations as the number of participating species increases. Such higher order interactions can nevertheless be stabilized by a network of reciprocal cross-feeding. We show how our results connect to the theory of nonequilibrium phase transitions and discuss the implications of our findings for the design of synthetic microbial communities.

4:54PM P63.00011: Dynamics of a predator-prey system with multiple predation strategies  RITWIKA VALLOMPARAMBATH PANIKKASSERYSU (Presenter), Physics, University of California, Merced, JUSTIN YEAKEL, Life and Environmental Sciences, University of California, Merced, AJAY GOPINATHAN, Physics, University of California, Merced — Predator foraging behavior includes hunting, scavenging, and stealing. Despite a wealth of literature about predator-prey dynamics, studies with different predator behavioral modalities are rare. We use non-linear dynamics to understand how populations evolve in predator-prey systems with multiple predator behaviors. Predator-prey interactions are summarized by coupled differential equations describing predator and prey population fluxes. The predator population is described by a single variable while the prey population is described by three – alive prey, prey being eaten by predators and is available for stealing, and dead prey available for scavenging. The size of each prey group serves as a proxy for the proportion of the relevant predator behavior. Fixed point analysis yields two trivial and one non-trivial fixed point, and the latter depends on predator death rate, prey growth rate, and relative strengths of different predator-prey interactions. Numerical simulations yield at least three distinct families of solutions depending on interaction strengths between prey types and predator – i.e., the system has multiple bifurcations. Finally, we show that hunting is more prevalent than scavenging or stealing.
5:06PM P63.00012: Investigating the role of pairwise interactions in microbial community assembly* JAMES BRUNNER (Presenter), NICHOLAS CHIA, Mayo Clinic — Using metabolic and ecological modeling, we investigate the question: is microbial co-occurrence in the human gut a result of pairwise interactions, or do higher order interactions play a significant role? We perform model fitting on data from pairwise bacterial growth experiments to produce deterministic and stochastic growth models for pairs and triplets of bacterial species. We measure the accuracy of the predictions given by the triplet models to assess the extent to which pairwise interaction parameters can explain triplet outcomes. We also use metabolic models to assess bacterial growth in pairs and triplets. Pairwise metabolic modeling can be used to determine interaction parameters between species, using for example dynamic flux balance analysis (dFBA). We compare the apparent pairwise interaction parameters derived from pair community models and triplet community models to determine whether or not constraint based metabolic modeling of communities depends strongly on only pairwise interactions, or if higher order interactions must be taken into account.

*We would like to thank the Jack DeWitt and Jackie Curtiss Foundation for their support.

5:18PM P63.00013: Immigration-induced phase transition in a regulated multispecies birth-death process* SONG XU (Presenter), Biomedical Informatics, Stanford University, THOMAS CHOU, Mathematics, UCLA — Power-law-distributed species counts or clone counts arise in many biological settings such as multispecies cell populations, population genetics, and ecology. This empirical observation that the number of species \( c_k \) represented by \( k \) individuals scales as negative powers of \( k \) is also supported by a series of theoretical birth-death-immigration (BDI) models. However, we show how a simple global population-dependent regulation in a neutral BDI model destroys the power law distributions. Simulation of the regulated BDI model shows a high probability of observing a high-population species that dominates the total population. Further analysis reveals that the origin of this breakdown is associated with the failure of a mean-field approximation for the expected species abundance distribution. We find an accurate estimate for the expected distribution \( \langle c_k \rangle \) by mapping the problem to a lower-dimensional Moran process, allowing us to also straightforwardly calculate the covariances \( \langle c_k c_l \rangle \). Finally, we exploit the concepts associated with energy landscapes to explain the failure of the mean-field assumption by identifying a phase transition in the quasi-steady-state species counts triggered by a decreasing immigration rate.

*NSF DMS-1814364

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P64 DBIO: Systems Biology and Stochasticity in Biological Networks BCEC 259B - Po-Yi Ho, Harvard University

2:30PM P64.00001: The effects of the circadian clock on cell cycle regulation in cyanobacteria PO-YI HO (Presenter), ARIEL AMIR, Harvard University — The circadian clock affects the timing of cell divisions in cyanobacteria such that cells tend not to divide near dawn or dusk. The mechanism underlying the coupling between the clock and division remains unclear. We developed a phenomenological model that captures the single-cell statistics of the timing of cell divisions in the cyanobacteria _Synechococcus elongatus_. The model reproduces experimental results for both the wildtype and a clock-deletion mutant, in constant as well as periodic environments. We further study, within the model, how coupling division to the clock may affect the fitness of the population as a whole.

2:42PM P64.00002: Molecular search for a target with a conformational change: First passage time approach* JAEOH SHIN (Presenter), ANATOLY BORIS KOLOMEISKY, Rice University — The process of a molecule search for its target is ubiquitous in Nature. During the process, the molecule is often moving in complex inhomogeneous environments with random transitions between different dynamic modes. A notable example is transcription factors searching for target sequences on a DNA. Here we study the search dynamics with stochastic transitions between two conformations in a one-dimensional lattice. Using the first passage time approach, we explicitly analyze the mean search time for arbitrary system parameters. We found that there are several dynamic regimes in the search dynamics, which are determined by the relative values of the relevant length scales in the system. Moreover, the search time can be minimized by the combination of two different modes. Intriguingly, a recent analysis of hOGG1 protein shows that the protein moves on a DNA in the optimal parameter range. Additionally, we construct a general dynamic phase diagram.

*The work was supported by the Welch Foundation (C-1559), by the NSF (CHE-1664218), and by the Center for Theoretical Biological Physics sponsored by the NSF (PHY-1427654).
Precise timing can be advantageous in many biological processes, whether to coordinate events in the cell cycle, determine the duration of cell states, or create reliable rhythms. However, it can be hard to achieve because chemical reactions often produce exponentially distributed waiting times for individual events even when the rates are perfectly constant. Here we develop mathematical theories to dissect classes of timing mechanisms in single cells -- derive fundamental limits and optimal strategies, and how simpler and realistic circuits would approach the optimal. For some broad but naturally occurring distributions, the noise is limited by the inverse quartic root of the average number of states, and even that requires intricate mechanisms. We discuss how known synthetic and natural genetic timers appear to employ these mechanisms to create precise rhythms or accurate multigenerational cell fate decisions.

*This work was supported by NSF award 1517372 and by DARPA Agreement HR0011-16-2-0049.

Exponential growth naturally arises in many biochemical, cellular, ecological and economic flux networks. While the majority of mathematical models focus on balanced, steady-state growth, the general existence criteria for a stable long-term growth rate remains unclear. Here, we introduce a theoretical framework by connecting ergodic theory to the long-term behavior of flux networks. We investigate the convergence of exponential growth rate for a broad class of nonlinear flux networks, constructed by scalable flux functions. Scalable networks expand our analytic tools for studying non-steady-state growing systems, including the cell cycle and oscillating ecosystems. We demonstrate how scalable networks facilitates the analysis of objective functions in flux optimization, and use them for characterizing the essential motif of autocatalytic flux networks. Overall, our theory allows systematic construction of nonlinear networks and investigate their growth rate under optimization, regulation and perturbation.

Cellular events such as cell migration, division, and cell differentiation rely on precise timing. Molecular events inside cells are highly stochastic, and yet cells trigger events with high timing precision. We explore the effect of gene regulatory networks on first passage timing precision. We devise a method to find the global regulation function between the regulator and target gene which optimizes the timing precision. This method can be applied to a range of networks involving two genes such as regulation by an external species combined with autoregulatory feedback on the target gene itself. We confirm that feedback alone is not helpful in increasing timing precision. However, if a regulator is present then the combination of feedback and regulation is more beneficial than regulation alone. Specifically, higher timing precision is achieved by positive feedback when the regulator is high and negative feedback when the regulator is low. Our results are relevant to experimental gene regulatory systems where high timing precision is crucial, such as neuroblast migration during Caenorhabditis elegans development.

We acknowledge the Human Frontier Science Program.

The ability to measure shallow gradients in a chemical concentration plays an important role in a number of cellular processes, from chemotaxis to wound healing and development. Berg and Purcell were the first to demonstrate that diffusion sets a fundamental physical limit to the accuracy with which a cell can measure chemical concentrations. There is a growing body of physical literature concerning many aspects surrounding cellular concentration sensing. This includes the effects of receptor cooperativity, cellular shape and memory, and collective effects in multicellular sensing. Notably absent from this list is the role of fluid flow. In this talk, we discuss the problem of a low Reynolds number spherical squirmer directly sensing spatial gradients in concentration. By constructing a renormalization group improved solution of the appropriate advection-diffusion equation, we derive physical limits to the accuracy of spatial gradient sensing by swimming cells. At small Péclet number, advection is a singular perturbation in the problem. As a result, the sensory limits differ qualitatively from the case of pure diffusion which neglects the effects of fluid flow.
on the energetic cost associated with each task and the benefit provided by the trait. We show the optimum initial ratio of these two subpopulations depends on conditions heterogeneity in communication networks and division of tasks between two different phenotypes representing a public good, can freely diffuse into the environment and breakdown a substrate. We verify under what conditions an exoenzyme under quorum sensing regulation can increase the growth rate of individuals. This exoenzyme, representing a public good, can freely diffuse into the environment and breakdown a substrate. We verify under what conditions heterogeneity in communication networks and division of tasks between two different phenotypes are metabolically beneficial for the whole population. We show the optimum initial ratio of these two subpopulations depends on the energetic cost associated with each task and the benefit provided by the trait.


*Financial support from DFG, grant ME-1332/28-1, is gratefully acknowledged.
4:30PM P64.00011: Optimal control of aging in complex networks  ERIC SUN (Presenter), THOMAS MICHAELS, L MAHDEVAN, Harvard University — Aging is a shared process of biological and technical systems. As structural and organizational complexity increases, the phenomenon of aging—the progressive increase in the probability of death or decay—arises as an emergent property. A key question is how to maximize longevity of an aging system at minimal cost of maintenance and intervention. Here, we answer this question using optimal control theory and machine learning on a network model of aging. We derive and numerically validate optimal protocols for repair that emerge from a balance between maximizing system healthspan and minimizing the overall cost of repair. These protocols may motivate the design of rational strategies for delaying aging in complex systems.

4:42PM P64.00012: Integrating epigenetics to construct gene regulatory networks  ABHIJEET SONAWANE (Presenter), KIMBERLY RENEE GLASS, Medicine, Harvard Medical School — The biological processes that drive cellular function can be modeled by a complex network of interactions between regulators (transcription factors) and their targets (genes), summarized by gene regulatory networks (GRNs). The cell’s “epigenetic state” governs the potential targeting of genes by influencing chromatin accessibility. However, integrating such information to construct GRNs remains a challenge. Here, we develop an approach SPIDER using epigenetic information (DNase-I Seq data) and message-passing algorithm to estimate networks between transcription factors and genes in multiple cell lines. We validate our predictions against public ChIP-Seq data. SPIDER was more accurate, in predicting GRNs that other methods that integrate epigenetics compared to existing methods and improved detection of cell-line specific interactions in respective GRNs. SPIDER was also able to identify indirect interactions when putative motifs are absent in the regulatory region of genes, but with ChIP-Seq evidence of regulation. The epigenetically-informed GRNs from SPIDER can be used to identify targets of key regulators, or regulators of important genes from an experiment, in the given context of the cell-type.

4:54PM P64.00013: Kinetic PDE models of cell size control: size blow-up and evolution of growth rate*  MINGTAO XIA, Mathematics, Peking University, THOMAS CHOU (Presenter), Mathematics, UCLA — We derive kinetic equations for the distribution of cells in age, size, and added size after birth. These kinetic PDE models incorporate timer, sizer, and adder mechanisms of cell division. After properly constructing cell division rates, we show that an sizer-adder PDE model can lead to diverging cell sizes, particularly if the distribution of daughter cells immediately after birth is broad. The kinetic models are also extended to include growth rate correlation between successive generations. As the population evolves, so does the distribution of cellular growth rates. Representative numerical solutions to our PDEs will be presented.

*NSF DMS-1814364

5:06PM P64.00014: Exploiting a Percolation Transition for the Clustering of Noisy Gene Expression Data*  STEFFEN WERNER (Presenter), TOM S SHIMIZU, AMOLF, GREG STEPHENS, Physics, Vrije Univ (Free Univ) Amsterdam — Gene expression largely determines the fate of individual cells and ultimately influences development and behaviour of entire organisms. Thus, the ability to assess the abundance of mRNA intermediates of gene expression on a genome-wide scale (down to single cell resolution) promises to revolutionize our understanding of biological processes. While the collection of such data is rapidly growing thanks to experimental innovations, researchers face the challenge of identifying meaningful patterns and often need to discriminate subtle signals from a high noise floor. Here, we describe a density-based clustering approach that takes advantage of a percolation transition generically arising in random data to help discriminate meaningful patterns of variation from noise. The method allows clustering parameters to be defined by statistical properties of the data itself, thus obviating arbitrary parameter choices or detailed knowledge of experimental noise sources. By applying this approach to data from single cells to whole organisms, we reveal known as well as unknown modules of co-regulated genes.

*This work is part of the research program (nr. 161) of the Foundation for Fundamental Research on Matter, financially supported by the Netherlands Organization for Scientific Research (NWO).
5:18PM P64.00015: Dynamical network formation of *C. elegans* KEN NAGAI (Presenter), School of Materials Science, Japan Advanced Institute of Science and Technology, HIROSHI ITO, Faculty of Design, Kyushu University, TAKUMA SUGI, Molecular Neuroscience Research Center, Shiga University of Medical Science — Ordered collective motions are ubiquitous among locally interacting living beings. Experimental systems have been developed for non-living self-propelled particles, bacteria, and mammalian cells on a substrate, but there have been no experimental systems of multicellular organisms, which have much more complex behaviours, with various controllable parameters over a wide range.

Here, we have constructed an experimental system in which *C. elegans* collectively forms dynamical networks. We investigated the dependence of our designed experimental system on the substrate, ambient humidity and density of worms. Taking advantage of *C. elegans* genetics, we also controlled genetically determined motility by mutations. Furthermore, we developed an agent-based model with simple rules that reproduced the dynamical network formation and its dependences on the parameters, suggesting that the key behaviours for the network formation were alignment of worms after collision and smooth turning. This result revealed that the collective motion of the living things with advanced information processing systems can be described by a simple minimal model in a broad area of parameter space.

*This work was supported by JSPS KAKENHI Grant Numbers JP17KT0016 and JP18H05474.

**Wednesday, March 6, 2019 2:30 PM - 5:30 PM**

**Session P65 DBIO: Active and Living Matter II** BCEC 260 - Azam Gholami, Max-Planck-Gesellschaft - Tag(s): Focus

2:30PM P65.00001: Tissue flow genetics: mapping the forces that shape complex organs* [Invited] SEBASTIAN STREICHAN (Presenter), Physics, University of California Santa Barbara — Developmental biology established principles of how the body plan is laid out, morphogens setup axes, and gene expression patterns determine cell fates - yet how the form of organs emerges from coordinated action of multiple domains of distinct cell types remains elusive. We combine *in toto* live imaging and automated data analysis with physical modeling to investigate the link between kinetics of global tissue transformations and patterns of force generation during *Drosophila* gastrulation. We find our visco-elastic model driven by stress proportional to the spatial distribution and anisotropy of two quantitatively measured myosin pools achieves a 90% accurate description of the measured tissue flow - using only 3 parameters. Our analysis shows (i) forces driving the flow arise from non-uniformity of stress, thus spatial myosin modulation is critical for dynamics. Long-range modulation of the anisotropic part along the Dorso-Ventral (DV) axis suggests a novel role for the DV patterning system in convergent extension. (ii) The relation between flow and myosin forcing is non-local, and a transition towards areal incompressibility during germband extension further enhances non-locality. (iii) Mutant analysis indicates mechanical feedback on myosin recruitment relating it to the local strain rate. We conclude that understanding morphogenetic flows requires a fundamentally global perspective.

*NIH 4R00HD088708-03

3:06PM P65.00002: Quantifying the changes in cell morphology with changes in cell state* ELAHEH ALIZADEH, Cell & Molecular Medicine, Univ. of Arizona, WENLONG XU, Chem & Bio Engr, Colorado State Univ, JORDAN CASTLE, Colorado State Univ, JACQUELINE FOSS, Biomedical Engr, Colorado State Univ, ASHOK PRASAD (Presenter), Chem & Bio Engr, Colorado State Univ — The shape of an adherent cell on a surface depends upon its active cytoskeletal properties and can change with a change in cell state. We have developed a large number of parameters to quantify cell shape and cytoskeletal morphology[1]. Using these to study different cell lines, as well as different experimental conditions, we show, with the help of statistical analysis and neural networks, that cell shape and cytoskeletal texture can discriminate between different states. Projections into lower-dimensional shape space allow us to distinguish between similar and dissimilar changes in shape, and identify similarities in shape changes between breast cancer and osteosarcoma cell lines accompanying the acquisition of invasive characteristics. We also discuss the similarities and differences between shape changes of different cell lines with similar experimental perturbations, as well as the heterogeneity in shape characteristics. Our data indicates that cellular morphology may be a powerful and sensitive window into the physiological state of the cell [2].


*NSF PHY-1151454
3:18PM P65.00003: Loss of vimentin intermediate filaments increases motility and nuclear damage in confining spaces* ALISON KOSER PATTESON (Presenter), Physics Department, Syracuse University, PAUL JANMEY, University of Pennsylvania — Cell migration is important to many biological processes, such as embryogenesis, wound healing, and cancer metastasis. The proper migration of cells is regulated by the mechanical properties of the cytoskeleton. The cytoskeleton is comprised of three main polymers, F-actin, microtubules, and intermediate filaments. When cells transition from stationary to migratory states, they often upregulate the intermediate filament vimentin. The viscoelasticity of vimentin networks in shear deformation has been documented, but its role in motility remains largely mysterious. Here, we used mouse embryo fibroblasts derived from wild-type and vimentin-null mice and examined their migration in microfluidic constrictions. We find that loss of vimentin increases 3D motility, unlike on rigid 2D substrates. Migrating through small constrictions leads to stress-induced nuclear damage in the form of blebs, nuclear envelope rupture, and double-stranded DNA breaks. These nuclear damage markers increase in the absence of a filamentous vimentin network. Our findings indicate that vimentin hinders 3D motility by providing mechanical resistance against large strains and thereby protects the structural integrity of the cell.

*NIH-NIGMS (P01 GM096971)

3:30PM P65.00004: Probing the mechanical organization of k-fiber microtubule bundles within the mammalian mitotic spindle via targeted laser ablation and speckle microscopy MARCUS A BEGLEY, ELIZABETH MAE DAVIS, MARY WILLIARD ELTING (Presenter), Physics, North Carolina State University — In dividing cells, a self-assembling microtubule-based machine called the mitotic spindle segregates chromosomes, ensuring that each new daughter cell has exactly one copy of its genetic information. Spindle microtubule organization imparts shape and structural robustness. For example, bundles of microtubules called kinetochore-fibers (k-fibers) attach chromosomes to the spindle and exert force to align and ultimately segregate them. Thus, the mechanical integrity of the k-fiber is critical to spindle function, yet its organization is not well-understood. For example, we do not fully understand how molecules that crosslink microtubules along k-fiber lengths contribute to overall k-fiber mechanics, nor whether k-fiber microtubules remain rigidly associated or fluidly slide past each other in response to spindle dynamics. To address these questions, we are probing the mechanics of inter-microtubule associations within the k-fiber by single-molecule speckle microscopy and by severing k-fibers via laser ablation. Our initial results suggest that k-fiber microtubules associate along their lengths and primarily act in the spindle as single rigid objects, but that connections between their microtubules are weak enough to be disrupted by our mechanical perturbations.

3:42PM P65.00005: Stress-stabilized sub-isostatic fiber networks in a rope-like limit* SADJAD ARZASH (Presenter), JORDAN SHIVERS, Department of Chemical & Biomolecular Engineering, Rice University, ALBERT JAMES LICUP, Department of Physics & Astronomy, VU University Amsterdam, ABHINAV SHARMA, Leibniz Institute of Polymer Research Dresden, FRED C. MACKINTOSH, Department of Chemical & Biomolecular Engineering, Rice University — Biological networks are common in both intercellular and extracellular environments. Mechanics of these disordered fibrous networks is strongly dependent on their local coordination number. It is observed that real biopolymer networks have connectivity between three and four. Such networks are sub-isostatic with only central force interactions, but exhibit a mechanical phase transition between floppy and rigid states under shear. Introducing weak bending interactions stabilizes these networks and decreases the critical signatures of this transition. We show that applying external stresses on a sub-isostatic network with only tensile central force interactions, i.e., a rope-like potential also stabilizes these systems. Moreover, we find that the linear shear modulus shows a power law scaling with the external normal stress, with a non-mean-field exponent. We also find a critical strain that shifts to lower values under prestress. Applied normal stress also suppresses criticality in these systems.

*This work was supported in part by the National Science Foundation (Grants DMR-1826623 and PHY-1427654).
3:54PM P65.00006: Mobility of Molecular Motors Regulates Contractile Behaviors of Actin Networks  ATSUSHI MATSUDA, Institute for Frontier Life and Medical Sciences, Kyoto University, JING LI, PETER BRUMM, Interdisciplinary Life Science - PULSe, Purdue University, TAJI ADACHI, YASUHIRO INOUE, Institute for Frontier Life and Medical Sciences, Kyoto University, TAEYOON KIM (Presenter), Interdisciplinary Life Science - PULSe, Purdue University — Cells generate mechanical forces primarily from interactions between F-actin, cross-linking proteins, myosin motors, and other actin-binding proteins in the cytoskeleton. To understand how molecular interactions between the cytoskeletal elements generate forces, a number of in vitro experiments have been performed but are limited in their ability to accurately reproduce the diversity of motor mobility. In myosin motility assays, myosin heads are fixed on a surface and glide F-actin. By contrast, in reconstituted gels, the motion of myosin and F-actin are both unrestricted. Since only these two extreme conditions have been used, the importance of mobility of motors for network behaviors has remained unclear. In this study, to illuminate the impacts of motor mobility on the contractile behaviors of the actin cytoskeleton, we employed an agent-based computational model based on Brownian dynamics. We found that if motors can bind to only one F-actin like myosin I, networks are most contractile at intermediate mobility. On the contrary, if motors can bind to a pair of F-actins, a network can exhibit larger contraction with higher motor mobility. Results from this study imply that mobility of molecular motors may critically regulate contractile behaviors of actin networks in cells.

4:06PM P65.00007: Mechanical and Kinetic Factors Drive Sorting of Actin Crosslinkers*  SIMON FREEDMAN (Presenter), Engineering Sciences and Applied Mathematics, Northwestern University, CRISTIAN SUAREZ, JONATHAN WINKELMAN, DAVID KOVAR, GREGORY A VOTH, AARON DINNER, University of Chicago, GLEN HOCKY, Chemistry, New York University — In cells, actin crosslinkers segregate to different cytoskeletal networks to perform distinct functions, such as forming filopodia to enable cell migration, or polarizing actin bundles to enable cell division. Recent experimental work revealed a passive mechanism that may control this spatial localization: the binding of a short crosslinker to two actin filaments can promote binding of other short crosslinkers and inhibit binding of longer crosslinkers. We hypothesize that this spatial localization is due to the fact that actin is semiflexible and cannot bend over short lengths. We develop a mathematical theory and a Monte Carlo simulation to elucidate the quantitative predictions of this hypothesis. Experiments confirm the predictions but reveal an unanticipated dependence of crosslinker domain size on the kinetics of actin filament polymerization and crosslinker binding affinity. We use simulations of a coarse-grained but molecularly explicit model to characterize the interplay of mechanical and kinetic parameters and understand the observed behavior. Our work demonstrates a physical mechanism by which cells can organize molecular material to drive biological processes, and it can guide the choice and/or design of crosslinkers for protein-based materials.

*NSF MRSEC + Simons Fdn

4:18PM P65.00008: Reconstitution of aster movement and cell division plane positioning mechanisms in Xenopus egg extract*  JAMES PELLETIER (Presenter), Physics, Massachusetts Institute of Technology, CHRISTINE FIELD, Systems Biology, Harvard Medical School, NIKITA FAKHRI, Physics, Massachusetts Institute of Technology, JOHN OAKLEY, Chemical Engineering, University of Wyoming, JAY GATLIN, Molecular Biology, University of Wyoming, TIMOTHY MITCHISON, Systems Biology, Harvard Medical School — During early development, microtubule asters move through the cytoplasm to position microtubule organizing centers (MTOCs) near the centers of subsequent cells. Aster movement is thought to depend on pulling forces by cytoplasmic dynein opposed by hydrodynamic drag; however, it remains unclear what are the cytoplasmic anchors, and how other cytoplasmic networks such as actin facilitate or hinder aster movement. We reconstituted aster growth, interaction, and movement in an actin-intact Xenopus egg extract system under quasi-2D confinement. We imaged microtubules, actin, and candidate cytoplasmic anchors. Asters interacted to generate dynamic Voronoi tessellations with edges corresponding to division planes. MTOCs moved toward the center of each polygon, mimicking their movement in vivo. Dynein inhibition blocked inward transport of cytoplasmic anchors. Actin depolymerization increased the rate of inward transport of anchors, but decreased the rate of aster movement. Actin depolymerized at Voronoi edges due to AukkB activity, resulting in aster movement away from edges. Our experiments inform how dynamic cytoplasmic networks interact to drive aster movement by dynein-dependent and -independent mechanisms.

*JFP was supported by a Fannie and John Hertz Foundation Fellowship.
4:30PM P65.00009: Chromatin Mechanics and the Biological Implication*  YAOJUN ZHANG (Presenter), DANIEL LEE, Princeton University, YIGAL MEIR, Ben Gurion University, CLIFF BRANGWYNNE, NED WINGGREEN, Princeton University — The nucleus of the cell is a dense repository of information. But the DNA of the genome is more than just a string of letters – it forms “chromatin” a protein-nucleic-acid fiber with complex organization. Increasingly, the spatial organization of the genome has come into focus based on a suite of new technologies. The emerging picture spans scales from nucleosomes to loop domains to phase-separated regions. In parallel, the mechanics of chromatin has been probed by passive and active rheology, with its own emerging picture of chromatin as a viscoelastic and heterogeneous material. How are these two pictures related? To address this question, we developed a mechanistic model of chromatin using coarse-grained molecular dynamics simulations. The model captures chromatin's central viscoelastic nature and its observed heterogeneity, and has revealed long-range cross-links as critical to reproduce experimental observations. Our results further elucidate the role of mechanics in fundamental biological processes taking place in the cell nucleus.

*This work was supported in part by the NSF, through the Center for the Physics of Biological Function (PHY-1734030), the Graduate Research Fellowship Program (DCE-1656466, D.S.W.L.), NIH Grants R01 GM082938, U01 DA040601, and the HHMI.

4:42PM P65.00010: Bacterial chromosome organization by collective dynamics of SMC condensins*  CHRISTIAAN A. MIERMANS (Presenter), CHASE P. BROEDERSZ, Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians University of Munich — Recent Hi-C experiments of many bacterial species indicate a juxtaposed organization of the two chromosomal arms. These features in Hi-C maps have been attributed to various nucleoid-associated proteins, including the highly conserved SMC condensin. Although the molecular structure of these ATPases has been mapped in detail, it has been unclear how only a small number of condensins orchestrates this remarkable spatial organization. To resolve this puzzle, we developed a computational model for the dynamic organization of DNA by condensins as active slip-links. We first consider a scenario in which the ATPase activity of slip-links regulates their DNA-recruitment near the origin of replication, while the slip-link dynamics is assumed to be purely diffusive. We find that such diffusive slip-links can organize the entire chromosome into a state with aligned arms, but not within physiological constraints. However, slip-links that include motor activity are far more effective at organizing the entire chromosome, dynamically driving an entire chromosome into the juxtaposed state at physiological densities. We expand on these insights by showing the relation between this out-of-equilibrium organization and chromosome segregation.

*DFG Grants TRR174 and GRK2062/1.

4:54PM P65.00011: Ionic Conductance of 1.5 nm Diameter Carbon Nanotube Porins*  ALEKSANDR NOY (Presenter), Lawrence Livermore Natl Lab — Controlling ion transport on a molecular scale is important for applications ranging from industrial water treatment, to membrane separations, to bioelectronic interface design. Carbon nanotube porins—pore channels formed by ultra-short carbon nanotubes assembled in a lipid membrane—exploit nanoscale confinement and unique structure of carbon nanotube walls to transport water, protons, and small ions with efficiency that rivals and sometimes exceeds that of biological channels. We report the ion conductance characteristics and ion selectivity of the individual 1.5 nm diameter carbon nanotube porins. The conductance follows the power law scaling that is distinct from the previously reported characteristics of carbon nanotubes. We will also discuss the physical mechanisms that lead to these conductance characteristics. Overall, carbon nanotube porins represent versatile biomimetic membrane pores that are ideal for studying nanoscale transport phenomena and building new separation technologies and bioelectronic interfaces.

*These studies were supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award SCW0972. Work at LLNL was performed under the auspices of the U.S. Department of Energy under Contract DE-AC52-07NA27344.
We propose an extremely simple but efficient self-propelled cruiser, able to travel freely in 2D granular materials made of bidisperse dissipative particles under gravity. The cruiser has a round shape and a square indentation on its edge. To move into a given direction, perpendicular or parallel to gravity, we orient the indentation in line with the desired direction, and the cruiser shifts the granular particles entering its indent-region to its rear-half by a prescribed distance and then ejects them backward to gain thrust for moving forward. Using frictionless molecular dynamics (MD) method, we identify three universal phases of the cruiser during one particle-ejection process: 1) acceleration due to the ejection-thrust, 2) deceleration by the compressed particles ahead and 3) relaxation with the decompressed particles. We also confirm that the cruiser can travel continuously within the granular medium by successive particle-ejection, and the cruising performance increases with the ejection-strength and decreases by the interference from gravity. We believe our study demonstrates a novel approach to engineer self-propelled machines in granular materials.

*Startup funding, Shizuoka University, Japan

We find the general solution to the Fokker-Planck equation using homotopic methods. This result is represented as a series solution in time. The series coefficients are determined as phase-space derive operators. In addition, the general formalism is used to find mean values (variance and mean-square displacements) for the case of active Brownian particles on Euclidian and non-Euclidian spaces and under external fields. The theoretical results are validated using Brownian Dynamics simulations.

**Session P66 DBIO: Force Generation, Biomechanics and Tissue Dynamics**

Wednesday, March 6, 2019 2:30 PM - 5:18 PM

[2:30PM P66.00001: Active wetting of epithelial tissues* [Invited] RICARD ALERT (Presenter), Princeton Center for Theoretical Science, Princeton University, CARLOS PEREZ-GONZALEZ, Institute for Bioengineering of Catalonia, CARLES BLANCH-MERCADER, University of Geneva, MANUEL GOMEZ-GONZALEZ, Institute for Bioengineering of Catalonia, TOMASZ KOLODZIEJ, Jagiellonian University in Kraków, ELSA BAZELLIERES, Institute for Bioengineering of Catalonia, JAUME CASADEMUNT, University of Barcelona, XAVIER TREPAT, Institute for Bioengineering of Catalonia — Development, regeneration, and cancer involve drastic transitions in tissue morphology. In analogy with the behavior of inert fluids, some of these transitions have been interpreted as wetting transitions. The validity and scope of this analogy are unclear, however, because the active cellular forces that drive tissue wetting have been neither measured nor theoretically accounted for. We show that the transition between two-dimensional epithelial monolayers and three-dimensional spheroidal cell aggregates can be understood as an active wetting transition whose physics differs fundamentally from that of passive wetting phenomena. By combining an active polar fluid model with measurements of physical forces as a function of tissue size, contractility, cell-cell and cell-substrate adhesion, and substrate stiffness, we show that the wetting transition results from the competition between active traction forces and contractile intercellular stresses. This competition defines a new intrinsic length scale of active polar fluids that gives rise to a critical size for the wetting transition: Tissues larger than the critical size wet the substrate whereas smaller tissues dewet — a striking feature that has no counterpart in classical wetting. Finally, we show that active fluctuations of the tissue shape are dynamically amplified during the dewetting process. Overall, we conclude that tissue spreading constitutes a prominent example of active wetting — a novel physical scenario that may explain morphological transitions during tissue morphogenesis and tumor progression.


*R. Alert was funded by Fundació 'La Caixa'.
A Computational Model of Calcium Signals Around Laser-Induced Epithelial Wounds

AARON STEVENS (Presenter), KAZI TASNEEM, JAMES OCONNOR, SHANE HUTSON, ANDREA PAGE-MCCAW, Vanderbilt University — Epithelial wounds heal in multiple stages that involve wound detection, cell migration, and cell proliferation. One of the earliest signals of wound detection is an increase in cytosolic calcium concentration. Laser-ablation wounds in Drosophila epithelia trigger complex calcium signaling dynamics on multiple spatiotemporal scales. Given multiple hypothesized mechanisms that may drive calcium signals, we have developed a computational model to test the plausibility of these hypotheses and further understand the underlying biology. The model consists of intracellular exchange of calcium between cytosol and endoplasmic reticulum (ER), as well as exchange of calcium and other ions with the extracellular space and neighboring cells. The model thus couples calcium concentrations and membrane potentials among gap-junction-connected epithelial cells. These ion exchanges are initiated in the model by microtears in the plasma membranes of cells near the wound and by the activation of G-protein coupled receptors via a wound-induced diffusible ligand. We will discuss the model in detail, evaluate the plausibility of its hypotheses, and describe its experimentally testable predictions.

*Funded by NIH/NIGMS grant 1R01GM130130

Controlling collective cell migration using geometric boundary perturbations

MATTHEW HEINRICH (Presenter), DANIEL COHEN, ANDREJ KOSMRLJ, Princeton University — We work at the intersection of the active matter and tissue engineering communities, where our goal is to learn more about emergent behaviors of cellular collectives in response to perturbations of the microenvironment and to exploit these to develop design rules for controlling tissues. Here, we try to bias MDCK tissue expansion using asymmetric geometric boundary perturbations, a known strategy for biasing transport in several active matter systems. We aim to find the minimal boundary perturbation that can influence behavior in the bulk of a cell collective. Using a high throughput, high-resolution tissue-patterning assay, we can study the effects of these patterns on tissue expansion, wound healing (tissue collisions), and collective cell migration in general without typical microfabrication processes.

Coupling between symmetry and motion in 3D printed microtissue arrays

SARAH ELLISON (Presenter), CHRISTOPHER O’BRYAN, CAMERON MORLEY, THOMAS ANGELINI, University of Florida — Symmetry plays a major role in the emergence of collective phases of inanimate materials. In magnetism, for example, geometric frustration leads to spin-glass phases. If similar principles could be leveraged to control collective phases of biological materials, like living cell assemblies, a new set of design strategies could be developed in tissue engineering applications. Building symmetry into biological systems is often challenging and is sometimes achieved through surface micropatterning; achieving such patterns in 3D is even more challenging. To fabricate 3D multi-cellular systems of designed symmetry and spatial patterning, we 3D print geometric patterns of collagen and 3T3 fibroblast cells. These cell/ECM patterns are printed directly into a 3D growth media made from jammed microgels, providing a well-defined yet reconfigurable environment on all sides of the structures. By comparing the collective motion arising in systems with hexagonal and square symmetries, we probe the potential role of geometric frustration in multicellular structure maturation. Preliminary data and analysis will be presented.

Instabilities on the leading front of collectively migrating tissue

YANJUN YANG (Presenter), HERBERT LEVINE, Rice University — Instabilities are often observed on the leading front of a collectively migrating cellular sheet both in vivo and in vitro. Instead of moving forward uniformly, the leading front often destabilizes into multicellular fingering-like structures. To decipher the mechanical origin of the instabilities, we develop a continuous model based on the Toner-Tu equations for active fluids, in which the collectively moving cells are modeled as a system of self-propelled particles. We perform different perturbations on the front edge and analyze the linear stability. We show the instabilities are due to some kinds of perturbations, for example, leader cells. Finally, we show our simulation of figuring-like protrusions with the guidance of leader cells.

*This work is supported by the National Science Foundation Center for Theoretical Biological Physics (NSF PHY-1427654), and NSF DMS-1361411.
3:54PM P66.00006: Different modes of fluidization in Human Bronchial Epithelial Cells -- the Unjamming Transition vs. the Epithelial-Mesenchymal Transition  
AMIT DAS (Presenter), Northeastern University, JENNIFER A MITCHEL, Harvard T.H. Chan School of Public Health, DAPENG BI, Northeastern University, JIN-AH PARK, Harvard T.H. Chan School of Public Health — Epithelial tissues are non-migratory and behave as a jammed system under homeostatic conditions. Using a jammed layer of human lung epithelial cells we compare a new mode of tissue fluidization, induced by mechanical compression, namely the unjamming transition (UJT) with the epithelial-mesenchymal transition (EMT). Our analyses of experimental data reveal the following: Strong cellular elongation and large fast moving Nematic swirls during the UJT while retaining epithelial nature. All these features are lost during the EMT when the cells become mesenchymal. To further our understanding we developed a dynamic vertex model (DVM) which differs from previous vertex models in that the cell edges can now become curved and can thus reflect the competition of the forces acting on the edge locally. These forces include cortical tension, intracellular-pressure differences, and polarized motility forces. We explore different paths of solid-to-fluid transitions based on different parameters in the model, such as individual cell motility and preferred cell shapes, and compare our predictions with the experimental observations on UJT and EMT. Based on our comparisons, we propose that the UJT could be an alternative route to fluidization of jammed epithelial tissues, independent of the EMT.

4:06PM P66.00007: How the mechanics of extracellular matrices interacts with cells*  
YOUYUAN DENG (Presenter), HERBERT LEVINE, Center for Theoretical Biological Physics, Rice University — In the last twenty years, we have seen all-round progress in modeling the mechanics of the biopolymer network. Its stability is understood based on Maxwell counting arguments. The lattice-based models numerically predict the phase diagrams and other bulk properties that are consistent with experimental observations. Other analytical theories, such as mean-field approximation and scaling laws, also enlighten our understanding.

Part of the reason behind it being so intensively investigated is that, a good example of biopolymer networks, extracellular matrices(ECM), plays a central role in many cellular processes. On the single-cell level, experiments have shown that the ECM interact with biochemical networks in a cell, e.g. inducing the epithelial-mesenchymal transition. On multi-cellular levels, the ECM modulates collective biophysical processes like the durotaxis. Deciphering the force pattern behind many collective cellular behaviors is still under its way. We hereby showcase our recent efforts in modeling the couplings between the mechanics of ECM and biology of cells embedded inside the former.

*This work was supported by the National Science Foundation Center for Theoretical Biological Physics (NSF PHY-1427654), and NSF DMS-1361411.

4:18PM P66.00008: The origin of solidity and fluidity in cellular materials and biological tissues.  
DAPENG BI (Presenter), Northeastern University, LE YAN, Kavli Institute for Theoretical Physics — Models for confluent biological tissues often describe the network formed by cells as a triple-junction network, similar to foams. However, higher order vertices or multicellular rosettes exist prevalently in developmental and in vitro processes and have been recognized as crucial in many important aspects of development, disease and physiology. In this work, we study the influence of rosettes on the mechanics of a confluent tissue. We find that the existence of rosettes in a tissue can greatly influence its rigidity. Using a generalized vertex model and effective medium theory we find a fluid-to-solid transition driven by rosette density and intracellular tensions. This phase transition exhibits several hallmarks of a second-order phase transition such as a growing correlation length and a universal critical scaling in the vicinity a critical point. Further, we elucidate the nature of rigidity transitions in dense tissues using a generalized Maxwell constraint counting to answer a long-standing puzzle of the origin of solidity in cellular materials.
4:30PM P66.00009: The dynamics of laminin-mediated red blood cell adhesion in sickle cell disease*  SHAMREEN IRAM (Presenter), Physics, Case Western Reserve University, UTKU GOREKE, Mechanical and Aerospace Engineering, Case Western Reserve University, GUNDEEP SINGH, Physics, Case Western Reserve University, JANE LITTLE, University Hospitals, UMIT GURKAN, Mechanical and Aerospace Engineering, Case Western Reserve University, MICHAEL HINCZEWSKI, Physics, Case Western Reserve University — Understanding red blood cell (RBC) adhesion to blood vessel walls is crucial to treat sickle cell disease. We have developed a microfluidic RBC adhesion assay [Alapan et al., Translational Research, 173, 74-91, (2016)] and performed experiments on clinical whole blood samples to probe RBC adhesion biomechanics. Microchannels functionalized with laminin (an endothelial protein) were integrated with a programmable syringe pump to mimic physiological flow conditions in microvessels. A novel set of methods for automated identification and tracking of adherent RBCs from video data was developed. We analyzed the dynamical data using a theoretical approach adapted from a prior study on heterogeneity in protein adhesion in Atomic Force Microscopy (AFM) experiments [Hinczewski et al., Proc. Natl. Acad. Sci., 113, E3852 (2016)]. Our analysis yielded a minimal physical model of the RBC detachment process, and comprehensively characterized the adhesion dynamics across patient samples. Model parameters also revealed statistically significant correlations with patient clinical data, opening the possibility of diagnostic applications suited to automated, high-throughput and low cost diagnostic platforms with clinical utility.

*NSF CAREER BIO/MCB 1651560
NSF CAREER ENG/CMMI 1552782
NIH R01 R01HL133574

4:42PM P66.00010: Shape Fluctuations and Curvature-Driven Mechanics of Heterogeneous Lipid Vesicles*  DAVID ROWER (Presenter), PAUL J ATZBERGER, Mathematics/Mechanical Engineering, UCSB — We investigate heterogeneous vesicles consisting of mixtures of different lipids. We develop single-bead implicit-solvent coarse-grained models based on anisotropic pair potentials to capture vesicle shapes arising from species with different preferred curvatures. We develop theory and methods for mapping our molecular results to continuum mechanics descriptions, useful for analysis of fluctuation spectra to estimate bending elasticities and other mechanical parameters. For mixed lipid species, we find that passive fluctuation spectra are significantly influenced by the formation of small curved segregated domains. We actively probe the vesicle mechanics with compression and narrow-passage transport experiments. When compressed, we find that high-curvature domains arrange circumferentially, leading to a smaller resistance force. When transporting through a narrow passage, we find that mixed vesicles are characterized by much higher variances in passage times. We also find that geometric effects can delay phase-separation in the bulk and promote phase-separation during channel transport, resulting in occasional budding events. Our results may have implications for biological systems, fluidics utilizing vesicles, and other experimental assays.

*NSF DMS-1616353, NSF DMS-0956210

4:54PM P66.00011: Theory of cytoskeletal rearrangement and force generation*  ADAM LAMSON (Presenter), SHANE FIORENZA, MATTHEW GLASER, M. BETTERTON, University of Colorado, Boulder — Cytoskeletal networks that include microtubules, crosslinkers, and kinesin motors are the basis of the mitotic spindle and cytoplasmic transport. The large separation of time scales between motor and crosslinker activity (sub-second to second) and network function (minutes to hours) is a challenge for theoretical approaches. We developed a minimal model, building on the separation of time scales between relatively fast crosslinker and motor rearrangement and relatively slow filament movement. The model reproduces experimentally measured force, torque, and self-organization in cytoskeletal networks of different length scales. With this model, we study mitotic spindle assembly from a monopolar initial condition and compare the mechanisms of motor- versus crosslinker-mediated spindle assembly. The results show how torque-balance and force-balance properly align microtubule bundles. In another study, we propose that oscillating optically trapped microtubule pairs crosslinked with motors and/or crosslinkers can be used to determine the kinetics and mechanics of crosslinking proteins.

*NSF grants DMR1725065(MDB), and DMS1620003 (MAG and MDB); NIH grants K25GM110486 (MDB), R01GM124371 (MDB); NIH/CU Boulder Biophysics Training Program (AL); and NSF grants ACI1532235 and ACI153223.
5:06PM P66.00012: Force Generation by Curvature-Generating Molecules* JONAH SCHER-ZAGIER (Presenter), Department of Physics, Washington University, St. Louis, ANDERS CARLSSON, Department of Physics and Center for Engineering Mechanobiology, Washington University, St. Louis — Curvature-generating molecules (CGMs) are central to a variety of biological processes. In particular, proteins such as clathrin help provide bending forces and moments to drive endocytosis. We develop a discrete mechanical model of the shape of a small CGM-membrane complex that incorporates the effects of cell wall elasticity and high turgor pressure. We study the dependence of the force generated by the CGMs on several parameters, including the bending modulus, the complex size, and the turgor pressure. We find evidence of transitions as a function of external turgor pressure and intrinsic curvature. This work also compares the discrete model to previous continuous models of CGM forces, finding that the distribution of the forces depends on the strength of the turgor pressure relative to the bending energy. The forces are localized at the edges for high turgor pressure, and more widely distributed for low turgor pressure. In addition, the energy exhibits a minimum at small numbers of molecules. Further, for realistic values of the bending rigidity and curvature, CGMs alone are insufficient to initiate endocytosis against turgor pressure, in agreement with previous findings.

*This work was supported by NIGMS Grants R01 GM107667 and T32 EB018266-03, and NSF Grant CMMI:15-458571.

Wednesday, March 6, 2019 2:30 PM - 5:30 PM

Session P67 DBIO: Physics of Neural Systems I BCCE 050 - Joshua Shaevitz, Princeton University - Tag(s): Focus

2:30PM P67.00001: What the odor is not: Estimation by elimination* [Invited] VIJAY SINGH (Presenter), Physics, University of Pennsylvania, Philadelphia, PA, USA, MARTIN TCHERNOOKOV, Physics, University of Wisconsin, Whitewater, WI, USA, VIJAY BALASUBRAMANIAN, Physics, University of Pennsylvania, Philadelphia, PA, USA — The olfactory system is thought to encode vast numbers of odors combinatorially in the responses of a much smaller number of broadly sensitive receptors. Here, we propose a method for decoding such a distributed representation. The main idea is that it is much easier to identify what the odor is not, rather than what the odor is. This is because a typical receptor binds to many odorants; so a response below threshold signals the absence of all such odorants. We demonstrate that, for biologically realistic numbers of receptors, response functions, and odor mixture complexity, this remarkably simple method of elimination turns an underdetermined decoding problem into an overdetermined one, allowing accurate determination of the odorants in a mixture and their concentrations. We give a simple neural network realization of our algorithm which resembles the known circuit architecture of the piriform cortex.

*VS: Computational Neuroscience Initiative Postdoctoral Fellowship (University of Pennsylvania); VS, VB: Simons Foundation grant in Mathematical Modeling for Living Systems 400425 for Adaptive Molecular Sensing in the Olfactory and Immune Systems

3:06PM P67.00002: Quantifying Multi-neuronal Olfactory Responses in C. elegans* ALBERT LIN (Presenter), Department of Physics, Harvard University, VIVEK VENKATACHALAM, Department of Physics, Northeastern University, WESLEY HUNG, MIN WU, MEI ZHEN, Samuel Lunenfeld Research Institute, Mount Sinai Hospital, ARAVINTHAN SAMUEL, Department of Physics, Harvard University — Complex animal behaviors arise in response to an organism’s environment, as perceived through its senses. Unlike other stimuli animals experience, such as light or sound, chemosensory stimuli form a high dimensional space, making the computational problem faced by organisms interpreting olfactory cues especially complex. The processes by which olfactory information is encoded are poorly understood. To better understand ensemble-level olfactory representation, we record from all sensory neurons in the nematode C. elegans simultaneously, while presenting stimuli in a highly controlled manner in a microfluidics environment. Observing the dynamics of these neurons in response to odors and odor mixtures of varying identity and strength has allowed us to build a quantitative and comprehensive picture of the way the olfactory system in C. elegans consolidates and represents high-dimensional sensory information. Our results suggest that olfactory stimuli are represented by distinct constellations of multiple chemosensory neurons, and that response characteristics of individual neurons is odor-dependent.

*This work was supported by an NSF BRAIN EAGER grant, the NSF Ideas Lab: Cracking the Olfactory Code, and an NIH PO1 grant.
Seizure Prediction with Machine Learning using Real and Simulated Electrocorticography Data*

LOUIS NEMZER (Presenter), Nova Southeastern University, ROBERT WORTH, Indiana University, GARY D CRAVENS, VICTOR CASTRO, ANDON PLACZEK, KRISTINA BOLT, Nova Southeastern University — Epilepsy is the most common chronic neurological disorder, affecting approximately one percent of people worldwide. Patients with symptoms not well controlled with medication often suffer significantly reduced quality of life due to the unpredictable nature of seizures, which are periods of pathological synchronization of neural activity in the brain. Using a surgically-implanted intracranial electrode grid, electrocorticography (ECoG) provides better spatial and temporal resolution of brain electrical activity, compared with conventional scalp electroencephalography (EEG). We combine this patient data with simulated output from a full Hodgkin-Huxley calculation using in silico neurons connected with a small-world network topology. Supervised Machine Learning, a set of powerful and flexible artificial intelligence techniques that allow computers to classify complex data without the need for explicit programming, along with topological data analysis methods, are employed with a goal of developing an algorithm that can be used for the real-time clinical prediction of seizure risk.

*This work is supported by Nova Southeastern University President's Faculty Research and Development Grant #335472

Attractor-state itinerancy in neural circuits with synaptic depression*

BOLUN CHEN (Presenter), PAUL MILLER, Brandeis University — Neural populations with strong excitatory recurrent connections support bistable states in their mean firing rates. Multiple fixed points in a network of such bistable units can be used to model memory retrieval and pattern separation. The stability of fixed points may change on a slower timescale than that of the dynamics due to short-term synaptic depression. This leads to state-transitions that depend on the history of stimuli. We study a minimal model which characterizes multiple fixed points and transitions in response to diverse stimuli. We show that the slow synaptic depression introduces multiple time-scales. The interplay between fast and slow dynamics of synaptic input and depression makes the system's response sensitive to the amplitude and duration of square-pulse stimuli in a history-dependent manner. Weak cross-couplings further deform the basins of attraction for different fixed points into intricate and even fractal-like shapes. Our analysis provides a natural explanation for the system's rich responses to stimuli with different duration and amplitudes while demonstrating the encoding capability of bistable neural populations for dynamical features.

*Supported by the Swartz Foundation.

Nonlinear Brain Dynamics via Neural Field Theory*

PETER ROBINSON (Presenter), School of Physics and Center for Integrative Brain Function, Univ of Sydney — Going beyond well-known nonlinear effects at the single-neuron level, nonlinear effects at the systems and whole-brain levels are manifest in epileptic seizures (Hopf bifurcations, limit cycles, saddle cycles), migraines and visual hallucinations (Turing and Hopf-Turing patterns), strong visual stimulation (harmonic and subharmonic generation, phase locking, entrainment), deep brain stimulation therapy of Parkinson's disease (entrainment, harmonic and subharmonic generation, resonance suppression), the natural 10 Hz alpha rhythm (bistability), and normal sleep-wake dynamics (near-criticality, hysteresis, critical slowing).

Recent analyses of the above nonlinear effects are surveyed here, showing that they can be explained by neural field theory, whose predictions reproduce experimental results on large-amplitude normal, abnormal, and driven brain oscillations.

*This work was supported by the Australian Research Council under Center of Excellence Grant CE140100007 and Laureate Fellowship Grant FL140100025.
3:54PM P67.00006: Dynamics of excitable tree networks: Application to sensory neurons* ALI KHALEDI NASAB (Presenter), Department of Physics and Astronomy, Ohio University, JUSTUS KROMER, Department of Neurosurgery, Stanford University, LUTZ SCHIMANSKY-GEIER, Department of Physics, Humboldt-Universität zu Berlin, ALEXANDER NEIMAN, Department of Physics and Astronomy, Ohio University — We study the collective dynamics of diffusively coupled excitable elements on small tree networks with regular and random connectivity, which model sensory neurons with branched myelinated distal terminals. Examples of such neurons include touch receptors, muscle spindles, and some electroreceptors. We developed a theory that predicts the collective spiking activity in the physiologically-relevant strong coupling limit. We show that the mechanism of coherent firing is rooted in the synchronization of local activity of individual nodes, even though peripheral nodes may receive random independent inputs. The structural variability in random tree networks translates into collective network dynamics leading to a wide range of firing rates and coefficients of variations, which is most pronounced in the strong coupling regime.

*AKN and ABN acknowledge support by the Neuroscience Program, by Quantitative Biology Institute and Ohio Material institute at Ohio University. LSG thanks Ohio University for hospitality and support.

4:06PM P67.00007: Role of geometrical cues in neuronal growth* CRISTIAN STAII (Presenter), Physics and Astronomy, Tufts University — I will present a systematic experimental and theoretical investigation of neuronal growth on micro-patterned surfaces. The experimental results show that neurons cultured on surfaces with periodic geometrical patterns display a significant increase in the total length of axons, as well as axonal alignment along preferred growth directions, which are controlled by the surface geometry. We demonstrate that axonal dynamics is governed by non-linear stochastic differential equations, and use this theoretical model to measure key dynamical parameters: angular distributions, correlation functions, diffusion coefficients and cell-surface coupling forces. Our results show that neuronal alignment on these surfaces is completely determined by the surface geometry, and that the growth dynamics can be quantified by a minimal set of experimentally measurable parameters. I will also discuss how to generalize this approach to include mechanical and biochemical external cues, and introduce a general framework for the quantitative description of neuronal growth and self-organization in complex environments.

*Tufts Faculty Research Grant

4:18PM P67.00008: Long-lasting desynchronization achieved by decoupling stimulation JUSTUS KROMER (Presenter), PETER A. TASS, Stanford University — Abnormally strong synchronization of neuronal activity is a hallmark of several brain disorders. In Parkinson's patients, deep brain stimulation is permanently delivered at high frequencies (> 100 Hz) to suppress symptoms. A qualitatively different, theory-based approach uses dedicated stimulus patterns to cause a desynchronization-induced decoupling of oscillatory neurons. Corresponding long-lasting desynchronizing effects were demonstrated in animal and clinical studies. However, parameters of desynchronizing stimuli, e.g. the stimulation frequency, have to be adapted to the dominant neuronal rhythm. This is an issue since different abnormal brain rhythms may coexist.

We here present a novel approach which causes long-term desynchronization by decoupling stimulation, primarily targeting the slow synaptic weight dynamics - Random Step (RS) stimulation. It ultimately leads to full-blown desynchronization by shifting neural networks from attractors with synchronized to attractors with desynchronized neuronal activity. Compared to desynchronizing stimulation techniques, the acute desynchronizing effect of RS stimulation is weaker, but the robust long-lasting effect does not require fine-tuning to the dominant neuronal rhythms. This may enable novel clinical applications.

4:30PM P67.00009: Cooling Reverses Pathological Bifurcations to Spontaneous Firing Caused by Mild Traumatic Injury* BENJAMIN BARLOW (Presenter), BELA JOOS, University of Ottawa, ANH-KHOI TRINH, McGill University, ANDRE LONGTIN, University of Ottawa — Experimental studies have revealed that mild trauma in the form of e.g. physical pressure or chemical stimuli can alter the properties of the main current (sodium) responsible for the voltage swings or “firings” of neurons. This leads to ongoing firings even when the cell should be quiescent. Such pathological firing interferes with the usual input integration properties of the cell, and in particular has been implicated in the genesis of pathological pain, which persists even after the injury-producing stimulus is removed. From a dynamical point of view, this mild trauma lowers the threshold for firing. This presentation explores the possibility of using temperature to offset this effect by raising the firing threshold back up (see Chaos, 28, 106328 (2018)). Our modeling study predicts that cooling the neuron by just a few degrees – as is possible e.g. for peripheral nerve cells – can counteract the pathological state. The sensitivity of the sodium current to temperature is the key determinant of this effect.

*This work was supported by the Natural Sciences and Engineering Research Council (Canada).
4:42PM P67.00010: Utilizing network analysis and fMRI to infer key language modules and their circuits from healthy human controls*  QIONGGE LI (Presenter), Physics, City College of New York, GINO DEL FERRARO, LUCA PASQUINI, KYUNG K. PECK, Radiology, Memorial Sloan Kettering Cancer Center, HERNÁN A. MAKSE, Physics, City College of New York, ANDREI I. HOLODNY, Radiology, Memorial Sloan Kettering Cancer Center — Traditional task-based functional Magnetic Resonance Imaging (tb-fMRI) statistical analysis has served as a powerful tool to identify brain areas associated with language. However, it does not provide an explanation of how different functional areas interact and integrate with each other to form comprehensive language tasks.

We abstracted task-correlated areas at different anatomical locations as network modules where each voxel within the module is a network node and utilized statistical inference methods to infer the links between each node pair from their correlation matrix. We applied this network analysis to language tb-fMRI scans acquired from 9 healthy right-handed individuals.

Our results show that a robust fully-connected functional language network exists across 8 out of 9 healthy individuals, which entangles the Brocas Area, Wernickes Area, Supplementary Motor Area, and Pre-Motor Area, all in the left hemisphere. Furthermore, we uncovered the functional connectivity of the anatomical sub-divisions (pars-opercularis and pars-triangularis) of the Broca's Area.

*NIH; NIH-NIBIB 1 R01 EB022720-01; U54 CA137788; U54 CA132378; P30 CA008748; NSF; NSF-IIS 1515022, ISSNAF imaging chapter award 2018 and ESOR Bracco clinical fellowship 2018.

4:54PM P67.00011: The effects of inhibitory neuron fraction on the dynamics of an avalanching neural network*  JACOB CARROLL (Presenter), ADA WARREN, UWE CLAUS TAUBER, Virginia Tech — The statistical analysis of the collective neural activity known as avalanches provides insight into the proper behavior of brains across many species. In this talk we present a neural network model based on the work of Lombardi, Herrmann, de Arcangelis et al. that captures the relevant dynamics of neural avalanches, and we show how the active neuron fraction can be used as a control mechanism to introduce exponential cut-offs in the distributions of avalanche strength and duration, transition the power spectral density of the network out of an epileptic regime, and drive the evolution of the network structure over time.

*Research was sponsored by the Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.

5:06PM P67.00012: Quantitative Characterization of Neuromorphic Neural Circuits  JASON PLATT (Presenter), JUN WANG, HENRY D. I. ABARBANE, GERT CAUWENBERGHS, University of California, San Diego — NeuroDyn is a neuromorphic very large scale integrated circuit (VLSI) capable of modelling four interconnected Hodgkin-Huxley like neurons coupled through twelve chemical synapses. The 384 digitally programmable parameter space specifies ion conductances, reversal potentials and ion channel gating variables. Errors during the manufacturing process can result in a large mismatch between a specified design parameter and the value realized in the hardware. Statistical data assimilation (SDA) is a technique that can estimate parameters in a non-linear dynamical system. By inputting a current designed to probe the full dynamical range of the chip and then measuring the four state variables of the NaKL Neuron (V, m, h, n) we can estimate the mismatch between the programmed and physical parameters. Characterization of the errors in the VLSI chip will help standardize and render useful all manufactured neuromorphic chips such that they can interchangeably be used for applications and research.

5:18PM P67.00013: Neural Correlates of Cognition in Primary Visual versus Downstream Posterior Cortices During Evidence Accumulation*  SUE ANN KOAY (Presenter), DAVID W TANK, CARLOS D BRODY, Princeton University — The ability of animals to accumulate sensory information across time is fundamental to decision-making. Using a mouse behavioral paradigm where navigational decisions are based on accumulating pulses of visual cues, I compared neural activity in primary visual (V1) to secondary visual and retrosplenial cortices. Even in V1, only a small fraction of neurons had sensory-like responses to cues. Instead, all areas were grossly similar in how neural populations contained a large variety of task-related information from sensory to cognitive, including cue timings, accumulated counts, place/time, decision and reward outcome. Across-trial influences were prevalent, possibly relevant to how animal behavior incorporates past contexts. Intriguingly, all these variables also modulated the amplitudes of sensory responses. While previous work often modeled the accumulation process as integration, the observed scaling of sensory responses by accumulated counts instead suggests a recursive process where sensory responses are gradually amplified. I show that such a multiplicative feedback-loop algorithm better explains psychophysical data than integration, particularly in how the performance transitions into following Weber-Fechner's Law only at high counts.

*NIH grants 5U01NS090541, 1U19NS104648
Wednesday, March 6, 2019 4:00 PM - 5:00 PM

Session Q80 APS: LGBTQ+ Roundtable Discussion  Westin Stone - Tag(s): Diversity, Undergraduate

4:00PM Q80.00001: LGBTQ+ Roundtable Discussion  — This roundtable discussion will focus on ways to improve the professional and educational climate within physics for those who identify as gender and sexual minorities (LGBTQQIAAP+). We will review the findings of the report, LGBT Climate in Physics: Building an Inclusive Community (https://www.aps.org/programs/lgbt/index.cfm), and brainstorm strategies to improve support for physicists across the spectrum of career stages and work environments. All are welcome to attend.

Wednesday, March 6, 2019 5:00 PM - 6:00 PM

Session Q81 APS: National Society of Black Physicists (NSBP) Meetup & Reception  Westin Quincy - Tag(s): Diversity

5:00PM Q81.00001: National Society of Black Physicists (NSBP) Meetup & Reception  — The National Society of Black Physicists (NSBP) Meetup will provide opportunities for NSBP members and those interested in the work of the societies to gather, network, and learn about NSBP initiatives. All are welcome. Students and postdoctoral researchers are especially encouraged to attend.

Wednesday, March 6, 2019 5:30 PM - 6:30 PM

Session Q34 FIAP: FIAP Business Meeting  BCEC 205A

5:30PM Q34.00001: FIAP Business Meeting  — FIAP Business Meeting

Wednesday, March 6, 2019 5:45 PM - 6:45 PM

Session Q18 DCOMP: DCOMP Business Meeting  BCEC 156B

5:45PM Q18.00001: DCOMP Business Meeting  — tbd

Wednesday, March 6, 2019 5:45 PM - 7:15 PM

Session Q21 GMED: GMED Business Meeting  BCEC 157B

5:45PM Q21.00001: GMED Business Meeting  — GMED Business Meeting

Wednesday, March 6, 2019 5:45 PM - 6:45 PM

Session Q51 APS: Scholarly Metrics in Research Assessment  BCEC 253A
5:45PM Q51.00001: Scholarly Metrics in Research Assessment — Scholarly metrics play a significant role in the way scientists and their research are assessed for funding, hiring, and promotion. The APS editors will host a special session in which three panelists with experience in university administration, bibliometrics research, computational social science, and science policy will present their perspectives on scholarly metrics and research assessment.

Topics will include:
Current metrics and tools for assessing the impact of researchers and journals
Best practices and responsible use of metrics
Potential adverse effects of evaluation on research
Latest developments on scholarly metrics and indicators

Panelists:
Johan Bollen, Professor of Informatics and Computing, Indiana University
Vincent Larivière, Associate Professor of Information Science, University of Montréal, Canada.
Rashid Zia, Dean of the College and Associate Professor of Engineering & Physics, Brown University

Moderator:
Manolis Antonoyiannakis, Associate Editor/Bibliostatistics Analyst, American Physical Society

Wednesday, March 6, 2019 5:45 PM - 6:45 PM

Session Q60 GSOFT: GSOFT Business Meeting BCEC 258A

5:45PM Q60.00001: GSOFT Business Meeting — GSOFT Business Meeting

Wednesday, March 6, 2019 6:00 PM - 7:00 PM

Session Q83 APS: National Society of Hispanic Physicists (NSHP) Meetup & Reception Westin Paine - Tag(s): Diversity

6:00PM Q83.00001: National Society of Hispanic Physicists (NSHP) Meetup & Reception — The National Society of Hispanic Physicists (NSHP) Meetup will provide opportunities for NSHP members and those interested in the work of the societies to gather, network, and learn about NSHP initiatives. All are welcome. Students and postdoctoral researchers are especially encouraged to attend.

Wednesday, March 6, 2019 7:00 PM - 8:30 PM

Session Q84 APS: Education & Diversity Reception Westin Sauciety - Tag(s): Diversity, Education

7:00PM Q84.00001: Education & Diversity Reception — Join us for an opportunity to learn about current diversity efforts spearheaded by the APS, the Committee on Minorities (COM), the Committee on the Status of Women in Physics (CSWP), and the LGBT+ physicists group. This is also a great time to network with colleagues. Light refreshments will be served.

Wednesday, March 6, 2019 7:30 PM - 8:30 PM

Session Q53 : Public Lecture: The Physics and Materials Science of Superheroes BCEC 253C - Tag(s): Invited

7:30PM Q53.00001: The Physics and Materials Science of Superheroes [Invited] JAMES KAKALIOS (Presenter), University of Minnesota — While physicists, engineers, and material scientists don't typically consult comic books when selecting research topics; innovations first introduced in superhero adventures as fiction sometimes find their way off the comic book page and into reality.

Wednesday, March 6, 2019 8:00 PM - 10:00 PM
Session Q85 APS: Imaginative Performances: Quantum Voyages and the History of Physics in 13 Songs  Westin Commonwealth A/B - Tag(s): Outreach, Undergraduate

8:00PM Q85.00001: Imaginative Performances: Quantum Voyages and the History of Physics in 13 Songs — Quantum Voyages: Two voyagers, guided by the spirit of wisdom, enter the microscopic realm of atomic landscapes and quantum conundrums to discover a magnificent and baffling world foreign to everyday human experience. The piece weaves together dramatic performance, movement, music, and guest appearances by physicists. The University of Illinois at Urbana-Champaign production team, includes Creative and Scientific Director, Smitha Vishveshwara; Performance Director, Latrelle Bright; Production Manager, Maddie Martin; and Principal Performers Kalan Benbow, Michael Highman, and Gloria Lee.

The History of Physics in 13 Songs: Highlights turning points in the history of Physics. The performance establishes theatrical interpretations by creating lyrics from the writings of some of the most prominent physicists and presents original songs based on these fragments. The University of Michigan team consists of lyricists and musician Alberto Rojo, percussionist Michael Gould, and narrator Malcolm Tulip.

Sponsored by the APS: Forums on History of Physics, Outreach and Engaging the Public, Physics and Society, and Education; Division of Condensed Matter Physics; and Committee on the Status of Women in Physics. Produced by Smitha Vishveshwara, University of Illinois, and Brian Schwartz, CUNY.

Wednesday, March 6, 2019 9:15 PM - 10:45 PM

Session Q86 APS: Rock-n-Roll Physics Sing-Along  Westin Marina Ballroom I-II - Tag(s): Outreach, Undergraduate

9:15PM Q86.00001: Rock-n-Roll Physics Sing-Along — Join us for an evening of fun physics tunes set to familiar rock, blues, and swing music. Light refreshments will be served.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R01 DCMP: Fractional Quantum Hall Effect: Novel States  BCEC 106 - Ravindra Bhatt, Princeton University

8:00AM R01.00001: Incompressible Even Denominator Fractional Quantum Hall States in the Zeroth Landau Level of Monolayer Graphene*  SUJIT NARAYANAN (Presenter), Physics, Simon Fraser University, BITAN ROY, Max Planck Institute for the Physics of Complex Systems, MALCOLM KENNED, Physics, Simon Fraser University — Incompressible fractional quantum Hall states at even denominator fractions (ν = 1/2, 1/4) have recently been observed in experiments in monolayer graphene. We use a Chern-Simons description of multicomponent fractional quantum Hall states in graphene to study these incompressible fractional quantum hall states in the zeroth Landau level and suggest variational wavefunctions that may describe them. We find that the experimentally observed even denominator fractions and standard odd fractions (such as ν = 1/3, 2/5, etc.) can be accommodated within the same flux attachment scheme and argue that they may arise from sublattice or chiral symmetry breaking orders (such as charge-density-wave and antiferromagnetism) of composite Dirac fermions. We also discuss possible experimental probes that can narrow down the candidate broken symmetry phases for the fractional quantum Hall states in the zeroth Landau level of monolayer graphene.

*This work was supported by NSERC

8:12AM R01.00002: Pfaffian paired states at filling factor 5/2  MILICA MILOVANOVIĆ (Presenter), JAKSA VUCICEVIC, Institute of Physics Belgrade, LUKA ANTONIC, Faculty of Physics, Belgrade — Within the Dirac composite fermion theory of fractional quantum Hall effect (FQHE), we investigate which Pfaffian paired state will dominate at a fixed value of a particle-hole (PH) symmetry breaking parameter - the mass of Dirac composite fermions. The Dirac mass mimics the presence of Landau level mixing in experiments. We demonstrate that the presence of mass stabilizes PH Pfaffian topological pairing contrary to our naive expectation that the PH Pfaffian will be relevant for the (zero-mass) PH symmetric case. Using only field theoretical means we show that, due to gauge field effects, there is a strong competition among Pfaffians; depending on the sign of mass, Pfaffian or anti-Pfaffian will dominate for small masses, consistent with numerical experiments at filling factor 5/2, and PH Pfaffian may be present for larger masses. L. Antonic, J. Vucicevic, and M.V. Milovanovic, Paired states at 5/2 : Particle-hole Pfaffian and particle-hole symmetry breaking, Physical Review B 98, 115107 (2018).
A Study of Reentrant Integer Quantum Hall States in High Landau Levels*
DOHYUNG RO (Presenter), NIANPEI DENG, MICHAEL MANFRA, Purdue University, LOREN PFEIFFER, KENNETH WEST, Princeton University, GABOR CSATHY, Purdue University — Reentrant integer quantum Hall states are widely thought to be realizations of the so-called electronic bubble phases, some of the most intricate electron solids forming in the two-dimensional electron gas. According to the predictions of the Hartree-Fock theory, different types of bubble phases may exist, as distinguished by the number of electrons per bubble. So far, in the third and higher Landau levels four reentrant integer quantum Hall states were seen. Here we report the observation of eight reentrant integer quantum Hall states developing in the fourth Landau level. Properties of these reentrant states will be discussed. Our observation highlights the development of correlated phases of increasing complexity in improved samples and support the bubble interpretation of the reentrant integer quantum Hall states.

*This work was supported by the NSF grant DMR 1505866. Sample growth effort of M.J.M. was supported by the DOE contract no. DE-SC0006671, while that of L.N.P. and K.W.W. by the Gordon and Betty Moore Foundation Grant GBMF 4420 and the National Science Foundation MRSEC Grant DMR-1420541.

Geometry of flux attachment in anisotropic fractional quantum Hall states*
RAVINDRA BHATT (Presenter), Electrical Engineering, Princeton University, MATTEO IPPOLITI, FREDERICK D HALDANE, Physics, Princeton University — We study the internal metric of fractional quantum Hall (FQH) states, a degree of freedom which allows them to variationally optimize their energy in the presence of competing geometries. In particular, we focus on incompressible FQH states in the presence of isotropic Coulomb interaction and anisotropic band mass [1]. We use an infinite-cylinder density matrix renormalization group method [2] to numerically simulate these states and access their internal metric through the long-wavelength limit of their static guiding center structure factor. We find the response to band mass anisotropy is approximately the same for all states belonging to the first Jain sequence (ν = 1/3, 2/5, ...). The ν = 1/5 state, on the other hand, exhibits markedly smaller anisotropy. The observed behavior is well captured by a two-body model of flux attachment.


*This research was supported by Department of Energy BES Grant DE-SC0002140.

Working principles of the short-period superlattice structure in GaAs quantum wells*
EDWIN CHUNG (Presenter), K. W. BALDWIN, KENNETH WEST, MANSOUR SHAYEGAN, LOREN PFEIFFER, Princeton University — We present the design rules of GaAs quantum wells that utilize the short-period superlattice (SPSL) structure to achieve a two dimensional electron system (2DES). By changing growth conditions such as doping density, barrier composition, and well width within the SPSL, we show that the density of the 2DES can be tuned from 2.0 x 10^11 cm^-2 to 4.5 x 10^11 cm^-2 even with a fixed spacer thickness. This implies we can prepare samples that have quite different 2DES density but rather similar scattering conditions. The magnetotransport is analyzed in detail and the influence of the change in 2DES density is discussed, with an emphasis on the strength of the fraction quantum Hall states.

*Work supported by the NSF (Grants DMR 1709076, ECCS 1508925, and MRSEC DMR 1420541), the DOE Basic Energy Sciences (Grant DE-FG02-00-ER45841), and the Gordon and Betty Moore Foundation (Grant GBMF4420).

A recursion approach to thin cylinder approximants for fractional quantum Hall states
MATHEUS SCHLOSSER (Presenter), SUMANTA BANDYOPADHYAY, ALEXANDER SEIDEL, Washington University, St. Louis — Aside from the beautiful many-body wave functions that have defined the field, recursive and/or second-quantized presentations of fractional quantum Hall states have played an increasingly important role in the past. Examples include the recent discovery of the MPS structure of many quantum Hall states, but also a recursion for the Laughlin state related to the “non-local order parameter” defined by Read, originally defined in a mixed first/second quantized manner. Such recursions have recently been generalized to all composite fermion states, and put into a purely second-quantized, “all guiding-center” form. Here we observe that these recursions commute with the expansion of cylinder fractional quantum hall states in a “thin-cylinder parameter”. This allows one to define not only the full quantum Hall state recursively, but also any “thin cylinder approximant”, to any order. Relations/differences with the MPS are discussed, and we speculate on broader implications for DMRG approaches to quantum Hall states, in particular the efficient evaluation of non-local order parameters.
9:12AM R01.00007: Evidence for an even-denominator fractional quantum Hall state in the ground Landau level of an anisotropic system  
MD. SHAFAYAT HOSSAIN (Presenter), MENG MA, EDWIN CHUNG, LOREN PFEIFFER, KENNETH WEST, K. W. BALDWIN, MANSOUR SHAYEGAN, Princeton University — Even-denominator fractional quantum Hall states (FQHs) are widely believed to host a novel class of matter that obey non-Abelian statistics and could be of potential use in topological quantum computing. Examples of such states include the $\nu = 5/2$ FQHS in GaAs two-dimensional (2D) electron systems. Even-denominator FQHs have also been reported in both 2D electron and 2D hole systems confined to wide GaAs quantum wells, in bilayer GaAs 2D electron systems and, more recently, in 2D electrons in ZnO and in graphene. We report here the observation of an even-denominator FQHS at filling factor $\nu = 1/2$ in a 2D electron system confined to a wide AlAs quantum well where the electrons can occupy multiple conduction-band valleys with an anisotropic effective mass. We observe phase transitions from a compressible Fermi liquid to an incompressible FQHS and then to an insulating phase as we tilt the sample in the magnetic field, thus rendering the electron charge distribution more bilayer-like.

9:24AM R01.00008: Hall viscosity of manifestly modular invariant composite fermion wave functions*  
SONGYANG PU (Presenter), JAINENDRA JAIN, Pennsylvania State University — The Hall viscosity has been proposed to be robust within a topological phase [1]. We perform a numerical calculation of the Hall viscosity of general fractional quantum Hall states by deforming the modular parameter $\tau$ on a torus. For this purpose, we follow the approach in [2] to construct composite fermion wave functions on a torus in terms of Haldane's modified sigma function [3] to achieve a manifestly modular invariant form. (Numerical calculations show that the wave functions in this new form are identical to those in Ref. [2], therefore proving modular invariance for the latter wave functions as well.) We compare our Hall viscosities with the orbital spins for various fractional quantum Hall states in a broad region of the modular parameter $\tau$.

*This work was supported by DOE under Grant no. DE-SC0005042.

9:36AM R01.00009: Kohn-Sham Theory of the Fractional Quantum Hall Effect*  
YAYUN HU (Presenter), JAINENDRA JAIN, Pennsylvania State University — The Kohn-Sham (KS) formulation of the density functional theory (DFT) fails for FQHE because the FQHE state cannot be mapped into a system of non-interacting electrons. We instead map the FQHE system into a system of non-interacting composite fermions, which experience an effective magnetic field that depends on density. We generalize the Hohenberg-Kohn theorem to systems with a density-dependent kinetic energy operator, and formulate the KS equations for the FQHE. We also show the equivalence of our formulation with the generalized Kohn-Sham scheme. Numerical results show that our method produces densities that are good approximations to those obtained from many-body wave functions for states with general occupation configurations. As two applications of our method, we (i) obtain the density profile at the edge of fractional quantum Hall states, finding edge reconstruction as the confinement potential becomes softer; and (ii) show how an external charge produces a screening cloud with a fractionally quantized charge accumulation. We speculate on the implications of our method for general strongly correlated systems.

*This work is supported in part by DOE under Grant no. DE-SC0005042 and by the China Scholarship Council.

9:48AM R01.00010: Fixed phase diffusion Monte Carlo study of finite width effect in FQHE*  
TONGZHOU ZHAO (Presenter), JAINENDRA JAIN, Department of Physics, Penn State University — In FQHE, it is customary to include finite width effects by calculating the transverse wave function at zero magnetic field in LDA, and assuming that it does not change as a high perpendicular magnetic field is applied. We instead determine the transverse density profile directly at a high magnetic field through the fixed phase diffusion Monte Carlo method, where the phase is fixed by the in-plane FQHE state. While the results are in qualitative agreement with those obtained from zero-field LDA, there are interesting quantitative deviations. We will discuss the implications of our study to experiments.

*Supported by DOE under Grant no. DE-SC0005042
10:00AM R01.00011: Composite fermions with quenched disorder at the half-filled Landau level*  PRASHANT KUMAR (Presenter), KEVIN SHENGYI HUANG, Physics, Stanford University, MICHAEL C MULLIGAN, Physics & Astronomy, University of California, Riverside, SRINIVAS RAGHU, Physics, Stanford University — The gapless state at the half-filled Landau level is approximately described in terms of nearly-free composite fermions. Within the mean-field approximation, it has recently been shown that the composite fermions describe a quantum phase transition between an insulator and an integer quantum Hall state when the effects of a quenched disorder are included. Here, we further characterize this random quantum critical point using the non-linear sigma model and network model approaches to disordered fermions.

*DOE Office of Basic Energy Sciences, contract DEAC02-76SF00515

10:12AM R01.00012: Observation of new plasmons in the fractional quantum Hall effect: interplay of topological and nematic orders(*)*  LINGJIE DU, Department of Applied Physics and Applied Mathematics, Columbia University, URSULA WURSTBAUER (Presenter), Walter Schottky Institut and Physik-Department, Nanosystems Initiative Munich, Technische Universität München, SAEED FALLAHI, GEOFFREY GARDNER, Department of Physics and Astronomy, Purdue University, MICHAEL MANFRA, Department of Physics and Astronomy, School of Materials Engineering and School of Electrical and Computer Engineering, Purdue University, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, ARON PINCZUK, Department of Applied Physics and Applied Mathematics and Department of Physics, Columbia University — Collective modes of exotic quantum fluids reveal underlying physical mechanisms responsible for emerging ground states. We observe unexpected collective modes in the fractional quantum Hall (FQH) regime of the second Landau level (LL): intra-Landau-level plasmons measured by resonant inelastic light scattering. The plasmons herald nematic phases in the second LL and uncover the nature of long-range translational invariance in these phases. The fascinating dependence of plasmon features on filling factor provides new insights on interplays between topological quantum Hall order and nematic electronic liquid crystal phases. At LL filling factor \( v = \frac{7}{3} \), a sharp and strong plasmon peak that links to emerging macroscopic coherence supports the proposed model of a FQH nematic state at this filling factor. A marked intensity minimum in the plasmon spectrum at \( v = \frac{5}{2} \) strongly suggests that the paired state overwhelms competing nematic phases, unveiling the robustness of the superfluid state.

(*) Supported by award NSF-DMR-1306976

10:24AM R01.00013: Half-filled Landau level in a honeycomb lattice: Chern insulator of composite fermions  SAURABH MAITI (Presenter), TIGRAN SEDRAKYAN, Physics, University of Massachusetts, Amherst — The study of electronic correlations in half-filled Landau level presents a challenge due to the massive degeneracy in the single-particle spectrum. The most successful description of this exotic state has been in terms of field theory of composite fermions: either the Halperin-Lee-Read (HLR) version where the composite fermions are the original electrons bound to some fluxes; or the Dirac composite fermion which exploits the duality of the field strength and density. In this work we demonstrate the construction of a lattice version of the long-wavelength field theories. We show that for a honeycomb lattice, a HLR type construction of composite fermions leads to a Chern insulator which reduces to the Haldane model at half-filling. As a result, the K and K' points are gapped out which can be measured in tunneling experiments.

10:36AM R01.00014: Probing the Melting of Two-dimensional Quantum Wigner Crystal via its Screening Efficiency*  HAO DENG (Presenter), MENG MA, LOREN PFEIFFER, KENNETH WEST, K. W. BALDWIN, MANSOUR SHAYEGAN, Princeton University — One of the most fundamental and yet elusive collective phases of an interacting electron system is the quantum Wigner crystal (WC), an ordered array of electrons dominated by Coulomb repulsion energy. In low-disorder, two-dimensional (2D) electron systems, the quantum WC is known to be favored at very low temperatures (T) and small Landau level filling factors (v). Pinned by the disorder potential, the WC phase exhibits an insulating behavior. An experimental determination of a T vs v phase diagram for the melting of the WC, however, has proved to be challenging. Here we use capacitance measurements to probe the 2D WC thorough its effective screening as a function of T and v. We find that, as expected, the screening efficiency of the pinned WC is very poor at very low T and improves at higher T once the WC melts. Surprisingly, the screening efficiency shows a well-defined maximum at a T which is close to the previously-reported melting temperature of the WC. Our experimental results suggest a new method to map out the T vs v phase diagram of the magnetic-field-induced WC precisely.

*Work supported by NSF (Grants DMR 1709076, ECCS 1508925, MRSEC DMR 1420541), the DOE (Grant DE-FG02-00-ER45841), and the Gordon and Betty Moore Foundation (Grant No. GBMF4420).
Aharonov-Bohm interference of integer and fractional quantum Hall edge modes in small electronic Fabry-Perot interferometers

JAMES NAKAMURA (Presenter), SAEED FALLAHI, SHUANG LIANG, GEOFFREY GARDNER, MICHAEL MANFRA, Purdue University — Electronic Fabry-Perot interferometers may be used to probe quantum Hall edge states; however, Coulomb charging effects complicate the operation of small devices. We implement a novel GaAs/AlGaAs heterostructure design in which Coulomb charging effects are suppressed, enabling operation of small interferometers in the Aharonov-Bohm regime with high quantum coherence. We present measurements of the selective interference of inner and outer edge states in the integer quantum Hall regime. Aharonov-Bohm oscillations are observed at the fractional quantum Hall states $\nu = 2/3$ and $\nu = 1/3$.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R02 DMP: Topological Materials -- New Materials II

- Tag(s): Focus

8:00AM R02.00001: Towards Topological States in Silver Bismuthates Synthesized under High-Pressure

MOHAMED OUDAH (Presenter), University of British Columbia, MINU KIM, Max Planck Institute for Solid State Research, DOUGLAS ANDREW BONN, University of British Columbia, BERNHARD KEIMER, HIDENORI TAKAGI, Max Planck Institute for Solid State Research — The stoichiometric silver bismuthate Ag$_2$BiO$_3$ typically contains equal amounts of bismuth in the Bi$^{+3}$ and Bi$^{+5}$ states, and this charge ordering renders Ag$_2$BiO$_3$ insulating [1]. Recent theoretical predictions of metal-insulator transition and Weyl semimetal state in Ag$_2$BiO$_3$ have revived the interest in this material [2]. However, such novel properties are only expected in the absence of the charge ordering of bismuth. Here, we examine the possibility of achieving a topologically nontrivial phase and suppressing the charge ordering in Ag$_2$BiO$_3$ via chemical substitution/doping. We present a new high-pressure synthesis route for Ag$_2$BiO$_3$, which we utilize for substituting/doping at the Ag site. Also, we explore the possibility of making Ag-deficient Ag$_{2-x}$BiO$_3$ phases using high pressure synthesis. In the presentation, we will discuss the specific synthesis conditions, Rietveld refinement, and some magnetic and transport properties in detail.


*This work is funded by the Stuart Blusson Quantum Matter Institute and Max Planck-UBC-UTokyo Centre for Quantum Materials.

8:12AM R02.00002: Controlled layer growth and topological states in stanene studied by STM

XIAOHU ZHENG (Presenter), JIANFENG ZHANG, RUI-RUI DU, Peking University — It is proposed that stanene (a single layer of Sn) is a two-dimensional topological insulator with a bandgap of more than 0.3 eV [1]. Moreover, its band structure and properties may be modulated with increasing thickness (layers), ranging from topological insulator, topological Dirac semimetal to zero gap semimetal [2-3]. We have grown high quality few layer Sn on B-faced InSb (111) through MBE and measured their structural and electronic properties by 400 mK STM. The topological properties of various trivial/non-trivial phases are also investigated in-situ in magnetic field. Main results and discussions will be presented.


*The work is supported by NBRPC (No. 2014CB920901), National Key R and D Program of China (No. 2017YFA0303301) and NSFC (No.11704010)
8:24AM R02.00003: Revealing Optical Transitions and Carrier Dynamics within the Bulk Band Structure of Chiral Tellurium Nanosheets* GIRIRAJ JNAWALI (Presenter), SAMUEL M LINSER, SEYYEDESADAF POURNIA, IRAJ ABBASIAN SHOJAEI, HOWARD E JACKSON, LEIGH SMITH, Department of Physics, University of Cincinnati, RUOXING WANG, School of Industrial Engineering, Purdue University, GANG QIU, School of Electrical and Computer Engineering, Purdue University, WENZHUO WU, School of Industrial Engineering, Purdue University, PEIDE (PETER) YE, School of Electrical and Computer Engineering, Purdue University — Tellurium is a chiral crystal consisting of helical chains arranged in a hexagonal array along the c-axis. The bulk band structure due to the spin-orbit interaction exhibits Weyl nodes with opposite chirality at the H and H’ points in the Brillouin zone. Here we use polarized mid-infrared pump-probe spectroscopy on nanosheets of tellurium to map the band-edge electronic structure and interrogate carrier relaxation processes over a wide energy range (0.3 to 1.2 eV). We observe a series of transitions between all three valence bands at H-point of the Brillouin zone (H4, H5 and H6 symmetries) with the doubly degenerate conduction band with Weyl points (H6 Symmetry) with dynamic response of polarization anisotropy. The main decay of photoexcited carriers occurs within the first 50 ps, followed by a weak long-lived decay of carriers. The carrier thermalization process varies with polarization state of the probe beam at different bands. Such knowledge of electronic structure and carrier dynamics provides a foundation for understanding the topological and anisotropic nature of the material.

*UC acknowledges NSF grants ECCS-1509706, DMR-1531373, and DMR-1507844. PY acknowledges NSF/AFOSR 2DARE, ARO and SRC. WZW acknowledges Purdue University and ORAU.

8:36AM R02.00004: Effects of Cu intercalation in Single Crystals of CuxBi2Te2Se* YANAN LI (Presenter), CHRISTIAN PARSONS, NATHANIEL SMITH, PRASENJIT GUPTASARMA, Department of Physics, University of Wisconsin Milwaukee, Wisconsin — Intercalation of Cu in Topological Insulators such as Bi2Se3 and Bi2Te3 is known to yield superconductivity. The fundamental origin of superconductivity in these systems, whose parent compounds have non-trivial topology, remains under intense scrutiny. Bi2Te2Se is believed to be a topological insulator with structure similar to Bi2Se3 and Bi2Te3, but with much higher bulk resistivity. Here, we report structure-property relationships of Cu-intercalation in single crystals of CuxBi2Te2Se (0<x<0.5) using X-ray Diffraction, Raman Spectroscopy and X-ray Photoemission Spectroscopy. For x<0.2, Cu intercalates in Bi2Te2Se as Cu1+. Increasing x results an increase in c-axis length along with a softening of A1g2 and Eg2 Raman modes. We observe a double-mode behavior in both A1g2 and Eg2 modes corresponding to the outer atoms of Bi and Te(1)/Se(1). Thus, Bi-Te(1) and Bi-Se(1) vibrations are decoupled from each other. For higher x, we observe a triple mode behavior in both A1g2 and Eg2 modes. We ascribe this to additional Cu atoms partially substituting at Bi sites and creating additional modes such as Cu-Se(1) and Cu-Te(1).

*AFOSR-MURI

8:48AM R02.00005: Collective magnon excitations observed in a dilute ferromagnetic topological insulator* ROBERT MCQUEENEY (Presenter), Ames Laboratory, DANIEL PAJEROWSKI, Oak Ridge National Laboratory, DEBORAH SCHLAGEL, DAVID VAKNIN, Ames Laboratory — Inelastic neutron scattering measurements are presented on ferromagnetic Mn-doped Bi2Te3 with a concentration of 0.1 Mn per formula unit. Susceptibility and neutron diffraction measurements find a Curie temperature (T_C) of 12 K and ordered moments oriented perpendicular to the quintuple-layer structure. Sharp magnetic diffraction peaks suggest long-ranged and homogeneous ferromagnetism. Despite the dilute nature of the magnetic constituents, collective ferromagnetic magnon excitations are observed below T_C with a bandwidth of ~3 meV, although the dispersive features are broadened by site disorder. The magnons are two-dimensional in character, indicating that the strongest magnetic interactions occur within the quintuple-layer with weaker interlayer interactions. In addition, sharp, low-energy (< 1 meV) localized excitations are observed which are consistent with free Mn pairs or small clusters separated from the main percolated ferromagnetic Mn network.

*Work at the Ames Laboratory was supported by the U. S. Department of Energy (DDOE), BES, Division of Materials Sciences and Engineering, under Contract No. DEAC02-07CH11358. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.
Topological Insulator Superlattices via Spinodal Decomposition*  
DEMET USANMAZ (Presenter), PINKU NATH, CORMAC TOHER, JOSE JAVIER PLATA, RICO FRIEDRICH, Center for Materials Genomics, Duke University, MARCO FORNARI, Department of Physics and Science of Advanced Materials Program, Central Michigan University, MARCO BUONGIORNO NARDELLI, Department of Physics and Department of Chemistry, University of North Texas, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics and Chemistry, Duke University — Advanced thermodynamic and electronic structure concepts are combined to define a design strategy for topological insulator superlattices – an alternative to the costly and time-consuming experimental artificial growth methods [1]. Stabilizing self-assembled interfaces between iso-structural and iso-valent topological insulators is possible through spinodal decomposition. To investigate the composition range guaranteeing the topologically protected gapless metallic states, various thermodynamically driven boundaries are designed between constituent materials. The dimensions and topological nature of the metallic channels are tracked by following the spatial distribution of the charge density and spin-texture. The results validate the proof of concept for obtaining spontaneously forming two-dimensional topologically protected metallic states embedded in a three-dimensional insulating environment without any vacuum interfaces.


*The authors acknowledge support by DOD-ONR (N00014-13-1-0635, N00014-15-1-2863, N00014-16-1-2326). R. F and S.C. acknowledges the Alexander von Humboldt Foundation for financial support.

Hybrid Quantum Anomalous Hall Effect at Graphene-Oxide Interfaces*  
ZEILA ZANOLLI (Presenter), Catalan Institute of Nanoscience and Nanotechnology (ICN2) — Interfaces are ubiquitous in materials science, and devices in particular. As device dimensions are constantly shrinking, understanding the physical properties emerging at interfaces is crucial to exploit them for applications. Using first principles techniques and Monte Carlo simulations, we investigate the mutual magnetic interaction at the interface between graphene and an antiferromagnetic semiconductor, BaMnO3 [1]. We find that graphene deeply affects the magnetic state of the substrate, down to several layers below the interface, by inducing an overall magnetic softening, and switching the in-plane magnetic ordering from anti- to ferromagnetic. The graphene-BaMnO3 system presents a Rashba gap 300 times larger than in pristine graphene, leading to a new flavor of Quantum Anomalous Hall effect (QAHE), a hybrid QAHE, characterized by the coexistence of metallic and topological insulating states. These findings could be exploited to fabricate novel devices that use graphene to control the magnetic configuration of a substrate [2].


*Ramon y Cajal (RYC-2016-19344), EC H2020-EINFRA-5-2015 MaX CoE (824143), Severo Ochoa (SEV-2013-0295), CERCA (2017SGR1506), MINECO (FIS2015-64886-C5-3-P)
After our first screening step, we use Wannier-interpolation to calculate the topological invariants and to search for band crossings in our candidate materials. We discuss some individual example materials, as well as trends throughout our dataset, that is available at JARVIS-DFT website: http://jarvis.nist.gov.

We demonstrate that in addition to Z2 topological insulators, this screening method successfully identifies many semimetals and topological crystalline insulators. Our approach is applicable to the investigation of disordered or nontrivial band structures.

Recently, transition metal silicides with B20 crystal structure have been found to belong to the class of topologically nontrivial materials. The electronic structure of CoSi contains linear dispersion branches with nodal points located near the Fermi level. Therefore, CoSi is an interesting candidate to study the correlation between electronic structure and thermoelectric properties.

Micro wires of CoFeSi were prepared by FIB from samples grown by Bridgeman method. The morphology and chemical composition was analysed by TEM, EDX and XRD. Furthermore, the micro ribbons were contacted via lithography patterning. Afterwards, the temperature and magnetic field dependent transport properties were characterized. The CoFeSi reveals a monocrystalline B20 crystal structure. We analysed the electrical transport for parallel and perpendicular field. In parallel field, we observe a positive magneto resistance switching to comparable high positive magneto resistance for low temperature. In perpendicular field, we see a positive magneto resistance increasing for low temperature.

*DFG/RSF (NI 616/22-1)

**9:36AM R02.00009: Discovery and Categorization of Topological Materials** [Invited] MAIA VERGNIORY (Presenter), Donostia International Physics Center, LUIS EL Coro, Condensed Matter Physics Department, University of the Basque Country, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, NICOLAS REGNAULT, ENS Paris-CNRS, ANDREI B BERNEVIG, ZHIJUN WANG, Princeton University — Topological Quantum Chemistry (TQC) links the chemical and symmetry structure of a given material with its topological properties. This field tabulates the data of the 10398 real-space atomic limits of materials, and solves the compatibility relations of electronic bands in momentum space. A material that is not an atomic limit or whose bands do not satisfy the compatibility relations, is a topological insulator/semimetal. We use TQC to find the topological stoichiometric non-magnetic, “high-quality” materials in the world. We develop several code additions to VASP which can compute all characters of all symmetries at all high-symmetry points in the Brillouin Zone (BZ).

Using TQC, we then develop codes to check which materials in ICSD are topological. Out of 26938 stoichiometric materials in our filtered ICSD database, we find around 7300 topological materials. For the majority of the “high-quality” topological materials, we compute: the topological class (equivalence classes of TQC elementary band representations - equivalent to the topological index), the symmetry(ies) that protects the topological class, the representations at high symmetry points and the direct gap (for insulators), and the topological index. For topological semimetals we then compute whether the system becomes a topological insulator (whose index/class we compute) upon breaking symmetries - useful for experiments. Our exhaustive results show that a large proportion of all materials in nature are topological. We confirm the topology of several new materials by Wilson loop calculations. I will also explain an open-source code and end-user button on the Bilbao Crystallographic Server (http://www.cryst.ehu.es/cgi-bin/cryst/programs/topological.pl) which checks the topology of any material.

*IS2016-75862-P national project of the Spanish MINECO

**10:12AM R02.00010: High-throughput discovery of topological materials using spin-orbit spillage** KAMAL CHOUHARY (Presenter), KEVIN GARRITY, FRANCESCA TAVAZZA, MML, National institute of standards and technology, MD, USA — We present the results of a high-throughput, first principles search for topological materials based on identifying materials with band inversion induced by spin-orbit coupling. Out of the currently available 30000 materials in our database, we investigate more than 4507 non-magnetic materials having heavy atoms and low bandgaps. We compute the spillage between the spin-orbit and non-spin-orbit wave functions, resulting in more than 1699 high-spillage candidate materials. We demonstrate that in addition to Z2 topological insulators, this screening method successfully identifies many semimetals and topological crystalline insulators. Our approach is applicable to the investigation of disordered or distorted materials, because it is not based on symmetry considerations, and it can be extended to magnetic materials.

After our first screening step, we use Wannier-interpolation to calculate the topological invariants and to search for band crossings in our candidate materials. We discuss some individual example materials, as well as trends throughout our dataset, that is available at JARVIS-DFT website: http://jarvis.nist.gov.
10:24AM R02.00011: Electrides as a New Platform of Topological Materials  MOTOAKI HIRAYAMA (Presenter), Center for Emergent Matter Science, RIKEN, SATORU MATSUISHI, HIDEO HOSONO, Materials Research Center for Element Strategy, Tokyo Institute of Technology, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology — Research on the topological properties of the wave function attracts a great deal of attention [1]. In our presentation, we show that electrides are suitable for achieving various topological insulating and topological semimetal phases [2]. In electrides, some electrons reside in the interstitial regions and act as anions to stabilize the structure. Since interstitial electrons have small work function, band inversion around the Fermi level is likely to occur. We find that Sc$_2$C shows nontrivial insulating phase characterized by the π Zak phase. This π Zak phase appears as a surface polarization charge, and we propose that this surface charge is useful for carrier doping by using the electride. We find various topological electrides such as Y$_2$C, Sr$_2$Bi (nodal-line semimetal), HfBr (quantum spin Hall system), and LaBr (quantum anomalous Hall insulator). We also discuss one-dimensional electride materials as topological electrides with corner charges.


10:36AM R02.00012: Restoring $E$ vs $k$ band structure dispersion in low symmetry disordered systems*  ZHI WANG (Presenter), Renewable and Sustainable Energy Institute, Univ of Colorado - Boulder, QIHANG LIU, Southern University of Science and Technology, ALEX ZUNGER, Renewable and Sustainable Energy Institute, Univ of Colorado - Boulder — Many target properties of materials are not readily available for pure components AX or BX but do exist in alloys of (AX)$_x$(BX)$_{1-x}$. Substitutional alloy disorder generally results in the distribution of local environments as well as symmetry-breaking atomic displacements as seen in EXAFS, leading to the removal of band degeneracies and meaning of sharp wavevectors $k$ hence $E$ vs $k$ band dispersion. These effects are not treatable by single-site disorder theories such as CPA. Supercells do retain atomic resolution of disorder but do not readily produce $E$ vs $k$ dispersion needed to judge topological properties. We combine supercells with band unfolding [1] in alloys, leading to Effective Band Structure which recognizes local symmetry yet informs about the extent to which the long-range translational symmetry is retained. We show how the scale of disorders in alloy systems, such as PbS-PbTe, PbSe-SnSe, CdTe-HgTe, PM phase Mott insulators and ABO$_3$ perovskites affects the topological properties, and how the restored band dispersion helps us to understand experimental observations.


*DOE-BES-MSE grant DE-FG02-13ER46959

10:48AM R02.00013: Flat Energy Bands within Antiphase and Twin Boundaries and at Open Edges in Topological Materials*  LINGHUA ZHU (Presenter), Department of Physics, New Jersey Institute of Technology, EMIL PRODAN, Department of Physics, Yeshiva University, KEUN HYUK AHN, Department of Physics, New Jersey Institute of Technology — We present a model of two-dimensional electronic, photonic, and mechanical metamaterial systems, which has flat one-dimensional zero-mode energy bands and stable localized states of a topological origin confined with twin boundaries, antiphase boundaries, and at open edges. Topological origins of these flat bands are analyzed for an electronic system as a specific example, using a two-dimensional extension of the Su-Schrieffer-Heeger Hamiltonian with alternating shift of the chains. It is demonstrated that the slow group velocities of the localized flat band states are sensitively controlled by the distance between the boundaries and the propagation can be guided through designed paths of these boundaries. We also discuss how to realize this model in metamaterials.

*E. Prodan acknowledges support from the W. M. Keck Foundation.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R03 DCMP: Topological Phases  BCEC 107B - Haruki Watanabe
Controlling topologically protected states by external fields and doping

ALVARO DIAZ FERNANDEZ (Presenter), FRANCISCO DOMÍNGUEZ-ADAME, ELENA DÍAZ, Materials Physics, Complutense University of Madrid — Topological materials often display topologically protected surface states with Dirac-like dispersions. Controlling their properties is desirable for their foreseen applications and a number of proposals have been put forward to this respect (e.g. [1,2,3,4]). In this contribution, the system I will consider is a topological boundary. I will discuss how applying uniform electric and magnetic fields that preserve the symmetries lead to an anisotropic reduction of the Fermi velocity as the fields are increased. [5,6]. I will also show how a δ-layer of donor atoms at the boundary can lead to a coexistence of a two-dimensional electron gas with the topological surface states. Moreover, the linear optical response is markedly reshaped by the presence of the topological state [7].


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Topological phases of the rainbow chain

GERMAN SIERRA (Presenter), Instituto de Física Teórica UAM-CSIC, Madrid, Spain — Inhomogenous quantum many body systems exhibit novel phenomena such as the breaking of the area law of entanglement entropy. A notable example is the so called rainbow model which consists of a XX spin chain where the exchange coupling constants decrease exponentially from the center towards the edges. This system has been analyzed in great detail using the strong disorder renormalization group method and conformal field theory. These methods explain the appearance of long range valence bonds across the spin chain, having the shape of a rainbow. In this talk, we shall explain another feature which is the appearance of topological order in the rainbow chain with an odd number of sites. In the particular case when there is rotational symmetry one obtains the Haldane phase. This result indicates that the short range entanglement characteristic of the SPT phases can be related to the long range entanglement of the critical phases by considering the inhomogenous deformation of the latters.


Topology and localization in the Kondo lattice model

YING SU (Presenter), SHIZENG LIN, Los Alamos National Laboratory — The Kondo lattice model describing the coupling between conduction electrons and localized magnetic moments is relevant for a large family of physical systems. Here we reveal that the one-dimensional Kondo lattice model with a magnetic elliptical spiral is a topological insulator with a Chern number 2Z in the two-dimensional space with one physical dimension and one ancillary dimension spanned by the Goldstone mode of the spiral. The 2Z topological classification can be reduced to Z if certain spin rotation symmetry is broken. Moreover, when the elliptical spiral is incommensurate, the electronic states can be localized for a strong local exchange coupling. The topological protected edge states are responsible for the pumping of electron charge, and give rise to multiferroic response. The coexistence of nontrivial band topology and Anderson localization results in a unique charge pumping. Our work uncovers hitherto undiscovered nontrivial topology and Anderson localization in the Kondo lattice model. Ref: Ying Su and Shi-Zeng Lin, arXiv:1809.06295 (2018).

*This work was carried out under the auspices of the U.S. DOE Award No. DE-AC52-06NA25396 through the LDRD program, and was supported by the Center for Nonlinear Studies at LANL.
8:36AM R03.00004: Topology of Quantum Systems Out of Equilibrium* MAX McGINLEY (Presenter), NIGEL R COOPER, Physics, University of Cambridge — We investigate the topological properties of many-body quantum systems undergoing unitary time-evolution. We find that it is possible for the topology of the wavefunction to change out of equilibrium, and accordingly establish the existence of a robust nonequilibrium topological classification which generally differs from equilibrium [1]. The classification naturally inherits phenomenology familiar from equilibrium – it is robust against disorder and interactions, and exhibits a nonequilibrium bulk-boundary correspondence, which we probe using the entanglement spectrum. We explicitly construct a nonequilibrium generalisation of the `ten-fold way', which applies to non-interacting fermionic systems with non-spatial symmetries in all dimensions [2]. The differences between equilibrium and nonequilibrium topology are shown to have directly observable consequences, in both bulk and boundary physics. In particular, we show that non-equilibrium topological effects have important ramifications for various Majorana fermion-based implementations of quantum memories.


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8:48AM R03.00005: Self-assembled Bismuth Selenide (Bi$_2$Se$_3$) quantum dots grown by molecular beam epitaxy* MARCEL CLARO, Chemistry, The City College of New York, ABHINANDAN GANGOPADHYAY, Engineering, Arizona State University, DAVID SMITH, Physics, Arizona State University, MARIA TAMARGO (Presenter), Chemistry, The City College of New York — Three-dimensional topological insulators (TIs) are insulators in the bulk with surface states that have spins locked with momentum and are protected by time-reversal symmetry. Control of these states can be useful for novel applications in quantum computing and spintronics. Some properties of these materials can be enhanced by electronic confinement in quantum dots (QDs)$^{1,2}$. Bi$_2$Se$_3$ is particularly interesting since its band gap is relatively large and the experimentally verified Dirac cone is in the Γ-point. Bi$_2$Se$_3$ has been grown successfully by molecular beam epitaxy (MBE) on different substrates, and a lithographically defined QD with quantum confinement was previously demonstrated$^3$. We report the growth of self-assembled Bi$_2$Se$_3$ QDs by MBE using the droplet epitaxy technique. The QDs form after anneal of Bi droplets under a Se flux. They are crystalline and have average dimensions of 12-nm height (12 quintuple layers) and 46-nm width, and a density of 8.5x10$^9$ cm$^{-2}$. The QD formation process developed is simple, reproducible and tunable.


*The authors acknowledge NSF grants no. HRD-1547830 and DMR-1420634.

9:00AM R03.00006: Quantization of Fractional Corner Charge in C$_n$-symmetric Topological Crystalline Insulators* WLADIMIR BENALCAZAR (Presenter), Physics, The Pennsylvania State University, TIANHE LI, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — We show that C$_n$ symmetries quantize the corner charge in crystalline topological insulators. We first classify two-dimensional crystalline insulators having time-reversal and C$_n$ symmetries and construct sets of primitive generator models that span these classifications. From these generators, we are able to characterize the existence of corner fractional charge systematically and relate it to the symmetry representations of the occupied energy bands. We find that C$_n$-symmetric crystalline insulators have fractional corner charges in multiples of e/n. Our findings are compiled in a set of topological indices that quantify the amount of charge robustly localized at corners. When an additional chiral symmetry is present, e/2 corner charges are accompanied by zero-energy corner-localized states. Finally, we discuss the role of fractional charges bound to disclinations as bulk probes for these topological insulators.

*W.A.B. was partially supported by the Eberly Postdoctoral Fellowship. W.A.B. and T.L.H. thank the U.S. National Science Foundation under grant DMR-1351895 and the Sloan Foundation for support. T.L. thanks US National Science Foundation (NSF) Emerging Frontiers in Research and Innovation (EFRI) grant EFMA-1627184.
causes the topological insulating phase to become stable at either a small or zero strain (with respect to the ground state impossible. We show that instead, chemical functionalization using -CX3 groups (X = F, Cl, Br, I) induces giant chemical strains (of 9.5%, 37.4%, 48.9% and 62.8%, respectively) on the germanene lattice, relative to GeCH3. For X = F and Cl, this causes the topological insulating phase to become stable at either a small or zero strain (with respect to the ground state geometry of GeCX3), respectively. When X = Cl, the system undergoes a symmetry-lowering distortion that shifts the valence band maximum and conduction band minimum away from the zone center, while preserving the topological insulator phase. For X = Br, we obtain a trivial insulator, and for X = I, the system is unstable. Our finding that monolayer GeCCl3 is a topological insulator under ambient conditions is of interest for possible applications in future devices.

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This work was supported by U.S. DOE-BES (Grant No. DE-FG02-04ER46148). The calculations were done on the CHPC at the University of Utah and the National Energy Research Scientific Computing Center (NERSC) at the Office of Science in the U.S. Department of Energy.

This work was supported by U.S. DOE-BES (Grant No. DE-FG02-04ER46148). The calculations were done on the CHPC at the University of Utah and the National Energy Research Scientific Computing Center (NERSC) at the Office of Science in the U.S. Department of Energy.

*HW acknowledges support from JSPS KAKENHI Grant Number JP17K17678. AM acknowledges support from the Materials Education program for the future leaders in Re- search, Industry, and Technology (MERIT).
10:00AM R03.00011: Inequivalent Berry Phases for the Bulk Polarization* HARUKI WATANABE (Presenter), Applied Physics, University of Tokyo, MASAKI OSHIKAWA, Institute for Solid State Physics, University of Tokyo — We discuss the characterization of the polarization for insulators under the periodic boundary condition in terms of the Berry phase, clarifying confusing subtleties. For band insulators, the Berry phase can be formulated in terms of the Bloch function in momentum space. More generally, in the presence of interactions or disorders, one can instead use the many-body ground state as a function of the flux piercing the ring. However, the definition of the Bloch function and the way of describing the flux are not unique. As a result, the value of the Berry phase and its behavior depend on how precisely it is defined. In particular, identifying the Berry phase as a polarization, its change represents a polarization current, which also depends on the definition. We demonstrate this by elucidating mutual relations among different definitions of the Berry phase and showing that they correspond to currents measured differently in real space. Despite the nonuniqueness of the polarization current, the total charge transported during a Thouless pumping process is independent of the definition, reflecting its topological nature.


*JSPS KAKENHI Grant Numbers JP17K17678 (H. W.) and JP16K05469 (M. O.).

10:12AM R03.00012: Magic-Angle Physics in Two-Dimensional Topological Insulators YIXING FU (Presenter), JUSTIN WILSON, JED PIXLEY, Rutgers University, New Brunswick — The Bernevig-Hughes-Zhang (BHZ) model is a quintessential model for a two-dimensional Z₂ topological insulator with topological and trivial insulator phases separated from each other by semimetallic critical points. We study the fate of the BHZ model in the presence of a quasiperiodic potential by using the kernel polynomial method to calculate the density of states and conductivity to determine the zero temperature phase diagram. The semimetal undergoes magic-angle transitions driven by the quasiperiodic potential, which generates flat bands at the transition to a metallic phase similar to other two-dimensional systems with Dirac nodes. Additionally, the topological insulating phases undergo quantum phase transitions into a metallic phase due to the quasiperiodic potential closing the insulating band gap. Lastly, we also study how the surface states strongly renormalize due to these unique quasiperiodic driven transitions.

10:24AM R03.00013: Disentangling interacting symmetry protected phases of fermions in two dimensions* TYLER ELLISON (Presenter), LUKASZ FIDKOWSKI, University of Washington — We explicitly construct the ground states of certain 2+1D fermionic symmetry protected topological (SPT) phases using finite depth circuits of local unitaries. We recover the classification of the so called supercohomology SPT phases and demonstrate that the composition of our unitaries captures the corresponding SPT group structure. Our strategy is to first build an auxiliary bosonic model from group supercohomology data and then employ the recently developed lattice-level fermionization duality to obtain the fermionic SPT. This construction both yields fixed point lattice Hamiltonians that can be defined on arbitrary triangulations and disentangles the roles of supercohomology data and spin structure in fermionic SPT phases. Further, the global symmetry of our circuits implies that these SPT phases can be many-body localized.

*LF is supported by NSF DMR-1519579.

10:36AM R03.00014: Symmetry and Topology in Non-Hermitian Systems HENGYUN ZHOU (Presenter), JONG YEON LEE, SHANG LIU, Department of Physics, Harvard University, BO ZHEN, Department of Physics and Astronomy, University of Pennsylvania — The ideas of topology have found great success in Hermitian physical systems, but the incorporation of non-Hermitian effects may lead to even richer possibilities. Here, we present two results regarding the roles of symmetry and topology in non-Hermitian physical systems. First, we provide a systematic classification of non-Hermitian symmetry protected topological phases in arbitrary spatial dimension, based on the Bernard-LeClair symmetry classes. We discuss the physical insights provided by such a classification, and how it can serve as an important guide for future searches of non-Hermitian topological systems. We then discuss how symmetries can protect the existence of a surface of exceptional points, which are a natural generalization of Hermitian topological nodal phases.
Topological crystalline insulator states in the Ca$_2$As family

XIAOTING ZHOU (Presenter), National Cheng Kung University, CHUANG-HAN HSU, National University of Singapore, TAY-RONG CHANG, National Cheng Kung University, QIONG MA, PABLO JARILLO-HERRERO, NUH GEDIK, Massachusetts Institute of Technology, ARUN BANSIL, Northeastern University, VITOR PEREIRA, National University of Singapore, SUYANG XU, Massachusetts Institute of Technology, HSIN LIN, Academia Sinica, LIANG FU, Massachusetts Institute of Technology — Topological crystalline insulators (TCIs) are insulating electronic phases of matter with nontrivial topology originating from crystalline symmetries. Recent theoretical advances have proposed new TCI states protected by rotational symmetries and provided powerful guidelines to search for TCIs in real materials. Building upon recent theoretical works, we demonstrate a feasible method to identify new TCI states based on first-principles calculations. We systematically unveil the topological properties of the TCI states in Ca$_2$As. On both top and side surfaces, we observe topological surface states protected independently by rotational and mirror symmetries. We show that a particular lattice distortion can single out the newly proposed topological protection by the rotational symmetry. As a result, the Dirac points of the topological surface states are moved to generic locations in momentum space away from any high-symmetry lines. Such topological surface states have not been seen before. Our work reveals rich and exotic TCI physics across the Ca$_2$As family of materials and demonstrates a complete roadmap for uncovering TCIs topological nature based on first-principles calculations. Such a method can be broadly applied in searching for new TCIs.

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R04 DCMP: Mechanical, Structural and Thermal Behavior of Metals

BCEC 107C - Avadh Saxena, Los Alamos National Laboratory

8:00AM R04.00001: Physical and Thermal Properties of Iron Meteorites below 300 K* MATTHEW BONIDIE (Presenter), CHRISTOPHER NOYES, Physics Department, Boston College, DANIEL BRITT, Physics Department, University of Central Florida, GUY CONSOLMAGNO, ROBERT MACKE, Specula Vaticana, GEORGE SCHMIEDESHOFF, Department of Physics, Occidental College, CYRIL OPEIL, Physics Department, Boston College — The iron meteorites Canyon Diablo [IAB-MG] and Agoudal [IIAB] are primarily kamacite or taenite based Fe-Ni polycrystalline alloys that solidify from planetary cores over a timespan of t > 10$^6$ years via thermal radiation into the vacuum of space. Depending on their Ni composition and cooling rates, iron meteorites crystallize into a fine octahedrite, coarse octahedrite, or hexahedrite crystal structure.

Using resonant ultrasound spectroscopy, the elastic constants (c$_{11}$, c$_{22}$, c$_{44}$) and Young's modulus were measured as a function of temperature from 10-300 K. These measurements allow a comparison of how Ni percentage, crystallographic structure, and impact history effect the mechanical behavior of these meteorites. Specific heat capacity and thermal expansion measurements permit an analysis of the Grüneisen parameter as a function of the same temperature range.

*NASA, SSERVI (Solar System Exploration Research Virtual Institute) and CLASS (Center for Lunar and Asteroid Surface Science) under grant No. NNA14AB05A.

8:12AM R04.00002: First-principles study for the enhancement of the stability of the precipitates in the Cu alloys EUN-AE CHOI (Presenter), SEUNG ZEON HAN, JEE HYUK AHN, Korea Institute of Materials Science, SATOSHI SEMBOSHI, Institute for Materials Research, Tohoku University — Cu is widely used as an electronic circuit component because of its high conductivity. However, in order to be used as connector materials, high strength as well as the high conductivity is required to maintain the desired shape. The Cu-Ti alloy is one of precipitation hardening alloys with the tensile strength of 800-1200MPa and the conductivity of 10-20%IACS. In general, the precipitation hardening alloys can be strengthened more by additional cold working after aging. However, we confirmed that these precipitates dissolve in Cu matrix during cold working, lowering the conductivity considerably. To obtain high conductivity and high strength simultaneously, it is essential to solve this problem. In this study, we tried to find a way to increase the stability of the precipitates in order to avoid dissolution of them during cold working. Using the density functional theory(DFT) calculations, we analyzed the characteristics of the precipitates in Cu-Ti alloy. To find additional elements to enhance the stability of the precipitates, we investigated the properties of them doped with 3d transition metals. Based on DFT results, we found a proper element stabilizing the precipitate and confirmed that the dissolution was inhibited after cold working in Cu-Ti alloys experimentally.
Metallic Refractory Titanium Nitride: An alternative stable metal with tunable optical properties for high temperature plasmonic applications

MENA N GADALLA (Presenter), ANDREW GREENSPON, MICHELE TAMAGNONE, FEDERICO CAPASSO, EVELYN L HU, John A. Paulson School of Engineering and Applied Sciences, Harvard University — The increasing demands of high temperature plasmonic applications require a refractory plasmonic material that is more stable than commonly used metals such as gold (Au). Although a dielectric, under different deposition conditions titanium nitride (TiN) can be converted into a metal-like material that is stable at high temperatures and with plasmonic performance similar to that of Au. We produce TiN films with tunable optical properties ranging from those characteristic of a dielectric to strong metallic behavior with high negative real part of its frequency dependent dielectric function. Various nanostructures formed from both Au and TiN were characterized and compared, using Fourier Transform Infrared Spectroscopy and Scanning Near Field Optical Microscopy. TiN nano-antennas show tunable and distinct localized surface plasmon resonances that are comparable to those of Au. Moreover, the TiN nano-antennas exhibit a significantly more robust optical response after being annealed at high-temperatures, demonstrating the suitability of TiN to act as a stable metal for high temperature plasmonic applications.

First-Principles Molecular Dynamics Simulation of a Liquid Li-Sn as a Plasma-Facing Component

BEATRIZ GONZALEZ DEL RIO (Presenter), Mechanical and Aerospace Engineering, Princeton University, EMILY K. DE JONG, Chemical and Biological Engineering, Princeton University, EMILY ANN CARTER, School of Engineering and Applied Science, Princeton University — Liquid metals, with inherent disorder, have long been suggested as plasma-facing components (PFC) in fusion reactors due to their imperviousness to mechanical damage, thereby allowing for a self-healing and self-replenishing surface. The most promising candidates for liquid PFCs are lithium (Li) and the lithium-tin alloys (Li30Sn70 and Li20Sn80) due to their low melting points and evaporation rates. Although liquid Li properties have been studied extensively, further research into the behavior of LiSn is needed.

We present results of first-principles molecular dynamics simulations of liquid Li30Sn70 and its interaction with various concentrations of deuterium from the melting point up to 970 K. Static and dynamic properties such as pair distribution functions, diffusion coefficients, and viscosities are evaluated. Moreover, deuterium retention in the liquid Li-Sn alloy is compared to that of pure liquid Li. Overall, we provide insight into the atomic-scale behavior of Li30Sn70, which will be useful for further research into PFCs for fusion reactors.

High Strength Al Alloy Thin Films: A Nanoscale Analysis of Microstructure and Interface Segregation

PRAKASH PARAJULI (Presenter), RUBEN MENDOZA-CRUZ, MIGUEL YACAMAN, ARTURO PONCE, Physics and Astronomy, University of Texas at San Antonio — Aluminum alloy (AA) 7075 is commonly used in industries for manufacturing highly stressed structural materials including various parts of commercial aircraft, aerospace and transportation equipment because of its extremely high strength to density ratio. This yield strength relies primarily on the microstructural properties, particularly the structure (types, frequency, and connectivity), geometry (inclination and dihedral angle), and chemistry (segregation and precipitation) of the grain boundaries. Herein, experimental results on the microstructural features and atomic scale Cu grain boundary segregation of high strength Al alloy 7075 thin films are analyzed in detail using advanced microscopic characterization techniques. Two distinct types (point and parallel array) of Cu grain boundary segregation behavior are demonstrated for the Al alloy GBs for the first time; GBs misoriented by less than 28° displayed point (highly segregated atomic column surrounded by low segregated columns) segregation behavior whereas more than the 28° displayed parallel array (two highly segregated columns opposite to each other across the interface surrounded by low segregated columns) segregation behavior.

Welch Foundation-Grant No. AX-1615
9:00AM R04.00006: Modeling dislocation evolution around precipitates in superalloy  
PARINIT ANGADI, DEBIPROSAD ROY MAHAPATRA (Presenter), Indian Institute of Science —  
In this paper we discuss a new approach to correlate the dynamic mechanical properties of Nickel based superalloys to their precipitate driven mechanism of dislocation evolution. These precipitates are responsible for arresting defects or dislocations and enhancing the life of a structural component. The mechanism of dislocation evolution across grain or phase boundaries give complex patterns whose initial stages can be correlated to strain rate dependent damping parameters. We show here molecular dynamic simulation of dislocation evolution under cyclic loading of Ni3Al precipitates in Ni matrix and make an attempt to relate the growth rate parameters to the size of the precipitate and damping constants. The mechanism of deformation under cyclic normal and shear loading are investigated. This is an ongoing effort to extend our understanding to more complex and realistic situation involving temperature effects and microstructure of the superalloys.

9:12AM R04.00007: Atomistic simulation of dislocation-assisted γ-precipitate nucleation in Mg-Al alloys  
PENG YI (Presenter), MICHAEL FALK, Johns Hopkins University —  
Magnesium has drawn increasing interests as a lightweight material for applications in transportation and aerospace industries. Mechanical processing methods like equal channel angular extrusion (ECAE) have shown potential in controlling the morphology of the precipitate particles for enhanced precipitation hardening performance. Understanding how deformation affects the precipitation process is crucial for processing condition optimization, property prediction, and materials design.  
We study the dislocation-assisted precipitate nucleation of Mg17Al12 precipitates in Mg-Al alloys. We determine the critical nucleus size under different composition and stress conditions. The critical nucleus size is very sensitive to the solute concentration. The local stress introduced by dislocations can significantly change the nucleation barrier and the nucleation path. The local stress not only affects the misfit strain energy, but also significantly alters the relative stability of the phases. As a result, although γ precipitate is denser than the α matrix, counter-intuitively nucleation is favored under tension conditions rather than compression conditions. We incorporate our results into continuum model and compare with recent ECAE experiments.

9:24AM R04.00008: Stabilizing the Simple Hexagonal Structure -- Alloys of Tin*  
MICHAEL MEHL (Presenter), MATEO RONQUILLO, United States Naval Academy, COREY OSES, STEFANO CURTAROLO, CORMAC TOHER, Duke University —  
Approximately thirty elements have ground state or room-temperature structures with only one atom in the unit cell: fcc (Cu, Ir, Pb, etc.), bct (Cr, Ta, W, etc.), bct (In), rhombohedral (Hg), and even simple cubic (Po) lattices. The simple hexagonal (sh) lattice is never seen, even though it has a higher symmetry than rhombohedral and the same number of near neighbors as the bcc lattice. Only element, tin, has even a relatively low-energy sh structure.  
Experimentally, the sh structure is found in mercury-tin alloys. To understand this, we performed a series of Density Functional calculations on HgxSn1-x and CdxSn1-x structures by the virtual crystal approximation (VCA); supercell calculations with ordered placement of the Cd/Hg atom (e.g., one impurity atom per unit cell); and using high-throughput AFLow calculations to sample larger supercells with random impurities.  
Both Cd and Hg stabilize the simple hexagonal structure against α- and β-Sn. The success of the VCA suggests that this is a density of states effect, and we examine the effect of alloying on the density of states using all of our techniques.  
*MJ Mehl is funded by the Kinnear Foundation and Duke University. Duke University research is funded by the US Office of Naval Research grant N00014-17-1-2090.
glass transition and primary crystallization of melt-spun Al₈₆Ni₆Y₄.₅Co₂La₁.₅ metallic glass have been investigated at modified description of the crystal growth kinetics in the whole temperature range is obtained. In the analysis a theoretical model is employed which takes into account equation for the description of the viscosity and the Maxwellian relaxation time. This result is confirmed by measurements of primary crystallization performed also over a wide range of scanning rates. The results reveal that the kinetics of crystallization follows a non-Arrhenius behavior. In the heating rate dependence of the glass transition temperature can be described by a generalization of the Bartenev-Ritland equation utilizing the Vogel-Fulcher-Tammann theory (DFT), molecular dynamics (MD), and high-throughput nanocalorimetry to study the Cu-Zr-X high-temperature shape memory alloy system (X= Ni/Co/Hf). Nanocalorimetry shows the martensite-austenite transformation temperature and stability on thermal cycling as a function of composition. DFT and MD are used to map out the martensitic transformation pathways. We found that the martensite-austenite energy difference and transformation temperature are positively correlated, while the martensite-austenite lattice mismatch and transformation hysteresis are negatively correlated. Our results provide a map of the shape-memory properties of Cu-Zr-X, and can be extrapolated to a larger compositional space to search for novel shape memory alloys.

This work was supported by the Air Force Office of Scientific Research under Grant No. FA9550-16-1-0180. It was performed in part at the Harvard University Center for Nanoscale Systems (CNS), which is supported by the National Science Foundation under NSF ECCS award no. 1541959.

Thermonelectance NICHOLAS VU (Presenter), RONALD WARZOH, ANDREW SMITH, BRIAN DONOVAN, United States Naval Academy, DARIN SHARAR, Army Research Laboratory — Shape Memory Alloys (SMAs) have a wide range of applications due to their unique thermal-mechanical properties caused by the austenitic-martensitic phase transformation. One of the most promising applications is in elastocaloric cooling, which has the potential to become a small, environmentally friendly, and efficient alternative to vapor-compression systems. The SMA with the most promise is Nickel Titanium (NiTi) due to its stability and thermal-mechanical performance. The mechanisms that govern the thermal properties of NiTi are not well characterized and may be affected grain size, strain, and temperature. Using the frequency-domain thermoreflectance (FDTR) method, the thermal properties of NiTi SMAs with different grain sizes will be determined as a function of strain and temperature. FDTR is a pump-probe non-contact optical technique that can accurately determine the thermal properties such as heat capacity, thermal conductivity, and thermal boundary conductance of thin films and bulk materials. It is expected that measuring the thermal properties of NiTi will help to determine its viability as a candidate material for strain-induced elastocaloric cooling.

Computational Investigation of the Mechanical Properties of Alloys MICHAEL WOODCOX (Presenter), JOSHUA YOUNG, MANUEL SMEU, Physics, State University of New York at Binghamton — The nature of alloying is to combine other elements with a metal in order to make a unique material that possesses desired properties that are lacking in the separate constituents. However, with these novel materials there are new and exciting physical implications that need to be studied in order to collectively understand the alloy process; which is also crucial for their use in industrial applications. We have used DFT to calculate the mechanical properties of several bulk materials to gain a quantitative understanding of the nature of ductility. Specifically, using the VASP code, we have been able to calculate the elastic tensor of different materials, which allows for the calculation of elastic properties: including the bulk, shear, and Young's moduli, Poisson's ratio, and the Pugh ratio. We have applied this process to previously unstudied alloy materials with the goal of offering a further insight into the nature of ductility and a means to quantify it. Through Bader charge analysis, and calculation of the density of states, we have also worked to understand the significance of ductility as it relates to bonding. We anticipate that the proposed technique will help guide experimentalists in the development of ductile materials, in the interest of replacing Pb based solders.

Glass transition and primary crystallization of Al₈₆Ni₆Y₄.₅Co₂La₁.₅ metallic glass at heating rates spanning over six orders of magnitude BIN YANG (Presenter), JÜRN W. P. SCHMELZER, Institute of Physics, University of Rostock, BINGGE ZHAO, YULAI GAO, Shanghai University, CHRISTOPH SCHICK, Institute of Physics, University of Rostock — The glass transition and primary crystallization of melt-spun Al₈₆Ni₆Y₄.₅Co₂La₁.₅ metallic glass have been investigated at continuous heating covering more than six orders of magnitude of heating rates (0.083 K/s to 40,000 K/s). Differential fast scanning calorimetry (DFSC) and conventional differential scanning calorimetry (DSC) were employed, by which the glass transition kinetics was analyzed. In particular, it is shown that the heating rate dependence of the glass transition temperature can be described by a generalization of the Bartenev-Ritland equation utilizing the Vogel-Fulcher-Tammann equation for the description of the viscosity and the Maxwellian relaxation time. This result is confirmed by measurements of primary crystallization performed also over a wide range of scanning rates. The results reveal that the kinetics of crystallization follows a non-Arrhenius behavior. In the analysis a theoretical model is employed which takes into account the effect of decoupling of viscosity and diffusion, i.e., the breakdown of the Stokes-Einstein equation. In this way, a modified description of the crystal growth kinetics in the whole temperature range is obtained.
Magnetic Shape Memory Alloys

JOSE MARIA PORRO AZPIAZU (Presenter), ANABEL PEREZ CHECA, BCMaterials, PATRICIA LAZPITA, JORGE FEUCHTWANGER, Departamento de electricidad y electrónica, University of the Basque Country, VOLODYMYR CHERNENKO, Ikerbasque, the Basque Foundation for Science — Magnetic Shape Memory Alloys (MSMAs) are a group of active materials that undergo phase transitions (resulting in large recoverable mechanical deformations) induced by temperature, stress and/or magnetic fields. Their superfast response and high energy density makes them ideal candidates to be implemented in the field of sensors and actuators. The magnetic properties of MSMAs depend on the magnetic coupling between atoms that, in turn, depends on the atomic positions within the lattice. We have performed powder neutron diffraction experiments in order to elucidate the crystal structure of the martensite phases of Ni\textsubscript{51}Mn\textsubscript{28-x}Ga\textsubscript{21}Y\textsubscript{x} MSMAs, where the doping element is Y=Co,Fe and x=0,1,3,5. The analysis of the diffractograms obtained in the experiment shows that the x=0 alloy has a mixture of modulated orthorhombic and tetragonal phases; the Co-rich samples tend to stabilize the tetragonal phase towards a non-modulated one; and the Fe-rich samples tend to stabilize the orthorhombic phase. We have determined the atomic site occupancies in both the martensite and austenite phases of all the alloys studied, and explored their relation with the changes on the magnetic properties of the alloys.

*JMPA acknowledges funding from the H2020 program under the MSCA-IF-EF-ST fellowship no.753025.

Spherical Nanomechanical Characterization of Novel Nanocrystalline Cu Cold Spray Manufactured Materials

BRYER SOUSA (Presenter), KRISTIN LUISE SUNDBERG, CHRISTOPHER J. MASSAR, Worcester Polytechnic Institute, VICTOR K. CHAMPAGNE, JR., US Army Research Lab, DANIELLE L. COTE, Worcester Polytechnic Institute — The novel mechanical, microstructural, and functional properties associated with nanocrystalline metal materials has brought about interdisciplinary interest and curiosity. Nanostructured metals can be manufactured by way of multiple methods; however, during the course of this research the method studied herein is employs severe plastic deformation processing via cold spray powder deposition. TEM and SEM analysis confirmed the noteworthy grain refinement brought about by cold spray for two copper feed stocks. More specifically, the two types of copper powders were that of conventional gas atomized Cu as well as nanostructured Cu powders produced by way of spray drying and agglomeration. As such, the classical nanoindentation properties of hardness and Elastic modulus are experimentally determined using both static and dynamic nanomechanical testing. Dynamic spherical nanoindentation methodologies are employed to unveil the cold spray consolidated coating's stress-strain response and flow behavior. The mechanical flow curves extracted herein suggest that the protocol refinements proposed by Leitner, Maier-Kiener, and Kiener may have fundamentally advanced spherical nanoindentation testing at large.

*US Army Research Laboratory grant W911NF-15-2-0024
Topological superconductivity revealed by scanning tunneling spectroscopy

DONGLAI FENG (Presenter), QIN LIU, RAN TAO, CHEN CHEN, YAJUN YAN, TONG ZHANG, Fudan University, QIANG-HUA WANG, Physics, Nanjing University, ZHIPING YIN, Beijing Normal University, XIAOLI DONG, Institute of Physics, CAS, YOICHI ANDO, University of Cologne, ZHONGXIAN ZHAO, Institute of Physics, CAS — CuₓBi₂Se₃ hosts both topological surface states and bulk superconductivity. It has been identified recently as a topological superconductor (TSC) with an extraordinary nematic, i.e. C₂-symmetric, superconducting state and odd-parity pairing. Using scanning tunneling microscopy (STM), we directly examine the response of the superconductivity of CuₓBi₂Se₃ to magnetic field. Under out-of-plane fields, we discover elongated magnetic vortices hosting a zero-bias conductance peak (ZBCP) consistent with the Majorana zero mode (MZM) expected in a TSC. Under in-plane fields (B//), the average superconducting gap exhibits two-fold symmetry with field orientation, the long C₂ symmetry axes are pinned to the dihedral mirror planes under B//=0.5 T but slightly rotate under B//=1.0 T. Moreover, a nodeless Δ₄ₓ gap structure is semi-quantitatively determined for the first time. Our data paint a microscopic picture of the nematic superconductivity in CuₓBi₂Se₃ and pose strong constraints on theory. [1]

The MZMs in CuₓBi₂Se₃ are neither clean nor robust, most likely due to contamination from impurity states or other closely-packed Caroli-de Gennes-Matricon (CdGM) states, which hampers further manipulations of Majorana fermions. We show that a ZBCP well separated from the other discrete CdGM states exists ubiquitously in all cores of free vortices in the defect free regions of (Li₀.₈₄Fe₀.₁₆)OHFeSe, which has a superconducting transition temperature of 42 K. Moreover, a Dirac-cone-type surface state is observed by angle-resolved photoemission spectroscopy, and its topological nature is confirmed by band calculations. The observed ZBCP can be naturally attributed to a MZM arising from this chiral topological surface states of a bulk superconductor. (Li₀.₈₄Fe₀.₁₆)OHFeSe thus provides an ideal platform for studying MZMs and topological quantum computing. [2]

References

Superconductivity in zerovalent copper intercalated Bi₂Se₃ crystals

MIN-NAN OU (Presenter), SHIH-HSUN YU, Institute of Physics, Academia Sinica, MITCH M. C. CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, YANG-YUAN CHEN, Institute of Physics, Academia Sinica — In order to understanding of the role of Cu atoms to the formation of superconducting quasiparticles. A series of CuₓBi₂Se₃ (x= 0~ 0.3) crystals prepared with Bridgman method followed by an electrochemical technique (EC method) at room temperature. The existence of copper confirmed by means of XRD, SEM and TEM EDS mapping as well. Where the obvious increasing on lattice c confirm the intercalating of copper atoms rather than the substitution. The further study on temperature dependent electrical resistance and magnetic susceptibility revealed a superconducting transition at about T_C = 3 ~ 3.5 K. As an illustration, optimized 10 at% of Cu, a clear superconducting transition at T_C = 3.4 K with large shielding fraction (volume susceptibility) of ~ 95% is observed. The characteristic peaks of the zerovalent chemical state of copper confirmed by x-ray photoelectron spectra (XPS) and Auger electron spectra (AES). By the electron energy loss spectroscopy (EELS), near-edge fine structure revealed the absence of Cu¹⁺ and Cu²⁺ characterization peaks, which confirmed the zerovalent of intercalated copper atom. The results of this work suggested that the formation of superconducting quasiparticles do not relate to the charge transfer of copper.
8:48AM R05.00003: Reproducible Growth of Superconducting Sr$_2$RuO$_4$ Films by Molecular-Beam Epitaxy*

NATHANIEL SCHREIBER (Presenter), HARI NAIR, JACOB P RUF, LUDI MIAO, YINGFEI LI, MORGAN GRANDON, DAVID BAEK, BERIT GOODGE, LENA FITTING KOURKOUTIS, KYLE M SHEN, DARRELL G. SCHLOM, Cornell University — The unconventional, likely chiral $p$-wave, superconductivity in Sr$_2$RuO$_4$ has been studied extensively in bulk single crystals since its discovery over 20 years ago. The superconducting state in Sr$_2$RuO$_4$ is extremely sensitive to defects and non-magnetic impurities, and therefore superconductivity has only been observed in very pure crystals with a midpoint $T_c$ of up to ~1.5 K [1]. Thin films of Sr$_2$RuO$_4$ have only recently been realized, and this advancement is important for both the study of the unconventional superconducting properties and for the implementation of Sr$_2$RuO$_4$ in any future practical applications. In this talk, we report a thermodynamic growth window, in which we can reproducibly grow superconducting Sr$_2$RuO$_4$ thin films by molecular-beam epitaxy with transition temperatures of up to 1.8 K on (110) NdGaO$_3$ substrates [2].


*N.J.S. acknowledges support from the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE-1650441.

9:00AM R05.00004: Effects of deep superconducting gap minima and disorder on thermal transport in Sr$_2$RuO$_4$*

ZHIQIANG WANG (Presenter), McMaster University, JOHN DODARO, Stanford University, CATHERINE KALLIN, McMaster University — Recent thermal conductivity measurements on Sr$_2$RuO$_4$ were interpreted as favoring a pairing gap function with vertical line nodes while conflicting with chiral $p$-wave pairing. Motivated by this work we study the effects of deep superconducting gap minima on impurity induced quasiparticle thermal transport in chiral $p$-wave models of Sr$_2$RuO$_4$. Combining a self-consistent T-matrix analysis and self-consistent Bogoliubov-de-Gennes calculations, we show that the dependence of the residual thermal conductivity on the normal state impurity scattering rate can be quite similar to the $d$-wave pairing state that was shown to fit the thermal conductivity measurements, provided the normal state impurity scattering rate is large compared with the deep gap minima. Consequently, thermal conductivity measurements on Sr$_2$RuO$_4$ can be reconciled with a chiral $p$-wave pairing state with deep gap minima. However, the data impose serious constraints on such models and these constraints are examined in the context of several different chiral $p$-wave models.

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9:12AM R05.00005: Superconducting Symmetries of Sr$_2$RuO$_4$ from Spin- and Charge-fluctuations*

OLIVIER GINGRAS (Presenter), RQMP, Université de Montréal, REZA NOURAFKAN, ANDRE-MARIE TREMBLAY, Institut quantique and RQMP, Université de Sherbrooke, MICHEL COTE, RQMP, Université de Montréal — Although the normal state of Sr$_2$RuO$_4$ is well understood, its pairing symmetry is still debated [1]. From its correlated multi-orbital normal state, we construct the spin- and charge-fluctuation pairing interactions. These interactions depend on the proximity to an instability and on the size of the screened Hund’s coupling. We present the leading gap function symmetries obtained by solving the frequency dependent linearized Eliashberg equation [2]. Close to magnetic instabilities, we find spin-singlet $d$-wave pairing. Away, where charge-fluctuations increase, we observe the emergence of two even-parity spin-triplet states: an odd in frequency $s$-wave and two degenerate momentum-independent states that pair electrons on different orbitals and are odd in orbital indices. We will explain by what means spin- and charge-fluctuations mediated pairing favors such symmetries, how to understand them from specific features of the correlated electronic structure and compare their gap value with experiments.


*NSERC grants RGPIN-2014-04584, RGPIN-2016-06666, FRQNT, CIFAR, Calcul Québec, Calcul Canada, CFREF, Research Chair in the Theory of Quantum Materials.
9:24AM R05.00006: STM study of impurity states in topological superconducting candidates Li(Fe,Co)As and PbTaSe$_2$*

SONGTIAN SONIA ZHANG (Presenter), JIAXIN YIN, Department of Physics, Princeton University, GENFU CHEN, Institute of Physics, Chinese Academy of Sciences, GUOQING CHANG, Department of Physics, Princeton University, TAY-RONG CHANG, Department of Physics, National Cheng Kung University, KUN JIANG, Department of Physics, Boston College, CHANGQING JIN, Institute of Physics, Chinese Academy of Sciences, ZIQIANG WANG, Department of Physics, Boston College — Introducing impurities, both magnetic and nonmagnetic, into superconducting systems via surface or bulk chemical substitution can both provide a wealth of information about the underlying system, as well as manipulate some of its crucial properties. Here, we use low temperature scanning tunnelling microscopy to study vortex core and impurity states in topological superconductor candidates Li(Fe,Co)As and PbTaSe$_2$ at 0.4K. We perform a systematic study in the Li(Fe,Co)As system of eight Co concentrations, spanning its entire superconducting phase diagram. Using a superconducting tip, we explore the impurity effects on the topological surface states as well as bulk superconductivity in PbTaSe$_2$. Our results not only provides strong constraints on their superconducting order parameters, but also sheds light on the interplay of magnetism and topological superconductivity.

*Work at Princeton was supported by the US DOE under Basic Energy Sciences programme (grant number DOE/BES DE-FG-02-05ER46200) and the Gordon and Betty Moore Foundation (GBMF4547/ Hasan).

9:36AM R05.00007: Rotational symmetry breaking in the upper critical field of topological superconductor candidate CaSn$_3$

YASUYUKI NAKAJIMA (Presenter), K A M HASAN SIDDIQUEE, RIFFAT MUNIR, CHARUNI DISSANAYAKE, PRIYANKA VAIDYA, CAMERON NICKLE, ENRIQUE DEL BARCO, University of Central Florida, DERRICK VANGENNEP, JAMES HAMLIN, University of Florida — Electronic nematicity is a quantum analogue to liquid crystals, breaking the rotational symmetry, but preserving the translational symmetry. The electronic nematic states emerge not only in strongly correlated systems, including quantum Hall liquids, high temperature cuprate and iron-based superconductors, and heavy fermion compounds [1], but also in weakly correlated systems, such as the superconducting states in doped-topological insulators known as nematic superconductivity [2]. Closely correlated with the topological nature, the nematic superconductivity in topological materials has attracted great interest. Here, we report systematic studies of the upper critical field of topological superconductor candidate CaSn$_3$, forming a cubic structure with point group Oh. We reveal two-fold symmetry in the anisotropy of upper critical field, breaking the underlying lattice structure. Similar to doped-topological insulator M$_x$Bi$_2$Se$_3$ (M=Sr, Cu and Nb), the rotational symmetry breaking indicates the realization of nematic superconductivity in CaSn$_3$. We will discuss the possible superconducting pairing state stabilized in this system.


9:48AM R05.00008: Band Structure Perfection and Superconductivity in Type-II Dirac Semimetal Ir$_{1-x}$Pt$_x$Te$_2$

FUCONG FEI (Presenter), FENGQI SONG, Nanjing University — Recent levels of interest in topological semimetals have stimulated a fruitful avenue of research in materials science. A new concept of type-II Dirac semimetal (DSM) with tilted Dirac dispersion has been predicted and confirmed by multiple experimental techniques in PdTe$_2$, PtTe$_2$ and PtSe$_2$. However, the Dirac points in these materials are far below the Fermi level and several trivial bands cross the Fermi level. Many exotic properties thus disappear or are concealed by trivial signals. Here we discover a new type-II DSM in Ir$_{1-x}$Pt$_x$Te$_2$ with optimized band structure. Pt dopants protect the 1T-phase crystal structure and tune the Fermi level close to the Dirac point. Type-II Dirac dispersion in Ir$_{1-x}$Pt$_x$Te$_2$ is confirmed by angle-resolved photoemission spectroscopy and first-principle calculations. Superconductivity is also observed and persists when the Fermi level aligns with the Dirac points. Ir$_{1-x}$Pt$_x$Te$_2$ is an ideal platform for further studies on the type-II DSMs, and opens up a new route for the possible topological superconductivity and Majorana physics.
10:00AM R05.00009: Topological superconductivity in full shell proximitized nanowires*  ROMAN LUTCYN (Presenter), GEORG W. WINKLER, BERNARD VAN HECK, TORSTEN KARZIG, Station Q, Microsoft Corp, KARSTEN FLENSBERG, University of Copenhagen, LEONID GLAZMAN, Yale University, CHETAN NAYAK, Station Q, Microsoft Corp — We consider a new model system supporting Majorana zero modes based on semiconductor nanowires with a full superconducting shell. We demonstrate that, in the presence of spin-orbit coupling in the semiconductor induced by a radial electric field, the winding of the superconducting order parameter leads to a topological phase supporting Majorana zero modes. The topological phase persists over a large range of chemical potentials and can be induced by a predictable and weak magnetic field piercing the cylinder. The system can be readily realized in semiconductor nanowires covered by a full superconducting shell, opening a pathway for realizing topological quantum computing proposals.

*This work was performed in part at Aspen Center for Physics, which is supported by National Science Foundation grant PHY-1607611.

10:12AM R05.00010: Topological superconductivity in full-shell nanowires: numerical results and phase diagrams ROMAN LUTCYN, GEORG W. WINKLER, BERNARD VAN HECK (Presenter), TORSTEN KARZIG, Microsoft Station Q, Microsoft Quantum, KARSTEN FLENSBERG, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, LEONID GLAZMAN, Departments of Physics and Applied Physics, Yale University, CHETAN NAYAK, Microsoft Station Q, Microsoft Quantum — We investigate numerically the Majorana topological phase appearing in semiconductor nanowires with a full superconducting shell. We consider both toy models and more realistic models where the electrostatic profile in the semiconducting core is computed self-consistently and the semiconductor and superconductor are treated on equal footing in the strong coupling regime. The topological phase diagram is computed for different core radii. This talk is a continuation of the previous talk on the same topic by R.M. Lutchyn.

10:24AM R05.00011: Josephson junctions with weak links of topological crystalline insulator nanowires*  CHRISTIE J TRIMBLE (Presenter), University of Maryland, College Park, PENGZI LIU, JUDY CHA, Yale University, JAMES R WILLIAMS, University of Maryland, College Park — Incorporating superconductivity in topological states of matter offers potential routes to novel excitations with properties essential to topological quantum computation. Topological crystalline insulators (TCIs) are topological states of matter protected by crystalline symmetry, in contrast to the more commonly used time-reversal invariant topological insulators. In this talk, we report on the fabrication of Josephson junctions using nanowires of SnTe, a TCI, as the weak link material. We show the divergence of our devices from standard Josephson junction behavior using DC techniques, highlighting intriguing novel behavior in the magnetic diffraction pattern, and discuss the origin of this behavior in terms of pi phase difference across the junction.

*NSF Award #1743913

10:36AM R05.00012: Is a quantum dot a good tool to detect the topological properties of a proximitized Rasba nanowire?  DENIS CHEVALLIER (Presenter), OLESIA DMYTRUK, DANIEL LOSS, JELENA KLINOVAJA, University of Basel — Recent experiments in developing Majorana qubits have focused on semiconductor-superconductor Rashba nanowire junctions. A quantum dot is located in the non-superconducting section of the nanowire and is used to probe its topological properties. Various phenomena can be understood with the transport measurement through the quantum dot such as the renormalization of the g-factor [1] as well as the flipping of the bulk band resulting from the topological transition [2,3]. However, the presence of such quantum dot can also mimic the zero-bias peak feature [4], questioning the presence of the topological phase and, as a consequence, temporarily blocking the road towards topological quantum computation.


10:48AM R05.00013: Andreev bound states and Fabry-Perot interference in InAsSb nanowires  FANMING QU (Presenter), JIANGBO HE, JIANGHUA YING, GUANGTONG LIU, JIE FAN, ZHONGQING JI, Institute of Physics, Chinese Academy of Sciences, DONG PAN, JIANHUA ZHAO, Institute of Semiconductors, Chinese Academy of Sciences, LI LU, Institute of Physics, Chinese Academy of Sciences — Andreev bound states (ABSs) are electronic analogues of Fabry-Perot interference. Signatures of Majorana zero modes have been demonstrated as merging of electron and hole ABSs as well as zero bias conductance peaks. We take the bottom-up route to study the ABSs and Fabry-Perot interference in InAsSb nanowires. The superconductor-InAsSb-superconductor device shows induced hard superconducting gap in the quantum dot regime. The g factor is extracted consistently from the evolution of both the excited states and the Kondo effect in magnetic field. Moreover, the device can be driven to the Fabry-Perot interference regime where ABSs are observed.
8:00AM R06.00001: Anomalous critical exponents in itinerant ferromagnets $\text{Ni}_{1-x}\text{Rh}_x$ ($x = 0.3 - 0.375$) close to a quantum phase transition*  
CHIEN-LUNG HUANG (Presenter), BIANCA SPIESS, Physics and Astronomy, Rice University, SEBASTIAN KUNTZ, KAI GRUBE, Institute fuer Festkoerperphysik, Karlsruhe Institute of Technology, ALANNAH HALLAS, KYLE BAYLIFF, Physics and Astronomy, Rice University, TIGLET BESARA, THEO SIEGRIST, National High Magnetic Field Laboratory, YIPENG CAI, JAMES BEARE, GRAEME LUKE, Department of Physics and Astronomy, McMaster University, EMILIA MOROSAN, Physics and Astronomy, Rice University — We studied the critical behavior of itinerant ferromagnets $\text{Ni}_{1-x}\text{Rh}_x$ with $x = 0.3 - 0.375$ based on the Arrott-Noakes scaling analysis. The ferromagnetic ordering temperature is continuously suppressed to zero at a critical concentration $x_c \sim 0.375$. For $x = 0.3$, mean-field like exponents $\beta \sim 0.5, \gamma \sim 1.5$, and $\delta \sim 3$ are observed. With increasing $x$, critical exponents vary smoothly and reach at $\beta \sim 0.6, \gamma \sim 0.7,$ and $\delta \sim 2.3$ for $x = 0.37$. The evolution of exponents with $x$ and the exponent values close to $x_c$ cannot be described by any known universality class for classical models. The possible explanation for the trend of exponents is that, close to $x_c$, strong quantum fluctuations enhance the role of disorder and drive the system to a new strong-coupling regime.

*We acknowledge support from the Gordon and Betty Moore Foundation EPIQS Initiative through grant GBMF4417.

8:12AM R06.00002: Search for a magnetic quantum critical point in LuFe$_2$Ge$_2$ substitution series*  
RAQUEL RIBEIRO (Presenter), Universidade Federal do ABC (Brazil), Iowa State University (USA), SERGEY BUDKO, PAUL CANFIELD, Iowa State University — As part of an extensive study of the RFe$_2$Ge$_2$ series [1] a SDW-like transition was discovered in LuFe$_2$Ge$_2$ near 9 K. Given that LuFe$_2$Ge$_2$ has the same structure as the AFe$_2$As$_2$ (A =Alkali and Alkali-Earth) Fe-based superconductors, the possibility of LuFe$_2$Ge$_2$ manifesting fragile magnetism [2], and even exotic, emergent states that could be revealed as T-SDW is suppressed toward zero, was enticing. To address this, a study of Y, Sc, Co and Ru substitutions into LuFe$_2$Ge$_2$ was made [3]. Although phase diagrams constructed down to 2-3 K failed to reveal emergent effects [3], in this talk we will present magnetization and specific heat data down to 400 mK and 100 mK respectively. Updated phase diagrams will be presented and discussed.


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8:24AM R06.00003: Hall Coefficient of Pure Chromium at Finite Temperatures and High Pressures  
STEPHEN ARMSTRONG (Presenter), Caltech, YISHU WANG, Johns Hopkins University, DANIEL SILEVITCH, Caltech, YEJUN FENG, Okinawa Institute of Science and Technology, THOMAS F ROSENBAUM, Caltech — Elemental chromium is a spin density wave antiferromagnet which may be tuned through a second order quantum phase transition by the application of pressure or by chemical doping with e.g. vanadium. For both routes, the Hall coefficient has proven to be a powerful probe of the quantum critical region. In the low temperature limit, the Hall coefficient varies rapidly through the transition due to Fermi surface reconstruction. However, critical scaling of the Hall coefficient differs between pressure and doping driven transitions, establishing disorder as a relevant parameter in defining the universality class of a quantum phase transition. For doped chromium, the measured finite temperature behavior of the Hall coefficient cannot be described by band theory, and instead has been interpreted as evidence of a pseudogap phase. Here, we examine the pressure-driven Hall coefficient in pure chromium at finite temperature in search of signatures of a pseudogap phase in the absence of disorder.
8:36AM R06.00004: Ferromagnetic quantum phase transition in compressed CePd$_2$P$_2$* TIMOTHY A ELMSLIE (Presenter), DERRICK VANGENNEP, Department of Physics, University of Florida, YOU LAI, DAVID E GRAF, RYAN BAUMBACH, National High Magnetic Field Laboratory, Florida State University, JAMES J. HAMLIN, Department of Physics, University of Florida — The correlated electron material CePd$_2$P$_2$ crystallizes in the ThCr$_2$Si$_2$ structure and orders ferromagnetically at 28 K. Recently, Y. Lai et al. [1] found evidence for a ferromagnetic quantum critical point induced by chemical compression via substitution of Ni for Pd. In this present work, we examine the T-H-p phase diagram of single crystalline CePd$_2$P$_2$ to 25 GPa using a combination of resistivity, magnetic susceptibility, and x-ray diffraction measurements. We find that the ferromagnetism is destroyed near 20 GPa. These results are compared to similar experiments on the ferromagnets CeTiGe$_3$ [2] and LaCrGe$_3$ [3].


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8:48AM R06.00005: Observation of Griffiths phase at an anti-ferromagnetic quantum critical point in Ce(Cu$_{1-x}$Co$_x$)$_2$Ge$_2$ RAJESH TRIPATHI (Presenter), Indian Institute of Technology Kanpur, DEBARCHAN DAS, CHRISTOPH GEIBEL, Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany, SUDESH KUMAR DHAR, DCMP and MS, Tata Institute of Fundamental research, Mumbai 400005, India, ZAKIR HOSSAIN, Indian Institute of Technology Kanpur — A comprehensive study has been carried out on polycrystalline samples of Ce(Cu$_{1-x}$Co$_x$)$_2$Ge$_2$ by means of electrical resistivity, magnetic susceptibility, specific heat and thermo electric power measurements. The long-range antiferromagnetic order, at $T_N = 4.1$ K in CeCu$_2$Ge$_2$, is suppressed by non-iso-electronic cobalt (Co) doping at a critical value of the concentration $x_c = 0.6$, accompanied by non-Fermi-liquid behavior. A power-law dependence of heat capacity and susceptibility i.e. $C(T)/T$ and $\chi(T)$ $\sim T^{-1+\lambda}$ down to 0.4 K are observed around $x_c = 0.6$ which is compatible with the quantum Griffiths phase scenario and attributed to an antiferromagnetic quantum critical point. Our results on Ce(Cu$_{1-x}$Co$_x$)$_2$Ge$_2$ manifest a complex magnetic phase diagram, where we have observed a continuous decrease of $T_N$ with large negative slope down to $T_N = 0.83$ K at $x = 0.1$, and then a comparatively small negative slope takes over. We conclude that the rapid decrease of $T_N$ upon Co-doping is mainly due to carrier concentration change and associated change of $T_K$ and $T_{RKKY}$. We have not seen any superconducting phase in the quantum critical regime down to 0.4 K

Pressure-induced quantum critical behavior and magnetic order in YbNi$_3$Ga$_9$ with a chiral crystal structure: AC-calorimetric measurements up to 12 GPa

KAZUNORI UMEO (Presenter), N-BARD, Hiroshima University, TAKUMI OTAKI, YUDAI ARAI, AdSM, Hiroshima University, SHIGEO OHARA, Graduate School of Engineering, Nagoya Institute of Technology, TOSHIRO TAKABATAKE, AdSM, Hiroshima University — YbNi$_3$X$_9$ (X=Al, Ga) crystallize in the trigonal ErNi$_3$Al$_9$-type structure with a chiral space group $R32$. YbNi$_3$Al$_9$ undergoes a magnetic transition at $T_M=3.4$ K. By substituting Cu for Ni, a chiral soliton lattice (CSL) is realized under magnetic fields $B_{\perp c}$. While YbNi$_3$Ga$_9$ resides in an intermediate-valence regime under ambient pressure, application of pressure $P$ is expected to drive this compound into a magnetic ordered state. Indeed, a magnetic order above $P_c=9$ GPa was inferred from the electrical resistivity and AC magnetic susceptibility measurements.

In this work, we have investigated the magnetic order in YbNi$_3$Ga$_9$ using AC-calorimetric measurements under $P$ up to 12 GPa. With applying $P$, the Sommerfeld coefficient dramatically increases and reaches to $1 J/K^2\text{mol}$ at 8.6 GPa=$P_c$. A broad maximum in $C/T$ at 1.6 K for $P=9.3$ GPa>$P_c$ shifts to higher temperatures and becomes a sharp $\lambda$-type peak at 5 K for $P\geq11$ GPa. The sets of data of $C(T, P)$ under $B//c$ and $B_{\perp c}$ at $P\geq11$ GPa revealed that another field-induced ordered phase (FIOP) appears only for $B_{\perp c}$. We discuss the origin of the FIOP in relation to the CSL for Yb(Ni$_{1-x}$Cu$_x$)$_3$Al$_9$ and A-phase for MnSi and EuPtSi.

*This work was partly supported by JSPS KAKENHI Grants No. JP16H01073 and No. JP18H04324, and JSPS Core-to-Core Program.

Tuning a quantum phase boundary with microwaves

MATTHEW LIBERSKY (Presenter), THOMAS F ROSENBAUM, DANIEL SILEVITCH, Caltech — The ferromagnet LiHoF$_4$ is a realization of the dipole-coupled transverse field Ising model with a Curie temperature of 1.53 K and a transverse-field-driven quantum phase transition (QPT) at 5 T. The strong hyperfine coupling of the Ho$^{3+}$ ion leads to an effective spin rescaling to $I+J$ below 400 mK, increasing the transverse field required to drive the QPT. This spin rescaling can be suppressed by exciting the nuclear moments into their highest spin states using a strong RF field in the microwave band as a pump. We employ a high-Q loop-gap resonator tuned to approximately 3 GHz to drive the nuclear spins and simultaneously perform dc magnetometry to probe the bulk magnetization. We tune the location of the phase transition as a function of microwave power, and explore the further possibility of studying quantum quench dynamics in a system with a thermodynamic number of spins.

Electrical transport near an Ising nematic quantum critical point

XIAOYU WANG (Presenter), James Frank Institute, University of Chicago, EREZ BERG, Weizmann Institute of Science — Electrical transport properties near an Ising-nematic quantum critical point are of both theoretical and experimental interest. The difficulty of the problem is in part due to the fact that the electronic scattering mediated by critical fluctuations are momentum-conserving, and that one needs to incorporate additional current relaxation mechanisms into the low-energy theory. In this talk, we discuss two mechanisms relevant in such systems, namely Umklapp scattering and compensated metal. We present a memory matrix calculation of the DC resistivity, which treats the quasiparticle density at each patch on the Fermi surface as a slow variable. We work in the temperature regime where electrons are coherent but the fluctuations are Landau-damped. We show that in the case of Umklapp scattering, resistivity shows a smooth crossover from $T^2$ at low temperatures to sublinear at high temperatures. For a compensated metal where current and momentum are orthogonal, resistivity shows a surprising T-linear behavior. Connections to recent numerical simulations and experiments will be discussed.

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The emergence of novel quantum phenomena is often shown in materials close to a zero temperature phase transition. Much of the effort to study these new effects, like Kondo entanglement and its breakdown in heavy-fermion metals, has been focused mainly in fermionic systems. Here, we demonstrate that a phonon (bosonic) system can exhibit a quantum phase transition with dislocations. The quantum critical point (QCP) reached by the phonons arises at a second-order transition between two-ground states corresponding to a conventional phonon state (symmetric phase) and a dynamically-induced dipole field (symmetry-broken phase), at zero temperature. The distinct ground states arise from a competition between the phonon-dislocation anharmonic interaction and the topological nature of the dislocation. Furthermore, through renormalization group analysis, this phonon system provides a very different type of quantum critically which can be used to tailor phonon transport at the single-mode level [arXiv:1809.06495].

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**VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744)
The Knut and Alice Wallenberg Foundation (2013.0096)
10:24AM R06.00013: Quantum Criticality and the Non-linear I-V Curve of Two-channel Kondo-Luttinger System*  
CHAO-YUN LIN, YUNG-YEH CHANG, Department of Electrophysics, National Chiao Tung University, COLIN RYLANDS, NATAN ANDREI, Department of Physics and Astronomy, Rutgers University, CHUNG-HOU CHUNG (Presenter), Department of Electrophysics, National Chiao Tung University — We theoretically study the quantum phase transition and non-linear I-V curve of a Kondo impurity in a Luttinger liquid wire. With decreasing Luttinger parameter K (or increasing electron interactions), it has been known since 1990s that the system undergoes a quantum phase transition from 1-channel (1CK) to 2-channel Kondo (2CK) ground states at K=1/2. However, the quantum critical properties near this transition is not known to date due to the lack of controlled theoretical tools to examine the physics near the strong coupling 2CK fixed point. Via bosonization-refermionization approach, we map the system near 1CK-2CK quantum critical point (QCP) and near the Toulouse limit onto an effective fermionic model in weak coupling regime subject to a bosonic bath. The 1CK-2CK QCP is identified via renormalization group technique. The analytical form of the non-linear differential conductance and various critical exponents near this novel QCP are obtained. Our results are relevant for the recent experiment in a dissipative quantum dot via a double-barrier potential.

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10:36AM R06.00014: Unconventional superconductivity driven by Kondo-destruction quantum criticality*  
ANG CAI (Presenter), Department of Physics and Astronomy, Rice University, JED PIXLEY, Department of Physics and Astronomy, Rutgers University, KEVIN INGERSENT, Department of Physics, University of Florida, QIMIAO SI, Department of Physics and Astronomy, Rice University — How quantum criticality affects superconductivity is a central issue in strongly correlated systems. Particularly pressing is for the beyond-Landau type quantum criticality, such as appearing in heavy fermion systems in the form of Kondo destruction [1]. This is exemplified by the heavy fermion superconductor CeRhIn5, which has an antiferromagnetic quantum critical point (QCP) accompanied by a sharp Fermi surface reconstruction, and in which d-wave superconductivity develops with a high Tc [2]. Here we address the pairing instabilities near a Kondo destruction QCP by studying the Anderson lattice model using the Cluster Extended-DMFT approach [3]. For extreme Ising anisotropic case, the pairing susceptibility is significantly enhanced near the QCP. Whereas for SU(2) symmetric case, we find superconducting order around the QCP [4]; Tc is comparably high as compared with the observation in CeRhIn5 under optimal pressure. In both cases, we find the paring tendency to be stronger for the Kondo destruction type QCP than for the spin density wave type.


*NSF Grant No. DMR-1611392 & Robert A. Welch Foundation Grant No. C-1411.

10:48AM R06.00015: Kondo destruction in multipolar order: Implications for heavy-fermion quantum criticality*  
HSIN-HUA LAI (Presenter), Rice University, EMILIAN NICA, University of British Columbia, WENJUN HU, Rice University, SHOUSHU GONG, Beihang University, SILKE PASCHEN, Vienna University of Technology, QIMIAO SI, Rice University — Motivated by the quantum-critical heavy-fermion systems [1,2] exhibiting multipolar orders, we theoretically study an effective field theory of a Kondo lattice model involving both spin and quadrupole degrees of freedom. The field theory contains a quantum non-linear sigma model of the antiferroquadrupolar (AFQ) phase in spin-1 systems, with Kondo couplings to conduction electrons. In the absence of the Kondo coupling, we demonstrate the stability of the AFQ phase using density matrix renormalization group analysis in the underlying spin model. We proceed to analyze the effect of the Kondo couplings, using a mixed fermion-boson renormalization group procedure [3]. We show that the Kondo couplings are exactly marginal, which implies a Kondo destruction in the multipolar phase. Our results provide theoretical basis for the recently advanced notion of sequential Kondo-destruction [1]. Implications of our results for the global phase diagram of the heavy fermion systems are discussed. [1] V. Martelli et al., arXiv:1709.09376. [2] J. Custers et al, Nat. Mater. 11, 189 (2012). [3] S. J. Yamamoto and Q. Si, Phys. Rev. B 81, 205106 (2010).

*NSF Grant No. DMR-1611392 & Robert A. Welch Foundation Grant No. C-1411

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R07 DCMP: Mott Insulators and the Hubbard Model  
BCEC 109B - Bruce Normand, Paul Scherrrer
Institute - Tag(s): Focus
8:00AM R07.00001: Finite-temperature charge dynamics and the melting of the Mott insulator* 

BRUCE NORMAND (Presenter), Paul Scherrer Institute, Switzerland, XING-JIE HAN, RWTH Aachen University, Aachen, Germany, CHUANG CHEN, JING CHEN, HAI-DONG XIE, RUI-ZHEN HUANG, HAI-JUN LIAO, ZI YANG MENG, TAO XIANG, Chinese Academy of Sciences (CAS), China — The Mott insulator is the quintessential strongly correlated electronic state. A full understanding of the coupled charge and spin dynamics of the Mott-insulating state is thought to be the key to a range of phenomena in ultracold atoms and condensed matter, including high-$T_c$ superconductivity. Here we extend the slave-fermion (holon-doublon) description of the two-dimensional Mott insulator to finite temperatures. We benchmark its predictions against state-of-the-art quantum Monte Carlo simulations, finding quantitative agreement. Qualitatively, the short-ranged spin fluctuations at any finite temperatures are sufficient to induce holon-doublon bound states, and renormalize the charge sector to form the Hubbard bands. The Mott gap is understood as the charge (holon-doublon) gap renormalized downwards by these spin fluctuations. With increasing temperature, the Mott gap closes while the charge gap remains finite, causing a pseudogap regime to appear naturally during the process of melting the Mott insulator.

*This work was supported by the National Natural Science Foundation of China, by the National Basic Research Program of China and by the Chinese Academy of Sciences.

8:12AM R07.00002: Local Density distribution of disordered Bose-Hubbard Model

K HETTIARACHCHILAGE (Presenter), Physics, The Collage of New Jersey, C MOORE, V. G ROUSSEAU ROUSSEAU, KA-MING TAM, MARK JARRELL, J MORENO, Physics, Louisiana State University — We study the local density of the Bose-Hubbard model in the presence of on-site disorder in the canonical ensemble. At incommensurate filling, our findings support the scenario of percolating superfluid clusters enhancing Anderson localization. Scaling analysis of the superfluid density at the incommensurate filling of $\rho=1.1$ and on-site interaction $U=80t$ predicts a superfluid-Bose glass transition at disorder strength of $\Delta_c\sim30t$. At this filling, the local density distribution becomes more skew with increasing disorder strength. In the Bose glass phase, the mode of the local density distribution approaches an integer value as expected from typical medium theory for the Anderson localization. On the other hand, the behavior at commensurate filling is rather different. Close to the tip of the Mott lobe $\rho=1$, $U=22t$ we find a Mott insulator-Bose glass transition at disorder strength of $\Delta_c\sim16t$. An analysis of the local density distribution shows Gaussian like behavior for a wide range of disorders above and below the transition.

8:24AM R07.00003: Resonant Driving induced Ferromagnetism in the Fermi Hubbard Model

NING SUN (Presenter), PENGFEI ZHANG, HUI ZHAI, Tsinghua University — In this letter we consider quantum phases and the phase diagram of a Fermi Hubbard model under periodic driving that has been realized in recent cold atom experiments, in particular, when the driving frequency is resonant with the interaction energy. Due to the resonant driving, the effective Hamiltonian contains a correlated hopping term where the density occupation strongly modifies the hopping strength. Focusing on half filling, in addition to the charge and spin density wave phases, large regions of ferromagnetic phase and phase separation are discovered in the weakly interacting regime. The mechanism of this ferromagnetism is attributed to the correlated hopping because the hopping strength within a ferromagnetic domain is normalized to a larger value than the hopping strength across the domain. Thus, the kinetic energy favors a large ferromagnetic domain and consequently drives the system into a ferromagnetic phase. We note that this is a different mechanism in contrast to the well-known Stoner mechanism for ferromagnetism where the ferromagnetism is driven by interaction energy.

8:36AM R07.00004: WITHDRAWN ABSTRACT

8:48AM R07.00005: The spectral function of Mott-insulating Hubbard ladders: From fractional excitations to coherent quasi-particles

CHUN YANG, ADRIAN FEIGUIN (Presenter), Physics, Northeastern University — We study the spectral function of two-leg Mott insulating Hubbard ladders using the time-dependent density matrix renormalization group method (tDMRG). The spectrum displays features of both spin-charge separation and coherent bound states. As the inter-leg hopping is increased, both spin and hole branches merge into a single coherent quasi-particle band and the spectrum undergoes a crossover from a regime with two incommensurate minima, to one with a single minimum. At the same time, the system shifts from a Mott insulator to a band insulator. Interestingly, while the bonding sector of the spectrum realizes quasi-particles, the anti-bonding one displays a broad low energy scattering continuum, which can be associated to the lack of quasi-particles. We identify the processes leading to quasiparticle formation by studying the time evolution of charge and spin degrees of freedom in real space after a hole is created. At short times, incoherent holons and spinons are emitted but charge and spin quickly form polarons that propagate coherently.
9:00AM R07.00006: The Hall conductivity in correlated electron systems  GEORG ROHRINGER (Presenter), ANTON MARKOV, ALEXEY RUBTSOV, Correlated Quantum Systems, Russian Quantum Center — The Hall conductivity describes the response current perpendicular to the direction of an applied electric field which occurs in many-electron systems exposed to a transverse magnetic field. It has been found that in lattice systems this quantity is typically quantized[1] and corresponds to a topological invariant[2], i.e., the so-called first Chern number. Such an exact correspondence holds for non-interacting systems at zero temperature and the effect of correlations on the quantized Hall conductivity is still unclear. We have calculated the Hall conductivity in the Hubbard model in a magnetic field by means of dynamical mean field theory (DMFT). Within this approach all purely local correlation effects are included by means of a local self-energy. We find that upon increasing the interaction strength between the particles the size of the quantized plateaus of the Hall conductivity is reduced and eventually vanishes. This reduction of the Hall conductivity can be explained by a correlation driven shift of spectral weight to the –otherwise gaped– Fermi level which destroys the exact correspondence to the topological invariant and, hence, the integer quantum Hall effect.


9:12AM R07.00007: Scaling theory for Mott-Hubbard transitions  ANIRBAN MUKHERJEE (Presenter), SIDDHARTHA LAL, Department of Physical Sciences, Indian Institute of Science Education and Research, Kolkata — We present a zero temperature nonperturbative analytical renormalization group (RG) investigation of the electronic Hubbard model in two dimensions on a square lattice. The source of quantum fluctuations in the occupation number of an electronic state is driven by elements of the Hubbard Hamiltonian that are off-diagonal in the Fock representation. Our RG resolves these quantum fluctuations via an iterative scheme involving the unitarily decoupling of an electronic state at every RG step. Stable fixed points of the RG identify effective Hamiltonians associated with various phases as a function of the fluctuation energy scale and doping. We find that the half-filled Mott transition involves passage from a gapless non-Fermi liquid to a gapped Mott liquid through a pseudogapped phase upon lowering the fluctuation scale. Upon doping, we show the collapse of the Mott liquid at a quantum critical point possessing d-wave structure in k-space: a nodal non-Fermi liquid with large superconducting fluctuations, and pre-formed Cooper pairs lying within spin-pseudogapped parts of k-space located away from the nodes. By allowing for symmetry breaking, we find an emergent d-wave superconducting phase surrounding the quantum critical point. This work is available at arXiv:1802.06528.

9:24AM R07.00008: Rectification in Mott-insulator p-n junctions  ZEKUN ZHUANG (Presenter), Brown University, JAIME MERINO, Universidad Autónoma de Madrid, JOHN MARSTON, Brown University — AC currents are typically rectified by semiconducting p-n junctions. Here, we theoretically explore the possibility of realizing a rectifier based on a doped Mott-insulator p-n junction. First, we obtain the time dependence of a dissipationless Mott p-n junction along one-dimensional chains modeled by a Hubbard model and an extended Hubbard model. We numerically integrate the many-body Schrodinger equation in time and show that rectification only occurs when both Coulomb repulsion and inversion symmetry breaking are simultaneously present. We then show how rectification is also captured when the Hubbard interaction is treated within a time-dependent Hartree-Fock (TDHF) approximation. Finally, we analyze the effect of dissipation in the Mott p-n junction by combining the time-dependent Hartree-Fock (TDHF) approximation with the Lindblad equation. This permits investigation of the transport properties of realistic three-dimensional junctions that can be compared to experimental observations.
9:36AM R07.00009: Prediction of Mott insulation and atomic displacements in 3d ABO₃ oxide perovskites without Hubbard U* JULIEN VARIGNON (Presenter), MANUEL BIBES, Unité Mixte de Physique CNRS Thales, ALEX ZUNGER, University of Colorado, Boulder, Colorado — The existence of insulating band gaps in both spin-ordered and disordered phases of 3d ABO₃ perovskite oxides has been traditionally ascribed within the Mott picture to the formation of a two-electron state on a 3d site and an empty 3d site; the separation between these upper-Hubbard and lower-Hubbard states is the interelectronic repulsion U. The observed structural distortions such as bond disproportionation or Jahn-Teller motions appear as secondary effects. The non-spin polarized DFT approach gives zero gap, a result that was used in the literature as a basis to argue that DFT fails. We apply to all ABO₃ 3d perovskites DFT with (i) fully relaxed large supercells (ii) using XC functionals that have small delocalization errors (DFT+U and SCAN without U) and (iii) occupying single partners in degenerate levels. We find DFT even without U capture gapping trends and structural distortions in ABO₃ materials ranging from titanates to nickelates in both AFM and PM phases. Our results thus suggest that dynamical correlations are not playing a universal role in gapping of 3d ABO₃ insulators, and demonstrate that DFT is a viable platform fully able to model their ground states.

*AZ supported by the DOE-BES-MSE grant DE-FG02-13ER46959
JV and MB supported by ERC grant MINT (Contract 615759)

9:48AM R07.00010: Mott transitions in a class of solvable models WAYNE ZHENG (Presenter), YUAN-MING LU, Department of Physics, Ohio State University — We construct a class of lattice models, where an electronic superconductor can be driven into a fractionalized Mott insulator by increasing the onsite Coulomb repulsion. We obtain the exact ground states of these models and study their quantum critical phenomena using quantum Monte Carlo simulations.

10:00AM R07.00011: Nature of Mott Insulator in 2D Hubbard Model by Eliashberg Theory* JOSE RODRIGUEZ (Presenter), GEOFANI A MONTOYA, Physics and Astronomy, California State University Los Angeles — We introduce an Eliashberg theory in the particle-hole channel for the Hubbard model over the square lattice that exploits the perfect nesting shown by the Fermi surface at half filling[1]. It results in Eliashberg equations for the wavefunction renormalization 1/Z and for the gap ΔSDW in quasi-particle excitations at half filling. They are solved within the approximation that the corners of the diamond Fermi surface control the physics at half filling. We find that the wavefunction renormalization 1/Z vanishes as (t/U)² at strong on-site repulsion U compared to the hopping matrix element t. By comparison with mean field theory, the SDW gap is accordingly reduced down in size by the wavefunction renormalization to ΔSDW ~ t²/U. In other words, the SDW gap is of order the antiferromagnetic exchange coupling constant J. These results will be checked against direct numerical solutions of the former Eliashberg equations.


*Research supported in part by the AFOSR and the NSF.

10:12AM R07.00012: Local entropies across the Mott transition in an exactly solvable model* LUKE YEO (Presenter), PHILIP PHILLIPS, Physics, University of Illinois at Urbana-Champaign — Spatial entanglement is a natural probe of delocalisation across metal-insulator transitions, but little is known of its behaviour in two or three dimensions near interaction-driven Mott transitions. We address this problem for the exactly solvable Hatsugai-Kohmoto model, whose Mott transition occurs at zero temperature between classically mixed states. We find that both its single-site entropy and its classical entropy density exhibit kinks at the Mott transition, only in one and two dimensions. Although the variation in entropy density across the transition dominates in the thermodynamic limit, the single-site entropy increases even as the degree of classical mixing is decreased. This suggests that the Hatsugai-Kohmoto model maintains quantum-coherent delocalisation even in the presence of classical mixing.

*NSF DMR-1461952 for partial funding of this project.
10:24AM R07.00013: Hidden spin current in doped Mott antiferromagnets

WAYNE ZHENG, Department of Physics, Ohio State University, ZHENG ZHU, Department of Physics, Massachusetts Institute of Technology, DONNA SHENG, Department of Physics and Astronomy, California State University, Northridge, ZHENG-YU WENG (Presenter), Institute for Advanced Study, Tsinghua University — We investigate the nature of doped Mott insulators using exact diagonalization and density matrix renormalization group methods. Persistent spin currents are revealed in the ground state, which are concomitant with a nonzero total momentum or angular momentum associated with the doped hole. The latter determines a nontrivial ground state degeneracy. By further making superpositions of the degenerate ground states with zero or unidirectional spin currents, we show that different patterns of spatial charge and spin modulations will emerge. Such anomaly persists for the odd numbers of holes, but the spin current, ground state degeneracy, and charge/spin modulations completely disappear for even numbers of holes, with the two-hole ground state exhibiting a d-wave symmetry. An understanding of the spin current due to a many-body Berry-like phase and its influence on the momentum distribution of the doped holes will be discussed.

10:36AM R07.00014: Doping a 2d Mott insulator – Study of a quantum dimer model

SEBASTIAN HUBER (Presenter), Arnold Sommerfeld Center, Ludwig-Maximilians University, 80333 Munich, Germany, FABIAN GRUSDT, Department of Physics and Institute for Advanced Study, Technical University of Munich, 85748 Garching, MATTHIAS PUNK, Arnold Sommerfeld Center, Ludwig-Maximilians University, 80333 Munich, Germany — Experiments with quantum gas microscopes have started to explore the antiferromagnetic phase of the Fermi-Hubbard model and effects of doping with holes away from half filling1. We show in this talk that the system averaged local two-spin density matrix enables to distinguish magnetically ordered and interesting topologically ordered spin-liquid phases, which might occur in the Hubbard model close to half filling. Fractionalized Fermi liquids (FL*) are a promising candidate for this parameter regime. The generalized quantum dimer model introduced in Ref. [2] is an effective lattice realization of such an FL* with a Hilbert space spanned by configurations of fermionic and bosonic short-range bound states. We construct a rather unconventional dynamical cluster approximation (DCA) by making explicit use of the dimer Hilbert space and show first results of spectral data for a minimal cluster of two lattice sites.

1A. Mazurenko, C. Chiu et al., Nature 545, 7655 (2017)
2M. Punk, A. Allais and S. Sachdev, PNAS 112, 31 (2015)

* S. Huber and M. Punk were supported by the German Excellence Initiative via the Nanosystems Initiative Munich (NIM). F. Grusdt acknowledges financial support by the Gordon and Betty Moore foundation under the EPIQS program.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R08 DCMP: Non-uniform states in Superconductors

BCEC 150 - Anton Vorontsov, Montana State University, Bozeman

8:00AM R08.00001: Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) State in a Strongly Correlated d-wave Superconductor

ANUSHREE DATTA (Presenter), Indian Institute of Science Education and Research Kolkata, Mohanpur, India-741246, KUN YANG, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA, AMIT GHOSAL, Indian Institute of Science Education and Research Kolkata, Mohanpur, India-741246 — The FFLO state is an unconventional superconducting (SC) state found under the influence of the Zeeman field. This is identified by finite center-of-mass momenta in the Cooper pairs which causes the pairing amplitude to modulate in real space. On the other hand, strong repulsion smears out spatial variations in the order parameters. We investigate the effects of strong correlation on the FFLO state in a d-wave superconductor within an integrated framework of Hartree-Fock-Bogoliubov theory and Gutzwiller approximation. Zeeman field causes a superconductor to undergo from BCS to FFLO and finally to a normal state with itinerant magnetism. We find that strong interaction enhances the phase space for the FFLO phase by shifting its boundaries significantly. With strong interaction, the density of states features a significantly sharper mid-gap peak in the FFLO phase creating strongly localized Andreev bound states. We discuss the fate of the FFLO phase in a competing ordered ground state (GS) by considering a GS with d-wave SC and antiferromagnetic (AFM) orders. Upon exposing such a GS to Zeeman field, we find that the FFLO modulation survives along with the AFM order with contrasting spatial features in the presence of strong correlation.
Surface pair-density-wave state and generalisation of Fulde-Ferrell-Larkin-Ovchinnikov state to chiral and nematic superconductors

MATS BARKMAN (Presenter), Theoretical Physics, Royal Institute of Technology, ALEXANDER ZYUZIN, Aalto University, EGOR BABAEV, Theoretical Physics, Royal Institute of Technology — The paramagnetic interaction between the applied magnetic field and the spin of the electrons in a superconductor may lead to the formation of Cooper pairs with non-zero momentum. This results in inhomogeneous superconducting states, breaking translational symmetry, which characterizes the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. We find that the transition from the FFLO to normal state is not direct. As temperature or applied magnetic field is increased, superconductivity vanishes first in the bulk while the pair-density-waves (PDW) exist on the boundaries. The surface PDW state can exist for significantly larger field and temperature than the FFLO state. I will also discuss generalisation of FFLO states to systems with unconventional pairing. One of the found states is a nematic superconductor where the nematicity vector breaks rotational and translational symmetries due to spontaneous spatial modulation. Another state is a chiral superconductor with spontaneously broken time reversal and translational symmetries, resulting in spatially alternating chirality.

References:
arXiv:1811.09590
arXiv:1811.10594

*The work was supported by the Swedish Research Council Grant No. 642-2013-7837 and by Göran Gustafsson Foundation for Research in Natural Sciences and Medicine.

Broken translational symmetry at edges of unconventional superconductors

PATRIC HOLMVALL (Presenter), Chalmers University of Technology, Sweden, ANTON VORONTSOV, Montana State University, Bozeman, MIKAEL FOGELSTROM, TOMAS LOFWANDER, Chalmers University of Technology, Sweden — Flat bands of zero-energy states at edges of $d$-wave superconductors have a topological origin. However, a mechanism that can shift the band to finite energies would lower the free energy, break the initial topological protection, and thereby enable a phase transition. We present results [1] for a second-order phase transition at $T\approx0.2T_c$, where $T_c$ is the superconducting transition temperature, where time-reversal and continuous translational symmetry along the surface are spontaneously broken. The order parameter, the superfluid momentum $p_s$, forms a non-trivial planar vector field with sources and sinks, that satisfies a generalized Poincaré-Hopf theorem, relating the sum of Poincaré indices to the Euler characteristics of the system. We discuss the robustness of this phase against an external magnetic field, mesoscopic surface roughness, and system size. We also present signatures for experimental verification by calorimetry and magnetometry.


*We thank the Swedish Research Council for financial support.

Phase crystallization near surfaces of unconventional superconductors

ANTON VORONTSOV (Presenter), Physics, Montana State University, PATRIC HOLMVALL, TOMAS LOFWANDER, MIKAEL FOGELSTROM, Microtechnology and Nanoscience - MC2, Chalmers University of Technology — We demonstrate that a pairbreaking surface leads to an instability in the phase of the superconducting order parameter. Initially uniform U(1) phase acquires spatial variation, and thus breaks the time-reversal symmetry, below a transition temperature $T^*$ that is only a few times smaller than the bulk $T_c$. The phase modulation appears through a second-order phase transition from the trivial superconducting phase. The most favorable phase distortion occurs at a finite wave vector, thus spontaneously breaking continuous translational symmetry along the surface, and generating periodic superflow and current patterns localized near the surface, which have been previously seen in numerical simulations. We analytically derive the non-local Ginzburg-Landau coefficient that is responsible for this transition, and clarify conditions under which this instability occurs, the reason for the periodic modulation, and the geometry of emerging superflow and current patterns.

*We thank the Swedish Research Council for financial support.
8:48AM R08.00005: Fine structure in the thermal conductivity of unconventional superconductor CeCoIn$_5$ in rotating magnetic field*  
ROMAN MOVSHOVICH, SHIZENG LIN, Los Alamos National Laboratory, DUK YOUNG KIM (Presenter), Institute for Basic Science, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory — Thermal-conductivity measurements are a powerful method of studying superconductivity. Cooper pairs of the condensate do not carry heat, and only unpaired electrons participate in a heat transport. We have measured the thermal conductivity of unconventional superconductor CeCoIn$_5$ in a rotating magnetic field. At a sufficiently low temperature below 100 mK, multiple features, including sharp resonances, are observed in the thermal conductivity as a function of the direction of the magnetic field. This fine structure of thermal conductivity may come from the interaction between the magnetic field and normal electrons in this multiband superconductor. Our measurements represent a new way of studying the superconducting state of a material.

* Work at Los Alamos was supported by the Los Alamos Laboratory Directed Research and Development program.

9:00AM R08.00006: Time-reversal symmetry breaking in superconductors through loop pair-current order*  
SUDEEP GHOSH (Presenter), JORGE QUINTANILLA, School of Physical Sciences, University of Kent, Canterbury, UK, JAMES ANNETT, H. H. Wills Physics Laboratory, University of Bristol, Bristol, UK — We propose a superconducting instability where microscopic loop pair-currents form spontaneously within a unit cell at the critical temperature, $T_c$. Such currents break time-reversal symmetry (TRS) without needing an unconventional pairing mechanism. Using Ginzburg-Landau theory we show how they emerge in a toy model and estimate an upper bound for the resulting magnetisation, which is consistent with recent muon-spin relaxation experiments. We discuss the crystal symmetry requirements and show that they are met by the Re6X (X=Zr, Hf, Ti) family of TRS-breaking, but otherwise seemingly conventional, superconductors.

*We acknowledge support from EPSRC (EP/P007392/1, EP/P00749X/1).

9:12AM R08.00007: Study of inhomogenous superconducting gap in titanium nitride (TiN) films measured by low-temperature STM*  
WAN-TING LIAO (Presenter), Physics, Univ of Maryland-College Park, KEVIN DANIEL OSBORN, ROBERT E BUTERA, Laboratory for Physical Sciences, CHRISTOPHER J LOBB, FREDERICK C WELLSTOOD, Physics, Univ of Maryland-College Park, MICHAEL DREYER, Laboratory for Physical Sciences — Titanium nitride films with low loss and high kinetic inductance show great promise for use in superconducting qubits and resonators. Here we report STM measurements performed at 500 mK on 25 nm and 50 nm thick films of TiN that have been prepared with oxygen. After gentle Ar-ion sputter cleaning of the surface, we observe a topographically rough surface with tip-sample current-voltage (I-V) characteristics that show a superconducting gap. We use both the Dynes model and the Blonder-Tinkham-Klapwijk (BTK) model to fit the I-V data. The Dynes model fits depend upon the superconducting gap and a quasiparticle lifetime (broadening) parameters, while the BTK model depends upon the gap, the temperature and the barrier transparency. Surprisingly, the two models yield strikingly different results and we present evidence that in these samples the BTK model yields the correct physical interpretation.

*We acknowledge support from the Laboratory for Physical Sciences. Parts of this work were supported by the NSF under DMR #1409925.
Spatially modulated superconductivity in CeIrIn$_5$ microstructures

GEORGE FERGUSON (Presenter), Laboratory of Atomic and Solid State Physics, Cornell University, MAJA BACHMANN, Max Planck Institute for Chemical Physics of Solids, FLORIAN THEUSS, Laboratory of Atomic and Solid State Physics, Cornell University, TOBIAS MENG, Institute for Theoretical Physics, Technical University Dresden, CARSTEN PUTZKE, TONI HELM, KENT SHIRER, YOU-SHENG LI, KIMBERLY MODIC, MICHAEL NICKLAS, MARKUS KOENIG, Max Planck Institute for Chemical Physics of Solids, DAVID LOW, SAYAK GHOSH, Laboratory of Atomic and Solid State Physics, Cornell University, ANDREW MACKENZIE, FRANK ARNOLD, ELENA HASSINGER, Max Planck Institute for Chemical Physics of Solids, ROSS MCDONALD, LAUREL WINTER, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory, BRAD RAMSHAW, Laboratory of Atomic and Solid State Physics, Cornell University, PHILIP MOLL, Swiss Federal Institute of Technology in Lausanne, KATJA NOWACK, Laboratory of Atomic and Solid State Physics, Cornell University — We present scanning SQUID microscopy of CeIrIn$_5$ Focused Ion Beam (FIB) defined microstructures. By imaging the diamagnetic response of the microstructure, we identify micrometer scale modulation in the superconducting transition temperature. We find that the rich spatial structure of the superconducting and metallic regions in the device is determined by a strain field generated by the thermal contraction mismatch between CeIrIn$_5$ and the sapphire substrate. By imaging microstructures with different FIB defined features, we demonstrate that the strain field and the geometry of the superconducting regions can be controlled with the FIB. Given that strain can serve as a clean tuning parameter for strongly correlated matter, our experimental approach illustrates a general approach to modulating the electronic properties of these materials on micrometer length scales.

Work at Cornell University was supported primarily by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Award DE-SC0015947 (scanning SQUID imaging, implementation of mK microscope). We also acknowledge funding from the Cornell Center of Materials Research with funding from the NSF MRSEC program under Award DMR-1719875 (SQUID and microscope design).

Topological Behavior of Pair Density Waves on a Kondo-Heisenberg Ladder

RYAN LEVY (Presenter), JULIAN MAY-MANN, BRYAN CLARK, EDUARDO HECTOR FRADKIN, University of Illinois at Urbana-Champaign — The pair density wave (PDW) phase, characterized by an oscillating superconductor order parameter, was proposed as part of the rich phase diagram of certain high temperature superconductors such as LBCO. One model exhibiting this phase in 1D is the Kondo-Heisenberg model (KHM). Past work has predicted that the PDW phase is topological, hosting protected edge modes. Using the density matrix renormalization group (DMRG), we explicitly illustrate the topological properties of the PDW phase of the KHM on finite systems. In particular, we show the emergence of half spin edge states within the PDW phase.

This research is part of the Blue Waters sustained petascale computing project, which is supported by the NSF (award no. OCI-0725070 & ACI-1238993) and the State of Illinois.

Suppression of superfluid stiffness near Lifshitz-point instability to finite momentum superconductivity

JONATAN WARDH (Presenter), University of Gothenburg, BRIAN ANDERSEN, Niels Bohr Institute, MATS GRANATH, University of Gothenburg — We derive the effective Ginzburg-Landau theory for finite momentum (FFLO/PDW) superconductivity without spin population imbalance from a model with local attraction and a repulsive pair-hopping. We find that the GL free energy must include up to sixth order derivatives of the order parameter, providing a unified description of the interdependency of zero and finite momentum superconductivity. For weak pair-hopping, there is a line of Lifshitz points with a continuous change from zero to finite momentum which for larger pair-hopping is replaced by a bicritical region where pair momentum changes discontinuously. Proximity to a Lifshitz point provides a mechanism for reduced superfluid stiffness and we discuss implications of the model for the cuprate superconductors.

This work was supported by MAX4ESSFUN.
Orbitally limited pair-density wave phase of multilayer superconductors* DAVID MÖCKLI (Presenter), The Hebrew University of Jerusalem, YOUICHI YANASE, Kyoto University, MANFRED W SIGRIST, ETH Zürich — We investigate the magnetic field dependence of an ideal superconducting vortex lattice in the parity-mixed pair-density wave phase of multilayer superconductors. In multilayer systems, due to local inversion symmetry breaking, a Rashba spin-orbit coupling is induced at the outer layers. This combined with a perpendicular paramagnetic limiting magnetic field stabilizes a layer dependent pair-density wave phase in the superconducting singlet channel. The high-field pair-density wave phase is separated from the low-field BCS phase by a first-order phase transition. The motivating guiding question in this paper is: what is the minimal necessary Maki value for the appearance of the pair-density wave phase of a superconducting trilayer system? To address this problem we generalize the circular cell method for the regular flux-line lattice of a type-II superconductor to include paramagnetic depairing effects. Then, we apply the model to the trilayer system, where each of the layers are characterized by Ginzburg-Landau parameter, and a Maki value. We find that when the spin-orbit Rashba interaction compares to the superconducting condensation energy, the orbitally limited pair-density wave phase stabilizes for Maki values above 10.

Mass hierarchy in collective modes of pair-density-wave superconductors SHAOKAI JIAN (Presenter), Tsinghua University, MICHAEL M SCHERER, Institute for Theoretical Physics, University of Cologne, HONG YAO, Tsinghua University — We study collective modes near the quantum critical point of a pair-density-wave (PDW) superconductor in 2+1 dimensions. The fate of gaps of various collective modes is investigated by functional renormalization. For incommensurate PDW superconductors, we show that the gapless Leggett mode, protected by the emergent U(1) symmetry, can induce an exponentially small Higgs mass compared to the superconducting gap. Further, for commensurate PDW superconductors, we find an emergent mass hierarchy in the collective modes, i.e., the masses of Leggett boson, Higgs boson, and the superconducting gap can differ by several magnitudes in the infrared. This may shed light to a mechanism underlying the hierarchy problem in the Standard Model of particle physics.

Study of over-doped thin film LSCO with scanning squid microscopy* RUBY SHI (Presenter), CAROLINA ADAMO, JOHN ROBERT KIRTLEY, Stanford University, J. STEVEN DODGE, Physics, Simon Fraser University, KATHRYN ANN MOLER, Stanford University — The high-temperature superconductor cuprates, with their complex phase diagram, offer an intriguing playground for testing new theories. It has recently been proposed that homogeneous, intermediate-strength disorder is responsible for several previously unexplained features of the superfluid density in the overdoped cuprates [1]. To test the validity of this picture, we have characterized the spatial homogeneity of zero-frequency superfluid density using scanning-SQUID microscopy. We performed simultaneous magnetometry and susceptometry scans of various-doped LSCO epitaxially grown on LSAO by MBE. We observed higher than expected critical temperature (45K for x=0.23) and spatial inhomogeneity of superfluid density (variation by a factor of 10 across 3mm). Therefore, local variation of superfluid density in these LSCO thin film samples has to be taken into account for future experiments.

Inhomogeneous superconductivity in PdTe2* GOUTAM SHEET (Presenter), ANSHU SIROHI, SHEKHAR DAS, AMIT VASHIST, Indian Institute of Science Education and Research, Mohali, PRIYO ADHIKARY, Indian Institute of Science, Bangalore, SIRSHENDU GAYEN, RAJESWARI ROY CHOWDHURY, YOGESH SINGH, Indian Institute of Science Education and Research, Mohali, TANMOY DAS, Indian Institute of Science, Bangalore — PdTe2 is a type II Dirac semimetal which also shows superconductivity below 1.7 K. We have performed scanning tunneling microscopy and spectroscopy on single crystals of PdTe2 and have shown that despite such unique co-existence of Dirac physics and superconductivity, the superconducting phase of PdTe2 is conventional in nature. As revealed by our magnetic field dependent STM experiments, the single crystals of PdTe2 display a type I-like behavior at certain points and type-II like behavior at certain other points. We will discuss the details of this inhomogeneous superconducting phase and comment on its relationship with the intrinsic electronic inhomogeneity that was also detected in the normal state of PdTe2.

*Israel Science Foundation, Grant No. 1287/15.

*Swarnajayanti fellowship under the grant number DST/SJF/PSA-01/2015-16.
Local versus Global Superconductivity in Atomic Layer Indium on Si(111)*

MENGKE LIU (Presenter), HYOUNGDO NAM, JUNGDAE KIM, CHIH-KANG SHIH, University of Texas at Austin — Superconductivity at the two-dimensional limit has attracted intense interest, and monolayer Indium on Si(111) provides a perfect platform for investigating this fascinating phenomenon. To better understand the role of defects in superconductivity, we studied superconducting monolayer Indium films by tailoring the step density of the substrate. We probed the superconductivity microscopically using scanning tunneling microscopy and spectroscopy. The macroscopic superconducting properties of the same sample were also probed using in-situ double coil mutual inductance measurements to determine the superfluid density and the transition temperature (Tc). By establishing local and global Tc correspondence, we uncover the intriguing nature of 2D superconductivity in indium atomic layer superconductors.

*This work was supported by Office of Naval Research (ONR), N-00014-14-1-0330, National Science Foundation (NSF), DMR-1506678, and Welch Foundation, F-1672.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R09 DCMP: Superconductivity: Proximity Effect and Josephson Junctions II BCEC 151A

8:00AM R09.00001: Ground-state Phase Oscillations in Josephson Junctions Containing Iron* ALEXANDER MADDEN (Presenter), BEN BYRD, REZA LOLOEE, NORMAN OWEN BIRGE, Physics and Astronomy, Michigan State University — Ferromagnetic Josephson junctions with a controllable ground-state phase difference are now well-established as a potential system for cryogenic memory applications. Many recent demonstrations of this phase control have used nickel as a fixed layer, with the phase controlled by the relative orientation of a magnetically soft layer. While nickel is a hard ferromagnet that allows high transmission of supercurrent, its multidomain structure and stray field have been obstacles to implementation in devices. Iron is another hard ferromagnet that has been investigated in S/F/S Josephson junctions and shown to undergo 0 – π phase oscillations with thickness [1]. We present a further investigation of iron Josephson junctions and their potential for use as memory devices. SQUID magnetometer measurements show that iron grown on a copper buffer layer gives a narrower magnetic transition and thinner magnetic dead layer than if grown directly on niobium. We also present junction transport measurements showing the critical current and 0 – π phase oscillations for a range of iron thickness grown on a 2nm copper buffer.


*This research is based upon work supported by the ODNI, IARPA, via ARO contract number W911NF-14-C-0115.

8:12AM R09.00002: Appearance of above the gap resonances in dirty Josephson junctions with epitaxial contact* SHAHRZAD ZARE (Presenter), WILLIAM ANDREW MAYER, FOSTER H SABATINO, Physics, New York University, CODY YOUMANS, Physics, City College of City University of New York, KAUSHINI WICKRAMASINGHE, JOSEPH YUAN, MATTHIEU DARTAILH, Physics, New York University, AARON SOMOROFF, POUYAN GAEMI MOHAMMADI, Physics, City College of City University of New York, JAVAD SHABANI, Physics, New York University — In Josephson junctions, when the separation of the superconducting contacts is made long enough, the system can be approximated with two superconducting-normal metal junctions connected with a normal link. In devices fabricated on InAs-Al materials, we observe oscillations of conductance with driving bias above the superconducting gap. The frequency of conductance oscillations as a function of the bias is determined by the geometric properties of the junction. We interpret these geometric oscillations (GO) in interference of quasi-particles with energies above the superconductivity gap. This can be compared with a simple quantum mechanical problem involving a particle in the box where the states with energy above the box wall solely gain a phase shift as they pass over the box potential. In the case of GO the variation of the superconducting gap size affect the phase of the quasi-particles as they pass through. We compare our data with our theoretical model and find agreement in dependence of the data to bias, magnetic field and temperature.

*NSF CREST Center for Interface Design and Engineered Assembly of Low Dimensional systems (IDEALS),grant number HRD-1547830
8:24AM R09.00003: Pair tunneling in La_{2-x}Sr_xCuO_4 junctions above T_c

PANPAN ZHOU (Presenter), LIYANG CHEN, Physics and Astronomy, Rice University, YUE LIU, Physics, Beijing University, ANTHONY TRAVIS BOLLINGER, XI HE, Condensed Matter Physics & Materials Science, Brookhaven National Lab, ILYA SOCHNIKOV, Physics, University of Connecticut, IVAN BOZOVIC, Condensed Matter Physics & Materials Science, Brookhaven National Lab, DOUGLAS NATELSON, Physics and Astronomy, Rice University — High temperature superconductivity remains challenging more than thirty years after its initial discovery. One of the most captivating ongoing debates is about the mechanism and the normal state above the critical temperature. Various experiments imply paired charge carriers persisting above the transition temperature T_c, but without direct signatures of pairing. Shot noise, the intrinsic current fluctuations that result from the discreteness of current-carrying excitations, probes the magnitude of the charge of carriers. We report measurements on the shot noise of the tunneling current in c-axis epitaxial structure of La_{2-x}Sr_xCuO_4/La_2CuO_4/La_{2-x}Sr_xCuO_4 for several doping levels. At temperatures far above T_c, the shot noise agrees quantitatively with independent tunneling of carriers with charge magnitude $e$.

Approaching but still above T_c, the noise exceeds the expectations of single charge tunneling, indicating pairing of carriers. Well below T_c the noise is greatly enhanced within the bias region of the superconducting gap, consistent with multiple Andreev reflection processes.

*Supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division and by Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4410.

8:36AM R09.00004: Infrared and THz Optical Nanoscopy of High-Tc Superconductor Devices

ADRIAN GOZAR (Presenter), QIANBO LU, Applied Physics, Yale University, ANTHONY TRAVIS BOLLINGER, IVAN BOZOVIC, Condensed Matter and Materials Science, Brookhaven National Laboratory — We use cryogenic atomic force microscopy (AFM) combined with scanning near-field optical microscopy (SNOM) to study thin films and nano-constriction devices in La_{2-x}Sr_xCuO_4 high-Tc cuprate superconductors. Using light in the mid-infrared region we demonstrate that our customized AFM-SNOM setup can provide three dimensional dielectric characterization of devices fabricated by tightly focused Helium ion beams. Light demodulation up to the 4th harmonic of the AFM tapping frequency allows us to observe in the dielectric response irradiation induced amorphization effects which extend on length scales that are orders of magnitude larger than the size of the focused ion beam. We ascribe this widespread damage to a Helium depth distribution substantially modified by internal device interfaces. Low-temperature data in the THz range enables detection of superconducting fluctuations in a 13 nm thick La_{2-x}Sr_xCuO_4 film with a superconducting critical temperature T_c ~ 31.5 K. Our results show that AFM-SNOM is a powerful technique for probing and characterizing superconducting interfaces and devices with nanometer scale resolution.

*Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4410

8:48AM R09.00005: Non-vanishing Fraunhofer Pattern in WTe_2 Josephson Junction

YONG-BIN CHOI (Presenter), Department of Physics, Pohang University of Science and Technology, CHUI-ZHEN CHEN, Department of Physics, Hong Kong University of Science and Technology, JINHO PARK, Department of Physics, Pohang University of Science and Technology, GAURAV RANA, Max Plank Institute for Microstructure Physics, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology, MAZHAR ALI, Max Plank Institute for Microstructure Physics, KAM TUEN LAW, Department of Physics, Pohang University of Science and Technology, KIN CHUNG FONG, Quantum Information Processing Group, Raytheon BBN Technologies, GIL-HO LEE, Department of Physics, Pohang University of Science and Technology — WTe_2 is predicted to host Weyl nodes at the contact of electron and hole pockets in a momentum space (Type-II Weyl semimetal) and exhibit novel transport properties. We fabricated proximity Josephson junctions based on mechanically exfoliated WTe_2 layers of thickness around 10-20 nm and studied their Josephson effects under magnetic field. Josephson critical current modulation as a function of perpendicular magnetic field, I_c(\mathbf{B}), (so-called Fraunhofer pattern) exhibited non-vanishing lobes up to ~300 Gauss when Josephson current direction is parallel to a-axis of WTe_2 crystal. This indicates that Josephson current through a-axis of WTe_2 layer has enhanced contribution from the edges of the flake. However, flowing Josephson current parallel to b-axis of WTe_2 resulted in ordinary Fraunhofer pattern. We will discuss about observed anisotropic quantum transport of WTe_2 Josephson junction in regard to its topological nature.
Interestingly, we observe an enhancement in the nonmonotonic dependence of the supercurrent on external pressure in the quantum critical superconductor CeRhIn5. This is a consequence of the interplay between the induced superconducting gap and the spin-orbit coupling in those structures. The high transparency of our contacts can arise from Landau-Zener transitions in our InAs structures.


*H2020-MSA-IF No.796603–EuSuper, ONR (N00014-16-1-2657) and NSF (DMR 1700137).

9:36AM R09.00009: Shapiro steps in InAs-based Josephson junctions with epitaxial Al contacts* MATTHIEU DARTAILLH (Presenter), JOSEPH YUAN, WILLIAM ANDREW MAYER, KAUSHINI WICKRAMASINGHE, DILLON LIU, ADITI MITRA, JAVAD SHABANI, Physics, New York University — Semiconductor-based Josephson junction provide a platform to study the proximity effect and can serve as a platform for the realization of in topological superconductivity. Recently our group has demonstrated the possibility to have a highly transparent contact between the superconductor and the semiconductor by combining InAs high mobility surface 2D-dimensional electron gases with epitaxially grown aluminum. The interplay between the induced superconducting gap and the spin-orbit coupling in those structure is still an on-going field of research. While DC measurements can allow to access the current-phase relation of those structure, some details could be masked by relaxation processes. We utilize microwave radiation on Josephson junctions to unmask the periodicity of the current phase relation. We study Shapiro steps that appear in the IV characteristic of a junction under microwave irradiation. We observe a missing first Shapiro step below 6 GHz that may point to a 4π component in the current-phase relation of those junctions. Similar signatures have been observed in HgTe (in the topological regime) but given the high transparency of our contacts they may arise from Landau-Zener transitions in our InAs structures.

*We acknowledge support from the US Army Office of Research.
9:48AM R09.00010: Ultrasensitive Calorimetry in an Al/InAs Josephson Junction  RAJ KATTI (Presenter), OLLI SAIRA, MATTHEW MATHENY, MICHAEL ROUKES, Caltech — Calorimetry allows for the detection of single-shot energy pulses over a wide bandwidth. Pushing the limits of energy resolution to the yoctojoule (1e-24 J) regime would allow detection of individual thermal phonons and monitoring of dynamics in open quantum systems. We present work toward development of a Josephson junction-based calorimeter fabricated from an Al/InAs superconductor-semiconductor heterostructure, a material system being developed for scalable topological quantum computation. Ongoing work seeks to demonstrate a device proof-of-principle while simultaneously characterizing fundamental thermal properties of this material system.

10:00AM R09.00011: Unconventional Josephson effect in 2D Josephson junctions based on In0.75Ga0.25As quantum wells  KAVEH DELFANAZARI (Presenter), PENGCHENG MA, University of Cambridge, IAN FARRER, University of Sheffield, DAVID A RITCHIE, HANNAH JOYCE, MICHAEL JOSEPH KELLY, CHARLES G SMITH, University of Cambridge — Here, we report on the discovery of an unconventional Josephson effect in hybrid In0.75Ga0.25As two-dimensional electron gas-Nb junctions that are designed and fabricated for scalable hybrid quantum circuit integration [1-3]. By sweeping the in-plane magnetic field, we observe a completely new type of oscillation mechanism in the differential conductance, that has not been identified before. We find that the differential conductance as a function of source-drain voltage shows two symmetric in-gap resonances, which are strongly temperature and magnetic field dependent. The resonances amplitudes enhance with increasing in-plane magnetic fields up to a critical field where they gradually suppress and disappear. The observed supercurrent also gradually increases with applied magnetic field up to the same critical field. We believe that these striking observed behaviours in our devices-that cannot be explained by the conventional Josephson effect phenomenon-may be related to the context of topological superconductivity in hybrid 2D systems.

Reference:

10:12AM R09.00012: Effect of Material Quality on Superconducting Proximity Effect in Al-InAs Heterostructures*  KAUSHINI WICKRAMASINGHE (Presenter), Physics, University of Maryland, College Park, WILLIAM ANDREW MAYER, JOSEPH YUAN, Physics, New York University, TRI NGUYEN, Physics, City University of New York, MATHIEU DARTAILH, Physics, New York University, KASRA SARDASHTI, Department of Science and Math, Fashion Institute of Technology, VLADIMIR MANUCHARYAN, Physics, University of Maryland, College Park, JAVAD SHABANI, Physics, New York University — Renewed theoretical and experimental interest in InAs heterostructure with two-dimensional electron systems (2DESs) confined to the surface is partly due to their potential applications in topological and superconducting quantum computation. Here we study Josephson junctions with epitaxial Al-InAs contacts and find large super currents and substantial product of ICRN in our high mobility wafers. We also compare the product of excess current and normal resistance, IexeRN of high mobility samples and low mobility samples. The excess current is negligible in the devices made of lower mobility Al-InAs samples whereas it is substantial and independent of gate voltages and junction length in high mobility sample. For the devices made with high mobility samples, we found that ICRN/Δ~2.2. Further we discuss how the above parameters are linked to the material quality of the samples.

*We acknowledge the support of US Army Office of Research and DARPA.

10:24AM R09.00013: Probing pair-breaking mechanisms in proximity-induced hybrid superconducting interfaces*  KARTHIK RAMAN (Presenter), Hyderabad, Tata Institute of Fundamental Research — Understanding depairing effects in a hybrid-superconducting interface utilizing high spin-orbit materials is an important study in proximity-induced superconductivity. Experimentally, proximity-induced superconductivity is found to suppress at much lower magnetic fields compared to the superconducting layer without a good understanding of its cause. Here, we provide a phenomenological tool to characterize different pair-breaking mechanisms, the ones that break or preserve time reversal symmetry, and show how they affect the differential tunneling conductance response. Importantly, we probe the properties of the SC layer at the hybrid interface and observe conductance peak pinning at zero bias in a larger field range with eventual signs of weak peak splitting. Further, the effect of varying the spin-orbit scattering and the Lande g-factor in tuning the conductance peaks show interesting trends. 


*We would like to thank SERB, DST and DAE, India for supporting our reseach funding.
10:36AM R09.00014: Wavefunction of Andreev bound states with topological Weyl singularity in multi-terminal Josephson junction*  
TOMOHIRO YOKOYAMA (Presenter), Graduate school of Engineering Science, Osaka University, SHIRO KAWABATA, Nanoelectronics Research Institute, National Institute of Advanced Industrial Science & Technology — We theoretically investigate a four-terminal Josephson junction. 
N superconductors can define N-1 independent superconducting phase differences. The spectrum of Andreev bound states (ABSs) in the junction is $2\pi$ periodic in all the phase differences $\{\varphi\}$ and can be regarded as the ``band structure'' in the $\{\varphi\}$-space. In a previous studies, we have exhibited that the band structure can have topologically protected singular points (Weyl points) at zero energy in the spectrum. \footnote{T. Yokoyama and Yu. V. Nazarov, Phys. Rev. B (bf 92), 155437 (2015).} In this study, we investigate the wavefunction of ABSs with and without the Weyl point.

For two-terminal junction, the ABS wavefunction is delocalized to connect the two terminals and does not show any structure except an oscillation associated to the coherence length in the normal region. For multi-terminal case, the wavefunction can be localized between only several terminals. This localization is relevant to the presence and absence of Josephson current between the terminals. At the Weyl points, the spectrum has singularity. We discuss the influence of this singularity on the current and the ABS wavefunction.

*This work has been partially supported by the Hattori Hokokai Foundation and the JSPS KAKENHI 18K13484.

10:48AM R09.00015: Reduced Parameter Spread in Arrays of Planar MgB2 Josephson Junctions Made by Focused Helium Ion Beam*  
LEILA KASAEI (Presenter), Temple University, MENGJUN LI, Rutgers University, THOMAS MELBOURNE, Temple University, LEONARD C FELDMAN, TORGNY GUSTAFSSON, Rutgers University, KE CHEN, XIAOXING XI, Temple University — Series arrays of up to 100 planar Josephson junctions on MgB2 film with less than 3 % spread in critical current at 10 K were successfully developed and characterized. This technique uses a 30 keV focused helium ion beam with nominal beam diameter less than 0.5 nm and range of dose from 0.9 to $3 \times 10^{16}$ (Ions/cm²)[1] to locally damage the 25 nm-thick MgB2 thin films grown by hybrid physical-chemical deposition (HPCVD) on SiC substrates to form the junction barriers. A typical single junction has an $I_c R_n$ of 70 μV at 20 K and RSJ-like current-voltage characteristics. Under microwave radiation, flat Shapiro steps up to 150 μA width appear at voltages $V_n = Nn(\Phi_0 f$, where $N$ is the number of junction in the array, $n$ is an integer representing Shapiro step index, and $f$ is the applied microwave frequency. The greatly reduced spread in critical current is a significant improvement over the previous studies. This technique may lead to applications including Josephson voltage standards and arbitrary function generators that can work at around 20 K.


*This work was supported by the National Science Foundation under Grant No. DMR-1310087.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R10 DMP: Fe-based Superconductors -- Nematicity I  
BCEC 151B - Cheng Cen, West Virginia University -
Tag(s): Focus

2269 of 3305
8:00AM R10.00001: ARPES of iron-based superconductors: how nematic order sets the stage for magnetic and superconducting ground states in NaFeAs and FeSe [invited] TIMUR KIM (Presenter), Diamond Light Source, MATTWATSON, School of Physics and Astronomy, University of St. Andrews, LUKE RHODES, Department of Physics, Royal Holloway University of London —

Angle-resolved photoemission spectroscopy (ARPES) gives a unique insight into the evolution of the electronic structure of iron-based superconductors. By varying the temperature and doping of the sample, one can investigate all regions of their phase diagrams, including the high-temperature normal state, the magnetic ground state, the so-called nematic state where four-fold symmetry is broken without magnetic order, and the superconducting state. For example, ARPES measurements of FeSe give an exclusive opportunity to investigate the electronic structure in nematic phase without magnetic order. In our measurements, we found substantial shifts of both the electron and hole bands associated with the onset of the nematic order, however the interpretation of these data has caused some controversy due to the formation of twin orthorhombic domains in samples. Our high-resolution ARPES results obtained on FeSe crystals detwinned by application of mechanical strain, reveal remarkable anisotropies hidden in the measurements of twinned samples. We observe that in the nematic phase the Fermi surface consists of one elliptical hole-like pocket and only one orthogonally oriented electron-like pocket. Moreover, we find the same effect in detwinned NaFeAs samples where the spectral weight from only one elliptical electron pocket is detected in the nematic phase.

Finally, we use synchrotron-based high-resolution ARPES to map the 3D momentum dependence of the superconducting gap in FeSe. We find that on both the hole and electron Fermi surfaces, the gap is highly anisotropic, with its magnitude following the distribution of \( d_{yz} \) orbital weight on each pocket. We show that this anisotropic gap structure can be naturally reproduced from theoretical calculations only when the one-electron pocket state, observed in the nematic phase, is taken into account. These results support the spin fluctuation mediated mechanism of superconductivity in FeSe.

8:36AM R10.00002: Characterizing the nematic phase in Ba122 iron arsenides with a SQCRAMscope FAN YANG (Presenter), STEPHEN TAYLOR, JOHANNA PALMSTROM, STEPHEN D EDKINS, IAN R FISHER, BENJAMIN LEV, Stanford University — Microscopic imaging of local magnetic fields provides a window into the organizing principles of complex and technologically relevant condensed matter materials. However, a wide variety of strongly correlated and topologically nontrivial materials exhibit poorly understood phenomena outside the detection capability of state-of-the-art high-sensitivity, high-resolution scanning probe magnetometers. We have recently introduced the Scanning Quantum Cryogenic Atom Microscope (SQCRAMscope), a quantum-noise-limited scanning probe magnetometer that can operate from room-to-cryogenic temperatures. By employing a magnetically levitated atomic Bose-Einstein condensate (BEC) that can be scanned near the surface of a cryogenically cooled material, the microscope achieves unprecedented DC-field sensitivity at micron-scale resolution. Combining this unique probe with optical polarimetry, we present recent work on characterizing the nematic phase transition in unstrained Ba122 iron-based superconductors. Domain structure is visualized through spatial mapping of the current density, from which resistivity anisotropy is extracted as a proxy for the nematic order parameter. The temperature dependence of nematicity is studied and compared to optical polarimetry results from the same sample.

8:48AM R10.00003: Observation of orbital ordering and origin of nematic order in FeSe* GUOQING WU (Presenter), RONGXING CAO, XIANGHUA ZENG, Y. F. XU, Yangzhou University, QIULIANG WANG, Chinese Academy of Science, BING WU, Fayetteville state University — Nematic order has being found to widely exist in the cuprates and in the Fe-based superconductors in most recent years. It is directly linked to the superconductivity because nematic instability is a characteristic feature of the normal state upon which at lower temperatures the superconductivity emerges. FeSe has been regarded as a model system for the study of the Fe-based superconductors. But it is highly controversial as to whether the nematic order is driven by spin order, AFM spin fluctuations, and/or orbital order. Here we report the experimental result of field-dependent \(^{77}\text{Se-NMR}\). Our results shows for the first time that the difference of the static internal field in the \( ab \)-plane in the orthorhombic phase at the Se-nucleus is predominantly from the Fe-ion 3d electron orbitals (essentially all orbital), not from the electron spins, and gain AFM spin fluctuations are gradually developed below \( T \sim 40 \text{ K} \) in the orthorhombic phase, which is far below the nematic order/structure phase transition temperature \( T_{\text{nem}} = T_{\text{s}} = 89 \text{ K} \), while AFM spin order is absent at all temperatures and at all fields. Therefore, for the first time we provide direct evidence that orbital ordering is unequivocally the origin of the nematic order in FeSe.

*China NSF #61474096, 1804291, 51477167 & 41527802
9:00AM R10.00004: Single Crystal Diffuse Scattering Investigation of Nematic Fluctuations in (Ba,Na)Fe$_2$As$_2$* 
RAYMOND OSBORN (Presenter), MATTHEW KROGSTAD, STEPHAN ROSENKRANZ, Materials Science Division, Argonne National Laboratory, OMAR CHMAISSEM, PUSPA R UPRETI, RYAN STADEL, Department of Physics, Northern Illinois University, KEITH TADDEI, Neutron Scattering Division, Oak Ridge National Laboratory — The phase competition between nematic order and superconductivity has been intensively investigated in iron-based superconductors. Recent neutron pair-distribution-function (PDF) measurements on polycrystalline samples provide evidence of dynamic orthorhombic distortions, even within the C$_4$ tetragonal magnetic phase of hole-doped compounds [1]. We present synchrotron x-ray measurements of diffuse scattering from single crystals of (Ba,Na)Fe$_2$As$_2$, which show that these nematic fluctuations are predominantly two-dimensional. The measurements cover a sufficiently large volume of reciprocal space that they can be transformed into real space, generating 3D PDFs, from which both in-plane and out-of-plane correlation lengths are determined as a function of temperature and dopant concentration. These results will be compared to other measurements of the nematic susceptibility.


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

9:12AM R10.00005: Quantum critical nematic fluctuations and spin excitation anisotropy in the iron pnictides* 
ELIHU ABRAHAMS (Presenter), University of California, Los Angeles, CHIA-CHUAN LIU, QIMIAO SI, Rice University — Quantum criticality in the iron pnictides involves the nematic and antiferromagnetic channels in a concurrent way [1,2]. To elucidate the nematic correlations, we study the spin excitation anisotropy defined by the difference between the dynamical spin susceptibilities at (π,0) and (0,π) [3]. We consider an effective Ginzburg-Landau theory involving spin and Ising-nematic degrees of freedom [1,2] in the presence of a small external C4-symmetry-breaking potential. Our analysis is carried out in a large N limit [2]. We establish a relation among the spin excitation anisotropy, the dynamical spin susceptibility and the nematic susceptibility, and then show how it can be used to extract the information of the nature of the quantum critical point. The relation we establish provides a means to understand the singular energy dependences observed for the spin excitation anisotropy in the avoided quantum critical regime of the optimally Ni-doped BaFe$_2$As$_2$ under a uniaxial strain. We also propose a mechanism accounting for these singular energy dependences.

References:

*DOE BES Award # DE-SC0018197.

9:24AM R10.00006: Origin of diverse nematic orders in Fe-based superconductors: 45 degree rotated nematicity in AFe$_2$As$_2$ (A=Cs, Rb) 
HIROSHI KONTANI (Presenter), SEIICHIRO ONARI, Nagoya University — The origin of nematicity and their order parameters in strongly correlated superconductors have been attracting increasing attention. Both the orbital order without magnetization in FeSe and d-wave bond order in cuprate superconductors are satisfactorily explained based on the spin-fluctuation-driven mechanism [1-3]. Recently, new type nematic order has been discovered in heavily hole-doped (n$_d$ = 5.5) compound AFe$_2$As$_2$ (A = Cs, Rb). The discovered nematicity has B$_{2g}$ symmetry, rotated by 45 degrees from the B$_{1g}$ nematicity in usual Fe-based superconductors. To reveal the origin of B$_{2g}$ nematicity, we analyze the spontaneous symmetry-breaking in the self-energy [2] based on the multiorbital Hubbard model. We predict that the ”nematic bond order”, given by the symmetry-breaking in the d$_{xy}$ orbital correlated hopping, is responsible for the B$_{2g}$ nematic order in AFe$_2$As$_2$. It is concluded that not only conventional B$_{1g}$ orbital order (n$_{x^2-y^2}$ ≠ n$_{xy}$), but also B$_{2g}$ bond order with respect to d$_{xy}$ orbital in AFe$_2$As$_2$ are caused by the same mechanism, that is, the charge-spin mode-coupling due to the Aslamazov-Larkin vertex correction. [1] S. Onari et al., PRL 116, 227001 (2016). [2] Y. Yamakawa et al., PRX 6, 021032 (2016). [3] M. Tsuchiizu et al., PRB 97, 165131 (2018).
9:36AM R10.00007: Orbital-selective superconductivity in the nematic phase of FeSe*  HAOYU HU (Presenter), Department of Physics and Astronomy, Rice University, RONG YU, Department of Physics, Renmin University of China, EMILIAN NICA, Department of Physics, Arizona State University, JIAN-XIN ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, QIMIAO SI, Department of Physics and Astronomy, Rice University — The considerations of the orbital-selective Mott physics in the normal state [1,2] motivated the theoretical proposal for orbital-selective pairing [3]. The experimental evidence for the latter has come from both the iron pnictides [4] and iron selenides [5]. We study the superconductivity in the presence of nematic order in a multi-orbital model with frustrated spin-exchange interactions [6]. We found that the electron correlation effects amplified by the nematic order [7] give rise to an enhanced orbital-selective pairing. The latter produces a large gap anisotropy on the Fermi surface which naturally explains the experimental observations.


*DOE BES Award # DE-SC0018197

9:48AM R10.00008: Basic principles of disorder-induced electronic nematicity  PANAGIOTIS KOTETES (Presenter), Niels Bohr Institute & ITP-CAS, DANIEL STEFFENSEN, Niels Bohr Institute, INDRANIL PAUL, Universite Paris Diderot-Paris 7 & CNRS, BRIAN M. ANDERSEN, Niels Bohr Institute — Resolving the phenomenon of nematicity, i.e., the breaking of fourfold-rotational (C4) symmetry, remains an outstanding problem in the field of iron-based superconductors. A wide range of techniques have provided experimental evidence for electronic nematic behavior, while more recently, the nucleation of local nematicity around impurities has been also detected. While some of these results may be attributable to residual sample strain, the possible induction of local nematicity due to disorder appears as a prominent and, at the moment, a poorly-explored phenomenon. To shed light on this physics, we perform a detailed theoretical study of the role of disorder in systems exhibiting an electronic nematic instability, with an emphasis on temperatures above the critical temperature at which the spontaneous C4-symmetry breaking sets in. We employ both a phenomenological Ginzburg-Landau theory, as well as a microscopic model, and identify the spatial profile generated by a disorder configuration which either respects or explicitly breaks the fourfold rotational symmetry. In the former case, we find that while such a potential cannot induce net nematicity, it still modifies the Stoner criterion for the nematic instability, thus, generally enhancing the nematic critical temperature.

10:00AM R10.00009: Emergent XY-nematic fluctuations in heavily-hole doped iron-based superconductors  KOUSUKE ISHIDA (Presenter), MASAYA TSUJII, SUGURU HOSOI, YUTA MIZUKAMI, Univ of Tokyo-Kashiwanoha, SHIGEYUKI ISHIDA, AKIRA IYO, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, KAI GRUBE, THOMAS WOLF, HILBERT LOEHNEYSEN, Karlsruhe Institute of Technology, RAFAEL M FERNANDES, University of Minnesota, TAKASADA SHIBAUCHI, Univ of Tokyo-Kashiwanoha — Electronic nematicity, rotational symmetry broken state originating from electronic mechanism, has been identified in several strong correlated systems. However, in contrast to its liquid crystal counterparts, the director of electronic nematic domains cannot point in an arbitrary direction (XY- nematic), but is confined to specific directions via non-negligible coupling to the lattice (Ising-nematic). Here we report the elastoresistance measurements in Ba1-xRbxFexAs2 and CsFexAs2, which can evaluate the nematic fluctuations from the change in the resistance induced by uniaxial strain. In RbFexAs2 and CsFexAs2, we found that B1g nematic fluctuations is more significant than B2g nematic fluctuations, providing the evidence for the nematicity along Fe-As direction in these compounds, 45 degree rotated from the unusual nematicity along Fe-Fe direction in the underdoped region. Furthermore, for the intermediate doping between these two distinct Ising-nematic phase, B1g and B2g nematic fluctuations exhibit identical Curie-Weiss behaviors, revealing that nearly XY-nematic fluctuation regime. This observation opens up a new route to realizing the novel electronic liquid crystal state in iron-based superconductors.
Nematic fluctuations close to quantum criticality: a new method for comparing simulations and experiments*

DANIEL JOST (Presenter), Walther Meissner Institute for Low Temperature Research, SAMUEL LEDERER, Cornell University, THOMAS U BOEHM, Walther Meissner Institute for Low Temperature Research, YONI SCHATTNER, Stanford Institute for Material and Energy Science, EREZ BERG, Chicago University, STEVEN KIVELSON, Stanford University, RUDOLF HACKL, Walther Meissner Institute for Low Temperature Research — The comparison of numerical simulations and spectroscopic results is notoriously difficult because of the analytic continuation in the complex energy plane. In addition to the analytic continuation, lifetime and mass enhancement factors must be extracted from the experimental spectra using, e.g., Kramers-Kronig transformation with the well-known problems resulting from the extrapolations to low and high energies. One way out of this dilemma is a transformation of the experimental results from real to imaginary frequencies which provides us with an imaginary-time-ordered correlation function $\Lambda(\tau)$. For determining $\Lambda(\tau)$, the cutoff is much faster. From this transformation, one can extract the quantity $\beta \Lambda(\beta/2)$ with $\beta=1/k_B T$. We show in this contribution how this quantity can be derived from the electronic Raman spectra of the iron pnictide Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ and varies with doping and temperature. We compare the results with those obtained via the Kramers-Kronig formalism at zero frequency. Additionally, we highlight the perspectives of this method with view on quantum criticality and the comparison of experiment and theory.

*German Research Foundation (DFG): SPP1458 (HA2071/7), TRR80; Friedrich Ebert Foundation; BaCaTeC.

The anomalous high magnetic field electronic state of the nematic iron-based superconductor FeSe$_{1-x}$S$_x$*

MATT BRISTOW (Presenter), PASCAL REISS, Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, U.K, AMIR HAGHIGHIRAD, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany, ALIX MCCOLLAM, High Field Magnet Laboratory (HFML-EMFL), Radboud University, 6525 ED Nijmegen, The Netherlands, WILLIAM KNAFO, Laboratoire National des Champs Magnétiques Intenses (LCMM), CNRS-UIF-UPS-INSA, Toulouse, France, AMALIA COLDEA, Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, U.K — Superconductivity is closely linked to the electronic states from which it emerges. Here we investigate the normal electronic state of the nematic superconductor FeSe$_{1-x}$S$_x$ using magneto-transport and Hall Effect studies in magnetic fields up to 35 T (Nijmegen) and 70 T (Toulouse) over a large temperature range. Inside the nematic phase we find anomalous magneto-resistivity behaviour in very high magnetic fields, well above the upper critical field. The behaviour changes outside the nematic phase, where we show that at low temperatures Fermi-liquid behaviour is recovered. We account for the multiband structure and trace the carrier densities and motilities across the nematic phase transition. We also investigate the regime of superconducting fluctuations, which is expected to varying significantly in this isoelectronic series. We will discuss our results in relation to both Fermi liquid and non-Fermi liquid behaviour, and superconducting fluctuations.

*This work was support by the Engineering and Physical Sciences Research Council (EPSRC, UK) (EP/I004475/1, EP/I017836/1, EP/M020517/1, EP/N01085X/1). Part of this research was also supported by the Oxford Centre for Applied Superconductivity (CFAS) and the John Fell Fund of the Oxford University.

Charge order and structural evolution in nematic superconductor Ba(0.33)Sr(0.67)Ni$_2$As$_2$

JOHN COLLINI (Presenter), CHRISTOPHER ECKBERG, Center for Nanophysics and Advanced Materials, University of Maryland College Park, SANGJUN LEE, STELLA SUN, PETER ABBAMONTE, University of Illinois Urbana-Champaign, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, University of Maryland College Park — Recent discoveries of charge order in the cuprates and electron nematic order in the iron-based superconductors has pointed towards the possibilities of both orderings being tied to mechanisms of high Tc superconductivity. The (Ba,Sr)Ni$_2$As$_2$ superconducting system has very recently been shown to exhibit both types of ordering without the presence of any magnetic order. Through single crystal x-ray diffraction reports, the Ba parent compound shows the emergence of an incommensurate charge density wave (CDW) before transitioning from a tetragonal structure to a triclinic structure with the emergence of a new commensurate triclinic CDW. We report single crystal x-ray observations how the charge order and structure of the system has evolved up through a Sr concentration of $x=.67$, just before the complete extinction of the triclinic phase and maximal superconducting Tc.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R11 DCMP: 2D Materials and Heterostructures BCEC 152 - Oscar Avalos Ovando, Ohio University
8:00AM R11.00001: A first-principles study of the ferroelectricity of two-dimensional IV-VI group compounds
FEN XIONG (Presenter), Department of Mechanical Engineering, The University of Hong Kong, XILIN ZHANG, College of Physics and Materials Science, Henan Normal University, ZHEN LIN, YUE CHEN, Department of Mechanical Engineering, The University of Hong Kong — Two-dimensional (2D) ferroelectric materials with atomic thickness have attracted much research interest due to their potential industrial applications. The recent successful synthesis of 2D SnTe, which exhibits a spontaneous polarization along the in-plane directions, motivates further studies of the related 2D IV-VI group compounds. In this work, we focus on the theoretical calculations of the stability and ferroelectricity of 2D IV-VI compounds based on density functional theory (DFT) and the Berry phase method. Firstly, the energies of the competing 2D crystal structures of the IV-VI compounds have been computed from DFT; it is found that different structures are adopted by the 2D IV-VI compounds. To facilitate the engineering of the crystal structure, the alloying effects on the phase stability and the corresponding electronic origins have been further studied. Secondly, the spontaneous polarization is calculated using the Berry phase approach, and it is found that some of the 2D IV-VI compounds have more robust ferroelectricity than others. Moreover, the manipulation of spontaneous polarization via external strain has also been discussed.

8:12AM R11.00002: Van der Waals induced rippling and anisotropy in the natural superlattice Franckeite
PABLO SAN-JOSE, RICCARDO FRIENDA, ICMM-CSIC, Consejo Superior de Investigaciones Científicas, IOANNA URBAN (Presenter), MICHAL BARANOWSKI, Laboratoire National des Champs Magnétiques Intenses, NIKOS PAPADOPOULOS, HERRE S.J. VAN DER ZANT, TU Delft, GABRIEL SÁNCHEZ-SANTOLINO, MAR GARCÍA-HERNÁNDEZ, ICMM-CSIC, Consejo Superior de Investigaciones Científicas, PAULINA PLOCHOCKA, Laboratoire National des Champs Magnétiques Intenses, ANDRES CASTELLANOS-GOMÉZ, ICMM-CSIC, Consejo Superior de Investigaciones Científicas — Franckeite, a naturally occurring van-der-Waals hetereostructure, is composed of alternating pseudohexagonal and pseudotetragonal two-dimensional layers. While both types of layers are in principle mechanically and electrically isotropic in the plane, Franckeite, like its cousin Cylindrite, exhibits a characteristic rippling pattern, the origin of which has remained unclear. Here we show, using continuum elasticity theory, that rippling is ultimately the result of a mechanical instability produced by a one-dimensional moiré superlattice forming in Franckeite's interlayer alignment. We also show that the ripples give rise to marked anisotropies in the electrical and optical sectors, as measured by differential reflectance, polarised Raman spectroscopy and electrical transport measurements. This picture connects the properties of bulk Franckeite to the basic mechanisms governing low-angle moiré multilayers, such as twisted graphene bilayers.

*We acknowledge funding from the European Research Council (ERC) (grant n° 755655, ERC-StG 2017 project 2D-TOPSENSE), the EU Graphene Flagship funding (Grant Graphene Core 2, 785219), the Netherlands NWO (program Rubicon, project 680-50-1515) and the Spanish MINECO/MICINN (Grant Nos. FIS2015-65706-P, FJCI-2015-25427).

8:24AM R11.00003: Layer Dependent MCD on Van der Waal-like 2D ferromagnetism
YU-CHE CHIU (Presenter), ZHENGUANG LU, National High Magnetic Field Laboratory, DANIEL A RHODES, Columbia University, YUXUAN JIANG, DMITRY SMIRNOV, National High Magnetic Field Laboratory, JAMES HONE, Columbia University, LUIS BALICAS, National High Magnetic Field Laboratory — The layered ferromagnetic semiconductor CrSiTe3 is a promising candidate for spintronic applications. According to DFT calculations, its bulk bandgap is predicted to be ~0.4 eV; meanwhile, a Curie temperature of ~33 K was reported, thus providing evidence for bulk ferromagnetism. More importantly, due to the van der Waal-like interlayer coupling, CrSiTe3 is exfoliable and possible to achieve monolayers through mechanical exfoliation making it appealing for 2D spintronics. However, the fundamental properties of CrSiTe3 have not been thoroughly studied, particularly in the few layers limit. A number of of theoretical reports, suggest that the monolayer could have a larger bandgap but the presence of magnetism is still debatable (FM or AFM order). Nonetheless, among these predictions, the common agreement is that the decisive factor causing FM- or AFM-exchange coupling is the distance between Cr-Te-Cr bonds, which indicates that the spin configuration is closely related to the lattice. Therefore, in order to study the presence of magnetism and to understand the role spin-phonon interaction, we performed layer-dependent magnetization measurements via the magnetic circular dichroism (MCD) and Raman spectroscopy at different Ts.

8:36AM R11.00004: Strain induced half-semiconductor to half-metallic transition in 2D magnet CrI3: A DFT approach
TISTA MUKHERJEE, Presidency University, SUMAN CHOWDHURY (Presenter), Bangabasi College, DEBNARAYAN JANA, University of Calcutta, LOK LEW YAN VOON, University of West Georgia —
In this work, compressive and tensile strain (uniaxial as well as biaxial) upto 12% have been applied to study the variation of the electronic and magnetic properties of CrI3 employing density functional theory in (LDA+U) exchange correlation scheme. The stability limits of the structures under the influence of strains have been carried out via the deformation potential and stress-strain relation. Using appropriate strains, the pristine half-semiconducting nature can be tuned to observe half-metallicity. Further, the indirect band gap in the half-semiconducting phase can be increased by the application of tensile strain. The magnetic moment computed from the density of states is enhanced significantly under the influence of compressive strain. However, it has been observed that after the application of strain in some specific crystal directions, the magnetic moment of monolayer CrI3 remains almost unchanged. Thus, with the help of strain, the tuned half-metallicity along with underlying characteristic ferromagnetism of this material can unfold a new avenue for potential usage in spintronic devices.

8:48AM R11.00005: Emission of Geometrically Modulated Monolayer Semiconductors*
I-TUNG CHEN (Presenter), CHUN AN CHEN, TUNG-HAN YANG, KUAN-CHANG CHIU, YING-YU LAI, YI-HSIEN LEE, National Tsing Hua University —
Emission, including light and electrons, of the monolayer 2D lattices offers significant scientific interests in materials sciences and potential optoelectronics applications. However, monolayers of transition metal dichalcogenides (TMDs) exhibit reduced efficiency on optical emission and electron field emission. Here, emission of the geometrically modulated monolayer semiconductors suspended with 1D nanoarrays is demonstrated. Synthesized TMD monolayers offer an ideal platform to explore the fundamental process of the emission of the TMD. Geometrical modulation and charge transfer of the semiconducting monolayers can be significantly tuned with the structural suspension with nanoarrays.

*We acknowledge support from AOARD grant (co-funded with ONRG) FA2386-16-1-4009, Ministry of Science and Technology (MOST-105-2112-M-007-032-MY3, MOST-106-2119-M-007-027), and Academia Sinica Research Program on Innovative Materials and Analysis Technology Exploration (AS-iMATE-107-11), Taiwan.

9:00AM R11.00006: Barrier tunneling for the dice lattice under linearly-polarized light
DIPENDRA DAHAL (Presenter), CUNY Graduate Center, GODFREY GUMBS, Physics and Astronomy, Hunter college, CUNY, ANDRII IUROV, DANHONG HUANG, Physics, University of New Mexico —
We have investigated electron tunneling across a square barrier under external off-resonance dressing fields in α-T3 lattices with variable interatomic coupling parameter α which yields the dice lattice limit (or T3 material) when α = 1. Our results show strong dependence on both the parameter α and the polarization of the imposed irradiation. In the absence of the irradiation, the low-energy pseudospin-1 Dirac-Weyl Hamiltonian which gives an energy spectrum consisting of a pair of Dirac cones and a dispersionless (at) band in the K and K' valleys is employed for these calculations. For the case of linearly-polarized dressing field, an asymmetric, or non-head on Klein tunneling has been discovered. We explore the dependence of Klein tunneling through rectangular electrostatic barriers as the irradiation intensity varies continuously. However, complete transmission is no longer observed for α ≠ 1 under all types of incident light polarization.
In this talk, we will highlight that nonreciprocity and mechanical motion are deeply intertwined. We will discuss some unusual features of the electrodynamics of moving media [1] and highlight that a translational motion can be mimicked with a drift-current [2]. In particular, we will show that a graphene sheet biased with a direct electric current is a very promising solution to break the Lorentz reciprocity and have a broadband regime of unidirectional propagation of surface plasmons protected against backscattering from obstacles and imperfections [3].


*This work is supported in part by Fundação para a Ciência e a Tecnologia with the grants PTDC/EEITEL/4543/2014 and UID/EEA/50008/2017.

**9:24AM R11.00008: Twisted-bilayer graphene devices fabricated with polymer-free graphene** RUJ LYU (Presenter), Physics and Astronomy, University of California, Riverside, DONGYING WANG, EMILIO A CODECIDO, Physics, the Ohio State University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, CHUN NING LAU, MARC BOCKRATH, Physics, the Ohio State University — The Mott-like insulator state and superconductivity realized by stacking two graphene sheets that are twisted near 1.1°, the "magic angle [1,2," has stimulated a new wave of interest in this newfound material in the two-dimensional material family. We will present our recent work in fabricating twisted bilayer graphene heterostructures. Instead of using graphene exfoliated by tape, we obtain the graphene sheets by scratching thin graphite flake deposited on wafer with a razor blade. Combining with the pick-up technique[3], the graphene is free from any tape or polymer residue. Atomic force microscope images and transport measurements results indicate a high quality in the devices we made. Low temperature magnetocconductance measurements are also performed and the latest results will be discussed. [1] Y. Cao et al, Nature 556, 80-84(2018), [2] Y. Cao et al, Nature 556, 43-50 (2018). [3] L. Wang et al., Science 342, 614-617 (2013).

**9:36AM R11.00009: Electronic and Magnetic Properties of Patterned Hydrogenated Graphene: A First-principles Study** BI-RU WU (Presenter), Department of Natural Science, Center for General Education, Chang Gung University — Graphene is recognized as a promising 2D material with abundant physical properties, and flexibility in designing, but the zero band gap limited its applications. Graphane, a fully hydrogenated graphene, opens a remarkable energy gap. Furthermore, the hydrogenation also provide magnetic configuration of partial hydrogenated graphene due to the unpaired or localized electrons of unhydrogenated carbon atoms. In hydrogenated graphene, the carbon atoms of missing hydrogen atom prefer aggregate and form a cluster or zigzag chains. The former establishes a graphene quantum dot (GQD) embedded in graphene; the later is as a bare carbon chain or chains in graphene. We found the bare carbon chains and embedded GQDs can interact with each other. Such an inter-chain interaction and inter-dot affect the band structure of patterned hydrogenated graphene, and the inter-dot interaction will further change the magnetic properties of the embedded GQDs. It is interesting that the interaction changes the spin orientation of the atoms in the adjacent triangular GQDs and alters the energy dispersions.

*This work was supported by the Ministry of Science and Technology of the Republic of China under grant numbers MOST 105-2112-M-182-002-MY3.

**9:48AM R11.00010: Transport measurement of twisted bilayer-bilayer graphene** THAO DINH (Presenter), ZHIREN ZHENG, QIONG MA, SUYANG XU, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, PABLO JARILLO-HERRERO, NUH GEDIK, Massachusetts Institute of Technology — The recent discovery of correlated insulator behavior and superconductivity in magic-angle graphene has attached tremendous interest in twisted van der Waals systems. So far, people have been focusing on the moiré superlattice and the flat band formed due to the interlayer coupling. In fact, twisting can be used to engineer the symmetry of a 2D system, which may lead to interesting phenomena that are not allowed in their natural form. In this work, we explore such broken symmetry effect in a twisted bilayer-bilayer graphene structure. The two bilayers are rotated with respect to each other by 180°. Based on the symmetry analysis, the twisted four-layer system is strongly inversion-broken and has an out-of-plane polar axis. We fabricated high quality dual-gated devices and we will report on the transport and optical behavior of this novel system.
10:00AM R11.00011: Inter-Landau-level Andreev Reflection at the Dirac Point in a Graphene Quantum Hall State Coupled to a NbSe2 Superconductor* MANAS SAHU (Presenter), department of physics, indian institute of science, bangalore 560012, India, XIN LIU, School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China, ARUP KUMAR PAUL, department of physics, indian institute of science, bangalore 560012, India, SOURIN DAS, Indian Institute of Science Education and Research, Kolkata, Mohanpur 741246, India, PRATAP RAYCHAUDHURI, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400 005, India, JAINENDRA JAIN, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, ANINDYA DAS, department of physics, indian institute of science, bangalore 560012, India — Superconductivity and the quantum Hall effect are distinct states of matter occurring in apparently incompatible physical conditions. Recent theoretical developments suggest that the coupling of the quantum Hall effect with a superconductor can provide fertile ground for realizing exotic topological excitations such as non-Abelian Majorana fermions or Fibonacci particles. As a step toward that goal, we report observation of Andreev reflection at the junction of a quantum Hall edge state in a single layer graphene and a quasi-twodimensional niobium diselenide (NbSe2) superconductor. Our principal finding is the observation of an anomalous finite-temperature conductance peak located precisely at the Dirac point, providing a definitive evidence for inter-Landau-level Andreev reflection in a quantum Hall system. Our observations are well supported by detailed numerical simulations, which offer additional insight into the role of the edge states in Andreev physics. This study paves the way for investigating analogous Andreev reflection in a fractional quantum Hall system coupled to a superconductor to realize exotic quasiparticles.

* A. D. thanks Department of Science and Technology (DST), Government of India, under Grants No. DSTO1470 and DSTO1597.

10:12AM R11.00012: Band structure tuning of doped Graphene/hBN heterostructure HONGYUN ZHANG (Presenter), ERYIN WANG, Tsinghua University, SHUOPEI WANG, XIAOBO LU, Chinese Academy of Science, JONATHAN DENLINGER, ALEXEI V FEDOTOV, Lawrence Berkeley National Labotatory, TAKASHI TANIGUCHI, National Institute for Material Science, GUANGYU ZHANG, Chinese Academy of Science, SHUYUN ZHOU, Tsinghua University — Tuning Dirac electrons by a periodic potential is an important scientific question and graphene/h-BN is a model van der Waals heterostructure for investigating this. Here we report our recent ARPES progress on the electronic band structure of doped graphene/BN, which shows intriguing band structure engineering of both the valence and conduction bands.

10:24AM R11.00013: Nonequilibrium noise measurements using hBN tunnel barriers XUANHAN ZHAO (Presenter), PANPAN ZHOU, LOAH STEVENS, DOUGLAS NATELSON, Rice University — Xuanhan Zhao1, Loah A. Stevens1, Panpan Zhou1, K. Watanabe2, T. Taniguchi2, Douglas Natelson1,3,4

1Department of Physics and Astronomy, Rice University, Houston, TX 77005
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Nonequilibrium (or “shot”) noise, which comprises the inherent fluctuations in the electrical current of system driven out of equilibrium, is predicted to be an outstanding experimental probe for underlying physics in many systems. Hexagonal boron nitride is a 2D material with atomically smooth surface available down to thicknesses of single atomic layers and possessing a large bandgap, which makes it an ideal choice for fabrication of tunnel junction. Here we report nonequilibrium charge current noise measurements in a variety of tunnel junctions prepared using different ways of transferring hBN as monolayer tunnel barriers. We will further discuss the prospect of making single-layer hBN a general tool for tunneling spectroscopy of materials.
10:36AM R11.00014: Imaging non-circular cyclotron orbits in a graphene/hBN superlattice  ARTHUR BARNARD
(Presenter), AARON SHARPE, Stanford University, USA, JOHN WALLBANK, University of Manchester, UK, KENJI WATANABE,
TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, VLADIMIR FALKO, University of Manchester, UK, DAVID
GOLDHABER-GORDON, Stanford University, USA — When graphene is rotationally aligned with an underlying hexagonal
boron nitride (hBN) substrate, a superlattice naturally forms. This drastically alters graphene's electronic band structure,
leading to minibands whose structure enables us to electrostatically tune the Fermi-surface size and shape. A striking
consequence of altering the Fermi-surface shape is that electrons are no longer expected to follow circular cyclotron
motion in the presence of a magnetic field. Transverse electron focusing (TEF) measurements have shown signatures of
these non-circular orbits in a graphene/hBN superlattice, however, a direct probe has been lacking.
Here, we image the shape of cyclotron orbits in an hBN/graphene superlattice by performing TEF measurements in a
cryogenic scanning gate microscope (SGM). We study a hall-bar device with collimating contacts and use a home-built
multi-terminal lock-in technique to efficiently determine where electrons are electrostatically deflected by the SGM tip.
With this system, we resolve both circular and triangular orbits, in good agreement with expectations from band structure
calculations.

10:48AM R11.00015: THz spectroscopy of graphene coupled to LaAlO3/SrTiO3 nanoscale junctions*  ERIN SUTTON
(Presenter), LU CHEN, JIANAN LI, QING GUO, University of Pittsburgh, HYUNGWOO LEE, JUNGWOO LEE, CHANG-BEOM EOM,
University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh —

We investigate the gate-dependent optical response of graphene using the broadband nonlinear generation and detection
capabilities of nanoscale junctions created at the LaAlO3/SrTiO3 interface [1]. Using the large non-resonant third-order
nonlinear susceptibility in SrTiO3, strong difference frequency mixing occurs when the junction is biased, leading to
induced polarization that can also be detected at the junction [2]. Here we discuss results of gate-dependent experiments
which interrogate the relationship between the THz signal and the gate location with respect to the Dirac point in devices
where graphene is coupled to the LaAlO3/SrTiO3 interface. Preliminary results suggest we may be detecting a surface
plasmon resonance or phonon mode. We will also discuss results indicating a gate-dependent enhancement of the
graphene absorption.


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(N00014-16-1-3152) (JL). C-BE acknowledges support from AFOSR (FA9550-15-1-0334), NSF DMREF (DMR-1629270), and
NSF MRSEC (DMR-1420645) (C-BE). ES acknowledges support from the NSF GRFP (1747452).

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R12 DCMP GMAG: 2D Materials: Magnetism and Optoelectronics BCEC 153A - Erik Henriksen,
Washington Univ - Tag(s): Focus

8:00AM R12.00001: Relative stability and magnetic ground state of all stacking patterns in bilayer chromium
trihalides from first principles*  MARCO GIBERTINI (Presenter), Department of Quantum Matter Physics, University of Geneva
— Chromium trihalides, CrX3 (X = Cl, Br, I), are layered magnetic materials that have recently attracted considerable
attention owing to their easy exfoliability. Their monolayers are ferromagnetic, with spins lying in-plane for CrCl3 and out-
of-plane for CrBr3 and CrI3. This difference is reflected also in distinct interlayer interactions when layers are stacked into
their bulk: antiferromagnetic for CrCl3, while ferromagnetic for the others. Still, even multilayers of CrI3 behave as
antiferromagnets, whereas CrBr3 remains ferromagnetic. Here, we address this controversy by studying bilayers of these
materials using density functional theory. We enumerate all possible stacking patterns with the smallest unit cell and
investigate their relative stability. We show that, depending on the stacking order, the magnetic ground state can be
different. In particular, we recover that the bulk stacking is indeed the most stable and it is correctly ferromagnetic for CrI3
and CrBr3, although there exist other low-lying metastable configurations that are antiferromagnetic. Based on our
findings, we speculate on how the apparent controversy could be resolved.

*Support from the Swiss National Science Foundation through the Ambizione program and the NCCR MARVEL is greatly
acknowledged.
8:12AM R12.00002: C1 vacancy in pentagraphene*  AADITYA MANJANATH (Presenter), CHAO-PING HSU, Institute of Chemistry, Academia Sinica, YOSHIYUKI KAWAZOE, Tohoku University, New Industry Creation Hatchery Center — Pentagraphene (PG), a two-dimensional allotrope of carbon with only five-membered rings, was recently predicted to exhibit exciting electronic and thermal properties with possible implications in nanoelectronics. However, its potential properties arising from defects have not been explored yet. Here, we explore the C1 vacancy in PG using first-principles density functional calculations. This defect introduces four midgap levels indicating the possibility of studying the charge states. The charged defect is amphoteric with deep donor and deep acceptor levels. Introducing the vacancy in the sheet renders it inherently ferromagnetic (FM) with a magnetic moment of 4 $\mu_B$. Upon further investigating spin polarization in PG, three possible unique magnetic configurations are found to exist: FM, anti-ferromagnetic (AFM)–dominant, and quenched-AFM. The energy differences between the FM and the AFM states are on an average ~2 meV/atom, indicating that reversible spin manipulation through thermal energy is possible.

*JSPS Kakenhi Grant no. 17H03384, HPCI project hp170190, Academia Sinica Investigator award AS-IA-106-M01 and MOST of Taiwan with project 105-2113-M- 001-009-MY4, and Academia Sinica Distinguished Postdoctoral Fellowship

8:24AM R12.00003: Magnon-assisted tunnelling in van der Waals heterostructures based on CrBr3  DAVIT GHAZARYAN (Presenter), Department of Physics, National Research University Higher School of Economics, MARK GREENAWAY, Department of Physics, Loughborough University, ZIHAO WANG, IVAN JESUS VERA MARUN, JUN YIN, Physics and Astronomy, The University of Manchester, SERGE MOROZOV, Institute of Microelectronics Technology and High Purity Materials, ALEXANDER LICHTENSTEIN, Institute of Theoretical Physics, University Hamburg, MIKHAIL KATSNELSON, Institute for Molecules and Materials, Radboud University, ARTEM MISHCHENKO, LAURENCE EAVES, ANDRE GEIM, KOSTYA NOVOSELOV, ABHISHEK MISRA, Physics and Astronomy, The University of Manchester — Recently, the family of two-dimensional materials has been expanded to include ferromagnets. It was shown that CrI3 exhibits ferromagnetism down to thicknesses of a single monolayer [Huang, B. et al. Nature 546, 270 (2017)]. CrI3 is part of a group of materials known as the chromium trihalides, CrX3 (where X=Cl, Br or I). I will report on a few layers of exfoliated CrBr3 (2-6 layers) that are also ferromagnetic by fabricating and characterising functional tunnelling devices where the CrBr3 layer is sandwiched in between two graphene electrodes. I will also report a new type of tunnelling mechanism in van der Waals heterostructures by demonstrating that electrons in our device tunnel between the graphene layers via the emission (and, at high temperature, absorption) of magnons in the CrBr3 barrier.

8:36AM R12.00004: Spin texture of a quasi-two-dimensional ferromagnetic kagome metal*  XIAO-MING MA, Physics, Southern University of Science and Technology, XIAO-BO WANG, Physics, Hong Kong University of Science and Technology, YU-JIE HAO, YUE FENG, JIE-MING YANG, TIAN-XIONG HAN, HUI-WEN SHEN, YI-MING XU, RONG-RONG SONG, Physics, Southern University of Science and Technology, HONG DING, Institute of Physics, Chinese Academy of Sciences, CHANG LIU (Presenter), Physics, Southern University of Science and Technology — The discovery of low dimensional, long range magnetic order and the study on accurate control of such order have led to the revolution of magnetic storage devices that reformed our daily lives. Two dimensional systems with underlying kagome symmetry is found to be one of the most convenient platforms for the creation and manipulation of various magnetic structures. For example, planar ferromagnetism and non-collinear antiferromagnetism are present in kagome metals Fe3Sn2 and Mn3Sn, respectively, both of which are also recently found to be topologically nontrivial. In this talk, we report our study on the spin texture of Fe3Sn2, using both spin-resolved ARPES and DFT calculations. Our results show that the topological Dirac bands at the K points of Fe3Sn2 originates from inner layers of the crystal, and are highly spin-polarized along a single spatial direction, realizing in-plane ferromagnetism. This study reveals the low-lying spin texture of a two dimensional topological metal, serving as guidance for spintronic applications on systems alike.

*This work was supported by the National Natural Science Foundation of China (NSFC) (No. 11504159), NSFC Guangdong (No. 2016A030313650), and the Technology and Innovation Commission of Shenzhen Municipality (No. JCYJ20150630145302240).
Layered transition metal dichalcogenides are currently intensively investigated due to their opto-electronic, superconducting and topological properties as well as their potential usage as mono-layer building blocks. However, despite their layered nature they often exhibit three dimensional (3D) properties in the bulk. Surprisingly, in semiconducting 2H-MoTe2 long-range magnetic order of unknown origin has recently been observed at low temperature [1]. Here we present the full 3D band structure of 2H-MoTe2, determined with soft X-ray ARPES. We find a pronounced $k_z$ dispersion in most bands, consistent with ab-inito calculations, proving the three dimensional character of this material. Furthermore, we present results of beta detected $^6$Li NMR measurements and show that the spin-lattice relaxation of the implanted Li ions is inconsistent with long range magnetic order, but supports the presence of magnetic fluctuations. We also find signatures of Li diffusion below room temperature, indicating a potential application in Li battery materials.


*This work is supported by the Swiss National Science Foundation (SNF-Grant No. 200021_165910).
9:12AM R12.00007: Interacting Rydberg Exciton-Polaritons in Two-Dimensional Transition Metal Dichalcogenides
JIE GU (Presenter), Department of Physics, City College of New York, 160 Convent Ave., New York, NY 10031, USA, LUTZ WALDECKER, Department of Applied Physics, Stanford University, Stanford, California, 94305 USA, DANIEL A RHODES, Department of Mechanical Engineering, Columbia University, New York, NY 10027 USA, ALEXANDRA BOEHMKE, RIAN KOUTS, Department of Physics, City College of New York, 160 Convent Ave., New York, NY 10031, USA, ARCHANA RAJA, Department of Applied Physics, Stanford University, Stanford, California, 94305 USA, JAMES HONE, Department of Mechanical Engineering, Columbia University, New York, NY 10027 USA, TONY F HEINZ, Department of Applied Physics, Stanford University, Stanford, California, 94305 USA, VINOD M MENON, Department of Physics, City College of New York, 160 Convent Ave., New York, NY 10031, USA — Strong optical nonlinearities play a central role in realizing quantum photonic technologies. In solid state systems, the exciton-polariton which result from the hybridization of material excitations and cavity photons are an attractive candidate to realize such nonlinearities. The interaction arising from the material component, excitons, forms the basis of the polaritonic nonlinearity. Several solid state systems have demonstrated nonlinear interaction of polaritons using the \( n = 1 \) excitonic state. However, the nonlinear interaction can be significantly enhanced if excited Rydberg excitonic states can be used instead of the ground state excitons. Recently such excited Rydberg excitonic states have been observed in monolayer transition metal dichalcogenides. Here we demonstrate the formation of Rydberg exciton-polaritons in monolayer WSe\(_2\) embedded in a microcavity. Owing to the larger wavefunctions of the Rydberg excitons, these polaritons show greater nonlinear response evidenced through the blue shift of the lower polariton branch under optical excitation. The demonstration of Rydberg exciton-polaritons in two-dimensional semiconductors and their enhanced nonlinear response may facilitate the realization of quantum photonic logic gates and processors.

9:24AM R12.00008: Room temperature dynamical control and electroluminescence from microcavity polaritons in monolayer transitional metal dichalcogenides* 
BISWANATH CHAKRABORTY (Presenter), JIE GU, PHYSICS, City College of New York, City University of New York, New York 10031, USA, ZHENG SUN, Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA, MANDEEP KHATONIAR, REZLIND BUSHATI, ALEXANDRA BOEHMKE, RIAN KOUTS, VINOD M MENON, PHYSICS, City College of New York, City University of New York, New York 10031, USA — We demonstrate modulation of exciton-photon interaction in strong coupling regime showing polariton branches at room temperature in monolayer WS\(_2\) field effect transistor embedded inside a microcavity. Transitions from strong to weak coupling happens when WS\(_2\) becomes electron doped under gating due to reduction in oscillator strength of the excitons arising from decreased Coulomb interaction. For polariton electroluminescence from a monolayer WS\(_2\) at room temperature we incorporate a tunnel field effect transistor with graphene-hBN-WS\(_2\)-hBN-graphene van der Waal heterostructure inside the microcavity. Injected electrons and holes tunnel through hBN barrier and recombine in the WS\(_2\) resulting in luminescence and shows clear polariton branches. Our findings with these new class of materials pave a novel way to realize low energy optoelectronic switches and possibly room temperature based polariton lasers through electrically controlled polariton luminescence.

*This work was supported by the NSF under EFMA-1542863 and MRSEC program1420634

9:36AM R12.00009: Collective electronic properties of an \( \alpha \)-\( T_3 \) lattice at finite temperatures* 
ANDRII IUROV (Presenter), University of New Mexico, GODFREY GUMBS, Hunter college, DANHONG HUANG, Air Force Research Labs., LIUBOV ZHEMCHUZHNA, Hunter college — Many-body electronic properties, including plasmons, their damping, static screening and transport coefficients have been calculated based on the finite-temperature polarization function for the \( \alpha \)-\( T_3 \) model. We have thoroughly investigated the role of the coupling strength parameter \( \alpha \) for the extra atom at the center of the honeycomb lattice, which in our case could be continuously varied from 0 (graphene) to 1 (the dice lattice). Specifically, we obtained and analyzed the dice lattice limit. We have derived several crucial semi-analytical approximations for the static and long wavelength limits, related to the finite-temperature behavior of the plasmon excitations in \( \alpha \)-\( T_3 \) materials.

*D.H. would like to acknowledge the support from the Air Force Office of Scientific Research (AFOSR). D.H is also supported by the DoD Lab-University Collaborative Initiative (LUCI) program. G.G. would like to acknowledge the support from the Air Force Research Laboratory (AFRL) through Grant #12530960.
CHENHAO JIN, EMMA REGAN (Presenter), DANQING WANG, IQBAL B UTAMA, JEFFREY CAIN, University of California, Berkeley, YING QIN, YUXIA SHEN, Arizona State University, ZHIREN ZHENG, University of California, Berkeley, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, SEFAATTIN TONGAY, Arizona State University, ALEX K ZETTL, FENG WANG, University of California, Berkeley — Moiré superlattices dramatically modify the properties of electrons and excitons in van der Waals heterostructures by introducing a new length and energy scale. The effect can be especially strong for interlayer excitons, where electrons and holes reside in different layers and are sensitive to the local atomic configuration. For example, it was recently predicted that moiré superlattices can host localized interlayer exciton states with distinct optical selection rules due to an emergent moiré angular momentum. In this talk, I will discuss our effort to observe distinct interlayer exciton states and to probe the possible effects of the moiré angular momentum on the interlayer exciton states.

ROBERT YOUNTS (Presenter), Research and Applied Sciences, Space and Naval Warfare Systems Center Atlantic — Recently, monolayer transition metal dichalcogenides (TMDs) have shown the ability to undergo a phase transition between an insulating gas of strongly bound excitons to a conducting electron-hole plasma (EHP). Typically, to reach this phase transition, ultrashort optical pulses are used to create a non-equilibrium high carrier density. However, this EHP state can also be reached via continuous wave (CW) excitation. In most semiconductors, the high carrier density needed for the EHP phase transition cannot be reached using CW light since nonlinear recombination processes limit the equilibrium carrier density. However, the mechanical properties of monolayer TMDs can be used to manipulate the electronic structure to change the carrier dynamics, allowing for high carrier densities to be reached through CW excitation. Specifically, by applying strain, the energy offset between direct K-K and indirect Γ-K transitions can be used to shift the carrier population between valleys. By interchanging different transition metals or chalcogens, we can change the indirect-direct energy offset creating an EHP predominately in the indirect transition or direct transition. This has a profound impact on the optical properties of the EHP, providing an avenue to engineer novel opto-electronic devices.

CHARLES SAYERS (Presenter), Centre Nanoscience and Nanotechnology (CNAN), Department of Physics, University of Bath, HAMOON HEDAYAT, DAVIDE BUGINI, CLAUDIA DALLERA, Dipartimento di Fisica, Politecnico di Milano, DANIEL WOLVERSON, Centre Nanoscience and Nanotechnology (CNAN), Department of Physics, University of Bath, TIM BATTEN, Renishaw plc, SARA KARBASSI, SVEN FRIEDEMANN, HH Wills Physics Laboratory, University of Bristol, University of Bristol, GIULIO CERULLO, Dipartimento di Fisica, Politecnico di Milano, JASPER VAN WEZEL, Institute for Theoretical Physics, Institute of Physics, University of Amsterdam, STEPHEN CLARK, Centre Nanoscience and Nanotechnology (CNAN), Department of Physics, University of Bath, ETTORE CARPENE, IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, ENRICO DA COMO, Centre Nanoscience and Nanotechnology (CNAN), Department of Physics, University of Bath — Using time- and angle-resolved photoemission spectroscopy (TR-ARPES), we have studied the femtosecond dynamics of the charge density wave (CDW) in 1T-TiSe₂. This material exhibits a commensurate CDW with a (2 x 2 x 2) lattice distortion below 200 K for which the mechanism is still debated today. One of the recurring problems is disentangling the contributions from the electronic and lattice-driven order. Here, we have observed the photo-induced suppression of the CDW in real-time by tracking the valence band maximum at the Γ-point following an intense laser pulse. The timescales of gap closing and band-replica unfolding (< 200 fs), and the relatively low fluence required for these processes are suggestive of an excitonic mechanism. During recovery, coherent oscillations of the CDW gap are observed relating to the Ã₁₈ (3.4 THz) mode. A detailed pump fluence dependence reveals several regimes, including impeded recovery at high fluence. This bottleneck coincides with a change in the dominant frequency seen in the oscillations. Using complementary time-resolved reflectivity, we have established the threshold fluence of this phenomenon to be F > 60 μJ cm⁻². Our work is supported by a rate equation model which highlights the crucial role of excitons and phonons in this complex system.
10:24AM R12.00013: Electromagnetic Field dependent Coulomb renormalisation in Dirac Materials*  
DI MAURO VILLARI LEONE (Presenter), IAN GALBRAITH, FABIO BIANCALANA, Heriot-Watt University — 
Condensed matter physics is witnessing a rapid expansion of materials with Dirac fermion quasiparticle excitations. In recent works it has been shown that a full understanding of the optical properties of such materials requires one to go beyond the standard approach of the semiconductor Bloch equations (SBEs). In his influential paper Ishikawa derived an extended version of the SBEs for graphene using the formalism of instantaneous eigenstates. More recently his approach was generalised further for the case of a gapped material. These generalised Dirac-Bloch (DBEs) equations reproduce novel and previously unexplained nonlinear optical properties of graphene and gapped graphene, however they do not include Coulomb interactions that are in general very strong in two dimensional semiconductors. Starting from the quantisation of the instantaneous Dirac field we include Coulomb interactions and provide a fully renormalised version of the DBEs. By solving these equations we account for the linear optical properties of 2D Dirac semiconductor. We discuss how the absorption spectrum evolves as the energy gap is reduced to zero. We then study the strong Coulomb coupling regime in which the excitons form a relativistic Bose-Einstein condensate.

*EPSRC (UK, Grant No. EP/L015110/1)

10:36AM R12.00014: Excited excitonic states in second harmonic spectra of 2D materials with \textit{ab-initio} many-body methods*  
KORY BEACH (Presenter), MICHAEL C LUCKING, HUMBERTO TERRONES, Rensselaer Polytechnic Institute, MARK BRONGERSMA, OZGUR BURAK ASIAN, Stanford University — First principles calculations of the second harmonic generation (SHG) of various semiconducting 2D materials including transition metal dichalcogenides (TMDs) are performed using a time-dependent Bethe-Salpeter Equation (TDBSE) nonequilibrium Green's function approach. It is shown that by increasing simulation time, spectral resolution can be improved, resolving features in the SHG spectrum that can be attributed to excited states of excitons. By comparing the differences in excited exciton energies to the differences observed experimentally, a calibration metric for the degree of over- or under-binding of the excitons can be formulated. Moreover, the degree to which substrate screening in these materials modifies not only the binding energy and the fundamental gap, but also the relative energies of excited states, is explored. The relative intensities of the excited exciton peaks in the SHG are also examined for the additional layer of information they can provide beyond corresponding peaks in the first-order spectra. This focus on a more precise understanding of excitonic resonances in the second harmonic spectrum lays the groundwork for a more systematic use of this TDBSE method for studying nonlinear optical properties in 2D materials.

*NSF (EFRI-1433311), XSEDE, RPI CCI

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R13 DMP: 2D Materials (General): Transport and Optical Phenomena -- Emerging Materials BCEC 153B - Judy Cha, Stanford University

8:00AM R13.00001: Optical conductivity of black phosphorus*  
SEONGJIN AHN (Presenter), Center for Correlated Electron Systems, Institute for Basic Science (IBS), JIHO JANG, HONGKI MIN, Department of Physics and Astronomy, Seoul National University — Black phosphorus (BP) is a two-dimensional layered material composed of phosphorus atoms. Recently, it was demonstrated that external perturbations such as electric field close the band gap or even induce a band inversion in few-layer BP, resulting in the insulator phase with a finite energy gap or the Dirac semimetal phase characterized by two separate Dirac nodes. At the transition between the two phases, a semi-Dirac state appears in which energy disperses linearly along one direction and quadratically along the other direction. In this work, we study the optical conductivity of few-layer BP using a lattice model and the corresponding continuum model, incorporating the effects of an external electric field and finite temperature. We find that the low-frequency optical conductivity scales as a different power-law depending on the phase, which can be used as an experimental signature. We also demonstrate the change of the material parameters as an external field increases and its consequence on the power law behavior of the optical conductivity.

*J.J. and H.M. were supported by the NRF grant funded by the Korea government (MSIT) (No. 2018R1A2B6007837) and Creative-Pioneering Researchers Program through Seoul National University. S.A. was supported by IBS-R009-D1 (G1, G2, G3, Y1).
8:12AM R13.00002: Bright Mid-Infrared Photoluminescence in Thin-Film Black Phosphorus*  CHEN CHEN (Presenter), FENG CHEN, XIAOLONG CHEN, BINGCHEN DENG, Electrical Engineering, Yale University, New Haven, CT, USA, BRENDAN ENG, Electrical and Computer Engineering, University of Illinois Urbana–Champaign, Champaign, IL, USA, DAEHWAN JUNG, Institute for Energy Efficiency, University of California Santa Barbara, Santa Barbara, CA, USA, QIUSHI GUO, SHAOFAN YUAN, Electrical Engineering, Yale University, New Haven, CT, USA, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan, MINJOO LAWRENCE LEE, Electrical and Computer Engineering, University of Illinois Urbana–Champaign, Champaign, IL, USA, FENGNIAN XIA, Electrical Engineering, Yale University, New Haven, CT, USA — In this work, we report bright mid-infrared photoluminescence (PL) emission from thin-film black phosphorus (BP). The intensity of the PL emission from a 46-nm thick BP is only seven times weaker than that of an indium arsenide (InAs) multiple quantum well (MQW) structure grown by molecular beam epitaxy, in which the total thickness of the quantum wells is of similar thickness to BP. The PL emission is further tunable by the temperature and layer number of thin-film BP. In the 46-nm thick BP, the PL spectra indicates a bandgap of 0.334±0.003 eV at 300 K, which decreases to 0.308±0.003 eV at 80K. The anomalous redshift of the BP bandgap with decreasing temperature agrees with previous theoretical and experimental results, while the overall energy shift is about 60% of the previously reported value obtained from photocurrent spectroscopy. We also measure the layer number dependence of PL spectra of the thin-film BP (6-to 46-nm), and we show that the emission peaks from around 3.3 to 4 mm at 80 K. Our results reveal the promising future of thin-film BP in mid-infrared light emitting and lasering applications.

*We acknowledge the financial support from the National Science Foundation EFRI-2DARE program (1542815).

8:24AM R13.00003: Barkhausen effects in the first order structural phase transition in type-II Weyl semimetal MoTe2*  CHUANWU CAO, XIN LIU, XIAO REN, Peking University, KENAN ZHANG, Physics, Tsinghua University, DONG SUN, Peking University, SHUYUN ZHOU, Physics, Tsinghua University, YANG WU, Tsinghua University, YUAN LI, JIANHAO CHEN (Presenter), Peking University — We report the first observation of the non-magnetic Barkhausen effect in van der Waals layered crystals, specifically, between the $T_d$ and $1T'$ phases in type-II Weyl semimetal MoTe2. Thinning down the MoTe2 crystal from bulk material to about 25nm results in a drastic strengthening of the hysteresis in the phase transition, with the difference in critical temperature increasing from ~40K to more than 300K. The Barkhausen effect appears for thin samples and the temperature range of the Barkhausen zone grows approximately linearly with reducing sample thickness, pointing to a surface origin of the phase pinning defects. The distribution of the Barkhausen jumps shows a power law behavior, with its critical exponent $\alpha = 1.27$, in good agreement with existing scaling theory. Temperature-dependent Raman spectroscopy on MoTe2 crystals of various thicknesses shows results consistent with our transport measurements. Reference: C. Cao et al., 2D Materials 5, 044003 (2018)

*This project has been supported by the National Basic Research Program of China (Grant Nos. 2014CB920900, 2018YFA0305604), and the National Natural Science Foundation of China (Grant Nos.11774010 (C. Cao, X. Liu and J.-H. Chen)) (Grant Nos. 11674013,11704012 (D. Sun)).

8:36AM R13.00004: Ferroelectric switching of a two-dimensional metal  WENJIN ZHAO (Presenter), ZAIYAO FEI, TAUNO PALOMAKI, BOSONG SUN, MOIRA K MILLER, University of Washington, ZHIYING ZHAO, JIAQIANG YAN, Oak Ridge National Laboratory, XIAODONG XU, DAVID HENRY COBDEN, University of Washington — In its 3D form the semimetal WTe2 has a polar space group, whereas an isolated monolayer of WTe2 is centrosymmetric. We find that when exfoliated down to two- or three-layer thickness, WTe2 exhibits a spontaneous out-of-plane electric polarization, while the monolayer does not. The polarization persists to room temperature and can be switched by a perpendicular electric field using graphite gate electrodes located above and below the sheet. We directly detect and quantify the polarization using graphene as an electric-field sensor. The polarization state can also be distinguished via the in-plane conductivity. The ferroelectricity persists even when the material is metallic in the plane; this is possible because the few-layer WTe2 is so thin that the applied electric field penetrates it.
8:48AM R13.00005: Nonlinear imaging of grain boundaries in monolayer semiconducting transition metal dichalcogenides*  
BRUNO R CARVALHO, Departamento de Física, Universidade Federal de Rio Grande do Norte, YUANXI WANG, MAURICIO TERRONES, Physics, The Pennsylvania State University, LEANDRO M. MALARD (Presenter), Universidade Federal de Minas Gerais — Locating and imaging defects in two-dimensional (2D) materials is a key challenge to probe the material quality for different target applications. Recently, second harmonic generation (SHG) has been used to characterise different 2D materials and defective regions like grain boundaries [1]. However it has been shown that these grain boundaries were revealed by interference between the two neighbouring domains, leading to a dark region (no SHG emission) between them [1]. Here we implemented a nonlinear dark-field SHG microscopy setup to accurately probe grain boundaries and edges from semiconducting transition metal dichalcogenide monolayers. The dark-field SHG efficiently separates the spatial components of the emitted light and accurately locates grain boundaries and edges as bright patterns. The far field SHG pattern is calculated considering the interference between two second harmonic dipoles, which is in agreement with our experimental finding. Therefore the dark field second harmonic imaging opens new opportunities to characterize defects in 2D materials [2].


*We Acknowledge funding from CNPq, CAPES, FAPEMIG, FINEP and INCT Nanocarbono, AFOSR grant 17RT0244 and NSF (2DARE-EFRI-1433311).

9:00AM R13.00006: Tightly Coulomb-bound four- and five-particle intervalley states in monolayer tungsten diselenide  
SHAO-YU CHEN (Presenter), THOMAS A GOLDSTEIN, Department of Physics, University of Massachusetts Amherst, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, JUN YAN, Department of Physics, University of Massachusetts Amherst — Tightly-bound excitonic complexes in atomically-thin semiconducting transition metal dichalcogenides (TMDCs) provide an appealing platform for studying many-body correlations. Here, we present the observation of the Coulomb-bound four-particle biexciton and five-particle exciton-trion in monolayer tungsten diselenide by the photoluminescence (PL) measurements. The ultrahigh quality sample enables us to resolve and assign several intrinsic emission features in the energy window right below the bright neutral exciton emission. Interestingly, we discover that the biexciton consists of a spin-zero bright exciton in one valley and a spin-one “dark” exciton in the other, which is confirmed by the magneto-PL measurements. The binding energy of these multi-particle states are further estimated as 18–23 meV and 13–20 meV for the biexciton and the exciton-trion, respectively, by charge doping and thermal activation measurements. The tightly bound nature of the multi-particle states in atomically-thin TMDCs offers opportunities for understanding many-body physics and for realizing interesting applications such as Bose-Einstein condensation, and quantum communication and teleportation.


9:12AM R13.00007: WITHDRAWN ABSTRACT —

9:24AM R13.00008: Layer number dependent barrier height of MoS2 on ultra-flat conducting surfaces*  
HAO LEE, Physics and Astronomy, San Francisco State University, SANCHIT DESHMUKH, Electrical Engineering, Stanford University, JING WEN, Chemical, Biological and Materials Engineering, University of Oklahoma, VIVIANE COSTA, Physics and Astronomy, San Francisco State University, ERIC POP, Electrical Engineering, Stanford University, BIN WANG, Chemical, Biological and Materials Engineering, University of Oklahoma, AKM NEWAZ (Presenter), Physics and Astronomy, San Francisco State University — Transition metal dichalcogenides (TMDs) are layered semiconducting van der Waal crystals and promising materials for wide range of electronic and optoelectronic devices. Realizing practical device application requires an understanding of nanoscale local electronic and optoelectronic properties on layered TMDs on a conducting metal surface. In this work, we have used conducting atomic force microscopy (CAFM) of layered MoS2 (1-5 layers) immobilized on two different ultra-flat conducting surfaces (RMS surface roughness <0.2 nm) Au and indium tin oxide (ITO) forming metal (conductive-tip)-semiconductor-metal devices. First, we have found that the edges of the different layers are insulating. Second, the current increases as the layer number increases. By applying Fowler-Nordheim tunneling theory, we have determined the barrier heights for different layers and observed that the barrier height decreases as the number of layers increases. Our study provides a fundamental understanding of the local electronic behavior of TMD depending on layer numbers and may pave an avenue toward developing nanoscale electronic devices with tailored properties of different layers.

*NSF ECCS-1708907
Second-harmonic generation in strained transition metal dichalcogenide monolayers

LUKAS MENNEL (Presenter), MATTHIAS PAUR, THOMAS MUELLER, Photronics Institute, Vienna University of Technology — Second-harmonic generation (SHG) is a powerful measurement technique to analyze the symmetry properties of crystals. Mechanical strain can reduce the symmetry of a crystal and even weak strain can have an immense impact on the SHG intensity along different polarization directions. The impact of strain on the SHG can be modeled with a second-order nonlinear photoelastic tensor. We determined the photoelastic tensors for four different transition metal dichalcogenide (TMD) monolayers: MoS$_2$, MoSe$_2$, WS$_2$ and WSe$_2$. We find that the photoelastic tensors depend highly on the excitation intensity along different polarization directions. The impact of strain on the SHG can be modelled with a second-order mechanical strain can reduce the symmetry of a crystal and even weak strain can have an immense impact on the SHG harmonic generation (SHG) is a powerful measurement technique to analyze the symmetry properties of crystals.

We acknowledge financial support by the European Union (grant agreement No. 785219 Graphene Flagship), the Austrian Science Fund FWF (START Y 539-N16), and the doctoral college program “TU-D Unravelling advanced 2D materials” funded by TU Vienna.

Computing nonlinear response to arbitrary order in the presence of electronic interactions via time-domain integration of polarizability

EMILIA RIDOLFI (Presenter), PAOLO EMILIO TREVISANUTTO, VITOR PEREIRA, Centre for Advanced 2D Materials, National University of Singapore, 6 Science Drive 2, Singapore 117546 — We describe a theoretical approach to study the nonlinear optical response of electronic systems based on a real-time solution of the electronic dynamics in the presence of time-dependent electromagnetic fields. Using accurately parameterized tight-binding models and electronic interactions, this allows expedite and accurate calculations of the nonlinear response to arbitrary order for realistic systems. We demonstrate its capabilities by computing the excitonic spectrum and high-harmonic generation (SHG, THG, FHG) in MoS$_2$ and BN monolayers. The linear optical conductivity is seen to reproduce exactly the Kubo-formula perturbative results based on the Bethe-Salpeter equation and, moreover, reproduces very well the experimental traces. Such benchmark against experiments in linear order allows us to confidently predict the frequency dependence of the higher-harmonic susceptibilities which, within our scheme, are obtained with no additional effort, in contrast to an order-by-order perturbative approach.

Growth of self-assembled graphene nanoribbons on SiC substrates

HANBYUL JIN (Presenter), MATTIAS KRUSKOPF, ALBERT RIGOSI, DINESH PATEL, SHAMITH PAYAGALA, ALIREZA PANNA, DEAN G. JARRETT, DAVID B NEWELL, RANDOLPH E ELMQUIST, National Institute of Standards and Technology — Graphene nanoribbons (GNRs) hold promise for future nanoelectronics due to their unique band structure. Quantum confinement effects are observed in GNRs, and their bandgap energies increase with inverse proportionality to the GNR width. However, existing lithographic patterning methods cause disordered edges to form during the etching process creating dangling bonds that degrade the electrical properties of the GNR. To overcome these problems, structured silicon carbide (SiC) has been used as a template for selective growth of GNRs, which show outstanding ballistic transport with an electronic mean free path up to 15 μm [1, 2]. In this study, we have demonstrated the growth of narrow GNRs (~40 nm width) with improved structural properties using a surface pre-treatment. This method restrains SiC terrace edge step-flow during the annealing process, helping to form GNRs with the shape of the patterned SiC. The longitudinal and Hall magnetoresistance of GNRs are measured at low temperature using a six-terminal Hall bar geometry and the structural characteristics are demonstrated with atomic force microscopy (AFM), conductive AFM, and field emission scanning electron microscopy.


Two-dimensional electrons electrostatically confined on the surface of graphite

JUN YIN (Presenter), SERGEY SLIZOVSKIIY, SHENG HU, YANG CAO, School of physics and astronomy, the University of Manchester, INNA LOBANOVA, BENJAMIN PIOT, Laboratoire National des Champs Magnétiques Intenses, France, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, KOSTYA NOVOSELOV, ANDRE GEIM, VLADIMIR FALKO, ARTEM Mishchenko, School of physics and astronomy, the University of Manchester — In the bulk of a crystal, charge carriers are described by the Bloch states. At the crystal surface, the lattice periodicity is disrupted transforming itinerant Bloch waves to evanescent states. While easily accessible in semiconductors due to the presence of band gap, surface states are prohibited in gapless metals due to the presence of massive Fermi sea. Here, using capacitance spectroscopy, we show that two-dimensional (2D) charge carriers can be confined on the surface of graphite and electronically decoupled from the bulk simply by electrostatic gating. In the presence of a magnetic field, perpendicular to graphite basal plane, the Landau bands of bulk graphite render to evanescent Landau levels, which, in high magnetic fields, show electron-electron interactions including fractional quantum Hall states and negative electronic compressibility. Our work provides an experimentally convenient and highly tunable system for exploring bulk-surface correspondence.
10:24AM R13.00013: Interlayer interaction and Davydov splitting in MoS₂ polytypes studied by Raman spectroscopy

WOONGKI NA (Presenter), KANGWON KIM, JAE-UNG LEE, HYEONSIK M CHEONG, Physics, Sogang University —

The dependence of the interlayer interaction on the stacking order of MoS₂ is investigated by Raman spectroscopy using three excitation energies of 2.81, 2.41, and 1.96 eV. The low-frequency Raman spectra show distinct correlation with the stacking type [1]. The A-like intra-layer vibration mode at 405 cm⁻¹ exhibit Davydov splitting due to interlayer interactions when the 1.96-eV excitation is used. The positions and the relative intensities of the Davydov-split peaks depend on the stacking type as well. By using the linear-chain model, the interlayer force constants are extracted and compared for 3-layer samples with different stacking types: the 3R-types have a larger force constant than the 2H-type. For the 2H-type, Davydov splitting is analyzed as a function of the number of layers. The force constants for the second-nearest-neighbor interaction are obtained and compared with other transition metal dichalcogenides [2, 3, 4].

References

10:36AM R13.00014: Current Transport and Phase Transition in MoTe₂

ZIJING ZHAO (Presenter), YUEMING YAN, WENJUAN ZHU, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign — MoTe₂ is an interesting two-dimensional (2D) material, which has small energy barrier between semiconducting 2H phase and metallic 1T′ phase, and has ambipolar transport with high carrier mobility, which makes it promising for phase-change memories and logic devices. In this work, we systematically studied the current transport and phase transition in MoTe₂. The spectral photocurrent measurement reveals that the bandgap of MoTe₂ is ~1eV. The bandgap of MoTe₂ was also extracted using temperature dependence of conductance. The mobility of MoTe₂ was characterized using Hall-bar devices. At low temperatures, the carrier mobility is limited by Columbic scattering, while at high temperatures, it is limited by phonon scattering. Vertical metal/MoTe₂/metal junctions were also fabricated. As the current or voltage applied to the junction increases, MoTe₂ exhibits two transitions: high-to-low resistance transition at medium current levels, and low-to-high resistance transition at high current levels. These two transitions in resistivity in MoTe₂ may correspond to the 2H-to-1T phase transition and 1T-to-amorphous state transition respectively.

*The authors would like to acknowledge ONR support under Grant NAVY N00014-17-1-2973 and NSF support under grant ECCS 16-11279.

10:48AM R13.00015: Impacts of h-BN Stacking Sequence and Layer Thickness on the Band Structure and Radiative Recombination

KELSEY MENGLE (Presenter), EMMANOUIL KIOUPAKIS, University of Michigan — We investigated the variation of the electronic and optical properties of h-BN as a function of stacking sequence and number of layers using first-principles calculations. Our study includes bulk and bilayer structures for the five possible stacking sequences, as well as monolayer and randomly stacked bulk structures (t-BN). Variations of the band structure were studied both at the density functional theory (DFT) and GW levels, with particular focus on the band extrema. The majority of the investigated structures were found to have indirect band gaps, with a few exceptions such as the AB₁ stacking sequence and t-BN. We further calculated the phonon-assisted optical matrix elements (S) for all structures to understand how the number of layers and stacking type influence light emission. Most of the ordered bulk and bilayer structures are capable of efficient light emission with values of S² ranging from ~10-1000× that of bulk Si, indicating that efficient phonon-assisted light emission is possible even though the gap is indirect.

*This work was supported by NSF DMREF program (1534221) and the NSF GRFP through Grant No. DGE 1256260. Computational resources provided by DOE NERSC (DE-AC02-05CH11231).

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R14 DMP: 2D Materials (Metals, Superconductors, and Correlated Materials) -- Twisted Graphene I BCEC 153C - Philip Kim, Harvard University - Tag(s): Focus
8:00AM R14.00001: A scanning tunneling study of twisted bilayer graphene at the first magic angle* YONGLONG XIE (Presenter), BERTHOLD JAECK, CHENG-LI CHIU, Physics department, Princeton University, KYOUNGHWAN KIM, YIMENG WANG, Electrical and Computer Engineering department, The University of Texas at Austin, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, EMANUEL TUTUC, Electrical and Computer Engineering department, The University of Texas at Austin, ALI YAZDANI, Physics department, Princeton University — Recently, bilayer graphene with small twist angle has been shown to be a valuable platform for correlated electron phenomena. Band structure calculations show that at certain twist angle values, labelled magic angles, the lowest band has a flat energy-momentum dispersion. Transport experiments find evidence for a correlated insulating phase when this flat band is exactly half filled. Furthermore, a small doping level away from half filling gives rise to a superconducting instability. In this talk, we will discuss how a scanning tunneling microscope can help to elucidate the electronic properties of twisted bilayer graphene close to the first magic angle.

*This work is supported by the DOE, Moore Foundation, NSF, and DOD-ARO.

8:12AM R14.00002: Atomistic study of electron-phonon coupling in magic-angle twisted bilayer graphene* YOUNG WOO CHOI (Presenter), HYOUNG JOON CHOI, Department of Physics, Yonsei University, Seoul 03722, Korea — We report strong electron-phonon coupling in magic-angle twisted bilayer graphene (MA-TBG) obtained from atomistic description of the system including more than 10,000 atoms in the moiré supercell. Electronic structure, phonon spectrum, and electron-phonon coupling strength λ are obtained before and after atomic-position relaxation both in- and out-of-plane. Obtained λ is very large for MA-TBG, with λ > 1 near the half-filling energies of the flat bands, while it is small (λ~0.1) for monolayer and unrotated bilayer graphene. Significant electron-hole asymmetry occurs in the electronic structure after atomic-structure relaxation, so λ is much stronger with hole doping than electron doping. Electron-phonon coupling is nearly isotropic and very weakly dependent on electron momentum, suggesting single-gap s-wave superconductivity. Relevant phonon energies are much larger than electron energy scale, going far beyond adiabatic limit. Our results provide fundamental understanding of electron-phonon interaction in MA-TBG, highlighting that it can contribute to rich physics of the system.

*This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2017-C3-0079). Y.W.C. acknowledges support from NRF of Korea (NRF-2017H1A2A1042152).

8:24AM R14.00003: Band Degeneracy and Normal State Properties of Twisted Bilayer Graphene at the Magic Angle CHENG LI (Presenter), TIN-LUN HO, Ohio State University — Recently, superconductivity is discovered in twisted bilayer graphene at a small twist angle. Associated this superconducting state is a whole host of unusual normal state properties: (i) that the band degeneracy between charge neutrality and the insulating phase is 4, instead of the expected 8-fold degeneracy by counting all the relevant quantum numbers (valley indices, two layers and two spins), (ii) the appearance of an insulating phase at a finite chemical potential below charge neutrality, (iii) that the insulating phase is destroyed by an in-plane magnetic field, (iv) a further reduction of the band degeneracy from 4 to 2 on at chemical potential away from the insulating phase, (v) a large asymmetry of the size of Fermi surfaces on different sides of the insulating phase as reveal by quantum oscillation measurements.

In this talk, we show how (i) can come about through coupling of Dirac cones of the opposite valley index in different layers. This reduction of degeneracy immediately provides a natural explanation for all other phenomena (ii) to (v); and that the insulating phase is associated with a spin density wave. Our picture also has implications on light scattering and Raman absorption experiments.
degrees twist mismatch between the layers hosts a low energy flat band in which the Coulomb interaction is large relative to the bandwidth, promoting correlated insulating states at half band filling, and superconducting (SC) phases with dome-like structure neighboring correlated insulating states. Here we show measurements of a dual-graphite-gated twisted bilayer graphene device, which minimizes charge inhomogeneity. We observe new correlated phases, including for the first time a SC pocket near half-filling of the electron-doped band and resistive states at quarter-filling of both bands that emerge in a magnetic field. Changing the layer polarization with vertical electric field reveals an unexpected competition between SC and correlated insulator phases, which we interpret to result from differences in disorder of each graphene layer and underscores the spatial inhomogeneity like twist angle as a significant source of disorder in these devices [1].


*The authors are grateful to the Brazilian funding agencies CAPES, CNPq, FAPERJ, and INCT-Nanomateriais de Carbone for financial support and to the High Performance Computing Center (NACAD), COPPE-UFRJ for the use of supercomputing facilities.

9:00AM R14.00006: Wigner Crystallization in Twisted Bi-layer Graphene BIKASH PADHI (Presenter), PHILIP PHILLIPS, CHANDAN SETTY, University of Illinois at Urbana-Champaign — Study of strongly correlated phases took an interesting turn recently by the surprising discovery of high-Tc superconductivity in twisted sheets of graphene. The electronic properties of each graphene-layer can be described by non-interacting electrons. However, in a twisted bi-layer graphene (TBLG), close to the 'magic angles', the kinetic energy of the electrons is heavily quenched. This causes interactions to dominate, paving way for strong correlation. In this talk, I discuss arXiv: 1804.01101 and 1810.00884. We first compute quasiparticle interaction energy and kinetic energy to obtain their ratio, \( r_s \), which quantifies the extent of strong correlation. This ratio crossing unity already signals departure from a perturbative regime (or Fermi liquid behavior). For \( r_s \) larger than 37, the system minimizes the strong Coulomb repulsion by forming electronic crystals, called Wigner crystals. We show that TBLG near magic angles exhibits \( r_s \) much larger than this critical value, facilitating a hierarchy of metal-insulator transitions. Pressure enhances such crystallization. In light of Wigner crystallization we discuss various aspects of the recent experiments and show remarkable agreement with this scenario.

9:12AM R14.00007: Emergent Flat band lattices in spatially periodic magnetic fields* MUHAMMAD TAHIR (Presenter), HUA CHEN, Department of Physics, Colorado state University, Colorado State Univ — Motivated by the recent discovery of Mott insulating phase and unconventional superconductivity due to the flat bands in twisted bilayer graphene, we propose more generic ways of getting two-dimensional (2D) emergent flat band lattices using either 2D Dirac materials or ordinary electron gas subject to moderate periodic magnetic fields with zero spatial average. We provide simple formulas for the "magic ratios" between the field strength and its wavenumber for getting flat bands, and give an intuitive explanation for their origin by constructing coarse-grained lattice models. Our work provides new, flexible platforms for exploring interaction-driven phases in 2D systems with arbitrary superlattice symmetries.

*MT and HC were supported by the start-up funding of CSU.
Tuning the electronic structure and electron correlation in 2D twisted massive Dirac system: the case of twisted bilayer hBN

LEDE XIAN (Presenter), Max Planck Institute for the Structure and Dynamics of Matter, DANTE KENNES, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, NICOLAS TANCOCGNE-DEJEAN, MASSIMO ALTARELLI, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter — Recent experiments have suggested that twisted bilayer graphene (TBG) near magic angles can be an ideal platform for the study of strong correlation effects and unconventional superconductivity. Interestingly, our density functional theory (DFT) calculations show that flat bands also develop at both the top of the valence bands and bottom of the conduction bands in bilayer hBN with a twist. But different from the case of TBG systems, the band width of these flat bands decreases monotonically with twist angles and there is no appearance of any magic angles. We further use functional renormalization group (FRG) method to show that the flat band at the top of the valence bands can host exotic strong-correlated physics, such as the appearance of Mott insulator phase and unconventional superconductivity. Our study suggests that the gapless and massless characters of graphene is not essential in the observed strong-correlated phenomena and many more other 2D materials can also be explored in the form of twisted bilayer system for the study of unconventional superconductivity.

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 709382 (MODHET).

Tunable spin-polarized Mott insulator in twisted bilayer-bilayer graphene

XIAOMENG LIU (Presenter), ZEYU HAO, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, PHILIP KIM, Harvard University — Twisted bilayer graphene, forming a flatband at the magic angle, has become a new platform to study correlated electron states. Superconductivity and Mott insulator phase have been demonstrated in this system. However, the flatband only occurs at a specific twist angle, which is both hard to achieve and lacks tunablity to enable other emergent phenomena.

Here we report experiments on twisted bilayer-bilayer graphene, where two Bernal-stacked bilayer graphene are placed together with a small twist angle. Due to the tunable band structure of bilayer graphene with displacement fields, we can achieve flatband structure in a large range of twist angles. At each twist angle, we observed Mott insulator phase at 1/2 filling in a specific range of displacement fields. Under a parallel magnetic field, additional insulating states emerge at 1/4 and 3/4 filling while the 1/2 filled insulating state become more robust. This suggest the 1/2 insulator is a spin-polarized state.

The nature of correlations in the insulating states of twisted bilayer graphene

MARÍA JOSÉ CALDERÓN (Presenter), JOSÉ MARÍA PIZARRO, ELENA BASCONES, Instituto de Ciencia de Materiales de Madrid, CSIC — The recently observed superconductivity in twisted bilayer graphene emerges from insulating states believed to arise from electronic correlations. While there have been many proposals to explain the insulating behavior, the commensurability at which these states appear suggests they are Mott insulators. We focus on the insulating states with ±2 electrons or holes with respect to the charge neutrality point. We show that the theoretical expectations for the Mott insulating states are not compatible with the experimental dependences on temperature and magnetic field if, as frequently assumed, only onsite (local) correlations are included. We argue that the inclusion of intersite correlations in the treatment of the Hubbard model can bring the predictions for the magnetic and temperature dependencies of the Mott transition to an agreement with experiments. The importance of these non-local correlations indicates that the observed insulating gap is not the one between the Hubbard bands and that antiferromagnetic-like correlations play a key role in the Mott metal insulator transition. arXiv:1805.07303.

On the nature of the correlated insulator states in twisted bilayer graphene

MING XIE (Presenter), ALLAN MACDONALD, Department of Physics, University of Texas at Austin — We use self-consistent Hartree-Fock calculations performed in the full π-band Hilbert space to assess the nature of the recently discovered correlated insulator states in magic-angle twisted bilayer graphene (MATBG). We show that at integer number of electrons per moiré period, the mean-field ground states break the combined two-fold rotation and time reversal symmetry $C_2T$ that protects the moiré-band Dirac points, inducing gaps and establishing valley projected bands that have non-zero Chern numbers. Broken spin/valley flavor symmetries then enable gapped states to form not only at neutrality but also at moiré band filling $n = \pm p/4$, where $p$ is the number of electrons per moiré period. We predict that the MATBG ground states at $n = \pm 1/4$ and $n = \pm 3/4$ have an anomalous Hall effect, and discuss the implications of our findings for theories of magic-angle superconductivity.
GREGORY HOLDMAN (Presenter), WYATT BEHN, ZACH KREBS, KEENAN SMITH, BENNY TOCK, VICTOR W BRAR, University of Wisconsin - Madison — Bilayer graphene (BLG) is known to have a dynamic electronic structure including a continuously tunable bandgap, and correlated electron behavior under a variety of conditions. To better understand these phenomena, it is important to develop local probes that can directly determine how these effects manifest in the presence of defects and impurities. In many semiconducting or metallic systems, scanning tunneling spectroscopy (STS) can serve as such a local probe. However, STS necessarily applies a local electric field to the system it measures. For BLG, this field can alter the local band structure by breaking the symmetry of the two layers and simultaneously doping the surface. This dynamic band structure modification makes STS measurements of BLG difficult to interpret and prevents straightforward extraction of the material parameters. In this talk, we show how these effects can be modeled and understood by computing the expected voltage-dependent tunneling spectrum of a BLG sheet between two gate electrodes. We compare this model to STS data taken from BLG/SiO₂ and BLG/h-BN systems under UHV conditions at a temperature of 4 K and show how to extract the BLG bandgap from STS measurements performed at different back-gate voltages.

10:24AM R14.00013: Graphene quasicrystal
PILKYUNG MOON (Presenter), Department of Physics, New York University Shanghai, MIKITO KOSHINO, Department of Physics, Osaka University, YOUNG-WOO SON, School of Computational Sciences, Korea Institute for Advanced Study — Quasicrystals have been used to study quantum states between the limits of periodic order and disorder. Recently, we reported that quasicrystals can be realized by stacking atomic layers at a specific configuration [1]. And, as a specific example of such designer quasicrystals, we reported a graphene quasicrystal composed of two graphene layers stacked at a rotation angle of 30°.
In this talk, I will discuss the theory of Dirac electrons in a graphene quasicrystal and show the characteristic features of this structure [2]. I will first report a rigorous effective model of the electronic structures of graphene quasicrystal. Then, I will show the emergence of the critical states, which are neither perfectly localized nor fully extended, and reveal the origin of these states as well as the minimum wave functions for describing the electronic structures. In addition, I will show that the wave functions show 12-fold rotational symmetry and report the band dispersion of graphene quasicrystal.

*P.M. was supported by NYU Shanghai Start-Up Funds, NYU-ECNU Institute of Physics, NYU Global Seed Grants for Collaborative Research.

10:36AM R14.00014: Flat bands due to twisted bilayer graphene: A coordinate transformation approach
DAVID SCHMELTZER (Presenter), City College of the City University of New York, AVADH SAXENA, Los Alamos National Laboratory — We consider two-layer graphene with one layer twisted by a small angle θ. This can be investigated using a coordinate transformation given by an angle θ with respect to the untwisted layer. For the untwisted layer two sublattices are a(\textbf{R}) and b(\textbf{R} + δ) and in the twisted layer we have A(\textbf{R}') and B(\textbf{R}' + δ). We consider hopping between the two layers −ta,A and −ta,B. As a result, we obtain four eigenvalues. Two eigenvalues have low energy with vanishing dispersion as a function of the angle. The solution is based on the replacement of the twisted coordinate in the momentum space by a spinor transformation B'σ(k'(\textbf{k})) = exp(iσ3θ/2) Bσ(\textbf{k}). In the presence of interaction the coordinates are affected by the transformation and thus contain the phase exp(iσ3θ/2).

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R15 DMP: 2D Materials (Semiconductors) -- Processing and Characterization
154 - Han Wang, University of Southern California - Tag(s): Focus

8:00AM R15.00001: Recent STM Studies of Gate-tunable 2D Material Devices
JIONG LU (Presenter), ZHIZHAN QIU, HANYAN FANG, Department of Chemistry, National University of Singapore — 2D materials with reduced dimensionality exhibit unprecedented tunability in both their electronic and optical, chemical properties due to the high susceptibility to the doping and the change of many-electron effects. Here we demonstrate a tunable band gap modulation in back-gated 2D material devices. Using low-temperature scanning tunnelling microscopy (LT-STM), we probed the quasiparticle electronic bandgap of recently emerged 2D materials such as black phosphorus (BP) and 2D TMDCs as a function of electrostatic gating. The demonstration of an electrical field tunable bandgap in 2D material devices paves the way to designing electro-optic modulators and photodetector devices that can be operated in a wider electromagnetic spectral range.

*Ministry of Education (Singapore): R-143-000-A06-112
**8:12AM R15.00002: Real-space Observation of Charge Separation in Mixed Dimensional InSe-C\textsubscript{70} van der Waals Heterojunctions**

SHAOWEI LI (Presenter), CHENGMEI ZHONG, ALEX HENNING, MARK HERSAM, Northwestern University —

Two-dimensional InSe is a direct bandgap semiconductor promising for high performance photodetectors and solar cells. Mixed dimensional p-n heterojunction between InSe and organic molecules integrates desirable properties of both. Electronic structure of surface states is critical for optimal band offsets at the heterojunction. Although there is no consensus on the type of intrinsic doping, few-layered InSe field-effect transistors showed exclusively n-type behavior. Here, we report that the atomically clean surface of mechanically exfoliated InSe is unintentionally p-doped. STS taken over the native surface selenium vacancies resolves occupied defect states near the valance band edge. These defect states lead to an upward band bending near the InSe surface, rendering InSe surface p-type. In prototype InSe/C\textsubscript{70} heterojunction, PL spectroscopy and STS both indicate formation of a type-II heterojunction. Electrons can transfer between InSe and C\textsubscript{70} evidence from mutual PL quenching of both InSe and C\textsubscript{70}. STS in vacuum and KPFM in the ambient consistently reveal the electron transfer from InSe to C\textsubscript{70} resulting in a photovoltage of \(\sim 0.25\) eV. This study reveals the unusual electron donor behavior of InSe in an organic-inorganic heterostructure.

**8:24AM R15.00003: Atomically thin dichalcogenide heterostructures and interfaces measured via cathodoluminescence in scanning transmission electron microscope**

AKSHAY SINGH (Presenter), HAEYEON LEE, SILVIJA GRADECAK, Massachusetts Institute of Technology — Atomically thin transition metal dichalcogenides (TMDs) and associated heterostructures have distinct opt-electronic properties including enhanced luminescence and high on-off current ratios. However, optoelectronic properties measured using conventional methods are limited to micro-milimeter scale and with no direct structural correlation, despite the fact that relevant property fluctuations can be caused by significantly smaller structural features. We use cathodoluminescence (CL) in a scanning transmission electron microscope (STEM) as a nanoscale probe that offers direct structure-optical correlation with high spatial resolution. We present the first, to our knowledge, STEM-CL measurements of monolayer tungsten disulfide (WS\textsubscript{2}) encapsulated between hexagonal boron nitride (HBN). We measure spatially inhomogeneous luminescence resulting from variations in the interface quality between layers, and provide a direct way to probe optical properties of TMD heterostructures on the nanoscale. We also discuss role of the electron beam and the ways to minimize it to measure intrinsic properties of TMDs. STEM-CL offers to be a powerful method to directly measure structure-optical correspondence, with applications in measuring lateral or vertical TMD heterostructures and alloys.

**8:36AM R15.00004: Carrier density tuning in single layers of WS\textsubscript{2} via photochlorination**

GEORGE KIOSEOGLOU (Presenter), IOANNA DEMERIDOU, IOANNIS PARADISANOS, Institute of Electronic Structure and Laser - FORTH, and University of Crete, Greece, PANOS PATSALAS, Department of Physics, Aristotle University of Thessaloniki, Greece, EMMANUEL STRATAKIS, Institute of Electronic Structure and Laser - FORTH, and University of Crete, Greece — Monolayers of Transition Metal Dichalcogenides (TMDs) of the form MX\textsubscript{2} (M=Mo or W and X=S or Se) are promising semiconducting materials for future 2D nanoelectronics due to their unique properties. Carrier modulation and doping reversibility are very important issues in the study of the electronic properties of TMDs and at the heart of many applications. We demonstrate electron density control in chlorine-doped WS\textsubscript{2} monolayers by pulsed laser irradiation in a precursor gas atmosphere [1]. The increase of the photochlorination time gives rise to a systematic red-shift in the PL energy of the neutral exciton indicating a reduction in the electron density. This electron withdrawing process enabled also the determination of the trion binding energy of the intrinsic crystal, found to be 20 meV, in accordance to theoretical predictions. At the same time, it is found that the effect can be reversed upon cw laser rastering of the monolayer in air. SAM and XPS reveal that chlorine physisorption is responsible for the e-density modulation induced by the pulsed laser photochemical reaction process and confirmed by DFT calculations. [1] I. Demeridou et al, 2D Mater. 6 (2019), 015003

*This work is supported by the GSRT Greece under the project FLAG-ERA II - JTC2017 - GRFAR - GRAPH-EYE*
Surface Oxidation Induced P-doping in Transition Metal Dichalcogenides

MINJU KIM (Presenter), JUNKYEONG JEONG, DONGGUEN SHIN, JEEHONG PARK, JAEHYUN YANG, SANGWAN CHO, Department of Physics, Yonsei University, HYUNBOK LEE, Department of Physics, Kangwon National University, YEONJIN YI, Department of Physics, Yonsei University — Transition metal dichalcogenides (TMDCs) has received tremendous attention due to their fascinating electrical properties, such as a high carrier mobility, high on/off ratio and tunable bandgap. However, TDMC-based electronic devices do not show their pristine properties due to the contact resistance between the metal electrode and TMDCs. Surface oxidation has been known to induce a p-doping and it improves the contact resistance. With optimum oxidation, highly improved contact was evidently observed in field-effect transistors, while it is rather worsen with non-optimum conditions. To elucidate the origin of improvement, the changes in the electronic structure of TMDCs upon the surface oxidation should be understood. In this regard, the electronic structure of TMDCs was studied with ultraviolet and x-ray photoemission and inverse photoemission spectroscopy (UPS/XPS/IPES). TMDCs were treated with UV-ozone and the changes in oxidation states of TMDCs were investigated with XPS. Then, the changes of work function and band edges were directly observed with UPS and IPES. The surface oxidation can control the position of band edges efficiently.

* NRF of Korea: SRC program (vdWMRS center)

Modulation doping in hexagonal BN atomic-layer semiconductor

SUSUMU SAITO (Presenter), YUUTO MATSUURA, YOSHITAKA FUJIMOTO, Tokyo Institute of Technology — We study the stable stacking sequences and the electronic properties of hexagonal BN (h-BN) trilayers within the framework of the density functional theory. Because of its lower-symmetry geometry of the h-BN sheet than that of graphene, there appear several different stable stacking sequences in the h-BN trilayers. Interestingly, most of stable stacking sequences of trilayers are found to be different from that of the bulk phase. It is also found that spatial distributions of both the valence-band top states and the conduction-band bottom states are rather confined to a certain specific layer in stable h-BN trilayers. By utilizing this fact, we design the C-doped h-BN trilayers where carriers conduct not in the doped layer but mostly in the undoped perfect layer. These systems are therefore considered to be the ultimate modulation-doped semiconductor heterostructure where both the doped region and the conducting region are only one atomic-layer thick. We also discuss several four-layer and five-layer h-BN systems which can host further clear spatial modulation doping.

*This work was partly supported by MEXT Element Strategy Initiative to From Core Research Center through Tokoday Institute for Element Strategy, JSPS KAKENHI Grant Numbers JP17K05053 and JP25107005.

Doping dependent magnetic properties in monolayer PdSe2

YOSEP CHO (Presenter), HYOUNG JOON CHOI, Physics, Yonsei University — In recent years, ferromagnetism in two-dimensional materials which is induced by charge doping drawn great interest. Density functional theory (DFT) calculations with changing the total number of electrons predict that increase of hole doping leads to ferromagnetism in monolayer (ML) PdSe\textsuperscript{2}. In this work, we investigate doping dependent magnetism in ML PdSe\textsubscript{2} using supercells with differently substituted impurities. Moreover, we performed virtual crystal approximations (VCA) for uniform and non-uniform doping to see doping method dependence for the magnetism. To understand the magnetism in this material, we discuss local-moment interactions and Stoner-type mechanism.

*This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2017-C3-0079).
**9:24AM R15.00008: All-optical quality assessment of 2D TMDs using polarization-resolved SHG**  
EMMANUEL STRATAKIS (Presenter), Institute of Electronic Structure and Laser - FORTH, and University of Crete, Greece, SOTIRIS PSILODIMITRAKOPoulos, LEONIDAS MOUCHLIADIS, IOANNIS PARADISANOS, ANDREAS LEMONIS, Institute of Electronic Structure and Laser - FORTH, Greece, GEORGE KIOSEOGLOU, Institute of Electronic Structure and Laser - FORTH, and University of Crete, Greece — While large-area crystal growth techniques, such as chemical vapor deposition (CVD), are successfully used to produce 2D transition-metal dichalcogenides, the presence of grain boundaries, vacancies and arbitrarily oriented grains, substantially affect their crystal quality. We demonstrate a fast, high-resolution non-linear optical method for the quality control of WS2 monolayers. Polarization resolved second harmonic generation (PSHG) imaging reveals with high-precision the orientation of the main crystallographic axis (armchair). By performing a pixel-by-pixel mapping of the armchair orientations on a CVD-grown sample area, we can distinguish between different domains, locate their boundaries and reveal their detailed structure. We fit experimental PSHG images of sub-micron resolution into a generalized theoretical model and we acquire the armchair orientation for every pixel. This allows us to measure the mean orientational average of armchair angle distributions from specific regions of interest and consequently to define the standard deviation of these distributions as a crystal quality factor. [1] S. Psilodimitrakopoulos, et al., Light Science & Applications 7, 18005 (2018).

*This work is supported by the GSRT Greece under the project FLAG-ERA II-JTC 2017-GRFAR-GRAH-EYE

**9:36AM R15.00009: Chemically Tunable 2D Layered Materials: Acoustic Phonons, Charge Density Waves, & Phase Transitions** [Invited] KRISTIE KOSKI (Presenter), University of California, Davis — I will present an innovative strategy to intercalate atomic species including heavy metals, semiconductors, and semimetals (Ag, Au, Bi, Cr, Cu, Ge, Mn, Mo, Ni, Os, Pb, Pd, Pt, Rh, Ru, Sb, W) into 2D layered materials. With intercalation of zero-valent elements, fundamentally new physical behaviors arise such as chemically-controllable commensurate and incommensurate charge density waves, altered acoustic phonons as measured with Brillouin scattering, and chemically-tunable pressure-dependent phase transitions. This strategy can be further used to achieve 2D metal-semiconductor heterostructures or 2D semiconductor heterostructures with unique physical properties. Chemically tunable physical properties of intercalated Bi2Se3, Si2Te3, GeS and MoO3 are demonstrated.

**10:12AM R15.00010: Understanding bound excitons in 2D monolayer semiconductors with nano-optical imaging and spectroscopy**  
NICHOLAS BORYS (Presenter), Physics, Montana State University, THOMAS DARLINGTON, Physics, University of California, Berkeley, JIM SCHUCK, Mechanical Engineering, Columbia University, ANDREY KRAYEV, Horiba Scientific — Bound excitons in 2D semiconductors are of interest as potential qubits as well as single-photon emitters for quantum computing and information applications. But our limited understanding of these states inhibits overcoming several challenges that they pose for integration into practical technological applications. One such issue is the suppression of bound excitons at temperatures above ~150 K. Employing a suite of time-resolved and nano-optical spectroscopy studies, we find that the thermally-activated process suppresses their formation and develop a nano-optical architectural motif to reverse this suppression and activate the states at room-temperature. Furthermore, using nano-optical imaging and spectroscopy, distinct bound exciton states are optically imaged within strain-induced potentials at resolutions down to 20 nm. This nanoscale resolution allows us to measure the extent to which these states are localized as well as identify how nanoscale strain controls their excited-state properties. From these studies, we can begin to envision how to use nano-optical antennas to integrate patterns of bound exciton states in two-dimensional monolayer semiconductors for model optoelectronic and room-temperature quantum devices.

**10:24AM R15.00011: Laser annealing for Large Excitonic Reflectivity from MoSe2 grown by Chemical Vapor Deposition**  
CHRISTOPHER ROGERS (Presenter), DODD J GRAY, NATE BOGDANOWICZ, HIDEO MABUCHI, Stanford University — We present data of a laser annealing procedure which drastically improves the quality of suspended monolayers of chemical vapor deposition grown MoSe2. Annealing with a green laser locally heats the suspended flake, which both removes contaminants and reduces strain gradients. At 4 K, we observe linewidths as narrow as 3.5 meV (1.6 nm) full width at half maximum for both photoluminescence and reflection. Large peak reflectances up to 47% are also observed. These values are comparable to those of the highest quality hexagonal boron nitride encapsulated samples. We demonstrate that this laser annealing process can yield spatially homogeneous samples where the length scale of the homogeneity is limited primarily by the size of the suspended area. Annealed regions are very stable, exhibiting negligible deterioration over 24 h at cryogenic temperatures. The annealing method is also very repeatable.

*This work was funded in part by the National Science Foundation (NSF) Award No. PHY-1648807, and by the NSF Award No. DMR-1838497.
Spontaneous Curvature of Janus Transition Metal Dichalcogenide Nanoribbons: Effects on Optoelectronic, Magnetic and Mechanical Properties  JARON KROPP (Presenter), FATIH ERSAN, CAN ATACA, University of Maryland, Baltimore County — Janus transition metal dichalcogenides (TMDs) are two-dimensional materials of the form MXY (M = Mo, W; X, Y = S, Se, Te). These materials are similar to traditional TMDs with structure MX₂, but with one chalcogen layer replaced by another chalcogen type. In this work, we study freestanding armchair and zigzag nanoribbons of the Janus materials Mo/WSSe, Mo/WSTe, and Mo/WSeTe using density functional theory. The lattice mismatch between the X and Y sides of the material causes curvature of the unsupported ribbons. We investigate the magnetic and electronic properties of these structures as a function of ribbon width and curvature angle. Zigzag nanoribbons are found to be metallic while armchair nanoribbons are semiconducting with a band gap that depends on the ribbon width. Additionally, all zigzag nanoribbons possess a magnetic moment while armchair ribbons may not. We also study the effects of edge passivation on both armchair and zigzag nanoribbons. Hydrogen passivation was found to increase the band gap, enhance the stability of nanoribbon edge and induce a magnetic moment in the armchair ribbons. This work sheds light on how the spontaneous curvature of the nanoribbons affect/enhance the optoelectronic, magnetic and mechanical properties.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R16 DMP: Transport in Nanostructures -- Electron-phonon Coupling and Phonon Transport in Nanostructures and Heterostructures BICEC 155 - Charles Harris, Sandia National Laboratories - Tag(s):
Focus

8:00AM R16.00001: Spatially-Resolved Non-Equilibrium Phonon Transport Across Nanoscale Interfaces* GEORGIOS VARNAVIDES (Presenter), Department of Materials Science, Massachusetts Institute of Technology, ADAM JERMYN, Kavli Institute for Theoretical Physics, University of California at Santa Barbara, POLINA ANIKEEVA, Department of Materials Science, Massachusetts Institute of Technology, PRINEHA NARANG, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Understanding phonon-mediated heat transfer at the nanoscale, to explain heat-dissipation in nanoelectronics, local temperature effects, and new phenomena probed my ultrafast coherent dynamics, presents a theoretical challenge. Further, nanoscale interfaces pose an exciting experimental frontier, with diverse applications from interface-engineering for thermoelectrics to catalytic interfaces and nanotheranostic agents. Despite the ubiquity of these applications, an accurate microscopic description of thermal interface resistance (TIR) remains elusive. To address this, we introduce a new theoretical and computational framework for semi-classical transport with position-, momentum-space, and scattering event resolution. We demonstrate the recursive formalism for phonon transport in a spherical nanoparticle, and highlight new insights made possible using this multi-dimensional resolution. We extend the formalism to handle interfaces explicitly to quantitatively capture TIR for the technologically relevant Si-Ge heterostructure. Finally, we will present preliminary results in coherent and driven phonon effects, now accesible via ultrafast spectroscopies.

*GV, PN acknowledge support from ONR: N00014-18-1-2691.
ASJ acknowledges support from GBMF: GBMF7392 and NSF : PHY-1748958.

8:12AM R16.00002: Unconventional Impact of Interfacial Thermal Coupling in Film-On-Substrate Systems KARTIK KOTHARI (Presenter), ABHINAV MALHOTRA, MARTIN MALDOVAN, Georgia Institute of Technology — An accurate determination of thermal transport in thin film-on-substrate (FOS) architectures is crucial to optimum performance of nanostructured optoelectronic devices. A rigorous treatment of the nanoscale interfacial coupling between materials accounting for dispersion mismatch, interfacial roughness and shadowing effects is imperative in studying the impact of substrates on thin-film heat conduction. In a unique finding, we discover an increase in thermal conductivity with a reduction in thin-film thickness attributed to phonon injection from the substrate layer. We examine the in-plane and cross-plane configurations of thermal conduction in Ge and Al₀.₁Ga₀.₉As thin-films mounted over Si and GaAs substrates respectively. We provide an extensive analysis of phononic coupling and contrast the results with bulk and isolated thin film values. We present a detailed microscopic and spectral analysis by investigating the spatial thermal flux distribution, modal thermal conductivity, and mean free path and frequency spectra in the FOS architecture. We demonstrate how interlayer phonon coupling opens new avenues for thermal conductivity manipulation in nanostructures and achieves desired thermal properties for rational thermal material design in microelectronics and optoelectronics.
8:24AM R16.00003: Modeling phonon transport in nanowires with rough surfaces  SID ABHINAV (Presenter), KHANDKER A MUTTALIB, University of Florida — We study phonon transmission in thin silicon nanowires where surface-roughness dominates over bulk disorder. Our previous study was based on an exact mapping of surface disorder, modeled as a random distribution of localized phonons\(^1\). Here we extend the idea to study its effects on transport of propagating acoustic phonons. We characterize the localized phonons by surface roughness parameters and study the effects using NEGF techniques. Non-linear heat current is evaluated for various couplings between the propagating phonons from the leads and the localized phonon in the central device. Numerical evaluation gives frequency dependence of heat current at various finite temperatures, where the difference in temperature between the two leads can be large under non-equilibrium conditions. We show that our simple model captures the qualitative features obtained in experiments, and suggests combination of surface parameters that can lead to a substantial reduction in thermal conductivity, as required for applications in thermoelectricity.

Reference: (1) https://doi.org/10.1103/PhysRevB.96.075403

8:36AM R16.00004: Phonon-dominated thermal transport in an ultrathin Au-Ni bilayer  ALEXEI MAZNEV (Presenter), Department of Chemistry, Massachusetts Institute of Technology, JAN-ETIENNE PUDELL, MARC HERZOG, Institut für Physik & Astronomie, Universität Potsdam, MATTHIAS KRONSEDER, Physics Department, Technical University Munich, CHRISTIAN BACK, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, GREGORY MALINOWSKI, Institut Jean Lamour, Université Lorraine, ALEXANDER VON REPPERT, MATIAS BARGHEER, Institut für Physik & Astronomie, Universität Potsdam — Thermal conductivity in metals is normally predominantly electronic. However, at small distances, the phonon contribution to thermal transport becomes increasingly important, especially in metals with weak electron-phonon coupling such as Au. In this report, we show that thermal transport in an Au-Ni bilayer becomes predominantly phononic when the Au thickness is ~6 nm or less. We analyze recent ultrafast x-ray diffraction measurements of heat transport in an ultrathin metal bilayer consisting of 5.6 nm Au and 12 nm Ni \(^1\) together with earlier measurements on a thicker bilayer \(^2\) and show that in the experiment \(^1\) more than 50% of the heat flow from the Ni lattice to Au lattice was carried by phonons, despite a high thermal boundary resistance for phonon heat transport due to a large mismatch of the phonon spectra. The measurements reported in Ref. \(^1\) offer a way to study heat transport by phonons in multilayer structures on the single digit nanometer scale and could be used for direct testing of non-equilibrium molecular dynamics simulations.

\(^1\) J. Pudell et al., Nature Commun. 9, 3335 (2018).

8:48AM R16.00005: Beyond diffusive scattering: Phonon coupling to reduce thermal conductivity  ABHINAV MALHOTRA (Presenter), KARTIK KOTHARI, MARTIN MALDOVAN, Georgia Institute of Technology — Diffusive scattering has remained the only mechanism to reduce thermal conduction at the nanoscale. In this talk, we show that phonon coupling in layered nanomaterials (bi-layers and tri-layers) can be engineered to reduce the thermal conductivity of a silicon thin-film below its free-standing value. We present a methodology to quantitatively evaluate the impact of phonon coupling on each layer in layered nanostructures. We evaluate the dependence of resultant thermal conductivity modulations on structural parameters and find that they are critically dependent on layer spacings and interface properties. The results of this work open new avenues within the rational thermal design by elucidating a new method that can be used to reduce thermal conductivities beyond the traditional diffusive scattering based approaches. The prospects of being able to modulate the thermal conductivity can radically change how we control heat flow in electronic, optoelectronic, and thermoelectric materials.

9:00AM R16.00006: Electronic Thermal Transport in h-BN/Graphene/h-BN heterostructures* [Invited]  MIR MOHAMMAD SADEGHI, LI SHI (Presenter), University of Texas at Austin — Using a sensitive differential electro-thermal measurement technique, we observe that the Lorenz number for the electronic thermal conductivity of h-BN/graphene/h-BN heterostructures is considerably lower than the Sommerfeld value in the single-band regime at room temperature and below. In the bi-polar regime near the Dirac point, a Lorenz peak well above the Sommerfeld value is observed at room temperature, and decreases with decreasing temperature. The deviation from the Wiedemann-Franz law and its temperature dependence provide insight into the unique transport behavior of Dirac Fermions in this system.

*This work is supported by Department of Energy Office of Basic Energy Science Award DE-FG02-07ER46377.
An Onsager reciprocity relation for ballistic phonon heat transport in anisotropic thin films of arbitrary orientation

GEOFF WEHMEYER (Presenter), Mechanical Engineering, Rice University, ANDREA D PICKEL, CHRIS DAMES, Mechanical Engineering, University of California, Berkeley — A classic Onsager reciprocity relation for Fourier heat conduction states that the thermal conductivity tensor in bulk anisotropic solids is symmetric. However, since Fourier's law fails in thin dielectric films due to ballistic phonon transport effects, it is natural to ask whether an analogous Onsager relation can be identified for thin films. To answer this question, we solve the Boltzmann transport equation (BTE) under the relaxation time approximation for in-plane and cross-plane heat transport in thin films with anisotropic phonon dispersion relations and scattering rates. These BTE solutions show that the effective thermal conductivity tensor of thin films is symmetric from the diffusive through the boundary scattering regime. We validate the BTE solution against previous atomistic simulations of arbitrarily aligned graphite thin films, and use published first-principles calculations to model anisotropic heat flow in black phosphorus thin films. This derivation shows how Onsager reciprocity for anisotropic heat conduction extends to the boundary scattering regime, and reduces the number of independent measurements required to characterize heat transport in anisotropic thin films.

Citation: G. Wehmeyer, A.D. Pickel, and C.Dames. PRB 98, 014304 (2018).

NSF #1106400

Surface Acoustic Wave Generation and Detection on LaAlO$_3$/SrTiO$_3$

DENGYU YANG (Presenter), YUN-YI PAI, YUHE TANG, YANG HU, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNGWOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — We aim to generate and detect surface acoustic waves (SAW) in LaAlO$_3$/SrTiO$_3$ heterostructures. Using a well-developed conductive-AFM lithography technique [1], we “sketch” interdigitated transducers (IDT) on LaAlO$_3$/SrTiO$_3$ “canvases”, which convert electronic signals into SAW and vice-versa. Two sets of IDTs are written on the structure to function as generator and detector. SAW can be used to generate dynamic potentials based on piezoelectric properties of LaAlO$_3$/SrTiO$_3$, and have the potential to drive electrons through nanostructures, a property that could be useful for quantum information applications.


JL acknowledges support from the Vannevar Bush Faculty Fellowship program, funded by ONR (N00014-15-1-2847). C-BE acknowledges support from NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-4046).

Electron Phonon Coupling in Metallic Superlattices

ANDRIUS BERNOTAS (Presenter), BRIAN DONOVAN, RONALD WARZOHA, Physics, United States Naval Academy, PATRICK HOPKINS, University of Virginia — Superlattices offer potential improvement in microelectronic transistor design as diffusion barriers between the silicon active layer and copper interconnects. While these materials provide a novel path forward in terms of electronic and atomic transport, more work must be done to understand potential thermal bottlenecks that could arise from their use in transistors. A major source of thermal buildup in microelectronic devices is the interaction between electrons and the surrounding atomic species in the form of electron-phonon coupling. In this project we explore the coupling between electrons and phonons as heat carriers in conductive multilayer superlattices of copper with tantalum, tungsten, and tantalum nitride. We use time domain thermoreflectance measurements and the two temperature thermal model to better understand the relationship between the electron phonon coupling in these materials and the physical parameters of the system. A greater understanding of this relationship will allow for greater control of the thermal properties of transistors, hopefully leading to increased thermal efficiency in microelectronics.
10:12AM R16.00010: Tuning the thermal boundary conductance at metal-dielectric interfaces by varying interlayer thicknesses  SHANY MARY OOMMEN (Presenter), Department of Physics and Astronomy, York University, Toronto, ON, Canada, SIMONE PISANA, Department of Electrical Engineering and Computer Science, York University, Toronto, ON, Canada — Interfaces play a significant role in the heat transport across boundaries at sub-micron length scales. Interfacial adhesion and phonon matching are important factors in determining the thermal boundary conductance, and the addition of an interlayer can be used to tune the heat dissipation. In this study, we analyze the modification of the thermal boundary conductance at metal-dielectric interfaces by insertion of metal interlayers with varying thicknesses from 2.5 Å to 100 Å. We show that the insertion of a tantalum interlayer at Al/Si and Al/sapphire interfaces hinders the phonon transmission across the interfaces and it plateaus at ~20 Å. We found that the addition of a nickel interlayer significantly increased the thermal interfacial conductance at both the Al/Si and the Al/sapphire interfaces. The nickel interlayer, having an intermediate Debye temperature as compared to the Aluminum layer and the substrates, increases the phonon transmission across the boundary. Thermal property measurements were performed through time domain thermoreflectance, and are in good agreement with a formulation of the diffuse mismatch model based on real phonon dispersions, accounting for anharmonic phonon scattering and phonon confinement within the interlayer.

10:24AM R16.00011: Lone-pair Electrons do not Necessarily Lead to Low Lattice Thermal Conductivity: an Exception of Two-dimensional Penta-CN$_2$  HUIMIN WANG (Presenter), Nanjing University — It has long been documented in literature that, the lone-pair electrons (LPE) are generally thought to lead to low lattice thermal conductivity ($\kappa_L$) of bulk materials by inducing strong phonon anharmonicity. Herein, we show an exceptional case of two-dimensional (2D) penta-CN$_2$ that possesses LPE but exhibits more than doubled $\kappa_L$ (660.71 W m$^{-1}$ K$^{-1}$) than the LPE free counterpart of penta-graphene (252.95 W m$^{-1}$ K$^{-1}$), which is unexpected and contradictory to the traditional theory of LPE leading to low $\kappa_L$. Based on the comparative study of four 2D systems possessing LPE and their respective LPE free counterparts (planar C$_3$N vs. graphene and penta-CN$_2$ vs. penta-graphene), the underlying mechanism is found lying in the bonds homogenization in penta-CN$_2$ due to the wide spatial extension of the non-symmetrically distributed LPE, which compensates the lattice anharmonicity due to LPE and is responsible for the opposite tendency of LPE affected $\kappa_L$ in the four 2D systems.

10:36AM R16.00012: Tuning thermal transport in nanostructures and nanostructured materials*  KONSTANTINOS TERMENTZIDIS (Presenter), CETHIL, INSA of LYON, CNRS — Due to the rapid evolution of nanomaterials elaboration the last decade a serie of nanostructures and nanostructured material like phononic-like crystals or nanowire networks are easily fabricated today. New physical phenomena are observed in such structures as ballistic phonon transport, phonon focusing, phonon tunneling and coherence effects. In general, nanostructured materials have a much lower thermal conductivity compared to bulk materials, due to phonon confinement and boundary scattering. Such phenomena will be presented with the present work. The thermal conductivity of a serie of structural, diameter, core/shell modulated and growth direction of silicon, silicon carbide and bismuth telluride nanowires and phononic like crystals and nanowire networks are easily fabricated today. New physical phenomena are observed in such structures as ballistic phonon transport, phonon focusing, phonon tunneling and coherence effects. In general, nanostructured materials have a much lower thermal conductivity compared to bulk materials, due to phonon confinement and boundary scattering. Such phenomena will be presented with the present work. The thermal conductivity of a serie of structural, diameter, core/shell modulated and growth direction of silicon, silicon carbide and bismuth telluride nanowires and phononic like crystals and parameters like neck distance, hole diameter, amorphisation of pores and filling of a second type of material will also be presented using atomistic and mesoscopic simulations. The purpose is to appraise the impact of surface roughness, amorphous parts integration, diameter modulation as well growth direction on the thermal conductivity reduction. The addition of both amorphous regions and nanoconstrictions hinder the thermal conductivity even under the amorphous limit, while preserving a large crystalline volume fraction.

*CNRS

10:48AM R16.00013: Calculating lattice thermal conductivity: A comparative study on carbon nanotubes.  DANIEL BRUNS (Presenter), JOERG G ROTTLER, A. SRIKANTHA PHANI, ALIREZA NOJEH, University of British Columbia — Carbon nanotubes (CNTs) are commonly utilized in nanoscale devices. High structural order, rigid sp$^2$-bonds and a low atomic mass result in an exceptionally high lattice thermal conductivity (TC), which motivates their use in applications demanding efficient heat removal. However, pinpointing exact TC values of individual defect-free CNTs remains a challenge both experimentally and computationally. The thermal transport properties of ideal CNTs are dominated by phonon-phonon scattering, and a theoretical prediction of TC has to include anharmonic terms in the interatomic potential energy which give rise to phonon-phonon interaction. Here we compare two computational frameworks that take into account lattice anharmonicity to predict TC: classical molecular dynamics (MD) vs. anharmonic lattice calculation (ALC). Taking the same empirical interaction potential as input to both MD and ALC, we contrast phonon-phonon scattering rates and TC results as a function of temperature. This comparison also allows us to critically evaluate several assumptions in the different methods, namely the description of anharmonicity by a truncated Taylor expansion of the interaction potential in ALC, the use of classical phonon statistics in MD, and the importance of Umklapp processes for the TC.
New directions for random search* [Invited]  
CHRIS PICKARD (Presenter), University of Cambridge —

Genuinely new knowledge and scientific insight can be obtained about dense matter by combining random numbers with reliable and efficient first principles methods. Diverse ensembles of initial structures can be generated, and structurally optimized. The resulting low energy structures are candidates for stable, and metastable, phases and/or defects that might be experimentally realized. This, of course, depends on a sufficiently broad and thorough sampling of configuration space.

Algorithms which attempt to learn from (computational) experience are necessarily sequential, and correlated. A purely random strategy, as employed by Ab Initio Random Structure Searching (AIRSS),[1,2] is entirely parallel, and a natural fit to the high throughput computation (HTC) paradigm. The absence of correlation between the independent random samples ensures that it is possible to estimate when a sufficiently dense sampling has been achieved (or at least, has not been achieved). Challenging cases can be tackled by designing the initial random structures so that they focus the search in regions of configuration space that are anticipated to yield success.

The design of these random “sensible” structures will be explored, along with some new directions which promise to accelerate random search, and recent applications to materials under extreme compression.

[2] Released under the GPL2 license: http://www.mtg.msm.cam.ac.uk/Codes/AIRSS

* C.J.P. is supported by the Royal Society through a Royal Society Wolfson Research Merit award and the EPSRC through Grants No. EP/P022596/1.

Theoretical Prediction of Superhard Materials with the XtalOpt Evolutionary Algorithm  
XIAOYU WANG (Presenter), PATRICK AVERY, Department of Chemistry, University at Buffalo, State University of New York, DAVIDE PROSERPIO, Università degli Studi di Milano, CORMAC TOHER, STEFANO CURTAROLO, Duke University, EVA ZUREK, Department of Chemistry, University at Buffalo, State University of New York —

The XtalOpt evolutionary algorithm for crystal structure prediction has been extended to enable the prediction of superhard stable materials. The hardness is calculated via a linear relationship with the shear modulus (originally discovered by Teter) as reported by Chen. The shear modulus is obtained via AFLOW-ML (Automatic FLOW for Materials Discovery - Machine Learning). A new fitness function has been implemented wherein the user can denote the percent contribution that hardness and enthalpy have on the fitness function. We have used XtalOpt to search for hard and stable carbon allotropes and found 44 hitherto unpredicted phases whose Vickers Harnesses were calculated to be greater than 45 GPa. The structural motifs in these phases were analyzed. We also discuss the thermodynamic and kinetic stability of the predicted structures, and potential ways in which they can be synthesized under pressure.
8:48AM R17.00003: Meta GGA (SCAN) + van der Waals functionals (rvv10) calculation for K-edge X-ray Raman Spectrum of the epsilon and zeta phase of solid oxygen* 

LE ANH (Presenter), Computational Applications Unit, RIKEN, Japan, MASAHIRO WADA, Graduate school of Material Science, University of Hyogo, Japan, ZHI LI, Xinjiang Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, China, HIROSHI FUKUI, Graduate school of Material Science, University of Hyogo, Japan, TOSHIAKI IITAKA, Computational Applications Unit, RIKEN, Japan — Previous theoretical studies could not predict precisely the epsilon-zeta transitional pressure which was measured at 96 GPa by experiments (Weck et al., PRL 2009, 102, 255503). The GW calculation showed the transitional pressure at 50 GPa (Kim et al., RPRB 2008, 77, 092104) while the B3LYP hybrid functional could estimate the co-existence range of epsilon-zeta from 75 GPa to 145 GPa (Ochoa-Calle et al., PRB 2015 92, 085148). The combination of meta GGA(SCAN) and van der Waals functional (rvv10) was demonstrated to enhance the direct epsilon-zeta transition at 70 GPa while the lattice parameters were very closed to the experimental data (in manuscript). On the other hand, the Inelastic X-ray Scattering (IXS) was successfully used to study epsilon phase of solid oxygen (Meng et al., PNAS 2008, 105, 33). In this talk, we will discuss the evolution of calculated IXS K-edge spectra from epsilon phase to zeta phase using SCAN+rvv10. The calculated spectra will be compared to the experimental data.

*This research was supported by MEXT as “Exploratory Challenge on Post-K computer” (Frontiers of Basic Science: Challenging the Limits) and the RIKEN iTHEMS Project and used the computational resources of the Hokusai supercomputer system provided by RIKEN Information Systems and Cybersecurity.

9:00AM R17.00004: Dynamic non-equilibrium chemical bonding pathways under thermomechanical compression

ANGUANG HU (Presenter), Defence Research and Development Canada — The most urgent need in the explosion science of chemical reactions is about time-resolved non-equilibrium processes on when and how mechanical work and thermal heat are deposited into molecules to initiate reactions. Using quantum solid-state chemistry calculations, multi-resolution and multi-scale dynamic non-equilibrium simulations were recently developed for chemical reactions under compression. The non-equilibrium reaction processes are characterized by the lowest resolution in reactant and resultant conformations, the intermediate resolution in energy, enthalpy, mechanical stress, and chemical shear flows, and the highest resolution in reactive modes selected by compression. The dynamic motion of these flows is governed by a number of equations with respect to time, including the conservation of momentum and energy together with effects of mechanical endothermic bond compression, thermal heat transfer, and exothermic energy release of bond breaking related to irreversible Arrhenius kinetics with volume change and energy barriers. It provides details of dynamic non-equilibrium chemical bonding pathways from quantum to continuum scales. Simulations agreed well with experimental observations such as shock compressed graphite transformed into hexagonal diamond.

9:12AM R17.00005: phq: a Fortran code to compute phonon quasiparticle properties and dispersions

ZHEN ZHANG (Presenter), Department of Applied Physics and Applied Mathematics, Columbia University, DONG-BO ZHANG, Beijing Computational Science Research Center, TAO SUN, Key Laboratory of Computational Geodynamics, Chinese Academy of Sciences, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics, Department of Earth and Environmental Sciences, Lamont-Doherty Earth Observatory, Columbia University — Intrinsic thermal shifts of phonon frequencies due to lattice anharmonicity may be significant in solids at high temperatures. As such, the calculation of phonon dispersions incorporating anharmonic effects is critical for predictive studies of vibrational, thermodynamic, and lattice transport properties. Here we introduce the phq code to compute anharmonic phonon dispersions of crystals that combines molecular dynamics (MD) and lattice dynamics calculations. The method invokes the concept of phonon quasiparticles to extract thermal shifts and phonon lifetimes from velocity autocorrelation functions projected into normal modes sampled by MD simulations. With the renormalized frequencies, it is possible to construct an effective harmonic force constant matrix that allows us to calculate the anharmonic phonon dispersion over the whole Brillouin Zone. Due to the nature of phonon quasiparticles, this approach is applicable not only to simply crystals, but also to complex crystal structures with many atoms per primitive cell with extra effort. We demonstrate successful applications of this code to weakly and strongly anharmonic systems. In addition to temperature-dependent anharmonic phonon dispersions, the vibrational entropy and free energy at constant volume can also be obtained.
9:24AM R17.00006: Evolutionary optimized PAW (EPAW) data-sets across the periodic table*  
KANCHAN SARKAR (Presenter), Department of Earth and Environmental Sciences, Lamont-Doherty Earth Observatory (LDEO), and Applied Physics and Applied Mathematics (APAM), Columbia University in the City of New York, RENATA WENTZCOVITCH, Department of Earth and Environmental Sciences, Lamont-Doherty Earth Observatory (LDEO), and Applied Physics and Applied Mathematics (APAM), Columbia University in the City of New York — We have recently designed and implemented a method named “Evolutionary Generator of projector augmented wave datasets” (EPAW-1.0) [1,2] to produce optimized projector augmented-wave (EPAW) data-sets. The generated EPAW data-sets are transferable and can be employed in Quantum ESPRESSO and ABINIT distributions for the accurate prediction of materials properties at the scalar relativistic level. The accuracy level is very close to the highly precise calculations by the all-electron full potential linearized Augmented-plane-wave (AE-FLAPW) approach as implemented in the WIEN2k code. The EPAW performance level in solid-state studies is nearly uniform over an enlarged pressure region and outperforms other standard PAW dataset libraries, ultra-soft, and norm-conserving pseudopotentials mentioned in the reported effort by Lejaeghere et al. [3]. Employing EPAW-1.0, we generate both LDA and GGA EPAW libraries especially for low-pressure calculations for elements across the periodic table.

2) K. Sarkar et al., COMPUT PHYS COMMUN,233 (2018), 110.
3) K. Lejaeghere et al., Science (80), 351 (2016).

*This work is supported primarily by grants NSF/EAR 1348066. NAWH is supported by NSF grant DMR-1507942.

9:36AM R17.00007: qha: A Python package for quasi-harmonic free energy calculation for multi-configuration system  
QI ZHANG (Presenter), Department of Applied Physics and Applied Mathematics, Columbia University in the City of New York, TIAN QIN, Department of Earth Sciences, University of Minnesota, KOICHIRO UMEMOTO, Earth-Life Science Institute, Tokyo Institute of Technology, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics, Columbia University in the City of New York — The quasi-harmonic approximation (QHA) offers an effective way of calculating the thermodynamic properties of many crystalline solids at high pressures and temperatures. In some cases, e.g., solid solutions or partially disordered systems such as H2O ice-VII, the system has numerous symmetrically distinct configurations. Here we present a Python package, qha, which can calculate the equation of state and various thermodynamic properties of both single- and multi-configuration crystalline systems in the framework of the QHA. This code has a wide range of applications, including, but not limited to, order-disorder phase transitions [1], solid solutions [2], complex defect stability [3], etc. Apart from its versatility, qha has been tested to be both accurate and computationally efficient. It can also be used as an all-in-one executable or taken apart into stand-alone functions, increasing its usability.


9:48AM R17.00008: Intrinsic Lattice anharmonicity and thermal conductivity of PbTe at High Temperature: Breakdown of the Phonon Minimal Mean Free Path Theory  
XINGJU ZHAO (Presenter), DONG-BO ZHANG, YONG LU, Beijing Computational Science Research Center, TAO SUN, Key Laboratory of Computational Geodynamics, University of Chinese Academy of Sciences, Beijing 100049, China — We investigated the vibrational property of lead telluride (PbTe) with a focus on lattice anharmonicity at relatively high temperatures using the phonon quasiparticle approach. The calculated anharmonic phonon dispersions are strongly temperature dependent and some phonon modes adopt giant frequency shifts. As a result, we witness the avoided crossing between transverse optical modes and longitudinal acoustic modes at elevated temperature, in good agreement with experimentation. These results reveal strong anharmonic effects in PbTe. The obtained phonon lifetimes allow studies of transport properties. For considered temperatures, the phonon mean free paths can be shorter than lattice constants at relatively high temperature, especially for optical modes. This finding goes against the widely employed minimal phonon mean free path concept. As such, the calculated lattice thermal conductivity of PbTe, which is indeed relatively small, does not have the prescribed minima at high temperature, showcasing the breakdown of the minimal mean free path theory. Our study provides a basis for delineating vibrational and transport properties of PbTe and other thermoelectric materials within the framework of the phonon gas model.
Predictions of materials properties at extreme conditions of pressures and temperatures are exceedingly important because it is challenging to obtain them experimentally. At the atomistic level, the accuracy of these predictions relies essentially on a satisfactory characterization of lattice anharmonicity which is generally pronounced at high temperatures. This has stimulated the development of several ab initio approaches to address anharmonic effects on lattice vibrations.

In this talk we present an overview of an ab initio method to address lattice anharmonicity based on the concept of phonon quasiparticles and illustrate its applications to some complex systems, e.g., (i) the vibrational and thermodynamic stabilization of cubic CaSiO3-pv at high temperatures, (iii) the hcp-bcc pre-melting transition in beryllium, and (iii) the irregular thermal shifts of IR frequencies and the breakdown of the well-known minimal phonon mean free path theory in MgSiO3-perovskite. We also introduce a computational package for high pressure and high temperature computational studies that interfaces with popular ab initio packages.

References:

*Dong-Bo Zhang was supported by NSFC under Grants Nos. 11674022 and U1530401, and by the Fundamental Research Fundsfor the Central Universities.

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R18 DCOMP: Frontiers in Theory of Physical Systems 8CEC 156B - Amy Liu, Georgetown University -
Tags: Focus

8:00AM R18.00001: Heterodimensional Plasmonic Stubs Enabling THz Electronics† MICHAEL SHUR (Presenter), ECSE and Physics, Rensselaer Polytechnic Institute, JOHN MIKALOPAS, GREGORY AIZIN, Physics, The City University of New York — Emerging TeraFET technology has yielded sensitive tunable detectors of terahertz (THz) radiation. Using plasmonic crystals incorporating TeraFETs to achieve the instability of the plasma waves enabling electronic THz sources could revolutionize the THz electronics. But this approach faces challenges related to matching the boundary conditions between dissimilar plasmonic regions. We report on using “plasmonic stubs” – the narrow regions of an increased width to match the conditions at the interfaces between different devices regions. The physics of the problem (explored using the hydrodynamic model) is similar to that of the water flow in a river of a variable width. The mathematics of the problem is based on the transmission line model. Our analysis shows how to achieve tunable plasmonic instability (supporting THz emission) using plasmonic stubs.

*This work was supported by the U.S. Army Research Laboratory Cooperative Research Agreement (Project Monitor Dr. Meredith Reed) and by the Office of Naval Research (Project Monitor Dr. Joe Qiu).

8:12AM R18.00002: Measurement and Analysis of Uncertainty in Mechanical Quality Factor and Implications for LIGO Thermal-Noise Estimation* IAN MACMILLAN (Presenter), GREGORY M HARRY, Physics, American University — With the continued push for more-sensitive gravitational wave interferometers, reducing coating Brownian thermal noise becomes increasingly essential. We report on the uncertainty in quality factor experiments, which are key measurements for predicting the thermal noise of the optics in gravitational wave detectors. Through repeated measurements, we investigate the distribution associated with quality factor measurements. We estimate these uncertainties in mechanical loss measurements and discuss their possible causes. Finally, we comment on the implications of our results for the Laser Interferometer Gravitational-Wave Observatory, LIGO.

*This research was made possible by the National Science Foundation grant 1453252, 1707920, and a grant from the NASA DC Space Grant Consortium.
8:24AM R18.00003: Diffusion of Multi-Speed Gear-Shifting Brownian Swimmers.∗ DON KRASKY (Presenter), DAISUKE TAKAGI, Mathematics, University of Hawaii at Manoa — We introduce a model for dispersion of independent swimmers jumping randomly between multiple translational velocities in arbitrary dimensions. Stochastic differential equations are introduced and used to produce simulations for comparison with theory. The associated Fokker-Planck equations are derived from the Langevin dynamics, giving an analytical prediction for the effective diffusion constant. This prediction is shown to be in good agreement with simulations, and is in a relatively simple form yielding a quick tool for experimentalists to obtain an accurate estimate of diffusion coefficient. A full analysis of the model is presented for the case with two velocities, and some extreme cases are discussed in the general model. We show adaptability of the model by fitting to three previous models of swimmers having two or three preferred velocities. These comparisons explore how stochastic vs. deterministic velocity changes and restricting certain velocity jumps result in different rates of dispersion.

∗This work was supported by the US ARO Grants W911NF-15-1-0608 and W911NF-17-1-0442

8:36AM R18.00004: Unification of Gas Breakdown and Electron Emission* AMANDA LOVELESS (Presenter), ADAM M DARR, SAMUEL DYNAKO, ALLEN GARNER, Purdue University — The miniaturization of technologies requires a deeper understanding of gas breakdown and electron emission at micro- and nanoscales. Previous work [A. M. Loveless and A. L. Garner, Phys. Plasmas, 24, 113522 (2017).] analytically unified Paschen's law (PL) for Townsend avalanche with field emission (FE) to show continuous reduction in breakdown voltage with decreasing gap size. Another study [G. Meng, et al., Phys. Plasmas, 25, 082116 (2018).] demonstrated this behavior experimentally and derived an analytic solution with a linear relationship between breakdown voltage and gap size in the field emission-Townsend regime. Further reductions in gap size result in the transitions to space-charge limited emission (SCLE). This paper assesses the transitions between FE and the Mott-Gurney (MG) law for collisional SCLE, MG to the Child-Langmuir (CL) law for vacuum SCLE, and CL to quantum scales with Schrödinger’s equation. These derivations yield a triple point, where FE, MG, and CL predict a common breakdown voltage at a specific gap size and pressure. The implications of these transitions will be discussed.

* This material is based on work supported by ONR under Grant No. N00014-17-1-2702, AFOSR under award number FA9550-18-1-0218, a DEPS Scholarship, and a Purdue Doctoral Fellowship.

8:48AM R18.00005: Nonlinear Evolution of Tearing Modes with Resistivity and Hyper-Resistivity* DING LI (Presenter), Chinese Academy of Sciences — The nonlinear resistive tearing modes with hyper-resistivity has been analytically investigated. In contrast to the flux average method used by previous works, in the present work the quasilinear method has been extended to obtain the time evolution equation for nonlinear tearing modes. This equation can describe the general evolution of nonlinear tearing modes with both plasma resistivity and hyper-resistivity effects, especially the transition between these two situations. It is difficult to obtain its analytical solution directly. One special solution has been obtained. It is found that the magnetic flux grows with time to the one third power. Some discussions about two limiting cases for resistivity or hyper-resistivity dominant will be presented.

*Supported by the National Natural Science Foundation of China under Grant Nos 11675257, and 11835016.

9:00AM R18.00006: A Coarse-Graining Procedure for Differential Equation Models PRANAV KANTROO (Presenter), BENJAMIN MACHTA, Yale Univ — The Renormalization Group framework gives a prescription to determine which macroscopic variables are relevant in a system and sufficient to describe large scale dynamics. Can we develop an analogous methodology to extract important parameters of dynamical systems in general? The Fisher Information Matrix (FIM) formalism measures the response sensitivity of a system to perturbations in its control parameters and has emerged as one way of extracting a hierarchy of relevant variables, even when renormalization isn’t straightforward. The relevant parameter directions are given by eigenvectors of FIM: the hierarchy of relevance is induced by the magnitude of their eigenvalues. This procedure has been done previously for discrete diffusion coarse-grained in time and for the lattice Ising model coarse-grained spatially (Machta et al 2013). Relevant parameters had Fisher information eigenvalues that remained large after microscopic data was discarded. We now extend this analysis to systems of stochastic differential equations utilizing a temporal coarse-graining scheme inspired from Compatible Monte Carlo: specific points in the system are held fixed while the rest of the system is free. Coarse-graining then corresponds to increasing the temporal separation between these fixed points.
Wiener-Khinchin theorem for Fourier-Laplace transformation; new derivation, and application to molecular simulations

AKIRA KOYAMA (Presenter), Department of General Education, National Institute of Technology, Toyota College, DAVID A NICHOLSON, MARAT ANDREEV, Department of Chemical Engineering, Massachusetts Institute of Technology, KOJI FUKAO, Department of Physical Sciences, Ritsumeikan University, TAKASHI YAMAMOTO, Graduate School of Science and Engineering, Yamaguchi University, GREGORY C RUTLEDGE, Department of Chemical Engineering, Massachusetts Institute of Technology — The Wiener-Khinchin theorem for Fourier-Laplace transformation (WKT-FLT) provides a general purpose method to calculate numerically the one-sided Fourier transformation of an arbitrary autocorrelation function (ACF) from molecular simulations. However, the existing derivation of the WKT-FLT equation includes some ambiguities. Moreover, the equation obtained always yields 2 artifacts in the data computed. In this work, we present a new derivation that eliminates these ambiguities and artifacts.

We define an ACF as a natural extension of the known ACF, and write its Fourier-Laplace transformation as the Fourier transformation of the product of the Heaviside unit step function and the ACF. As the result, we successfully obtain an equation for the WKT-FLT. Then, we discretized the WKT-FLT equation to compute the frequency-domain correlation function (FDCF) from numerical simulations. It is found that a correction term is needed in order to avoid over-counting and to satisfy the sum rule. With the correction term, an artifact previously observed in the real part of the FDCF disappears. On the other hand, another artifact still remains in the imaginary part of the FDCF. We will discuss the cause of this artifact.

Radiofrequency Bremsstrahlung of Electrons and Nanoparticles of Heterogeneous Plasma with a Condensed Dispersed Phase

VLADIMIR MARENKOV (Presenter), Odessa Mechnikov National University, Ukraine, SERGIY MOKHOV, University of Central Florida — The mechanism of braking radiation generation in the bulk of heterogeneous plasma formations has been studied in the framework of the statistical “cell” approach to the description of the ionization in heterogeneous plasma (HP). In our description of the effective interaction between microfields and charges in plasma, the stochastic motion of charged particles in HP is considered as an evolution of anharmonic oscillations executed by separate charges in an instant field of electric forces in the electroneutral cell. Effective values of frequency and the specific integral power of the braking radiation from HP in the radiofrequency spectral range are calculated by averaging over the ensemble of cells. The amplitude-frequency function and relative contributions of separate oscillation modes of plasma charges to the emitted radiation intensity are determined in the random phase approximation. A comparative analysis of the modeling data and the experimental data obtained for plasma with aluminum oxide nanoparticles was carried out in the space of key HP parameters. A good agreement between numerical results and experimental data was obtained at both qualitative and quantitative levels. Possible applications for telediagnostics of heterogeneous plasma formations were discussed.

Supernova, fluid instabilities, and interfacial mixing

SNEZHANA ABARZHI, Univ of Western Australia, AKLANT BHOWMICK, Carnegie Mellon University, ANNIE NAVEH (Presenter), Univ of Western Australia, ARUN PANDIAN, Carnegie Mellon University, ROBERT F STELLINGWERF, Stellingwerf Consulting, DAVID ARNETT, University of Arizona — Supernovae and their remnants are a central problem in astrophysics due to their role in the stellar evolution and nuclear synthesis. A supernova’s explosion is driven by a blast wave causing the development of Rayleigh–Taylor and Richtmyer–Meshkov instabilities and leading to intensive interfacial mixing of materials of a progenitor star. Rayleigh–Taylor and Richtmyer–Meshkov mixing breaks spherical symmetry of a star and provides conditions for synthesis of heavy mass elements in addition to light mass elements synthesized in the star before its explosion. By focusing on hydrodynamic aspects of the problem, we identify the properties of Rayleigh–Taylor and Richtmyer–Meshkov dynamics with variable acceleration, discover subdiffusive character of the blast wave-induced interfacial mixing, and reveal the new mechanism of energy accumulation and transport at small scales in supernovae.

*The work is supported by the University of Western Australia (AUS) via project grant 10101047, and the National Science Foundation (USA) via award 1404449.
9:48AM R18.00010: Validation of classical mixing rule coupled with van der Waals type equation of state for sound speed of non-ideal gas mixture*  
RYUJI TAKAHASHI (Presenter), NOBUYUKI TSUBOI, Department of Mechanical and Control Engineering, Kyushu Institute of Technology, TAKASHI TOKUMASU, Institute of Fluid Science, Tohoku University, SATOSHI WATANABE, SHIN-ICHI TSUDA, Department of Mechanical Engineering, Kyushu University — In the CFD analyses for the combustion chamber of liquid rocket engine, classical mixing rule (CMR) has been often applied to van der Waals (vdW) type equation of state (EOS) such as Soave-Redlich-Kwong (SRK) EOS for prediction of the thermodynamic properties of non-ideal gas mixture. However, the CMR has hardly been validated because of the lack of experimental data. In the present study, for validation of the CMR coupled with SRK EOS for sound speed, which is important to compute the flow field in the combustion chamber, we applied molecular dynamics (MD) method to a Lennard-Jones fluid with modified Lorentz-Berthelot rules that simulates oxygen-hydrogen gas mixture. For the computation of sound speed, NVEPG ensemble proposed by Meier and Kabelac (Meier, K. and Kabelac, S., J. Chem. Phys., 2006.) was employed. As a result, the sound speed from the CMR coupled with SRK EOS agreed with that from MD simulation: it was suggested that the CMR can be applied to sound speed of oxygen-hydrogen mixture system in supercritical condition corresponding to the inlet region of combustion chamber.

*This study has been supported by the Collaborative Research Project of the Institute of Fluid Science, Tohoku University.

10:00AM R18.00011: Nucleation of Quantized Vortices within a Quantum-Mechanical Compton Generator*  
MARTIN KANDES (Presenter), San Diego Supercomputer Center, University of California, San Diego, RICARDO CARRETERO, Department of Mathematics & Statistics, San Diego State University — In 1913, Arthur Compton invented a simple way to measure the rotation rate of the Earth with a tabletop-sized experiment. The experiment consisted of a large diameter circular ring of thin glass tubing filled with water and oil droplets. After placing the ring in a plane perpendicular to the surface of the Earth and allowing the fluid mixture to come to rest, he then abruptly rotated the ring, flipping it 180 degrees about an axis passing through its own plane. The result was that the fluid acquired a measurable drift velocity due to the Coriolis effect of the Earth. Compton measured this induced drift velocity by observing the motion of the oil droplets in the water with a microscope. This device, which is now named after him, is known as a Compton generator. The fundamental research objective of this project is to explore the dynamics of a quantum-mechanical analogue to the classical Compton generator experiment through the use of numerical simulations. Here, we present the first definitive results on the nucleation of quantized vortices within a quantum Compton generator and discuss future directions of the project.

*This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1053575.

10:12AM R18.00012: Using Monte Carlo and self-consistency to solve Newton's 2nd Law  
JAVIER HASBUN (Presenter), University of West Georgia — In working with Newton's 2nd law, given a force, one seeks to solve for the position, x(t), and the velocity, v(t), as a function of time, t. Obtaining an analytic solution is, of course, of great value, when the problem is solvable. However, a numerical solution is a common route to difficult problems and methods to effect them exist. Two different numerical approaches of interest here are a Monte Carlo (MC) approach [1] and a self-consistent (SC) method. The idea, in the MC case, is to make a random guess for the acceleration, a(t), and to use the trapezoid method to get the velocity versus time, v(t). The time dependent position, x(t), follows by standard numerical integration of v(t). Depending on the situation, sometimes this method is not very efficient. In the SC method, one starts by making an initial numerical guess for a(x(t)) to obtain a v(t), which is used to obtain an x(t), which results in a new a(x(t)), etc. The process is repeated until there is no change in x(t). Here both methods are applied to simple systems and compared to the known analytic solutions for comparison and assessment purposes.


10:24AM R18.00013: Dispersion dynamics applications*  
ANTONY BOURDILLON (Presenter), retired — One starting point is the Klein Gordon equation and the stable wave packet [1]. Simpler is relativity: insert Planck's law and the de Broglie hypothesis. In simple units, angular frequency = \(\omega = (k^2 + m_0^2)^{1/2}\), with \(m_0\) the rest mass. Now differentiate with respect to wave vector \(k\). Three related velocities are the phase velocity, the group velocity and the speed of light. Dispersion dynamics requires consistently, negative mass in the antiparticle, with negative kinetic energy, negative momentum and negative angular velocity. These properties have widespread application in: the Hall effect; superconductivity; the switching principle; galactic rotational velocities; event horizons, uncertainty, intrinsic spin, etc.


*none
In Cosmology, both de Sitter space and Anti-de Sitter (AdS) space are both named after the astrophysicist de Sitter. In Einstein's General Theory of Relativity (GR), space and time are on an equal footing, and we have a unified geometry of space-time, instead of a separate space and a separate time. This yields three cases of constantly curved space-time: de Sitter space with positive curvature; Minkowski space with zero curvature; and anti-de Sitter space with negative curvature. Very conveniently, the Anti-de Sitter space can be extended to any number of dimensions, with n representing the number of dimensions. A combination of classical General Relativity (GR) and Quantum Field Theory (QFT) provides an interesting thermodynamic description of black holes. We use an algorithm proposed by Nemati et al. (2013). In this formalism, we start with a hypercube with each of its vertices labeled with black hole binaries. The back holes are associated with probability functions, and the black holes move based on the probabilities. Our research has applications both Quantum Gravity (QG) and in Black Hole Physics (BHP).

*Financial support from the New Mexico Alliance for Minority Participation (NM-AMP) program of the National Science Foundation (NSF)

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R19 DMP DCOMP: Computational Materials Design and Discovery -- Catalysis and Electronic Structure

8:00AM R19.00001: Computational design of (electro-)catalysts [Invited] ANDREW PETERSON (Presenter), School of Engineering, Brown University — Catalysts are crucial in energy conversion technologies, and electrocatalysts directly allow the interconversion of electrical and chemical energy carriers. Here, I will discuss atomistic approaches to describe and design catalyst materials from a computational framework. We have recently developed techniques to control the workfunction (and thus, the potential) of simulations in a "Solvated Jellium" approach. We will show how this allows for the inclusion of reaction barriers and the direct deduction of electrocatalytic mechanisms. We will use this to explain the unique reactivity of Pt that has not been accessible from a traditional "volcano plot" approach, and shed insights for the design of earth-abundant materials with high activities.

8:36AM R19.00002: Two-Dimensional Phases of Robust CO2 Reduction Photocatalysts* STEVEN TORRISI (Presenter), Physics, Harvard University, ARUNIMA SINGH, Physics, Arizona State University, JOSEPH MONTOYA, KRISTIN PERSSON, Energy Technologies Area, Lawrence Berkeley National Laboratory — Two-dimensional materials are increasingly popular for applications in catalysis due to useful properties like high surface area, differing surface reactivity from bulk counterparts, and their ability to be formed into nanostructures. This motivates our first-principles based study of the structure and electronic properties of 2D phases of several binary semiconductor materials which have been identified as promising CO2 reduction photocatalysts in the bulk [1]. Using van der Waals corrected functionals as well as HSE06, we identify suitable stable structures with reasonable band gaps for visible light absorption. Finally, we qualitatively evaluate the compounds’ catalytic efficiency by computing the adsorption energy of reaction intermediates on each respective surface.


*S.B.T. was supported by the Dept. of Energy (DOE) Computational Science Graduate Fellowship. Computational work was supported by the Materials Project (Grant No. EDCBEE) Predictive Modeling Center through the U.S. (DOE), Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-05-CH11231: Materials Project program KC23MP.
8:48AM R19.00003: Computational Dissection of Two-Dimensional Rectangular Titanium Mononitride TiN: Auxetics and Promises for Photocatalysis* LIUJIANG ZHOU (Presenter), SERGEI TRETIAK, Los Alamos National Laboratory — Recently, two-dimensional (2D) materials with a negative Poisson's ratios (auxetics) have triggered an enormous interest for their potential applications in the next-generation readable/writeable memory and optoelectronic technologies. Here, by using a broad range of first-principles calculations, we report a systematic study of 2D rectangular materials of titanium mononitride (TiN), exhibiting high energetic and thermal stability due to in-plane d–p orbital hybridization and synergetic out-of-plane electronic delocalization. The rectangular TiN monolayer also possesses enhanced auxeticity and ferroelasticity with an alternating order of Possion's Ratios, stemming from the competitive interactions of intra- and inter-Ti—N chains. Such TiN nanosystem is a n-type metallic conductor with specific tunable pseudogaps. Halogenation of TiN monolayer downshifts the Fermi level, achieving the optical energy gap up to 1.85 eV for TiNCl(Br) sheet. Overall, observed electronic features suggest that the two materials are potential photocatalysts for water splitting application.

*LANL LDRD program

9:00AM R19.00004: Exploring PtXnY(2-n) (X, Y= S, Se and Te ; 0≤n≤2) monolayers: Is Janus PtXY the most favorable one? FATIH ERSAN (Presenter), CAN ATACA, University of Maryland, Baltimore County — In this study, we investigated Janus and alloy structures of PtXnY(2-n) (X,Y=S,Se,Te; 0≤n≤2) materials on the basis of first-principles plane-wave simulations. Using cluster expansion theory for studying alloys of PtXnY(2-n) monolayers at various concentrations, for half coverage (n=1), our results indicated that Janus type structures are not energetically the most favorable for PtXY monolayers, however they are dynamically and thermally stable. In order to distinguish Janus PtXY structures, we reported the Raman active modes and compared them with bare PtX2 monolayers. Calculated electronic band gap values using hybrid functionals are on-par with available experimental data. It is also reported that spin-orbit coupling significantly modified the electronic band structure of PtXY monolayers. Due to the electronegativity differences of different chalcogen atoms on each surfaces of Janus PtXY structures, the arising dipole moment significantly modified the band alignments on both surfaces. We found that hydrogen evolution and oxygen reduction happen on different surfaces and applied strain enhanced the catalytic activity. Our results indicated that due to their intrinsic dipole moments and band gaps, Janus PtXY monolayers are the perfect candidates for water splitting reactions.

9:12AM R19.00005: Computational design of bimetallic core-shell nanoparticles for hot-carrier photocatalysis* LUIGI RANNO, STEFANO DAL FORNO (Presenter), JOHANNES LISCHNER, Imperial College London — Modelling nanoplasmonic devices with tailored properties for photocatalytic, optoelectronic and photovoltaic applications is an important and interesting research field that can lead to groundbreaking technological discoveries. However, developing a quantitative description of nanoplasmonic systems is challenging as quantum-mechanical theories of electrons in large nanoparticles must be combined with nanophotonic approaches.

In this talk, we present an approach which combines a material-specific effective mass theory for the electrons in core-shell nanoparticles with a quasi-static description of the plasmon potential. We studied 100 different combinations of bimetallic core-shell nanoparticles and found that systems with alkali-metal cores and transition-metal shells exhibit the highest figure of merit for water splitting. We discovered that the electronic structure of such systems features a two-dimensional electron gas in the shell which accounts for their high photocatalytic efficiency.

*Authors aknowledge EPSRC under Grant No. EP/N005244/1 and the Thomas Young Center under Grant No.TYC-101. This work used the ARCHER UK National Supercomputing Service, which is funded by EPSRC (EP/L000202).

9:24AM R19.00006: Electronic and optical properties of 3d-4d double perovskite Sr2VNbO6: a first-principles DFT+DMFT study* ARPITA PAUL (Presenter), TURAN BIROL, University of Minnesota — Double perovskite oxides (A2BB'O6) have drawn enormous interest due to their large variety of emergent properties. We use first-principles DFT+DMFT method to study the electronic and optical properties of Sr2VNbO6, which has both 3d (V) and 4d (Nb) electrons with varying degree of on-site interaction strengths. With both parent compounds SrVO3 and SrNbO3 shown to be promising transparent conductors on the opposite ends of the visible spectrum, we explore the optical properties of the ordered double perovskite Sr2VNbO6. We show that the electronegativity difference and the resulting possibility of charge transfer between the two transition metal cations affect the electronic structure and optical properties such as plasma frequency.

*The authors were supported by NSF DMREF program under the award NSF DMREF project DMREF-1629260.
9:36AM R19.00007: Combined DFT & STM Study of Fe/Ir(111) Surface States*  STEPHEN GANT (Presenter), JACOB REPICKY, ROLAND KAWAKAMI, JAY A GUPTA, Ohio State University — Chiral spin structures like those present in Fe/Ir(111) are playing an increasingly important role as processor and device size continue to shrink to length scales where quantum effects are relevant. Here, we present density functional theory (DFT) calculations of the Fe/Ir(111) and Ir(111) surfaces and compare them with experimental scanning tunneling microscopy (STM) images and spectroscopy. We performed our calculations using a fully relativistic projector augmented-wave (PAW) approach in conjunction with spin-orbit coupling (SOC) to produce band structures, surface local density of states (LDOS), and simulated STM topography. Experimental STM studies were performed at low temperature in an ultrahigh vacuum environment. Ir(111) was prepared via Ar sputtering, while a monolayer of Fe was deposited in bare Ir(111) via molecular beam epitaxy (MBE). We find good agreement between our DFT calculations and STM data. Of particular interest is the correspondence in Ir(111)'s surface state at the Γ point. Additionally, we present an analysis of how this state is affected by a pseudomorphic monolayer of Fe.

*Funding by NSF MRSEC DMR-1420451 and by DARPA-18AP00008

9:48AM R19.00008: First-Principles Study of Magnetism in Bilayer Manganese Phthalocyanine*  HAECHAN PARK (Presenter), HAI-PING CHENG, JAMES NATHAN FRY, SHUANGLONG LIU, YUN-PENG WANG, University of Florida — Magnetism in two dimensional materials has recently become a hot research topic due to its potential applications in spintronics and physical properties that arise from low dimensionality. Previously, monolayer manganese phthalocyanine (MnPc) has been synthesized experimentally, and theoretical studies have revealed that its magnetic properties can be tuned by substituting cations, applying biaxial strain, and imposing a gate voltage. In this first-principles study we examine the properties of bilayer MnPc using density functional theory (DFT). According to our simulations, Mn-to-Mn on-top stacking is found to be energetically less favorable, and we determine the stable position of the top layer relative to the bottom layer. When bilayer MnPc is in its ground state, both MnPc layers are in the Neel anti-ferromagnetic (NAF) state, although the ground state of monolayer MnPc is Collinear Antiferromagnetic (CAF), indicating that the interlayer magnetic coupling is very important. We will discuss further the nature of intra- and inter-layer magnetic couplings.

*This work was supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), under Contract No. DE-FG02-02ER45995. Computations were done using the utilities of NERSC and UFRC.

10:00AM R19.00009: Contrasting Ferromagnetism in FeS2 Pyrites Induced by Cobalt Doping and by Electrostatic Gating  EZRA DAY-ROBERTS (Presenter), RAFAEL M FERNANDES, TURAN BIROL, University of Minnesota — Pyrites are a family of transition metal disulfides that host a wide variety of electronic ground states. In particular, the ferromagnetic transition in Co-doped FeS2 has been studied as a source of variable, experimentally accessible electron spin polarizations. Advances in ionic liquid gating have provided an alternative way to change the electron concentration via electrostatic gating instead of chemical doping, thus avoiding the introduction of impurity scattering centers. We use Density Functional Theory combined with a tight-binding model to compare electrostatic gating and chemical doping with cobalt. Using maximally localized Wannier functions to construct a tight-binding model, we calculate the magnetic susceptibility across the entire range of compounds Fe1-xCoxS2. We find that electrostatic gating requires a higher electron concentration than the equivalent in Co-doping to induce ferromagnetism via a Stoner-like mechanism. We attribute this behavior to the formation of a narrow cobalt band near the bottom of the conduction band under doping. This band is not formed for electrostatic gating and wide, low DOS sulfur states are filled instead.
Ab initio Informed Tight Binding Theory of Axis-dependent Conduction Polarity in Goniopolar Materials

YAXIAN WANG (Presenter), JOSEPH P C HEREMANS, JOSHUA E. GOLDBERGER, WOLFGANG WINDL, Ohio State University — We have recently shown that NaSn$_2$As$_2$ exhibits opposite conduction polarities along in-plane and cross-plane directions, defined as “goniopolarity”. On the lowest level of theory, we can show that this novel phenomenon originates from a special topology of the Fermi surface, which is essentially determined by the nature of the bonding states in this layered crystal. In this paper, we present an improved fundamental understanding of goniopolarity based on a novel formulation of goniopolarity within the tight-binding model. The tight-binding matrix elements are calculated from GW calculations based on Density Functional Theory (DFT) via maximally localized Wannier functions. Considering a minimum-basis set with sp$^3$ orbitals for both Sn and As, the 64 hopping integrals are evaluated. Within our model, we provide a new tight-binding based formulation for both Seebeck and Hall coefficients for NaSn$_2$As$_2$ and can show that critical ratios of hopping and on-site matrix elements exist that pose limits for goniopolarity to appear in materials. Based on that, additional candidate materials for goniopolarity can be proposed, and the design space for goniopolar materials in general will be defined.

*Y. W., J. G. and W. W. acknowledge NSF-MRSEC and AFOSR; and J. H. acknowledge NSF-EFRI.

Effects of Si Doping on the Electronic Structure and Conductivity of Pure and Off-Stoichiometric Ge$_2$Sb$_2$Te$_5$ Cystrals: First-Principles Investigation

RAJARSHI SINHA-ROY, ANTONIN LOUISET, MAGALI BENOIT, LIONEL CALMELS (Presenter), CEMES, Université de Toulouse, CNRS, 29 rue Jeanne Marvig, 31055 Toulouse, France — We calculate the electronic structure and electrical conductivity of pure and Si-doped off-stoichiometric Ge$_2$Sb$_2$Te$_5$ cubic crystals, using the relativistic Korringa-Kohn-Rostoker method based on the multiple-scattering theory. These crystals are described by a rock-salt unit cell, in which the chemical disorder is taken into account through the coherent potential approximation. The accuracy of the results is verified by comparing, for several compositions, the density of electronic states calculated with this method and with a method that uses Kohn-Sham wave functions in big supercells. The calculated Bloch spectral function shows the dispersion of the electron states and its modification with the atomic disorder. We show the chemical-composition dependence of the electrical conductivity, and discuss it in terms of the concentration of carriers and of the modification of their scattering by atomic disorder. These results can be used to model Ge-Sb-Te phase-change-material samples, the microstructure of which consists of grains with different compositions, each grain being described by a different value of the conductivity.

*We acknowledge the “Programme des Investissements d’Avenir” (grant NEXT n° ANR-10-LABX-0037) and HPC supercomputing centre CALMIP.

Electrical Conductivity of Graphene-Polymer Composite Foam

ZILU WANG (Presenter), The University of Akron, ADAMSON H DOUGLAS, Institute of Material Science, University of Connecticut, ANDREY DOBRYNIN, The University of Akron — Graphene-polymer composites have potential applications in energy storage, oil absorption, and sensing. Here, we focus on dependence of the electrical conductivity of the composite graphene-polymer foams as a function of their composition and deformation. Using a combination of the coarse-grained simulations and analytical calculations we developed a bottom-up approach which allows us to express the macroscopic sample conductivity in terms of conductivity of the graphene layers coating the foam's shells. In particular, we propose a close packing shell model to describe the conductivity of the graphene shells with multiple contact points. This shell conductivity model is used to calculate the change in foam conductivity upon deformation which could be induced either by solvent absorption or by external foam compression/elongation. The model predictions are compared with the experimental data on conductivity of composite poly(butyl acrylate)/graphene foams.

*NSF DMR 1535412

Density matrix renormalization group study of Hubbard ladders

YILIN ZHAO (Presenter), Chemistry, McMaster University, LING WANG, Corresponding author, CSRC, GAYANATH FERNANDO, University of Connecticut — Motivated by exact diagonalization work on small Hubbard clusters$^1$, we focus on Hubbard ladder systems using the DMRG method. The exact diagonalization work has yielded an extremely rich variety of results related to the physics of the minimal orbital Hubbard clusters and the present study will attempt to elucidate related size and other effects.

8:00AM R20.00001: Ionic Transport in Materials with Substitutional Disorder [Invited]  ALEXANDER URBAN (Presenter), Department of Chemical Engineering, Columbia University — Substitutional disorder can have a profound impact on the ionic transport properties of crystalline solids, such as the solid electrolytes of solid oxide fuel cells or cation-disordered cathode materials for lithium ion batteries (LIBs). However, the direct experimental investigation of disorder on the atomic scale is challenging, and (conventional) first-principles computational techniques cannot be directly applied to disordered materials.

Here I will show how relatively simple computational models can provide useful insight into the interplay of substitutional disorder and ionic conduction in cation-disordered LIB cathode materials. Over the last years, computational modeling has contributed to the understanding of this new class of materials and has guided the discovery of several new high-energy density cathode materials.

8:36AM R20.00002: Tunable band-gap engineering of ZnSnN$_2$ via cation disorder from first-principles calculations*  ZIHAO DENG (Presenter), LOGAN WILLIAMS, CHRISTINA JONES, EMMANOUIL KIOUPAKIS, University of Michigan — Heterovalent ternary alloys offer a rich space to search for the next-generation optoelectronic materials. Unlike their III-V counterpart, cation disorder can greatly alter the electronic properties of II-IV-V$_2$ compounds by breaking the octet-rule locally. Thus, intentional introduction of cation disorder can provide a new route to tune the electronic band gap of heterovalent ternary compound besides conventional alloying. To demonstrate this possibility, we performed first-principles calculations based on hybrid density functional theory to study the cation disorder effect in ZnSnN$_2$, which is a promising solar material in the II-IV-V$_2$ family. We found a direct relationship between the band gap of ZnSnN$_2$ and the long-range order parameter S, which characterizes the Zn/Sn disorder. Such band gap variations arise from the presence of octet-rule breaking motifs in the lattice (Zn$_3$Sn, ZnSn$_3$, Zn$_4$, Sn$_4$). Our findings reveal the correlations between cation disorder and the band gap of ZnSnN$_2$, and suggest the possibility of alloy-free band gap tuning in heterovalent ternary compounds.

*This work was supported by NSF DMR-1254314. Computational resources provided by DOE NERSC (DE-AC02-05CH11231).

8:48AM R20.00003: Pristine electronic properties in multinary semiconductor alloys at magic compositions  JIE PAN (Presenter), National Renewable Energy Laboratory, JACOB CORDELL, Colorado School of Mines, ANDRIY ZAKUTAYEV, ADELE TAMBOLI, STEPHAN LANY, National Renewable Energy Laboratory — The materials electronic structure is usually very sensitive to topological distribution of atoms in the materials. Generally, the electronic integrity is easily destroyed by defects and disorder causing charge localization. The design of multinary materials has attracted a great interest for its wide tunability in properties. This functional versatility is rooted in many-fold degrees of freedom in composition and atomic distribution. At some “magic” compositions, the disordered material system can exhibit perfect short range ordered (SRO) ionic distributions that conserve the local octet rule despite the absence of long range order. In this contribution, we study the dual sublattice mixed semiconductor alloy (ZnSnN$_2$)$_{1-x}$(ZnO)$_{2x}$ in which perfect SRO are observed when $x=0.0$ and 0.25.

Disordered structures were generated from Monte Carlo simulations and the energies were calculated from first principles. At the magic composition, these SRO conserving systems have a much reduced mixing enthalpy and increased band gap. More importantly, these SRO structures do not have charge localization effects near band edges, as seen in the inverse participation ratio, thereby maintaining a pristine electronic structure.
9:00AM R20.00004: Lattice Constant and Band Gap Tuning in BInGaN Alloys for Next-Generation LEDs* KEVIN GREENMAN (Presenter), LOGAN WILLIAMS, EMMANOUIL KIOUPAKIS, University of Michigan — InGaN light-emitting diodes (LEDs) have enabled significant energy and cost savings, and further savings can be realized by operating at the same efficiency at higher power. However, the efficiency of currently available InGaN LEDs is lowered by the loss of carriers to Auger recombination when operating at high power. The Auger loss can be reduced by increasing the active-region volume, but the lattice mismatch between thick InGaN active layers and underlying GaN layers cause performance-degrading dislocations. Previous work has shown that this problem can be addressed by co-alloying InGaN with BN. Doing so can produce alloys that maintain an approximate lattice match to GaN while allowing for a band gap that is adjustable throughout the visible range. In this work, we expand on previous hybrid density functional theory calculations to explore the thermodynamic, structural, and electronic properties of a larger area of the BxInyGa1-x-yN composition space and examine the wurtzite, zinc blende, and planar hexagonal phases. A more thorough understanding of these properties will help to direct efforts to fabricate thick active regions for more cost-effective BInGaN LEDs.

*This work was supported by NSF DMREF (1534221). Computational resources provided by DOE NERSC (DE-AC02-05CH11231).

9:12AM R20.00005: High precision detection of the change in intermediate range order of amorphous thin films due to annealing  KIRAN PRASAI (Presenter), E. L. Ginztion Laboratory, Stanford University, JUN JIANG, ALEC MISHKIN, Department of Physics and Quantum Theory Project, University of Florida, SARAH HOBACK, Department of Physics, American University, DAVID A DRABOLD, Department of Physics and Astronomy, Ohio University, ERIC KEITH GUSTAFSON, LIGO Lab, California Institute of Technology, MARIANA FAZIO, Department of Electrical and Computer Engineering, Colorado State University, GREGORY M HARRY, Department of Physics, American University, APURVA MEHTA, SLAC National Accelerator Laboratory, CARMEN SUSANA MENONI, Department of Electrical and Computer Engineering, Colorado State University, CARL LÉVESQUE, Department of Physics, Université de Montréal, IAN MACLAAREN, School of Physics & Astronomy, University of Glasgow, STEVEN D PENN, Department of Physics, Hobart and William Smith Colleges, FRANÇOIS SCHIETTEKATTE, ROSALIE SHINK, Department of Physics, Université de Montréal, BADRI SHYAM, University of Dayton Research Institute, GABRIELE VAJENTE, LIGO Lab, California Institute of Technology, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, MARTIN FEJER, RICCARDO BASSIRI, E. L. Ginztion Laboratory, Stanford University — Future gravitational wave detectors, such as Advanced LIGO +, will be limited in sensitivity by thermal noise associated with mechanical loss in the detectors’ amorphous mirror coatings. In order to reduce mechanical loss, we aim to understand the atomic level structures responsible for it and take a directed design approach to suggest improved coatings. Through studies on thin films of amorphous zirconia-doped-tantala (ZrO2-Ta2O5), a potential coating for LIGO mirrors, we present high precision detection of the change in the intermediate range order (IRO) as a function of post-deposition annealing, using grazing incidence x-ray scattering measurements carried out at the Stanford Synchrotron Radiation Lightsource. For the first time, our atomic modeling based on x-ray scattering data is able to capture the changes in IRO. We show that the primary structural units (PSUs), which are disordered oxygen octahedra centered around the metal atoms, remain largely unchanged after annealing. We explain the observed structural changes in terms of the IRO, specifically, the change in metal-oxygen-metal bond angles at the bridging oxygen sites, and the way neighboring PSUs share bridging oxygens. Finally, we discuss correlations between the observed changes in the IRO and mechanical loss.

9:24AM R20.00006: Temperature-dependent properties of thermoelectric clathrates*  MARIA TROPPENZ (Presenter), SANTIAGO RIGAMONTI, CLAUDIA DRAXL, Humboldt University of Berlin — Intermetallic clathrate compounds, among them the type-I clathrate Ba8AlxSi46-x, are promising candidates for high-efficiency thermoelectric applications. They exhibit a strong dependence of the electronic properties on the atomic arrangement of the substitutional Al atoms in the crystal framework [1]. At the charge-balanced composition (x=16), the ground-state configuration is semiconducting, however, configurations higher in energy are metallic. Understanding the temperature-dependent properties is essential, as semiconducting behavior is a prerequisite for thermoelectric applications. By employing the cluster expansion technique combined with Monte-Carlo samplings and the Wang-Landau method [2] we find a semiconductor-to-metal transition at around 600 K which is driven by a partial order-disorder transition. Signatures of this phase transition are observed in the temperature-dependent band structure, specific heat, and partial occupations.


* M.T. acknowledges funding from the Elsa-Neumann Scholarship of Berlin.
Beyond the constant relaxation time*

ILARIA SILOI (Presenter), ANOOJA JAYARAJ, Physics, University of North Texas, Denton, TX, USA, ANDREW R SUPKA, Department of Physics and Science of Advanced Materials Program, Central Michigan University, Mt. Pleasant, MI, USA, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, Durham, NC, USA, MARCO BUONGIORNO NARDELLI, Physics, University of North Texas, Denton, TX, USA, MARCO FORNARI, Department of Physics and Science of Advanced Materials Program, Central Michigan University, Mt. Pleasant, MI, USA —

Over the years, first principles calculations have become a complementary tool for the experimental research aiming to discover high-performance thermoelectrics. This has greatly improved the understanding of the transport properties and has advanced optimization strategies based on “band engineering” [1,2]. In most cases, the constant relaxation time approximation has been used without much analysis. We investigated the limits of the approximations for the relaxation time in the electronic transport coefficients properties of well know TE materials by considering different models that include energy and temperature dependence. Transport coefficients have been computed using the recently developed PAOFLOW package (http://aflowlib.org/src/paoflow/).

*We acknowledge collaboration within the AFLOW Consortium (www.aflow.org) under the sponsorship of DOD-ONR (Grants N000141310635 and N000141512266).

Potential Candidate for Thin-Film Photovoltaics: Alloyed Semiconductor Cu2BaGe1-xSnxSe4

TONG ZHU (Presenter), GARRETT C. WESSLER, JON-PAUL SUN, ALEXIS HARRELL, WILLIAM P. HUHN, VOLKER BLUM, DAVID MITZI, Mechanical Engineering & Materials Science, Duke University — Cu2BaGeSe4 (CBGSe) was previously identified as a potential thin-film photovoltaic (PV) candidate based on computationally scanning the I2-II-IV-VI4 (I = Cu, Ag; II = Ba, Sr; IV = Ge, Sn; VI = S, Se) materials family and successful experimental synthesis. This material avoids difficulties of competing PV materials like toxicity (Cd) or scarcity (In, Te) of constituent elements in Cu(In,Ga)(S,Se)2 and CdTe. Moreover, the similar ionic sizes and coordination preferences compared to the recently identified PV material Cu2BaSn(S,Se)4 may provide a potential avenue to overcome the unavoidable antisite disordering that limits the competing material Cu2ZnSn(S,Se)4. In this work, hybrid density functional theory (HSE06) including spin-orbit coupling is used to explore the electronic properties of three cation alloying approaches (Ag for Cu, Sr for Ba, and Sn for Ge ) for unalloyed CBGSe, which has a relatively large band gap (1.91 eV). The largest band gap decrease can be achieved by Sn/Ge alloying. The minimum band gap occurs at 1.57 eV for x≈0.70 in alloyed Cu2BaGe1-xSnxSe4. The minimum occurs just prior to a structural transition from the P31 to the Ama2 space group just above x=0.7; the P31 phase is associated with a significantly lower band gap.

First-principles study of photochromic material YHxOy

YI-YANG SUN (Presenter), State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, CAS — Photochromic materials refer to the materials that change color under light illumination, particularly visible light. Organic materials dominate the photochromic materials due to their highly tunable properties. However, inorganic photochromic materials are attractive for their stability and possibly high resistance to fatigue. YHxOy is a new photochromic material found a couple of years ago. However, its chemical composition, atomic structure, electronic properties have not been completely studied so far. The mechanism of the photo-induced color change is still elusive too. In this work, using first-principles calculations based on the density functional theory, we aim to provide a comprehensive understanding on this new material. Possible strategies on how to tune the properties, such as its band gap, through oxygen concentration will be discussed.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R21 DCOMP: Emerging Trends in Molecular Dynamics Simulations and Data Analytics IV
Menichetti, Kanekal, Bereau, arXiv:1805.10158

*This work was supported by the Emmy Noether program of the Deutsche Forschungsgemeinschaft (DFG).

8:36AM R21.00002: Simultaneous structure exploration and machine-learned potential fitting* NOAM BERNSTEIN (Presenter), United States Naval Research Laboratory, GÁBOR CSÁNYI, VOLKER L DERINGER, Cambridge University — Defining interatomic potentials using ideas from machine learning that treat the problem as a high-dimensional fit of the reference (usually density functional theory) potential energy surface is an exciting new approach for developing accurate potentials. However, because of their variational freedom such potentials require large fitting datasets, with large amounts of manual selection and tuning of configurations by the researcher. We present an iterative method, where a preliminary potential is used to carry out a number of random-structure searches, and selected configurations from the searches are used to fit the next iteration’s potential. We test the method on a number of elements with different bonding types, including an insulator, a semiconductor, and a metal. We show how the process converges in a few iterations, and how the resulting potentials reproduce the reference DFT values on a number of bulk and defect properties.

*N.B. was supported by the Office of Naval Research through the U. S. Naval Research Laboratory’s core basic research program. V.L.D. was supported by a Leverhulme Early Career Fellowship and support from the Isaac Newton Trust.

8:48AM R21.00003: Adaptive multiple time scales mapping in heterogeneous molecular simulation, a hierarchical domain decomposition approach HORACIO ANDRES VARGAS GUZMAN (Presenter), Theory, Max Planck Institute for Polymer Research, HIDEKI KOBAYASHI, Theory Research Interest Group, University of Cambridge — Heterogeneous molecular systems are mostly inspired by natural phenomena, such as, phase segregation, evaporation, among others. Those systems can be modeled by means of advanced molecular simulations methods, as it is done in multiscale concurrent and non-equilibrium simulations. Interestingly, the heterogeneity of the mentioned systems has a huge potential to map and span time and length scales beyond fully atomistic simulations, because a subdomain of the simulation box can be tackled with slowly diffusive regime, while other remains in a faster diffusive regime. From this description, a decisive question arises on how to map those heterogeneous time scales without losing the theoretical speedup planned from the method development perspective. Here, we introduce the heterogeneous time-spatial domain decomposition approach which is a combination of an heterogeneity sensitive spatial domain decomposition with a time evolution average of particles’ diffusion domainwise estimated. Within this approach, the spatial domain decomposition is theoretically modeled and results in scaling-laws for the force calculation time, while timewise the subdomains with different diffusivity are adapted by means of the number of neighboring shells to a unique frequency of neighbors list updates.

8:48AM R21.00004: Identifying 1H/2T Phases and Defects in MoS2 Using Boltzmann Machines JEREMY LIU (Presenter), RAJIV KALIA, University of Southern California, KE-THIA YAO, Information Sciences Institute — We use Boltzmann machines (BMs), an energy-based learning model, to identify semiconducting (2H) and metallic (1T) phases and defects in molecular dynamics (MD) simulations of strained MoS2 monolayer. We compare various BM models, i.e. Restricted BMs (RBM) versus Limited BMs (LBM) with intra-layer couplings, and measure their performances. Our use of BMs gives insight into the structure of the underlying MD data and is amenable to implementation using sampling via an adiabatic quantum annealer. We show our LBMs have superior performance over RBMs, examine connectivity within our BM variants, explore hardware qubit mapping schemes, and discuss what performance differences may imply about locality within the data without prior knowledge.

HAIXIN WEI (Presenter), Materials Science and Engineering, University of California, Irvine, JUNMEI WANG, Pharmaceutical Sciences, University of Pittsburgh, PIOTR CIEPLAK, SBP Medical Discovery Institute, YONG DUAN, University of California, Davis, RAY LUO, University of California, Irvine — Electrostatic interactions are of fundamental importance to the structures and functions of biomolecules. Their accurate modeling is crucial in the design and development of physical models in computational studies of biomolecules. It is known that widely used point-charge models cannot capture the subtle short-range interactions and molecular anisotropicity. Recently emerged point multipole models, in the meantime, face the so-called “polarization catastrophe” difficulty that requires artificial truncation and omission of important short-range interactions. Considering these limitations, we are developing a new polarizable Gaussian multipole (pGM) framework, which is capable of describing the short-range interactions more accurately without greatly increasing computational cost. Our data shows that the new model greatly improves the modeling of molecular anisotropicity. We are also developing a new set of algorithms for more efficient modeling electrostatics interactions within the pGM scheme. With all its advantages, we believe that the pGM model will positively impact the field of the biomolecular simulations.


REBECCA LINDSEY (Presenter), LAURENCE FRIED, NIR GOLDMAN, SORIN BASTEA, Lawrence Livermore Natl Lab — Understanding chemistry at extreme conditions is crucial in fields including geochemistry, astrobiology, and alternative energy. First principles (quantum-mechanical) methods can provide valuable microscopic insights into such systems while circumventing the risks of physical experiments, however the time and length scales associated with chemistry at high temperature and pressure (i.e. ns and μm, respectively) largely preclude extension of such models to molecular dynamics. In this work, we discuss development of ChIMES, a generalized n-body force field comprised of linear combinations of Chebyshev polynomials. ChIMES models are machine-learned to selected configurations from short Density Functional Theory (DFT) molecular dynamics simulations and are refined through active learning. ChIMES models are found to retain much of the accuracy of DFT at a fraction of the cost and exhibit linear size scalability.

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9:36AM R21.00007: Quantum-simulation-informed machine learning of dynamic properties of two-dimensional and layered materials*

LINDSAY BASSMAN (Presenter), ARAVIND KRISHNAMOORTHY, PANKAJ RAJAK, University of Southern California, FUYUKI SHIMOJO, Kumamoto University, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Two-dimensional and layered transitional metal dichalcogenides are emerging as promising materials for the electronic and optoelectronic devices of tomorrow due to the large space of design variables (such as configuration of dopant atoms, sequence of stacking along the van der Waals direction etc.) that can be used to tune dynamic properties of the material. The primary challenge for rational design of these materials is navigating this complex design space to identify optimal structures and compositions that possess desired properties. In this work, we show that machine-learning methods applied to atomistic data from quantum mechanical simulations are highly suitable for predicting optimal structures with respect to dynamic properties like thermal, charge and spin transport, electron-phonon coupling and non-equilibrium phonon distributions, and propensity for structural and phase transformations.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607. Simulations were performed at the Argonne Leadership Computing Facility under the DOE INCITE program and the Center for High Performance Computing of the University of Southern California.
LINFENG ZHANG (Presenter), Princeton University, DE-YE LIN, Institute of Applied Physics and Computational Mathematics, HAN WANG, Laboratory of Computational Physics, ROBERTO CAR, WEINAN E, Princeton University — We propose an active learning procedure called Deep Potential Generator (DP-GEN) for the construction of accurate and transferable potential energy surface (PES) models. This procedure has three major components: exploration, labeling, and training. As an important application, we use DP-GEN to generate an ab-initio trained reactive force field for water that describes both the molecular and the dissociated water phases.

*The work of L.Z. and W.E is supported in part by Major Program of NNSFC under grant 91130005, ONR grant N00014-13-1-0338 and NSFC grant U1430237.
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The work of H.W. is supported by the National Science Foundation of China under Grants 11501039, 11871110 and 91530322, and the National Key Research and Development Program of China under Grants 2016YFB0201200 and 2016YFB0201203.
The work of D.Y.L. and H.W. is supported by the Science Challenge Project No.-JCKY2016212A502.

10:00AM R21.00009: Metallization of the Si(001) surface: An atomistic study using a neural network potential*
SONALI JOSHI (Presenter), DUY LE, TALAT S. RAHMAN, University of Central Florida — Despite being one of the widely studied surfaces because of its technologically importance, the nature of the metallization of Si(001) at high temperatures is still an open question. The semiconductor-metal transition of the surface occurring at 900 K is often linked to the transformation from asymmetric to symmetric structure of the Si dimers at the surface [1]. In this work, we apply a neural network derived interatomic potential to perform molecular dynamics simulations of Si(001) for a large temperature range. This potential was developed with input from ab initio molecular dynamics simulations of Si(001) and validated to be as accurate as density functional theory. Our simulations show that the asymmetric, buckled structure of the dimer still exists at higher temperatures, but the increased dimer flipping rate makes them spend more time in the symmetric configuration making the surface metallic. Our results also suggested that such phenomenon is appreciable even at temperatures lower than 900 K, in agreement with angle-resolved photoemission spectroscopy data [2].


*This work is support in part by DOE grant DE-FG02-07ER46354.

10:12AM R21.00010: Datasets of Unusual Size: Benchmark Databases of Non-Covalent Interaction Energies of CCSD(T)/CBS Accuracy
ELIZABETH DECOLVENAERE (Presenter), ROBERT T MCGIBBON, ANDREW GARVIN TAUBE, ALEXANDER G DONCHEV, JOHN L KLEPEIS, DAVID E. SHAW, D. E. Shaw Research — We present a new benchmark collection, DES360K, containing interaction energies for 366,117 dimer geometries computed using coupled-cluster with single, double, and perturbative triple excitations [CCSD(T)] extrapolated to the complete basis set (CBS) limit, considered the “gold standard” of quantum chemistry. Our collection spans 392 unique small molecules in 3,697 combinations, and explores both energetically minimized dimers and dimers extracted from molecular dynamics simulations. We extend our dataset using SNS-MP2-Ext, a neural network-based method for predicting CCSD(T) interaction energies from MP2 inputs trained on the DES360K dataset. SNS-MP2-Ext revises our original SNS-MP2 approach to be extensive by construction, resulting in significantly reduced prediction errors and narrower confidence intervals than the original SNS-MP2. More importantly, SNS-MP2-Ext eliminates the large variations in predictive performance shown in SNS-MP2 for different chemical classes and energy scales. We have used both SNS-MP2 and SNS-MP2-Ext to expand our dataset to contain another 5 million unique data points with minimal computational expense while maintaining CCSD(T) levels of accuracy. The resulting collection, DESSM, is the largest-ever available collection of gold standard data.
10:24AM R21.00011: Accelerating atomistic modelling with active learning* JONATHAN VANDERMAUSE (Presenter), STEVEN TORRISI, SIMON BATZNER, Harvard University, ALEXIE M KOLPAK, Massachusetts Institute of Technology, BORIS KOZINSKY, Harvard University — Machine learning provides a path toward fast, accurate, and large-scale materials simulation, promising to combine the accuracy of ab initio methods with the computational efficiency of analytical potentials. However, training current state-of-the-art models, which include Neural Network Potentials and Gaussian Approximation Potentials, often requires hundreds of CPU hours and databases containing tens of thousands of chemical environments. Moreover, these potentials are trustworthy only for chemical configurations that fall within the training set and have so far been restricted to single- or few-component systems. In this talk, we present a multi-component on-the-fly learning scheme that refines the machine learned force-field when a new chemical configuration is encountered, opening the door to ML-driven molecular dynamics that can capture complex many-body dynamics spanning previously unprecedented length- and time-scales.

*S.B.T. acknowledges support from the DOE Computational Science Graduate Fellowship. S.B. acknowledges support from the Skoltech-MIT Center for Electrochemical Energy Storage.

10:36AM R21.00012: Designing High-strength Carbon-nanotube Polymer Composites Using Reinforcement Learning Algorithms Integrated with Molecular Dynamics Simulations* AOWABIN RAHMAN (Presenter), Department of Mechanical Engineering, University of Utah, MATTHEW RADUE, GREGORY ODEGARD, Department of Mechanical Engineering-Engineering Mechanics, Michigan Technological University, MICHAEL CZABAJ, Department of Mechanical Engineering, University of Utah, PRATHAMESH DESHSPANDE, Department of Mechanical Engineering-Engineering Mechanics, Michigan Technological University, ASHLEY SPEAR, Department of Mechanical Engineering, University of Utah — Carbon-nanotube (CNT)-based composites have great potential in modern aerospace applications requiring high-strength, lightweight structural materials. However, one factor that limits the potential of CNT composites is the inefficiency in load transfer between CNTs using a polymeric resin, arising due to low CNT/polymer interfacial strength. This talk presents a modeling framework that uses a reinforcement learning (RL) algorithm along with molecular dynamics (MD) simulations to make design modifications at the CNT/polymer interface for improving the interfacial strength of CNT/polymer composites. The proposed framework uses a modular approach consisting of: (i) reinforcement learning model to recommend design modifications, i.e. inserting reactive groups and dopants, to the CNT/polymer model; (ii) method for rapidly implementing the recommendations by modifying the MD model structure; and (iii) methodology to reduce computational time for performing MD simulations of CNT pullout after making these modifications. The proposed framework would enable fundamental exploration of design space to develop high-strength CNT-based composites and could potentially be extended or adapted for a more general integration of data-driven techniques with MD for design applications.

*NASA NNX17AJ32G

10:48AM R21.00013: "Azide and Alkyne CHARMM Parameterization with the Force Field took kit (ffTK) and Unnatural Amino Acid (uAA) Protein Simulation" ADDISON SMITH (Presenter), THOMAS KNOTTS IV, Brigham Young University — Drug-like small molecules that contain azido and alkynyl groups are structurally unique because they contain linear angles useful in therapeutics and bioconjugation reactions. The bioconjugation "click" reactions has been useful in drug design and uAA research; however, these technologies rely heavily on molecular modeling.

CGenFF and CHARMM are common force fields for drug-like molecules; however, this force field lacks parameters for linearangle molecular moieties and current literature does not contain any solution. We propose a method that (1) develops CHARMM parameters for four small molecules that contain terminal azido and alkynyl groups using ffTK, (2) addresses linearity issues, and (3) validates ffTK results via in silico MD simulation. We then combine these parameters with CGenFF to generate parameters for uAA MD simulation.

In this presentation we prove that the physics of the linear terminal dihedral angles are well-represented by multiple parameter sets as long as they maintain the linear structures. We then show the reliability of our parameter set by running MD simulations to prove our modeled structures match those found in literature and quantum theory. Finally, protein MD compares simulation with crystallographic data using a protein that contains an azide uAA.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R22 DCOMP DCOMP: Electrons, Phonons, Electron-Phonon Scattering and Phononics V BCEC 157C - Mu Wang, American Physical Society - Tag(s): Focus
In this talk, I will discuss our recent theoretical effort towards ultrafast control of dielectric response through the excitation of infrared active phonons. I will highlight cases where the induced unidirectional Raman response is comparable to the dielectric response dictated by the symmetry and amplitude of the excited phonons. This provides a strategy for selective, ultrafast control of dielectric properties through infrared phonon excitation.

Recent developments in the generation and control of intense ultrashort infrared radiation have provided a new approach to nonlinear optics through the coherent excitation of infrared active phonons to large amplitudes. Due to the large oscillating displacement of excited infrared phonons, Raman active phonons can be unidirectionally displaced through special nonlinear coupling terms. In contrast to the typical considerations of nonlinear optics where crystalline symmetry and light intensity dictate the dielectric response of the material, in this “nonlinear phononics” process alteration of the dielectric response is dictated by the symmetry and amplitude of the excited phonons. This provides a strategy for selective, ultrafast control of dielectric properties through infrared phonon excitation.

In this talk, I will discuss our recent theoretical effort towards ultrafast control of dielectric response through the excitation of infrared active phonons. I will highlight cases where the induced unidirectional Raman response is comparable to the excited infrared phonon amplitude.

*DMR-1719875

8:36AM R22.00004: From electron-phonon transport properties to computational discovery of new materials for energy conversion. [Invited] BORIS KOZINSKY (Presenter), Harvard University, GEORGY SAMSONIDZE, Bosch Research — We introduce a novel simplified approach for computing electronic transport properties of complex semiconductors and low-dimensional quantum materials, without empirically fitted parameters. Using this method allowed us to discover new thermoelectric alloy compositions with leading performance and stability. The computational approach achieves good accuracy and transferability while greatly reducing complexity and computation cost compared to the existing methods. The first-principles calculations of the electron-phonon coupling demonstrate that the energy dependence of the electron relaxation time varies significantly with chemical composition and carrier concentration, suggesting that it is necessary to go beyond the commonly used approximations to screen and optimize materials' composition, carrier concentration, and microstructure. The new method is verified using high accuracy computations and validated with experimental data before applying it to screen and discover promising compositions in the space of half-Heusler alloys. We discuss the universality of the Wiedemann-Franz law and deviations from it in semiconductors, computing the Lorenz number from first principles.
9:12AM R22.00005: Influence of Oxygen Phonon Coupling on Fluctuating Stripes in the Three-band Hubbard Model
TIANYI LIU (Presenter), EDWIN HUANG, Stanford University, BRIAN MORITZ, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory — The normal state of high-\( T_c \) cuprate superconductors is characterized by competition between multiple ordered states such as antiferromagnetism, charge-density-waves, and stripes. We use determinant quantum Monte Carlo (DQMC) simulations of the three-band Hubbard model with oxygen phonon coupling to investigate how electron-phonon coupling influences high-temperature fluctuating stripes, in relation to doping level, phonon properties and electron-phonon coupling strength. Quantities such as the spin-spin and density-density correlation functions are extracted from the simulations to illustrate the influence of electron-phonon coupling on stripes.

9:24AM R22.00006: Pressure enhanced superconductivity in MoTe\(_2\)^*
HARI PAUDYAL (Presenter), Department of Physics, Applied Physics, and Astronomy, Binghamton University-SUNY, SAMUEL PONCE, Department of Materials, University of Oxford, ELENA R MARGINE, Department of Physics, Applied Physics, and Astronomy, Binghamton University-SUNY — Molybdenum ditelluride (MoTe\(_2\)) has attracted significant research interest due to the discovery of exotic topological states and pressure-driven superconductivity. First-principles calculations combined with the anisotropic Migdal-Eliashberg formalism have been carried out to investigate the role of electron-phonon interaction and the superconducting pairing mechanism in the two structurally similar phases, T\(_d\) and 1T\(_'\), under pressure. We find that both phases are superconducting, with the centrosymmetric 1T\(_'\) phase displaying a slightly larger electron-phonon coupling strength compared to the non-centrosymmetric T\(_d\) phase due to the softening of the low-energy phonon modes and a small increase in the density of states at the Fermi level.

*H. P. and E. R. M. acknowledge the NSF support (Award No. OAC-1740263) and the computational resources provided by XSEDE (TG-DMR180047).

9:36AM R22.00007: A comparison of molecular dynamics and Boltzmann transport equation approaches for lattice thermal conductivity^*
MARCELLO PULIGHEDDU (Presenter), University of Chicago, YI XIA, Argonne National Lab, Northwestern University, MARIA CHAN, Argonne National Lab, GIULIA GALLI, University of Chicago, Argonne National Lab — The predictive modeling of lattice thermal conductivity \( \kappa_L \) is of importance for both fundamental understanding and materials design. Molecular dynamics (MD) and Boltzmann Transport Equation (BTE) are the two most common approaches used to predict \( \kappa_L \). In this work, we perform a comprehensive comparison between MD and BTE approaches, on two model systems (MgO and PbTe), using interatomic potentials. Comparisons between MD and lifetimes from three- and four-phonon scattering, and between different treatment of statistics, are made. The sources of agreement and differences between MD and BTE are discussed.

^*This work was supported by the Midwest Integrated Center for Computational Materials (MICCoM) as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division (5J-30161-0010A).

9:48AM R22.00008: Four-phonon scattering-dominated linewidth of optical phonons^*
XIAOLONG YANG, Mechanical Engineering, Purdue University, TIANLI FENG, Oak Ridge National Laboratory, XIULIN RUAN (Presenter), Mechanical Engineering, Purdue University — Optical phonon linewidth is crucial to infrared optical properties of polar materials and thermal conductivity of certain materials that have a large number of optical phonon branches. The current understanding is, however, still limited to the lowest order phonon scattering, and the predicted linewidths often have large discrepancy with experiment. In this work we show the significance of four-phonon scattering in determining infrared optical properties for a range of important materials, including cubic boron arsenide (BAs), cubic silicon carbide (3C-SiC), and \( \alpha \)-quartz. Strikingly, We find that four-phonon scattering generally dominates optical phonon linewidths at elevated temperatures over three-phonon scattering. In large band gap-materials, e.g., BAs and AlSb, four-phonon scattering rates are found to be orders of magnitude higher than three-phonon scattering rates even at room temperature. The predicted infrared optical properties of \( \alpha \)-quartz after including four-phonon scattering show good agreements with experimental measurements.

^*We acknowledge the partial support from the National Science Foundation (Award No. 1150948) and Defense Advanced Research Projects Agency (Award No. HR0011-15-2-0037).
10:00AM R22.00009: First-principles calculation of ballistic photocurrents

We apply this methodology to BaTiO$_3$, a typical ferroelectric which displays the BPVE. These results clarify density functional perturbation theory, to find the carrier distribution functions and the magnitudes of ballistic scattering processes. We calculate the amplitudes of these processes using electron-phonon interactions derived from the unbalanced momentum space distribution of carriers, which results from the interference of multiple carrier-phonon scattering processes. These ballistic currents arise from an asymmetry in the phonon-induced ballistic current contribution. These ballistic currents arise from asymmetric phonon scattering, and shift currents, which are displacements of electrons upon photoexcitation, have been proposed as mechanisms responsible for the BPVE under linearly polarized light. However, only the shift current contribution has been routinely studied with first-principles calculations. In this work, we present first-principles calculations of the phonon-induced ballistic current contribution. These ballistic currents arise from an unbalanced momentum space distribution of carriers, which results from the interference of multiple carrier-phonon scattering processes. We calculate the amplitudes of these processes using electron-phonon interactions derived from density functional perturbation theory, to find the carrier distribution functions and the magnitudes of ballistic photocurrents. We apply this methodology to BaTiO$_3$, a typical ferroelectric which displays the BPVE. These results clarify the origin of the BPVE, and the relative importance of shift and ballistic currents.

10:12AM R22.00010: First-principles study of structural phase transition and thermal transport in halide perovskite CsPbBr$_3$

We applied the recently developed self-consistent phonon (SCP) scheme [1] to investigate the three different phases of all-inorganic perovskite CsPbBr$_3$, and calculated the thermal conductivity $\kappa_0$ and vibrational free energy from first principles. The SCP theory incorporates the anharmonic effect non-perturbatively and enables us to obtain well-defined phonons of the high-temperature phases. Also, we predicted the structural phase-transition temperatures $T_c$ of CsPbBr$_3$ by comparing the anharmonic free-energy of the three phases. We will demonstrate the validity of our approach by comparing the predicted $\kappa_0$ and $T_c$ values with available experimental data and discuss the origin of the low $\kappa_0$.


10:24AM R22.00011: Lattice thermal conductivity calculations of $\alpha$-quartz and $\alpha$-cristobalite

Although $\alpha$-quartz and $\alpha$-cristobalite have similar phonon densities of states, phonon frequency dependencies of phonon group velocities and lifetimes are dissimilar, which results in largely different anisotropies of the lattice thermal conductivities. For $\alpha$-quartz and $\alpha$-cristobalite, distributions of the phonon lifetimes effective to determine the lattice thermal conductivities are well described by energy and momentum conservations of three phonon scatterings weighted by phonon occupation numbers and one parameter that represents the phonon-phonon interaction strengths.


Phonon anharmonicity is essential for explaining phenomena such as thermal conductivity, thermal expansion, and the change in phonon frequencies with strain. In particular, strain dependence of phonon frequencies can be expressed through Grüneisen parameters, which are often used as a heuristic to quantify anharmonicity in general for a given system. However, the exact nature by which a system departs from anharmonicity is important - third, fourth, and higher order terms in the atomic potential play different roles in different situations. Are the same higher order force constants that contribute to Grüneisen parameters the ones involved in, for example, thermal transport processes, or are the ones that cause the quasiharmonic approximation to fail at high temperature? Using both analytic methods and density functional theory to inform and understand the underlying features of anharmonicity for a variety of systems, we find that while Grüneisen parameters provide valuable insight for how phonon modes couple to strain, one must take care in relating this quantity to other anharmonic effects. We further explore the relationship between phonons and strain, and other couplings between periodic eigenfunctions and aperiodic perturbations.

*NASA-NNX13AL39H; NSF-DMR-1550347, XSEDE-DMR-160052
Thermal Transport in a Substrate with Periodic Nanoscale Heat Sources

XINPENG ZHAO (Presenter), RONGGUI YANG, Mechanical Engineering, University of Colorado, Boulder — Understanding thermal transport from nanoscale heat sources to a substrate is crucial for the thermal management of high power electronics. When the size of a heat source is in comparison with or smaller than the phonon mean free path, the thermal transport in the substrate would deviate from the diffusive heat transfer described by the Fourier's law of heat conduction. Recent experimental results have shown that the thermal transport in a substrate with periodic nanoscale heat sources could be ballistic or diffusive-like by tailoring the size of the heat source and the distance between neighboring heaters. In this work, heat transport in a substrate with periodic nanoscale heating sources is simulated by solving the frequency-dependent phonon Boltzmann transport equation (BTE) using the Monte Carlo simulations. The effects of geometric sizes such as heat source size and spacing of heat sources on the heat dissipation efficiency are evaluated quantitatively. The results from the simulations could be used to understand the quasi-ballistic phonon transport mechanism in a substrate with periodic heating and to guide the design of the nanostructures for efficient thermal transport.

Thursday, March 7, 2019 8:00 AM - 9:48 AM

Session R23 GIMS: Acoustics, Noise and Damping BCEC 158

8:00AM R23.00001: Particulate dampers for absorption of structural vibrations at audible frequencies. Hasson M. Tavossi, Ph.D., Savannah State University, Department of Engineering Technology, 3219 College St., Savannah, GA 31404.* HASSON TAVOSSI (Presenter), Savannah State University — Absorption of mechanical vibrations by particulate material versus frequency are investigated, with the goal of reduction of transmission of vibrations into building structures. Attenuation of vibration by particulates depend mainly on their mechanical properties, shape, size-distribution, and degree of compression. Structural vibrations can be damped by surrounding them with particulate materials. Experimental results show that, particulate dampers behave as band-pass filters for vibrations that pass through them. The frequencies outside their passband range are strongly absorbed. Some particulate materials have a frequency band-gap, where frequencies in the bandgap range are strongly attenuated by scattering, absorption, or localization of vibrational energy. Samples of uniform size are coupled to mechanical vibrations at different frequency and amplitude. Their vibration absorption versus frequency are determined. Effects of layer thickness, particulate size, orientation, at different frequencies, in the audible range, are measured. The goal is to determine optimal vibration dampers to mitigate the transmission of external mechanical vibrations into the buildings.

*NA

8:12AM R23.00002: Cancelling Ambient Noise in Spectroscopic Images on a Scanning Tunneling Microscope* ALBERT CHIEN (Presenter), BRYCE PRIMAVERA, HARRIS PIRIE, JENNY HOFFMAN, Harvard University — Scanning tunneling microscopy (STM), a technique to measure the electronic structure of condensed matter systems with atomic resolution, requires an extremely stable environment to operate. Modern ultra-quiet STMs typically employ a combination of pneumatic suspensions and massive inertial blocks to reduce ambient vibrations to the sub-nanometer scale. Yet the tip-sample junction still experiences picometer vibrations that limit the signal-to-noise ratio in the tunneling current. Here we demonstrate a measurement scheme and software algorithm that reduces the effects of residual sub-picometer vibrations by order 50% in both topographic and spectroscopic images. We first calibrate a transfer function between a sensitive geophone on the STM head, and the STM tip-sample distance itself. We then use the simultaneously measured geophone output and tunneling current to cancel the effects of vibrations in the STM data in a 300Hz bandwidth.

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

8:24AM R23.00003: Design and Characterization of a Cylindrical Inertia Block for an Ultra-Low-Vibration Laboratory WENJIE GONG (Presenter), YU LIU, Harvard University, JOSEPH D. GIBBONS, Wilson HGA Architects, JENNIFER HOFFMAN, Harvard University — Typical low-vibration facilities employ a rectangular concrete inertia block supported on pneumatic isolators that damp vertical oscillation. However, it has been shown that when the inertia block sides are parallel to the surrounding room walls, acoustic standing waves can exert pressure on the parallel faces of the slab that causes measurable motion. To address this problem, we have designed a new low-vibration laboratory room housing a cylindrical inertia block, with no parallel faces. Here we simulate and measure the acoustic modes of the room and place limits on their coupling to the cylindrical inertia block. We further measure the transfer function from the building foundation to the inertia block. Finally, we drive the flexural resonance modes of the cylindrical inertia block and compare their frequencies to more traditional block shapes.
8:36AM R23.00004: Imaging Sound Waves in Phononic Metamaterials

WILLIAM FU (Presenter), NATHAN DRUCKER, HARRIS PIRIE, JENNIFER WANG, WOLFGANG RUECKNER, JENNIFER HOFFMAN, Harvard University — Phononic and photonic metamaterials have recently been proposed as analogs for topologically insulating structures, with a variety of potential applications. Most of these systems have been analyzed by simulation only (e.g. in COMSOL Multiphysics), but it has remained challenging to construct them experimentally and to measure their dynamics. Here we demonstrate two approaches to experimentally characterize real systems of topological phononic metamaterials using schlieren optics and a scanning microphone. In the schlieren setup, a mirror with long focal length is used to detect small changes in the refractive index of air using strobed light, which allows dynamic imaging of sound pressure [1]. Furthermore, we have developed a computer numerical control (CNC) scanning microphone with 6 degrees of freedom for dynamic imaging. Our sound wave imaging enables characterization of a topological phononic waveguide and other devices [2].


*This work was supported by the Science and Technology Center for Integrated Quantum Materials under NSF DMR-1231319. HP was funded by the Gordon and Betty Moore Foundation's EPiQS Initiative, Grant GBMF4536.

8:48AM R23.00005: Observation of GHz Modes in Quartz Circular Surface Acoustic Wave Resonator

JOEL THERRIEN (Presenter), SAISRIDEVESH KADAMBARI, ECE, University of Massachusetts Lowell — A novel form of Surface Acoustic Wave (SAW) resonators functions by exciting SAW modes in a circular acoustic cavity formed on a ST-cut quartz substrate. The resonant and harmonic frequencies of these devices is dependent on the diameter of the cavity. Based on the acoustic properties of ST quartz, devices with dimension in the range of 100's of μm are expected to have resonant frequencies in the range of 10's to 100's of MHz. These modes are indeed observed, however additional modes with frequencies in the GHz range (between 1-8 GHz) have also been observed. These modes do not appear to be part of the harmonic series associated with the MHz range modes. Moreover, specific aspects of these modes are inconsistent with the known acoustic properties of ST-cut quartz. Progress on understanding these modes will be presented.

9:00AM R23.00006: Regenerative Acoustofluidic NanoFilters for Biomolecular Purification and Quantification

WEIWEI CUI (Presenter), State Key Laboratory of Precision Measuring Technology & Instruments, Tianjin University, SHARI YOSINSKI, Biomedicine Engineering, Yale University, XUEXIN DUAN, State Key Laboratory of Precision Measuring Technology & Instruments, Tianjin University, MARK A REED, Yale University — Precise manipulation of target molecules is critical for microfluidic applications, such as molecular purification, target enrichment, and biosensing. Here, we report a microfluidic-based regenerable nanoscale filtration technique for purification and detection of target molecules from complex samples. By assembling specific functionalized nanoparticles (SFNPs) in an acoustofluidic vortex chip, an array of nanofilters is constructed. The acoustofluidic vortex is produced by a gigahertz bulk acoustic wave resonator, which allows for simple regeneration. Additionally, the acoustofluidic vortex increases SFNP-target interactions, overcoming diffusion limits. We demonstrate this nanofiltration method for rapid and effective purification of targets in both buffer and serum samples. We studied the molecular capturing dynamics using the biotin-SAv complex as a model, where we demonstrate a rapid (within 60 seconds) and accurate (with a detection limit of 170ng/mL) molecular quantification biosensor. The approach has the advantages of non-clogging high-throughput capability, as well as excellent flexibility, enabling wide biomedical applications.

9:12AM R23.00007: Non-invasive, non-destructive characterization of subsurface weld defects via directed ultrasound

JOHN GREENHALL (Presenter), ALAN LYMAN GRAHAM, CRISTIAN PANTEA, DIPEN N SINHA, Los Alamos National Laboratory — Directed ultrasound is employed to identify defects in subsurface welded joints and to characterize the defects as either inclusions or voids. We scan over the welded joint with a single ultrasound transducer, which transmits an ultrasound burst, and then we measure the burst after it reflects from the subsurface weld defects. In contrast with existing ultrasound characterization techniques we do not require a mechanical connection between the ultrasound transducer and the welded specimen, which facilitates implementation in the field. We utilize a correlation envelope to identify and locate defects in the presence of noise, and we distinguish between voids and inclusions based on phase change in the measured burst after reflection from a weld defect. We demonstrate the directed ultrasound technique for identifying subsurface defects in a tungsten alloy with a square joint. In contrast with X-ray imaging techniques, which cannot penetrate tungsten alloys, we identify, locate, and characterize known defects at depths of >10 mm. This directed ultrasound technique enables non-invasive, non-destructive inspection of a wide range of materials, and finds application in numerous applications including welding, printed circuit board fabrication, and sintered 3D printing.
9:24AM R23.00008: Ultrasonic Collimated Beams in Elastic Solids*  
VAMSHI KRISHNA CHILLARA (Presenter), CRISTIAN PANTEA, Los Alamos National Laboratory — Ultrasonic collimated beams are directed beams that propagate in materials with very little angular spread. Generation of such beams in solids enable high resolution imaging of heterogeneous and attenuating materials like concrete and noninvasive materials characterization of anisotropic materials like composites. We present a simple approach to generating ultrasonic collimated beams that relies on a novel approach to generating Bessel beams using radial modes of piezoelectric disc transducers. We first discuss the resonance and vibration characteristics of radial modes of piezoelectric discs using numerical and experimental studies. Then, analytical and numerical results on ultrasonic Bessel beam generation in elastic solids will be presented. Finally, a technique for the reduction of side lobes in Bessel beams will be discussed and numerical results on ultrasonic collimated beam generation in elastic solids will be presented.

*This research was funded by DOE office of Energy Efficiency and Renewable Energy (EERE).

9:36AM R23.00009: Multiscale porosity measurements of Shale rocks using multiple gas adsorption and mercury intrusion porosimetry  
NICOLAS CHANUT (Presenter), THIBAUT DIVOUX, RÉNAL BACKOV, CEE, Massachusetts Institute of Technology, JEFF KENVIN, Micromeritics, ROLAND JM PELLENQ, CEE, Massachusetts Institute of Technology — Unconventional oil and gas production from shale has revolutionized the world energy landscape. Shale is a fine-grained sedimentary rock, composed of solid organic matter (OM) scattered in a mineral framework. The decomposition of this OM at high temperature leads to the generation of hydrocarbons during a process known as maturation. The resulting organic matter develops a nanoscale porosity that governs the ability of a shale petroleum reservoir to store and then to yield oil and gas. The mineral matrix also contributes to the overall porosity leading to a pore size distribution spanning from a few Å to the µm range. In this work, we have combined gas adsorption of multiple gases (CO2, H2, N2, and Ar) and mercury intrusion porosimetry to study the pore system of 5 samples from the Vaca Muerta formation that differ in maturities. Indeed, while gas adsorption allows probing the micro and mesoporosity (< 50nm), mercury intrusion allows for the characterization of the macroporosity (10nm to 500µm). Rather than using a fragmented approach of simple overlays from individual techniques, a unified approach that utilizes a kernel constructed from model isotherms and model intrusion curves is used to calculate the complete pore size distribution and the total pore volume of the material.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R24 DAMOP DQI: Hybrid/Macroscopic Quantum Systems, Optomechanics, and Interfacing AMO with Solid State/Nano Systems III  
BCEC 159 - Nathan Schine, University of Chicago

8:00AM R24.00001: Controlling thermal fluctuation of phonon modes with nonreciprocal dynamics in an optomechanical system*  
HAITAN XU (Presenter), LUYAO JIANG, Physics, Yale University, AASHISH CLERK, Institute for Molecular Engineering, University of Chicago, JACK HARRIS, Physics, Yale University — Nonreciprocal dynamics in optomechanical systems is of rising interest in the past several years. While earlier works mainly focused on photonic modes, here we study nonreciprocal dynamics for phonon modes. We have realized nonreciprocal coupling between phonon modes, which leads to nonreciprocal phonon transfer. We achieved phonon isolation which can be tuned continuously over a wide range from -30dB to 30dB. We show the nonreciprocal phonon transfer as a new way to control the thermal fluctuation of phonon modes by controlling laser phases.

*This work is supported by AFOSR grant FA9550-15-1-0270, AFOSR MURI FA9550-15-1-0029, ONR MURI N00014-15-1-2761, and the Simons Foundation (Award Number 505450).
8:12AM R24.00002: Diamond optomechanical crystals with embedded nitrogen-vacancy centers* JEFF CADY (Presenter), OHAD MICHEL, KENNETH LEE, ANIA CLAIRE JAYICH, University of California, Santa Barbara — Hybrid mechanical systems, in which qubits are coupled to mechanical degrees of freedom, have recently emerged as a promising alternative and supplement to traditional photonic systems. Recent experiments\(^1\) have demonstrated such a hybrid system with diamond mechanical resonators and embedded nitrogen-vacancy (NV) centers, which interact with one another via crystal strain. While previously realized devices have enabled, for example, extension of coherence using mechanically-dressed spin states and frequency and polarization tuning of the NV center excited state transition, NV-phonon coupling rates have not approached the high quantum cooperativity regime necessary for such applications as phonon-mediated spin-spin interactions and NV-assisted mechanical cooling. As a preliminary step toward the high cooperativity regime in NV center-based hybrid mechanical devices, we design and fabricate single-crystal diamond optomechanical crystals (OMCs), which host GHz-scale mechanical modes and telecom-band optical modes and contain embedded NV centers. Importantly, the spin coherence of these NV centers has been preserved through the fabrication process, with \(T_2^-\) exceeding 1 μs and \(T_2\) exceeding 70 μs.

\(^1\) D. Lee, \textit{et al.}, \textit{J. Opt.} \textbf{19} 033001 (2017)

*NSF CAREER Award DMR1352660

8:24AM R24.00003: Persistent and Reversible Frequency Tuning in Graphene/Hexagonal Boron-Nitride Nanomechanical Resonators DAVID MILLER (Presenter), ANDREW BLAIKIE, BENJAMIN J ALEMAN, University of Oregon — Persistent and reversible methods for tuning the resonance frequency of a nanomechanical resonator are essential for fields ranging from quantum information to ultra-sensitive force and mass sensing. However, reliable methods to achieve this tuning have been difficult to realize.

Here, we demonstrate that the resonance frequency of nanomechanical resonators can be persistently and reversibly tuned using photoelectric doping[1]. We demonstrate this effect in drumheads made from heterostructures of hexagonal boron-nitride (h-BN) and graphene. However, this technique could potentially be extended to electromechanical resonators made from any material that can be photoelectrically doped. We observe tuning that is robust over weeks, can occur at rates as fast as \(-1\) GHz/s, and has a tuning range of greater than 250%. This could enable future applications which need large numbers of individually tunable nanomechanical elements, such as chip-scale optomechanical circuits.


8:36AM R24.00004: Cooling and amplifying motion of a diamond nanobeam via translation of a focused laser beam* HARISHANKAR JAYAKUMAR (Presenter), BEHZAD KHANALILOO, DAVID LAKE, PAUL BARCLAY, Department of Physics and Astronomy, University of Calgary — Controlling the dynamics of mechanical resonators is central to many quantum science and metrology applications. Optomechanical control of diamond resonators is attractive owing to diamond’s excellent physical properties and its ability to host electronic spins that can be coherently coupled to mechanical motion. Using a confocal microscope, we demonstrate tunable amplification and damping of a diamond nanomechanical resonator’s motion. Observation of both normal mode cooling from room temperature to 80K, and amplification into self-oscillations with 60 μW of optical power is observed via waveguide optomechanical readout. This system is promising for quantum spin-optomechanics, as it is predicted to enable optical control of stress-spin coupling with rates of \(-1\) MHz (100 THz) to ground (excited) states of diamond nitrogen vacancy centers.

*NSERC (Discovery and Research Tools and instruments), CFI, AITF and NRC.

8:48AM R24.00005: Measuring the Casimir torque* JEREMY MUNDAY (Presenter), University of Maryland, College Park — It is well-known that the confinement of quantum electromagnetic fluctuations between two macroscopic objects can result in a force, known as the Casimir force. However, in addition to this force, a torque has been predicted between optically anisotropic materials. In this presentation I will discuss counter-intuitive ways to increase the torque (e.g. placing the objects in a dielectric medium rather than vacuum) and our recent experiments that confirm its existence.

*This work was supported by the National Science Foundation under Grant No. PHY-1506047 and PHY-1806768.
Optomechanics for NEMS based Mass Spectrometry  
EWA REJ (Presenter), JARVIS LI, WARREN FON, MATTHEW MATHENY, MICHAEL ROUKES, Caltech — NANOeLectromechanical systems (NEMS) provide an ideal platform for single molecule sensing applications due to their minute size and high quality factors. One application is the measurement of the mass of individual adsorbed molecules, such as single proteins. The mass resolution is governed by the uncertainty in the measured resonance frequency, with contributions from the mechanics (e.g. thermomechanical noise), readout circuitry noise, and the intrinsic instability of the resonator. As a result, a detailed understanding of phase noise is necessary for improved sensor performance. Here we detail a new scheme for NEMS mass sensing based on superconducting microwave cavity optomechanics. The optomechanical transduction scheme is expected to improve the phase noise and resulting mass resolution of NEMS sensors.

Search for light scalar dark matter using optomechanical systems  
SWATI SINGH (Presenter), University of Delaware — Although the existence of dark matter (DM) has been indisputably proven by a range of cosmological and astronomical measurements, there is no viable candidate for dark matter in the Standard Model. In this talk, we will explore optomechanical resonators as detectors of scalar dark matter in the $10^{-12} - 10^{-6}$ eV regime. Light DM particles have large occupation numbers and can be phenomenologically described as a classical field. Irrespective of the model used to produce them, such a classical field can have consequences that can be measured by precision measurement setups, such as varying $\alpha$ or $m_e$ at the frequency associated with DM mass. This effect is enhanced in a solid, and variations in the size of an elastic medium lead to a new force just like the tidal force due to a passing gravitational wave. Moreover, the resonant enhancement over a localized frequency provided by these devices enhances sensitivity to such fields. We will discuss the scalar field parameter space than can be explored by current and future optomechanical devices. Finally, we will comment on how these searches can complement the existing precision measurement based searches based on atomic clocks, spin precession or equivalence principle tests.

Enhanced Optomechanics with Nanostructured Material*  
LI-FAN YANG, ANURUP DATTA, YUCHUN HSUEH, XIANFAN XU, KEVIN WEBB (Presenter), Purdue University — The maximum pressure on a planar surface is understood to be twice the incident wave power density normalized by the background velocity. We demonstrate for the first time that this pressure can be exceeded by a substantial factor by structuring a surface. Experimental results for direct optomechanical deflection of a nanostructured gold film on a silicon nitride membrane illuminated by a laser beam are shown to significantly exceed those for the planar surface. This enhanced pressure can be understood as being associated with an asymmetric optical cavity array realized in the membrane film, and a simple one-dimensional model explains the basic picture. Force control depends on the material properties and the geometrical parameters of the structured material. The interplay between material, structure at the nanometer-scale, and optical force should have substantial consequences in applications that include all-optical communication, remote actuation, propulsion, and biophysics.

Cryogenic Optical and Spin Characterization of Tin-Vacancy Centers in Diamond*  
MATTHEW TRUSHEIM (Presenter), Electrical Engineering and Computer Science, Massachusetts Institute of Technology, BENJAMIN PINGAULT, Cavendish Laboratory, University of Cambridge, NOEL WAN, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, MUSTAFA GUNDOGAN, Cavendish Laboratory, University of Cambridge, LORENZO DE SANTIS, KEVIN CHEN, MICHAEL WALSH, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, JOSHUA ROSE, Cavendish Laboratory, University of Cambridge, JONAS BECKER, Clarendon Laboratory, University of Oxford, ERIC BERSIN, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, GIRISH MALLADI, HASSARAM BAKHRU, College of Nanoscale Science and Engineering, SUNY Poly, IAN A WALMSLEY, Clarendon Laboratory, University of Oxford, METE ATATURE, Cavendish Laboratory, University of Cambridge, DIRK R. ENGLUND, Electrical Engineering and Computer Science, Massachusetts Institute of Technology — Color centers in diamond are promising quantum systems that can combine long-lived spin degrees of freedom with coherent optical transitions. Recently, emitters based on Group IV-vacancy complexes, including the silicon- and germanium-vacancy, have garnered interest as their inversion symmetry protects the optical line from environmental noise. Here, we will discuss cryogenic resonant spectroscopy of tin-vacancy (SnV) center in diamond. Specifically, we will describe its electronic structure, optical signatures of spin, and coherent optical and spin properties. We find that the SnV is a candidate quantum memory that can operate at liquid helium temperatures, potentially enabling scalable quantum networks.

*M.T. acknowledges support by an appointment to the Intelligence Community Postdoctoral Research Fellowship Program at MIT, administered by Oak Ridge Institute for Science and Education through an interagency agreement between the U.S. Department of Energy and the Office of the Director of National Intelligence.
9:48AM R24.00010: Utilizing the nonlinear dynamical response of an optically damped mechanical oscillator*
KJETIL BORKJE (Presenter), University of South-Eastern Norway — We consider a standard cavity optomechanics setup where a mechanical oscillator is coherently driven at its resonance frequency. The cavity mode is driven below its resonance, providing optical damping of the mechanical oscillations. We study the nonlinear coherent response of the mechanical oscillator in this setup. For large mechanical amplitudes, we find that the system can display dynamical multistability if the optomechanical cooperativity exceeds a critical value. We investigate the effect of thermal and quantum noise and estimate the noise-induced switching rate between the stable states of the system. Finally, we discuss how this system can be used as bifurcation amplifiers for the detection of small mechanical or optical signals.

*The author acknowledges funding from the QuantERA ERA-NET Cofund in Quantum Technologies (project QuaSeRT) implemented within the European Union's Horizon 2020 Programme.

10:00AM R24.00011: Ground-state cooling of a mechanical resonator enabled by critical coupling and dark entangled states*
CRISTIAN CORTES (Presenter), MATTHEW OTTEN, STEPHEN K GRAY, Nanoscience and Technology Division, Argonne National Laboratory — Over the past ten years, there has been tremendous interest in achieving ground-state cooling in mechanical resonators in order to enhance the performance characteristics of mechanical-based sensors, quantum memories, and quantum transducers. While there have been successful demonstrations of ground-state cooling using optomechanical systems, an outstanding challenge remains in reaching the ground state using solid-state defects. In this work, we present a novel approach for resonant phonon cooling using the concept of critical coupling, subradiance, and many-body entanglement within an ensemble of two-level systems. We reveal that carefully engineering the strain profile of the mechanical resonator allows phonon cooling to proceed through the dark entangled states of an interacting ensemble, thereby enabling ground-state cooling in spite of the small spin-strain coupling strengths encountered in real systems. Our work provides a new avenue for phonon cooling and should be accessible for experimental demonstrations.

*This work was performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, and supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

FREDERIC PEYSKENS (Presenter), Massachusetts Institute of Technology, DRIES VAN THOURHOUT, Ghent University, DIRK R. ENGLUND, Massachusetts Institute of Technology — Localized quantum emitters in certain 2D materials show great promise to realize single photon sources on top of photonic integrated circuits, as these materials allow easy and scalable integration with such circuits. Most research so far was however devoted to the study of free-space quantum emitters. We will present our work on the integration of 2D materials on top of a mature silicon nitride photonic platform and moreover elaborate on our analytical framework to describe the interaction of a 2D-material-based cavity-emitter system with a dielectric photonic waveguide. Rather than minimizing the cavity modal volume, our analysis predicts an optimum modal volume to maximize the single photon generation efficiency into the guided mode of the waveguide, thereby balancing waveguide coupling and spontaneous emission rate enhancement. Numerical simulations on realistic systems allow us to extract optimal parameters for the design of integrated quantum photonic circuitry.

*F.P. acknowledges support from a BAEF, Fulbright, and FWO postdoctoral fellowship. D.E. and F.P. acknowledge partial support from the CDQI and the NSF EFRI-ACQUIRE program.

10:24AM R24.00013: Cavity optomagnonics with magnetic textures: coupling a magnetic vortex to light
JASMIN GRAF (Presenter), HANNES PFEIFER, FLORIAN MARQUARDT, SILVIA VIOLA-KUSMINSKIY, Max Planck Institute for the Science of Light — Efforts so far in cavity optomagnonics, where light couples coherently to magnons in a solid state cavity system, have focused on systems with a homogeneous magnetic background. We propose a cavity-optomagnonic system with a non homogeneous magnetic ground state, namely a vortex in a magnetic microdisk. We study the coupling between optical whispering gallery modes to gyrotrropic and flexural magnon modes localized at the vortex. We show that the optomagnonic coupling has a rich spatial structure and that it can be tuned by an externally applied magnetic field. Our results predict cooperativities at maximum photon density of the order of $C \sim 0.01$ by proper engineering of these structures.
10:36AM R24.00014: Nonlinear dynamics in disordered optomechanical arrays  THALES FIGUEIREDO ROQUE (Presenter), FLORIAN MARQUARDT, VITTORIO PEANO, Max Planck Institute for the Science of Light, OLEG YEV TUSHENKO, Ludwig-Maximilians-University — Optomechanical arrays (OMA) have already offered a playground for the theoretical investigation of a broad range of phenomena including synchronization, many-body dynamics, quantum control and topological effects. The implementation of these investigations requires a degree of control on the dispersion of the parameters of the individual optomechanical cells. However, the most promising platforms for OMA are based on nanoscale on-chip technologies such as microdisks and optomechanical crystals. This represents a challenge because fabrication imperfections are difficult to control on the nanoscale. Conversely, disorder can be viewed as a resource which gives rise to interesting physical phenomena. In this talk, we focus on the nonlinear dynamics of disordered OMA. This regime displays a number of nontrivial and yet not explored phenomena involving the interplay of Anderson localization, dissipation and strong nonlinearities.

10:48AM R24.00015: Modeling the Adsorption-Desorption Phase Noise in Optomechanical Oscillators  CIJY MATHAI (Presenter), SIDDHARTH TALLUR, Indian Institute of Technology Bombay — Optomechanical oscillators (OMOs) exhibit self-sustained mechanical oscillations, driven by optical pumping through radiation pressure or optical gradient force. Due to the lack of externally applied feedback, prior theoretical models and experiments have reported that such oscillators are free of 1/f^3 (pink noise) and higher order slopes in the phase noise spectrum [Opt. Exp. 2011;19:24522-29]. However, most OMO results reported at sub-atmospheric temperatures and pressures exhibit significant 1/f^4 phase noise (brown noise), that is not explained by conventional models. In this work, we study the impact of adsorption and desorption (of gas molecules on the resonator surface) on phase noise in OMOs, based on noise analysis in mechanical oscillators [IEEE TUFFC. 1989;36(4):452-8]. Experimental data recorded for a chip-scale silicon OMO (obtained in a liquid nitrogen cooled vacuum ambience) fits well with the theoretical prediction. An additional insight drawn from the model is that unlike phase noise originating from thermal noise sources, the brown phase noise is independent of the mechanical mode shape, as validated through observation of similar magnitude of 1/f^4 noise in oscillations of a radial breathing mode at 70MHz and wineglass mode at 58MHz in the same device.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R25 DAMOP DCMP: Disorder and Localization in AMO Systems III: Many-body Localization  BCEC 160A - Fernando Sols, Complutense University

8:00AM R25.00001: Long-range resonances and the meltdown of many-body localization*  BENJAMIN VILLALONGA (Presenter), BRYAN CLARK, University of Illinois at Urbana-Champaign — Closed, quantum systems with interactions can transition to a many-body localized (MBL) phase in the presence of disorder. In this work, we attempt to numerically identify the presence of resonances in the ergodic-MBL transition. We find evidence for the proliferation of resonances around the transition, where the resonance structure becomes scale invariant. In addition, we consider how the resonances induce the buildup of entanglement and spectral statistics observed in the system through collisions between energy levels. We explore this both in the real-space basis as well as an adiabatic 1-bit basis.

*This research is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.
8:12AM R25.00002: Critical Dynamics at the Many-Body-Localized Phase Transition*  MATTHEW RISPOLI (Presenter), ALEXANDER LUKIN, ROBERT SCHITTKO, SOOSHIN KIM, JOYCE KWAN, MING E TAI, JULIAN LEONARD, MARKUS GREINER, Harvard University — When an isolated quantum system is prepared far from equilibrium, transport of its constituent particles allows it to relax by energy exchange throughout the remaining system. However, the addition of strong disorder in these interacting systems breaks down transport at a critical disorder strength as a consequence of many-body localization (MBL). Here, we study many-body localization in a 1-D system of interacting bosons with quasi-periodic disorder. Through the site-resolved, correlated density fluctuations, we extract a dynamic transport length and observe exceptionally slow transport near this critical disorder strength. We additionally verify the critical nature of the system’s dynamics by tuning the total system size. Finally, we identify a microscopic mechanism of the interaction-driven delocalization via a sparse-resonant structure. This sparse structure persists into higher-order correlation functions and additionally identifies the many-body critical nature. These results and observed mechanism lay a foundation for characterizing dynamic many-body phases and studying other proposed microscopic mechanisms in interacting, disordered systems.

*We are supported by the NSF, the Moore Foundation, AFOSR MURI, and ARO MURI.

8:24AM R25.00003: Avoiding Ergodicity: Localization in Clean Interacting Systems YUVAL BAUM (Presenter), EVERT VAN NIEUWENBURG, GIL REFAEL, Caltech — Since the phenomenon of many-body-localization (MBL) was re-postulated more than a decade ago, it has attracted a great deal of attention. A key ingredient for achieving the MBL phase is disorder (randomness). The roots of this phase lie within the phenomenon of Anderson localization, where non-interacting particles form a localized non-ergodic phase. It is the question regarding the fate of Anderson localization in the presence of interactions that plants the seed for the discovery of the MBL phase.

We wish to go beyond the conventional paradigm and ask whether randomness is indeed an essential ingredient in achieving generic non-ergodic interacting phases.

We proposed the idea that the essential ingredient for MBL is localization, which does not necessarily mean disorder. We analyze the spectral and the dynamical properties of one-dimensional interacting fermions and spins in the presence of both disorder and linear potential. We show that by considering these two different localizing mechanisms, i.e., disorder and linear fields, one may construct a two-dimensional phase diagram which hosts a connected non-ergodic (MBL) phase.

8:36AM R25.00004: Dephasing Beyond the Markovian Limit; Implications for Many-Body Localization SETH DAVIS (Presenter), MATTHEW FOSTER, Rice University — Despite progress in understanding many-body localization (MBL) in one-dimension, many questions remain with respect to the nature of the transition and the stability of the MBL phase. We envision approaching the MBL transition from the high-temperature ergodic phase. We search for signatures of the transition as a failure of dephasing, which prevents the infrared divergence of quantum conductance corrections in the ergodic phase in 1D and 2D.

For an isolated fermion system with short-ranged interactions, dephasing is due to diffusive (strongly non-Markovian) thermal density fluctuations. A previous study identified a nontrivial RG fixed point in \(4 - \epsilon\) dimensions, at which the dephasing time diverges (Liao and Foster, PRL 2018). By contrast, long-range Coulomb interactions provide an approximately Markovian bath. A perfectly Markovian bath dephases at any nonzero temperature (Altshuler, Aronov, Khmelnitsky 1982).

We perturb about the exactly solvable Markovian limit, which we re-interpret as an exact, infinite-order diagrammatic summation. Using explicit calculations and scaling arguments, we will describe results beyond the Markovian limit in 1D and 2D.

8:48AM R25.00005: Many Body Localization Transition in Systems with Correlated Disorder* RAJDEEP SENSARMA (Presenter), ABHISEK SAMANTA, AHANA CHAKRABORTY, Tata Institute of Fundamental Research — We study the transition from many body localized to ergodic transitions in disordered spin chains where the disorder at different sites are correlated. In the uncorrelated limit, the system has a well studied transition between many body localized to ergodic phase as a function of increasing disorder strength. On the other hand, in the extremely correlated limit, we essentially obtain a translation invariant system. We use two different models of correlated disorder and map out the phase diagram in the correlation-disorder plane.

*We acknowledge use of computational facilities in Department of Theoretical Physics, TIFR Mumbai
Activating many-body localization in solids by driving

ZALA LENARCIC (Presenter), EHUD ALTMAN, University of California, Berkeley, ACHIM ROSCH, University of Cologne —

Coupling to phonons prevents many-body localization (MBL) from occurring in disordered solids even when the disorder is strong. This is because phonons mediate non-local interaction which weakly breaks local conservation laws characteristic for the MBL phase. Nevertheless, I will show that decay of local conservation laws can be compensated when the system is driven out of equilibrium. We propose to detect the fingerprints of an underlying MBL phase by measuring the variation of local temperatures in the resulting steady state.

The concrete example I will consider is a one-dimensional disordered spin-chain which is weakly coupled to a phonon bath and weakly irradiated by white light. The irradiation has weak effects in the ergodic phase. However, if the system is in the MBL phase irradiation induces strong temperature variations. Temperature variation can be used similar to an order parameter to detect MBL phases, the phase transition, an MBL correlation length and even the critical exponents. Finite coupling strengths broaden the transition into a crossover, potentially containing information on the Griffiths effects. I will address this using tensor network and variational ansatz approaches.


Flow Equations for Many-Body Localisation: Dynamics and Dimensionality*

STEVEN THOMSON (Presenter), MARCO SCHIRO, Institut de Physique Théorique — Once thought to destroy localisation completely, we now know that adding interactions into disordered quantum matter can lead to the formation of a many-body localised phase. This phase is characterised by an extensive number of local conserved quantities and a failure to thermalise. Consequently it cannot be described by conventional equilibrium quantum statistical mechanics: new theoretical tools are required. Here, we present a semi-analytic flow equation approach that is capable of simulating large system sizes and of computing the real-time dynamics of observables and correlation functions. We employ a continuous unitary transform to diagonalise the Hamiltonian of a gas of interacting spinless fermions, show how local integrals of motion naturally emerge from this method, and go on calculate time evolution and localisation properties in the strongly-disordered regime in both one and two spatial dimensions. We further comment on ongoing work extending the method to incorporate additional features, including spin, as well as three-dimensional systems.


*This work was supported by the grant "Investissements d'Avenir" from LabEx PALM (ANR-10-LABX-0039-PALM) and by the CNRS through PICS-USA-14750.

Localization in Fractonic Random Circuits

SHRIYA RAMACHANDRAN PAI, MICHAEL PRETKO (Presenter), RAHUL NANDKISHORE, University of Colorado, Boulder — In this talk, I will describe a new mechanism for many-body localization, making use of ideas drawn from the field of fractons. Specifically, I will present results on the spreading of initially local operators under random unitary evolution in spin chains subject to fracton conservation laws, such as conservation of dipole moment. We find that fractons remain permanently localized at their initial positions, providing a crisp example of a non-ergodic dynamical phase of random unitary evolution. These results can be interpreted as a consequence of the properties of low-dimensional random walks. This mechanism for localization remains robust in one and two dimensions, but breaks down in three-dimensional fracton systems. We argue that these results extend to Floquet and Hamiltonian time evolution, even in the absence of disorder, thereby providing a mechanism for many-body localization in a translationally invariant system.

Statistics of entanglement spectrum across MBL to ergodic transition.

ABHISEK SAMANTA (Presenter), KEDAR DAMLE, RAJDEEP SENSARMA, Tata Institute of Fundamental Research — We show how the statistics of entanglement spectra change across the transition between a many body localized phase and an ergodic phase of an interacting disordered system. Using a disordered spin chain as a model, we numerically construct various measures and try to find an "order parameter" for the transition. The transition point obtained from this construction matches with those obtained from other indicators like the distribution of many-body energy gaps.
Localization in an interacting system with two degrees of freedom per site: Is charge disorder alone sufficient to localize the Hubbard model or is spin disorder also necessary?* RACHEL WORTIS (Presenter), BRANDON LEIPNER-JOHNS, Physics & Astronomy, Trent University — Many-body localization, the inability of some isolated quantum systems with both interactions and disorder to achieve thermal equilibrium, has been studied primarily in systems with one degree of freedom per site. The addition of a second degree of freedom creates a new avenue for exploration and connects to the Hubbard model, a launch point for the study of a wide range of systems of current interest including transition metal oxides and cold atoms in optical lattices. With both charge and spin degrees of freedom at each site, is disorder in just one of these channels sufficient to cause the full system to be localized? Alternatively, does the degree of freedom without disorder delocalize the one which sees disorder? To what extent is the level of localization in one channel related to the disorder in the other channel? We consider the Hubbard model with both charge and spin disorder. We employ several measures of localization designed to treat spin and charge on equal footing. We find measures based on the local integrals of motion are consistent with those based on the dynamics. For sufficient disorder in one degree of freedom, only a small amount of disorder in the other degree of freedom localizes both degrees of freedom.

*Supported by NSERC of Canada.

Many-body localization in a multifractal fermionic chain* NICOLAS MACÉ (Presenter), NICOLAS LAFloRENCIE, FABIEN ALET, Laboratoire de Physique Théorique, Université de Toulouse — We study the many-body localization (MBL) properties of a chain of interacting fermions subject to a deterministic quasiperiodic on-site potential following the Fibonacci sequence. With this choice, the single-particle eigenstates are delocalized and multifractal, no matter how strong the potential is. Contrary to naive expectations, adding interactions in this system does not enhance delocalization, and a MBL transition is observed. Due to the highly correlated nature of the potential, the MBL phase presents features which differ from those encountered for the more documented random-box potential. We observe for example extra peaks in the fermion density distribution which we can relate to the occurrence of specific local patterns in the quasiperiodic potential. Furthermore, in the ergodic phase, non-trivial properties of the single-particle density matrix are observed, compatible with a persistence of the free fermions multifractality. Our analysis is based on exact numerical studies of eigenstates and dynamical properties after a quench.

*We acknowledge support from the French ANR (THERMOLOC ANR-16-CE30-0023-02), Investissements d'Avenir (ANR-11-IDEX-0002-02, ANR-10-LABX-0037-NEXT), PRACE (grant 2016153659), CALMIP (2017-P0677 and 2018-P0677) and GENCI (x2018050225).

Many body localization in the presence of a central qudit* NATHAN NG, Physics, UC Berkeley, MICHAEL KOLODRUBETZ (Presenter), University of Texas at Dallas — We consider a many-body localized system coupled globally to a central d-level system. Under an appropriate scaling of d and system size, we find evidence that the localized phase survives. We argue for two possible thermalizing phases, depending on whether the qudit becomes fully ergodic. This system provides one of the first examples of many-body localization in the presence of long-range (non-confining) interactions. We discuss possible anomalous behavior in the system, such as an inverted mobility edge - localized at high temperature, but ergodic at low temperature.

*We acknowledge support from the U.S. Department of Energy Basic Energy Sciences (BES) TIMES initiative and UTD Research Enhancement Funds.

Stability of quasiperiodic chains to quantum avalanches* ANUSHYA CHANDRAN (Presenter), PHILIP CROWLEY, Boston University — In one dimension, it is conjectured that full many-body localization is unstable if the localization length exceeds a threshold value. The instability is due to the presence of rare ergodic Griffiths regions; each such region thermalizes its environment and grows, resulting in a (slow) avalanching process of thermalization. We show that weakly interacting chains with quasiperiodic potentials violate this conjecture because the sparse local structure of the l-bits prevents thermalization near an ergodic region. Our work identifies the first qualitative difference between random and quasi-periodic localization and suggests new experimental tests of avalanche instabilities.

*AC acknowledges support from the Sloan Fellowship and from the NSF through the grant DMR-1752759.
10:36AM R25.00014: Hilbert space properties of the many-body localization problem: from full ergodicity to multifractality* NICOLAS MACÉ, FABIEN ALET, NICOLAS LAFLORENCIE (Presenter), CNRS, Université Paul Sabatier, Laboratoire de Physique Théorique, Toulouse — In contrast with Anderson localization where a genuine localization is observed in real space, the many-body localization (MBL) problem is much less understood in the Hilbert space, support of the eigenstates. In this work, using exact diagonalization techniques up to L=24 spin-1/2 particles (i.e. Hilbert space of size N=2.7 millions) we address the ergodicity properties in the underlying N-dimensional complex networks spanned by various computational bases. We report fully ergodic eigenstates in the delocalized phase (irrespective of the computational basis), while the MBL regime features a generically (basis-dependent) multifractal behavior, delocalized but non-ergodic. The MBL transition is signaled by a non-universal jump of the multifractal dimensions.

*This work benefited from the support of the project THERMOLOC ANR-16-CE30-0023-02 of the French National Research Agency (ANR) and by the French Programme Investissements d'Avenir under the program ANR-11-IDEX- 0002-02, reference ANR-10-LABX-0037-NEXT. We acknowledge PRACE for awarding access to HLRS's Hazel Hen computer based in Stuttgart, Germany under grant number 2016153659, as well as the use of HPC resources from CALMIP (grants 2017-P0677 and 2018-P0677) and GENCI (grant x2018050225).

10:48AM R25.00015: Entanglement, dynamics and breakdown of many-body localization in current driven system* SUMILAN BANERJEE (Presenter), ANIMESH PANDA, Center for Condensed Matter Theory, Department of Physics, Indian Institute of Science — What is the fate of a many-body localized system under a voltage bias between two ends? Can the system undergo a transition to a current carrying non-equilibrium steady state and how the entanglement properties of the quantum states change across the transition? Motivated by these questions, we model a current driven interacting disorder system through a non-Hermitian Hamiltonian and study the entanglement properties of its eigenstates. We also discuss the dynamics, entanglement growth and long-time fate of a generic initial state under an appropriate time-evolution of the system governed by the non-Hermitian Hamiltonian. Our study reveals rich entanglement structures of current driven states and multiple dynamical transitions as a function of disorder and the strength of the non-Hermitian term, that is related to the external bias.

*SB is supported by The Infosys Foundation, India through Infosys Young Investigator Award, AP by UGS-CSIR, India

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R27 DQI: Quantum Error Correction Theory and Experiment II BCEC 160C - Christopher Chamberland, IBM Thomas J Watson Research center - Tag(s): Focus

8:00AM R27.00001: The boundaries and topological defects of the color code* [Invited] MARKUS KESSELRING (Presenter), FU Berlin — We give a thorough exploration of the color code phase to find all of its boundaries and domain walls. This gives us a new playground to discover new quantum error correcting codes and ways of performing gates. Our exploration uncovered improved methods for performing quantum computations by code deformation, a new four-qubit error-detecting code, as well as families of new quantum error-correcting codes we call stellated color codes, which encode logical qubits at the same distance as the next best color code, but using approximately half the number of physical qubits.

*MSK is supported by the DFG (CRC183, project B02). FP was supported by the Alexander von Humboldt Foundation. JE is supported by DFG (CRC 183, project B02, El 519/14-1, and El 519/7-1), the ERC (TAQ), the Templeton Foundation, and the BMBF (Q.com). BJB is supported by the University of Sydney Fellowship Programme, the Australian Research Council via the Centre of Excellence in Engineered Quantum Systems(EQuS) project number CE170100009, and the Villum Foundation.

8:36AM R27.00002: Connecting discrete and continuous variable quantum codes LINSHU LI (Presenter), Yale Univ, VICTOR ALBERT, Caltech, KYUNGJOO NOH, LIANG JIANG, Yale Univ — We consider the connection between discrete variable (DV) codes based on qubit/qudit systems and continuous variable (CV) codes based on bosonic systems. Specifically, we study generalization of quantum parity codes (QPCs) that allows multiple excitations in each mode and fills in the gap between DV quantum parity codes and single-mode binomial codes. The connection offers an alternative perspective to understand these two types of quantum codes, and can hopefully shed light upon generic connections between the two regimes.
8:48AM R27.00003: Braiding via symmetry transformation: universal transversal gate set for topological codes
GUANYU ZHU (Presenter), MAISSAM BARKESHLI, University of Maryland, College Park — Recent studies of the relationship between symmetry and topology have stimulated a series of new discoveries. A recently developed theory of "quantum origami" revealed the deep relation between mapping glass group, topological symmetry and transversal gates in fault-tolerant quantum computation (arXiv:1711.05752). Motivated by this finding, here we show that elements in the spherical braid group with n punctures (anyons) can be completely generated with two isometries related to different rotational symmetries of the punctured surface. By folding the surface to 2n layers connected with gapped boundaries, we acquire a "folded fan" model for quantum computers in reminiscence of the "pancake" model consisting of multiple disconnected layers. The two isometries in the unfolded manifold can be mapped into onsite symmetry in the folded fan, corresponding to fault-tolerant transversal logical gates which can be used to perform quantum computation. For the non-abelian Fibonacci-Turaev-Viro code, these transversal gates form a universal set, along with a constant-depth circuit switching the symmetry. In contrast to the code switching approach to circumvent the Eastin-Knill no-go theorem, we achieve the circumvention using a symmetry switching approach with constant time overhead.

9:00AM R27.00004: Depth reduction for quantum Clifford circuits through Pauli measurements* YI-CONG ZHENG (Presenter), Quantum Lab, Tencent, CHING-YI LAI, Institute of Communications Engineering, National Chiao Tung University, TODD BRUN, Electrical Engineering, University of Southern California, LEONG-CHUAN KWEK, Centre for Quantum Technologies, National University of Singapore — Clifford circuits play an important role in quantum computation. Gottesman and Chuang proposed a gate teleportation protocol so that a quantum circuit can be implemented by the teleportation circuit with specific ancillary qubits. In particular, an n-qubit Clifford circuit U can be implemented by preparing an ancillary stabilizer state $I \otimes U |\Psi\rangle^\otimes n$ for teleportation and doing a Pauli correction conditioned on the measurement. In this paper, we provide an alternative procedure to implement a Clifford circuit through Pauli measurements, by preparing O(1) ancillas that are Calderbank-Shor-Steane (CSS) stabilizer states. That is to say, O(1) CSS states are sufficient to implement any Clifford circuit. As an application to fault-tolerant quantum computation, any Clifford circuit can be implemented by O(1) steps of Steane syndrome extraction if clean CSS stabilizer states are available.

2. National Research Foundation of Singapore and Yale-NUS College (through grant number IG14-LR001 and a startup grant)
3. Ministry of Science and Technology, Taiwan under Grant No. 107WIA0110106,
4. NSF Grants No. CCF-1421078 and No. MPS-1719778
5. An IBM Einstein Fellowship at the Institute for Advanced Study

9:12AM R27.00005: A Systematic Construction of Clifford Perfect Tensors MENGZHEN ZHANG (Presenter), LIANG JIANG, Yale Univ — Perfect tensors are essential building blocks for holographic quantum states, which provide an intriguing platform of combining quantum information theory and physics of spacetime. Network of perfect tensors generated from stabilizer codes can be efficiently analyzed. To our knowledge, the full classification of such perfect tensors is still unknown. In this work, we demonstrate a systematic approach of constructing a large class of perfect tensors, with some existing construction schemes as special cases. Moreover, we investigate their operator generalization to continuous variable systems and identify the differences between the construction schemes in discrete variable and continuous variable systems.

9:24AM R27.00006: Calderbank-Steane-Shor Holographic Quantum Error Correcting Codes* THOMAS STACE (Presenter), Univ of Queensland — We expand the class of holographic quantum error correcting codes by developing the notion of block perfect tensors, a wider class that includes previously defined perfect tensors. The relaxation of this constraint opens up a range of other holographic codes. We demonstrate this by introducing the self-dual CSS heptagon holographic code, based on the 7-qubit Steane code. Finally we show promising thresholds for the erasure channel by applying a straightforward, optimal erasure decoder to the heptagon code and benchmark it against existing holographic codes.

* Australian Research Council, US Air Force

9:36AM R27.00007: Good quantum subsystem codes in 2-dimensions THEODORE YODER (Presenter), Research, IBM Tj Watson — Given any two classical codes with parameters $[n_1, k_1, d_1]$ and $[n_2, k_2, d_2]$, we show how to construct a quantum subsystem code in 2-dimensions with parameters $[[N, K, D]]$ with $N = n_1 n_2$, $K = k_1$, and $D = \min(d_1, d_2)$. These quantum codes are in the class of generalized Bacon-Shor codes introduced by Bravyi. Then, using constructions of good families of classical expander codes, we give constructive families of good quantum subsystem codes in 2-dimensions, that is, families saturating Bravyi's bound $KD = O(N)$. While such codes were known to exist via counting arguments, this is the first explicit construction of them. Additionally, we provide a linear-time decoder for these subsystem codes.
9:48AM R27.00008: Dynamically protected qubit based on high-impedance superconducting circuits*  
PHILIPPE CAMPAGNE-IBARCQ (Presenter), Applied Physics, Yale University, MAZAYAR MIRRAHIMI, Quantic Team, INRIA Paris, MICHEL H. DEVORET, Applied Physics, Yale University — Quantum information encoded in a physical system is submitted to decoherence induced by interaction with uncontrolled degrees of freedom in the environment of the system. However, these interactions are local in the sense that they only induce continuous evolutions of the system in its phase space. One can thus protect quantum information by storing it “non-locally”, i.e. in the correlations between distant phase space regions. Here, we propose to combine a high impedance superconducting resonator with a Josephson junction whose energy is stroboscopically modulated. This system simulates the dynamics of a LC oscillator combined with a Josephson junction and a Quantum Phase Slip element. In presence of these two non-locally acting noiseless elements, the ground states are degenerate non-local grid states of the resonator and are expected to provide a fully protected logical qubit.

*Work supported by ARO, AFOSR and YINQE

10:00AM R27.00009: Natural quantum error-correction in many-body dynamics implies stability of volume-law entangled states against projective measurements  
SOONWON CHOI (Presenter), YIMU BAO, Physics, University of California Berkeley, XIAOLIANG QI, Physics, Stanford University, EHUD ALTMAN, Physics, University of California Berkeley — In a generic isolated quantum many-body system, entanglement entropy of any subsystem grows linearly in time until saturated to a value proportional to its volume. Random projective measurements, however, can severely affect such dynamics by disentangling the measured parts from the rest of the system. In this work, we investigate this interplay between entangling dynamics and projective measurements from the perspective of quantum information theory. We show that volume-law entangled states can remain stable even when a substantial fraction of the system is measured in every time unit. Our key observation, based on the quantum decoupling theorem, is that a sufficiently scrambling unitary can hide quantum correlations in a non-local form such that local measurements cannot decrease entanglement. Such dynamics is generic and can be explicitly demonstrated in a toy model involving random local unitary gates acting on a chain of qubit clusters followed by probabilistic measurements. Our work suggests that the stability of the volume-law entangling phase originates from the effective quantum error correcting feature of scrambling dynamics, which protects quantum entanglement from the noisy environment.

10:12AM R27.00010: Quantum simulation of fermions: geometric locality and error mitigation  
ZHANG JIANG (Presenter), JARROD MCCLEAN, RYAN BABBUSH, HARTMUT NEVEN, Google — We consider mappings from fermionic systems to spin systems that preserve geometric locality in more than one spatial dimension. Such mappings are useful for simulating lattice fermion models (e.g., the Hubbard model) on a quantum computer. Locality-preserving mappings avoid the overhead associated with non-local parity terms in conventional mappings, such as the Jordan-Wigner transformation. As a result, they often provide solutions with lower circuit depth. Moreover, locality-preserving mappings are likely to be more resistant to qubit noises by avoiding encoding the fermionic correlation functions in non-local Pauli operators. Here, we discuss how to detect/correct single-qubit errors with two known locality-preserving maps. We then go beyond that by constructing new mappings with better error detecting/correcting performance than the existing ones. Our methods do no introduce extra physical qubits beyond those required by the original mappings. Being able to detect/correct errors in initial state preparations is crucial to the success of near-term quantum algorithms such as the variational quantum eigensolver. Our results also provide systematic methods to constructing quantum error-detecting/correcting codes with Majorana fermion operators.

10:24AM R27.00011: Approximate stabilizer rank and improved weak simulation of Clifford-dominated circuits for qudits*  
YIFEI HUANG (Presenter), PETER J LOVE, Tufts University — Bravyi and Gosset recently gave classical simulation algorithms for quantum circuits dominated by Clifford operations. These algorithms scale exponentially with the number of T-gate in the circuit, but polynomially in the number of qubits and Clifford operations. Here we extend their algorithm to qudits of odd prime dimensions. We generalize their approximate stabilizer rank method for weak simulation to qudits and obtain the scaling of the approximate stabilizer rank with the number of single-qudit magic states. We also relate the canonical form of qudit stabilizer states to Gauss sum evaluations. We give an O(n^3) algorithm to calculating the inner product of two n-qudit stabilizer states.

*This work is supported by the National Science Foundation award number PHY 1720395 and from Google Inc.
10:36AM R27.00012: Direct Measurement of a Very Small Logical Qubit's Observables* NICHOLAS MATERISE (Presenter), ELIOT KAPIT, Colorado Sch of Mines — We extend recent longitudinal readout schemes to the very small logical qubit (VSLQ) architecture. The two photon X-operators in the VSLQ are read out by borrowing principles from the longitudinal approach, although the operator itself is transverse. Our results follow those of previous studies of coupling between a single cavity mode and superconducting qubit, where high measurement fidelities are realized for shorter measurement pulses compared to dispersive readout. In the interest of minimizing microwave circuit resources per VSLQ unit cell, we have investigated the use of the higher modes of the same resonator for error correction. We demonstrate use of the fundamental resonator mode for fast readout of an inductively coupled VSLQ with improved fidelities compared to the dispersive case. By measuring along the X-axis, we benefit from the added protection of the passive error correction during readout, reducing potential state preparation and measurement error.

*We acknowledge funding support from the National Physical Sciences Consortium graduate fellowship and ARO grant W911NF-18-1-0125.

10:48AM R27.00013: Graph convolutional network for topological stabilizer codes YASUNARI SUZUKI (Presenter), NTT Secure Platform Laboratories, AMARSAANAA DAVAASUREN, University of Tokyo, KEISUKE FUJII, Kyoto University, MASATO KOASHI, YASUNOBU NAKAMURA, University of Tokyo — As quantum computers are close to realization, a fast, versatile, and high-performance decoder for quantum error correction is demanded. In recent years, several machine-learning-based decoders have been proposed, and are expected to enable fast decoding with near-optimal performance for an arbitrary topological code. Since local Pauli errors only flip local syndromes in topological codes, a convolutional neural network is used for explicitly extracting local features in topological codes. However, the filter shapes for the convolution only match to the qubit allocation of [2d^2-2d+1, 1, d]-surface code. It has been not known how we can naturally extract local features of other topological codes.

In this talk, we propose a novel construction of a machine-learning-based decoder with a model known as graph convolutional network. This decoder enables us to utilize local features of an arbitrary topological stabilizer code. With numerical results, we show that our model achieves similar performance to minimum distance decoder, which is known to be inefficient but near-optimal, for several topological codes and noise models using practical size of training datasets.

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R28 DQI: Distributed Quantum Computation, Networking and Information Security II BCEC 161 - Victoria Lipinska, Delft University of Technology - Tag(s): Focus

8:00AM R28.00001: Entanglement cost of quantum state preparation and channel simulation* XIN WANG (Presenter), University of Maryland, College Park, MARK M WILDE, Louisiana State University — We study various aspects of the entanglement cost of quantum state preparation and quantum channel simulation. First, we establish that the exact entanglement cost of any bipartite quantum state under PPT-preserving operations is given by a single-letter formula, here called the κ-entanglement of a quantum state. This formula is calculable by a semidefinite program, thus allowing for an efficiently computable solution for general quantum states. Notably, this is the first time that an entanglement measure for general bipartite states has been proven not only to possess a direct operational meaning but also to be efficiently computable, thus solving a question that has remained open since the inception of entanglement theory over two decades ago. Second, we study the exact entanglement cost of quantum channel simulation in the parallel setting. In particular, the largest κ-entanglement that can be established via a quantum channel remarkably gives a single-letter formula for the exact parallel PPT-entanglement cost of simulating this channel, and it is also efficiently computable by a semidefinite program.

*XW acknowledges support from the Department of Defense. MMW acknowledges support from the National Science Foundation under Award no. 1350397.
8:12AM R28.00002: Communicating via Ignorance* KAUMUDIKASH GOSWAMI (Presenter), JACQUILINE ROMERO, ANDREW WHITE, Univ of Queensland — Communication through a sequence of two identical, noisy, depolarising channels is impossible in conventional information theory. Surprisingly, it has been shown in the paper [1] communication becomes possible if the depolarising channels are within a quantum switch, where the order of the channels is in a quantum superposition [2,3]. We experimentally demonstrate this counterintuitive result in a quantum switch that uses polarisation to coherently control the order of two depolarising channels acting on the transverse spatial mode of a photon. We send $(3.41\pm0.15)\times10^{-2}$ bits of information through two fully depolarising channels that are in an indefinite causal order. [4]

References:

*This work has been supported by the ARC by Centre of Excellence for EQUS.

8:24AM R28.00003: Quantum Link Prediction in Complex Networks YASSER OMAR (Presenter), Instituto Superior Tecnico, JOÃO MOUTINHO, ANDRÉ MELO, BRUNO COUTINHO, Physics of Information and Quantum Technologies Group, Instituto de Telecomunicações, ISTVAN KOVACS, ALBERT BARABASI, Northeastern University — Predicting the existence of a link in a complex network is a non-trivial task, namely for large social and biological networks, with important applications. Experiments to map the full structure of biological networks (e.g. protein-protein interactions) are very challenging, costly and time consuming, and large amounts of data is still missing. Link prediction methods are not only a key computational tool to aid these efforts in understanding complex biological systems, but also very useful for other studies of time-varying complex networks, as for example social networks.

In this work we present a novel method for link prediction in complex networks based on continuous-time quantum walks. The control of a relative phase allows our method to be used in different types of networks (physical, biological, social, etc.). By exploiting quantum coherence we are able to outperform the state of the art classical methods, indicating that our method is also able to capture complex local patterns (such as local communities around paths of length 3) without the need to impose a specific pattern structure. Our results indicate there is a strong potential for combining quantum algorithms with complex network research to produce tools with direct and immediate experimental relevance.

8:36AM R28.00004: Indefinite Causal Order* JACQUILINE ROMERO, KAUMUDIKASH GOSWAMI, CHRISTINA GIARMATZI, MICHAEL KEWMING, FABIO COSTA (Presenter), School of Mathematics and Physics, University of Queensland, CYRIL BRANCIARD, Institut Neel, CNRS, ANDREW WHITE, School of Mathematics and Physics, University of Queensland — Quantum mechanics allows events to happen with no definite causal order: this can be verified by measuring a causal witness, in the same way that an entanglement witness verifies entanglement. Here we realise a photonic quantum switch, where two operations, A and B, act in a quantum superposition of their two possible orders. The operations are on the transverse spatial mode of the photons, while polarisation coherently controls their order. Our implementation ensures that the operations cannot be distinguished by spatial or temporal position. It also allows qudit encoding in the target. We confirm our quantum switch has no definite causal order by constructing a causal witness and measuring its value to be 18 standard deviations beyond the definite-order bound.

*Australian Research Council
John Templeton Foundation
Advance Queensland
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French National Research Agency
8:48AM R28.00005: Counterfactual Quantum Superdense Coding*  
FAKHRAR ZAMAN (Presenter), YOUNGMIN JEONG, HYUNDONG SHIN, Kyung Hee University — Quantum superdense coding (QSC) is one of the most striking effects in quantum communication. It enables one to transmit a two-bit classical message by sending only one qubit using initially shared entanglement. In this article, we present a counterfactual QSC scheme that enables remote parties to accomplish this task without prior entanglement but no physical particle is found in the transmission channel. We consider two remote parties, namely Alice (sender) and Bob (receiver), have untangled particles—an electron and a photon. First, we generate entanglement between the electron and photon without transmitting any physical particle over the channel. Alice performs one of the four unitary operations $\mu \in \{I, \sigma_x, \sigma_y, \sigma_z\}$ on her entangled particle. Instead of transmitting her entangled particle to Bob, Alice and Bob perform counterfactual Bell-state analysis based on the chained quantum Zeno effect to distinguish between the four Bell-states under local operations and enable Bob to decode the two-bit classical message.  
*This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2016R1A2B2014462), and by the Basic Science Research Program through the NRF funded by the Ministry of Education (No. 2018R1D1A1B07050584).

9:00AM R28.00006: Drone-based Quantum Key Distribution*  
ANDREW CONRAD (Presenter), DALTON CHAFFEE, JOSEPH CHAPMAN, CHRIS CHOPP, KYLE HERDON, ALEXANDER HILL, University of Illinois at Urbana-Champaign, DANIEL SANCHEZ-ROSALES, JOSEPH SZABO, DANIEL J GAUTHIER, Dept. of Physics, OSU, PAUL G KWAT, University of Illinois at Urbana-Champaign — Recent advances in quantum memories point to the future viability of quantum networking, including quantum cryptography. To be truly multi-purpose, future quantum communication networks should consist of a variety of platforms, e.g., airplanes, drones, and ships, though the motion of these platforms precludes the use of fiber-based approaches to quantum cryptography; free-space quantum key distribution (QKD) systems have historically been rather bulky. Small moving platforms, such as multirotor drones, are ideal for reconfigurable networks in both urban and rural environments but are only capable of supporting lightweight payloads (< 10 kg). Here we discuss our current progress in developing a reconfigurable network of two or more small multi-rotor drones implementing a modified BB84 quantum key distribution protocol over a free-space optical channel. This requires the development of fast and lightweight sources of polarized photons with no side channel leakage, miniaturization of time-tagging electronics and single-photon detectors, and the development of a robust signal acquisition and pointing and tracking system.  
*This work is supported by the ONR MURI program on Wavelength-Agile Quantum Key Distribution in a Marine Environment, Grant #N00014-13-1-0627.

9:12AM R28.00007: Quantum Internet Applications  
[Invited] ELHAM KASHEFI (Presenter), edinburgh — The long-term ambition of the community is to build a Quantum Internet that enables any distributed quantum communication applications (beyond QKD) between any points on Earth. In this talk I will present a set of useful applications that could be executed on the quantum nodes with various hardware capabilities presenting a blueprint for a quantum client-server platform. I will also present the Quantum Protocols Wikipedia, a QIA lead community effort in developing and curating a comprehensive software library for a list of relevant quantum network protocols achieving various functionalities.

EMIL KHABIBOULLINE (Presenter), Harvard University, JOHANNES BORREGAARD, University of Copenhagen, KRISTIAAN DE GREVE, MIKHAIL LUKIN, Harvard University — Quantum networks provide a platform for astronomical interferometers capable of imaging faint stellar objects. We present a protocol with efficient use of quantum resources and modest quantum memories. In our approach, the quantum state of incoming photons along with an arrival time index is stored in a binary qubit code at each receiver. Nonlocal retrieval of the quantum state via entanglement-assisted parity checks at the expected photon arrival rate allows for direct extraction of phase difference, effectively circumventing transmission losses between nodes. Compared to prior proposals, our scheme, based on efficient quantum data compression, offers an exponential decrease in required entanglement bandwidth. We show that it can be operated as a broadband interferometer and generalized to multiple nodes. We also analyze how imaging based on the quantum Fourier transform provides improved signal-to-noise ratio compared to classical processing. Finally, we discuss physical realizations including photon detection-based quantum state transfer. Experimental implementation is then feasible with near-term technology, enabling optical imaging of astronomical objects akin to well-established radio interferometers and pushing resolution beyond what is practically achievable classically.
necessary to realize experimentally desirable levels of non-classical correlations. We present the requirements to quantify the nonclassical correlations that are realized. Analyzing these measures reveals that the key rate of RFI-MDI-QKD can be improved for a large misalignment of the reference frame.

Please see the Reference [H.-W. Liu et al., Optica 5, 902 (2018)] for more information about the results of our paper.

*This work is supported by National Natural Science Foundation of China (NSFC) (11674397); State Key Laboratory of Information Photonics and Optical Communications (Beijing University of Posts and Telecommunications (BUPT)) (IPOC2017ZT04).

10:12AM R28.00010: Entangled-pulse generation inside coherent Ising machines using entanglement swapping* RYOTATTSU YANAGIMOTO (Presenter), PETER McMATHON, TATSUHIRO ONODERA, EDWIN NG, HIDEO MABUCHI, Stanford University — Coherent Ising machines (CIMs) have been proposed and demonstrated as heuristic solvers of hard combinatorial optimization problems. In current measurement-feedback-based CIMs (P.L. McMahon 2016), interactions between pulses (spins) are mediated via a classical feedback mechanism, and consequently no entanglement among pulses is generated. In this research, we investigate the use of entanglement swapping to introduce inter-pulse entanglement into such CIM-like architectures, using an external source of independently squeezed pulses. We develop models to describe the resulting intracavity dynamics as a function of system parameters, which can be numerically simulated to characterize the quantum noise and correlations in the pulse train. We also introduce and employ several measures of inseparability to quantify the nonclassical correlations that are realized. Analyzing these measures reveals trade-offs between system parameters and produces metrics useful for optimizing them. We present the requirements necessary to realize experimentally desirable levels of non-classical correlations.

*This work is supported by Masason foundation and National Science Foundation under award PHY-1648807.

10:24AM R28.00011: Maximal LELM Distinguishability of Qubit and Qutrit Bell States using Projective and Non-Projective Measurements NATHANIEL LESLIE (Presenter), Physics, UC Berkeley, JULIEN DEVIN, Physics, Stanford University, THERESA WLYNN, Physics, Harvey Mudd College — Numerous quantum information protocols make use of maximally entangled two-particle states, or Bell states, in which information is stored in the correlations between the two particles rather than their individual properties. Retrieving information stored in this way means distinguishing between different Bell states, yet the well known no-go theorem establishes that projective linear evolution and local measurement (LELM) detection schemes can only reliably distinguish three of the four qubit Bell states. We present newly-established maximum distinguishability bounds for the qutrit Bell states of bosons via projective LELM measurements; only three of the nine Bell states can be distinguished. Next, we extend to the case of non-projective measurements. We present newly-established maximum distinguishability bounds for the qutrit Bell states of bosons via projective LELM measurements; only three of the nine Bell states can be distinguished. We extend to the case of non-projective measurements. We present a strengthened no-go theorem, which shows that general LELM measurements cannot reliably distinguish all four qubit Bell states. We also establish that at most five qutrit Bell states can be distinguished with generalized LELM measurements.

10:36AM R28.00012: Generating accessible entanglement in bosons via pair-correlated tunneling TYLER VOLKOFF, Konkuk University, CHRIS HERDMAN (Presenter), Middlebury College — We consider an extended Bose-Hubbard model that includes pair-correlated tunneling. We demonstrate that a minimal four-mode implementation of this model exhibits a pair-correlated regime in addition to Mott insulator and superfluid regimes. We propose a low complexity variational subspace for the ground state of the system in the pair-correlated regime, which we find to be numerically exact in pure pair-tunneling limit. Additionally, we propose a parameter-free high fidelity model wave function that qualitatively captures the features of the ground state in the pair-correlated regime. Due to particle number conservation, the operationally accessible entanglement vanishes deep inside the Mott insulator and superfluid regimes, however in the pure pair-correlated tunneling limit we find that the accessible entanglement entropy grows logarithmically with the number of particles. Additionally, we demonstrate that upon application of a unitary beamsplitter operation, the pair-correlated ground state is transformed into a state with completely accessible entanglement that is not limited by superselection rules.
8:00AM R29.00001: Quantum control of spins in silicon carbide with photons and phonons* [Invited] DAVID AWSCHALOM (Presenter), University of Chicago — There is a growing interest in exploiting the quantum properties of electronic and nuclear spins for the manipulation and storage of quantum information. Here we focus on recent developments in controlling and connecting individual spins in silicon carbide (SiC) using photons and phonons. We find that defect-based electronic states in SiC [1] can be isolated and optically probed at the single spin level with surprisingly long spin coherence times and high-fidelity control within non-isotopically purified, commercial-grade wafers operating at near-telecom wavelengths. Moreover, a detailed study of the defect spin-photon interface yields efficient quantum control in various polytypes along with near-unity electronic and nuclear polarization, highlighting the potential of SiC for photon-mediated entanglement. In addition, we use Gaussian surface acoustic wave resonators to exploit both the piezoelectric and isotropic phonon dispersion properties of SiC to demonstrate Autler-Townes splittings, mechanically driven Rabi oscillations, and explore spin-strain coupling contributions from all mechanical degrees of freedom, including shear [2]. The spatial confinement of phonons is mapped using a synchrotron-based x-ray diffraction real-space microscopy technique with 25 nm spatial resolution [3]. This work expands the versatility of optically and mechanically driven spins in a material with well-developed device and fabrication capabilities and shows promise towards integrating quantum states with hybrid quantum systems for both control and communication.


*This work was supported by AFOSR, ARO, DOE BES, NDSEG, NSF GRFP, and UChicago MRSEC.

8:36AM R29.00002: Quantum network nodes with silicon-vacancy center and coupled nuclear spins in diamond nanocavities DENIS SUKACHEV (Presenter), MIHIR K BHASKAR, CHRISTIAN T NGUYEN, RUFFIN EVANS, BARTHOLOMEUS MACHIELSE, HONGKUN PARK, MARKO LONCAR, MIKHAIL LUKIN, Harvard University — We realize quantum-network nodes based on silicon-vacancy color centers in diamond nanocavities coupled to nearby nuclear spins. A high cooperativity SiV-cavity interface and efficient tapered-fiber collection allows for single-shot readout of the SiV electronic spin. With dynamical decoupling sequences, we measure a coherence time of 400μs. We observe coupling to nearby 13C spins and demonstrate coherent control of the SiV-13C register. By using these nuclear spins, we realize a quantum memory exceeding 1ms. Together with our previous work, these results pave the way for quantum computation based on 2D cluster states with more than 10 photons, and quantum communication based on quantum repeaters.

8:48AM R29.00003: Resonant optical spin initialization and readout of single silicon vacancies in silicon carbide* ONEY SOYKAL (Presenter), United States Naval Research Laboratory, HUNTER BANKS, NRC Postdoc at Naval Research Laboratory, SAMUEL CARTER, THOMAS REINECKE, United States Naval Research Laboratory — The silicon mono-vacancy defect in 4H-SiC is a promising candidate for solid-state quantum information processing. Recent high-resolution resonant optical spectroscopy on single defects have shown favorable low temperature optical properties, i.e., two narrow and nearly lifetime-limited optical transitions with no discernable zero-field splitting fluctuations or spectral diffusion. We present a theoretical fine structure model that describes the energy level structure and reveals all intersystem crossing and spin polarization time constants of the V2 defect, shedding light on its optical and spin characteristics. In particular, we show that the silicon mono-vacancy is described well by a four-level optical structure assisted by additional non-radiative transitions leading to rich dynamical spin pumping behavior. Our calculated rates result in an overall fluorescence lifetime of 5.8 ns in good agreement with measurements. Based on this model, we show that initialization fidelities exceeding 99% are theoretically attainable at low resonant laser powers. Further, we describe the differences in optical properties between the cubic and the hexagonal defect sites due to dynamic and pseudo Jahn-Teller effects.

*This work was supported by the U.S. Office of Naval Research and the OSD QSEP.
Fault-Tolerant Quantum Metrology with High-Density Spin Ensembles: Theory

JOONHEE CHOI (Presenter), HENGYUN ZHOU, Harvard University, SOONWON CHOI, UC Berkeley, RENATE LANDIG, HELENA KNOWLES, Harvard University, JUNICHI ISOYA, University of Tsukuba, FEDOR JELEZKO, Ulm University, SHINOBU ONODA, Takasaki Advanced Radiation Research Institute, HITOSHI SUMIYA, Sumitomo Electric Industries Ltd., MIKHAIL LUKIN, Harvard University — One of the most promising routes towards high-sensitivity quantum metrology is to utilize high density spin ensembles. Here, spins are typically periodically manipulated in order to both extend coherence and detect an external signal at a particular frequency. However, spin-spin interactions and on-site disorder may severely limit the coherence time and the achievable sensitivities under such dynamical protocols. In addition, control imperfections pose a significant challenge to the effectiveness of decoupling and sensing sequences. Here, we present a novel formalism for the fault-tolerant design of sensing sequences that simultaneously decouples interactions and suppresses the effects of disorder and imperfect controls, while maximizing sensitivity to an external signal. In addition to the broad applicability to different decoupling and sensing scenarios, this formalism could also serve as a powerful tool for the engineering of Hamiltonians to study many-body physics.

Fault-Tolerant Quantum Metrology with High-Density Spin Ensembles: Experimental Results

HELENA KNOWLES (Presenter), HENGYUN ZHOU, JOONHEE CHOI, Harvard University, SOONWON CHOI, UC Berkeley, RENATE LANDIG, Harvard University, JUNICHI ISOYA, University of Tsukuba, FEDOR JELEZKO, Ulm University, SHINOBU ONODA, Takasaki Advanced Radiation Research Institute, HITOSHI SUMIYA, Sumitomo Electric Industries Ltd., MIKHAIL LUKIN, Harvard University — High density solid-state spin ensembles have shown great promise as high-sensitivity magnetometers on the nanoscale. However, further increases in sensitivity require techniques to overcome the limits to coherence times imposed by spin-spin interactions. Here, using a dense ensemble of Nitrogen-Vacancy centers in diamond, we experimentally demonstrate fault-tolerant decoupling of spin-spin interactions, achieving a ten-fold enhancement of spin coherence times. This was made possible by introducing novel dynamical decoupling sequences that simultaneously suppress disorder, interactions, and imperfections in controls. We utilize the prolonged coherence time to perform quantum metrology, demonstrating an increase in sensitivity compared to conventional sensing protocols such as the XY-8 sequence. These results thus demonstrate a significant enhancement beyond the interaction limit, crucial for high-sensitivity magnetometers in high-density interacting spin ensembles.

Multi-qubit registers with solid-state defect centers

ERIC BERSIN (Presenter), MATTHEW TRUSHEIM, KEVIN CHEN, MICHAEL WALSH, SARA MOURADIAN, TIM SCHRÖDER, DIRK R. ENGLUND, Massachusetts Institute of Technology — Medium-scale ensembles of qubits offer a platform for near-term quantum technologies, as well as studies of many-body physics. Atom-like emitters in solids have emerged as promising candidates for this application, with long coherence times, coherent optical transitions, the ability to couple to long-lived nuclear spins for extended storage, and a path towards scalability. A prerequisite for generating such clusters is subdiffraction localization, necessary to achieve strong spin-spin coupling for efficient state transfer and gates operations.

In this work, we present progress made towards producing such ensembles. We demonstrate subdiffraction registers of multiple nitrogen vacancy centers in diamond that maintain individual control and readout of each constituent spin. We further discuss recent work towards scalable creation of such clusters and techniques for producing systems of coupled spins.

*This work was supported by a NASA Space Technology Research Fellowship; AFOSR grants FA12-1-0025, FA9550-14-1-0052, and FA9550-16-1-0391; NSF grants 0551153, 1231319, and 1641064; ARL grant 2875-Z8401005; and DOE grant DE-SC0014664.
The negatively charged nitrogen-vacancy (NV⁻) center in diamond is emerging as a powerful quantum magnetometer. As an atomic size sensor, an NV⁻ center incorporated into a scanning probe microscope has the potential of imaging molecular structure. To achieve the requisite sensitivity and spatial resolution, it is crucial that NV⁻ centers are located within nanometers from the surface; however, the diamond surface is known to reduce the spin coherence and charge stability of NV⁻ centers, compromising the capacity of single-spin sensitivity. Here, we address charge state instability of single shallow NV⁻ centers both under illumination and in the dark [1]. We identify tunneling to a local electron trap as the mechanism for charge ionization in the dark and develop techniques to control and readout the trap charge state. We demonstrate experimental protocols to mitigate the detrimental effects, and we present progress towards imaging single molecules.


** NSF CAREER Grant No. DMR-1352660 and Air Force Office of Scientific Research PECASE Award

High sensitivity quantum limited electron spin resonance spectroscopy**

Following recent advances in circuit quantum electrodynamics, we have employed high quality factor superconducting resonators to reduce the mode volume around the spins and operate ESR in so-called Purcell regime [1,2] where a larger $g$ not only leads to a larger signal but also provides a high repetition rate. In particular with a nanometric inductor, we show $g/2\pi$ of 3 kHz, which together with Josephson parametric amplifier pushes the spin sensitivity to be 10 spins for unit signal to noise ratio per second of averaging.


*Research supported by ERC, CNRS.

Enhanced spin-squeezing using a parametrically-driven cavity

Entangled spin-squeezed states allow the possibility of sensing beyond the standard quantum limit, and have been pursued using a variety of different physical mechanisms. In this talk, we will describe and analyze a new, highly-efficient method for generating spin squeezing that exploits a cavity subject to a two-photon (parametric) drive. Unlike standard methods that use a detuned cavity to induce spin-spin interactions (the “one-axis twist” Hamiltonian), our approach employs a resonant interaction and counterdiabatic driving, leading to a more rapid protocol. Our technique can also achieve true Heisenberg-limited scaling, unlike the standard one-axis twisting approach. We will discuss the main properties of the protocol, and explore its performance in realistic parameter settings. The outlined scheme could be implemented in systems where spin ensembles are coupled to superconducting microwave cavities (e.g. [1]), as well as in systems where spins are strain-coupled to the motion of a nanomechanical resonator (e.g. [2,3]). In both cases, the required resource of a parametric drive is experimentally accessible.

10:12AM R29.00010: All-optical cryogenic thermometry based on NV centers in nanodiamonds* MASAYA FUKAMI (Presenter), CHRISTOPHER G YALE, PAOLO ANDRICH, XIAOYING LIU, Institute for Molecular Engineering, University of Chicago, JOSEPH HEREMANS, Materials Science Division, Argonne National Laboratory, PAUL F NEALEY, DAVID AWSCHALOM, Institute for Molecular Engineering, University of Chicago — Nitrogen vacancy (NV) centers in nanodiamonds (NDs) have been shown to provide an excellent nanometer-scale high-sensitivity thermometry platform. Here we demonstrate a cryogenic-compatible, all-optical thermometry technique based on the emission spectrum of an ensemble of NV centers in NDs that operates from room-temperature to liquid nitrogen temperatures. The sensitivity is found to be slightly improved at cryogenic temperatures, in contrast to the conventional thermometry technique based on the temperature-dependent zero-field splitting of NV centers. We use this all-optical thermometer at T=170 K to measure the surface temperature of a ferromagnetic insulator, yttrium iron garnet (YIG), over tens of microns with the use of an array of NDs on a flexible polydimethylsiloxane (PDMS) sheet, where the YIG is thermally driven by a resistive heater. We directly observe a thermal gradient over micrometers in YIG, indicating that the technique is independent of magnetic noise and microwave resonances.

*This work is supported by ARO MURI and UChicago MRSEC.

10:24AM R29.00011: Optically coherent NV centers in um-thick etched diamond membranes for quantum applications MAXIMILIAN RUF (Presenter), MARK IJSPEERT, SUZANNE VAN DAM, MATTHEW WEAVER, Delft University of Technology, NICK DE JONG, *Netherlands Organisation for Applied Scientific Research (TNO, HANS VAN DEN BERG, JASPER FLIPSE, MARTIN ESCHEN, *Netherlands Organisation for Applied Scientific Research (TNO), SANTI SAGER LA GANGA, GUUS EVERS, RONALD HANSON, Delft University of Technology — Future quantum networks depend on efficient entanglement generation between nodes. Recently, we have generated entanglement between nitrogen-vacancy (NV) center nodes with a success rate of up to 40 Hz. This rate is now limited by the zero-phonon-line emission probability as well as the photon collection efficiency. Embedding a diamond slab containing individually resolvable NV centers between two highly reflective mirrors can address both challenges, benefiting from large Purcell enhancement due to a low optical mode volume.

Until now, cavity-enhanced entanglement generation between NV centers has not been achieved, predominantly due to poor optical properties of NV centers close to the diamond surface. Via a combination of electron irradiation and an optimized etch sequence, we have fabricated a 3.5 um thick membrane that combines low surface roughness (< 0.4 nm) and narrow optical NV transitions (<100 MHz). We incorporate such devices in an open, tunable micro-cavity setup, with the potential for a two orders-of-magnitude increase in remote entangling rates.

10:36AM R29.00012: CMOS-Integrated Diamond Nitrogen-Vacancy Quantum Sensor* CHRISTOPHER FOY (Presenter), MOHAMED IBRAHIM, DONGGYU KIM, MATTHEW TRUSHEIM, DIRK R. ENGLUND, RUONAN HAN, EECS, MIT — We report the first on-chip quantum sensor which combines CMOS integrated circuit technologies with nitrogen-vacancy (NV) centers in diamond. We will discuss how this system performs two critical functions for quantum magnetometry with NV centers: strong generation and efficient delivery of microwave for quantum-state control, and optical filtering/detection of spin-dependent fluorescence for quantum-state readout. We demonstrate on-chip optically detectable magnetic resonance (ODMR) for the first time. I will then discuss, some of our more recent efforts toward increasing the capabilities of this system to coherently control the NV's spin state.

*This research is supported in part by the Army Research Office Multidisciplinary University Research Initiative (ARO MURI) biological transduction program, Kwanjeong Educational Foundation, Singaporean-MIT Research Alliance (SMART), MIT Center of Integrated Circuits and Systems, and Master Dynamic Limited. It is also supported by the Intelligence Community Postdoctoral Research Fellowship Program at MIT, administered by Oak Ridge Institute for Science and Education through an interagency agreement between the U.S. Department of Energy and the Office of the Director of National Intelligence.

10:48AM R29.00013: Scanning Nitrogen-Vacancy Center Magnetic Imaging SUSANNE BAUMANN (Presenter), ALEC JENKINS, SIMON A MEYNELL, ANIA CLAIRE JAYICH, University of California, Santa Barbara — The NV center is a quantum probe that is sensitive to a variety of fields (magnetic, electric, thermal, strain), can achieve nanoscale spatial resolution, is non-invasive, and can operate over a wide range of temperatures; hence it is an ideal tool for studying novel phases of matter that often emerge only below a critical temperature. Here we use a cryogenic scanning NV magnetometer to probe materials that exhibit nanoscale magnetic phenomena often inaccessible to other experimental tools over a variety of temperatures.

Thursday, March 7, 2019 8:00 AM - 10:48 AM
8:00AM R30.00001: Mechanically Guided Assembly of Bio-Inspired 3D Mesoscale Frameworks [Invited] JOHN ROGERS (Presenter), Materials Science and Engineering, Northwestern University —
Complex, three dimensional (3D) assemblies of micro/nanomaterials form naturally in biological systems, where they provide sophisticated function in even the most basic forms of life. In spite of their potential utility in man-made devices, design options for analogous abiotic 3D mesostructures are severely constrained by the comparatively primitive capabilities that are available with established techniques for materials growth, assembly and 3D printing. This talk summarizes progress in strategies that rely on geometric transformation of preformed 2D functional micro/nanostructures into 3D architectures by controlled processes of actively induced compressive buckling. The emphasis will be on the foundational physics principles, computational approaches that enable inverse design, and examples of applications in areas ranging from thermoelectrics to microelectromechanical systems to biologically inspired open mesoscale networks as active cellular interfaces.

8:36AM R30.00002: Spatial control of frost formation on hydrophobic surfaces with millimetric serrated features YUEHAN YAO (Presenter), EMMA FELDMAN, KYOO-CHUL (KEN) PARK, Northwestern University — Numerous studies have focused on a low surface energy coating and a micro/nanoscale surface texture to design functional surfaces that delay frost formation and reduce ice adhesion. However, the scientific challenges for long-term icephobic surfaces have not been fully addressed because of degradation such as mechanical wearing. Inspired by the suppressed frost formation on concave regions of natural leaves, here we report findings on the frosting process on hydrophobic surfaces with various serrated structures. Dropwise condensation, the first stage of frosting, is enhanced on the peaks and suppressed in the valleys when the wavy surface is exposed to humid air, causing frosting to initiate from the peak. The condensed droplets in the valley are then evaporated, resulting in a non-frost band. The effects of surface topography on the frost pattern are systematically studied by varying the serrated geometry defined as the vertex angle, and numerically modeling the spatial distribution of diffusion flux of water vapor on the wavy surface. Under different ambient humidity levels, the magnitudes of diffusion flux at the non-frost boundaries of the surfaces are nearly identical, implying that the critical value of diffusion flux is the key to understand the non-frost pattern.

8:48AM R30.00003: Understanding Nanostructured Topography on Flower Petals: Hierarchical Wrinkles in Soft Multilayers* CHAO CHEN (Presenter), ALFRED CROSBY, Polymer Science and Engineering Department, University of Massachusetts Amherst — Hierarchical wrinkles on flower petals enable unique iridescence to attract pollinators. Although similar patterns have been observed on graded elastomers, mimesis of the natural patterns and relative dimensions with a controllable and tunable manner is challenging. Inspired by the multiple-layered structure of petal skins, here we present a physical model and a corresponding numerical model based on three-layered thin films. The layer-by-layer integration provides accuracy in controlling thickness and mechanical properties of thin films, thus enabling quantitative relations between physical and numerical models. We quantify the sequential development of a hierarchical structure, consisting of small wrinkles coupled with larger sinusoidal deformations. We found their wavelength follows the bilayer wrinkling theory; whereas the amplitudes of small wrinkles have a systematic spatial distribution largely controlled by larger wrinkles. We also discovered a collapse from the dual-wrinkling mode to a single-wrinkling mode, which depends upon thickness and mechanical properties of top layers. A phase map of the two wrinkling modes is constructed to guide the design of hierarchical wrinkles.

*This material is based upon work supported by Human Frontier Science Program (No. RGP0019/2017)

9:00AM R30.00004: Mechanics of Elephant Trunk Wrinkles ANDREW SCHULZ (Presenter), DAVID L HU, Georgia Institute of Technology — Elephant skin is obviously wrinkled, but no quantitative measurements have been made of why the trunk has such wrinkly skin. Through videos of trunk movement at Zoo Atlanta and dissections of a trunk from the Smithsonian Institute we report the geometry of the wrinkles and rationalize their function. Elephants can elongate their trunk by over 40%, but have little or no compression capability. Skin at the trunk's root forms square-waved wrinkles and is twice as thick as the skin at the tip which forms sinusoidal wrinkles. We rationalize that elephants use these wrinkling properties to perform incredible bending, elongation, and strength with their trunk. The energy of wrinkling will be compared to wrinkling phenomenon in the biological world. This work will relate to biologically inspired soft robotic manipulators.
Bioinspired materials with self-regulating mechanical properties upon loading/damages

SANTIAGO ORREGO, ZHEZHI CHEN, DECHING HOU, Mechanical Engineering, Johns Hopkins University, URSZULA KREKORA, Chemical and Biomolecular Engineering, Johns Hopkins University, SUNG KANG (Presenter), Mechanical Engineering, Johns Hopkins University — Nature produces outstanding materials for structural applications such as bones and coral reefs that can adapt to their surrounding environment and repair damages. This leads to the formation of mechanically efficient structures for optimal biomechanical and energy-efficient performance and long-term durability. However, it has been a challenge for synthetic materials to change and adapt their structures and properties to address the changes of loading conditions or damages. To address the challenge, we report a bioinspired material system that triggers mineral synthesis from ionic solutions on organic scaffolds upon mechanical loadings and/or damages so that it can self-adapt to mechanical loadings and regenerate upon damages. The mechanism also allows the formation of functionally graded materials using a simple one step process. We envision that our findings can open new strategies for making synthetic materials with self-regulating mechanical properties.

*We would like to thank the financial support from the Johns Hopkins University Whiting School Start-Up Fund and the Air Force Office of Scientific Research Young Investigator Program Award (Award number: FA9550-18-1-0073, Program manager: Dr. Byung-Lip (Les) Lee).

Fog collection on wire arrays

YOUHUA JIANG (Presenter), CHRISTIAN MACHADO, SHAAN SAVARIRAYAN, KYOO-CHUL (KEN) PARK, Northwestern University — The upright, wire-like leaves of Stipagrostis sabulicola, a grass species in the Namib Desert, shows excellent fog collection performance. Inspired by such wire geometry, we aim to understand the mechanism of fog collection on individual vertical wires and multiple-wire arrays. We visualized how fog droplets are collected on a wire and measured the resulting fog-collection rate while varying wire diameter, surface wettability, and wind speed. Results show that fog-collection rates on a single wire are determined by deposition efficiency, an aerodynamics-related parameter. Surface wettability has a negligible effect on the fog collection rate at low wind speeds (e.g., 0.5 m/s). By contrast, there appears to be a strong effect of wettability at high wind speeds (e.g., 3 m/s), where surfaces with the lowest droplet adhesion performs worst. Such phenomenon is explained by the competition between the air drag force and the droplet retention force on a surface, both of which are determined by surface wettability and wire diameter. Building on the knowledge gained from individual wires, we optimize the design of multiple-wire arrays, which shows a four-fold enhancement in fog-collection rate compared to a single wire of the same surface area.

Siderophore Inspired Molecules to Mediate Collagen Thin Film Adhesion

ROBERTO ANDRESEN EGUILUZ (Presenter), GEORGE DEGEN, ERIC VALOIS, GARRETT LINDSEY, KAI KRISTIANSEN, University of California, Santa Barbara — Adhesion in biological environments (aqueous ionic solutions) is challenged by the high dielectric constant of water which reduces van der Waals interactions, ions in solution which screen electrostatic interactions, and the hydration layers both on hydrophilic substrates and surface-bound ions which discourage adhesive contact between glues and the substrate. In this study, we investigated adhesion between symmetric thin films of collagen type-1 (Col-1), a major component of the extracellular matrix (ECM), mediated by synthetic analogs of siderophores (small molecule bacterial iron chelators).

Our SFA measurements indicate that Col-1 films remain strongly bound to the underlying mica substrate, even after repeated loading-unloading cycles. For only Col-1 films, we observed very weak adhesion forces, $F_{ad} < 5$ mN/m. Adsorption of TLC-adhesive molecules to the Col-1 films significantly increased the force of adhesion, $F_{ad}$, to $> 50$ mN/m. This adhesion remained constant over several hours.

These findings suggest that siderophore inspired molecules might be an improved alternative to existing bio-adhesives, as they have been proven to strongly bridge mineral surfaces (mimicking prosthesis metal surfaces) and now interacting with the main ECM component of mammal tissues, Col-1.
required to make specific colors and explore the range of hues that can be achieved with colloidal glasses.

experimental reflectance spectra and the model. We also develop an optimization algorithm to find the parameters

multiple scattering, we use a Monte Carlo approach to simulate photon trajectories. We find good agreement between

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2009,

observer owing to the glassy arrangement of air spheres in keratin in the feather barb (E. R. Dufresne et al,

internal structure of the feathers. In blue Cotinga birds, the colors are independent of the angle between light source and

species of birds display structural colors that arise from the constructive interference of light that is scattered from the

use colloidal glasses as a model system to study the physics in structurally-colored systems in nature, such as the blue

feather barbs of the plum-throated Cotinga. Both are composed of spheres in an arrangement with short-range order and

long-range disorder, and in both cases the color results from interference rather than absorption. Unlike biological

systems, however, colloidal glasses can be fabricated in the lab, and we can tune their reflectance spectra. While the

location of the primary structural resonance in their spectra can be predicted using a single-scattering theory, other

features of the spectra, such as the increase in reflection at short wavelengths, cannot be explained by single scattering

alone. To understand the effect of multiple scattering on the color, we do co- and cross-polarized measurements of the

reflection spectra, and we interpret these measurements using Monte Carlo simulations of photons scattering inside the

disordered structure.

Surface segregation of binary particles in photonic colloidal assemblies

Surface segregation also influences the structural colors of these supraballs. In addition, melanin is a multifunctional biological pigment and the control of its segregation at supraball surface leads to novel ways to modulate unique surface properties of colloidal assemblies.

*Air Force Office of Scientific Research (FA9550-13-1-0222) and National Science Foundation (EAR-1251895, DMR-1105370, DMR-1609543)

The prediction and design of bio-inspired structural colors using colloidal glasses

Many species of birds display structural colors that arise from the constructive interference of light that is scattered from the internal structure of the feathers. In blue Cotinga birds, the colors are independent of the angle between light source and observer owing to the glassy arrangement of air spheres in keratin in the feather barb (E. R. Dufresne et al, Soft Matter, 2009, 5, 1792-1795). Such colors can be mimicked in colloidal glasses, but while the locations of the peaks in reflectance spectra are accurately predicted by single-scattering models, weak multiple scattering also contributes to the reflected intensity. We develop a model that quantitatively predicts the reflectance spectra of colloidal glasses. To model the multiple scattering, we use a Monte Carlo approach to simulate photon trajectories. We find good agreement between experimental reflectance spectra and the model. We also develop an optimization algorithm to find the parameters required to make specific colors and explore the range of hues that can be achieved with colloidal glasses.

*MRSEC, NSF GRFP, NSERC

The physical origin of the reflectance features of structurally-colored colloidal glasses

We use colloidal glasses as a model system to study the physics in structurally-colored systems in nature, such as the blue feather barbs of the plum-throated Cotinga. Both are composed of spheres in an arrangement with short-range order and long-range disorder, and in both cases the color results from interference rather than absorption. Unlike biological systems, however, colloidal glasses can be fabricated in the lab, and we can tune their reflectance spectra. While the location of the primary structural resonance in their spectra can be predicted using a single-scattering theory, other features of the spectra, such as the increase in reflection at short wavelengths, cannot be explained by single scattering alone. To understand the effect of multiple scattering on the color, we do co- and cross-polarized measurements of the reflection spectra, and we interpret these measurements using Monte Carlo simulations of photons scattering inside the disordered structure.

*MRSEC, NSF GRFP, NSERC

Learning from butterflies: Folding lipid membranes to build photonic-crystal materials

In some butterfly wing scales, a cellular membrane is folded into a periodic nanostructure which generates color and iridescence by constructive interference of visible light. Inspired by this biological achievement, where protein binding is thought to mediate the energetics and dynamics of membrane folding, we aim to build photonic-crystal materials from self-assembly of small particles on artificial membranes. We start by characterizing the interactions between colloidal particles and a supported phospholipid membrane. We graft single-stranded DNA onto them, so that hybridization of complementary strands generates a specific, attractive force between the particles and the membrane. Using a total internal reflection microscope, we measure interactions with femtonewton resolution and kilohertz dynamics. We find that ligand-receptor affinity dramatically affects the energetics and dynamics of particle-membrane interactions: over a temperature range of a few degrees Celsius, adhesion strength varies by about 10 kT, while bound lifetimes and particle mobility change by orders of magnitude. These results may lead to better understanding of self-assembly of particles on fluid membranes, and ultimately enable self-assembling, membrane-based materials with remarkable optical properties.

*MRSEC, NSF GRFP, NSERC
To achieve this goal, we need to understand and re-design the rules used by nature to encode specificity in protein interactions. Sophisticated techniques for designing proteins de novo have been developed recently in David Baker’s lab. These proteins interact via designed hydrogen-bonding networks and can be used as building blocks to fabricate functional materials. The drawback is the enormous space of interactions that can be designed. In order to explore this space and identify the interactions which lead to specific mechanical properties, we need to understand the link between the protein building blocks and the target structures to assemble. In this talk I will present a theoretical/computational model to predict the yield of some simple protein-made structures as a function of few controlling parameters, such as the binding energies and the concentration of the building blocks.
8:48AM R31.00003: Diffusion Monte Carlo study of hydrogen adsorption on silicon carbide nanotube  GENKI IMAM PRAYOGO (Presenter), KENTA HONGO, Japan Advanced Institute of Science and Technology, HYEONDEOK SHIN, Computational Science Division, Argonne National Laboratory, RYO MAEZONO, Japan Advanced Institute of Science and Technology, ANOUAR BENALI, Computational Science Division, Argonne National Laboratory — Hydrogen is one of the candidates for environmentally friendly energy carriers. Although it has a high energy density per unit weight, its volumetric energy density is rather low, making its compact storage difficult. This is rather important when storage volume is paramount, such as in automobile and aviation industries. Physisorption of hydrogen molecules on materials with high surface area to volume ratio like nanotubes is one of the strategies to increase this volumetric efficiency. Along with carbon nanotube (CNT) and boron nitride nanotube (BNNT), silicon carbide nanotube (SiCNT) is one of the candidate materials for this use. Although it has yet to be experimentally synthesized in single-walled form, larger silicon carbide nanotubes have shown promising gains compared to carbon nanotubes in terms of storage capacity and lack of sorption hysteresis. Theoretical studies point to a stronger binding energy and the existence of point charges naturally occurring on alternating Si-C surface. We present our initial Diffusion Monte Carlo (DMC) results of the adsorption of molecular hydrogen on single walled SiCNT surface. DMC is a stochastic method solving the many-body Schrödinger equation and has demonstrated accuracies below the Kcal/mol for a wide range of materials.

9:00AM R31.00004: Band gaps and excitons in quantum Monte Carlo  MICHAEL BENNETT (Presenter), Department of Physics, North Carolina State University, MATEJ DITTE, Department of Physics, University of Ostrava, CODY MELTON, Department of Physics, North Carolina State University, MATUS DUBECKY, Department of Physics, University of Ostrava, LUBOS MITAS, Department of Physics, North Carolina State University — Using the fixed-node approximation, quantum Monte Carlo (QMC) allows for calculations of both ground and excited energy levels with explicit electron correlations. For example, in periodic systems, one can estimate band gaps by promoting an electron from the valence to conduction band or alternatively from the ionization potential and electron affinity. Since fixed-node QMC’s accuracy depends on the quality of trial functions this tacitly assumes that the relevant states are close to single reference states and well represented by single orbital promotions in the Slater determinant. However, this becomes more challenging for excitations that appear in the gap and are not representative of typical conduction states such as significantly localized excitonic states, impurity or defect levels that are not captured by ordinary band theories. Here the construction of the corresponding trial functions requires more elaborate schemes that might involve multi-reference forms, geometry relaxation and/or additional considerations depending on experiment that one compares with such as optical, conductivity or photoemission measurements. We study a few such cases, eg, benzene molecule and crystal and other systems to capture and illustrate these effects using QMC calculations.

9:12AM R31.00005: Ab Initio Finite Temperature Auxiliary Field Quantum Monte Carlo for Solids*  BRENDA RUBENSTEIN (Presenter), YUAN LIU, Department of Chemistry, Brown University, HANG ZHANG, Department of Chemistry, University of Science and Technology of China — Predicting the finite temperature properties of molecules, and especially, solids is critical for understanding many physical phenomena. Nevertheless, developing accurate, yet efficient methodologies for finite temperature applications remains an outstanding challenge. In this work, we present an Auxiliary Field Quantum Monte Carlo method with an $O(N^2)$ scaling for studying the finite temperature electronic structure of any system that can described by an $ab$ $initio$ Hamiltonian. The algorithm marries the $ab$ $initio$ phaseless auxiliary field quantum Monte Carlo algorithm known to produce high accuracy ground state energies of molecules and solids with its finite temperature variant, long used by condensed matter physicists for studying model Hamiltonian phase diagrams, to yield a phaseless, $ab$ $initio$ finite temperature method. We demonstrate the accuracy of this approach for benchmark solids, including hydrogen chains and networks, and compare to it more popular mean field treatments of real materials. Our method serves as a new, robust tool for studying low, but finite temperature phase transitions in models and solids, ultracold chemistry, and warm dense matter.

*We acknowledge support from the NSF DMR-1726213 and DOE DE-SC0019441 grants.
Multi-determinant Diffusion Monte Carlo in solids at the thermodynamic limit

KEVIN GASPERICH, Department of Chemistry, University of Pittsburgh, THOMAS APPLENCOURT, YE LUO, Argonne National Laboratory, QIMING SUN, California Institute of Technology, KENNETH D JORDAN, Department of Chemistry, University of Pittsburgh, LUKE SHULENBURGER, Sandia National Laboratories, ANTHONY SCEMAMA, MICHEL CAFFAREL, Universite Paul Sabatier Toulouse, ANOUAR BENALI (Presenter), Argonne National Laboratory — In the past decade, fixed-node diffusion Monte Carlo using a single determinant Slater-Jastrow trial wavefunction as proven to systematically reproduce (within 5-10Kcal/mol) the energies of a wide range of molecules and solids. While it has been demonstrated for molecular systems that the path to chemical accuracy (<1Kcal/mol) can be realized by improving the nodal surface using for example multideterminant trial wavefunctions generated with MCSCF or Selected CI. Reaching the same level of accuracy for solids in the thermodynamic limit has proven harder due to the exponential scaling of these wavefunction generation methods. In this talk, we will discuss the effect of using a multi-determinant Slater-Jastrow trial wavefunction with complex k-points and twist averaging in combination to reach chemical accuracy in the thermodynamic limit for solid carbon.

* A.B, L.S and Y.L were supported by US DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, part of the Computational Materials Sciences Program and Center for Predictive Simulation of Functional Materials.

Progress towards finite temperature density matrix quantum Monte Carlo calculations on solids

HAYLEY PETRAS, JAMES SHEPHERD (Presenter), Chemistry, University of Iowa — There has been a recent surge in interest in finite temperature calculations on molecules driven by methods such as FCI, CC, MP2, and AFQMC. By means of a follow-up to recent work on the uniform electron gas, we here present density matrix quantum Monte Carlo (DMQMC) calculations on molecular Hamiltonians. We compare and contrast molecular diatomics with the electron gas to make comment on the scope for performing periodic calculations with DMQMC. We also describe how DMQMC can contribute to the study of finite temperature ab initio Hamiltonians with other methods.

* We thank the University of Iowa for funding.

Difficulty to capture non-additive enhancement of stacking energy by conventional ab initio methods

KEN QIN (Presenter), TOMOHIRO ICHIBHA, KENTA HONGO, RYO MAEZONO, Japan Advanced Institute of Science and Technology — We evaluated the non-additive contributions in the inter-molecular interactions in B-DNA stacking by using diffusion Monte Carlo (DMC) methods. It is found that only DMC can capture the sign inversion in the contribution (i.e., the non-additivity enhances or reduces the interaction depending on the base pairs of DNA), which is never predicted by any other ab initio methods. Even by CCSD(T), the inversion is found to be difficult to be captured because of the practical handling of CBS (complete basis set correction) at the feasible level with MP2. The predicted non-additivity turns out to be several times larger (~8 kcal/mol) than those by other methods. The importance of the hydrogen bondings between the bases horizontally on the inversion is also clarified.

A simpler twist averaging for the uniform electron gas designed for finite basis set calculations such as coupled cluster and full configuration interaction quantum Monte Carlo

TINA MIHM (Presenter), University of Iowa, ALEXANDRA MCISAAC, Chemistry, MIT, JAMES SHEPHERD, University of Iowa — As a long term aim, we would like to improve the efficiency of wavefunction calculations for solids. An important step is the elimination of finite size error, and it is common for continuum quantum Monte Carlo to use twist averaging. Here, we describe and analyze a simple twist averaging scheme as applied to coupled cluster and full configuration interaction quantum Monte Carlo calculations of the uniform electron gas.

* We thank University of Iowa for their funding.
A diffusion Monte Carlo study of point defect diffusion in rutile TiO$_2$ bulk

TOM ICHIBHA (Presenter), Information Science, Japan Advanced Institute of Science and Technology, ANOUAR BENALI, Argonne Leadership Computing Facility, Argonne National Laboratory, KENTA HONGO, Research Center for Advanced Computing Infrastructure, Japan Advanced Institute of Science and Technology, RYO MAEZONO, Information Science, Japan Advanced Institute of Science and Technology — TiO$_2$ is one of the most popular photocatalysts. The diffusion of point defects (Ti interstitial/O vacancy) is responsible for charge transport. We investigated the diffusion mechanism of the point defects in rutile TiO$_2$ bulk using diffusion Monte Carlo (DMC). There are two issues related to the point defect diffusion: (a) The diffusion of positively charged defects from the bulk inside to the (101) surface promotes the surface oxidation reaction. Then, which type of defect transfers positive charges faster? (b) There are two known diffusion paths for Ti interstitial defects, one parallel to the c-axis and the other perpendicular. In which direction are the defects easier to diffuse? Our DMC calculations established that (a) Ti interstitial defects transfer a larger amount of positive charges to the surface and (b) the primary diffusion direction of Ti interstitial defects changes from `perpendicular to c-axis' to `parallel', along with the change of defect charge, 0 to +4. Both conclusions qualitatively support the previous GGA-DFT work. Yet, the barrier energy prediction is quantitatively much different by ~2eV at the maximum. We will discuss this huge difference and justify the barrier energies predicted by DMC, based on Bader charge analysis and electronic density prediction.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R32 DCP: Solvation and Nanofluidics

8:00AM R32.00001: The Intrinsic Density of a Nanoconfined Liquid* SAMUEL COHEN (Presenter), University of Maryland, College Park; Université Grenoble Alpes and CNRS, JOHN S BENDER, University of Maryland, College Park, BENOIT COASNE, Université Grenoble Alpes and CNRS, JOHN T FOURKAS, University of Maryland, College Park — Liquids confined to nanoscale geometries are ubiquitous in nature and important in many areas of science and technology. However, connecting the microscopic structure and dynamics of a confined liquid to its macroscopic behavior is a fundamental, unsolved problem in liquid-state physics. One key macroscopic property, the density, is highly fluid-dependent, and there is currently no rigorous way of assessing a confined liquid’s accessible volume. Here we present our work using the spectrum of intermolecular vibrational modes to probe the intrinsic density of a confined liquid. In particular, molecular simulations to probe the density will be discussed.

*This material is based upon research supported by the Chateaubriand Fellowship of the Office for Science & Technology of the Embassy of France in the United States and by the National Science Foundation, grant CHE-1362215.

8:12AM R32.00002: Uniaxial-deformation behavior of Ice Ih, as described by the TIP4P/Ice and mW water models

MAURICE DE KONING (Presenter), PEDRO ANTONIO SANTOS-FLÓREZ, Universidade Estadual de Campinas, CARLOS JAVIER RUESTES, CONICET and Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Cuyo — Using molecular dynamics simulations we assess the uniaxial deformation response of ice Ih, as described by two popular water models, namely the all-atom TIP4P/Ice potential and the coarse-grained mW model. In particular, we investigate the response to both tensile and compressive uniaxial deformations along the [0001] and [0-110] crystallographic directions for a series of different temperatures. We classify the respective failure mechanisms and assess their sensitivity to strain rate and cell size. While the TIP4P/Ice model fails by either brittle cleavage under tension at low temperatures or large-scale amorphization/melting, the mW potential behaves in a much more ductile manner, displaying numerous cases in which stress relief involves the nucleation and subsequent activity of lattice dislocations. Indeed, the fact that mW behaves in such a malleable manner even at strain rates that are substantially higher than those applied in typical experiments indicates that the mW description of ice Ih is excessively ductile. One possible contribution to this enhanced malleability is the absence of explicit protons in the mW model, disregarding the fundamental asymmetry of the hydrogen bond that plays an important role in the nucleation and motion of lattice dislocations in ice Ih.
8:24AM R32.00003: Theory of freezing point depression and materials damage by nano-fluidic salt trapping∗
EDMOND ZHOU (Presenter), MOHAMMAD MIRZADEH, ROLAND JM PELLENQ, MARTIN BAZANT, Massachusetts Institute of Technology — The electrolyte solution inside the pore space of many functional materials are subjected to freeze-thaw cycles in a cold season, often undermining the material structure and eventually leading to failure. For more durable designs, it is crucial to understand the interplay between pore surface charge, salt ions and pore connectivity during freezing. We present a continuum theory to distinguish nano-fluidic confined freezing from open systems, and calculate freezing point depression, supercooling and pressure in both limits. As an example application, we provide a possible explanation for the mechanism of freeze-thaw damage in cement paste. Our findings could also provide some insights for cryopreservation and survival of species in winter.

∗This work is supported by CSHub at MIT.

8:36AM R32.00004: Nuclear quantum effects on the liquid–liquid phase transition of a water-like monatomic liquid
NICOLAS GIOVAMBATTISTA (Presenter), Physics, City University of New York (CUNY) - Brooklyn College, GUSTAVO E LOPEZ, BINH NGUYEN, Chemistry, City University of New York (CUNY) - Lehman College — Polyamorphic substances have the ability to exist in more than one liquid and/or glass states. Examples include water, silicon, and hydrogen. In many of these substances, nuclear quantum effects may become important in the proximity of the liquid–liquid and glass–glass transformation. Here, we study the nuclear quantum effects on a monatomic liquid that exhibits water-like anomalous properties and a liquid–liquid phase transition (LLPT) ending at a liquid–liquid critical point (LLCP). By performing path integral Monte Carlo simulations with different values of the Planck's constant \( \hbar \), we are able to explore how the location of the LLCP/LLPT in the P–T plane shifts as the system evolves from classical, \( \hbar = 0 \), to quantum, \( \hbar > 0 \). We find that, as the quantum nature of the liquid (as quantified by \( \hbar \)) increases, and the atoms in the liquid become more delocalized, the LLCP pressure increases, the LLCP temperature decreases, and the LLCP volume remains constant. In addition, the crystallization temperature decreases with increasing \( \hbar \). For large values of \( \hbar \), the LLCP is not accessible due to rapid crystallization. The structure of the liquids studied at different values of \( \hbar \) are also investigated.

8:48AM R32.00005: Strain-Induced Raman Shifts Due to Ice Adhesion∗
SUBASH KATTEL (Presenter), JOSEPH MURPHY, MARINA MACHADO DE OLIVEIRA, SAMUEL PASCO, JOHN ACKERMAN, VLADIMIR ALVARADO, WILLIAM RICE, University of Wyoming — Ice formed on a material creates a strain that is indicative of the adhesive strength between the ice and substrate. Previous determinations of ice adhesion strength, a critical parameter for understanding icing physics, have proven to be both challenging and highly dependent on experiment-specific conditions (surface roughness, icing conditions, water purity, etc.). In this work, we use Raman spectroscopy to contactlessly and non-destructively measure ice-induced strain on silicon and single-layer graphene. To isolate the ice-material interface, we measured the vibrational modes of graphene from 20°C to -30°C with and without ice. Along with the well-known temperature-dependent Raman shift of graphene, a clear, ~3 cm\(^{-1}\) change in the G-mode (~1590 cm\(^{-1}\)) frequency developed upon ice formation. We found this change in the Raman shift tracked closely to the temperature-dependent density of ice, suggesting that we are optically measuring ice-created strain in graphene. When correlated with mechanical adhesion measurements, our non-destructive optical technique provides a way to measure ice adhesive strength, which can be extended to various materials.

∗We acknowledge support from NASA through Grant No. WY-80NSS17M0049 and through the University of Wyoming School of Energy Resources.

9:00AM R32.00006: Size and Aggregation of Ice-binding Proteins Control Their Ice Nucleation Efficiency∗
YUQING QIU (Presenter), ARPA HUDAIT, VALERIA MOLINERO, Chemistry, University of Utah — Ice-binding proteins are the common name shared by antifreeze proteins (AFPs) and ice nucleating proteins (INPs). It has been proposed that the size of ice-binding surface determines the function of these proteins, as INPs or AFPs. Aggregation of proteins can create large ice-binding surfaces, stabilize larger ice nucleus and enhance ice nucleation. However, the quantitative dependence of ice nucleation ability on the size and aggregation of the ice-binding surfaces has not yet been elucidated. We use molecular dynamic simulations to show that the ice nucleating ability of a ice-binding protein increases with their length and saturates at an ice freezing temperature lower that that induced by INP aggregates, because the short dimension of small ice-binding surface limits the formation of ice nucleus. We further demonstrate that INPs dimer with specific separation distance enhances the ice nucleating ability of INPs. We conclude that the size and aggregation of ice-binding proteins control their efficiencies.

∗This work was supported by the National Science Foundation through award CHE-1305427 “Center for Aerosols Impacts on Climate and the Environment”. We thank the Center for High Performance Computing at the University of Utah for technical support and a grant of computer time.
Wetting state transition of water droplet on graphene surface with nanoscale pillars*  

HONGRU REN (Presenter), CHUN LI, Northwestern Polytechnical University — The regulation of solid surface wettability can be effectively achieved by controlling surface microstructure and external electric fields. Here, the wetting properties of graphene textured with nanoscale square, circular and cone pillars are systematically investigated by using molecular dynamics simulation. It is shown that the transition of water droplet located on periodic pillars from Wenzel state to Cassie state is highly sensitive to the height of pillars and the hydrophilic-to-hydrophobic switch is achievable by decreasing the inter-pillar spacing. In addition, the behaviors of water droplets situated on graphene under external electric fields are also discussed. The configuration of water droplet performs a hemispherical-conical-ordered cylindrical shape variation with the increase of external electric fields. Notably, the orientations of water dipoles experience remarkable change from disorder to order in the process of increasing electric fields due to the polarization of water molecules induced by static electric fields. These findings could shed some light on future applications of graphene-based devices with controllable wettability.

*National NSF of China (11572251,11872309)

Surface Adsorption and Encapsulated Storage of H2 Molecules in a Cagelike (MgO)12 Cluster*  

YAN ZHANG (Presenter), Beijing Computational Science Research Center, HONGSHAN CHEN, Northwest Normal University — The cluster with a cagelike structure could enable the storage of H2 molecules via surface adsorption and encapsulated storage. Surface adsorption involves the interaction between H2 and host clusters. Encapsulated storage involves the storage of H2 in the interior space of the cagelike structure. The latter is essential for practical applications of cagelike clusters because the interior space is retained when they are assembled into solid-state materials, although many surface adsorption sites are occupied. Here, we report an investigation on surface adsorption and encapsulated storage of H2 molecules in the cagelike (MgO)12 cluster based on a dispersion-corrected density functional theory calculation. The results revealed that the cagelike (MgO)12 cluster surface can adsorb 24 H2 molecules with an average adsorption energy of 0.116 eV/H2, which brings about a gravimetric density of 9.1 wt%. Inside the cagelike (MgO)12 cluster, a maximum capacity of six H2 molecules could be stored according to symmetric configurations. The encapsulated H2 molecules are trapped by energy barriers no more than 2.55 eV, although the storage is an endothermic process.

*This work is financially supported by the National Natural Science Foundation of China (Grant Nos. 11504298 and 11664034).

Kosmotrope and Chaotrope Salts Influence on Water Structural Relaxation and hydrogen Bond Dynamics Investigated by Coherent Quasielastic Neutron Scattering  

ANTONIO FARAONE (Presenter), NIST Center for Neutron Research, National Institute of Standards and Technology, ERKAN SENSES, Department of Chemical and Biological Engineering, Koc University, EUGENE MAMONTOV, Neutron Scattering Division, Neutron Sciences Directorate, Oak Ridge National Laboratory — Salts can either increase or decrease the viscosity when dissolved in water. This phenomenon has been traditionally interpreted within the classification of the solutes as kosmotropes (structure makers) and chaotropes (structure breakers), with reference to their hypothesized property of enhancing or weakening the hydrogen bond network. However, at the molecular level the distinction is less clear as both kosmotropes and chaotropes affect the structure of the surrounding water molecules. Using coherent quasielastic neutron scattering, we have investigated the dynamics of NaCl/D2O and KCl/D2O, NaCl being a kosmotrope and KCl being a chaotrope, respectively. By probing the dynamics of these systems at the structure factor peak, we measured how different salts affect the structural relaxation of water. At the same time, by collecting data at the second peak in the deuterium intermolecular partial structure factor, the hydrogen bond dynamics was probed. Whereas the hydrogen bonding dynamics is largely unchanged by the presence of the salts, NaCl and KCl affect the structural relaxation differently: the former slows down the dynamics whereas the latter mostly leaves the relaxation unchanged.
Agregation Induced Emission (AIE) colloids with enhanced fluorescence activity. Concerning fluorophore encapsulation, it is also possible to control the core-confined crystallization of these to generate capsules loaded inside or on its outskirt with different interesting actives (dyes, meal nanoparticles, biotin...). In this presentation, we show how combining the phase diagrams of simple solutes (oils or solid fluorophores) with hydrophilic polymers (polysaccharides, PVA, pluronics) allows picking a domain where both species co-precipitate into a final capsular object (namely the solute surrounded by the polymer). By crosslinking the shell and functionalize it, one obtains capsules loaded inside or on its outskirt with different interesting actives (dyes, meal nanoparticles, biotin...). Concerning fluorophore encapsulation, it is also possible to control the core-confined crystallization of these to generate Aggregation Induced Emission (AIE) colloids with enhanced fluorescence activity.

*ANR Preproposal ANR-15-CE09-0021

**10:00AM R32.00011: Blue Shift of a Molecular Crystal Phonon at the Solid to Liquid Phase Transition**  
ALEX DAVIE (Presenter), Department of Physics, University at Buffalo, Buffalo, New York, United States, FARAH VANDREVALA, Department of Electrical Engineering, University at Buffalo, Buffalo, New York, United States, YANTING DENG, DEEPU GEORGE, Department of Physics, University at Buffalo, Buffalo, New York, United States, ERIC SYLVESTER, Department of Chemistry, University at Buffalo, Buffalo, New York, United States, TIMOTHY KORTER, Department of Chemistry, Syracuse University, Syracuse, New York, United States, ERIK EINARSSON, Department of Electrical Engineering, Department of Materials Design and Innovation, University at Buffalo, Buffalo, New York, United States, JASON BENEDICT, Department of Chemistry, University at Buffalo, Buffalo, New York, United States, ANDREA MARKELZ, Department of Physics, University at Buffalo, Buffalo, New York, United States — We investigate the dielectric response from the optically active phonons of single-crystal fructose using terahertz (THz) spectroscopic techniques. All samples were indexed by x-ray diffraction with space group of P2₁2₁2₁, lattice constants a = 8.09 Å, b = 9.21 Å, c = 10.03 Å and α = β = γ = 90°. Anisotropic THz absorbance unambiguously assigns the measured resonances to specific lattice vibrations calculated by density functional theory. Using [101] face polished crystals, the lowest frequency resonance polarized along the b axis at 1.70 THz is found to continuously red shift with heating to 1.59 THz at the melting temperature 103°C. As the sample is maintained at 103°C the resonance continues to red shift, broaden and decrease in amplitude with melting. Using [010] face polished crystals, the lowest frequency resonance polarized along the c axis at 1.31 THz is found to red shift with heating to 1.25 THz at 103°C, but then blue shifts to 1.26 THz as the temperature is held at 103°C. The peak then remains at this frequency, broadens and decreases in amplitude as the sample enters the liquid phase. The result is inconsistent with expected softening of intermolecular forces during the phase transition.

*This work was supported by a grant from LANL Award# 71842 and NSF MCB #161652.

**10:12AM R32.00012: Caged Contact Pair Formation in Cooled Triiodide-Ethanol Solutions**  
FRANK YI GAO (Presenter), YU-HSIANG CHENG, KEITH ADAM NELSON, Massachusetts Institute of Technology — We have conducted spectrally-resolved optical pump-probe experiments following the photodissociation of triiodide (I₃⁻) in cooled ethanol solutions from 300 K to 80 K. After being excited by a UV pump pulse at 400 nm, I₃⁻ dissociates into I₂⁻ and I fragments, the former of which is monitored by its broad absorption in the 660-870 nm range. Primary geminate recombination occurs within 4 ps over the temperature range studied and occurs in an increasing fraction of photofragments as the solution is cooled. Following an initial period of vibrational relaxation, the observed spectra continuously red-shifts with decreasing temperature before saturating near 800 nm below 160 K. The red-shifted band appears on a timescale similar to geminate recombination. These results are consistent with the increased formation of a caged contact pair species at low temperatures.

**10:24AM R32.00013: Capillary condensation in the atomic-scale slits**  
QIAN YANG (Presenter), ANDRE GEIM, Physics and Astronomy, University of Manchester — Capillary condensation determines fundamentally the adhesion, nucleation, adsorption and friction processes in all granular and porous materials, micromechanical devices and nanotechnology, even in living systems. Its theoretical basis—the Kelvin equation, whose cogency has long been questioned on the nanoscale, is under continuously debate. Consensus has been reached on the validity of the Kelvin equation down to 4 nm, but pores and cracks in nature do not stop their extending to the molecular dimensions. Up to now, little information, at least experimentally, is available at the molecular scale. Here we report water condensation in ultimately thin capillaries, which is capable of accommodate only one layer of water molecules. Pronounced deviations are observed under strong confinement less than 2 nm. Theoretical interpretation of changes in the solid-liquid surface energy resulting from rearranging the water structure near a particular surface complements the Kelvin equation in the ultimate limit of the atomic-scale confinement.
10:36AM R32.00014: Thermodynamics-based electrochemistry transport models: theory and applications  MAXIM ZYSKIN (Presenter), University of Oxford — I will describe Newman-Monroe thermodynamics-based electrochemical transport models and new results on numerical modeling and molecular dynamics based parameter estimation in such models. This work has applications to modeling multiphysics processes in solid electrolytes and is a part of a program of research on electric batteries.

10:48AM R32.00015: Curvature Dependence of Surface Tension and Test of Kelvin Equation at Molecular Scale* SEONGSOO KIM, DOHYUN KIM (Presenter), Seoul National University, JONGWOO KIM, Korea Research Institute of Chemical Technology, SANGMIN AN, WONHO JHE, Seoul National University — Capillary condensation is the vapor-to-liquid phase transition occurring in confined geometries. Such heterogeneous nucleation has been well described by the Kelvin equation, but its applicability at nanoscale is still unresolved. We show it is valid down to 0.5 nm scale when the curvature dependent surface tension is considered. Our results that unify the validity of the Kelvin equation and the curvature effect of surface tension may provide a better understanding of nucleation phenomena.

*This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (2016R1A3B1908660) and Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2017R1A6A3A1103301).

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R33 FIAP: Semiconductors and Applications I

8:00AM R33.00001: Local Magnetic Imaging of Epitaxial Magnetic Insulator on Semiconductor Nanowire* ZHENG CUI (Presenter), SEAN J HART, Stanford University, LIU YU, SAULIUS VAITIEKENAS, CHARLES M MARCUS, PETER KROGSTRUP, Niels Bohr Institute, University of Copenhagen, KATHRYN ANN MOLER, Stanford University — The observation of properties related to Majorana bound states in indium arsenide (InAs) nanowire-epitaxial aluminum hybrid structure has been encouraging, but the need for a large external magnetic field makes their control and application very challenging. To locally introduce a magnetic exchange field, a single-crystalline ferromagnetic insulator europium sulfide (EuS) has been grown directly onto the InAs nanowire. Using a scanning Superconducting QUantum Interference Device (SQUID) microscope, we study the local magnetization and susceptibility of the hybrid magnetic structure on a sub-micron scale. Imaging local magnetic properties as a function of temperature and external field on multiple devices allow us to characterize homogeneity, anisotropy and domain formation, which will be crucial to further develop these topological superconducting devices.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02- 76SF00515

8:12AM R33.00002: Magnetic Field Dependent Transport Measurements on High Quality InAs Nanowires MARKUS RITTER (Presenter), IBM Research - Zurich, 8803 Rüschlikon, Switzerland, ZIJIN LEI, Solid State Physics Laboratory, ETH Zürich, 8093 Zürich, Switzerland, BENJAMIN MADON, M A MUEED, AAKASH PUSHP, IBM Research - Almaden, San Jose, California 95120, United States, HEINZ SCHMID, IBM Research - Zurich, 8803 Rüschlikon, Switzerland, THOMAS IHN, KLAUS ENSSLIN, Solid State Physics Laboratory, ETH Zürich, 8093 Zürich, Switzerland, HEIKE RIEL, FABRIZIO NICHELE, IBM Research - Zurich, 8803 Rüschlikon, Switzerland — Semiconductor nanowires with strong spin-orbit interaction are attracting considerable interest as potential platform for spintronic and topological quantum computing applications. However, future progress will require scalability and integration concepts that go well beyond the single nanowire level. We present the low temperature characterization of InAs nanowires grown via the template assisted selective epitaxy (TASE) technique [1]. The TASE approach allows for the deterministic growth of semiconducting nanowires, networks and branched geometries on a two-dimensional silicon platform. Furthermore, structures grow encapsulated in a silicon oxide shell which preserves them from undesirable doping and surface oxidation. The high quality of TASE grown InAs nanowires was recently demonstrated by the observation of ballistic electron transport over length scales approaching one micrometer [2, 3]. In this work we additionally show quantized conductance measurements in a magnetic field and transport spectroscopy of Coulomb island devices for characterization of Landé g-factor and spin-orbit coupling strength.

8:24AM R33.00003: Strain-induced Gunn Effect in Silicon Nanowires

DARYOUSH SHIRI, Department of Microtechnology & Nanosciences, Chalmers University of Technology, Gothenburg, Sweden, AMIT VERMA, REZA NEKOYEV (Presenter), Department of Electrical Engineering & Computer Sciences, Texas A&M University-Kingsville, Kingsville, TX, USA, ANDREAS ISACSSON, Department of Physics, Chalmers University of Technology, Gothenburg, Sweden, SELVA SELVAKUMAR, Department of Electrical & Computer Engineering, University of Waterloo, Waterloo, ON, Canada, ANANT ANANTRAM, Department of Electrical Engineering, University of Washington, Seattle, WA, USA — Gunn (or Gunn-Hilsum) Effect and its associated negative differential resistivity (NDR) does not exist in bulk silicon. This effect which is due to transfer of electrons between two different energy subbands, is very pronounced in direct bandgap semiconductors like GaAs which makes them favorable for microwave Gunn-diode based oscillators.

In stark contrast to GaAs, bulk silicon has a very high energy spacing (~1 eV) which renders the initiation of transfer-induced NDR unobservable. However using Density Functional Theory (DFT), Tight Binding and Ensemble Monte Carlo (EMC) methods we show for the first time that: (1) Gunn Effect can be induced in silicon nanowires (SiNW) under 3% tensile strain and an electric field of 5000 V/cm,

(2) the onset of NDR in I-V characteristic is reversibly adjustable by strain, and (3) strain modulates the resistivity by a factor 2.3 for SiNWs of normal I-V characteristics i.e. those without NDR. Results of this study promise applications of SiNW-based Gunn diodes in microwave oscillators. The observed NDC is different in principle from Esaki-Diode and Resonant Tunneling Diodes (RTD) in which NDR originates from tunneling effect not electron transfer between subbands of different effective mass.

8:36AM R33.00004: The effect of ultrasmall grain sizes on the thermal conductivity of nanocrystalline silicon thin films

XIAO LIU (Presenter), United States Naval Research Laboratory, BATTOTOKH JUGDERSUREN, KeyW Corporation, BRIAN T KEARNEY, NRC Research Associate, JAMES CLIFFORD CULBERTSON, CHRISTOPH N CHERVIN, RHONDA MICHELE STROUD, United States Naval Research Laboratory — We report on the thermal conductivity of nanocrystalline silicon thin films with average grain sizes varying from 3 nm to 10 nm. The films were prepared by plasma-enhanced chemical-vapor deposition. The crystallinity and grain sizes of the films are controlled by hydrogen dilution during growth. Thermal conductivity was measured from 80 K to room temperature. The thermal conductivity of the film with 10 nm grain size roughly follows the minimum thermal conductivity predicted for amorphous silicon. As the grain size decreases to 3 nm, its thermal conductivity is reduced to one third of the minimum thermal conductivity. We extend the model of grain boundary scattering of phonons with Debye and Born-von Karman dispersion relations to explain our results. Although our results can still be explained by strong grain boundary scattering, we find the phonon mean-free-path would have to decrease at a faster rate than the reduction of grain size to explain the strong dependence of thermal conductivity on grain size.

*Work supported by the Office of Naval Research

8:48AM R33.00005: First-principles calculation of the dynamic heat current in semiconductors under the application of a thermal gradient

ÉAMONN MURRAY (Presenter), Department of Physics and Department of Materials, Imperial College London, IVANA SAVIC, Tyndall National Institute, Cork, Ireland, STEPHEN B FAHY, Department of Physics, University College Cork, Cork, Ireland — We present calculations of the time evolution of the thermal transport through a material following the application of a thermal gradient. This involves the calculation of the anharmonic force constants from first principles, which are used to find the scattering between phonon modes of different energies and wavelengths. We can then use this to find the dynamical heat current from the Boltzmann transport equation, going beyond the single mode relaxation time approximation and allowing us to see how the heat current evolves in time once the thermal gradient is applied or changes. We present results of this analysis as applied to several semiconductor systems.

9:00AM R33.00006: Ginzburg-Landau-Langevin theory and SSH model for Peierls transition in In/Si(111)

YASEMIN ERGUN (Presenter), Institut für Theoretische Physik, Leibniz Universität Hannover — Motivated by the thermal and photo-induced first-order Peierls transitions observed in atomic wires on semiconducting surfaces [1], we use the Ginzburg-Landau (GL) theory for charge-density-wave systems to investigate the dynamics of collective excitations in Peierls insulators. This formalism allows us to study the vibrations and the non-equilibrium dynamics of the amplitude modes (lattice distortion and density modulation) which are involved in a Peierls transition. We include no phase mode but amplitude modes for the commensurate Peierls system. The Langevin formalism is used to simulate finite temperature and thermalisation. The GL parameters are determined from the 1D Su-Schrieffer-Heeger (SSH) model in the grand canonical ensemble [2]. Next goals are the extension to coupled chains and the inclusion of non-adiabatic effects between electrons and phonons. Ultimately, we want to simulate the nonequilibrium dynamics of the SSH model for wires on substrates.

References:
First-principles calculations of second order nonlinear optical coefficients in the static limit and Pockels coefficients in III-N and II-IV-N₂ compounds

SAI LYU (Presenter), WALTER R L LAMBRECHT, Case Western Reserve University — The second order nonlinear optical coefficients in the static limit are evaluated using density functional perturbation theory from the electronic response to a static electric field for the group III nitrides and several II-IV-N₂ ternary nitrides. They are compared with literature results using the sum over states approach including local field effects. The effects of the scissor correction are evaluated. Good agreement is obtained for GaN, AlN and w-BN. For InN, the small or even negative gap in in the LDA at Γ causes an extreme sensitivity to the k-point summation and pseudopotentials. Similar problems occur for other very small gap II-IV-N₂ semiconductors. The nonlinear optics coefficients are showing a general trend of increasing values with smaller gaps but no clear scaling relation with the direct gaps is obtained. The Pockels coefficient, which include in addition to the electronic response, also the phonon and piezoelectric response and are also evaluated. They show that the phonon and electronic contributions to the response in these materials are comparable in magnitude.

This work was supported by National Science Foundation, Division of Materials research under grant No. 1533957.

Crystal free energy of SiC polytypes and stacking faults formation energy from DFT-based lattice-dynamics approach.

EMILIO SCALISE (Presenter), ANNA MARZEGALLI, FRANCESCO MONTALENTI, LEONIDA MIGLIO, Materials Science, University of Milano Bicocca — Despite a rising impact of SiC technology in the power electronics industry, some fundamental aspects of this material lack physical understanding. Particularly polytypism and growth of SiC polytypes have been discussed as a paradox from about thirty years because of an evident discrepancy between theory and experiments, not yet elucidated. SiC has more than 200 polytypes and few of them (i.e. 3C, 6H, 4H) are commercially available and used for power devices. Besides the scientific interest, investigating SiC polytypism and understanding its driving force is crucial to correctly predict the energetics of extended defects in SiC, which are one of the main concerns of this wide band gap semiconductor. We perform first-principle calculations, including long range interactions and based on a lattice dynamics approach, we predict the temperature dependent thermodynamic stability of different SiC polytypes which may explain their growth at different temperature. Finally, we estimate the formation energy of stacking faults in SiC and the effect of Van Der Waals corrections are proved to be key for reproducing experimental observations.

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High-mobility InAs two dimensional electron systems on GaSb substrates

ANTHONY HATKE (Presenter), Station Q Purdue and Department of Physics and Astronomy, Purdue University, CANDICE THOMAS, AYMERIC TUAZ, RAY KALLAHER, Birck Nanotechnology Center, Purdue University, TIALUNG WU, Station Q Purdue and Department of Physics and Astronomy, Purdue University, TIAN WANG, ROSA DIAZ, GEOFFREY C. GARDNER, MIKE CAPANO, Birck Nanotechnology Center, Purdue University, MICHAEL MANFRA, Station Q Purdue and Department of Physics and Astronomy, Purdue University — The two dimensional electron gas in InAs quantum wells grown on nearly lattice-matched GaSb substrates is an attractive stage for mesoscopic device physics. However, use of this system has remained difficult due to outstanding challenges. Here we report on heterostructure design optimization and device fabrication that satisfies three main criteria for mesoscopic device operation: electrical isolation from the semiconducting substrate, ability to fully deplete the charge carriers and control residual sidewall conduction with lithographic gates, and high mobility to ensure ballistic transport over mesoscopic length scales [1]. In addition, we discuss our current progress in realization of mesoscopic devices including quantum point contacts and quantum dots.

9:48AM R33.00010: High thermal conductivity in cubic boron arsenide crystals  SHENG LI (Presenter), Department of physics, University of Texas at Dallas, QIYE ZHENG, Department of Materials Science and Engineering and Materials Research Laboratory, University of Illinois at Urbana-Champaign, YINCHUAN LV, Department of Physics, University of Illinois at Urbana-Champaign, XIAOYUAN LIU, Department of physics, University of Texas at Dallas, XIQU WANG, Department of Chemistry, University of Houston, PINSHANE HUANG, DAVID G CAHILL, Department of Materials Science and Engineering and Materials Research Laboratory, University of Illinois at Urbana-Champaign, BING LV, Department of physics, University of Texas at Dallas — We report our experimental efforts on the high thermal conductivity above 1000 W/m/K in the zinc blende cubic BAs crystals. First principle calculations have predicted the thermal conductivity of BAs, is second only to that of diamond at room temperature, which may constitute a useful thermal management material for high-power density electronic devices. Herein, we reported our experimental efforts to grow single domain, defect-free, and large size BAs crystals, evidenced by both single crystal diffraction and scanning transmission electron microscopy (STEM) studies, through test and optimization various single-crystal growth methods. Furthermore, the time-domain thermoreflectance (TDTR) measurement of the BAs crystal gives a high thermal conductivity ~1000 W/m K which is consistent with the predicated value based on four phonon calculations, representing BAs as a new class of ultrahigh thermal conductivity materials.

10:00AM R33.00011: Interplay between molecular packing and charge transfer states in 6,13-bis(trisopropylsilylthynyl)-pentacene (TIPS-pentacene) organic semiconductor thin films*  YANG LI (Presenter), JING WAN, University of Vermont, DETLEF-M SMILGIES, Cornell University, JOHN M. HUGHES, RANDALL HEADRICK, University of Vermont — The optical properties of organic semiconductors are influenced by interference between neutral molecular excitations and charge transfer excitations. We present a comprehensive study of this effect for TIPS-pentacene in the temperature range from 25°C to 140°C via the influence of molecular packing on the optical and electronic properties, utilizing in-situ x-ray diffraction, polarized optical spectroscopy and density functional theory. In TIPS-pentacene, anisotropic thermal expansion causes neighboring molecules to “slide” relative to each other. Since charge transfer effects depend sensitively on the nodal structure of the highest occupied and lowest unoccupied molecular orbitals, optical excitations are modulated as the relative displacement is varied. We find that the transition energies of the lowest energy optical excitations are dramatically blue shifted as the temperature is increased, and that changes in the charge transfer integrals can be correlated with an enhancement of field-effect transistor mobility. These results suggest a new approach to improve carrier mobility in strained thin films by decreasing the sensitivity of the charge transfer integrals to dynamic disorder.

*This work was supported by the National Science Foundation under grant DMR-1701774.

10:12AM R33.00012: Overcoming bismuth saturation in GaAsBi by manipulating film strain  MARGARET STEVENS (Presenter), KEVIN GROSSKLAUS, JOHN MCELEARNEY, THOMAS VANDERVELDE, Tufts University — Epitaxially grown III-V-Bismides offer new band gap and lattice constant combinations for near- and mid-IR device applications on GaAs and InP substrates. High bismuth content GaAsBi is typically grown compressively strained on GaAs, though droplet-free thick films have been difficult to realize in that system. Surface Ga-Bi droplets inhibit bismuth incorporation and cause vertical phase separation, yielding films unusable for optoelectronic applications. To produce bismide films that are suitable for IR optoelectronics, we explored the growth of increasingly Bi-rich GaAsBi compounds under a variety of strain conditions ranging from highly compressively strained on GaAs to tensile strained on InGaAs buffer layers. High resolution x-ray diffraction and Rutherford backscatter spectrometry showed higher Bi content can be achieved without droplet formation by reducing film compressive strain. Atomic force microscopy and phase contrast microscopy showed reduced surface droplet density, indicating bismuth is being incorporated in the film rather than surface segregating. Overall, we show that reducing the compressive strain in GaAsBi films is a successful method for reducing droplet formation and enabling increased Bi incorporation.
ALBERT CHANG (Presenter), Duke University, PHILLIP M. WU, IOP, Academia Sinica, Taiwan (ROC) and GUS Technology, Taiwan/San Mateo CA, USA, HAO ZHANG, Tsinghua University, Beijing, China — We present evidence that quantum point contacts (QPCs) fabricated on a high mobility (~$10^6 \text{ cm}^2/\text{Vs}$) GaAs/AlGaAs heterstructure crystal with doping close to the 2D interface exhibit quantum transport conductance which is strongly dependent on the QPC geometry. In particularly, asymmetrically shaped, T-junction QPCs nearly always exhibit strong conductance resonances as well as anomalies in the conductance plateaus, whereas symmetrically shaped QPCs, designed with smooth entrance and exit regions joining to wide 2D regions, are largely devoid of such resonances. The dramatic difference in the conductance traces between the two types of geometries suggest that disorder does NOT play a dominant role in the transport characteristics. Furthermore, this implies that unusual features, including resonances, suppression of quantum plateaus[1,2], and novel differential conductance oscillations [3] previously reported in asymmetric QPCs could arise instead from intrinsic mechanisms, e.g. geometry and/or interaction effects.


*Funding: NSFDMR-0701948 and IOP, Academia Sinica, Taipei.

RASTHEL PRENTKI (Presenter), Physics, McGill University, FEI LIU, Institute of Microelectronics, Peking University, JIAN WANG, Physics, The University of Hong Kong, HONG GUO, Physics, McGill University — Power dissipations are to blame for part of the recent deceleration in the exponential growth rate of the transistor count on integrated circuits predicted by Moore's law. A relevant metric at the device level is the subthreshold swing (S) - the increment in gate voltage required for a tenfold increase in drain current - which is commensurate with energy losses during switching. For the ubiquitous Si Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET), thermodynamics and electrostatics impose that $S \geq 60 \text{ mV/dec}$ at room temperature. Phenomena beyond MOSFET physics thus need to be exploited to design a low S device; we show how ballistic transport can be used towards this end. In the resulting device, known as the cold source FET, thermionic emission is suppressed in the OFF-state by means of density-of-states engineering, thereby enabling low S while maintaining a high ON-state current. Deviations from the approximation of ballistic transport need to be considered for real-world implementations; we show how rethermalization due to inelastic scattering affects S.

*Supported by Fonds de recherche du Québec - Nature et technologies (FRQNT) and the Area of Excellence grant under project number AoE/P-04/08-1 from the Research Grant Council of Hong Kong.

HUIXIA FU (Presenter), Weizmann Institute of Science — Recently an air-stable layered semiconductor Bi$_2$O$_2$Se was discovered to exhibit an ultrahigh mobility in transistors fabricated with its thin layers. In this work, we explored the mechanism that induces the high mobility and distinguishes Bi$_2$O$_2$Se from other semiconductors. We found that the electron donor states lie above the lowest conduction band. Thus, electrons get spontaneously ionized from donor sites (e.g., Se vacancies) without involving the thermal activation, different from the donor ionization in conventional semiconductors. Consequently, the resistance decreases as reducing the temperature as observed in our measurement, which is similar to a metal but contrasts to a usual semiconductor. Furthermore, the electron conduction channels locate spatially away from ionized donor defects (Se vacancies) in different van der Waals layers. Such a spatial separation can strongly suppress the scattering caused by donor sites and subsequently increase the electron mobility, especially at the low temperature. We call this high-mobility mechanism self-modulation doping, i.e. the modulation doping spontaneously happening in a single-phase material without requiring a heterojunction. Our work paves a way to design novel high-mobility semiconductors with layered materials.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R34 FIAP FED: Live Long and Prosper as Physicist, Innovator, and Entrepreneur
BCEC 205A - Chuhee Kwon, Cal State Univ- Long Beach - Tag(s): Careers, Education, Industry, Invited, Undergraduate
Physicists as Master Innovators: Why Innovation and Entrepreneurship should be highlighted in physics education* [Invited] DOUGLAS ARION (Presenter), Carthage College — Physicists are positioned to be some of the most effective innovators - solving real-world problems by applying their broad knowledge and understanding of how the world works, and contributing to all sorts of organizations through an entrepreneurial mindset. How can we make that happen more often, and how can we leverage this to attract a larger and more diverse body of students into the field? Innovation and entrepreneurship education components - whether implemented in curriculum directly, co-curricular programs, or experiential learning opportunities - can be utilized to achieve these goals. Let's consider why we should take this on as an important part of physics education - as important as the canon of content we've always delivered.

*This work supported in part by NSF Grant number 1624822.

Live Long and Prosper as Physicist, Innovator, and Entrepreneur* [Invited] CRYSTAL BAILEY (Presenter), American Physical Society — Physics graduates are among the most employable in the world, with 96% of graduates finding successful employment, mostly in private sector settings. While employers value the technical skills and ability to engage in continued learning that are hallmarks of physics graduates, physics majors also have the potential to become impactful, positive agents of change in the world as effective innovators and entrepreneurs. In this talk, I will explore the skills, knowledge and mindset that are essential to entrepreneurship, and describe national efforts that are taking place to make innovation and entrepreneurship education a regular part of physics students' experience.

*Support for this work is provided by the National Science Foundation's IUSE program under Award No. 1624882 ("The PIPELINE Network").

Understanding the Value of Intellectual Property in Entrepreneurship: Finding Your Path Down the Yellow Brick Road [Invited] CYNTHIA PILLOTE (Presenter), Snell & Wilmer — You're done the hard work and you've got a brilliant idea for an invention. Now what? We'll discuss considerations for faculty and students when developing intellectual property (IP), including university policies and procedures, grant provisions, and getting the most value for your IP.

Making the Shift from Research to Revenue: Skills that Physicists Need to be Successful in Business [Invited] SAM WURZEL (Presenter), None — Physicists bring with them many useful skills for starting businesses: the ability to develop innovative ideas, a comfort with technology and mathematics, and the grit required to solve hard problems. However there are key skills that physicists often lack: sales, marketing, accounting, law, and interpersonal skills key to business. Luckily these skills are learnable. In my talk I will discuss my long path to learning them when I left physics to start Octopart and how this process can be accelerated for physicists starting businesses today.

Academia to Entrepreneurship- A Multi-pronged Journey [Invited] THIRUMALAI VENKATESAN (Presenter), National University of Singapore — There has been a sea change over the last few decades in the way academic institutions view entrepreneurial activities of the faculty and the role of the Institution in fostering an ecosystem conducive to such activities. This has become a global phenomenon and many of the leading Institutions in Europe and Asia are also beginning to replicate the model of the Boston or Silicon Valley academic Institutions. This clearly presents a wonderful opportunity for those who want to strike out on their own as opposed to waiting for someone else to offer them a job. This is the transition from a job seeker to a job creator. This is a multi-pronged journey with differing levels of risks and rewards. In my talk I will discuss a variety of models that are available to the academic entrepreneur, their pluses and minuses and also some of the critical knowledge one needs to understand about the world of entrepreneurship in general. I will use examples from several of my colleagues' startups and my own experience in running a company for over three decades maintaining an academic life.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R35 DQI: Read-out and Measurement of Superconducting Qubits BCEC 205B - Zlatko Minev, Yale Univ - Tag(s): Focus
Reducing measurement errors is critical for performing any quantum algorithm, especially those requiring feedback. In certain situations, e.g. in quantum experiments that only require averaged measurements, errors can be corrected using post-processing techniques. These experiments include any that only require operator expectation value measurements, such as tomography or variational quantum eigensolvers. Here we will present one such method, which involves calibrating these errors via measurements of prepared computational states which are used to feed a neural network. In this way we reduce the experimental overhead from exponential to polynomial scaling. We will present experimental demonstrations of this technique on IBM Q devices.

*This work was supported by the Army Research Office under contract W911NF-14-1-0124

Fault-tolerant quantum computing requires repetitive high-fidelity quantum parity measurements. In quantum processors based on circuit QED, the fidelity of indirect quantum parity measurements using an ancillary qubit is compromised by errors induced in the coherent interaction step and in the ancilla measurement. Here, we improve upon the state of the art by combining two techniques to reduce ancilla measurement time and measurement-induced cross-dephasing of data qubits: dedicated Purcell filtering for each qubit and active photon depletion. We find the parity measurement speed limit by minimizing the parity measurement error rate as a function of the cycle time. We individually quantify the error contributions of one- and two-qubit gates, residual interactions, cross-talk, parasitic measurement-induced dephasing, and quantum demolition.

*This research is funded by IARPA (U.S. Army Research Office Grant W911NF-16-1-0071). Additional funding is provided by Intel Corporation (N.M.).

High-fidelity readout of the state of a qubit is an indispensable part of a quantum computer. Progress in implementation of controllable large-scale quantum computers calls for implementation of a scalable high fidelity multi-qubit readout scheme. In a typical transmon superconducting qubit, measurement is implemented by applying a microwave drive to a readout resonator dispersively coupled to the qubit. Recent experiments demonstrated that despite detuning between the drive and qubit frequencies, measurement renormalizes the spectrum of the combined qubit-resonator system and induces cross-talk between nearby qubits resulting in reduced fidelity. A starting point is to develop an optimized readout scheme for a two-qubit system. With both numerical and approximate analytical analysis, we were able to identify the source of spurious transitions and explore qubit parameters optimal for scalable multi-qubit readout scheme.

*USRA Feynman Quantum Academy Program and NASA Academic Mission Service contract number NNA16BD14C.
High-fidelity, quantum non-demolition qubit measurement is a vital prerequisite for robust, large-scale quantum machines. In superconducting quantum circuits, the typical information carriers for qubit readout are coherent states of light, which must be amplified before they can be efficiently recorded in room-temperature electronics. Typically, these amplifiers consist of one, or two, microwave modes linked by a parametrically driven coupling. Such amplifiers regularly approach the quantum limit for amplification, allowing us to closely track qubits’ states. However, conventional parametric amplifiers lack almost every other desirable property, including high saturation power, large bandwidth, and directional operation. I’ll discuss our recent efforts to address these shortcomings by suppressing unwanted terms in the device’s Hamiltonian and combining multiple, simultaneous parametric drives between a pair of microwave modes. In a single device by varying the parametric drives, we can produce desired behaviors including transmission-only phase-sensitive amplification, input match, and gain-independent bandwidth. We have used observation of quantum jumps and weak measurements of superconducting qubits to benchmark the device’s performance. I will discuss the prospects for adding the final desired property, directionality, via further parametric couplings to a third microwave mode. Another route to higher measurement fidelity is to replace coherent states with squeezed light as the information carrier. I will present data from a recent experiment which uses an interferometric scheme for qubit readout with two-mode squeezed light, achieving a voltage signal-to-noise ratio improvement of ~25 % versus coherent state readout. I will also discuss the prospects for using two-mode squeezed light to remotely entangle distant qubits.

*This work is partially supported by the ARO, NSF, and the Kaufman Foundation.

In this work, we present a filter design allowing multiplexed qubit readout with Purcell protection. The design is composed of four quarter-wave stubs, providing a bandstop filter whose bandwidth is up to 1~GHz at the qubit frequency. Using a three-port scattering matrix formalism, we show that the qubit emission into the readout line is suppressed by more than 75~dB, while the readout line transmission is reduced by less than 3~dB. We then show that in situ tunability of the filter can be obtained by terminating the stubs with RF-Squids. Our results pave the way to large-scale qubit readout with high fidelity and flexibility.

We experimentally test this measurement protocol using a superconducting qubit coupled to a resonator mode. Compared to the conventional dispersive readout, we observe that our protocol yields higher fidelity for a given integration time. Finally, we use an additional resonator drive to leave the resonator state in vacuum if qubit is in the excited state before the measurement protocol. This suggests that the proposed technique may become useful in unconditionally resetting the resonator to a vacuum state after the measurement pulse.

*Financial support by European Research Council (681311 QUESS) and Marie Sklodowska-Curie Grant (795159), Academy of Finland (312300, 312059, 265675, 305237, 305306, 308161, 312300, 314302, 316551, 319579), the Jane and Aatos Erkko Foundation, and the Technology Industries of Finland Centennial Foundation.
9:36AM R35.00007: Fast Measurement of a Tunable Superconducting Flux Qubit via a Driven Nonlinear Resonator with Applications in Quantum Annealing* DANIEL TENNANT (Presenter), DENIS MELANSON, ANTONIO MARTINEZ, Institute for Quantum Computing, Department of Physics and Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo, MUHAMMET ALI YURTALAN, Institute for Quantum Computing, Department of Electrical and Computer Engineering, and Waterloo Institute for Nanotechnology, University of Waterloo, YONGCHAO TANG, Institute for Quantum Computing, Department of Physics and Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo, DAVID K KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, JONILYN L YODER, STEVEN WEBER, Lincoln Laboratory, Massachusetts Institute of Technology, ADRIAN LUPASCU, Institute for Quantum Computing, Department of Physics and Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo — Development of readout schemes of flux qubits in the persistent current basis is important for quantum annealing applications. High fidelity detection, controlled backaction on the qubit, as well as rapid acquisition, are all relevant for flexible quantum annealing. In order to accommodate these requirements, we develop a readout based on the use of metastable oscillation states in a nonlinear oscillator detection circuit specifically tailored for capacitively shunted flux qubits. In this work, we discuss the design as well as preliminary results for a device specifically designed for tunable capacitively shunted flux qubits specifically designed for use in quantum annealers.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).

9:48AM R35.00008: Realizing a Catch-Disperse-Release read-out of a qubit* PERONNIN THEAU (Presenter), Univ Lyon, ENS de Lyon, Univ Claude Bernard Lyon 1, CNRS, Laboratoire de Physique, F-69342 Lyon, Franc, DANIJELA MARKOVIC, Laboratoire Pierre Aigrain, Ecole Normale Supérieure, PSL Research University, CNRS, Université Pierre et Marie Curie, Sorbonne Universités, Université Paris Diderot, Sorbonne Pa, QUENTIN FICHEUX, Univ Lyon, ENS de Lyon, Univ Claude Bernard Lyon 1, CNRS, Laboratoire de Physique, F-69342 Lyon, Franc, ZAKI LEGHTAS, Centre Automatique et Systèmes, Mines-ParisTech, PSL Research University, 75006 Paris, France, BENJAMIN HUARD, Univ Lyon, ENS de Lyon, Univ Claude Bernard Lyon 1, CNRS, Laboratoire de Physique, F-69342 Lyon, Franc — Fast read-out is an essential piece of measurement based error correction codes. The usual technique of driving a dispersively coupled resonator presents some limitations such as finite reset time. To overcome these limits Sete and al. [1] proposed a catch, disperse and release scheme that we recently realized.

It uses a resonator with a tunable coupling to the transmission line. That resonator is coupled to the qubit in the dispersive coupling limit. First, we do brief unconditional coherent displacement of the resonator. Then the phase of the stored coherent state grows linearly in time at a rate depending on the state of the qubit. Finally, we release the resonator's state into the transmission line and measure the phase of the outgoing signal.

Our experiment implements that scheme by using a Josephson Parametric Converter as a tunable coupler between a low and a high Q factor resonator [2] to measure a transmon qubit in CPW geometry.

We demonstrate a state-of-the-art read-out with a fidelity of 97.5% in a total of 240 ns. The fidelity is limited by the qubit lifetime. We demonstrate the quantum non-demolition, reset, and Purcell protection granted by this scheme.


*Funded by the QMiCS project of the European Quantum Flagship

10:00AM R35.00009: ABSTRACT WITHDRAWN
10:12AM R35.00010: Tracking non-Markovian quantum dynamics of a superconducting qubit with a recurrent neural network filter*

NOAH STEVENSON (Presenter), BRADLEY MITCHELL, Univ of California - Berkeley, SHIVA BARZILI, RAZIEH MOHSENINIA, JUSTIN G. DRESEL, Chapman Univ, IRFAN SIDDIQI, Univ of California - Berkeley — Determining the time-dependent Hamiltonian for control pulses of superconducting quantum circuits is critical for their use in reliable quantum information processing; however, interactions between coupled qubits and nearby resonators can cause transient dynamics to become non-Markovian. We use quantum state tracking with continuous weak measurement to experimentally investigate non-Markovianity in a transmon superconducting qubit coupled to a readout resonator. By weakly measuring the state of the transmon qubit undergoing tunable Rabi oscillations comparable to the cavity linewidth, we isolate dynamics that are difficult to describe with single-qubit trajectory theory. We address this difficulty by training a recurrent neural network to reconstruct the quantum trajectories, motivated by such a network's demonstrated ability to learn long-time correlations in sequential data. Here we detail the experimental protocol and present preliminary data.

*This work was supported by the Army Research Office.

10:24AM R35.00011: Quantum non-demolition detection of single itinerant microwave photons*

JOHN MARK KREIKEBAUM (Presenter), Univ of California – Berkeley, KEVIN P O'BRIEN, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, BAPTISTE ROYER, Université de Sherbrooke, ARNE GRIMSMO, The University of Sydney, ALEXANDRE BLAIS, Université de Sherbrooke, IRFAN SIDDIQI, Univ of California – Berkeley — The detection of microwave photons is an important capability for superconducting quantum information processing and microwave quantum optics but remains challenging due to the small energy of photons at this frequency. Our circuit quantum electrodynamics (cQED) based detector [1] exploits the superradiant ‘bright’ and subradiant ‘dark’ states that are formed when transmons are coupled an appropriate distance from each other on a waveguide [2]. Detuning each transmon inhomogeneously from the operating frequency leads to coupling of the bright and dark states which allows for absorbed photons to be trapped for longer than the inverse of the absorption bandwidth. We utilize this long interaction time to achieve high-fidelity measurements of the photon number in the ensemble. Using a single photon source, we benchmark the performance of this protocol.


*This work was supported by the Army Research Office and the Department of Energy.

10:36AM R35.00012: Pulsed reset protocol for fixed-frequency superconducting qubits

DANIEL EGGER (Presenter), MAX WERNINGHAUS, MARC GANZHORN, GIAN SALIS, ANDREAS FUHRER, PETER MUELLER, STEFAN FILIPP, IBM Research - Zurich — Improving coherence times of quantum bits is a fundamental challenge in the field of quantum computing. With long-lived qubits it becomes, however, inefficient to wait until the qubits have relaxed to their ground state after completion of an experiment. Moreover, for error-correction schemes it is important to rapidly re-initialize syndrome qubits. We present a simple pulsed qubit reset protocol based on a two-pulse sequence. A first pulse transfers the excited state population to a higher excited qubit state and a second pulse into a lossy environment provided by a low-Q transmission line resonator, which is also used for qubit readout. We show that the remaining excited state population can be suppressed to 1.7 ± 0.1% and that this figure may be reduced by further improving the pulse calibration. We also show that the reset protocol can be used for cooling by removing the thermal qubit population.

10:48AM R35.00013: Diagnostic Single-Qubit Gate Monitoring with Continuous Measurements*

JOHN STEINMETZ (Presenter), ANDREW N JORDAN, University of Rochester — The physical implementation of a quantum gate generally deviates from the desired qubit operation. In order to improve the gate fidelity, we use continuous weak measurements to track the quantum map as it develops in time, so as to identify the origin of any deviations from the desired evolution. This gives insight into how to modify the qubit design as well as the controls applied. We test this diagnostic method on single qubit gates with both correlated and uncorrelated noise.

*US Army Research Office
IT-TaS$_2$ has been studied for a long time as a charge density wave system. The new unit cell consists of 13 site "star of David" clusters forming a triangular lattice. It was proposed 40 years ago that these cluster give rise to a Mott insulator state with $S=1/2$ per cluster. However, the expected local moments have never been observed and no magnetic ordering has been found. We proposed [1] that this material may be an example of the quantum spin liquid that has somehow gone unnoticed for 45 years. Recent experiments have provided strong evidence that this is indeed the case, and that the low energy excitations are characterized by a spinon Fermi surface. We propose that the mechanism has to do with the proximity to the Mott transition, which can be modelled by a spin model with NN exchange $J$ and a 4 site ring exchange term $K$. We performed DMRG calculations on this model [2], extending earlier work to 6 and 8 wide cylinders and found that a modest $K/J$ ratio is sufficient to stabilize a spin liquid ground state with Fermi surface. A strong signature is that the peaks in the spin-spin correlator lie on a circle with radius $2k_F$. We have also performed doping studies on the spin liquid and found that the leading pair correlation is oscillatory in space, ie, a pair density wave. [3] It will be very interesting to dope this and related systems very gently (less than 1% carrier per Ta) by gating to minimize localization of the doped carriers.


Evidence for a quantum spin liquid in single-layer 1T-TaSe$_2$

Quantum spin liquids are a novel state of matter predicted to arise in quantum antiferromagnets where magnetic frustration or quantum fluctuations are strong enough to prevent magnetically ordered states even down to the lowest temperatures. Quantum spin liquids are believed to exist in strongly correlated Mott insulators, and are thus related to unconventional superconductivity. Much work on quantum spin liquids has focused on triangular and kagome lattices where frustration is strong. An example is the bulk Mott insulator 1T-TaS$_2$ which has attracted attention as a quantum spin liquid candidate due to localized $d$-orbitals in the Ta atoms that form a triangular lattice in this material. This scenario, however, is complicated by interlayer coupling and possible different stacking orders in the bulk, thus motivating investigation into related single-layer materials.

I will discuss recent studies that we have performed on single-layer 1T-TaSe$_2$ that provide evidence for 2D spin liquid behavior. We have characterized the electronic structure of single-layer 1T-TaSe$_2$ (grown via molecular beam epitaxy) by means of scanning tunneling microscopy/spectroscopy (STM/STS), angle-resolved photoemission spectroscopy (ARPES), and first-principles calculations. We observe Mott insulating behavior in single-layer 1T-TaSe$_2$, including novel orbital texture not seen in bulk samples. Vertical heterostructures formed by a single 1T-TaSe$_2$ layer placed on top of metallic 1H-TaSe$_2$ exhibit Kondo behavior, providing direct evidence for a triangular array of local magnetic moments in single-layer 1T-TaSe$_2$. Evidence for a spin-liquid-based spinon Fermi surface is observed in both STM and ARPES measurements of single-layer 1T-TaSe$_2$. These results will be discussed in the context of recent theoretical predictions.
Half-integer thermal quantum Hall effect in a Kitaev spin liquid: A signature of Majorana edge modes and non-Abelian excitations

Yuichi Kasahara (Presenter), Department of Physics, Kyoto University — Kitaev quantum spin liquid (QSL) displays the fractionalization of quantum spins into Majorana fermions. In magnetic fields, the emergence of Majorana edge current is predicted to manifest itself in the form of thermal quantum Hall effect. Here we report on thermal Hall conductivity $\kappa_{xy}$ measurements in $\alpha$-RuCl$_3$, a candidate material for Kitaev QSL on two-dimensional (2D) honeycomb lattice. In magnetic field perpendicular to the 2D honeycomb planes, positive $\kappa_{xy}$ develops in a spin-liquid state below the temperature characterized by the Kitaev interaction $J_K/k_B \sim 80$ K, demonstrating the presence of highly unusual itinerant excitations. Although the zero-temperature property is masked by the magnetic ordering at $T_N = 7$ K, the sign, magnitude, and $T$-dependence of $\kappa_{xy}$ at $T_N < T < J_K/k_B$ follows the predicted trend of the itinerant Majorana fermion excitations. The application of a tilted magnetic field suppresses the AFM order, leading to a field-induced QSL ground state. In this QSL state, the 2D thermal Hall conductance per honeycomb plane $\kappa_{xy}^{2D}/T$ shows a plateau behavior as a function of applied magnetic field and has a quantization value of $\pi^2 k_B^2/6h$, which is exactly half of $\kappa_{xy}^{2D}/T$ in the integer quantum Hall state and fractional quantum Hall state that hosts Abelian anyons. This half-integer thermal Hall conductance provides direct evidence of a non-Abelian phase and topologically protected chiral edge modes of charge neutral Majorana fermions (particles that are their own antiparticles), which have half degrees of freedom of conventional fermions. Above a critical field, the quantization disappears and $\kappa_{xy}^{2D}/T$ goes to zero rapidly, indicating a topological phase transition.


Numerical Studies of Quantum Spin Liquids in Kitaev and Heisenberg Models

Donna Sheng (Presenter), California State University, Northridge — Rapid advancement in large-scale numerical simulations for strongly correlated systems has led to great progress in identifying and characterizing emerging new states of matter in realistic many-body systems in past a few years. I will report some of exciting advances including the identification of magnetic fields driven quantum spin liquids in the honeycomb Kitaev model and spin liquids in frustrated kagome and triangular lattice Heisenberg models. Based on the state of the art density matrix renormalization group simulations, we show that the non-Abelian chiral spin liquid emerges for the Kitaev model with antiferromagnetic Kitaev interactions, and remains robust up to a critical magnetic field that is an order of magnitude larger than the corresponding critical field for a ferromagnetic Kitaev model signaling the importance of frustration in such systems. Interestingly, an intermediate gapless spin liquid phase emerges with the increase of the magnetic field, which may be relevant to the experimental system RuCl$_3$ under magnetic fields. For spin Heisenberg lattice models, besides previous discovered robust chiral spin liquid and time-reversal invariant spin liquid, we also establish a new chiral gapless spin liquid on triangular lattice $|1\text{-}j_2\text{-}j_3|$ model. Furthermore, we explore the nature of different quantum spin liquids for kagome systems in the presence of DM interactions based on the dynamic structure factor simulation, which demonstrates consistency with observations in inelastic neutron scattering measurements of herbertsmithite.

Research was supported by the U.S. Department of Energy, the DOE Office of Basic Energy Sciences under the grant No. DE-FG02-06ER4630.
8:00AM R37.00001: Refined spin Hamiltonian for Yb2Ti2O7 and its two competing low field states* [invited] ALLEN SCHEIE (Presenter), JONAS KINDERVATER, Johns Hopkins University, GABRIELE SALA, GEORG EHLERS, Oak Ridge National Lab, SEYED KOOHPAYEH, COLLIN BROHOLM, Johns Hopkins University — We present a neutron scattering study of pyrochlore Yb2Ti2O7 in a [111] magnetic field using high-quality stoichiometric single crystals. High magnetic fields (1.5 T) reveal sharp spin wave modes, which we use to further refine the magnetic Hamiltonian, offering corrections to previous Hamiltonian refinements. Low magnetic fields reveal diffuse features which suggest an unconventional ground state, and we discuss mechanisms explaining how such a spectrum can be caused by proximity to a ferromagnetic-antiferromagnetic phase boundary. We present a model which accounts for the observed spectrum, and resolves several long-standing questions concerning the ground state of Yb2Ti2O7 [1].


*This work was supported through the Institute for Quantum Matter at Johns Hopkins University, by the U.S. Department of Energy, Division of Basic Energy Sciences, Grant DE-FG02-08ER46544. AS and CB were supported through the Gordon and Betty Moore foundation under the EPIQS program GBMF4532.

8:36AM R37.00002: Semiclassical simulation of quantum spin ice: seeing beyond the light* CLAUDIO CASTELNOVO (Presenter), ATTILA SZABÓ, University of Cambridge — We devise a semiclassical numerical method to investigate quantum spin ice, based on classical Monte Carlo and dynamical simulations of the effective ring exchange Hamiltonian in the large-$S$ limit. At low temperatures, this approach is asymptotically equivalent to a path integral field theory, and indeed we find excellent agreement with known results from the latter regarding the dispersion of the photonic modes of the system. We further argue that our method samples the finite-temperature path integral formulation of the quantum spin ice problem accurately, and thus allows us to go beyond the results attainable using the field theoretic description, and study also the isolated as well as collective behaviour of vison excitations.

*This work was supported in part by Engineering and Physical Sciences Research Council (EPSRC) Grants No. EP/P034616/1 and No. EP/M007065/1

8:48AM R37.00003: Vison and photon electrodynamics in quantum spin ice* ATTILA SZABÓ (Presenter), CLAUDIO CASTELNOVO, University of Cambridge — We investigate quantum spin ice on the pyrochlore lattice using semiclassical Monte Carlo and dynamical simulations of the effective ring exchange Hamiltonian. The model exhibits normal modes equivalent to photons as well as gapped vortices of the emergent magnetic field analogous to visons. Contrary to the behaviour of spinons in classical spin ice, we find that visons form a weak electrolyte; that is, their strong interaction makes the energy cost of a bound pair lower than that of an isolated vison. This leads to a qualitatively different temperature dependence of the pinch points in the corresponding emergent magnetic field. Finally, we observe that the thermal bath of photons dresses the visons and drastically reduces their energy. This suggests that visons may hybridise with the photon spectrum in quantum spin ice, which has potential implications on detecting them experimentally.

*This work was supported in part by Engineering and Physical Sciences Research Council (EPSRC) Grants No. EP/P034616/1 and No. EP/M007065/1.

9:00AM R37.00004: Probing the magnetic excitations in the quantum magnet Yb2Ti2O7 XINSHU ZHANG (Presenter), Johns Hopkins University, STEFFEN SÄUBERT, Technische Universität München, SEYED KOOHPAYEH, PETER ARMITAGE, Johns Hopkins University — The pyrochlore magnet Yb2Ti2O7 has shown exotic magnetic properties and has been considered to be a quantum spin ice although there is still considerable uncertainty about its Hamiltonian parameters. We study the evolution of its magnetic excitations as function of magnetic field and temperature using time-domain terahertz spectroscopy. We perform a thorough sum rule analysis of the low energy excitations by combining time domain terahertz spectroscopy and magnetization measurements. The distribution of spectral intensity indicates strong quantum fluctuations and short range spin correlations in Yb2Ti2O7 at low magnetic field. It also shows the very different manifestation of thermal fluctuations vs. quantum fluctuations in this compound.
9:12AM R37.00005: Capacitive Torque Magnetometry: Study of field-induced magnetic transitions and transient states in the Spin-Ice Material Ho$_2$Ti$_2$O$_7$* KEVIN BARRY (Presenter), Physics, Florida State University; NHMFL, Tallahassee, FL, United States, NAWEEN ANAND, NHMFL, Tallahassee, FL, United States, JENNIFER NEU, Physics, Florida State University; NHMFL, Tallahassee, FL, United States, HAIDONG ZHOU, Physics, University of Tennessee, Knoxville, TN, United States, DAVID E GRAF, NHMFL, Tallahassee, FL, United States, THEO SIEGRIST, CHRISTIANNE BEEKMAN, Physics, Florida State University; NHMFL, Tallahassee, FL, United States — We used capacitive torque magnetometry to compile phase diagrams that show the field-induced magnetic transitions between specific spin textures of the spin ice state. High quality single crystals have been measured at 500 mK in applied fields up to 11 T applied along various crystallographic directions. Utilizing reported results from neutron scattering as our starting point we have developed a phenomenological model that fully characterizes the anisotropic magnetic phase diagram of the system. This model clearly shows the evolution of the spin textures between the previously identified $Q = 0$, $Q = X$, and 3-in/1-out states, and it shows the existence of transient states between them. These transient states are characterized by spin flip excitations taking the spin ice away from the well-defined spin textures. Activation energies associated with these excitations have been extracted. This study demonstrates the applicability of torque magnetometry in probing specific spin textures hosted by the spin ice state.

*A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreements No. DMR-1157490 and No. DMR-1644779, and the State of Florida. JN and TS acknowledge support from NSF DMR-1506952.

9:24AM R37.00006: Investigations of scaling and dynamics in the kagome ice phase of Ho$_2$Ti$_2$O$_7$* ALEXANDRA TURRINI (Presenter), Paul Scherrer Institute, SEAN GIBLIN, EDWARD RIORDAN, School of Physics and Astronomy, Cardiff University, PETER C. W. HOLDSWORTH, Laboratoire de Physique, Ecole Normale Superieure de Lyon, PATRIK HENELIUS, Kondenserade Materiens Teori, Royal Institute of Technology Stockholm, TOM FENNELL, Paul Scherrer Institute — Applying a medium strength field along the [111] direction of the geometrically frustrated spin ices Ho$_2$Ti$_2$O$_7$ and Dy$_2$Ti$_2$O$_7$ results in a magnetization plateau called kagome ice. Competition between the ice rules and applied field separates the pyrochlore structure into alternating kagome and triangular planes, creating a quasi-two dimensional analog of spin ice with distinct spin correlations [1]. The concentration of spin flip excitations (recontextualized as magnetic monopole quasiparticles [2]) experiences various crossovers with increased field and temperature visible as critical inflections in the magnetization, specific heat [3] and susceptibility [4]. As the energy of spin flip excitations in the kagome plane changes with field, the mobility of monopole quasiparticles is constrained further from their spin ice counterparts. Using diffuse neutron scattering and high frequency susceptibility measurements on a Ho$_2$Ti$_2$O$_7$ single crystal, alongside Monte Carlo simulations, we have observed and characterized signals of scaling and crossovers attributed to changing monopole density above the critical point.


*SNF grant 200020_162626

9:36AM R37.00007: Fitting crystal field excitations using point-charge model -- application to rare earth pyrochlore, Kagome, and triangular magnets* ZHILING DUN (Presenter), XIAOJIAN BAI, Georgia Institute of Technology, JOSEPH PADDISON, University of Cambridge, MATTHEW BRANDON STONE, Oak Ridge National Lab, HAIDONG ZHOU, University of Tennessee, MARTIN MOURIGAL, Georgia Institute of Technology — Determining the single ion crystal field (CF) Hamiltonian is usually an indispensable step to understand the collective low-temperature magnetism in rare earth magnets. This sometimes becomes challenging in low-symmetry systems due to the limited experimental observables compared to a large number of fitted CF parameters. Here I describe a general method to fit neutron CF excitation spectrum using point charge models. By benchmarking with the existing inelastic neutron scattering measurements of pyrochlore oxides (R$_2$X$_2$O$_7$), we achieve a simple and universal point-charge model. This model is then modified and applied to the newly discovered tripod Kagome magnets (R$_2$Mg$_2$Sb$_3$O$_{14}$), through which the principal axes and local g-tensor in the pseudo-spin basis can be determined and diagonalized. Finally, we apply the point-charge calculation to the triangular lattice magnet YbMgGaO$_4$ and relates its mysterious extra CF levels to the local structure disorder.

*The work at Georgia Tech was sponsored by the Department of Energy under grant DE-SC-0018660. The work at U. Tennessee was supported by NSF-DMR-1350002.
Correlated Quantum Tunnelling of Monopoles in Spin Ice*

Bruno Tomaseullo (Presenter), Theory Group, Institut Laue-Langevin, Claudio Castelnovo, Cavendish Laboratory, University of Cambridge, Roderich Moessner, MPIPKS, Max Planck Institute, Jorge Quintanilla, SPS, University of Kent — The spin ice materials Ho$_2$Ti$_2$O$_7$ and Dy$_2$Ti$_2$O$_7$ are by now perhaps the best-studied classical frustrated magnets. A crucial step towards the understanding of their low temperature behaviour – both regarding their unusual dynamical properties and the possibility of observing their quantum coherent time evolution – is a quantitative understanding of the spin-flip processes which underpin the hopping of magnetic monopoles. We attack this problem in the framework of a quantum treatment of a single ion subject to the crystal, exchange and dipolar fields from neighbouring ions. By studying the fundamental quantum mechanical mechanisms, we discover a bimodal distribution of hopping rates which depends on the local spin configuration, in broad agreement with rates extracted from experiment. Applying the same analysis to Pr$_2$Sn$_2$O$_7$ and Pr$_2$Zr$_2$O$_7$, we find an even more pronounced separation of time scales signalling the likelihood of coherent many-body dynamics that is likely to have signatures in the behaviour of these systems.

*Institut Laue-Langevin,
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- EPSRC NetworkPlus on “Emergence and Physics far from Equilibrium”

Spectroscopy of Spin Fluctuations in Spin Ices*

Ritika Dusad (Presenter), Cornell University, Franziska Kirschner, Oxford University, Jesse Hoke, Benjamin Roberts, Anna Eyal, Cornell University, Felix Flicker, Oxford University, Graeme Luke, McMaster University, Stephen Blundell, Oxford University, James C Davis, Cornell University — In the past decade, the theoretical prediction of emergent magnetic charges in several lanthanide-pyrochlore magnetic insulators has spawned renewed experimental interest in the study of these elusive particles, albeit in a condensed matter system. Thermodynamic and transport studies of of the spin ice of Dy$_2$Ti$_2$O$_7$ and Ho$_2$Ti$_2$O$_7$ are the focus of research. We report new studies of the spin fluctuation spectrum in these materials and analyze the data in the context of theories for thermally generated magnetic monopole pairs.


*Gordon and Betty Moore Foundation’s EPiQS Initiative

Monopole equilibration in spin ice

David Tennant (Presenter), MSTD, Oak Ridge National Laboratory, Anjana Samarakoon, NSCD, Oak Ridge National Lab, Santiago Grigera, CONICET La Plata Argentina, Qiang Zhang, NSCD, Oak Ridge National Lab, Bastian Klemke, Helmholtz Center Berlin, Alexander Kirste, PTB Berlin, Claudio Castelnovo, Dept of Physics, University of Cambridge, Roderich Moessner, MPIPKS Dresden — Spin ice shows remarkably rich behavior due to its monopole quasiparticles and coulombic interactions. In actual materials quantum tunneling provides millisecond spin flip times which bring out-of-equilibrium states into reach for experimental and computational study. Recently there has been interest in using neutrons and noise as probes of such behaviors. We present computational and experimental studies of the magnetic states in Dy$_2$Ti$_2$O$_7$ under out-of-equilibrium conditions. These cover the feasibility of noise and neutron measurements to assess the states in the material under thermal and field quenching.
10:24AM R37.00011: Anomalous magnetic ground state behaviour of the mixed B-site pyrochlore Dy$_2$ScNbO$_7^*$
MEGAN RUTHERFORD (Presenter), Physics and Astronomy, McMaster University, COLE D MAUWS, Chemistry, University of Manitoba, CASEY MARJERRISON, Physics and Astronomy, McMaster University, SARA HARAVIFARD, Duke University, JAMES BEARE, GRAEME LUKE, Physics and Astronomy, McMaster University, HAIDONG ZHOU, University of Tennessee, Knoxville, CHRISTOPHER R WIEBE, Chemistry, The University of Winnipeg — The spin ice state, which is of great interest due to observed residual Pauling entropy, has been observed in rare-earth pyrochlores such as Dy$_2$Ti$_2$O$_7$, and Dy$_2$Sn$_2$O$_7$. In an effort to explore the robustness of the spin ice state in dysprosium based pyrochlores, a new species Dy$_2$ScNbO$_7$ has been synthesized and single crystals have successfully been grown. Early physical characterization has shown unique behaviour arising from the disordered b-site, with faster spin dynamics and an anomalous low ordering temperature. In an effort to further explore the unique behaviour of Dy$_2$ScNbO$_7$, heat capacity measurements have been performed with an applied magnetic field along the [111] kagomé ice plane and the [110] direction of the cubic unit cell. The phase diagrams constructed from these measurements and other recent physical characterization results show an unexpected divergence from spin ice behaviour, which is the focus of this presentation.

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Canadian Research Chairs

10:36AM R37.00012: The magnetism of novel pyrochlores with a known muon site studied using muon-spin rotation*
STEPHEN BLUNDELL (Presenter), FRANZ LANG, University of Oxford, TOM LANCASTER, Department of Physics, Durham University, DHARMALINGAM PRABHAKARAN, University of Oxford — Pyrochlore oxides with the formula A$_2$B$_2$O$_7$ display a rich variety of ground states and novel magnetic phenomena, encompassing cooperative paramagnetism, all-in-all-out (AIAO) states and spin-ice behaviour. The magnetic ions on the A or B sites occupy sublattices of corner sharing tetrahedra. In muon experiments on pyrochlores, it is important to consider the extent to which an implanted muon may perturb its local environment and whether it is capable of altering the intrinsic properties of the material under investigation, a significant effect for Pr-based pyrochlores [1]. We have determined the muon site in the pyrochlore structure and use this to understand experimental data obtained on Tm$_2$Ti$_2$O$_7$ (singlet ground state), Y$_2$V$_2$O$_7$ and Lu$_2$V$_2$O$_7$ (candidate topological magnon insulator), and Lu$_2$Ir$_2$O$_7$ (insulator, with AIAO structure). [1] F. R. Foronda, F. Lang, J. S. Möller, T. Lancaster, A. T. Boothroyd, F. L. Pratt, S. R. Giblin, D. Prabhakaran and S. J. Blundell, Phys. Rev. Lett. 114, 017602 (2015)

*We thank EPSRC (UK) under grant EP/N023803/1.

10:48AM R37.00013: Antisymmetric transport coefficients of magnetic monopoles in quantum spin ice under an electric field*
SHIGEKI ONODA (Presenter), RIKEN — Unambiguously detecting magnetic monopoles in classical or quantum spin ice has been an intriguing issue. Of our interest is the bosonic U(1) quantum spin liquid phase of quantum spin ice, which accommodates emergent magnetic monopoles as fractionalized quasiparticles and hosts deconfined emergent U(1) gauge fields. It has recently been recognized that the emergent electric gauge flux in this quantum spin liquid can be generated by a real electric field and electric polarization [1,2]. Here, solving the Harper equation [3] for a prototypical quantum spin ice, we show that magnetic monopoles can form Landau levels under an electric field, bending the orbital motion of magnetic monopoles and thus producing antisymmetric transport coefficients in response to the temperature gradient and the magnetic field gradient [4]. Possible experimental setups are also discussed.


*The work was partially supported by the JSPS Grant No. 15H03692 and by the RIKEN iTHEMS project. Calculations were partly performed on HOKUSAI at RIKEN.

Thursday, March 7, 2019 8:00 AM - 10:48 AM
8:00AM R38.00001: First-principles Study on Ferromagnetism in Two-dimensional Fe$_3$GeTe$_2$  
JINGZHAO ZHANG (Presenter), The Chinese University of Hong Kong, JING WANG, YUANBO ZHANG, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, JUNYI ZHU, The Chinese University of Hong Kong — Identifying new magnetic materials is key to better device performance and new device paradigm. Recently, the discoveries of two-dimensional (2D) ferromagnetic (FM) insulators have drawn a lot of attention to the searching of 2D magnetic materials. Here, by density functional theory calculation with different functionals as well as effective Hubbard U parameters, we symmetrically studied layered metallic magnet Fe$_3$GeTe$_2$ (FGT) from bulk to monolayer. Generally, LDA functional can give a correct description of the interlayer FM coupling, which is consistent with our experimental results. We simulated the ionic gate by electron doping in tri-layer FGT, explaining the mechanism of $T_C$ dispersion as a function of doping level revealed in experiments, by applying Stoner model. Moreover, by obtaining the intralayer and interlayer exchange parameters, we found that the itinerant ferromagnetism persists in FGT down to monolayer with an out-of-plane magnetocrystalline anisotropy. Finally, the calculated $T_C$ by mean field calculation is consistent with the experimental value.

*Acknowledge financial support from Chinese University of Hong Kong (CUHK) under Grant No 4053084, from University Grants Committee of Hong Kong under Grant No 24300814, and the Start-up Funding of CUHK.

8:12AM R38.00002: Above-room-temperature Ferromagnetism in Wafer-scale Two-dimensional Fe$_{3+x}$GeTe$_2$ Films  
SHANSHAN LIU (Presenter), ZI Han LI, KE YANG, HUA WU, FAXIAN XIU, Fudan University — Recently, 2D ferromagnetic materials have been discovered with tunable magnetism and nodal-line features. Controlling 2D magnetism in exfoliated nanoflakes via electric-field enables the boosted Curie temperature ($T_C$). One of the most intriguing challenges, however, is the realization of high $T_C$ materials that are tunable, robust and compatible with the commercial-level manufacturability. Here, we report the above-room-temperature ferromagnetic order in wafer-scale 2D Fe$_{3+x}$GeTe$_2$ films through a non-equilibrium growth process in molecular beam epitaxy. The perpendicular magnetic anisotropy in Fe$_{3+x}$GeTe$_2$ is found to persist up to 320 K, significantly higher than the stoichiometric bulk counterpart (Fe$_3$GeTe$_2$, $T_C$~220 K). By controlling the atomic ratio, we found a largely-modulated $T_C$ that depends on carrier density. Corroborated with DFT calculations, we demonstrated that the higher atomic ratio further stabilizes the FM ground state by yielding a larger energy difference of $E_{AFM}$-$E_{FM}$, therefore enabling the enhanced ferromagnetic order in this system. Our results show an effective approach, i.e., the element doping, to produce a robust ferromagnetic order beyond room temperature in wafer-scale Fe$_{3+x}$GeTe$_2$ films, which may render practical applications for 2D spintronic devices.

8:24AM R38.00003: Anomalous magnetotransport in Van der Waals ferromagnet Fe$_2$GeTe$_3$  
SIQI WANG (Presenter), YANG XIA, University of California at Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, YUAN WANG, XIANG ZHANG, University of California at Berkeley — Ferromagnetic Van der Waals (VdW) materials have been discovered with tunable magnetism and nodal-line features. Controlling 2D magnetism in exfoliated 2D magnet with an intrinsically-high Curie/Neel temperature remains a challenge. Here we show experimental evidence of ferromagnetic ordering around temperature in thin flakes of cleavable van der Waals magnet Fe$_2$GeTe$_2$. Anomalous Hall effect measurements and magneto-optic Kerr effect point towards out of plane anisotropy. Furthermore, our devices exhibit high metallicity and a rich phase diagram.

8:36AM R38.00004: Magnetism near room temperature in thin flakes of Fe$_5$GeTe$_2$  
DMITRY OVCHINNIKOV (Presenter), University of Washington, ANDREW MAY, Oak Ridge National Laboratory, BEVIN HUANG, ZAIYAO FEI, University of Washington, QIANG ZHENG, MICHAEL A MCGUIRE, Oak Ridge National Laboratory, XIAODONG XU, University of Washington — Two-dimensional (2D) magnets are an emerging class of materials that exhibit intrinsic magnetic order in the ultrathin limit. An immediate challenge is to realize 2D magnetic order at high temperature. Indeed, molecular beam epitaxy has successfully synthesized monolayers that are magnetically ordered at room temperature. Controlled intercalation of Li ions into a few layers of Fe$_5$GeTe$_2$ also increases magnetic order from low temperature up to room temperature. However, obtaining an exfoliated 2D magnet with an intrinsically-high Curie/Neel temperature remains a challenge. Here we show experimental evidence of ferromagnetic ordering around temperature in thin flakes of cleavable van der Waals magnet Fe$_5$GeTe$_2$. Anomalous Hall effect measurements and magneto-optic Kerr effect point towards out of plane anisotropy. Furthermore, our devices exhibit high metallicity and a rich phase diagram.
Imaging magnetic structure in Van der Waals ferromagnets using nanoSQUID microscopy

CHARLES TSCHIRHART (Presenter), MAREC SERLIN, JIACHENG ZHU, University of California, Santa Barbara, AVI G SHRAGAI, Physics, Cornell University, YU SAITO, University of California, Santa Barbara, MARTIN E HUBER, Physics, University of Colorado, Denver — Van der Waals ferromagnets have been shown to host a variety of magnetic phenomena, including gate-and-magnetic field-tunable transitions between ferromagnetic and layer antiferromagnetic states. I will present high resolution spatial maps of magnetic structure in exfoliated chromium iodide heterostructures, obtained using a scanning nanoscale SQUID on tip microscope, which provides sub-100 nm spatial resolution of magnetic domains across a wide range of magnetic fields spanning the coercive fields of these materials.

Prediction of a two-dimensional intrinsic ferromagnetic and half-metallic material MnSiTe₃

DECHEN ZHANG (Presenter), AZIZUR RAHMAN, WEI QIN, PING CUI, ZENGMING ZHANG, ZHENYU ZHANG, University of Science and Technology of China — Two-dimensional (2D) transition metal trichalcogenides (TMT) have recently been extensively studied due to their intriguing electronic and magnetic properties. Here, based on first-principles calculations, we predict a new 2D TMT material MnSiTe₃, which possesses both ferromagnetism and half-metallicity. The cleavage energy of the bulk MnSiTe₃ is found to be very low, suggesting its monolayer counterpart can be obtained via direct mechanical exfoliation. More intriguingly, we demonstrate that both the ferromagnetism and half-metallicity are preserved when reducing the dimensions from the bulk to monolayer. For the monolayer MnSiTe₃, we calculate the strengths of exchange interactions between nearest, next-nearest and next-next-nearest neighbors of Mn ions. The long-range ferromagnetic order is further confirmed by Monte Carlo simulations within the Heisenberg model, and the Curie temperature $T_c$ is shown to be $\sim$70K. Apart from the exchange interactions between magnetic atoms, the Ruderman-Kittel-Kasuya-Yosida interaction mediated by itinerant carriers also plays a crucial role in determining the ferromagnetic ground state. These findings provide a new 2D material for exploring applications in nano spintronics.

2D Ferromagnetism in Silicene Materials

DMITRY AVERYANOV, ANDREY TOKMACHEV, OLEG PARFENOV, IGOR KARATEEV, IVAN SOKOLOV, ALEXANDER TALDENKOV, VYACHESLAV STORCHAK (Presenter), NRC "Kurchatov Institute" — The appeal of ultra-compact spintronics drives intense research on magnetism in low-dimensional materials. Recent years have witnessed remarkable progress in engineering two-dimensional (2D) magnetism via defects, edges, adatoms and magnetic proximity. However, intrinsic 2D ferromagnetism remained elusive until recent discovery of magneto-optical response in Cr-based layers[1,2], stimulating the search for novel 2D magnets with tunable properties. We employ a bottom-up approach to produce layered structures of silicene (a Si counterpart of graphene) functionalized by rare-earth atoms, ranging from the bulk down to one monolayer. We track the evolution from the antiferromagnetism of the bulk to intrinsic 2D ferromagnetism of ultrathin layers of GdSi₂ and EuSi₂ [3]. Remarkably, the charge transport is found to be layer-dependent once silicene structures are scaled to a few-monolayers limit: it evolves from a Kondo-like trend to an insulating behavior once a gap opens up in its charge excitation spectrum. The discovery of a class of robust 2D magnets, compatible with the mature Si technology, is instrumental for engineering new spintronic devices.


*We acknowledge support from NRC "Kurchatov Institute" (1381) and RFBR (19-07-00249, 16-29-03027 and 17-07-00170).
**9:48AM R38.00008: Interplay between charge density wave phases and magnetism in transition metal diselenides**

**ADOLFO O. FUMEGA, VICTOR PARDÓ (Presenter)**, University of Santiago de Compostela — In this talk we will describe a series of density-functional-theory-based ab initio calculations carried out on structurally two-dimensional transition metal diselenides. VSe₂ has been reported to show robust magnetism[1], yet ab initio calculations[2] show that the coexistence of a charge-density-wave (CDW) phase with a ferromagnetic one is doubtful, even at the monolayer level. We will analyze how the interplay between magnetism and CDW phase occurs in VSe₂, what effects can cause the material to stabilize a long-range ferromagnetic order, how the magnetic properties change from the 1T-phase to the 2H-phase and also how the properties of the Peierls phase observed at the monolayer limit compare to the small-gap phase in isostructural TiSe₂.


*This work has received financial support from Ministerio de Economía y Competitividad (Spain) under project No. MAT2016-80762-R and (A.O.F. only) via FPU scholarship no. FPU16/02572.

**10:00AM R38.00009: Magnetic interfaces of MnSe₂ monolayers**

**TOMAS ROJAS (Presenter)**, Ohio University, ANH T NGO, Materials Science Division, Argonne National Laboratory, SERGIO E ULLOJA, Ohio University — Until recently, 2D magnetism was thought to occur together with defects or doping on different substrates. This situation changed drastically, as intrinsic Cr-based ferromagnetic monolayer materials were discovered, namely CrI₃ and Cr₂Ge₂Te₆. A different material, MnSe₂, was predicted as stable ferromagnetic monolayer by first-principles calculations, and it has been successfully grown on several substrates [1].

In this study, the authors confirm the intrinsic ferromagnetism of the monolayer, while for thicker samples they report an interface of the MnSe₂ monolayer with bulk α-MnSe(111). This phase of the material is non-magnetic, and yet the observed magnetic moments are of up to twice the value of those in the monolayer alone.

In this work, we present a detailed analysis of the interactions at this interface between the two phases, using the Heyd-Scuseria-Ernzerhof hybrid functional. We have studied the effects on the electronic and magnetic structure of both phases of the material, and the dependence on the sample thickness. We study the role that strain plays at the interface, and how it affects the magnetic moments of the structure.


*Supported by NSF-DMR 1508325, and Ohio Supercomputer Center

**10:12AM R38.00010: Emergent Transition Metal Dichalcogenide Monolayer Ferromagnetism at Terminated Edges**

**VIJAYSANKAR KALAPPATTIL, SADHU KOLEKAR, MANUEL BONILLA, RAJA DAS, TATIANA M EGGER,** University of South Florida, KHANG HOANG, North Dakota State University, MATTHIAS BATZILL, MANH-HUONG PHAN (Presenter), University of South Florida — The recent discoveries of the strong room-temperature ferromagnetism in epitaxially grown transition metal diselenide XSe₂ (X = V, Mn) monolayers have effectively heated up the field of two-dimensional (2D) van der Waals magnets [1,2]. However, the origin of the ferromagnetism in these nanosystems has remained an open question. In this talk, we demonstrate that chalcogenide (Se) atoms at terminated edges play a dominant role in the XSe₂ monolayer magnetism, regardless of the transition metal being a non-magnetic element (X = W, Ti) or a magnetic element (X = V). The ferromagnetic Se edge is responsible for the observed large magnetic moment, which decreases as the size of XSe₂ islands or the number of XSe₂ layers increases. The role played by the magnetic transition metal (X = V) on the ferromagnetic ordering of monolayer XSe₂ is also elucidated. Density functional theory (DFT) based calculations support the experimental findings. This understanding enables controlled nanoengineering of novel two-dimensional van der Waals magnets for next-generation spintronic devices and storage information applications.

**References**


*The U.S. DOE under Award No. DE-FG02-07ER46438.
**10:24AM R38.00011: Flat bands and Dirac cones in magnetic 2D metal-organic frameworks**

TOMOHIRO SOEJIMA (Presenter), Physics Department, UC Berkeley, RU CHEN, Molecular Foundry, Lawrence Berkeley National Laboratory, CHRISTOPHER H. HENDON, Chemistry Department, University of Oregon, JEFFREY B NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Metal-organic frameworks (MOFs) are interesting crystals for exploring new physics due to their tunable structure and chemical composition. 2D magnetic MOFs are of particular interest, and a composite kagome-honeycomb lattice was recently realized in a reported ferrimagnetic iron-semiquinone MOF [1]. Via molecular orbital and tight-binding analysis, and with density functional theory-based calculations, we study the iron-semiquinone MOF and show that its band structure contains multiple flatbands as well as multiple Dirac cones. We find that the MOF is semimetallic, with the Fermi level at a Dirac point; and the calculated magnetization is consistent with the reported experimental value. We also explore the effects of spin-orbit coupling and comment on the magnetism of related 2D MOFs; we also discuss how our tight-binding model might be generalized to other 2D MOFs of interest.


*Portions of this work is supported by the DOE.

**10:36AM R38.00012: Tuning surface properties of 2D magnetic coordination polymers**

SAMUEL MAÑAS-VALERO (Presenter), JAVIER LÓPEZ-CABRELLES, GUILLERMO MÍNGUEZ-ESPALLARGAS, EUGENIO CORONADO, University of Valencia — Magnetism has been an elusive property in the 2D-land up to date. There are only few recent reports regarding inorganic monolayers of antiferromagnets (FePS₃) [1, 2] and highly unstable ferromagnets such as CrI₃ [2] or Fe₃GeTe₂ [3]. To overcome the present unstabilities of 2D magnetic materials, we take advantage of layered molecular magnets since, thanks to the chemical design, they are excellent candidates in order to bring new magnetic scenarios as well as to overcome the present unstabilities of 2D magnetic materials. Here [4] we present a pre-synthetic method based on the use of magnetic coordination polymers that affords the isolation of crystalline functionalized monolayers. This involves functionalization of the ligand prior to the formation of the 2D material. The concept is illustrated using layered coordination polymers formed by reacting various benzimidazole derivatives with ferrocene. This surface tuneability, together with the robust magnetic and mechanical properties of these 2D materials, make them exceptional candidates for studying the magnetism in the 2D limit, as well as for developing membranes for selective molecular sensing.

[1] 2D Mat. 3, 031009 (2016)
**8:00AM R39.00001: Investigation of Diverse Magnetic Materials via Acoustically Driven Ferromagnetic Resonance**
PIYUSH SHAH, DEREK BAS, VLADIMIR SAFONOV, Materials and Manufacturing Directorate, Air Force Research Laboratory, MAKSYM POPOV, Department of Physics, Oakland University, ALEXEI MATYUSHOV, Department of Electrical and Computer Engineering, Northeastern University, ANNE KITTMANN, VIKTOR SCHELL, ECKHARD QUANDT, Institute for Materials Science, Chair for Inorganic Functional Materials, Kiel University, D-24143 Kiel, Germany, NIAN XIANG SUN, Department of Electrical and Computer Engineering, Northeastern University, GOPALAN SRINIVASAN, Department of Physics, Oakland University, BRANDON HOWE, MICHAEL E MCONNEY, MICHAEL PAGE (Presenter), Materials and Manufacturing Directorate, Air Force Research Laboratory — Magnetoelastic coupling has been exploited to detect FMR using surface acoustic waves (SAWs), a technique known as ADFMR. GHz-frequency SAWs are produced and detected electrically using pairs of interdigital transducers (IDTs). A magnetic film is placed in the path of the SAWs, which can then interact with magnetic moments via magnetoelastic coupling. Absorption of the SAWs occurs at FMR, modulating the measured output. Landau-Lifshitz-Gilbert theory describes the interaction in terms of the external magnetic field with a characteristic four-lobe pattern, from which the magnetic anisotropy field, FMR resonance field, and magnetoelastic coupling coefficient can be inferred.

We study the effects of a variety of magnetic materials including Ni, FeCo, FeGaB, and FeCoSiB, to examine the dependence of ADFMR patterns on material parameters and geometries. We use a range of SAW frequencies from ~300 to 2000 MHz to explore spectral effects of the IDT design on transduction efficiency, and the frequency dependence of the resonance field. We also calculate the FMR linewidth and quality factor—figures of merit useful for determining the efficacy of future ADFMR devices.

*This material is based on work supported by the Air Force Office of Scientific Research under project number FA9550-15-R-COR198

**8:12AM R39.00002: Enhanced-Spectral-Range Brillouin Light Spectroscopy by sub-diffraction confinement of light**
RYAN FREEMAN (Presenter), ROBERT LEMASTERS, FENG WANG, Emory University, VLADISLAV DEMIDOV, SERGEJ DEMOKRITOV, University of Münster, HAYK HARUTYUNYAN, SERGEI URAZHDIN, Emory University — Microfocus Brillouin Light Spectroscopy (BLS) is a standard optical technique which allows for the direct observation of quasiparticles such as phonons or magnons in magnetic films. A major limitation of the technique is that due to the small wavevector of light, the technique is only sensitive to the dynamical modes near the center of the Brillouin zone, making a large part of the spectrum optically inaccessible. We show that by using a nanoscale optical mask on top of the magnetic film, the BLS signal from short-wavelength spin waves can be enhanced by an order of magnitude. The enhancement is consistent with the broadened distribution of wavevectors caused by the spatial confinement of light, analogous to the uncertainty principle. Additionally, by engineering the geometry of the optical mask, we selectively enhance the sensitivity to specific spin wave modes, allowing us to reconstruct the spin wave dispersion.

*Supported by NSF ECCS-1804198

**8:24AM R39.00003: Coupling of Nitrogen Vacancy Centers to Pinned Domain Walls in Magnetic Nanowires**
JEFFREY RABLE (Presenter), ERIC KAMP, BENJAMIN S PIAZZA, NITIN SAMARTH, Pennsylvania State University — Nanodiamonds containing nitrogen vacancy (NV) centers have emerged as a robust system for measuring magnetic structures on the nanoscale. In addition to their use in studying static magnetic structures, such as stationary domain walls[1], they have recently been used to probe dynamic phenomena, such as ferromagnetic resonance[2] and spin wave propagation[3]. Here, we investigate the coupling of NV centers to pinned domain wall oscillations in a notched ferromagnetic nanowire made of permalloy. To design a nanowire that oscillates at NV resonance frequencies, we used micromagnetic simulations to test various wire sizes and notch geometries. Next, we used a pick-and-place method to position the nanodiamonds at the domain wall pinning site using an atomic force microscope. We then performed measurements using microwaves and a homebuilt confocal microscope. These methods pave the way for future measurements of domain wall dynamics with NV centers and more advanced methods of NV qubit control.


*Supported by the University of Chicago
8:36AM R39.00004: NV Diamond Based Broadband Readout of FMR from Organic Magnetic V[TCNE]2 Thin Film*  
BRENDAN MCCULLIAN (Presenter), MICHAEL CHILCOTE, Department of Physics, Ohio State University, VIDYA P BHALLAMUDI, Department of Physics, Indian Institute of Technology Madras, CAROLA PURSER, EZEKIEL JOHNSTON-HALPERIN, P CHRIS HAMMEL, Department of Physics, Ohio State University — Low damping magnetic thin films will play a key role in realizing nanoscale spin based computational elements. Organic-based magnetic films have shown high-quality resonance properties which rival the best oxides, and can be deposited across a wide range of substrates. A local probe of magnetic resonance is desirable for nanoscale characterization since inductive based techniques typically require large samples and can be spatially insensitive. The Nitrogen-Vacancy (NV) defect in diamond can serve as a platform for local, broadband, optical readout of magnetic resonance from a proximal magnetic film. We report broadband optically detected ferromagnetic resonance (ODFMR) from a micron-thick layer of the high quality organic-based ferrimagnet Vanadium Tetracyanoethylene (V[TCNE]2) grown on a diamond substrate. The locally probed FMR exhibits linewidths on the order of 1 Gauss, indicating both the high quality of the VTCNE on the micron scale and of the ability of the NV as a sensor for low damping materials. This work demonstrates the utility of the NV center to measure FMR of low Ms and organic systems.

*This work was supported by the Army Research Office under grant W911NF-16-1-0547, with partial support from NSF EFMA-1741666 and DMR-1507775.

8:48AM R39.00005: THz Spectrum Analysis Using an Antiferromagnetic Tunnel Junction as a Signal Mixer  
STEVEN LOUIS (Presenter), Electrical and Computer Engineering, Oakland University, PETRO ARTEMCHUK, OLGA SULYMENKO, Radio Physics, Taras Shevchenko National University of Kyiv, VASYL S TYBERKEVYCH, Department of Physics, Oakland University, JIA LI, Electrical and Computer Engineering, Oakland University, OLEKSANDR PROKOPENKO, Radio Physics, Taras Shevchenko National University of Kyiv, ANDREI SLAVIN, Department of Physics, Oakland University — We propose a novel, all-electrical method of performing spectrum analysis between 0.1 THz to 1.0 THz (in the “THz gap”). The method features an antiferromagnetic (AFM) tunnel junction that consists of 4 thin layers (Pt, AFM, MgO, Pt) and functions as follows [1]. First, an in-plane dc bias current \( I(t) \) in the Pt layer creates perpendicular spin Hall current, which excites rotation of the AFM sublattices with a frequency \( f(t) \approx I(t) \). When the bias current \( I(t) \) increases with time, \( f(t) \) can be linearly swept over the THz gap. Due to the tunneling magnetoresistance effect, the resistance \( R(t) \) of the MgO/Pt structure oscillates with the same frequency \( f(t) \). Oscillating resistance \( R(t) \) is mixed with an input signal producing low-frequency output voltage \( V(t) \) that temporally encodes the input spectrum. The spectrum can be extracted from \( V(t) \) using signal processing method described in [2].


9:00AM R39.00006: Incoherent ferromagnetic spinwave spectroscopy using defect spins in diamond*  
CAROLA PURSER (Presenter), Department of Physics, Ohio State University, VIDYA P BHALLAMUDI, Department of Physics, Indian Institute of Technology Madras, DENIS PELEKHOV, Department of Physics, Ohio State University, QIAOCHU GUO, GREGORY FUCHS, School of Applied and Engineering Physics, Cornell University, P CHRIS HAMMEL, Department of Physics, Ohio State University — Optically detected spin transitions in nitrogen vacancy (NV) centers in diamond sensitively detect fluctuating fields at NV transition frequencies. Applied to ferromagnetic dynamics, this has enabled sensing of thermally occupied spinwaves as well as broadband, off-resonant spectroscopy of driven uniform-mode ferromagnetic resonance. We measure the relaxation rates of NV sensor spins to detect thermally excited spinwaves from a thin film of permalloy (Py). Analytical calculations and micromagnetic simulations demonstrate good agreement with measured NV relaxation rate as a function of NV-Py separation and applied field strength. Notably, NV sensors detect field noise from Py at a separation of up to 450 nm, thus demonstrating the suitability of NV probes in the GHz frequency range and submicron length scales of interest for communication and information devices.

*The Ohio State University: ARO (#W911NF-16-1-0547) and the Center for Emergent Materials, NSF MRSEC (#DMR-1420451). Cornell University: AFOSR (#FA9550-14-1-0243) and the Cornell Center for Materials Research (#DMR-1120296).
A single electron spin to study magnons in a magnetic insulator

TONY X. ZHOU (Presenter), Applied physics, Harvard University; JORIS CARMIGGELT, LISA GACHTER, AMIR YACOBY, Physics, Harvard University — A single electron spin as a quantum sensor is an ideal tool to study novel condensed matter physics. Recently, NV center in diamond has been used as a single electron spin sensor to explore topics of skyrmion\cite{ref1} and spin chemical potential in ferromagnetic insulator\cite{ref2}. In this work, we use a single NV center in scanning probe microscope\cite{ref3} to study magnons in yttrium iron garnet (YIG).

References:

Crossover of tip-sample magnetic couplings in an in-field spin-polarized scanning tunneling microscopy

SOOHYON PHARK (Presenter), Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), DIRK SANDER, Experiment 1, Max-Planck-Institute of Microstructure Physics — We report a crossover between long- and short-range magnetic couplings in an atomic scale magnetic tunnel junction (MTJ), measured from a tip-sample distance $d_{TS}$-resolved spin-polarized scanning tunneling microscopy of a Co nanoisland with Fe tips. We show that superparamagnetic response of tip magnetization \cite{ref1} quantitatively measures the sample-induced field at the tip position $\mu_0 H_S(d_{TS})$, which results in non-zero field offset $H_{off}$ in the field-dependent differential conductance hysteresis. The $H_{off}(d_{TS})$ with a varying $d_{TS}$ quantitatively characterizes a dipole filed of $\sim 60$ mT. On the other hand, a short range coupling, which is characterized as an antiferromagnetic tip-sample coupling, is observed at a small $d_{TS}$. This strongly increases for a decreasing $d_{TS}$ and competes with the dipole field, resultantly, leading to a crossover of the magnetic couplings from parallel to antiparallel. Our works demonstrate a novel method for quantitative measurement of magnetic couplings in an atomic scale MTJ under a simple and precise control of its tunnel barrier thickness.

References:

Spin polarized scanning tunneling microscopy with EuS coated W tip

HOYEON JEON (Presenter), MINJUN LEE, Seoul National University, YOUNG KUK, Center for Quantum Nanoscience, Institute of Basic Science, Ewha Womans University, Seoul, Korea — Various kinds of ferromagnetic or antiferromagnetic tips have been used to measure local magnetic properties of surfaces in spin polarized scanning tunneling microscopy technique. In this study, europium sulfide (EuS) coated tungsten tip is used because EuS coated tip is known to have a Sherman factor of 0.85 due to its exchange splitting \cite{ref1,ref2}. With this tip, we have imaged different magnetic domains on iron islands grown on W(110) surface. The differential conductance was mapped at liquid helium temperature because Curie temperature of EuS is 16K. We were able to manipulate the magnetization orientation of a ferromagnetic domain of Fe island by spin polarized tunneling current. We measured magnetic properties of single-layer FeSe film on SrTiO$_3$ to confirm a theory that predicted antiferromagnetic order on Fe layer in the film.

References:

Determination of $^{167}$Er:YSO Spin Hyperfine and Quadrupole Tensors using Josephson Bifurcation Amplifier

RANGGA BUDOYO (Presenter), KOSUKE KAKUYANAGI, HIRAKU TOIDA, YUICHIRO MATSUZAKI, WILLIAM JOHN MUNRO, SHIRO SAITO, NTT Basic Research Labs — Using an ESR spectrometer based on Josephson Bifurcation Amplifier, we performed spectroscopy of Erbium-doped Y$_2$SiO$_5$ crystal at various magnetic field orientations and strengths. By fitting the resulting spectra, we extracted the ground state hyperfine and quadrupole tensor values for $^{167}$Er:YSO. We discuss these tensor values, and compare them with values obtained using other methods, including conventional ESR spectroscopy, tunable resonators, and optical methods.
10:00AM R39.00011: Neutron Depolarization Microscope for Imaging of Ferromagnetic Phase Transitions: Ni$_3$Al and HgCr$_2$Se$_4$ under pressure* BORIS KHAYKOVICH (Presenter), Massachusetts Institute of Technology, PAU JORBA, MICHAEL SCHULZ, Technische Universitat Munchen, DANIEL HUSSEY, National Institute of Standards and Technology, MUHAMMAD ABIR, Massachusetts Institute of Technology, MARC SEIFERT, Technische Universitat Munchen, VLADIMIR TSURKAN, ALOIS LOIDL, University of Augsburg, CHRISTIAN PFLEIDERER, Technische Universitat Munchen — We performed spatially resolved neutron depolarization imaging of a large Ni$_3$Al crystal, and a small HgCr$_2$Se$_4$ spinel under pressure, to probe bulk magnetic inhomogeneities in the ferromagnetic phase and the transition temperature with the spatial resolution of 100 μm. To obtain such resolution, we employed a new technique, a neutron microscope based on image-forming Wolter optics and a focusing guide. The depolarization images of Ni$_3$Al show that the sample doesn’t homogeneously go through the ferromagnetic transition; the improved resolution allows us to identify previously unidentified high-TC regions. The results on HgCr$_2$Se$_4$ highlight the advantage of this technique especially for complex sample environments such as pressure cells. The improved resolution allows to image domain formation in the sample while decreasing the acquisition time. The novel optical design that enabled acquisition of the high spatial resolution neutron depolarization images is described in detail and image results are compared to a conventional radiography setup without a lens.

*The work at MIT was supported by the award 60NANB15D361 from U.S. Department of Commerce, National Institute of Standards and Technology. Work partly supported by the DFG via the Transregional Collaborative Research Center TRR 80.

10:12AM R39.00012: Imaging Nanoscale Magnetism and its Dynamics at CSX Beamline* WEN HU (Presenter), FELIX BUETTNER, CLAUDIO MAZZOLI, ANDI BARBOUR, STUART B WILKINS, Brookhaven National Laboratory — Imaging magnetic materials and structures as a function of external parameters, including magnetic and electric fields, and temperature will provide detailed insight into their dynamics and behavior. Coherent soft x-ray scattering (CSX) beamline at NSLS-II provide researchers a world leading coherent high photon flux with full polarization control. Coherent diffraction imaging, such as resonant soft x-ray ptychography and holography, are under commissioning at CSX and welcome new users. Very recently, we monitored thermal motions of magnetic domain wall with high magnetic contrast and 10nm spatial resolution using holography imaging. Moreover, a new holography chamber has been developed and installed at CSX beamline and it provided holography imaging capability to study magnetic materials as a function of temperature under in-situ condition (current injection and in-vacuum magnetic field).

Here, we highlight current achievements and discusses the future potential of magnetic soft X-ray imaging with a spatial resolution of sub-10nm at CSX beamline.

*This work was done at CSX beamline of NSLS II, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Brookhaven National Laboratory under Contract No. DE-SC0012704.

10:24AM R39.00013: Extracting equivalent circuit model of magnetoelectric gyrator using vector network analyzer CHENG TU (Presenter), XIANFENG LIANG, CUNZHENG DONG, HUAIHAO CHEN, ZHAOQIANG CHU, NIAN XIANG SUN, Northeastern University — The magnetoelectric (ME) effect is a polarization change induced by an applied magnetic field, or conversely a magnetization change induced by an applied electric field. The giant ME effect found in coil-wrapped magnetostrictive/piezoelectric laminated composites can be utilized to realize gyrators. Until now, there is little reported work regarding how to extract the equivalent circuit model of such ME gyrator from measurement. In this work, we report an effective method to accurately extract the equivalent circuit model from the measured impedance parameters using a vector network analyzer (VNA). The two-port ME gyrator under investigation consists of a plate type piezoelectric/magnetostrictive laminate, in which the piezoelectric layer (PZT) is sandwiched between two magnetostrictive layers (metglass). A 30-turn coil is wrapped around the laminate serving as port 1. The metal electrodes on the surfaces of PZT layer are used as port 2. All the model parameters of the gyrator were extracted from the measured impedance parameters using a VNA. Good agreement between the model and measured results proves that the proposed extraction method is valid and accurate.
Capturing Nucleation at 4D Atomic Resolution* YONGSOO YANG (Presenter), JIHAN ZHOU, YAO YANG, DENNIS S KIM, ANDREW YUAN, XUEZENG TIAN, Physics and Astronomy, University of California, Los Angeles, COLIN OPHUS, Molecular Foundry, Lawrence Berkeley National Laboratory, FAN SUN, Physics, University at Buffalo, ANDREAS SCHMID, Molecular Foundry, Lawrence Berkeley National Laboratory, MICHAEL NATHANSON, HENDRIK HEINZ, Chemical and Biological Engineering, University of Colorado, Boulder, QI AN, Chemical and Materials Engineering, University of Nevada, Reno, HAO ZENG, Physics, University at Buffalo, PETER ERCIUS, Molecular Foundry, Lawrence Berkeley National Laboratory, JIANWEI MIAO, Physics and Astronomy, University of California, Los Angeles — Nucleation is a ubiquitous phenomenon in many physical and biological processes. However, it is a challenging process to study nucleation due to the lack of experimental tools to directly measure the 3D atomic structure of nuclei. Here, we further advance atomic electron tomography to study the early stage nucleation of FePt nanoparticle system at 4D atomic resolution [1]. We reveal that early stage nuclei are irregularly shaped, each has a core of a maximum order parameter, and an order parameter gradient points from the core to the boundary of the nucleus. We also capture the 3D atomic structure and dynamics of the same nuclei undergoing growth, fluctuation, dissolution, merging and/or division. We find that nucleation dynamics is regulated by the distribution of the order parameter and its gradient. These experimental results differ from classical nucleation theory (CNT), and we propose an order parameter gradient nucleation model which is thermodynamically more favorable than CNT. We further corroborate this model using molecular dynamics simulations of the liquid-solid phase transition of Pt.


*STROBE: NSF STC (DMR-1548924), US DOE (DE-SC0010378), the NSF DMREF (DMR-1437263), and the Molecular Foundry (US DOE DE-AC02-05CH11231)

Cryogenic Amplification of Magnetoresistance in Magnetic Tunnel Junctions with the Aid of SiGe-HBT* JASON DARK (Presenter), HANBIN YING, GRANT H NUNN, JOHN CRESSLER, DRAGOMIR DAVIDOVIC, Georgia Institute of Technology — Cryogenic amplification has been used for qubit readout, single electron transistor operation, and charge sensing with quantum point contacts; however, this useful tool has been missing from electron transport measurements in the broad field of magnetism. Silicon-Germanium Heterojunction Bipolar Transistors were used for cryogenic preamplification of nanoscale magnetic tunnel junctions at 8 K. The preamplification system increased the signal-to-noise ratio of the tunneling magnetoresistance signal by a factor of 6.62. The current gain provided by the preamplification also allowed for a higher bandwidth measurement limited by the external transimpedance amplifier, rather than cryogenic wiring. The high impedance (≈1 MΩ) of the junctions allow for easy migration to study the magnetodynamics of more interesting samples.

*This research was supported in part (J. Dark, G. Nunn, and D. Davidovic) by DOE contract DE-FG0206ER46281, and (H. Ying and J. D. Cressler) by the Laboratory Directed Research and Development (LDRD) Program at Sandia National Laboratories (operated by NTES of Sandia, a wholly owned subsidiary of Honeywell International Inc., for DOE's NNSA under contract DE-NA-0003525).

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R40 GMAG DMP DCOMP: Complex Oxide Films and Heterostructures III BCEC 208 -

Zhigang Chen, San Francisco State Univ - Tag(s): Focus
8:00AM R40.00001: Phase transitions and magnetic domain coexistence in Nd$_{0.5}$Sr$_{0.5}$MnO$_3$ thin films  I-TING CHIU
(Presenter), Chemical Engineering, University of California, Davis, APURVA MEHTA, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, ALEXANDER MICHAEL KANE, Materials Science and Engineering, University of California, Davis, RAJESH V CHOPDEKAR, Advanced Light Source, Lawrence Berkeley National Laboratory, CHRISTOPHER ROULEAU, The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, ALPHA N’DIAYE, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, YAYOI TAKAMURA, Materials Science and Engineering, University of California, Davis — We present a study of the physical properties of perovskite oxide Nd$_{0.5}$Sr$_{0.5}$MnO$_3$ (NSMO) thin films grown on (110)-oriented SrTiO$_3$ substrates. In bulk form, NSMO displays magnetic and electronic transitions from paramagnetic/insulator to ferromagnetic (FM)/metal and then to antiferromagnetic (AFM)/charge-ordered insulating phase with decreasing temperature. In thin films, AFM ordering only occurs in an anisotropic strain state such as those obtained in (110)-oriented substrates which allows for Jahn-Teller distortions of the MnO$_6$ octahedral and MnO$_6$ bond length distortions [1]. In this work, resonant x-ray reflectivity and magnetometry measurements showed that the NSMO film breaks up into three layers with different density and magnetic properties. X-ray magnetic circular dichroism confirmed the FM-AFM transition occurs between 80 K and 160 K for the main portion of the NSMO film, while x-ray magnetic linear dichroism provided a clear signature of the AFM phase at 80 K. At an intermediate temperature of 110 K, photoemission electron microscopy demonstrated the coexistence of FM and AFM domains. These temperature-dependent transitions have strong potential applications in next generation memory devices.


8:12AM R40.00002: Growth and Physical properties of full chemically ordered manganites  LINA DENG (Presenter), Department of Physics, Fudan University — Chemical doping is a widely used method to control materials’ physical properties. The dopants are usually randomly distributed. This unavoidably introduces disordering into the materials, which may affect the physical properties of the materials. This is especially true for electronic phase separation (EPS) phenomena in manganites, which is known to have a close correlation with disordering. In this work, we use superlattice growth to form chemically ordered manganites, and compare with conventional manganites whose chemical dopants are randomly distributed. Specifically, one unit cell LaMnO$_3$ / one unit cell PrMnO$_3$ / one unite cell CaMnO$_3$ tricolor superlattices have been grown on NGO (110) and STO (100) substrates by laser molecular beam epitaxy, forming chemically ordered La$_{1/3}$Pr$_{1/3}$Ca$_{1/3}$MnO$_3$ (O-LPCMO) thin films. In stark contrast to the conventional La$_{1/3}$Pr$_{1/3}$Ca$_{1/3}$MnO$_3$ (R-LPCMO) thin films which are characterized by large scale EPS, the O-LPCMO films show no signs of EPS. This indicates that dopants induced disordering plays a critical role in large scale EPS in manganites. Our experimental results show that the O-LPCMO system is in a charge-ordered insulating state which is consistent with the first principle calculations.

8:24AM R40.00003: The role of extreme configurational disorder in entropy stabilized single crystal perovskite oxides*  THOMAS WARD (Presenter), YOGESH SHARMA, Oak Ridge National Laboratory, ALESSANDRO MAZZA, University of Missouri — The ABO$_3$ perovskite and its derivatives are broadly important to a range of fundamental and applied interests. Modification of the A and B sites through substitutional doping allows for a wide variety of distortions and charge states to be tuned. Local distortions arising from cation size variance are balanced by internal changes to Jahn-Teller distortions and octahedral tilts and rotations. In strongly correlated systems, these shifts to local environment are often central to the emergence of important macroscopic functionalities. In this talk, we will describe our recent work using entropy stabilization to synthesize single crystal ABO$_3$ perovskite films possessing 6 or more cations to begin to explore how extreme levels of microscopic disorder might be used to generate unexpected long-range ordering responses. We will discuss how the element specific magnetic and charge states of the cations in La(Cr$_{0.2}$Mn$_{0.2}$Fe$_{0.2}$Co$_{0.2}$Ni$_{0.2}$)O$_3$ films are impacted by the extreme site to site disorder. Experimental results from STEM-EELs, XRD, XMCD, neutron diffraction, and SQUID magnetometry will be presented.

*This work was supported by the DOE Office of Science, Early Career Research Program and Basic Energy Sciences, Materials Sciences and Engineering Division.
8:36AM R40.00004: Charge order and phase separation nature of the insulating La$_{0.67}$Ca$_{0.33}$MnO$_3$ thin film on NdGaO$_3$ substrate*  
MINGQIANG GU (Presenter), JAMES M RONDINELLI, Department of Materials Science and Engineering, Northwestern Univ — Doped manganite systems have been intensively studied due to their rich phase diagrams at different temperature, strain, pressure, and composition conditions. La$_{0.67}$Ca$_{0.33}$MnO$_3$ thin film grown on NdGaO$_3$ substrate has found to exhibit abnormal antiferromagnetic (AFM) insulating ground state, which violates the bulk phase diagram. The puzzle that why the ground state of this $g^{3.67}$ system becomes insulating is studied with density functional theory (DFT) calculation. Several potential scheme has been examined, including substrate strain, pinning of Jahn-Teller distortion, and charge order (CO), within different magnetic configurations. We find that without charge order, neither substrate strain nor increased Jahn-Teller distortion are sufficient to induce the insulating state. With Mn$^{4+}$/Mn$^{3+}$ valence states ordered in a stripe type pattern along the $b$ lattice vector, the AFM insulating state can be observed. However, an unrealistic large uniaxial strain is required to assist this phase to beat the ferromagnetic (FM) phase. Further study suggests mixture of the CO [Mn$^{4+}$]$_{0.5}$/[Mn$^{3+}$]$_{0.5}$ and pure LaMnO$_3$ micro regions in the sample.

*M.G. and J.M.R. acknowledge financial support from the U.S. Department of Energy (DOE) under Grant No.DE-SC0012375.

8:48AM R40.00005: Studying Influence of Normal Metal on Magnetic Properties of Y$_3$Fe$_5$O$_{12}$ Thin Film Locally Using Scanning Ferromagnetic Resonance Force Microscopy  
GUANZHONG WU (Presenter), SHANE WHITE, WILLIAM RUANE, JACK T BRANGHAM, YANG CHENG, FENGYUAN YANG, P CHRIS HAMMEL, Department of Physics, The Ohio State University — We image the boundary separating regions of altered internal magnetic fields in Y$_3$Fe$_5$O$_{12}$(YIG) thin films arising from patterning metal films on the YIG film surface. High quality YIG thin films have proven to be useful for spintronics research. However, detailed investigations of internal magnetic variations in patterned devices are still lacking. Spatial maps of the internal fields were acquired using ferromagnetic resonance force microscopy(FMRFM); a technique allowing for nano to micro-scale spatial resolution and high sensitivity to magnetic fields within the film. FMRFM scans laterally across the YIG-YIG/M (M = Au, Pt) boundary indicate an internal field step that is tens of Gauss. Micromagnetic simulations assuming the presence of uniaxial anisotropy in both the bare YIG and the YIG/M bilayer qualitatively match experimental measurements. We discuss possible physical causes of this field shift, methods used to image the spatial magnetization profile, and implications for future spintronic devices.

9:00AM R40.00006: Effects of the apical-oxygen vacancy and magnetism on the ultra-thin LaNiO$_3$ layer studied using DFT+DMFT  
XINGYU LIAO (Presenter), HYOWON PARK, University of Illinois at Chicago — While the bulk LaNiO$_3$ remains metallic at all temperatures, the ultrathin films of LaNiO$_3$ shows a metal-insulator transition as the layer thickness reduces to 2 unit cells. Recent experiment shows that the NiO$_2$ surface layer without top LaO layer can have higher resistivity than the same NiO$_2$ layer with apical oxygens. In this talk, I will present the density functional theory plus dynamical mean field theory (DFT+DMFT) calculations for the one-layer LaNiO$_3$ slab including the LaAlO$_3$ substrate and the vacuum. The slab geometry with the capping LaO layer is metallic even with DFT+DMFT although Ni eg orbitals are renormalized compared to DFT bands. We also move the top LaO layer away from the surface layer to simulate the effect of apical oxygens on the electronic structure. As the apical oxygen moves away from the Ni ion, an effective charge transfer occurs toward the dz$^2$ orbital and the Wannier orbital level is shifted below the dx$^2$-y$^2$ orbital. Moreover, the DMFT self energy makes the dz$^2$ orbital more incoherent and it eventually becomes Mott insulating in the absence of apical oxygens. We also simulate the antiferromagnetic calculations with the up-up-down-down spin structure as measured in experiment. The results will be also compared with the above paramagnetic calculations.
Synthesis and Characterization of Ru-doped BaSnO$_3$ Thin Films and Heterostructures*  
EMILY LINDGREN (Presenter), URUSA S ALAAN, Materials Science & Engineering, Stanford University, YURI SUZUKI, Department of Applied Physics, Stanford University — Epitaxial doped stannate thin films have been identified recently as high mobility oxide semiconductors that could form the foundation of an all-oxide electronics. Adding magnetic functionality to this class of materials may provide for a spin-based electronics. Toward this end, we have grown epitaxial thin films of Ru doped BaSnO$_3$(BSO) and multilayers of alternating La doped and Ru doped BaSnO$_3$ on (001) SrTiO$_3$ substrates using pulsed laser deposition. X-ray photoelectron spectroscopy was used to verify successful incorporation of both La and Ru into the BSO lattice. X-ray diffraction measurements confirm epitaxial growth of the single layer and multi-layered films. Both single layer and multi-layered films are under epitaxial tensile strain according to X-ray diffraction. Omega rocking curves of both types of samples show excellent crystallinity with typical FWHM values of 0.096° and 0.073°. Both types of films exhibit a paramagnetic response which saturates at approximately 1μ$_B$/Ru$^{4+}$, thus indicating paramagnetism but no ferromagnetic order. Single layer Ru doped BSO films exhibit insulating behavior while layered films have a typical mobility value of 37 cm$^2$/Vs, carrier concentration of $110^{19}$ cm$^{-3}$ and resistivity of 0.4 mΩcm at 300K.

*National Science Foundation grant #1762971.

Structural, Electrical and Magnetic Properties of Solid Solution Films between SrRuO$_3$ and BaSnO$_3$  
PINGCHUN WU (Presenter), YING-HAO CHU, National Chiao Tung University — A series of SrRuO$_3$/BaSnO$_3$ solid solutions have been fabricated via laser molecular beam epitaxy. With the help of high-energy electron beam reflection, the ratio of SRO/BSO is precisely controlled in the scale of monolayer. The epitaxial relation was analyzed by x-ray diffraction and transmission electron microscopy. The lattice constants of c-axis varied with the change of the ratio between SRO and BSO, which is consistent with the results calculated by Vegard's law. After successfully fabricate a series of SRO/BSO, temperature-dependent resistances measurement has been carried out. It was found that electrical behavior of SRO/BSO was varied from pure metallic to insulating while the ratio of BSO increased in the solid solutions. A metal-insulating transition can also be found in specific ratio. Further, the increase of BSO will result in an enlarged magnetoresistance in the solid solutions. In the magnetic hysteresis loops, the decrease in saturated magnetic moment, coercivity and the change in anisotropy can also be found. This experiment realizes an accurately control of solid solutions in the scale of monolayer. The structural, electrical and magnetic properties of SRO/BSOs have been systematically analyzed and the origin of these differences has also been discussed.

Magnetic Field Control of the Fermi Surface Topology in EuTiO$_3$  
KAVEH AHADI (Presenter), University of California, Santa Barbara, XUEZENG LU, Northwestern university, SALVA SALMANI-REZAIE, PATRICK MARSHALL, University of California, Santa Barbara, JAMES M RONDINELLI, Northwestern university, SUSANNE STEMMER, University of California, Santa Barbara — Spin-orbit coupling plays a central role in the anomalous Hall effect (AHE) of itinerant ferromagnets and in materials with topologically non-trivial electronic states. Recently, AHE attracted significant attention in antiferromagnetic metals and semiconductors. For example, significant AHEs in non-collinear antiferromagnets have been discovered. The degenerately doped antiferromagnetic semiconductor EuTiO$_3$ is a unique testbed for these ideas for several reasons. Despite a small net magnetization, it exhibits an intrinsic AHE that changes sign as a function of the carrier density. We report on the symmetry of the anisotropic magnetoresistance (AMR) in doped EuTiO$_3$ films as a function of the applied magnetic field. Multiple transitions in the AMR symmetry are observed and are attributed to magnetic field induced changes in the band topology. At high fields a transition from positive to negative magnetoresistance coincides with change from four-fold to two-fold symmetry in the AMR. This indicates a non-trivial phase transition in the electronic structure. We discuss the results in the context of Weyl points that form in the band structure of the EuTiO$_3$. 

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9:48AM R40.00010: Electronic wave function spatial extension of the oxygen vacancies on EuO$_{1-x}$ surface.*

TE-YU CHIEN (Presenter), AARON WANG, University of Wyoming, GAURAB RIMAL, Rutgers University, ROBERT NIELSEN, YURI DAHNOVSKY, JINKE TANG, University of Wyoming — EuO$_{1-x}$ thin films deposited by pulsed laser deposition on Si(100) were studied by scanning tunneling microscopy and spectroscopy at room temperature. Oxygen vacancies in EuO$_{1-x}$ are visualized through dI/dV mapping and the apparent sizes of the oxygen vacancies are found to be 1.8 nm ± 0.5 nm. These apparent sizes are considered as the spatial extension of the electron wave function originated from the oxygen vacancies. It is further argued that this observed electronic wave function might be the precursor of the bound magnetic polaron formation occurred at lower temperature. Moreover, some of the oxygen vacancies were found (1) hopping to adjacent site; (2) emerging (vacancy creation); and (3) disappearing (vacancy annihilation), indicating that the oxygen vacancies on the EuO$_{1-x}$ surface at room temperature are not extremely stable.

*This work is financially supported by the U.S. National Science Foundation, Division of Materials Research (DMR) (Grants No. DMR-1710512).

10:00AM R40.00011: Magnetic phase transitions in thin films of the near-itinerant spinel CoV$_2$O$_4$*  

CHRISTIE J THOMPSON, Materials Science and Engineering Program and National High Magnetic Field Laboratory, Florida State University, CHRISTIANNE BEEEKMAN (Presenter), Physics and National High Magnetic Field Laboratory, Florida State University — Spinel vanadates are frustrated antiferromagnets, of interest due to the orbital physics that can be tuned via structural perturbations. The V-V distance determines proximity of the system to a localized-itinerant crossover, with CoV$_2$O$_4$ the closest known material to this transition. Previously, we have shown that CoV$_2$O$_4$ films are orthorhombic rather than cubic. The films undergo a spin canting/orbital order transition at low temperature, i.e., they show very different magnetic properties compared to bulk [1]. Based on recent magnetization measurements as a function of temperature we find signatures of three distinct magnetic transitions in the films. We investigate temperature, field, and film thickness dependence of these transitions, and we discuss the roles that single-ion anisotropy and shape anisotropy play.


* A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490, No. DMR-1644779, and the State of Florida.

10:12AM R40.00012: Room-temperature ferromagnetic insulating state in highly cation-ordered Sr$_2$Fe$_{1+x}$Re$_{1-x}$O$_6$ films*  

CHANG HEE SOHN (Presenter), ELIZABETH SKOROPATA, Materials Science and Technology Division, Oak Ridge National Laboratory, YONGSEONG CHOI, Advanced Photon Source, Argonne National Laboratory, XIANG GAO, ANKUR RASTOGI, Materials Science and Technology Division, Oak Ridge National Laboratory, AMANDA HUON, Department of Materials Science & Engineering, Drexel University, MICHAEL A MCGUIRE, Materials Science and Technology Division, Oak Ridge National Laboratory, LAUREN NUCKOLS, Department of Materials Science and Engineering, University of Tennessee, YANWEN ZHANG, Materials Science and Technology Division, Oak Ridge National Laboratory, JOHN WILLIAM FREELAND, DANIEL HASKEL, Advanced Photon Source, Argonne National Laboratory, HO NYUNG LEE, Materials Science and Technology Division, Oak Ridge National Laboratory — Ferromagnetic insulators with high Curie temperatures are critical components for developing quantum electronic/spintronic devices. However, since ferromagnetism generally accompanies metallicty, ferromagnetic insulators have been very limited in nature. Here, we report a highly insulating ferromagnetic state found in 3d-5d double perovskite Sr$_2$Fe$_{1+x}$Re$_{1-x}$O$_6$ (-0.2<x<0.2) epitaxial films by modifying the Fe/Re ratio. Beyond the original ferromagnetic metallic ground state in a stoichiometric film, Fe-rich films showed demanding ferromagnetic insulating states with three orders of higher room-temperature resistance than that of the metallic film, a high Curie temperature about 400 K, and a large saturated magnetization about 1.8 uB/f.u. In this presentation, we discuss about the growth, related physical properties, and the origin of the emerging ferromagnetic insulating state based on x-ray and optical spectroscopy.

* This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
10:24AM R40.00013: Observation of Compensation Temperature in Epitaxial Tm$_3$Fe$_5$O$_{12}$ Thin Films by Polar Magneto-Optic Kerr Effect  

YANJUN MA (Presenter), CHENG CEN, West Virginia University — Since ferrimagnetic rare-earth iron garnets (RIG) R$_3$Fe$_5$O$_{12}$ are excellent insulators with Curie temperatures well above room temperature, such materials have been extensively exploited in spintronics, leading to novel discoveries such as anomalous Hall effect in the heterostructure formed by topological insulator and Tm$_3$Fe$_5$O$_{12}$ (TmIG). While the recent research on TmIG thin films has been focusing on the behavior of their perpendicular magnetic anisotropy (PMA) in high temperature region, the magnetic properties of TmIG thin films at lower temperatures are elusive. In this report, we measured the low temperature magnetic properties of epitaxial TmIG films by polar magneto-optic Kerr effect. The divergence of the out-of-plane coercive filed and the reverse of the sign of out-of-plane magnetization were observed consecutively, indicating the existence of compensation temperature in TmIG. Further investigation showed that the temperature making divergent was dependent on the thickness and strain state of the film. Since the compensation temperature in bulk TmIG has never been established, our findings demonstrate that it is worth investigating low temperature magnetism in low dimensional rare-earth iron garnets to advance the research of RIG-based spintronics.

10:36AM R40.00014: Exotic Ferroelectric and Multiferroic Properties in Epitaxial YFeO$_3$ Thin Films and YFeO$_3$-CoFe$_2$O$_4$ Nanocomposites  

SHUAI NING (Presenter), CAROLINE ANNE ROSS, MIT — Multiferroics have been attracting considerable interest in the past decades, and researchers never stop searching for materials exhibiting multiferroic behavior. For orthoferrites, there should be no ferroelectricity in theory due to their centrosymmetric structure. However, when epitaxially grown, the strain can significantly modify the symmetry and physical properties. Here, we present the exotic ferroelectric properties of epitaxial YFeO$_3$ (YFO) thin films on perovskite substrates prepared by pulsed laser deposition (PLD). A nearly single-domain structure is observed in as-grown 40 nm-thick YFO thin films characterized by Piezoresponse force microscopy (PFM), and it can be fully switched suggested by the ideal ferroelectric hysteresis loop and by domain patterns written by a bias of +/- 8 V. The spontaneous polarization direction is highly dependent on the epitaxial strain, which could be tuned either out-of-plane or in-plane. Via co-deposition by PLD, the nanocomposites consisting of YFO and CoFe$_2$O$_4$ (CFO) have been prepared, in which phase separation is successfully achieved. Both ferroelectricity and ferromagnetism are observed originating from YFO and CFO respectively, indicating a promising magnetoelectric coupling in this 2-phase multiferroic nanocomposite.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R41 GMAG DMP: Spin Dynamics II  

8:00AM R41.00001: Nanometer-Thick YIG-Based Magnonic Crystals with Large Tunable Bandgaps  

HUAJUN QIN, GERT-JAN BOTH, SAMPO J. HÄMÄLÄINEN, SEBASTIAAN VAN DIJKEN (Presenter), Department of Applied Physics, Aalto University, Finland — Control of information-carrying spin waves in magnonic crystals is essential for the development of magnon-based computing. Crystals comprised of a periodic array of ferromagnetic metals offer versatility in band structure design, but strong magnetic damping restricts their transmission efficiency. Yttrium iron garnet (YIG) with ultralow damping is the palpable alternative, yet its small magnetization limits dynamic dipolar coupling between discrete units in the technological imperative Damon-Eshbach (DE) geometry. Here, we experimentally demonstrate low-loss spin-wave manipulation in one-dimensional magnonic crystals of physically separated nanometer-thick YIG stripes. We enhance the transmission of DE spin waves in allowed minibands by filling the gaps between the stripes with CoFeB. The thus-formed magnonic crystals exhibit tunable bandgaps of 50 MHz - 200 MHz with nearly complete suppression of the spin-wave signal. We also show that efficient Bragg scattering on just two airgaps or two CoFeB stripes already produces clear frequency gaps in spin-wave transmission spectra.
**8:12AM R41.00002: Ferromagnetic resonance and proximity effect in WTe$_2$/magnetic insulator heterostructure**

PENG LI (Presenter), Department of Applied Physics, Stanford University, EDBERT JARVIS SIE, Department of Materials Science and Engineering, Stanford University, JACOB WISER, LAUREN RIDDIFORD, AARON ALTMAN, Department of Applied Physics, Stanford University, AARON LINDENBERG, Department of Materials Science and Engineering, Stanford University, YURI SUZUKI, Department of Applied Physics, Stanford University — Integration of FMI films with 2D materials or topological insulators has proven to be promising for the demonstration of spin-orbit torque switching and more efficient spintronic devices. As an alternative to YIG, we have identified spinel ferrite MgAl$_{0.5}$Fe$_{1.5}$O$_4$ (MAFO) for the spin source material. The Gilbert damping constant of MAFO is 0.001, similar in magnitude to typical YIG. In this work, we have realized bilayer structures of exfoliated nanometer thick WTe$_2$ flakes on top of low damping MAFO thin films. The samples were post-annealed at 300 $^\circ$C for 5 h at a vacuum pressure, giving rise to strong exchange coupling between the 2D and the MAFO layers. Raman spectroscopy showed that WTe$_2$ maintained the desired phase after processing. Together with atomic force microscopy, the thickness of WTe$_2$ was estimated to be several atomic layers. Magnetoresistance measurements revealed a hysteresis loop that was correlated with the magnetization curves of MAFO. These results suggest proximity-induced ferromagnetism in the WTe$_2$ atoms at the interface. We characterized our samples with spin-torque ferromagnetic resonance. This new WTe$_2$/magnetic insulator system is promising for future spinel ferrite insulator based spin current devices.

**8:24AM R41.00003: The Effect of Defects on Precessional Dynamics in a Magnetic Field and Resulting Spin Wave Modes in Elliptical Nanomagnets with In-Plane Anisotropy**

MD AHSANUL ABEED, Electrical and Computer Engineering, Virginia Commonwealth University, SOURAV SAHOO, Condensed Matter Physics and Materials Science, S. N. Bose National Center for Basic Sciences, DAVID WINTERS, Electrical and Computer Engineering, Virginia Commonwealth University, ANJAN BARMAN, Condensed Matter Physics and Materials Science, S. N. Bose National Center for Basic Sciences, SUPRIYO BANDYOPADHYAY (Presenter), Electrical and Computer Engineering, Virginia Commonwealth University — We have simulated the precessional dynamics of magnetization in elliptical nanomagnets biased with an in-plane magnetic field along the minor axis and perturbed by a small out-of-plane magnetic field. The precessional dynamics gives rise to spin wave modes in the nanomagnets. We first calculate the time-dependent out-of-plane component of the magnetization at a fixed plane of the magnet at various coordinate points and also the spatially averaged magnetization as a function of time. We then find the Fourier transform of the spatially averaged component to find the dominant precessional frequencies (which do not necessarily correspond to the Kittel frequencies) and calculate the power and phase profiles of the spin wave modes at those frequencies. We find that the spin wave modes are significantly affected by the presence of defects in the nanomagnets. We have studied six different types of defects arising from material voids and thickness variations which are realistic defects that arise during fabrication processes. Our results show that the spin wave modes are significantly affected by defects. This has a serious implications for devices that rely on spin wave modes such as oscillators and neuromorphic computers based on phase locked oscillators.

*NSF ECCS 1609303, CCF 1815033.

**8:36AM R41.00004: Spin-current-mediated rapid magnon localization and coalescence after ultrafast optical pumping of ferrimagnetic alloys**

EZIO IACOCCA (Presenter), University of Colorado, Boulder, ALEX REID, SLAC National Accelerator Laboratory, ALEXEY KIMEL, THEO RASING, Radboud University, ROY CHANTRELL, University of York, MARK A HOEFER, University of Colorado, Boulder, THOMAS SILVA, NIST, HERMANN DÜRR, Uppsala University — We find evidence of rapid magnetic order recovery via nonlinear magnon processes after ultrafast demagnetization of amorphous GdFeCo thin films with perpendicular magnetic anisotropy. The spatial evolution of the magnetization is measured by time-resolved resonant X-ray scattering and modelled by atomistic and multiscale micromagnetic simulations. We identify both localization and coalescence processes. During localization a paramagnetic state evolves into a collection of localized textures while coalescence describes their growth, break-up, and merging. The characteristic length scale during coalescence is found to grow according to a power law in both experiments and simulations. Our results shed light into the physical mechanisms that are important for the picosecond recovery of magnetic order.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number 0000231415 and is partly supported by the European Research Council ERC Grant agreement No. 339813 (Exchange) and the Netherlands Organisation for Scientific Research (NWO). Operation of LCLS is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under contract No. DE-AC02-76SF00515.
Magnon-mediated Neel torques and magnonic responses to Neel order dynamics

Using the Neel ground state, we formulate a microscopic linear response theory of magnon-mediated Neel torques generated by the thermal gradient in collinear antiferromagnets. We also describe the inverse effects in which spin and heat currents are induced by the Neel order dynamics. We obtain the extrinsic and intrinsic contributions where the intrinsic contributions are related to the mixed space Berry curvature. We derive a closed equation of motion of Neel dynamics in antiferromagnets related to thermal Neel torque from linearized LLG equation. We confirm that the Neel torque effect is related to the inverse effect by the Onsager relations. We apply our theory to honeycomb antiferromagnet and confirm that a net magnon-mediated heat current can be induced by the Neel order precession.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. de-sc0014189.

General method for atomistic spin-lattice dynamics with first principles accuracy

A computationally efficient general first-principles based method is presented, with applications for spin-lattice simulations for solids and clusters. The method is based on a combination of atomistic spin dynamics and molecular dynamics, expressed through a spin-lattice Hamiltonian where the bilinear magnetic term is expanded to second order in displacement. The effect of first-order spin-lattice coupling on the magnon and phonon dispersion in bcc Fe is reported as an example, and is seen to be in good agreement with previous simulations performed with an empirical potential approach. In addition, we also illustrate the abilities of our method on a more conceptual level, by exploring dissipation free spin and lattice motion in small magnetic clusters.

Magnetic Vortex as a Spin Wave Filter

In the Landau state, the Néel wall is divided into two regions of opposite magnetization, separated by a vortex. In this work, we show, through micromagnetic simulations, that excitations performed at one region are mostly reflected by the vortex, but they can be transmitted at specific frequencies.

The frequency of the maximum transmitted wave (FTW) can be tuned by changing the uniaxial or shape anisotropy of the system. Considering a (4x1) μm² permalloy rectangle, the FTW has a quadratic behavior with the uniaxial anisotropy energy of the system, passing through a minimum of 500 MHz at 100 kJ/m³. By fixing the aspect ratio of the rectangle, if the area is increased, the FTW decreases exponentially. E.g., for a fixed 4 μm length, the FTW can be tuned between 800 MHz and 2 GHz by varying the width. Therefore, the vortex acts a tunable frequency filter for the channeled spin-waves.

1 - Garcia-Sanchez, et al. (2015) Narrow Magnonic Waveguides Based on Domain Walls

ABSTRACT WITHDRAWN
9:36AM R41.00009: Dynamical amplification of magnetoresistances and Hall currents up to the THz regime* FILIPE GUIMARAES (Presenter), MANUEL DOS SANTOS DIAS, JUBA BOUAZIZ, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, ANTONIO COSTA, ROBERTO B. MUNIZ, Instituto de Física, Universidade Federal Fluminense, SAMIR LOUNIS, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich — The quest for device miniaturization, decreased energy consumption, and improved speeds of processing and storage units naturally led to exploiting the connection between electric currents and magnetization dynamics. In this presentation, I demonstrate that ferromagnetic and antiferromagnetic excitations can be triggered by the dynamical spin accumulations induced by the bulk and surface contributions of the spin Hall effect [1]. I also analyze the general concepts of magnetoresistance and Hall effects together with spin-orbit-related mechanisms to demonstrate how dynamical currents can be dramatically enhanced and precisely controlled by applying ac electric fields and static magnetic fields, in a materials-specific approach [2]. This work may also impact experimental techniques that use currents to probe and quantify magnetization precession and the torques that induce it.


*Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 -- DYNASORE)

9:48AM R41.00010: Bound-state spin-wave spectroscopy exploiting nonlinear three-magnon processes ZHENYU WANG, BEINING ZHANG, YUNSHAN CAO, PENG YAN (Presenter), University of Electronic Science and Technology of China — One recent breakthrough in the field of magnonics is the experimental realization of reconfigurable spin-wave nanochannels formed by a magnetic domain wall with a width of 10–100 nm. This remarkable progress enables an energy-efficient spin-wave propagation with a well-defined wave vector along its propagating path inside the wall. In the mentioned experiment, a microfocus Brillouin light scattering spectroscopy was taken in a line-scans manner to measure the frequency of the bounded spin wave. Due to their localization nature, the confined spin waves can hardly be detected from outside the wall channel, which guarantees the information security to some extent. In this work, we theoretically propose a scheme to detect/eavesdrop on the spin waves inside the domain-wall nanochannel via nonlinear three-magnon processes [1]. The approach can be parallely applied for probing the Dzyaloshinskii-Moriya interaction in narrow magnetic stripes [2]. The idea is analytically formulated with micromagnetic simulations performed to verify the theoretical predictions.


10:00AM R41.00011: Transverse spin currents carried by surface spin waves in obliquely magnetized magnetic films CODY TREVILLIAN (Presenter), VASYL S TYBERKEVYCH, Oakland University — Properties of spin waves (SWs) are well-studied in perpendicular and in-plane magnetized magnetic films, but are understood much worse in the case of oblique magnetization (OM). Recent studies [1, 2] show an unexpected and interesting effect in OM films, namely, an appearance of transverse spin currents (TSCs) carried by SWs propagating in the backward-volume-type geometry. Here, we theoretically study this effect for surface SWs propagating approximately perpendicularly to the bias magnetic field (Damon-Eschbach-type geometry). We show, that the TSC resonantly depends on the direction of SW propagation, reaching maximum when SWs propagate several degrees away from the normal to the bias field. The maximum TSC of surface SWs significantly exceeds that of volume SWs, which makes surface SWs preferable for experimental study of TSCs.

10:12AM R41.00012: Off-resonance excitation of spin waves by a four-magnon process  ROBERT MCMICHAEL  (Presenter), PAUL HANEY, National Institute of Standards and Technology — Recent experiments have shown that driving ferromagnetic resonance in thin films generates noisy stray fields over a broad frequency spectrum [1-3]. The noise has been attributed to spin waves excited through a four-magnon mechanism, although the specifics of the mechanism have not been identified. In this paper we present modeling of one such mechanism that relies on nonuniform fluctuations in $M_s$ owing to thermal excitation. With $M_s$ fluctuating, a uniform driving field at frequency $f_0$ will excite spin waves at frequencies $f_k$. The uniform processional mode adds a resonant amplification of the driving field. The predicted spin wave noise power is proportional to input microwave power, $T^2$, and $1/f_k^4$ (temperature $T$, spin wave frequency $f_k$). We find the most relevant spin waves for this process are near the bottom of the spin wave band. Numerical evaluation yields spin wave noise power that is roughly a factor of $10^2$ weaker than the noise power due to pure thermal excitation. However, this result can be regarded as a lower bound. The effect may be much larger if the $M_s$ fluctuations are due to spin waves that are excited above equilibrium [3].


10:24AM R41.00013: Berry curvature and topological edge modes for coupled waves between magnons and electromagnetic waves*  AKIHIRO OKAMOTO (Presenter), SHUICHI MURAKAMI, Physics, Tokyo Institute of Technology, RYUICHI SHINDOU, School of Physics, Peking University — The Chern number characterizes existence of the chiral topological edge modes inside the gap. The chiral topological edge modes are well studied in electronic systems, and they can be realized in photonic crystals and magnonic crystals, in which the time-reversal symmetry is broken. In addition to systems with a single kind of particles, systems consisting of more than two kinds of particles or quasiparticles attract much attention recently, in the context of topological phases.

In this presentation, we consider coupled waves between magnons and electromagnetic waves in a ferromagnet. The Berry curvature is enhanced at the crossing point of dispersions, as is the case for other coupled waves such as magnons with the dipolar hybridization and magnetoelastic waves. The Chern number, i.e. the integral of the Berry curvature for the coupled waves between the magnon and the electromagnetic wave is quantized. We find that the hybridization gap in this case is topological. Therefore, there exist topological chiral edge modes inside this gap. We also present an emergence of edge modes at an interface between two topologically different regions.

*This work was partly supported by a Grant-in-Aid for Scientific Research on Innovative Area, “Nano Spin Conversion Science” (Grant No. 26100006).

10:36AM R41.00014: Effects of Carbon Content on Magnetic and Microwave Properties of Iron Gallium Carbon Thin Films  XIANFENG LIANG (Presenter), CUNZHENG DONG, NIAN XIANG SUN, Northeastern University — A systematic investigation of the soft magnetism, delta E effect, magnetostriction, and microwave properties has been carried out on iron gallium carbon (Fe-Ga-C) thin films over a wide carbon content range. The phase transformation of the Fe-Ga-C films from bcc polycrystalline to amorphous phase leads to excellent magnetic softness with a low coercivity of less than 1 Oe, high 4pMs, narrow ferromagnetic resonance (FMR) linewidth at 10 GHz of 20~30 Oe and ultra-low Gilbert damping constant of 0.0027. A record high piezomagnetic coefficient of 9.71 ppm/Oe, high saturation magnetostriction constant of 81.2 ppm, and large delta E effect of -120 GPa at 500 nm are also achieved. The soft magnetism, large delta E effect and piezomagnetic coefficient combined with ultra-low Gilbert damping constant make Fe-Ga-C thin film an attractive alloy for magnetoelectric and other voltage tunable RF/microwave device applications.
It has attracted great interests to explore efficient methods to control both the polarity and chirality of magnetic vortex in last decades. Here we report a new mechanism to control both the vortex chirality and polarity by electrical current, which is through the formation, decoupling and fusion of edge solitons. Our micromagnetic simulation show that the dynamics of the edge solitons at the disk edge can lead to selective switching of the vortex chirality and polarity. A way to directly write any of the four vortex states from any random states is proposed based on the switching diagram. The switching phase diagram as a function of disk diameters shows that the vortex chirality and polarity switching process is highly size-dependent. As the disk diameter scales down to below 160 nm, the vortex chirality and polarity are coupled together and always switch at the same time, resulting in an unchanged handedness before and after switch. Furthermore, the critical switch current can be as low as $3 \times 10^6$ A/cm$^2$. Our work offers an efficient way to control vortex chirality and polarity, which may have great application potential in the low-energy and high-density memory application.

*National Natural Science Foundation Of China, Grants No. 11604066

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R42 DQI: Quantum Annealing: Theory BCEC 210A

8:00AM R42.00001: Adaptive quantum annealing based on weak measurements to suppress the errors due to Landau-Zener transitions* YONGCHAO TANG (Presenter), ANTONIO MARTINEZ, University of Waterloo, SONG ZHANG, JUAN ATALAYA, BIRGITTA K WHALEY, University of California, Berkeley, ADRIAN LUPASCU, University of Waterloo — Quantum annealing is undermined by Landau-Zener transitions from the ground to the first excited state around small energy gaps. This kind of error can be suppressed by slowing down quantum annealing near the minimum gap. We study the relationship between the minimum gap and potential observables that can be used to gain information on the minimum gap using weak measurements. The measurement of energy curvature is promising as a measure of the location of the minimum gap. We apply master equations for the quantum annealing monitored by weak measurements to study the impacts of noise. The simulations show that Landau-Zener type errors can be suppressed by making the rate of quantum annealing dependent on monitoring with weak measurements.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).

8:12AM R42.00002: Feedback control of a monitored system evolving adiabatically* KA WA YIP (Presenter), DANIEL ALIDAR, University of Southern California — Time evolution of a system evolving adiabatically while coupled weakly to a thermal bath can be described by a quantum adiabatic master equation in Lindblad form. In quantum annealing it is desirable is to maintain the state as the ground state of the time-dependent Hamiltonian. This is difficult due to diabatic or thermal transitions. We devised a quantum feedback control method to reverse the effect of thermal excitation. Under specific continuous measurement schemes, quantum trajectories of the measurement records can be obtained and feedbacks conditioned on these records can be applied to increase the ground state population. We derived the feedback master equation for markovian feedback (feedback delay $\tau \to 0$) and further gave the timescale condition for feedback Markovianity. However, realistic feedbacks are non-markovian and subjected to non-negligible feedback delay, detector efficiency and restrictions of the form of the feedback Hamiltonian. We studied the effectiveness of feedback control under such limitations and explored how the optimized feedback delay time depends on the annealing schedule.

*Based upon work (partially) supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA).
Many-body quantum systems provide a mechanism for robust and efficient quantum search

KOSTYANTYN KECHEDZHI (Presenter), VADIM SMELYANSKIY, Google Inc., LARA FAORO, LPHE, CNRS, SERGIO BOIXO, HARTMUT NEVEN, Google Inc., LEV B IOFFE, Department of Physics, University of Wisconsin, BORIS ALTSHULER, Physics Department, Columbia University — Searching low energy subspace of a classical spin glass is computationally hard due to landscape of deep local minima separated by barriers. Applying a transverse field gives rise to tunneling between the quantum states defined within individual spin-glass minima. The number of transitions from a state grows exponentially with the number d of spin flips during the transition. This growth can compensate the decrease of the matrix elements with d leading to a transition from many-body localized to non-ergodic extended phase, where eigenstates are sparse superpositions of spin configurations corresponding to local minima within a narrow energy belt. We demonstrate a remarkable structure in the low energy eigenspectrum: it is partitioned into the alternating sequence of bands of two qualitatively different types, x- and z-, which retain characteristics of transverse field eigenstates and classical spin glass, respectively. We demonstrate this novel intermittency in a "wide band" impurity model with a bi-modal classical density of states with a delta-peak at zero energy containing most states and the second peak containing an exponentially smaller number of states lying at low energy. This non-ergodic structure of the eigenspectrum provides a mechanism for efficient quantum search.

Control of Phase Transitions in Wajnflasz–Pick model

YUYA SEKI (Presenter), Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and Technology, SHU TANAKA, Green Computing Systems Research Organization, Waseda University, SHIRO KAWABATA, Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and Technology — We construct a quantum Wajnflasz–Pick model, and investigate a nature of quantum phase transitions of the model. Quantum phase transition phenomena have drawn attention in the field of quantum computing as well as condensed matter physics, since the phenomena are closely related to the performance of quantum annealing (QA) and quantum adiabatic computation (QAC). Adding a driver Hamiltonian that causes spin flip and state transitions within upper and lower states to the Hamiltonian of classical Wajnflasz–Pick model, we construct the quantum model where phase transitions are controllable. Numerical analysis showed that the model undergoes first-order phase transitions whereas a corresponding spin-1/2 model does not undergo first-order phase transitions. In particular, we observed an anomalous phenomenon that the system undergoes first-order phase transitions twice under certain conditions. The results indicate that the performance of QA and QAC can be affected by the choice of the number of upper and lower states and the parameter in the driver Hamiltonian.

Energy gap scaling of quantum annealing based on Wajnflasz–Pick model

SHOHEI WATABE (Presenter), Tokyo University of Science, YUYA SEKI, SHIRO KAWABATA, Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and Technology — The conventional quantum annealer, transverse field Ising model, is known to suffer from the energy gap shrinkage for the scalable system, which may not provide the solution of the optimization problem within the realistic time scale. An idea for possibly overcoming this problem proposed by Seki, Tanaka, and Kawabata is to employ the Wajnflasz–Pick model, i.e., a qudit. By analyzing the order of the phase transition within the mean-field approach with the uniform interaction, they have found that the performance of quantum annealing is controlled by the number of upper and lower states of the spin. In this study, in order to confirm their claim, we revisit the energy gap of the finite size Wajnflasz–Pick model with all-to-all random interaction.

*This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO), Japan.
FERGUSON, SERGEY NOVIKOV, Northrop Grumman, HUO CHEN, DANIEL A LIDAR, University of Southern California — Annealing terms, as well as the values of the ferromagnetic couplings to be used in the minor embedding problem. In this talk I will focus on the parameter setting problem, that is how to find the optimal weights to be used in penalty hosted at NASA Ames with different values of the parameters will be discussed. Hamiltonian corresponds to the solution of the original problem. Finally, benchmark results using the D-Wave 2000Q chip implemented topology of the chip. These results show how state-of-the-art statistical learning algorithms can quantify the performance of physical quantum annealers, suggest a path towards mitigating the effects of persistent biases inevitably present in every analog device, and guide the design of new hardware architectures.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) through the Army Research Office (ARO) Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).

HAYATO GOTO (Presenter), TARO KANAO, Toshiba Corporation — Adiabatic quantum computation (AQC) with Kerr-nonlinear parametric oscillators, or KPOs for short, has been proposed [1-3], which is called bifurcation-based AQC [1]. The Hamiltonian used there is an effective one in a rotating frame and in the rotating-wave approximation. This is a notable difference between this approach and standard AQC using real Hamiltonians. Based on this difference, here we propose a method to improve the performance of bifurcation-based AQC, which is not applicable to standard AQC using real Hamiltonians.


ANDREA DI GIOACCHINO (Presenter), University of Milan - Quantum Artificial Intelligence Lab (QuAIL) @ NASA Ames - Stinger Ghaffarian Technologies (SGT), SALVATORE MANDRA, Quantum Artificial Intelligence Lab (QuAIL) @ NASA Ames - Stinger Ghaffarian Technologies (SGT), ELEANOR RIEFFEL, Quantum Artificial Intelligence Lab (QuAIL) @ NASA Ames — Solving a combinatorial optimization problem with the current generation of adiabatic quantum devices, as the D-Wave 2000Q, requires to express the cost function of the optimization problem in the QUBO form, which in many cases includes penalty terms to enforce hard constraints. A similar problem appears when a minor embedding is necessary to map the QUBO Hamiltonian on a specific hardware graph. Interestingly, the performance of both classical and quantum heuristics is very sensible to the choice of such penalty terms and an optimal choice of parameters could result in much faster computations than those ones performed with sub-optimal parameter values.

In this talk I will focus on the parameter setting problem, that is how to find the optimal weights to be used in penalty terms, as well as the values of the ferromagnetic couplings to be used in the minor embedding problem.

I will also present a method to find the minimum parameter values which guarantee that the ground state of the QUBO Hamiltonian corresponds to the solution of the original problem. Finally, benchmark results using the D-Wave 2000Q chip hosted at NASA Ames with different values of the parameters will be discussed.

*This project has received funding from Università degli Studi di Milano and NASA Ames Research Center.

ANDREY LOKHOV (Presenter), Los Alamos National Laboratory, YAROSLAV KHARKOV, University of New South Wales, CARLETON COFFRIN, MARC VUFFRAY, Los Alamos National Laboratory — Quantum annealers have a potential to provide a breakthrough in hard optimization and machine learning problems. Emerging physical implementations of quantum annealers are extremely sophisticated from the engineering point of view, and prediction of their performance remains a challenging problem. Here, we uncover the probabilistic relation between input and output of quantum annealers using the novel rigorous statistical learning tools. Extensive analysis of the output data allows us to check whether it satisfies the desired features assumed in the initial design of the device, to learn the machine's global response function, and to detect the echo of the chip architecture. In particular, our tests on D-Wave 2X and 2000Q quantum annealers revealed the presence of multi-body interactions and spurious next-nearest neighbor couplings between qubits as compared to the hardware-implemented topology of the chip. These results show how state-of-the-art statistical learning algorithms can quantify the performance of physical quantum annealers, suggest a path towards mitigating the effects of persistent biases inevitably present in every analog device, and guide the design of new hardware architectures.
9:48AM R42.00010: Quantum annealing and thermalization: insights from integrability*  
FUXIANG LI (Presenter), School of Physics and Electronics, Hunan University, NIKOLAI SINITSYN, Theoretical division, Los Alamos National Lab, VLADIMIR Y CHERNYAK, Department of Chemistry and Department of Mathematics, Wayne State University — We solve a model that has basic features that (are desired for quantum annealing computations: entanglement in the ground state,) controllable annealing speed, ground state energy separated by a gap during the whole evolution, and programmable computational problem that is encoded by parameters of the Ising part of the spin Hamiltonian. Our solution enables exact nonperturbative characterization of final nonadiabatic excitations, including scaling of their number with the annealing rate and the system size.

*Support of DOE at LANL with Contract No. DE-AC52-06NA25396 (N.A.S. and F. Li); NSF Grant No. CHE-1111350 (V.Y.C.); LDRD program at LANL

10:00AM R42.00011: The computational complexity of optical quantum annealers and Ising machines*  
RAPHAEL POOSER (Presenter), RYAN BENNNK, Computational Sciences and Engineering Division, Oak Ridge National Laboratory — Quantum annealers hold promise as optimization platforms for quantum machine learning applications and as layered neural networks. Recently, Optical Ising Machines (OIM) have been presented as a straight forward method to achieve this computational model. Relying on optical nonlinearities inside resonators, these devices are a network of coupled optical parametric oscillators (OPOs), a mature and practical technology in the field of continuous-variable quantum computing (CVQC). Despite the use of a key ingredient of CVQC (the second order nonlinearity which facilitates entanglement), the computational model of OIMs remains an open question. Here, we present a study of three different computational models based on physics of increasing complexity. We outline a fully classical nonlinear system of coupled oscillators, a semiclassical model of OPOs in the truncated Wigner representation, and a fully quantum treatment in the positive P representation. We present benchmarks of each model and outline their relative capability to capture the relevant physics responsible for practical computation in OIMs. Using these benchmarks, based on known quadratic optimization problems, we determine the computational complexity of these devices.

*ORNL Lab Directed Research and Development program.

10:12AM R42.00012: The power of pausing: advancing understanding of thermalization in experimental quantum annealers*  
JEFFREY MARSHALL (Presenter), University of Southern California and NASA Ames Research Center, DAVID VENTURELLI, NASA Ames Research Center, ITAY HEN, University of Southern California, ELEANOR RIEFFEL, NASA Ames Research Center — We investigate annealing schedules involving an intermediate pause, on the current generation of quantum annealing hardware: the D-Wave 2000Q. We show that a pause mid-way through the anneal can cause a dramatic change in the output distribution, and we provide evidence suggesting thermalization is occurring during such a pause. We demonstrate that upon pausing the system in a narrow region shortly after the minimum gap, the probability of successfully finding the ground state of the problem Hamiltonian can be increased by several orders of magnitude. We relate this effect to relaxation, after excitations occurring in the region near to the minimum gap. For a set of problems of size 500 qubits we demonstrate that the distribution returned from the annealer very closely matches a classical Boltzmann distribution of the problem Hamiltonian, albeit one with a noticeably higher temperature than that of the device.


10:24AM R42.00013: Understanding the Role of Non-stoquastic Catalysts in Quantum Adiabatic Optimization*  
TAMEEM ALBASH (Presenter), University of Southern California — The viability of non-stoquastic catalyst Hamiltonians to deliver consistent speedups in quantum adiabatic optimization remains an open question. Several studies (Crosson et al. (2014), Hormozi et al. (2017)) on random Ising problems have shown that stoquastic catalysts typically outperform non-stoquastic ones. A stark counterexample to this is the exponential speedup of non-stoquastic catalysts over stoquastic ones for infinite-range ferromagnetic p-spin models with p > 3 (Seki & Nishimori (2012)). We provide details on how the non-stoquastic catalyst provides an advantage in these models. We use this insight to then construct a geometrically local 2-body example that exhibits a similar exponential advantage for a non-stoquastic catalyst over a stoquastic one, up to the maximum system size we are able to study.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.
10:36AM R42.00014: Gap-independent cooling and hybrid quantum-classical annealing (HQCA)*
LUKAS S THEIS, PETER SCHUHMACHER (Presenter), MICHAEL MARTHALER, FRANK K WILHELM, Theoretische Physik, Saarland University — We present an efficient gap-independent cooling scheme for a quantum annealer that benefits from finite temperatures. We choose a system based on superconducting flux qubits as a prominent example of current quantum annealing platforms. We propose coupling the qubit system transversely to a coplanar waveguide to counter noise and heating that arise from always-present longitudinal thermal noise. We provide a schematic circuit layout for the system and show how, for feasible coupling strengths, we achieve global performance enhancements. Specifically, we achieve cooling improvements of about 50% in the adiabatic and a few hundred percent in the non-adiabatic regime, respectively.

*The research is based upon work (partially) supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.

10:48AM R42.00015: Enhancing quantum adiabaticity in adiabatic quantum computers with multiple local minima*
LIN TIAN (Presenter), University of California, Merced — The adiabatic criterion is a key requirement for the successful implementation of adiabatic quantum computing. However, in interacting many-body systems, the energy gap often decreases quickly with the number of qubits, which results in the violation of the adiabatic criterion and diabatic transition to the excited states. In a recent work [1], we presented an approach to enhance quantum adiabaticity that does not require the spectral knowledge of the adiabatic quantum computers or the construction of unphysical many-body interactions. In this talk, we show that this approach can be applied to adiabatic quantum computers with multiple local minima in the energy separation between the ground and the excited states. We demonstrate this approach with numerical simulation. [1] L. Tian, arXiv:1802.02285.

*This work is supported by the UC Lab Fee Program under Award No. LFR-17-477237 and the UC Merced Faculty Research Grants 2017.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R43 DCMP: Discrete Time Crystal Signatures in Driven Spin Systems BCEC 210B - Tag(s): Invited

8:00AM R43.00001: DTC signatures in NV Centers: Initial Discovery and Late-breaking Results [Invited] MIKHAIL LUKIN (Presenter), Harvard University — TBD

8:36AM R43.00002: Can Prethermal Regimes explain the latest observations of DTC signatures in driven spin systems? [Invited] CHETAN NAYAK (Presenter), Microsoft — TBD
9:12AM R43.00003: Observation of Discrete-Time-Crystal Signatures in an Ordered Dipolar Many-Body System*  
[Invited] JARED ROVNY, ROBERT BLUM, SEAN BARRETT (Presenter), Physics Dept., Yale Univ. — The rich dynamics and phase structure of driven systems include the recently described phenomenon of the discrete time crystal (DTC), a robust phase which spontaneously breaks the discrete time translation symmetry of its driving Hamiltonian. Experiments in trapped ions and diamond nitrogen vacancy centers have recently shown evidence for this DTC order. Here, we report nuclear magnetic resonance (NMR) observations of DTC signatures in a third, strikingly different, system: an ordered spatial crystal. This system is expected to be even farther from the regime of many-body localization (MBL) than those studied in the earlier experiments. We study the 100% occupied crystal lattice of spin-1/2 $^{31}$P nuclei in ammonium dihydrogen phosphate (ADP), with chemical formula NH₄H₂PO₄. ADP also contains spin-1/2 $^1$H nuclei (99.98% abundant) and spin-1 $^{14}$N nuclei (99.64% abundant). Implementing the DTC pulse sequence on the $^{31}$P spins, we observe robust oscillations at half the drive frequency ("DTC oscillations" for brevity) across orders of magnitude in interaction time. We also study the decay mechanism of the DTC oscillations, with two results. First, we show by generating a time-reversed DTC echo that the density matrix is more coherent than the original DTC sequence reveals. Second, we show that the effect of interactions during the nonzero pulse duration of the DTC sequence limits our ability to observe the intrinsic lifetime of the DTC oscillations [1,2]. In this work, we exploited both the long coherence times of our sample, and our ability to use NMR pulse sequences to edit the spin Hamiltonian. This suggests that NMR can be a useful probe of the physics of out-of-equilibrium, driven many-body systems.


*Supported by NSF Grant No. DMR-1610313. R.L.B. was supported by the NSF GRFP, Grant No. DGE-1122492.

9:48AM R43.00004: What NMR detection of DTC signatures may be telling us. [Invited] VEDIKA KHEMANI (Presenter), Harvard University — TBD

10:24AM R43.00005: Temporal Order in Periodically Driven Spins in small NMR spin Clusters*  
[Invited] SREEJITH GANESH JAYA (Presenter), SOHAM PAL, NAVEEN NISHAD, MAHESH T S, Physics, Indian Institute of Science Education and Research - Pune — We present the results of experimental studies on the magnetization response of star-shaped clusters of initially unentangled N=4, 10, and 37 nuclear spin-1/2 moments when subjected to inexact pi-pulse sequences. We find that an Ising coupling between the center and the satellite spins results in robust period-2 magnetization oscillations. On the other hand, control experiments (using alternate Isotopes ) without the Ising coupling do not show a robust time period. The period is stable against bath effects, but the amplitude decays with a timescale that depends on the inexactness of the pulse. Numerical simulations of the system reveal a simple semiclassical picture in which the rigidity of the period is due to a randomizing effect from the Larmor precession due to the magnetization of the surrounding spins. The timescale with stable periodicity increases with the net initial magnetization, even in the presence of perturbations and absence of disorder, indicating a robust temporal ordered phase for large systems with finite magnetization per spin. We also present results of numerical simulations of the system with simple model couplings to a bath.


*DST/SJF/PSA-03/2012-13  
CSIR 03(1345)/16/EMR-II

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R44 DCMP: Heavy Fermion Systems as a Platform for Strongly Correlated Electronic Topology  
BCEC 210C - Piers Coleman, Rutgers University - Tag(s): Invited
8:00AM R44.00001: Weyl-Kondo semimetals: Symmetries, signatures and nearby quantum phases* [Invited] SARAH GREFE (Presenter), Department of Physics and Astronomy and Rice Center for Quantum Materials, Rice University — In the last few years, manifestations of the long-anticipated Weyl semimetal have been observed in weakly correlated materials. In the context of a global phase diagram for strongly correlated systems with a large spin-orbit coupling, the prototypical heavy fermion systems have emerged as an important platform for topological metals. We have recently advanced a strongly correlated topological phase, the Weyl-Kondo semimetal (WKSM) [1], which exhibits Kondo effect-driven nodal quasiparticles. The Weyl nodes are pinned near the Fermi energy by strong correlations along with space group symmetry. One signature of this WKSM phase is a specific heat varying as $T^3$ below the Kondo temperature, with a colossal prefactor, as observed in the noncentrosymmetric heavy fermion semimetal Ce$_3$Bi$_4$Pd$_3$ [2]. Experiments on Ce$_3$Bi$_4$Pd$_3$ have also demonstrated a nonlinear spontaneous Hall response and an even-in-field Hall resistivity, which are attributed to the large Berry curvature dipole of a WKSM with tilted nodes [3]. Both illustrate that signatures of topological phases driven by strong correlations are often distinct from those typical for weakly correlated systems. Finally, in related models we have found how the WKSM connects with proximate topologically distinct phases, such as a Kondo Insulator and a Dirac-Kondo semimetal, as well as magnetic states. I will present these results, and discuss their place in the heavy fermion global phase diagram that the topological paradigm has enriched.


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8:36AM R44.00002: Kondo-Weyl semimetal behavior in Ce$_3$Bi$_4$Pd$_3$* [Invited] SAMI DZSABER (Presenter), GAKU EGUCHI, DIEGO A ZOCCO, ANDREI SIDORENKO, XINLIN YAN, ANDREY PROKOFIEV, LUKAS PROCHASKA, Institute of Solid State Physics, , Wiedner Hauptstr. 8-10, 1040 Vienna, Austria, Vienna University of Technology, T. SHIROKA, ETH Zurich, Paul Scherrer Institut, Switzerland, P. BLAHA, Institute of Materials Chemistry, Vienna University of Technology, 1040 Vienna, Austria, O. RUBEL, Department of Materials Science and Engineering, McMaster University, 1280 Main Street West, Hamilton, Ontario, Canada L8S 4L8, S.E. GREFE, H. H. LAI, Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA, QIMIAO SI, Department of Physics and Astronomy, Houston, Texas 77005, USA, Rice University, SILKE BUEHLER-PASCHEN, Institute of Solid State Physics, , Wiedner Hauptstr. 8-10, 1040 Vienna, Austria, Vienna University of Technology — In heavy fermion systems the Kondo effect stabilizes strongly renormalized heavy electronic bands, and promotes novel quantum phases and excitations. Recently, the discovery of topologically non-trivial insulators, as well as Dirac and Weyl semimetals with 3D bulk linear electronic dispersion has triggered a lot of interest. So far, investigations have focused on non-interacting settings, but it is of great interest to also explore the interplay of strong correlations and topology. For this purpose we have searched for topologically non-trivial phases in heavy fermion systems. Indeed, by tuning the spin-orbit coupling strength by Pt-Pd substitution in Ce$_3$Bi$_4$(Pt,Pd)$_3$, we have discovered a transformation from a Kondo insulator in Ce$_3$Bi$_4$Pt$_3$ to a semimetal in Ce$_3$Bi$_4$Pd$_3$ [1]. The latter shows the thermodynamic hallmark of strongly renormalized linear electronic bands [1], as recently predicted for a Weyl-Kondo semimetal [2]. Strikingly, as full Kondo coherence sets in, a large spontaneous Hall effect appears. As the material is entirely nonmagnetic, this is direct evidence of a huge Berry curvature dipole in the absence of time-reversal symmetry breaking. We attribute this effect to the topological nature of this noncentrosymmetric material, in the form of tilted Kondo-driven Weyl nodes [3].


*Financial support from the Austrian Science Fund (P29296-N27 and DK W1243) is gratefully acknowledged.
9:12AM R44.00003: Evidence for Weyl fermions in a heavy fermion semimetal YbPtBi* [Invited] CHUNYU GUO (Presenter), FAN WU, ZHONGZHENG WU, MICHAEL SMIDMAN, Zhejiang University, CHAO CAO, Department of Physics, Hangzhou Normal University, 310036 Hangzhou, China., AARON BOSTWICK, CHRIS JOZWIAK, ELI ROTENBERG, Advanced Light Source, E.O. Lawrence Berkeley National Lab, Berkeley, CA 94720, USA, YANG LIU, Zhejiang University, FRANK STEGLICH, Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany, HUIQIU YUAN, Zhejiang University — Materials with non-trivial band topology have been extensively studied in weakly correlated electron systems. Consequently, it is of great interest to test the existence of Weyl fermions when the electronic correlations are strong. Here, we report electronic structure calculations, ARPES, magneto-transport and calorimetric measurements of the canonical heavy fermion semimetal YbPtBi[1], we find triply degenerate points existed in band structure, which split into pairs of Weyl nodes under applying magnetic field. At high temperatures, the chiral anomaly effect is detected in the magneto-transport measurements, which becomes negligible when the electronic correlations become stronger at lower temperatures. However, the topological Hall effect and the temperature dependence of specific heat still demonstrate the existence of Weyl nodes. These results suggest that YbPtBi is a Weyl heavy fermion semimetal, where the bands hosting Weyl nodes are strongly renormalized at low temperatures due to the Kondo effect. Our findings provide a suitable platform to explore the interplay between topology and strong electronic correlations.


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9:48AM R44.00004: Excitons in topological Kondo insulators: Theory of thermodynamic and transport anomalies in SmB6 [Invited] JOHANNES KNOLLE (Presenter), Blackett Laboratory, Imperial College London — Kondo insulating materials lie outside the usual dichotomy of weakly versus correlated—band versus Mott—insulators. They are metallic at high temperatures but resemble band insulators at low temperatures because of the opening of an interaction-induced band gap. The first discovered Kondo insulator (KI) SmB6 has been predicted to form a topological KI (TKI). However, since its discovery thermodynamic and transport anomalies have been observed that have defied a theoretical explanation. Enigmatic signatures of collective modes inside the charge gap are seen in specific heat, thermal transport, and quantum oscillation experiments in strong magnetic fields. Here, we show that TKIs are susceptible to the formation of excitons and magnetoexcitons. These charge neutral composite particles can account for long-standing anomalies in SmB6.

10:24AM R44.00005: Topological Kondo insulators and semimetals* [Invited] ONUR ERTEN (Presenter), Department of Physics, Arizona State University — The electrons in heavy fermion materials experience strong spin-orbit coupling interactions that greatly exceed their kinetic energy. It has long been known that the spin-orbit coupling stabilizes new kinds of heavy fermion metals, superconductors and Kondo insulators and semimetals. In this talk, I will discuss the new realization that spin orbit coupling changes the topology leading to new kinds of topological orders. I will mainly focus on SmB6, CeNiSn and time permitting CeSb. In particular, I will discuss the puzzling experimental results on topological Kondo insulators and the possibility of a Skyrme insulating phase in SmB6 [1]. Next I will discuss how non-symmorphic symmetries can lead to Mobius-twisted surface states in failed Kondo insulators[2]. Time permitting, I will discuss recent ARPES experiments on gapless Kondo-Weyl semimetals[3].


*Supported by ASU startup grant.
8:00AM R45.00001: Photoemission Spectroscopy Experiments on Metalloporphyrin Architectures for Molecular Electronics  RADWAN ELZEIN (Presenter), RUDY SCHLAF, Electrical Engineering, University of South Florida — Metal Organic Frameworks (MOFs) based on metalloporphyrin architectures combine advantages of both organic and inorganic materials and therefore are interesting candidates for next generation molecular electronic devices and applications. They exhibit unique properties such as highly ordered structures, ultrahigh surface area, tunable nanopore size, and more interestingly tailorable electronic, and ionic properties.

In this work, we present Liquid Phase Epitaxy method to fabricate self-assembled monolayers on gold surfaces which enabled to host conductive MOFs with their ability to facilitate charge transfer and control the growth of the MOF thin films.

We used Photoemission Spectroscopy (PES) to reveal the electronic properties which is crucial for the construction of energy band diagrams of various metalloporphyrin derivatives coordinated to either copper or zinc based metal ions. The energy band diagrams revealed interesting details about the electronic properties when changing various metal ions or conductive ligands. The obtained results show the fabricated films exhibit semiconductor tunability of either p-type or n-type behavior as conducting medium of charge carrier transport which is a key prerequisite to build molecular electronic junctions and elaborated devices.

8:12AM R45.00002: Ultrafast electron dynamics in a thin C60 films observed with time and angle resolved photoemission*  PENG ZHAO (Presenter), CHRISTOPHER CORDER, JIN BAKALIS,MICHAEL GEORGE WHITE, THOMAS ALLISON, Stony Brook University — C60 derivatives are common acceptor materials for organic solar cells. Time- and angle-resolved photoelectron spectroscopy (tr-ARPES) is a powerful way to study the electron dynamics in these systems. However, experiments on perturbatively excited systems are very demanding. By combining an 88 MHz ultrafast XUV source [1] with time-of-flight momentum microscopy [2], we are able to perform experiments at high speed and low excitation fluence. Here we present first demonstration results on C60 films with this technique.


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8:24AM R45.00003: Waves guided by the surface of a Lorentz model dielectric medium*  S.R. SESHADRI (Presenter), 4502 Phyllis Court, Livermore, CA, Independent Researcher — The wavenumber, the phase velocity, the wave packet velocity, the energy transport velocity, and the attenuation coefficient are obtained for the wave guided by the surface of a Lorentz model dielectric medium.

*None

8:36AM R45.00004: The TEM Studies of Tungsten Irradiated by Helium*  KANGWEI ZHU (Presenter), RUILONG YANG, WENYUAN WANG, YIN HU, Institute of Materials, China Academy of Engineering Physics — Tungsten (W) as one of the potential plasma-facing materials (PFMS) would suffer severe irradiation in nuclear fusion reactor which can results in deterioration of the related mechanical and physical properties. Understanding the irradiation effects on PFMS is then critical to improve their performances. Here, we studied the He ions irradiation effects by focusing on microstructures of the the W surfaces. As the irradiation time increased, the surface morphologies changed from smooth to full of nano-structures. TEM images show that the nano-structures contain lots of He voids, it is noted that the shapes of the he bubbles are faceted, which pointed out that the system prefers to develop low surface energy bubbles. And the nano-structures show good deformation feature although micro-carcks are developed inside.

*This work was supported by National Science Foundation of China (No. 11305148), Foundation of Key Laboratory (XKFZ101606), Foundation of President of China Academy of Engineering Physics (YZjJlX2016006).

8:48AM R45.00005: Electronic Structure of Phase Separated Material Revealed by Nanospot Angle-Resolved Photoemission Spectroscopy  CHANGHUA BAO (Presenter), HONGYUN ZHANG, HAOXIONG ZHANG, KENAN ZHANG, YANG WU, Department of Physics, Tsinghua Univ, CHAOYU CHEN, JOSE AVILA, MARIA C. ASENSIO, Synchrotron SOLEIL, SHUYUN ZHOU, Department of Physics, Tsinghua Univ — Phase separation frequently occurs in strong correlated materials. The electronic structures of different phases are very important but difficult to access due to very small grain size. As an electronic structure microscopy, nanospot angle-resolved photoemission spectroscopy (NanoARPES) can measure the electronic structure both in real and momentum spaces and provides the unique ability to measure the electronic structures of different phases in phase separated materials. Here I will present our recent experimental results on the electronic structure of phase separated material by using NanoARPES.
9:00AM R45.00006: Optimization and Characterization of Dip-Coated PEDOT:PSS on CdTe Solar Cells* MICHAEL PATULLO (Presenter), NNAMDI ENE, DANIEL ROGERS, MEHMET ALPER SAHINER, Seton Hall University — Organic thin film solar cells have been identified as viable photovoltaic technology alternatives to conventional power production methods. In this work, we optimize the thin film deposition conditions for high-conductive grade poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) on pulsed laser deposited cadmium sulfide/cadmium telluride/indium tin oxide substrates. In our previous studies, we have determined that this particular substrate and polymer combination significantly improves the photovoltaic conversion efficiency due to a reduction of the Schottky barrier resistance. In this study, we focus on applying a uniform layer of the PEDOT:PSS back contact by optimizing thin film dip-coating parameters such as pulling rate, temperature, application duration, and drying procedures. The resultant back contacts are characterized by scanning electron microscopy, energy dispersive x-ray spectroscopy, and ellipsometry techniques. Electrical conductivity tests on full cells are also performed using a Keithley SourceMeter, and structure and efficiency results are discussed.

*All Advanced Materials Synthesis and Characterization Laboratory Members
New Jersey Space Grant Consortium (NASA)

9:12AM R45.00007: Effect of illumination on the interplay between Dresselhaus and Rashba spin-orbit coupling in InAs quantum wells* ELENA CIMPOIASU (Presenter), BENJAMIN DUNPHY, Physics, United States Naval Academy, Annapolis MD 21402, SHAWN MACK, JOSEPH A. CHRISTODOULIDES, BRIAN R BENNETT, Naval Research Laboratory, Washington DC 20375 — Illumination of variable wavelength was used to study the dependence on the carrier concentration of the spin-orbit coupling and the semiconducting properties of a thin n-type InAs quantum well. Measurements of the sheet and Hall resistance were performed in variable magnetic field, field orientation, temperature, and under illumination with wavelengths of 400 nm up to 1300 nm. Beats in the Shubnikov-de Haas oscillations indicated the presence of strong spin-orbit coupling and the FFT of the oscillations points towards the presence of both Rashba and Dresselhaus spin-orbit interactions. Here we have used simulations to extract the dependence of the spin-orbit strengths on the carrier concentration. The simulations are based on the Hamiltonian of a 2D electron system with both types of spin-orbit interactions and subject to a perpendicular magnetic field. The results indicate that the Rashba coefficient decreases with increasing the carrier concentration, while the Dresselhaus coefficient remains mainly constant. These results are consistent with observations on similar materials where the carrier concentration was varied using applied gate voltage.

*This work was funded by ONR.

9:24AM R45.00008: Band Structure engineering in epitaxial LuSb thin films via dimensional confinement and bi-axial strain SHOUVIK CHATTERJEE (Presenter), Electrical & Computer Engineering, University of California, Santa Barbara, HADASS INBAR, Materials Department, University of California, Santa Barbara, SHOAIB KHALID, Department of Physics & Astronomy, University of Delaware, ARANYA GOSWAMI, Electrical & Computer Engineering, University of California, Santa Barbara, FELIPE CRASTO DE LIMA, ABHISHEK SHARAN, FERNANDO SABINO, Department of Physics & Astronomy, University of Delaware, TOBIAS L BROWN-HEFT, YU-HAO CHANG, Materials Department, University of California, Santa Barbara, ALEXEI V FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, DANIEL READ, School of Physics & Astronomy, University of Cardiff, ANDERSON JANOTTI, Department of Physics & Astronomy, University of Delaware, CHRIS PALMSTROM, Electrical & Computer Engineering, University of California, Santa Barbara — Observation of extreme magnetoresistance (XMR) in rare-earth monopnictides has raised strong interest in understanding the role of its electronic structure. Here, the first demonstration of epitaxial synthesis of LuSb thin films on GaSb (001) substrates will be presented. Combining the techniques of molecular-beam epitaxy, low-temperature magnetotransport, angle-resolved photoemission spectroscopy, and hybrid density functional theory, we have unveiled the bandstructure of LuSb, where electron-hole compensation is identified as a mechanism responsible for XMR. However, by fabricating ultra-thin films, it is possible to controllably create an imbalance in the band fillings of electron and hole-like carriers in this otherwise compensated semimetal. Moreover, magnetoresistance behavior can also be tuned by application of bi-axial strain by synthesizing thin films of LuSb on lattice mis-matched substrates. Our work demonstrates the efficacy of epitaxial synthesis of rare-earth monopnictides to control its electronic structure, and thereby its physical properties.
9:36AM R45.00009: High quality Bi$_2$Se$_3$ thin films grown on Van der Waals substrate BiInSe$_3$* XIONG YAO (Presenter), Center for Quantum Materials Synthesis and Department of Physics and Astronomy, Rutgers, the State University of New Jersey, RONGWEI HU, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers, the State University of New Jersey, JISOO MOON, Department of Physics and Astronomy, Rutgers, the State University of New Jersey, SANG-WOOK CHEONG, SEONGSHIK OH, Center for Quantum Materials Synthesis and Department of Physics and Astronomy, Rutgers, the State University of New Jersey — We grew high quality BiInSe$_3$ single crystals and developed an exquisite process to prepare these crystals as substrates. Well cleaved BiInSe$_3$ single crystals with subsequent in-situ thermal treatment can obtain atomically flat surface, which is evidenced by the sharp streaky reflection high energy electron diffraction (RHEED) patterns. By optimizing the growth recipe, we successfully grew high quality Bi$_2$Se$_3$ thin films on BiInSe$_3$ single crystal substrates. Owing to the weak Van der Waals bonding between the interlayers of BiInSe$_3$ substrates, we can easily transfer the Bi$_2$Se$_3$ thin films grown on these substrates. The high quality surface morphology and electrical transport characteristics, together with the transferrable feature all prove that BiInSe$_3$ could be a promising substrate for TI films growth. Our discovery could pave a new pathway for improving the sample quality of topological insulator thin films.

*This work is supported by the center for Quantum Materials Synthesis (cQMS), funded by the Gordon and Betty Moore Foundation's EPiQS initiative through grant GBMF6402, and by Rutgers University.

9:48AM R45.00010: Very different adsorption pathways of triatomic molecule H$_2$O on isolated and domains of dangling bonds on the Si(100) surface* CHANG-YUAN CHANG, DENG-SUNG LIN (Presenter), National Tsing Hua University — On the ideal clean Si(100) surface, dangling bond pairs (DBPs, denoted as -Si-Si-) cover the entire surface. Each dangling bond is an active adsorption site for adsorption of a gas molecule. In this study, isolated DBPs are prepared on a Si(100) surface as well-defined chemically-reactive sites for chemisorption of the prototypical H$_2$O triatomic molecules. The surrounding dangling bonds are passivated by chlorine-termination. Following saturation exposure to H$_2$O molecules at room temperature, the adsorbate configurations on these reactive sites as well as on the clean surface have been examined in atomic resolution using scanning tunneling microscopy.

The results show that, while the H-Si-Si-OH adsorbate configuration is common on a DBP, other configurations such as H-Si-O-Si-H and H-Si-Si-H are observed. These findings indicate that a seemingly simple chemisorption reaction on reactive sites involves not only the sites themselves but also the relevant surrounding bonds and adatoms.

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10:00AM R45.00011: Reversible and Efficient Photo-Switching of Azobenzene Derivatives on an Insulator Surface Investigated by nc-AFM SIMON JAEKEL (Presenter), Institute of Chemistry, University of Graz, ANITJE RICHTER, ROBERT LINDNER, Institute of Physical Chemistry, University of Mainz, CHRISTOPHE NACCI, Institute of Chemistry, University of Graz, ANGELIKA KÜHNLE, University of Bielefeld, STEFAN HECHT, Department of Chemistry, Humboldt-Universität zu Berlin, LEONHARD GRILL, Institute of Chemistry, University of Graz, RALF BECHSTEIN, University of Bielefeld — Studying single molecular switches is of interest for a better understanding of fundamental physical and chemical processes, but also in view of their possible use in smart materials and molecular nanotechnology.

Azobenzene is a prototypical molecular switch, which changes between trans and cis isomers at the central N=N bond upon an external stimulus. Adsorption on solid substrates allows the study on the single molecule scale using scanning probe microscopy, but it has been shown that metallic substrates strongly influence the switching properties[1,2]. Here, we report non-contact atomic force microscopy (nc-AFM) results on the switching of individual Azobenzene derived molecules on an insulating calcite surface. It is demonstrated that unlike on metals [3] the molecules retain their efficient photoisomerization properties known from solution. Furthermore, the photoisomerization is shown to be reversible and selective, depending on the exciting wavelength.

10:12AM R45.00012: Theory of coupled deposition and dissolution of solids, with focus on corrosion  INGE BELLEMAN, Department of Materials, Textiles and Chemical engineering, Ghent University, DIMITRIOS FRAGGEDAKIS (Presenter), Chemical Engineering, MIT, MARTIN BAZANT, Chemical Engineering & Math, MIT — Corrosion affects the durability of metals and structures and has important economic consequences, such as the continuous inspection for and replacement of damaged material. Corrosion often initiates locally and therefore, to increase the sustainable use of metals, a thorough knowledge of corrosion and its localized initiation is crucial. One technique to investigate this experimentally is the gold nanoplating technique on pure copper. This study investigates the pattern formation in this concurrent deposition-corrosion system. First we derive the general model for deposition-dissolution systems and then apply this to the gold-nanoplating example. This is the first model to implement non-linear reaction kinetics based on far-from equilibrium thermodynamics. Effects related to curvature induced diffusion and/or effective phase-separation upon deposition/dissolution are inherently included, phenomena which affect the formation dynamics of deposited film and the corroded bulk material-film interface. Other applications of the model are the passivation of stainless steels, the galvanization protection of Zn with respect to iron, and Li plating during continuous cycling of Li-Ion batteries.

10:24AM R45.00013: Morphological Instability of Grain Boundary under Lateral Applied Strain*  MING-WEI LIU (Presenter), KUO-AN WU, National Tsing Hua University — The morphological instability of symmetrical high-angle tilt grain boundary induced by lateral applied strain is investigated using the phase field crystal model in two dimensions. By studying the growth rate of perturbations, we discover a threshold value of the applied strain below which the instability disappears. Furthermore, we construct the phase diagram of instability which is classified into two groups, namely the grain boundary structural transformation or the dislocation emission, based on the late stage behavior of the grain boundary. A theoretical model is proposed by taking into account a relatively soft solid-solid interface, the elasticity of solid grains, and the interfacial energy of grain boundary. The theoretical prediction of the growth rate and the phase diagram is in quantitatively good agreement with the simulation result. In addition, the theory also explains the inhomogeneous strain distribution observed in simulations.

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Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R46 DMP: Complex Oxide Interfaces & Heterostructures -- Strong correlations
BCEC 212 - Hyowon Park, University of Illinois at Chicago - Tag(s): Focus
8:00AM R46.00001: Magnetism and topology in SrRuO$_3$- and SrVO$_3$-based heterostructures: from DFT via DMFT to DΓA*[Invited] KARSTEN HELD (Presenter), Institute for Solid State Physics, TU Wien — Oxide heterostructures based on SrRuO$_3$ are promising candidates for thin film ferromagnetism, but experiments showed time and again that ferromagnetism breaks down below a critical thickness. By means of density functional theory (DFT) plus dynamical mean field theory (DMFT), we show [1] that growing SrRuO$_3$ in the (111) direction instead yields a half-metallic ferromagnetic state with an ordered magnetic moment of 2 $\mu$B/Ru and survives the ultimate dimensional confinement down to a bilayer -- even at elevated temperatures of 500 K. This ferromagnetic state has been confirmed by experiment and also hosts Haldane's quantum anomalous Hall state, without any external magnetic field or magnetic impurities [1]. Similar physics with an even larger gap is also observed in SrRhO$_3$ (111) but not in LaNiO$_3$ (111) [2] bilayers.

For SrRuO$_3$ grown in the (001)-direction, DFT+DMFT instead only yields ferromagnetism if the Ru is doped away from 4 d-electrons. This is possible by applying a gate voltage or, as we will show, by growing SrRuO$_3$ on an appropriate substrate that induces a self-doping between different SrRuO$_3$ layers.

For SrVO$_3$-based heterostructures, on the other hand, the metallic bulk behavior turns insulating below a thickness of 3 SrVO$_3$ layers, which has been proposed to be utilized as a Mott transistor [3]. Using DFT+DMFT and beyond that the dynamical vertex approximation (DΓA) [4], we here show that this insulating state is actually antiferromagnetic at low temperatures and can be switched to a ferromagnetic metallic state through a gate voltage, actually making it a Mott magnetotransistor. Here, strong non-local correlations further induce a Lifshitz transition at low temperatures.


*European Research Council (ERC) Grant No. 306447; Austrian Science Fund (FWF) SFB ViCoM F41 and P 30997.

8:36AM R46.00002: Designing new metastable nickelate thin films isostructural to the cuprates QI SONG (Presenter), GRACE PAN, CHARLES BROOKS, Harvard University, HANJONG PAIK, Cornell University, JULIA MUNDY, Harvard University — Despite over thirty years of intense experimental and theoretical effort, there remain outstanding questions on the origin of superconductivity in the cuprates. One strategy for gaining insight into this phase has been to probe materials which are isoelectronic to the cuprates and contain many of the same characteristics of the known high-TC superconductors. Recent work on bulk crystals of layered square planar nickelates, $R_nNi_{3-n}$O$_8$ ($R$ = La, Pr) has re-ignited interest in nickelates for this purpose [1]. Here, we use atomically-precise synthesis to construct a full series of $R_nNi_{n+1}$O$_{3n+1}$ ($n$ = 1 – 5) thin films which we then reduce to form $R_nNi_{n+2}$O$_{2n+2}$. We aim to develop a systematic understanding of these different nickelate thin films and to correlate the electronic behavior with the local crystal structure and nickel valence state.


8:48AM R46.00003: BoSS: Boson Slave Solver software for correlated electrons* SOHRAB ISMAIL-BEIJI (Presenter), MINJUNG KIM, Yale Univ, ALEXANDRU BOGDAN GEORGESCU, Center for Computational Quantum Physics, The Flatiron Institute — We describe the recent release of the open source software "BoSS" or Boson Slave Solver (bitbucket.org/yalebosssolver/boss), written in MATLAB, which solves extended Hubbard models using the slave boson approach. The primary intended application is to study the electronic structure of transition metal oxides which are often affected significantly by strong and localized electron-electron interactions. Examples include renormalization of the mass and spectral weight of low energy quasiparticles and the formation of Hubbard bands: these dynamical effects can not be described by band theory approaches (e.g., DFT, DFT+U or hybrid methods). Slave-boson approaches represent computationally efficient electronic structure methods that can explicitly include such effects. We present an overview of our recent slave boson methodology [1,2], show applications to some transition metal oxides where we can compare to experimental and dynamical mean field theory (DMFT) results.


*This work was supported by the NSF via grants MRSEC DMR-1119826 and ACI-1339804.
**9:00AM R46.00004: Study of infinite layer CaCuO$_2$/SrTiO$_3$ interfaces**  
ADRIEN WAELCHLI (Presenter), HUGO MELEY, STEFANO GARIGLIO, JEAN-MARC TRISCONE, Department of Quantum Matter Physics, University of Geneva — Thirty years after its discovery, superconductivity in cuprates still remains a lively field of research since the microscopic mechanisms leading to high $T_c$ are not yet fully identified and understood. Recent work on the infinite layer CaCuO$_2$ [1,2] has shown that superconductivity can occur at the interface with SrTiO$_3$. The conduction at the interface has been related to a chemical doping mechanism with O atoms inserting into the apical position above Cu. We present results on the study of CaCuO$_2$/SrTiO$_3$ bilayer structure. We investigate the influence of different growth parameters on the film quality and electrical properties explored through transport measurements.


**9:12AM R46.00005: Effects of epitaxial strain and oxygen underdoping on superconductivity in manganite/cuprate thin-film heterostructures**  
CHAO ZHANG (Presenter), HAO ZHANG, Department of Physics, University of Toronto, ANH NGUYEN, THOMAS GREDIG, Department of Physics and Astronomy, California State University Long Beach, MIN GU KANG, RICCARDO COMIN, Massachusetts Institute of Technology, Department of Physics, JOHN Y.T. WEI, Department of Physics, University of Toronto — To distinguish the role of magnetism from other factors that affect superconductivity in $c$-axis La$_{2/3}$Ca$_{1/3}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-δ}$ (LCMO/YBCO) heterostructures, we grow and characterize various perovskite/YBCO/perovskite trilayers, using ferromagnetic LCMO, paramagnetic LaNiO$_3$ (LNO), and orthorhombic PrBa$_2$Cu$_3$O$_{7-δ}$ (PBCO) as the sandwiching layers. LCMO and LNO trilayers show similarly large superconducting $T_c$ reductions with decreasing YBCO layer thickness, whereas this $T_c$ reduction is not seen in the PBCO trilayers. Our results indicate that epitaxial strain has a stronger effect on the $T_c$ of LCMO/YBCO heterostructures than any long-range magnetic proximity effect present. [1] Using this system, we also study how the $T_c$ reduction varies with oxygen underdoping by deoxygenating the cuprate layer. We discuss our results in the wider context of multiple competing orders, in particular the recent observation by resonant x-ray scattering of robust charge-density-wave order in LCMO/YBCO multilayers. [2] [1] H. Zhang et al., arXiv:1710.10668v1 [cond-mat.supr-con]  

*Work supported by NSERC, CFI-OIT and the Canadian Institute for Advanced Research

**9:24AM R46.00006: Multi-band, two-dimensional superconductivity above the Pauli limit in Sr$_{1-x}$Nd$_x$TiO$_3$**  
YILIKAL AYINO (Presenter), JIN YUE, TIANQI WANG, BHARAT JALAN, VLAD S PRIBIAG, University of Minnesota — We present evidence of two-dimensional, multi-band superconductivity in Sr$_{1-x}$Nd$_x$TiO$_3$ thin films from the temperature dependence of the resistive upper critical field. The out-of-plane upper critical field shows pronounced positive curvature, which extends substantially below the critical temperature, and further exhibits a change in curvature at low temperatures. Quite unusually, the out-of-plane upper critical field exceeds the Pauli paramagnetic limit, by almost a factor of two. We attribute this unusual observation to the enhancement of critical field due to two-band superconductivity and the presence of strong spin-orbit coupling. We propose a model for the critical field of a two-band superconductor that includes paramagnetic breaking of Copper pairs and spin-orbital coupling in the dirty limit and find good agreement of this model with our data. Our results suggest that in SrTiO$_3$ intra-band superconducting coupling dominates over inter-band coupling.

*NSF (UMN MRSEC) and DOE Center for Quantum Materials
9:36AM R46.00007: Prospects for creating complex oxide quantum electronic heterostructures via solid phase epitaxy: PrAlO3/SrTiO3 model system  YAJIN CHEN (Presenter), Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA, WATHSALA WADUGE, Department of Chemistry, Wayne State University, Detroit, MI 48202, USA, PENG ZUO, Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA, THOMAS F. KUECH, Department of of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA, SUE E. BABCOCK, Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA, CHUCK H. WINTER, Department of Chemistry, Wayne State University, Detroit, MI 48202, USA, PAUL G EVANS, Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA — Various oxide interfaces with composition \( \text{RAlO}_3/\text{SrTiO}_3 \) (\( \text{R} = \text{La, Pr, Nd} \)) can produce a two-dimensional electron gas (2DEG). Crystallization from amorphous precursors, termed solid phase epitaxy (SPE), is an approach for synthesizing these interfaces that complements vapor-phase epitaxy techniques. Atomic layer deposition (ALD) is a promising route for forming the amorphous films because it allows oxide interfaces to be created in non-planar geometries. SPE can be used with patterned substrates to grow epitaxial thin films in complex geometries, which may enable the creation of 2DEG beyond planar geometries. The creation of PrAlO3 thin films via SPE has required developing new ALD procedures, understanding crystallization kinetics, and probing the microstructure and interface structures of the crystallized thin films. Nearly stoichiometric amorphous PrAlO3 thin films were grown via ALD at 300 °C using tris(isopropylcyclopentadienyl)praseodymium, AlMe3, and water with a growth rate of 2.0 Å/cycle on TiO2-terminated STO (001) substrates. The as-deposited amorphous PrAlO3 crystallized via SPE to form an epitaxial layer on STO upon annealing at 800 °C for 3h. Our work provides new opportunities to form polar/nonpolar oxide interfaces, and the accompanying 2DEG in novel geometries.

9:48AM R46.00008: Suppression of Metal-Insulator Transition in VO2 by Interfacial Oxygen Migration  QIYANG LU (Presenter), CHANGHEE SOHN, Materials Science and Technology Division, Oak Ridge National Laboratory, GUOXIANG HU, PANCHAPAKESAN GANESH, PAUL KENT, Center for Nanophase Materials and Sciences, Oak Ridge National Laboratory, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory, GYULA ERES, Center for Nanophase Materials and Sciences, Oak Ridge National Laboratory, HO NYUNG LEE, Materials Science and Technology Division, Oak Ridge National Laboratory — Oxygen defects are essential building blocks for designing functional oxides with remarkable properties, ranging from electrical and ionic conductivity to magnetism and ferroelectricity. Oxygen defects therefore can profoundly alter crystal and electronic structures and enables emergent phenomena. In this work, we achieved tunable metal-insulator transition (MIT) in oxide heterostructures by inducing interfacial oxygen vacancy migration. We chose VO2-x as a model system due to its near room temperature metal-insulator transition temperature. We found that depositing a TiO2 capping layer on an epitaxial VO2 thin film can effectively suppress the MIT in VO2. We systematically studied the TiO2/VO2 heterostructures by structural and transport measurements, resonant inelastic x-ray scattering, X-ray photoelectron spectroscopy, and first principles calculations and found that that oxygen vacancy migration from TiO2 to VO2 is responsible for the suppression of MIT. Our findings underscore the importance of the interfacial oxygen “diode” effect in determining electronic structure and functionality, and provide new pathways of designing oxide heterostructures for novel ionotronics and computing devices.

10:00AM R46.00009: Tailoring the low-energy physics of RuO2 by epitaxial strain  JACOB RUF (Presenter), HANJONG PAIK, JASON KAWASAKI, BETUL PAMUK, HARI NAIR, NATHANIEL SCHREIBER, LUDI MIAO, DARRELL G. SCHLOM, KYLE M SHEN, Cornell University — Rutile ruthenium dioxide (RuO2) was long presumed to be a paramagnetic metal with weak electronic correlations, until recent measurements of antiferromagnetism in bulk single crystals by Berlijn et al. Motivated by this discovery to better understand its electronic structure, we synthesized RuO2 thin films by molecular-beam epitaxy on rutile TiO2 substrates and characterized these films using \textit{in situ} angle-resolved photoemission spectroscopy (ARPES). Comparing our ARPES data with density-functional calculations, we find that: (1.) electron-phonon coupling accounts for most of the modest quasiparticle mass renormalizations observed in RuO2, and (2.) a sizable crystal field splitting in the rutile structure lifts the threefold degeneracy of the t_{2g} manifold spanning the Fermi level (\( E_F \)), causing strong departures from the prototypical Hund's metal behavior observed in perovskite-based ruthenates, despite having the same electron count of 4d^4. Guided by this understanding of the effective low-energy physics, we explain how epitaxial strain modifies the orbital occupations in RuO2 films grown on different orientations of TiO2 substrates, and discuss how concomitant changes to the density of states near \( E_F \) feed back into the instability of strained RuO2 towards superconductivity.
10:12AM R46.00010: Physical properties of LaFeO$_3$ and Pr$_{2-x}$Ce$_x$CuO$_4$ superstructures* GUILLAUME HARDY, PRIYANKA BROJABASI, PATRICK FOURNIER (Presenter), Universite de Sherbrooke — Charge transfer in electron-doped Sm$_2$CuO$_4$ (SCO) and LaFeO$_3$ (LFO) superstructures (SS) grown by RF sputtering was predicted based on their band structure. STEM-EELS measurements revealed the presence of extra electrons at the interface between SCO and LFO[1]. However, the growth conditions left open questions regarding the actual doping of the SCO layers. We have grown SS of electron-doped Pr$_{2-x}$Ce$_x$CuO$_4$ (PCCO) and LaFeO$_3$ by pulsed-laser deposition with various thicknesses and annealing conditions. X-ray diffraction confirms the coherent growth of PCCO/LFO SS. Superconductivity is confirmed for selected samples by magnetic susceptibility and resistivity measurements, while the Hall Effect of low resistivity samples was carried out for all temperatures. A strong dependence of carrier density and the critical temperature as a function of annealing conditions and thickness of the SS subcomponents is observed. Our results indicate that charge transfer might not be the only source of charge carriers in these structures as annealing conditions are playing a central role in our PLD-grown superstructures.


*We acknowledge the technical support of B. Rivard and the financial support from NSERC, FRQ-NT, CFREF and CFI.

10:24AM R46.00011: X-ray imaging of ionically-controlled nanoscale phase separation in cobaltites* GEOFFERY IAN RIPPY, LACEY L TRINH, ALEXANDER MICHAEL KANE, ALEKSEY IONIN, MICHAEL STEVEN LEE, RAJESH V CHOPDEKAR, Materials Science and Engineering, University of California Davis, DUSTIN GILBERT, ALEXANDER GRUTTER, NIST Center for Neutron Research, NIST Gaithersburg, PEYTON MURRAY, Physics, University of California Davis, MARTIN HOLT, ZHONGHOU CAI, Advanced Photon Source, Argonne National Laboratory, KAI LIU, Physics, University of California Davis, YAYOI TAKAMURA, ROOPALI KUKREJA (Presenter), Materials Science and Engineering, University of California Davis — Controlling ionic distributions and stoichiometry provides a unique way for manipulating functional properties in perovskite oxides (ABO$_3$). This talk will focus on Gd/La$_{0.67}$Sr$_{0.33}$O$_3$ (LSCO) heterostructures due to high oxygen ion conductivity, as well as the coupled magnetic and electronic properties of LSCO, which are strongly dependent on the oxygen stoichiometry. This enables the ionic control of the functional properties of LSCO thin films through the presence of oxygen getter layers such as Gd. We utilize x-ray nanodiffraction to directly image the nanoscale morphology of LSCO thin films as they are progressively transformed from the equilibrium perovskite phase to the metastable brownmillerite (ABO$_{2.5}$) phase with increasing Gd thickness. Our studies show the coexistence of perovskite and brownmillerite phases with a critical oxygen vacancy concentration threshold which leads to the formation of extended brownmillerite filaments. In addition to lateral phase separation, we observed phase separation along the thin film thickness due to pinning of perovskite or brownmillerite by substrate/LSCO or Gd/LSCO interface respectively. Our measurements highlight local structural effects and provide insights into nanoscale strain behavior in Gd/LSCO heterostructures

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10:36AM R46.00012: Lifshitz transition and emergence of Van Hove singularity at the complex oxide heterostructure* RYO MORI (Presenter), University of California, Berkeley, PATRICK MARSHALL, KAVEH AHADI, University of California, Santa Barbara, JONATHAN DENLINGER, Lawrence Berkeley National Laboratory, SUSANNE STEMMER, University of California, Santa Barbara, ALESSANDRA LANZARA, University of California, Berkeley — Electronic correlations strongly depend on the topology of a given electronic structure. A Van Hove singularity (VHS), where the curvature of the electronic bands has opposite sign in two orthogonal directions, is a critical point for a change in electronic topology (Lifshitz transition). It has been considered to be the key to inducing many new unconventional states, especially when it is close to the Fermi level. By using angle-resolved photoemission spectroscopy, we will show the direct evidence of Lifshitz transition and an emergence of VHS in the oxide heterostructures with the different quantum well structures, revealing a new pathway to tune VHS and the corresponding electronic topology at a complex oxide heterointerface.

*This work was primarily supported by the Quantum Materials Program at LBNL, funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Science and Engineering Division, under Contract No. DE-AC02-05CH11231.
8:00AM R47.00001: Mapping experimental electronic transport measurements on appropriate band structure models*  
T. ETHAN STEARNS (Presenter), ANDREW R SUPKA, Department Physics and Science of Advanced Materials Program, Central Michigan University, NICHOLAS A MECHOLSKY, Department of Physics, Catholic University of America, MARCO BUONGIORNO NARDELLI, Department of Physics, University of North Texas, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science, Duke University, MARCO FORNARI, Department Physics and Science of Advanced Materials Program, Central Michigan University — For several years, established guiding principles based on effective masses, carrier density, and constant relaxation time have been heuristically used to interpret trends in the power factor. In spite of many simplifying assumptions, the Sommerfeld model has became a standard for thermoelectricity. To verify and validate this interpretative approach we have developed a software tool that, using experimental electronic transport data, leads to band structure parameters that can then be compared with first principles calculations. We present our software tool by illustrating few specific examples for complex sulfides.

*We acknowledges collaboration within the AFLOW Consortium (www.aflow.org) under the sponsorship of DOD-ONR (Grants N000141310635 and N000141512266).

8:12AM R47.00002: Selective breakdown of phonon quasiparticles across superionic transition in CuCrSe2*  
OLIVIER DELAIRE (Presenter), Duke University, JENNIFER L NIEDZIELA, Oak Ridge National Laboratory, DIPANSHU BANSAL, Duke University, ANDREW MAY, Oak Ridge National Laboratory, JINGXUAN DING, TYSON LANIGAN-ATKINS, Duke University, GEORG EHLERS, DOUGLAS L ABERNATHY, Oak Ridge National Laboratory, AYMAN SAID, Argonne National Laboratory — Superionic crystals exhibit ionic mobilities comparable to liquids while maintaining a periodic crystalline lattice. The atomic dynamics leading to large ionic mobility have long been debated. A central question is whether phonon quasiparticles - which conduct heat in regular solids - survive in the superionic state, where a large fraction of the system exhibits liquid-like behaviour. Here we present the results of energy- and momentum-resolved scattering studies combined with first-principles calculations and show that in the superionic phase of CuCrSe2, long-wavelength acoustic phonons capable of heat conduction remain largely intact, whereas specific phonon quasiparticles dominated by the Cu ions break down as a result of anharmonicity and disorder. The weak bonding and large anharmonicity of the Cu sublattice are present already in the normal ordered state, resulting in low thermal conductivity even below the superionic transition. These results demonstrate that anharmonic phonon dynamics are at the origin of low thermal conductivity and superionicity in this class of materials.

*INS/IIXS supported by S3TEC EFRC, DOE BES #DESC0001299. First-principles modeling supported by US DOE BES Early Career Award #DESC0016166. Sample synthesis supported by US DOE BES, MSED.

8:24AM R47.00003: Is AgCrSe2 really a phonon-liquid electron-crystal?  
SERCAN ARSLAN (Presenter), Physics Department, Royal Holloway University of London, DAVID VONESHEN, ISIS Pulsed Neutron and Muon Source, Science and Technology Facilities Council, PAUL STEFFENS, Institut Laue-Langevin, UTHAYAKUMAR SIVAPERUMAL, Physics Department, Royal Holloway University of London, ROBIN S. PERRY, Physics Department, University College London, JON GOFF, Physics Department, Royal Holloway University of London — The phonon liquid concept, in which superionic diffusion prevents the propagation of transverse acoustic phonons, has proved a popular view in the hunt for materials with ultra-low thermal conductivity. Recent inelastic neutron scattering results on AgCrSe2 have found a quasielastic signal (QENS) around 2 Å\(^{-1}\), and suppression of the transverse phonons above the superionic transition. The QENS scattering has been attributed to the melting of the Ag lattice and it is observed to increase dramatically above the superionic transition. Now, using polarised inelastic neutron scattering we determine the origin of this QENS below and above the superionic transition. The validity of a phonon-liquid in AgCrSe2 will be discussed in light of these results.

8:36AM R47.00004: Nanoscale thermal metrology using SEM, TEM, and confocal microscopy [Invited]  
CHRIS DAMES (Presenter), University of California, Berkeley — Nanoscale thermal transport plays a fundamental role in several current research directions in thermoelectric materials, from nanocrystalline composites to transport in thin films and nanowires. However, experimental measurements of the thermal properties of such materials at the nanoscale is challenging. In this talk I will present several collaborative efforts to develop new non-contact methods for heating and thermometry at the nanometer scale, techniques which could eventually be applied to characterize thermoelectric materials. Examples to be discussed include methods based on SEM (e-beam as a point heater; secondary electron yield as a thermometer), TEM (thermometry using the Debye-Waller effect), and confocal microscopy (luminescence thermometry of individual nanoparticles).
Thermoelectric Properties of Carbon-rich Boron Carbide Nanocomposites* YUCHENG LAN, JESSE DAMPARE, MOBOJAJI ZONDODE, Department of Physics and Engineering Physics, Morgan State University, HUA DENG, Department of Chemistry, Morgan State University, SZ-CHIAN LIOU, Advanced Imaging and Microscope Laboratory, Maryland NanoCenter, University of Maryland, SAROJ PRAMANIK, Department of Biology, Morgan State University, ABDELLAH LISFI, Department of Physics and Engineering Physics, Morgan State University, CHUNDONG WANG, School of Optical and Electronic Information, Huazhong University of Science and Technology, YONG-LE PAN, U. S. Army Research Laboratory, WINNIE WONG-NG (Presenter), Materials Measurement Science Division, National Institute of Standards and Technology — Boron carbide is widely used in industry and military because of its low mass-density, super high hardness, good electric conductivity, and excellent mechanical properties. The material is also one high-temperature thermoelectric compound capable for applications above 1000 °C. However, its thermoelectric properties, such as Seebeck coefficient and figure-of-merit, are low and need to be enhanced significantly for high-efficiency energy applications. Nanostructuring is an effective approach to improve thermoelectric properties. Here boron carbide nanomaterials with various chemical composites are prepared and their physical properties (crystallinity, chemical composition, band-gap, defects etc) are characterized. The as-synthesized nanomaterials are then bottom-up-ed to bulk nanocomposites. Thermoelectric properties of the bulks are measured. Their microstructures are characterized by X-ray powder diffraction, scanning electron microscopy, transmission electron microscopy, Raman scattering, and UV-vis spectroscopy etc. The enhanced performances of the carbide nanocomposites are like a result of their unique nanostructures.

*The work is partially supported by W911NF-12-2-0022 and NSF DMR 1206380.

Resolving Thermal Conductivity Spectrums through Time-resolved Spatial-Temporal Imaging* DING DING (Presenter), KEDAR HIPPALGAONKAR, Institute of Materials Research and Engineering — With the advent of nano-engineered and 2D materials, quasiballistic and anisotropic effects have become more commonplace in thermal properties of these material systems. However, current methods to measure these properties through thermal conductivity generally requires variation of spatial or temporal parameters, or measurement of multiple samples with tedious fabrication procedures. Here, we numerically propose an optical pump-probe technique that uses time-resolved spatial and temporal temperature profile to characterize both quasiballistic and anisotropic thermal transport with no variation of experimental parameters. By performing heat-flow analysis of the thermal profile with multi-parameter optimization, we are able to obtain the thermal conductivity spectrums of both the in-plane and cross-plane heat transport as a function of temporal and spatial frequencies, respectively. Such spectrums can then be used to derive the anisotropy in thermal conductivity and the phonon mean-free-path spectrums within a single experiment. We believe that this technique can enable high throughput screening of thermal properties for nano-engineered and 2D materials.

*This work was supported by AME Programmatic Fund by the Agency for Science, Technology and Research under Grant No. A1898b0043.

Right Definition of Thermoelectric Figure of Merit toward the Thermoelectric Efficiency Prediction for Segmented Devices* BYUNGGI RYU (Presenter), JAYWAN CHUNG, SUDONG PARK, Korea Electrotechnology Research Institute — The dimensionless figure of merit zT has been considered as a good metric for thermoelectric efficiency. But, due to the strong temperature dependence of material properties, the relation between the material properties and device performances is not clear. Here, we generalize the definition of device figure of merit $Z_{gen}T$. Since the thermoelectric leg acts as a electric and a thermal circuit, the $Z_{gen}$ should be written as $Z_{gen} = (V/\Delta T)^2/RK$, where V, R, and K are generated voltage, electric resistance, and the thermal conductance. Thus V, R, and 1/K should be computed as integrals of material properties ($-\alpha, \rho, \kappa$) on position x, not on temperature T. Using the temperature approximation of zero-electric-current condition, the $Z_{gen}$ is simply approximated as $Z_{gen}^{(0)} = <\alpha^2>/<\rho\kappa>$, where <> is a temperature average. Also we reveal that the $Z_{gen}^{(0)}$ is a good rank-preserving-parameter for efficiency prediction even for the segmented devices.

*This work was supported by KERI Primary research program through the NST funded by the MSIP (No. 18-12-N0101-34).
9:48AM R47.00008: NMR investigation of filled skutterudites \(\text{Ba}_x\text{Yb}_y\text{Co}_4\text{Sb}_{12}\) and \(\text{A}_x\text{Co}_4\text{Sb}_{12}\) (\(A = \text{Ba, Sr}\)) \(^{*}\)  

YEFAN TIAN (Presenter), ALI SIRUSI, Department of Physics and Astronomy, Texas A&M University, SEDAT BALLIKAYA, Department of Physics, Istanbul University, NADER GHASSEMI, Department of Physics and Astronomy, Texas A&M University, CTIRAD UHER, Department of Physics, University of Michigan, JOSEPH HANSBRO ROSS, Department of Physics and Astronomy, Texas A&M University —

Considered as one of the most promising thermoelectric families, skutterudite \(\text{CoSb}_3\) shows a high \(ZT\) value when prepared with filler atoms such as \(\text{Ba, Sr, Yb, etc.}\) We report \(^{59}\text{Co}\) NMR and transport measurements on \(\text{BaxYbyCo}_4\text{Sb}_{12}\) and \(\text{AxCo}_4\text{Sb}_{12}\) (\(A = \text{Ba, Sr}\)) as promising thermoelectric candidates. To analyze the experimental results, we developed a formalism for the NMR shifts and \(T_1\), allowing for arbitrary carrier densities rather than treating the extreme metallic or non-degenerate limit. We find that a model in which a large density of defect states located just below the conduction band edge dominate the electrical behavior works very well, providing a consistent picture of both the NMR and transport results. The carrier effective masses and \(g\)-factors estimated from NMR fitting results are in close agreement with each other. Additional contributions observed in shift and \(1/T_1\) measurements are shown to correspond to the susceptibility of electrons in localized states.

\(^*\)This work was supported by the Robert A. Welch Foundation, Grant No. A-1526. Synthesis of skutterudites samples at the University of Michigan was supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Award DE-SC-0000957.

10:00AM R47.00009: Rattling dynamics under a planar coordination in tetrahedrites  

CHUL-HO LEE (Presenter), National Institute of Advanced Industrial Science and Technology, KOICHIRO SUEKUNI, Kyushu University, EIJI NISHIBORI, University of Tsukuba, HITOSHI MORI, HIDETOMO USUI, MASAYUKI OCHI, Osaka University, TAKUMI HASEGAWA, Hiroshima University, MITSUTAKA NAKAMURA, SEIKO OHIRA-KAWAMURA, KOJI KANEKO, Japan Atomic Energy Agency, KATSUAKI HASHIKUNI, Hiroshima University, KAZUHIKO KUROKI, Osaka University, TOSHIRO TAKABATAKE, Hiroshima University — Suppressing lattice thermal conductivity \((k_L)\) as low as possible is essential to achieve high thermoelectric performance. One of effective methods is to use the rattling which is large anharmonic vibration of atoms. Typically, rattling atoms locate in oversized atomic cages of caged compounds. Recently, we found several new thermoelectric materials that contain rattling atoms without oversized cages. In \(\text{LaOBiS}_{2}\) and tetrahedrites, \(\text{Bi}\) and \(\text{Cu}\) atoms having a planar coordination vibrate largely toward out of plane [1-3]. We investigated crystal structures and phonon dynamics of tetrahedrites to clarify the driving force for the occurrence of rattling in a planar coordination. We found that the amplitude of \(\text{Cu}\) rattling increases with decreasing \(\text{S}_3\)-triangle area. The rattling energy observed by inelastic neutron scattering decreases with decreasing the \(\text{S}_3\)-triangle area and finally damped demonstrating an enhancement of anharmonicity. The results suggest that chemical pressure is essential for the appearance of planar rattling in contrast to caged compounds where free space is essential. [1] Y. Mizuguchi et al., J. Appl. Phys. 119, 155103 (2016). [2] C. H. Lee et al., Appl. Phys. Lett. 112, 023903 (2018). [3] K. Suekuni, C. H. Lee et al., Adv. Mater. 30, 1706230 (2018).

10:12AM R47.00010: Enhancement of thermoelectric figure of merit by pressure-driven electronic topological transition  

LIUCHENG CHEN (Presenter), Center for High Pressure Science and Technology Advanced Research, PEI-QI CHEN, Science, Mathematics, Computer Science Program,Poolesville High School, VIKTOR V STRUZHKA, ALEXANDER GONCHAROV, Geophysical Laboratory, Carnegie Institution of Washington, QIAN ZHANG, ZHIFENG REN, Department of Physics and TcSUH University of Houston, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research — The world is currently facing a state of energy shortage, and thus the alternative green energy is ultimately in demand. Thermoelectric generators, which can generate electricity directly from waste heat with the advantages of reliability and compactness, are considered as potential devices for waste heat recovery. The thermoelectric performance is usually evaluated by a parameter named as the figure of merit \(ZT\). So far, the maximum \(ZT\) at room temperature has remained around 1.0 over sixty years. For practical technological applications, it is highly desired to break this barrier. Here, we choose a Cr doped PbSe with the maximum \(ZT\) less than 1.0 at high temperature of about 700 K. By simply applying external pressure, we obtain the record high \(ZT\) value of 1.74 at room temperature. Pressure-driven electronic topological transition is proposed to account for such a huge enhancement. These results and findings point to a new direction in the improvement of \(ZT\) in the existing thermoelectric materials through the lattice compression.
10:24AM R47.00011: Impressive enhancement of thermoelectric performance in CuInTe2 upon compression  
HAO YU (Presenter), LIUCHENG CHEN, HONGJIE PANG, Center for High Pressure Science & Technology Advanced Research, XIAOYING QIN, Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, PENGFEI QIU, XUN SHI, LIDONG CHEN, Chinese Academy of Sciences, XIAO-JIA CHEN, Center for High Pressure Science & Technology Advanced Research — Thermoelectric materials can directly generate electric power by converting waste heat, and the efficiency is appraised by the figure of merit $zT$. A high $zT$ value larger than 3 is required to achieve comparable efficiency of the traditional heat engines. Despite great efforts over a century, the desired value of 3 is seemingly an upper limit and many existing thermoelectric materials have the $zT$ values less than 1. If their $zT$ values can be improved for several times to break through the upper limit, the energy revolution could be expected. Here, a p-type CuInTe2 is chosen as an example to show the extremely important role of pressure played in enhancing the thermoelectric performance. Over 5 times increase of the $zT$ value is realized by the application of pressure. Both the enhancement of the power factor and the reduction of the thermal conductivity account for this impressive enhancement. The former is due to the optimization of the carrier concentration and band structure, and the latter is attributed to the enhanced phonon anharmonicity. Our results offer an effective method to improve $zT$ of the existing materials for the future technological applications.

10:36AM R47.00012: Thermoelectric sulfides with the colusite structure: theory and experiments*  
VENTRAPATI PAVAN KUMAR, ENSICAEN, UNICAEN, CNRS, CRISMAT, Normandie Univ, ANDREW R SUPKA, Dept. of Physics and Science of Advanced Materials Program, Central Michigan University, PIERRIC LEMOINE, CNRS, ISCR, Univ. Rennes, OLEG I. LEBEDEV, BERNARD RAVEAU, ENSICAEN, UNICAEN, CNRS, CRISMAT, Normandie Univ, KOICHIRO SUEKUNI, Dept. of Applied Science for Electronics and Materials, Kyushu University, VIVIAN NAASSIF, CNRS, Univ. Grenoble Alpes, RABIH AL RAHAL AL ORABI, MARCO FORNARI (Presenter), Dept. of Physics and Science of Advanced Materials Program, Central Michigan University, EMMANUEL GUILMEAU, ENSICAEN, UNICAEN, CNRS, CRISMAT, Normandie Univ — We have achieved extraordinary power factors in bulk thermoelectric sulfides with the colusite structure without compromising the low lattice thermal conductivity. Using a synergy between high-throughput calculations and experiments we learned a possible strategy to engineer the electron relaxation time. The protocol is based on the “conductive network paradigm”, it has been applied to a variety of compositions and lead to power factors up to 1.86 mW m$^{-1}$ K$^{-2}$ at 700K and $zT$=0.86 before any optimization procedure.

*French Agence Nationale de la Recherche (ANR), through the program Energy Challenge for Secure, Clean and Efficient Energy (Challenge 2, 2015, ANR-15-CE05-0027); International Joint Research Program for Innovative Energy Technology funded by the Ministry of Economy, Trade and Industry (METI), Japan. The AFLOW Consortium (http://www.aflow.org) under the sponsorship of DOD-ONR (Grants N000141310635 and N000141512266).

10:48AM R47.00013: Thermoelectric transport properties with non-parabolicity, degeneracy and multiplicity of band edges: The case of anisotropic p-type SnSe*  
ANDERSON CHAVES (Presenter), John A. Paulson School of Engineering and Applied Sciences, Harvard University, JUAN J MELENDEZ, Physics Department, University of Extremadura, ROBERT L GONZALEZ-ROMERO, Departamento de Sistema Físicos, Químicos y Naturales, Universidad Pablo de Olavide, ALEX ANTONELLI, Gleb Wataghin Institute of Physics, University of Campinas — Efficient ab initio computational methods for the evaluation of transport properties of thermoelectric (TE) materials, are highly important for the development of energy harvesting technologies. The BOLTZTRAP code [1] has been widely used for this aim. However, its current version relies only on the constant relaxation time (RT) approximation, within the Boltzmann transport equation. Here, we extend the implementation of the BOLTZTRAP code by incorporating realistic k-dependent RT models of the main scattering processes, namely, screened polar and nonpolar scattering by optical phonons, scattering by acoustical phonons, and scattering by screened ionized impurities. The RT models are based on a smooth Fourier interpolation of the Kohn-Sham eigenvalues and its derivatives, thus, taking into account non-parabolicity, degeneracy and multiplicity of the band edges on equal footing, at a very low computational cost. To test our approach, we determined the anisotropic TE transport properties of the Pnma phase of p-type SnSe. Our results for the evolution of TE coefficients with both temperature and chemical potential are in agreement with the experimental data.


*This work was supported by Fapesp grant 2015/26434-2.
**Thursday, March 7, 2019 8:00 AM - 10:00 AM**

**Session R48 DFD GSOFT GSNP: Drops I** BCEC 251 - Daniel Harris, Brown University - Tag(s): Focus

8:00AM R48.00001: Marangoni convection in an evaporating sessile droplet depending on the substrate temperature.* LEV BARASH (Presenter), Landau Institute for Theoretical Physics, ALEXANDRA GAVRILINA, National Research University Higher School of Economics — We investigate numerically quasi-steady internal flows in an axially symmetrical evaporating sessile droplet of capillary size. The hydrodynamics of an evaporating sessile drop and effects of the thermal conduction in the droplet and substrate have been taken into account jointly. The equations have been solved by finite element method using ANSYS Fluent. Temperature distributions and the corresponding vortex structures in evaporating sessile droplets are obtained. The phase diagrams containing information on the number and orientation of the vortices depending on the ratio of substrate to fluid thermal conductivities and the contact angle, are presented and analyzed for different values of parameters. Depending on the substrate temperature, we obtain both axisymmetric and asymmetric fluid flow patterns.

*This work was supported by the Russian Science Foundation (project No. 18-71-10061).

8:12AM R48.00002: Spreading and contracting three-component droplets for cleaning high energy surfaces DIETER BAUMGARTNER (Presenter), ETH Zurich, SHAYANDEV SINHA, NATE J. CIRA, Rowland Institute at Harvard — Marangoni flows are a well established mechanism for inducing droplet spreading and contraction. In this work, we study the behavior of a three-component mixture (ethanol, water, and propylene glycol) on high energy surfaces. Evaporation of the ethanol (most volatile, lowest surface tension) results in a higher surface tension around the perimeter of the droplet and rapid spreading. After ethanol evaporation, water evaporation (next most volatile component, highest surface tension) from the perimeter induces a reversal in the direction of Marangoni flow and droplet contraction. We investigate this ternary parameter space to unravel the interplay of Marangoni flow, capillary flow, and evaporation. The self-expansion and contraction of these droplets make them suitable for cleaning even high energy surfaces.

8:24AM R48.00003: Binary Droplets Walking With Their Feet.* JEHAN CHARLIER (Presenter), ALEXEY REDNIKOV, SAM DEHAECK, PIERRE COLINET, DENIS TERWAGNE, Universite libre de Bruxelles — We shed new light on paramount but so far highly elusive morphological features of perfectly wetting binary sessile droplets evaporating into air with a more volatile component possessing higher surface tension (water + propylene glycol). By both interferometric measurements of the detailed shapes of the drops and theoretical developments, we show that there is a narrow high-curvature zone due to the solutal Maranoni effect localized near the edge (foot) of the droplet that dictates the overall droplet shape and behavior by means of induced apparent contact angles. The phenomenon is studied as a function of the mass fraction of the components in the droplet and the ambient relative humidity. We devise a local model, based on the lubrication approximation and Marangoni-flow-related Taylor dispersion, that enables to predict the apparent contact angles without any fitting parameters or invoking any microphysics. Motion dynamics of such droplets in a humidity gradient is also studied.

*We are grateful for the support from BELSPO PRODEX and ESA MAP projects and the Fond de la Recherche Scientifique – FNRS

8:36AM R48.00004: Tears of Wine PRERANA RATHORE (Presenter), CHENXIAN XU, VIVEK SHARMA, University of Illinois at Chicago — `Tears of wine` refer to the rows of wine-drops that spontaneously emerge within a glass of strong wine. Evaporation-driven Marangoni flows near the meniscus of water-alcohol mixtures drive liquid upward forming a thin liquid film, and a rim or ridge forms near the moving contact line. Eventually, the rim undergoes an instability forming drops, that roll back into bulk reservoir forming so-called tears or legs of wine. Most studies in literature argue the evaporation of more volatile, lower surface tension component (alcohol) results in a concentration-dependent surface tension gradient that drives the climbing flow within the thin film. Though it is well-known that evaporative cooling can create temperature gradients that could provide an additional contribution to the climbing flows, the role of thermocapillary flows is less well-understood. Furthermore, the patterns, flows and instabilities that occur near the rim, and determine the size and periodicity of tears, are not well-studied. Using experiments and theory, we visualize and analyze the formation and growth of tears of wine. The sliding drops, released from the rim towards the bulk reservoir, show oscillations and a cascade of fascinating flows that are analyzed for the first time.
Efforts to numerically model droplet-resolved, nonwetting emulsions in complex environments have been stymied, chiefly as multiphase flow through fibrous materials, packed beds with complex pellet shapes, and tortuous subsurface settings. Emulsions are encountered in a variety of environments, such as multiphase flow through fibrous materials, packed beds with complex pellet shapes, and tortuous subsurface settings. Efforts to numerically model droplet-resolved, nonwetting emulsions in complex environments have been stymied, chiefly due to the extremely close approach of fluid-fluid interfaces to solid surfaces. A multimesh desingularization technique is introduced to model the flow of tight-squeezing drops through arbitrary Lyapunov surfaces, i.e., smooth solid obstacles, using a boundary-integral formulation. The method utilizes a hierarchy of embedded mesh resolutions to approximate analytical single- and double-layer contributions from solid particles, for use by the high-order singularity subtraction scheme introduced by Zinchenko and Davis (2006). We present a fully three-dimensional study of drop squeezing through parallel cylindrical particles. Squeezing behavior through a fibrous material using this model is characterized with respect to capillary number, viscosity ratio and droplet size. The critical capillary number, below which trapping occurs, is found to lie between those of two-sphere and three-sphere constrictions.

9:36AM R48.00009: A versatile 3D-printed droplet-on-demand generator NIKOLAY P IONKIN (Presenter), DANIEL M HARRIS, School of Engineering, Brown University — There is a rapid and persistent growth in the study of dynamical behavior of droplets, however, the precise generation of these droplets over a range of sizes can be challenging. A versatile 3D-printed droplet-on-demand generator is presented for laboratory use. The design is modeled off of an existing design [Harris et al., Experiments in Fluids, 56:83 (2015)] but is tested with an extended range of working fluids and the manufacturing process is greatly simplified by 3D-printing the principal components. The present device is tested with deionized water and water-glycerol mixtures, and was reliably able to produce single droplets-on-demand of diameters 0.65-1.32 mm with an overall variability of less than 1%. Tips for fabrication, operation, and maintenance as well as potential applications will be discussed throughout.
9:48AM R48.00010: Axisymmetric Ellipsoidal Droplet Impact on a Horizontal Solid Surface*  XUAN ZHANG (Presenter), XIN LIU, XIAOMIN WU, JINGCHUN MIN, Tsinghua University — Droplet impact process on a solid surface exists in fields such as coating chemistry, inkjet printing, aerospace, etc. In many cases, the initial shape before a droplet impacts on the surface will be effected by the surroundings including flow, gravity and electric field and so on. Thus, a droplet with irregular initial shape will have a quite different impact process from a spherical droplet. In this work, the impact processes of spherical droplets are first simulated using VOF multiphase model coupled with Kistler's dynamic contact angle model, which is verified by the results in our experiment and reference. Then, simulations are conducted on the impact processes of axisymmetric ellipsoidal droplets with different aspect ratios (0.5~2.0) under serials of contact angle (30°~150°) and We number (10~90). It is found that the maximum spreading factor and its corresponding time increases with increases of We number and aspect ratio and decrease of contact angle. Based on an approximate theoretical analysis, an correlation between the maximum spreading factor and We number, contact angle and aspect ratio is proposed, aimed to improve the understanding of the mechanism of droplet impact.

*This work is funded by the National Key Basic Research Program of China (No. 2015CB755800).

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R49 DPOLY DBIO DFD GSNP: Polymer and Polyelectrolyte Rheology I: Molecular Sequence and Architecture  BCEC 252A - Samanvaya Srivastava, University of California, Los Angeles - Tag(s): Focus

8:00AM R49.00001: Elasticity of Self-Assembled Block Copolymers in Water and Oil Mixtures*  SAHAR QAVI (Presenter), Chemical and Materials Engineering, New Mexico State University, MILLICENT FIRESTONE, Los Alamos National Laboratory, REZA FOUDAIZI, Chemical and Materials Engineering, New Mexico State University — Amphiphilic block copolymers self-assemble at water/oil interface and form different mesomorphic structures such as lamellar, micellar cubic, normal hexagonal and reverse hexagonal. Usually, these structures are polycrystalline and their elasticity depends on the orientation of their constituent's single crystals. We provide a model to predict the elasticity and yielding of mesophases from their characteristic length and intermicellar interactions. Shear modulus of each structure has been calculated as a function of deformation (strain) applied in one direction. Zero shear modulus, G0, depends on the inverse of intermicellar distance with a power-law model. The power-law index for each structure is about n+2 where n is the degree of confinement in mesophase. Rheological properties of different mesophases of Pluronic P84 in the presence of water and p-xylene are used as case study. Our model is in good agreement with experimental data in the linear viscoelastic region. However, the yield strain value of experimental data is slightly lower than that of the model. Frequency sweep measurements were done to further characterize each mesophase structure and cooperative model was used to fit the frequency sweep data of mesophases.

*This work was supported by BoR, CINT, and NSF.

8:12AM R49.00002: Exploring dynamics of polymerlike wormlike micelles in high shear flow*  PAUL SALIPANTE, ALEX CONTE, VISHNU DHARMARAJ, STEVEN HUDSON (Presenter), National Institute of Standards and Technology — Wormlike micelle solutions entangle and flow like polymers, yet micelles can break and reform. Stress may influence breakage dynamics and the microscopic behavior of these fluids at high stress is not understood. We explore this behavior in pressure-driven microchannel flow. Velocity profiles are measured with high resolution using holographic 3D microparticle tracking velocimetry, to determine the relationship of stress and shear rate. As reported by others, this relationship depends on wall stress and channel dimensions and suggests diffusive processes whose rate depends on channel dimension. We therefore are measuring the local solution concentration with fluorescence microscopy, to explore molecular diffusion. We compare our velocity and concentration profiles to theoretical models that include a diffusive term in the stress balance, which becomes relevant at small channel dimensions.

*The National Institute of Standards and Technology on a Chip funding is gratefully acknowledged.
observed, demonstrating high fiber stiffness (increased by 104) with minimal water consumption. The fibers swell to a diameter of 600% in a gel-like structure at low pH. At neutral pH, the ionization degree is at least 79% and deswelling is along the fibers. The fibers demonstrate pH-responsive behavior with 17% ionization degree and an increase in fiber macromolecular orientation along the fiber axis which implies a better packing of macromolecules due to their orientation confining this solution by electrospinning results in 300-600 nm fibers. Polarized FTIR demonstrates preferred The PECs in aqueous medium was opaque but at 40% ethanol solution was transparent. Extensive stretching and of water/ethanol. Rheological investigation of semi-dilute solution demonstrated maximal relative viscosity at 40% ethanol. studied with 1:1 (by monomer ratio) poly(acrylic acid) (PAA) and poly(allylamine hydrochloride) (PAH) dissolved in a mixture (solid) to coacervates (elastic liquid) to dissolved solutions with increasing salt concentration. In case one of the PEs is dilute solutions of highly charged oppositely polyelectrolytes (PEs) generally yields compositions spanning complexes (solid) to coacervates (elastic liquid) to dissolved solutions with increasing salt concentration. In case one of the PEs is weakly charged, the PE pair can be dissolved without salt by adding an organic co-solvent. Such a system was recently studied with 1:1 (by monomer ratio) poly(acrylic acid) (PAA) and poly(allylamine hydrochloride) (PAH) dissolved in a mixture of water/ethanol. Rheological investigation of semi-dilute solution demonstrated maximal relative viscosity at 40% ethanol. The PECs in aqueous medium was opaque but at 40% ethanol solution was transparent. Extensive stretching and confining this solution by electrospinning results in 300-600 nm fibers. Polarized FTIR demonstrates preferred macromolecular orientation along the fiber axis which implies a better packing of macromolecules due to their orientation along the fibers. The fibers demonstrate pH-responsive behavior with 17% ionization degree and an increase in fiber diameter of 600% in a gel-like structure at low pH. At neutral pH, the ionization degree is at least 79% and deswelling is observed, demonstrating high fiber stiffness (increased by $10^4$) with minimal water consumption.

*This work is funded by ACS PRF Award # 54633-ND7.
Effect of edge disturbance on shear banding in polymeric solutions

SEUNGHWAN SHIN (Presenter), KEVIN DORFMAN, XIANG CHENG, University of Minnesota — Edge-induced instabilities have been suggested as one of the possible causes of experimentally observed shear-banding in well-entangled polymer solutions/melts. Using a high-aspect-ratio planar-Couette shear cell, we study the penetration length ($L$) of edge disturbance and the development of bulk shear profiles in highly entangled DNA solutions by measuring shear profiles while varying the locations from near-edge to center of the shearing plates. Under a weak oscillatory shear flow, where the corresponding Weissenberg number ($Wi$) > 1 and the DNA solutions display linear shear profiles with strong wall-slip, we find that $L$ is comparable to the gap ($H$) between the plates. On contrary, under a stronger oscillatory shear ($Wi$ > 1) that produces shear-banding profiles, $L$ is an order-of-magnitude larger than $H$ and the region of the stabilized shear-banding profiles becomes anisotropic. Moreover, a well-developed shear-banding profile persists farther away from the edge, where the edge effect is negligible, which implies its true bulk nature. Our results clarify a surprisingly long penetration of the edge disturbance and the bulk nature of shear-banding flows in entangled polymeric solutions under large amplitude oscillatory shear.

*This work was supported by NSF Grant No. CBET-1700771.

Viscoelastic Response of Branched Polyethylene Combs: A Molecular Dynamics (MD) Simulation Study

SIDATH WIJESINGHE (Presenter), Department of Chemistry, University Of North Carolina, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National Laboratories — Polymers exhibit distinctive rheological behavior depending on their architecture. Addition of small number of branches is sufficient to affect the rheology of polymers compared to their linear counterpart with the same molecular weight. Here, using coarse grained molecular dynamics simulations we resolve the effects of the branch length and branch density on the viscoelastic response of entangled polyethylene (PE) melts with branch lengths above and below the entanglement length. The stress relaxation behavior is measured following a small perturbation and from the stress autocorrelation function using the Green-Kubo relation. We find that the plateau modulus is sensitive to both branch length and branch density and decreases with decreasing branch length, consistent with reduction in entanglement length and increase in tube diameter. This study contributes to the nanometer level insight into long-lived problems in viscoelastic responses of polymers.

We kindly acknowledge NSF DMR 1611136

Flow behavior and impact of shear fields on structural transitions in diblock and triblock copolymer aqueous solutions

CONNOR S VALENTINE, LYNN WALKER (Presenter), Carnegie Mellon University — Low molecular weight diblock and triblock polymers in selective solvents form disordered micellar phases at low concentration and liquid crystal phases at high concentration (or low solvent to amphiphile molar ratio in the case of water). The energetic barriers between different lyotropic states and structures are large enough for systems to become kinetically trapped, but low enough for weak external fields to alter the nanoscale structure. We have been able to align ordered structures and anneal out defect texture in polycrystalline materials. Results for two different block copolymers in aqueous solution will be shown and rheological features correlated with structural measurements (through SANS and SAXS). The use of weak shear fields to align lyotropic structures and then transition to other low and high symmetry structures will be demonstrated.

Accelerated diffusion and entanglement evolution during relaxation of aligned polymer melts

MARCO GALVANI (Presenter), AUSTIN HOPKINS, Johns Hopkins University, THOMAS O’CONNOR, Sandia National Laboratories, MARK OWEN ROBBINS, Johns Hopkins University — The dynamics of entanglement formation and loss has long been recognized as a fundamental mechanism behind the macroscopic rheological properties of polymer melts. Models based on entanglements and a confining tube have been very successful in describing equilibrium diffusion and low rate viscous flow, but it is not yet clear how to extend these tube models to highly aligned states produced by shear or elongational flow and experiments cannot directly measure entanglements. Here we use molecular dynamics simulations to follow the motion of monomers and chains and the evolution of entanglements during relaxation from highly aligned states produced by shear and elongational flow. Polymers are modeled with the coarse-grained FENE potential with varying chain stiffness and entanglements are followed with both Primitive-Path Analysis and the Z1 code. Chain retraction occurs over the equilibrium Rouse time and chains reorient on the equilibrium disentanglement time. In sharp contrast to existing theories, the entanglement density does not decrease during chain retraction. A monotonic increase in entanglement density is observed that can be understood from the chain dynamics.

Material based upon work supported by the NSF under Grant CMMI-1628974.
10:24AM R49.00011: Filled Rubbers Missing High Harmonics in LAOS  SHAN JIANG (Presenter), School of Chemical Science and Engineering, Tongji University, XIAORONG WANG, Institute for Advanced Study, Tongji University — In the present work, the rheological properties of a number of filled elastomers under large amplitude oscillatory shear conditions are investigated. In the nonlinear regime the stress outputs of filled rubbers are surprisingly sinusoidal and essentially absent of any high harmonics. Fourier transform analysis shows that the ratio of the third to the first harmonic responses (I₃/I₁) in the range when G’ loses 70% of its original value and G” passes through its maximum is typically less than 4%. As the strain amplitude increases the ratio I₃/I₁ also displays a maximum and can be linearly corrected with the damping factor tanδ. Such a relationship is independent of the filler content and may reveal some important fundamentals behind this phenomenon.

10:36AM R49.00012: The positions and trajectories of deformed polymers and networks  KAIAI ZHENG (Presenter), YIFAN ZHANG, Institute for Basic Science, LINGXIANG JIANG, Jinan University, JIANG ZHAO, Chinese Academy of Sciences (CAS), STEVE GRANICK, Institute for Basic Science — This laboratory is interested to understand the heterogeneity that underpins an overall rheological response. To this end, we are integrating fluorescence and phosphorescence imaging with controlled rheological polymer deformations. Integrating epifluorescence imaging with a rheometer, we image individual molecules. Integrating new mechanophores with polymerized networks, we image individual stressed chains. Integrating polymer deformation with a newly-designed approach for fast STED (super-resolution) imaging, we also go below diffraction limitations. Result findings will be discussed.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R50 DPOLY: Ion Transport Mechanisms in Poly(ionic liquids) and Polymer Electrolytes BCEC 252B - Pinar Akcora, Stevens Institute of Technology - Tag(s): Focus

8:00AM R50.00001: Decoupling Conductivity and Segmental Motion in Polymerized Ionic Liquids*  JORDAN KEITH (Presenter), VENKATRAGHAVAN GANESAN, University of Texas at Austin — We characterize diffusion trends in polymerized ionic liquids using atomistic molecular dynamics simulations of a number of anion species and imidazolium cations, both tethered to and implanted in poly-alkyl backbones, to develop design guidelines for polymerized ionic liquids with highly decoupled conductivity and polymer segmental dynamics. We use glass-transition-normalized temperature to compare conductivity for similar segmental dynamics behavior across a variety of chemical species. Results suggest that ion mobility decoupling depends on two distinct modes: 1) a small-ion ion-pairing mode where conduction relies heavily on an ion-hopping mechanism that has been explored previously, and 2) a large-ion free-volume diffusion mode that utilizes large, interconnected gaps in the polymer matrix for diffusion in the absence of segmental motion.

*The authors acknowledge the Texas Advanced Computing Center (TACC) at The University of Texas at Austin, and funding in part by grants from the Robert A. Welch Foundation (Grant F1599), the National Science Foundation (DMR-1721512 and CBET-1706968), and the Donors of the American Chemical Society Petroleum Research Fund (56715-ND9).

8:12AM R50.00002: Molecular design of precise network polymerized ionic liquids to control aggregation and conductivity  QIUJIE ZHAO (Presenter), Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, CHENTHIAN SHEN, Department of Chemistry, University of Illinois at Urbana-Champaign, CHRISTOPHER EVANS, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Polymerized ionic liquids (PILs) are promising energy storage materials due to their high ionic conductivity and great thermal stability. The structure-property relationships of linear PILs have been extensively studied, yet little is known about other polymer architectures such as networks. We synthesized linear and network PILs containing precise linker lengths between charges using step-growth polymerization. Two different linkers were incorporated, either an 11 carbon chain (C11) or a tetra(ethylene oxide) chain (EO, also 11 atoms), to vary the network polarity. Wide-angle X-ray scattering measurements showed that the ion aggregation peaks were less intense in the EO systems, suggesting that the polar backbone provides better ion solvation. Network PILs had more pronounced ion aggregation peaks than their linear counterparts, indicating a role of polymer architecture on ion clustering. In addition, the EO network showed a two orders of magnitude increase in conductivity relative to the linear analogue at Tg+10°C. We hypothesize that the cross-linked structure provides greater correlation of conduction pathways. This systematic study provides a fundamental understanding on how polymer architecture and polarity can influence the aggregation and transport of ions in PILs.
8:24AM R50.00003: Competitive structural and cooperative dynamical heterogeneities of hydrogen bonding and π-type interactions in imidazolium bis(oxalato)borate and polymers  YONGLEI WANG (Presenter), AATTO LAAKSONEN, Department of Materials and Environmental Chemistry, Stockholm University, MICHAEL DAVID FAYER, Department of Chemistry, Stanford University, JIAYIN YUAN, Department of Materials and Environmental Chemistry, Stockholm University — Delicate intermolecular features like hydrogen bonding (HB) and π-type interactions play pivotal roles in stabilizing molecular structures in ionic liquids (IL) bearing ring planes and HB sites. The nature of these interactions is distinct depending on specific ion types. HB and π-type interactions simultaneously occur in ILs consisting of imidazolium cations coupled with small anions. However, both HB and π-type interactions are considerably weakened when imidazolium cations are associated with large anions. The trade-off between HB and π-type interactions becomes more complicated if anions are featured with ring planes. We performed first-principles and atomistic simulations to explore HB and π-type associations in imidazolium bis(oxalato)borate ILs. Preferential HBs and π-type coordinations among ring planes coexist in ILs. Lengthening alkyl chains in cations leads to a substantial increase in HB strength but decrease in π-π stacking stability between ring structures, indicating a competitive structural feature between HB and π-type associations. A cooperative character is observed in HB dynamics and in reorientations of rings with lengthening alkyl chains in cations. We will explore additional structural and dynamical heterogeneities in polymerized ILs in our ongoing work.

8:36AM R50.00004: The Role of Polymer Backbone Chemistry on Ionic Aggregation and Conductivity in Metal-Ligand Coordinating Polymers*  NICOLE MICHENFELDER-SCHAUSER (Presenter), University of California, Santa Barbara, MY LINH LE, Mount Holyoke College, RAM SESHAHRI, RACHEL SEGALMAN, University of California, Santa Barbara — Polymeric ionic liquids capable of conducting multivalent ions are based on metal-ligand coordination interactions. This work explores the roles of polymer backbone chemistry, metal-ligand coordination, and ion concentration on ionic conductivity. In these systems, multivalent ion transport is facilitated via ligands pendant to the polymer backbone. While previous results suggest the matrix dielectric constant affects ion dissociation and aggregate structure, this has been studied only in systems where ions interact directly with the polymer backbone. In the case of pendant ligands, it is not clear immediately that the dielectric constant of the backbone would be relevant in determining ion transport. We show for polymers with pendant imidazole ligands, the local dielectric properties of the polymer backbone, based on either poly(ethylene oxide) (PEO) or poly(butadiene) (PBD), still affect ion aggregation and ionic conductivity. While no aggregation is observed at low salt concentration for the PEO-based polymer, Li+, Zn2+ and Cu2+ show aggregation in the PBD polymer resulting in reduced ionic conductivity. This highlights the importance of backbone dielectric properties even in polymer electrolytes with tethered solvating groups.

*This work is funded by an NSF MRSEC (DMR 1720256).

8:48AM R50.00005: Polymerization of a Imidazolium Ionic Liquid Under 2D Confinement and the Resulting Effects on Ion Dynamics*  THOMAS KINSEY (Presenter), KAITLIN GLYNN, JOSHUA SANGORO, University of Tennessee — We have employed broadband dielectric spectroscopy to probe ion dynamics in 1-ethyl-3-vinylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid (IL) under confinement within ~7nm nanoporous silica membranes. The IL was then polymerized within the pores to a maximum monomer conversion of ~70% as determined using Raman spectroscopy. Compared to the pure systems in bulk, the confined PIL displayed increased ionic conductivity, while the IL displayed decreased ionic conductivity under confinement. To unravel the effects of unconverted monomer and the effects of confinement on the increased ion conduction in the PIL system, a blend of the IL and PIL was prepared at the same monomer to polymer ratio as was achieved during polymerization within the membranes. Decreased conductivity in bulk compared to confinement is described due to aggregation of the IL in the blend with that does not occur within the membranes due to free volume effects. These results are also compared to recent theoretical results from the literature.

*The authors acknowledge financial support through the National Science Foundation, Division of Chemistry through grant CHE-1753282.
**9:00AM R50.00006: Polymer-Grafted Nanoparticles in Ionic Liquids**

SIQI LIU (Presenter), Stevens Institute of Technology, NARESH OSTI, Chemical and Engineering Materials Division, Oak Ridge National Laboratory, CLEMENS LIEDEL, Max Planck Institute of Colloids and Interfaces, PINAR AKCORA, Stevens Institute of Technology — The newly synthesized zwitterionic liquid (ZIL) 1-butyl-3-methyl imidazole-2-ylidene borane, has superior properties to existing ionic liquids such as good stability in ambient environment. Because it is a zwitterion, there is no self-dissociation of ions, the ion transport and conductivity measured will be due to dynamics of zwitterionic molecule. In this work, deuterated PMMA-grafted nanoparticles with two grafting densities were synthesized. Their dispersion in aprotic ZIL and protic ionic liquid (1-hexyl-3-methylimidazolium bis(trifluormethylsulfonyl)imide) (IL) were investigated in high resolution electron microscopy. We measured dynamics of IL and ZIL with the addition of grafted particles in quasi-elastic neutron scattering experiments. We found translational ionic diffusion of IL slowed down as result of the good mixing and coupling of IL with grafted chains. With the aggregated system, diffusion was similar in bulk, which was due to the phase separation between IL and particles. Interestingly, diffusivity of ZIL increased with the inclusion of particles, particularly with the particles of higher graft density. The increased diffusivity is explained by the confinement of ZIL within structures of grafted nanoparticles.

*This work is funded by NSF-DMR-Polymers Grant #1807802

**9:12AM R50.00007: Effects of Molecular Architecture on the Simultaneous Enhancement in Modulus and Ionic Conductivity in Polymer Solid Electrolytes**

SPIROS ANASTASIADIS (Presenter), EMMANUIL GLYNOS, PARASKEVI PETROPOULOU, LAMPROS PAPOUTSAKIS, Foundation for Research and Technology-Hellas and Univ. of Crete, Heraklion Crete, Greece, EMMANOUIL MYGIAKIS, ALKMINI D. NEGA, GEORGIOS SAKELLARIOU, National and Kapodistrian University of Athens, Greece, WENYANG PAN, EMMANUEL P. GIANNELIS, Cornell University, USA — In an effort to develop solid polymer electrolytes (SPEs) with enhanced mechanical modulus and ionic conductivity, we utilize PMMA stars with high functionality as rigid nanoparticle additives to a liquid PEO electrolyte, doped with LiTFSI. The resulting SPEs exhibit two orders of magnitude higher conductivity and one order of magnitude higher mechanical strength compared to their linear PMMA blend analogues. In addition, the former remain solid-like over an extended temperature range. This performance is due to the SPE morphology of dispersed PMMA nanoparticles within the liquid electrolyte host, which allows for the formation of a highly interconnected network of pure liquid electrolyte that leads to high ionic conductivity (comparable to that of the neat PEO electrolyte).

*This research has been co-financed by the General Secretariat for Research and Technology (Action KRIPI, project AENAO, MIS: 5002556).

**9:24AM R50.00008: Increasing Permittivity in Ion-Containing Polymers: Influence of Zwitterion Additives on Ion-Conduction**

WENWEN MEI (Presenter), JOSH M RINEHART, JOSH E BOSTWICK, ROBERT HICKEY, RALPH H COLBY, Materials Science & Engineering, Pennsylvania State University — An effective approach to improve the ionic conductivity in ion-containing polymers is to increase the dielectric constant of the host, by adding molecules with large dipole moments. With covalently bonded cation and anion on a single molecule, zwitterions are promising candidates. Despite the high ionic conductivity observed by zwitterion addition in polymerized ionic liquids (PILs), the underlying mechanism remains misunderstood. Here, we studied the change in dielectric constant for a series of sulfonate-imidazolium-based zwitterions blended with glycol solvents using dielectric relaxation spectroscopy (DRS). Adding zwitterions drastically increases the permittivity compared with that of the pure glycol solvents. The Landau-Lifshitz mixing rule describes well the measured permittivities of the blends and was further used to extrapolate to the permittivities of pure zwitterions based on their blend behavior. The dependence of measured permittivity on zwitterion structure, composition, and temperature will be discussed in the context of ion conduction in polymeric materials. The work presented here highlights the exceptional ability of zwitterions to increase permittivity and their potential to boost conductivity of PILs by creating a more polar environment.
9:36AM R50.00009: Quantitative Evidence of Mobile Ion Hopping in Polymerized Ionic Liquids*  HONGJUN LIU (Presenter), ALEXEI P SOKOLOV, STEPHEN J PADDISON, University of Tennessee —
We demonstrate the dynamical heterogeneity and cooperative motion of ion transport in polymerized ionic liquids using atomistic molecular dynamics simulations and establish quantitative evidence of mobile ion hopping for the first time. The hopping of anions is dominantly interchain in nature and is generally facilitated by five associating cations from two chains. Intrachain hopping was found to be much less significant being mediating with fewer chains. The mobile anions tend to form string-like structures and move cooperatively; and the string length of concerted motion of mobile anions increases with decreasing temperature. Our results reveal the important role of a distance criterion in defining hopping events to elucidate the ion transport mechanism which has a significant consequence on rationalizing experimental observations and the design of novel polyILs.

* Financial support of the U.S. Army Research Office under Contract No. W911NF-15-1-0501 and W911NF-16-1-0402 is greatly acknowledged. Computing resource was provided through XSEDE allocation DMR130078 at Stampede2 of TACC.

9:48AM R50.00010: Ion Transport in Precise Sulfonate Ionomers with Layered, Cylindrical, and Gyroid Morphologies*  LU YAN (Presenter), Department of Chemical and Biomolecular Engineering, University of Pennsylvania, U.S., CHRISTINA RANK, STEFAN MECKING, Department of Chemistry, University of Konstanz, Germany, KAREN WINEY, Department of Materials Science and Engineering, University of Pennsylvania, U.S. — Precise spacing of ionic pendant groups along linear polymers produces well-defined nanoscale ion-aggregate morphologies and allows new insights into the ion transport mechanism. In this study, we investigate a series of new ionomers synthesized by polycondensation having sodium (Na\(^+\)) or tetrabutylammonium ([N(C\(_4\)H\(_9\))\(_4\)]\(^+\)) sulfosuccinate segments precisely placed every 23 or 48 backbone carbons of a linear backbone. X-ray scattering studies suggest that these precise semicrystalline ionomers containing sodium sulfosuccinate segments form layered or bicontinuous cubic gyroid ionic nanochannels at room temperature and transition to hexagonal symmetry upon heating. In contrast, those containing tetrabutylammonium sulfosuccinate segments exhibit layered ionic aggregates and transition to liquid-like morphologies upon heating. The temperature dependence of ion transport includes both VFT and Arrhenius behavior and varies with ion aggregate morphology. Overall, increasing cation size from Na\(^+\) to [N(C\(_4\)H\(_9\))\(_4\)]\(^+\) leads to faster ion transport due to the enhanced ion dissociation. These precise ionomers provide a promising way to design solid polymer electrolytes with interconnected ionic nanochannels for fast ion transport.

*We acknowledge NSF Grant DMR (15-06726).

10:00AM R50.00011: Nanostructured Polymer Particles for High Modulus and High Conductivity Polymer Electrolytes*  EMMANOUIL GLYNOS (Presenter), LAMPROS PAPOUTSAKIS, SPIROS ANASTASIADIS, Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, WENYANG PAN, EMMANUEL P. GIANNELIS, Department of Materials Science and Engineering, US, Cornell University, PETRA BACOVA, VAGELIS HARMANDARIS, Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, EMMANOUIL MYGIAKIS, ALKMINI D. NEGA, GEORGIOS SAKELLARIOU, Department of Chemistry, National and Kapodistrian University of Athens — We will present a facile new approach for the synthesis of all-polymer nanostructured solid electrolytes that exhibit unprecedented combination of high modulus and ionic-conductivity at room temperature. Novel nanostructured polymer particles, composed of mikto-arm star-shaped copolymers, were synthesized and used as additives to liquid electrolytes. The mechanical properties of the resulting SPEs are dramatically improved compared to the pure liquid electrolyte (the shear modulus increased by up to 8-orders of magnitude), while the ionic conductivity was maintained close to that of the pure liquid electrolyte. Key to their performance is their morphology that stems from the ability of the mikto-arm copolymers to self-assembly in highly interconnected structures within the liquid electrolytes host. With the help of atomistic molecular dynamics we will show that our strategy offers a tremendous potential for the design of nanostructured polymeric materials where the morphology of the nanostructured SPEs could be precisely controlled as is encrypted within the macromolecular characteristics of the star-shaped nanoparticles.

*Action: EREYNW-DHMIOYRGW-KAINOTOMW, project: SOLIDEL, MIS: 5033805
Multivalent cation conduction in dual cation-exchanged polyanions

BUMJUN PARK, JENNIFER SCHAEFER (Presenter), University of Notre Dame — Batteries based on active multivalent metal cations are the topic of research worldwide due to the high abundance of these metals. Unfortunately, transport of hard multivalent cations such as Mg$^{2+}$ and Al$^{3+}$ in polymers is known to be very slow, due to the strong interactions of these ions with the polar constituents on solvating polymers resulting in chain crosslinking and sluggish coordination site exchange rates. Here we report on the transport of multivalent cations in certain poly(ionic liquids). The inclusion of bulky organic cations is found to reduce the glass transition temperature of the matrix and screen metal multivalent cation interactions, resulting in enhanced ion transport. Characterization of the structure and dynamics of a family of materials incorporating varying organic cation types will be discussed.

* A portion of this work was supported by the National Science Foundation though grant number DMR-1654162.

Poly(ionic liquid)s: marriage of ionic liquids and polymers for better materials

JIAYIN YUAN (Presenter), Department of Materials and Environmental Chemistry, Stockholm university — This talk will focus on poly(ionic liquid)s (PILs), a class of multifunctional ionic polymers made up from ionic liquid (IL) monomers. The covalent linkage of IL species into polymeric chains or networks incorporates some unique properties of ILs into that of macromolecular architectures. This innovation in structure design catalyzes new chemistry and physics, and in turn expands the property and function window of ILs and traditional polyelectrolytes. However, PILs initially played a merely supplementary role to ILs, the rapid advance in PIL research in the past decade has created a large toolbox of innovative polyelectrolyte structures, making the study of PILs far beyond the scope of IL research. They are of fundamentally important to polymer chemistry and physics, as they offer new elements and features. Meanwhile, benefiting from a large number of cations and anions in IL chemistry, PILs provide a variety of structure choices and materials solutions in other fields. This lecture highlights the behavior and function of ions in PIL bulk or solution, illustrating the importance of ion motion and ion-guest molecule interaction to determine their global materials property and function.

References

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Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R51 DBIO: Artificial Intelligence, Data, and Dynamics: Learning Physical Models of Living Systems

Machine Learning, Statistical Physics, and Ecological Dynamics

PANKAJ MEHTA (Presenter), Boston University — In this talk, I will start by giving an overview of Machine Learning from a physics perspective and highlight open problems where physicists can contribute. I will then discuss the many connections between the statistical physics of disordered systems and ML. Building on this discussion, I will argue that, somewhat surprisingly, ML is also intimately related to ecological dynamics. I will show how many ML methods and concepts have natural counterparts and ecology and argue that these fields can and should cross-fertilize each other.

*The work was supported by NIH NIGMS grant 1R35GM119461, Simons Investigator in the Mathematical Modeling of Living Systems (MMLS) to PM, and the Scialog Program sponsored jointly by Research Corporation for Science Advancement (RCSA) and the Gordon and Betty Moore Foundation.
8:36AM R51.00002: Principles and Possibilities in the Phase Space of Animal Behavior* [Invited] GREG STEPHENS (Presenter), Physics, Vrije Universiteit & OIST Graduate University — We all instinctively recognize behavior: it’s what organisms do, from the motility of single cells to the stunning displays of bird flocks. To understand behavior, however, we must characterize complex, living movement as precisely and completely as its underlying molecular, cellular and network mechanisms. Here, we leverage a low-dimensional but complete representation of the posture of nematode worm C. elegans to reconstruct a continuous 6D phase space of crawling behavior. The reconstruction separates short and long-time dynamics, untangles subtle movement trajectories, and offers a quantitative arena for examining variability and stereotypy. We find that the phase space is organized into 3 conjugate dynamics containing 2 positive Lyapunov exponents which are approximately balanced by dissipative directions. We suggest that a near-Hamiltonian dynamics of coupled, chaotic oscillators underlie the motor control of C. elegans.

*This work was supported by the research program of the Foundation for Fundamental Research on Matter (FOM), which is part of the Netherlands Organization for Scientific Research (NWO), and by funding from OIST Graduate University.

9:12AM R51.00003: The difference between memory and prediction in recurrent networks [Invited] SARAH MARZEN (Presenter), Massachusetts Institute of Technology, ALEXANDER HSU, Mathematics, Claremont McKenna College — Recurrent networks are trained to memorize their input better, often in the hopes that such training will increase the ability of the network to predict. We show that networks designed to memorize input can be arbitrarily bad at prediction. We also find, for several types of inputs, that one-node networks optimized for prediction are nearly at upper bounds on predictive capacity given by Wiener filters, and are roughly equivalent in performance to randomly generated five-node networks. Our results suggest that maximizing memory capacity leads to very different networks than maximizing predictive capacity. We also discuss how well trained recurrent networks can predict, compared to the optimal.

9:48AM R51.00004: Hybrid Forecasting of Complex Systems: Combing Machine Learning with Knowledge-based Models [Invited] MICHELLE GIRVAN (Presenter), University of Maryland, College Park — In recent years, machine learning methods such as "deep learning" have proven enormously successful for tasks such as image classification, voice recognition, and more. Despite their effectiveness for big-data classification problems, these methods have had limited success for time series prediction, especially for complex systems like those we see in weather, solar activity, and brain dynamics. In this talk, I will discuss how a Reservoir Computer (RC) - a special kind of machine learning system that offers a "universal" dynamical system - can draw on its own internal complex dynamics in order to forecast systems like the weather, beyond the time horizon of other methods. The RC provides a knowledge-free approach because it builds forecasts purely from past measurements without any specific knowledge of the system dynamics. By building a new hybrid approach that judiciously combines the knowledge-free prediction of the RC with a knowledge-based, mechanistic model, we demonstrate a further, dramatic, improvement in forecasting complex systems. This hybrid approach can give us new insights into the weaknesses of our knowledge-based models and also reveal limitations in our machine learning system, guiding improvements in both knowledge-free and knowledge-based prediction techniques.

10:24AM R51.00005: Measuring the hidden dynamics of animal behavior* [Invited] GORDON BERMAN (Presenter), Emory University — When we think of animal behavior, what typically comes to mind are actions – running, eating, swimming, grooming, flying, singing, resting. Behavior, however, is more than the catalogue of motions that an organism can perform. Animals organize their repertoire of actions into sequences and patterns whose underlying dynamics last much longer than any particular behavior. How an organism modulates these dynamics affects its success at accessing food, reproducing, and myriad other tasks essential for survival. Animals regulate these patterns of behavior via many interacting internal states (hunger, reproductive cycle, age, etc.) that we cannot directly measure. Studying these hidden states' dynamics, accordingly, has proven challenging due to a lack of measurement techniques and theoretical understanding. In this talk, I will outline our efforts to uncover the latent dynamics that underlie long timescale structure in animal behavior. Looking across a variety of organisms, we find the existence of a non-trivial form of long timescale dynamics that is unexplainable in standard Markovian frameworks. I will present how temporal coarse-graining can be used to understand how these dynamics are generated and how the found course-grained states can be related to internal states governing behavior. Inferring these hidden dynamics presents a new opportunity to generate insights into the neural and physiological mechanisms that animals use to select actions.

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HSFP RGY0076/2018

Thursday, March 7, 2019 8:00 AM - 11:00 AM
8:00AM R52.00001: STRESS RELAXATION IN EPOXY NANOCOMPOSITES*  SURESH AHUJA (Presenter), xerox corporation — Nanocomposites are formed by the intercalation or exfoliation of nano inorganic fillers into polymers resulting in improvement of physical and mechanical properties relative to the unmodified polymer. In intercalated nanocomposite, the polymer is inserted between the silicate layers forming well-ordered multi-layers, whereas in exfoliated nanocomposite the silicate layers break into single platelets and orient themselves forming a random pattern. The effect of nano filler on strength and toughness appears to depend on the polymer filler interaction, dispersion on the polymer matrix and aggregation of the filler. In terms of polymer chain mobility in a nanocomposite, glass transition has been reported to increase, decrease, or remain unaffected, in comparison with that of the pure polymer, and sometimes a second glass transition has as well been observed. The molecular structure is modeled using a combination of the classical network theory and the elastic dumbbell model for polydispersed polymer segments and localized junctions.

Stress relaxation modulus of epoxy nanocomposites is analyzed. Qualitatively, FENE models can adequately explain experimental results.

* none

8:12AM R52.00002: Coarse-grained Molecular Dynamics Modeling of Epoxy/CNT Nanocomposites*  RALPH ROMERO (Presenter), HAYDEN HOLLENBECK, CHENGYUAN WEN, GARY SEIDEL, SHENGFENG CHENG, Virginia Tech — Modeling fracture in a polymer nanocomposite presents a big challenge at the moment. To enable us to model larger systems over longer time scales that can be bridged to those in continuum mechanics models such as peridynamics, we have developed a coarse-grained molecular dynamics (MD) model of epoxy/carbon nanotube (CNT) nanocomposites. The polymer is described as bead-spring chains with bonded and nonbonded interactions parametrized with atomistic MD simulations. A CNT is represented similarly as a bead-spring chain but with each bond treated as a rod with finite length and radius. Such a treatment leads to a jointed-tube model in which the corrugation issue associated with traditional coarse-grained models of CNTs is removed and the represented CNT behaves as a filament with finite radius. The CNT-CNT and CNT-polymer interactions are further trained with atomistic MD modeling. Using the coarse-grained model, we study the behavior of CNTs in an epoxy matrix including dispersion and bundling and the fracture properties of the epoxy/CNT nanocomposites.


8:24AM R52.00003: QM/MM hybrid simulations of critical failure at the interface in CNT/polymer nanocomposites.  JACEK GOLEBIOWSKI (Presenter), ARASH A MOSTOFI, PETER HAYNES, Imperial College London, JAMES R KERMODE, Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick — Functionalized carbon nanotube (CNT)/polymer composites have received significant interest as promising structural materials with applications in the most demanding areas of industry such as aerospace and ballistic protection. Developing a fundamental understanding of failure mechanisms at the CNT/polymer interface is essential to improving their properties. Here, we use a quantum mechanics/molecular mechanics (QM/MM) hybrid approach to show how chemical structure at the CNT/polymer interface determines its strength and propose candidate chemistries to guide further experimental work.

Computational investigation of interfacial failure in composite materials is challenging because it is inherently multi-scale: the bond-breaking processes that occur at the covalently bonded interface and initiate failure involve QM phenomena, yet the mechanisms by which external stresses are transferred through the matrix occur on length and time-scales far in excess of anything that can be simulated with QM. Here, we demonstrate and validate an adaptive QM/MM simulation method that can be used to address these issues. We demonstrate that the hybrid method results are in excellent agreement with fully-QM benchmark simulations and offers qualitative insights missing from classical simulations.
8:36AM R52.00004: A new strategy for tire tread stocks with high performances*  
AIHUA HE (Presenter), XINPING ZHANG, Shandong Provincial Key Laboratory of Olefin Catalysis and Polymerization, Key Laboratory of Rubber-Plastics (Ministry of Education), School of Polymer Science and Engineerin, RIGUO WANG, HAO WANG, Shandong Huaju Polymer Materials Co. Ltd. — The desire tire tread stocks require satisfied comprehensive performances including good wet-skid resistance, low rolling resistance, good abrasion resistance and excellent anti-fatigue property. In our work, trans-1, 4-poly (butadiene-co-isoprene) copolymer rubber (TBIR) as novel reactive functional rubber is introduced into traditional SSBR and SSBR/BR recipes. Owing to the reinforcement effect of TBIR on the blended polymer matrix, TBIR inclusion could not only inhibit the aggregation of silica during ageing process, but also improve the filler dispersion in the rubber matrix. Furthermore, the TBIR in the form of lamellar fibrils could inhibit crack initiation and deviate crack propagation direction. Consequently, the vulcanized elastomer nanocomposites exhibit significantly improved comprehensive properties, such as enhanced mechanical strengths, outstanding fatigue resistance, improved abrasion resistance and lower rolling resistance with other properties remaining unchanged.

*Thanks to the National Basic Research Program of China (No.2015CB654700 (2015CB654706)), the National Natural Science Foundation of China (No.51473083), the Significant Basic Research Program of Shandong Province(ZR2017ZA0304) and Taishan Scholar Program.

8:48AM R52.00005: The Linear-Nonlinear Dichotomy Behavior for Filled Rubbers in LOAS  
SHAN JIANG, School of Chemical Science and Engineering, Tongji University, XIAORONG WANG (Presenter), Institute for Advanced Study, Tongji University — Filled rubbers display an unusual linear-nonlinear dichotomy of their rheological responses under large amplitude oscillatory shears, where the amplitude of stress output deviates strongly from the linear dependence of strain, but the time-dependence of stress remains sinusoidal. Increasing the cross-linking density in the rubber matrix tends to favor this quasi-sinusoidal responses. Rising the usage of processing oil in a rubber compound tends to disfavor this dichotomy behavior. Varying the amount of reinforcement fillers seems to be ineffective, as long as the filler loading exceeds its percolation threshold. These observations suggest that the topological structure of polymer chain network in the matrix plays an important role in the linear-nonlinear dichotomy rheology. The agglomeration of fillers and the overall characteristics of the fractal structures of filler clusters may have a less important influence on this phenomenon. A summary of recent research activities at Tongji on this subject will be given.

9:00AM R52.00006: Controlling Microstructure in Thermoplastic Polyurethane/Graphene Oxide Nanocomposites via Rigid Segment Length*  
BRANDY GROVE (Presenter), SHAGHAYEGH KHANI, Case Western Reserve University, RICARDO ANDRADE, GUILHERMINO FECHINE, MackGraphe, Mackenzie Presbyterian University, JOAO MAIA, Case Western Reserve University — Thermoplastic Polyurethane (TPU) is a commercially and academically interesting polymer with a wide range of applications. Engineering the micro-structure of the block-copolymers is of crucial importance for achieving desired mechanical properties. Incorporation of nanofillers such as graphene and graphene oxide platelets provides a means to control the phase separation for this material. Dissipative Particle Dynamics (DPD) are preformed to study the phase separation of systems with these nanofillers and determine how much difference functionality makes in a variety of TPUs with hard segments of different lengths. Platelet nanofillers act as a nucleating agent in TPUs with shorter hard segments, inducing local order; as the hard segment length becomes longer, the ordered local structures formed by hard segments break down. Functionalized nanofillers do not aid or hinder the nucleation in TPUs with short hard segments, but may enhance order in TPUs with moderately longer segment length, particularly with a hard segment to nanofiller length that is 1/3 the length of the nanofiller size.

*US - Brazil Exchange Program from APS and SBF
Interphases in polymer nanocomposites - recent insights from NMR studies

— The outstanding performance of modern elastomers is dominated by reinforcement arising from nanometric fillers. The compounds’ peculiar thermo-mechanical properties cannot be explained without consideration of an interphase, i.e., a region of polymer with modified properties [1]. Our, and many others’, work supports a consensus picture of adsorbed components with locally increased $T_g$, reaching the bulk value over a gradient zone of a few nm [1-3]. This talk focuses on more recent results, mostly obtained by proton low-resolution NMR, that challenge the generality of this picture.

First, we present a more detailed investigation of a specific system, poly(ethylene oxide) – silica, which only superficially follows the above rationale [4]. While we do find rigid components forming a layer of up to 2 nm thickness around the particles, the layer thickness is not a function of temperature, and the chains in this layer feature rather fast, possibly uniaxial dynamics [5]. Moreover, small particles with diameters down to 10 nm exhibit much reduced layer thickness that depends on the end groups [5]. For a more complete picture, we have extended this study to a wider range of particle sizes, polymer molecular weight, and preparation conditions.

Second, spin-diffusion NMR experiments, which probe the size of nanometric domains with distinct mobility, indicate that the smooth-mobility-gradient picture of the “glassy layer” must be replaced by a scenario ruled by dynamic heterogeneities associated with the increased glass transition. We find intriguing similarities of filler-related species and interphase components in semicrystalline polymers and block copolymers [6].


Compatibility/Dispersion in Multi-Hierarchical Polymer Nanocomposites

— Commercial polymer nanocomposites such as reinforced elastomers differ significantly from model nanocomposites. Successful commercial products display a complex multi-level hierarchical, nano- to macro-scale structure. We have studied these structures using TEM, small-angle x-ray scattering, and rheology. The multi-hierarchical structure in carbon black reinforced polybutadiene will be described as a function of processing conditions. The filler network in this compound displays a nanoscale aggregate network within nano-clusters that percolate on the micron scale. The nanoscale network develops due to thermodynamic incompatibility of carbon black and polybutadiene which is mitigated by the accumulated strain. The network clusters are limited in size due to incompatibility. On increasing concentration, percolation of these network clusters is observed in scattering, TEM and dynamic rheology. Through this work control over this complex multi-hierarchical structure will be achieved through manipulation of compatibility/incompatibility and processing history.

A. Mulderig et al. Langmuir 33(2017) 14029

NSF CMMI-1635865, 1636036, DOE APS DE-AC02-06CH11357
10:00AM R52.00009: Fabricating Polymer Network Nanocomposites for Recyclability with Full Property Recovery and the Sometimes Complex Roles of Polymer-Nanofiller Interfaces  
XI CHEN (Presenter), LINGQIAO LI, JOHN TORKELSON, Northwestern University — Polymer network nanocomposites cannot be recycled for high-value applications because permanent covalent cross-links prevent melt-state reprocessing. We have developed novel dynamic covalent cross-linking methods that yield recyclability of polymer networks with full recovery of cross-link density. In the fabrication of network nanocomposites, filler surface functionality can provide challenges. With addition-type reversible covalent cross-linking, e.g., a controlled radical polymerization method, surface functionality (e.g., hydroxyl groups) has no significant effect on reprocessability. However, with step-growth-type dynamic covalent cross-linking, e.g., a hydroxyurethane cross-link, surface functionality has deleterious effects. With hydroxyl or amine functionality which can participate in hydroxyurethane chemistry, silica nanoparticles speed the reprocessing but modestly reduce cross-link density and property recovery. Silica nanoparticles with superhydrophobic surfaces (absence of functionality) impact reprocessing kinetics but not recovery of cross-link density. We will also discuss how filler surface functionality combined with dynamic covalent cross-linking may yield novel, well-dispersed nanocomposite networks with especially robust properties.

*Supported by the National Science Foundation through grants CMMI-1635865 and CMMI-1636036. This research used resources of the Advanced Photon Source under Contract No. DE-AC02-06CH11357.

10:12AM R52.00010: Intrinsic temperature dependence of plasmonic resonances in gold nanorod polymer nanocomposites  
DAVID LIOI, SARAH IZOR, VIKAS VARSHNEY, WILLIAM KENNEDY (Presenter), Air Force Research Laboratory — Optical scattering in plasmonic polymer nanocomposites is strongly influenced by the dielectric properties of both matrix and particles. Since changes in temperature can affect each constituent in fundamentally different ways, interpretation of optical scattering spectra as a function of temperature is not straightforward. Here we present a systematic experimental and analytical study of the optical scattering of gold nanorods embedded in an epoxy matrix. We demonstrate that the temperature dependence of scattering spectra from gold-polymer nanocomposites depends on the relative thickness of the surrounding ligands or inorganic coatings that are typically used to stabilize nanorods in polymer matrices. Using empirical fits for the dielectric functions of gold, epoxy, and coating materials we show that it is possible to correct for temperature effects in the interpretation of scattering spectra. This can greatly enhance the precision and accuracy of material state sensing applications that rely on the plasmonic response of gold nanorods in polymers.

*Funding for this project was provided by AFOSR 13RX02COR, Dr. Byung-Lip "Les" Lee, Program Officer.

10:24AM R52.00011: The Impact of an Emergent Hierarchical Filler Network on Nanocomposite Dynamics  
KABIR RISHI (Presenter), GREG BEAUCAGE, Chemical and Materials Engineering, University of Cincinnati, VIKRAM K KUPPA, Nonstructural Materials Division, University of Dayton Research Institute, ALEX MCGGLASSON, Chemical and Materials Engineering, University of Cincinnati, JAN ILAVSKY, Advanced Photon Source, Argonne National Laboratory — The performance of nanoscale-filled elastomers is related to the structure of the aggregated filler network in addition to interfacial chemical affinity and filler dispersion. This structure emerges due to a competition between the thermodynamically driven filler immiscibility and the kinetically driven mixing process. A hierarchical filler network model evidenced in x-ray scattering is linked to the dynamic response at low strains in the linear viscoelastic regime. The primary nanoscale network that percolates locally at ~5 vol % displays a mesh-size, which is related to the changes in the dynamic spectrum at frequencies below the Einstein-Smallwood enhancement associated with the elastomer within the network pores in the high frequency region. The secondary micron-scale network associated with the Payne effect and bulk electrical conductivity that percolates globally at ~20 vol %, influences the gel-like dynamic response at very low frequencies. The hierarchical filler network is described by two crossover frequencies in the dynamic spectrum and two related structural scaling regimes.

10:36AM R52.00012: Defect-Mediated Assembly of Liquid Crystal Elastomer Nanocomposites  
XINFANG ZHANG (Presenter), HAO YU, YUBING GUO, TARAS TURIV, O D LAVRENTOVICH, QI-HUO WEI, Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, Ohio, 44242, USA — One holy grail in making polymer nanocomposites is to be able to place the filling particles into designable positions or orientations. In this talk, we will present a new strategy to self-assemble liquid crystal elastomer nanocomposites by employing topological defects in liquid crystals. We show that topological defects with pre-designed shapes and topology can be created by using a photopatterning technique to control the molecular orientations at the boundaries. Nanoparticles dispersed in the liquid crystals are attracted and self-assembled to these topological defects to minimize the elastic energy of the system. With carefully designed molecular orientations, we show the self-assembly of the nanoparticles into loops and web-networks in liquid crystal polymers.

*NSF CMMI-1436565 and DOE, Office of Sciences, DE-SC0019105
10:48AM R52.00013: **Mesoscale modeling of polymer bigels using Janus particles**  SHENSHENG CHEN (Presenter), XIN YONG, Binghamton University — Polymeric gels composed of chemical-distinct networks may have unique mechanical properties and potential applications in various areas. Nanocomposites of polymer and colloidal particles also draw great attention due to their enhanced strength, stimuli responsiveness, and rheology. To guide the rational design for a bigel contains hydrophilic and hydrophobic networks with predictive properties, we utilize dissipative particle dynamics (DPD) to simulate a model system that incorporate chemistry, physical absorption, and material characterization. To enable the coexistence of hydrophilic and hydrophobic networks, we use Janus particle with corresponding surface chemistries to attract different polymers. A bell model is used to simulate the reversible physical absorption and desorption. Our results show that a bigel is formed when the hybrid polymers are integrated with a high concentration of Janus particles. The bigel exhibits increased Young's modulus and shear thinning behavior. More importantly, the bigel recovers to a homogenous network in a short time after deformation. This integrated approach provides a general path towards functional network materials with enhanced mechanical properties and potential applications in drug delivery and wound dressing.

### Thursday, March 7, 2019 8:00 AM - 11:00 AM

**Session R53 GSNP: Flow Driven Pattern Formation in Wet Granular Medium I**  BCEC 253C - Arshad Kudrolli, Clark University - Tag(s): Invited

**8:00AM R53.00001: On flow, fracture and getting jammed – Failure modes in dense suspensions**  [Invited] IRMGARD BISCHOFBERGER (Presenter), DOMENICO CAMPANARO, LEOPOLD BEUKEN, Massachusetts Institute of Technology, IVO PETERS, University of Southampton — Dense suspensions are a class of complex fluids that exhibit both shear-thickening and shear-jamming behavior as a response to an applied stress. These dynamic liquid-to-solid transitions have important consequences for the displacement of a dense suspension by another fluid: upon the injection of air, intricate patterns arise in the suspension, leading to flow or fracture of the material. We displace a cornstarch suspension by a pressure-controlled injection of air in a quasi-2D geometry. Depending on the concentration of cornstarch and the applied stress, we observe a variety of patterns: smooth fingering in the fluid regime and different modes of fractures, ranging from slow branched cracks to single fast fractures. Remarkably, there is a regime where, despite the application of pressure, the suspension cannot be displaced. Only upon an increase to a higher pressure, air injection occurs, leading to very thin fractures in the suspension. We hypothesize that in this regime the suspension is in the shear-jammed state. This would imply a novel way of investigating the mechanical properties of a shear-jammed material by probing its fracture behavior.

**8:36AM R53.00002: Multiphase flow in porous media: wetting, disorder, and pattern formation**  [Invited] RUBEN JUANES (Presenter), Massachusetts Institute of Technology — The displacement of one fluid by another in a porous medium gives rise to a rich variety of hydrodynamic instabilities. Beyond their scientific value as fascinating models of pattern formation, unstable porous-media flows are essential to understanding many natural and man-made processes, including water infiltration in the vadose zone, carbon dioxide injection and storage in deep saline aquifers, methane venting from organic-rich sediments, and fracturing from fluid injection. Here, we review a handful of these hydromechanical instabilities, elucidate the key physics at play, and point to modeling frameworks that permit quantitative assessments of their impact at the geologic scale.

**9:12AM R53.00003: Stressing gels out: exploiting gradients in shrinkable packings**  [Invited] H. JEREMY CHO, MICHAEL P HOWARD, NANCY B LU, SUJIT DATTA (Presenter), Princeton University — Diverse biological systems, ranging from actuation to drug delivery, rely on how soft gels respond to environmental stresses. In this talk, I will describe how we combine experiments and poroelasticity theory to investigate the influence of osmotic stresses in hydrogel packings. In some cases, the stresses that develop cause packings to crack. We show how cracking behavior depends on gradients in the stress profile, suggesting a way to control material behavior in this complex system. Ultimately, our work stimulates new findings and questions at the interface of Physics, Biology, Materials Science, and Engineering.

**9:48AM R53.00004: Granular erosion in Stokes flow**  [Invited] NICK MOORE (Presenter), Florida State University — Fluid-mechanical erosion of solid material occurs across many scales, from massive geological structures down to tiny granular constituents. Here, we numerically examine the erosion of a granular medium in the Stokes limit — the regime of groundwater flow. We combine a highly accurate boundary-integral formulation of the Stokes equations with stable interface-evolution methods. A single body erodes into a slender, for-aft-symmetric morphology which can be described analytically. Using the fast multipole method allows the simulation of 10-100 bodies. Many-body erosion naturally leads to the formation of channels and anisotropy in the medium conductivity.

*Simons Foundation Collaboration Grants for Mathematicians 524259
Pattern formation of frictional fingers in a gravitational potential

KNUT MÅLØY (Presenter), JON ALM ERIKSEN, PoreLab, The Njord Center, University of Oslo, RENAUD TOUSSAINT, Institute de Physique de Globe de Strasbourg, University of Strasbourg, EIRIK GRUDE FLEKKØY, OLIVER GALLAND, PoreLab, The Njord Center, University of Oslo, BJØRNAR SANDNES, College of Engineering, Swansea University — This work concerns experiments and simulations of slow drainage in a deformable quasi 2D porous media Hele Shaw. We introduce gravity as a parameter in the experiments where air displaces a liquid–granular mixture during drainage of a Hele-Shaw cell, by imposing shallow tilt angles. The receding interface accumulates a front of granular material, and an instability caused by a competition between surface tension and frictional forces results in an emerging pattern of frictional fingers, canals of air separated by branches of compacted grains, as also observed in horizontal systems. Aligned finger structures, with a characteristic width, emerge during the slow drainage. A transition from vertical to horizontal alignment of the finger structures is observed as the tilting angle and the granular density are varied. An analytical model is presented, demonstrating that the alignment properties are the result of the competition between fluctuating granular stresses and the hydrostatic pressure. The dynamics is reproduced in simulations. We also show how the system may explain patterns observed in nature, created during the early stages of a dike formation.

*We are grateful to the late Henning Knudsen, who made important contributions to the understanding of frictional fingers. We thank Gidon Baer, Einat Aharonov, and Benjy Marks for discussions. J.A.E. acknowledges support from the Campus France Eiffel Grant and Unistra. This work was partly supported by the Research Council of Norway through the Center of Excellence funding scheme, Project No. 262644, and the NFR Project No. 200051/S60. B.S. acknowledges support from the EPSRC Grant No. EP/L013177/1 and Sêr Cymru National Research Network in Advanced Materials Grant No. NRN141. R.T., K.J.M., and E.F. acknowledge support from EU FP7 Grant No. 316889-ITN FlowTrans and from the LIA France-Norway D-FFRACT. R.T. also acknowledges additional support from UiO, Unistra, and the INSU ALEAS risk program.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R54 DPOLY GSOFT GSNP: Confined Polymer Glasses III: Elasticity, Nanoparticles, and Brushes

Enhanced Thermal Stability of Polymers under Extreme Nanoconfinement

HAONAN WANG (Presenter), JYO LYN HOR, AIXI ZHANG, University of Pennsylvania, PRANTIK MAZUMDER, Corning Research and Development Corporation, DAYEON LEE, ZAHRA FAKHRAAI, University of Pennsylvania — It has been shown that the properties of polymers in weakly-interacting polymer nanocomposites (PNCs), such as Polystyrene(PS) and SiO₂ nanoparticles (NP), can deviate from bulk due to segmental and chain confinement. Capillary Rise Infiltration (CaRI) of polymers into densely-packed NP films can produce PNCs with ultra-high NP loadings. Depending on the degree of confinement, the glass transition temperatures ($T_g$) of PS/SiO₂ CaRI films can increase up to ~57 K. In this study, unentangled PS/SiO₂ CaRI films were used to study the thermal degradation of polymers under extreme nanoconfinement. The degree of confinement was controlled by using NPs with different diameters, thus adjusting the effective pore diameter by 3–30 nm. We show that the thermal stability of PS is significantly increased in smaller pores under both thermo-oxidative and pyrolytic conditions. The characteristic degradation time during isothermal degradation at high temperatures is proportional to the viscosity of PS at lower temperatures, indicating an entropic origin of the improved stability. The details of the kinetics of the degradation process through surface or bulk is also explored.

*We acknowledge University of Pennsylvania MRSEC grant (NSF DMR-1720530) for the funding of this study.
8:12AM R54.00002: Unexpected strengthening effect in brush particle-based hybrid materials with intermediate grafting density* JAEJUN LEE (Presenter), Department of Materials Science and Engineering, Carnegie Mellon University, ZONGYU WANG, Department of Chemistry, Carnegie Mellon University, JIANAN ZHANG, School of Chemistry and Chemical Engineering, Anhui University, TINGWEI DENG, Department of Materials Science and Engineering, Carnegie Mellon University, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, MICHAEL R BOCKSTALLER, Department of Materials Science and Engineering, Carnegie Mellon University — Surface functionalization of nanoparticles with polymers has emerged as a versatile platform to enable hybrid building blocks that can be assembled into functional nanocomposites with controlled microstructure and enhanced mechanical properties. However, the dense functionalization by conventional method presents a barrier to the utilization of this concept due to the limited inorganic content. This contribution will present a systematic analysis of the role of brush architecture on the elastic properties of brush particle films. Material systems with continuous variation of the grafting density as well as bimodal graft architectures were synthesized using modified atom transfer radical polymerization and films were characterized using indentation and thermal analysis. The results reveal that chain interdigitation plays a dominant role for the modulus and strength of the films. In particular, the results demonstrate an ‘optimum degree of functionalization’ to maximize cohesive interactions as a consequence of the enhanced dispersion interactions in interdigitated brush particle assemblies. The results are used to postulate design guidelines for the synthesis of brush particles capable of forming hybrid materials with enhanced performance.

*DOE (CMMI-1662305), NSF (DE-EE0006702)

8:24AM R54.00003: Dramatic Modification of Nanoparticle Surface Mobility in Polymer Colloids with a Core-Shell Structure HOJIN KIM (Presenter), Department of Chemical and Biomolecular Engineering, University of Delaware, EUNSOO KANG, BARTLOMEJ GRACZYKOWSKI, Max Planck Institute for Polymer Research, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University, ERIC M FURST, Department of Chemical and Biomolecular Engineering, University of Delaware, GEORGE FYTAS, Max Planck Institute for Polymer Research — Advances in polymer nanoparticle synthesis and assembly techniques have enabled new applications, from drug delivery carriers to novel coatings. However, the thermal transition of polymer dynamics, especially at the particle surfaces, must be understood in order to realize their potential. Using Brillouin light scattering as a direct probe of the particle surface mobility via polymer nanoparticle vibrations, recent experiments confirm the correlation between the glass transition behavior and surface dynamics of polymer nanoparticles. This raises a challenge of how the glass transition dynamics of polymer nanoparticles can be engineered. To address this need, we modify the surface condition of polystyrene nanoparticles with different shell architecture layers. We demonstrate that a shell layer composed of two polyelectrolytes, as thin as a single polymer chain, is able to eliminate the effect of enhanced particle surface mobility. Other shell structures, such as a single polyelectrolyte layer, enables tailoring the glass transition temperature, softening behavior, and elasticity of the nanoparticles.

8:36AM R54.00004: Materials by Design for Stiff and Tough Nanoparticle Assemblies with Polymeric Hairs* SINAN KETEN (Presenter), Northwestern University — In this work, a computational methodology for predicting the mechanical behavior of assembled hairy nanoparticle systems (aHNPs) using coarse-grained molecular dynamics simulations coupled with Gaussian process metamodeling will be presented (Hansoge et al. ACS NANO,2018). The coarse-graining approach for the polymeric hairs involves systematic parameter development based on the energy renormalization approach, which allows us to describe the behavior of the glassy nanocomposites with greater accuracy at larger length-scales. Simulations reveal that for cellulose nanocrystal-PMMA aHNPs, the Pareto frontier, which marks the optimal trade-offs between modulus and toughness within the design parameter space, can be reached when the weight percentage of nanoparticles is around 60% and the grafted chains exceed the critical length scale governing transition into the semidilute brush regime. A theoretical model with computationally determined parameters based on the Daoud–Cotton model adequately explains the dependence of the critical length scale on graft density and nanoparticle size. The computational results agree well with recent experiments and suggest that high stiffness and high toughness could be achieved by carefully tuning the molecular design parameters, most notably by keeping a relatively low grafting density while having high graft length and nanoparticle volume fraction.

*The authors acknowledge funding from a DoD PECASE award.
Diminishing Interfacial Effects with Decreasing Nanoparticle Size in Polymer-Nanoparticle Composites

HAMED EMAMY (Presenter), Columbia University, FRANCIS STARR, Wesleyan University, SANAT KUMAR, Columbia University — Using molecular simulations on model polymer nanocomposites at fixed filler loading we show that interfacial polymer dynamics are affected less with decreasing nanoparticle (NP) size. However, the glass transition temperature \( T_g \) changes substantially more for extremely small NP. The reason for this apparent contradiction is that the mean NP spacing decreases with decreasing particle size. Thus, all polymers are effectively interfacial for sufficiently small NP, resulting in relatively large \( T_g \) shifts. For larger NP, interfacial relaxations are substantially slower than the matrix for favorable NP-polymer interactions. The minority "bound" polymer dynamically decouples from the polymer matrix, and we only find small changes in \( T_g \), relative to that of the bulk polymer for large NP. These results are used to organize a large body of relevant experimental data, and we propose an apparent universal dependence on the ratio of the face-to-face distance between the NPs and the chain radius of gyration.

Disentangling the Role of Chain Conformation on the Mechanics of Particle Brush Materials

YU CANG, Max Planck Institute for Polymer research, JIARUL MIDYA, Institute of Physics, Johannes Gutenberg University Mainz, SERGEI EGOROV, Department of Chemistry, University of Virginia, KRZYSZTOF MATYJASZEWSKI, Chemistry Department, Carnegie Mellon University, MICHAEL R BOCKSTALLER, Department of Materials Science and Engineering, Carnegie Mellon University, ARASH NIKOUBASHMAN, Institute of Physics, Johannes Gutenberg University Mainz, GEORGE FYTAS (Presenter), Max Planck Institute for Polymer research — The modification of particle surfaces with polymeric ligands is widely used to enhance the interactions between particles, to allow their integration in polymeric matrices or for the processing of particulate materials through techniques such as molding or extrusion. A critical question that is of both fundamental and applied relevance pertains to the role of polymer architecture in controlling the interactions and resulting mechanical properties of polymer-tethered particles. Because of its ability to resolve the mechanical characteristics on submicrometer scale without sample destruction, Brillouin light scattering (BLS) has become an important analytical tool to elucidate the connection between structure, dynamics and macroscopic response in hybrid material systems. In this contribution a combined approach of experimental BLS analysis and coarse-grained simulations is presented to identify the respective contribution of grafting density and degree of polymerization on the macroscopic mechanical properties of films from polystyrene tethered silica colloids. The bulk modulus is maximized in intermediate to low grafting density systems, where the hard silica cores are partially exposed due to conformational fluctuations of the grafted polymers.

Interfacial entropic interactions tunes fragility and dynamic heterogeneity of confined polymer glasses with embedded nanoparticles.

NAFISA BEGAM, NIMMI DAS ANTHUPARAMBIL (Presenter), Department of Physics, Indian Institute of Science, Bangalore., SIVASURENDER CHANDRAN, Institute of Physics, University of Freiburg, 79104 Freiburg, Germany, MOHD IBRAHIM, Department of Physics, Indian Institute of Science, Bangalore., VENKAT PADMANABHAN, Department of Chemical Engineering, Tennessee Technological University, Cookeville, TN 38505, USA., MICHAEL SPRUNG, Deutsches Elektronen Synchrotron DESY, Notkestrasse 85, 22607 Hamburg, Germany., JAYDEEP K BASU, Department of Physics, Indian Institute of Science, Bangalore. — The nature of nanoparticle-polymer interfacial layer is known to play a vital role in determining various physical properties of polymer glasses. The influence of interfacial interactions on viscosity, fragility and dynamical heterogeneity of athermal melts are explored in this study\(^1\). Dynamical parameters are studied using X-ray photon correlation spectroscopy and results are corroborated with molecular dynamics simulations. Influence of various microscopic parameters such as interfacial layer diffusivity, matrix chain penetration depth etc on fragility of polymer glasses are demonstrated combining experiment and simulation results. Thin film-substrate interface adsorbed layer effects on dynamical properties of confined glasses are also investigated. Reduction (enhancement) in viscosity is observed for melts with low (high) entropic compatibility parameter, \( f \) (molecular weight ratio of graft to matrix chains). Fragility is found to increase with increasing \( f \). Anticorrelation between fragility and dynamical heterogeneity is found in these systems, which are contrary to various earlier studies on glass forming polymers.


Authors would like to thank the DST-Nanomission, India for the financial support.
9:48AM R54.00008: Interactions of Ligand-Coated Nanoparticles at a Liquid Surface*  
DAVID HOAGLAND (Presenter), PAUL KIM, YIGE GAO, ALEXANDER RIBBE, THOMAS RUSSELL, University of Massachusetts Amherst — The pair interaction potential of ligand-coated silica nanoparticles (NPs) at a liquid surface were determined by scanning electron microscopy, exploiting the nonvolatility of ionic liquids to stabilize the liquid specimens against microscope vacuum. Even at near contact, individual, two-dimensionally well-dispersed NPs were resolved. The potential of mean force, reduced to the pair interaction potential for dilute NPs, was extracted with good accuracy from the radial distribution function as both NP diameter and poly(ethylene glycol) ligand length varied. While NP polydispersity broadened the core repulsion, the pair potential well-approximated a hard sphere interaction. For short (5 kDa) ligands, a weak (<kT) long-range attraction was discerned, and for ligands of identical length, the potentials overlapped for NPs of different diameter; the attraction is suggested to arise from ligand-induced menisci. To probe the factors underlying the potential, NP surface-binding energies were measured by interfacial tensiometry, and NP contact angles were assessed by new atomic force microscopy and transmission electron microscopy methods.

*NSF/DMR-1807255

10:00AM R54.00009: Switching mixed polymer brushes surfaces through external stimulation  
MINGXIAO LI, CHRISTIAN PESTER (Presenter), Pennsylvania State University — Binary and mixed brushes are comprised of two (or more), chemically distinct polymers randomly grafted to a surface in close proximity. This approach is considered a potent means to manufacture responsive surfaces with tunable physical properties. We highlight recent work in using orthogonal polymerization techniques to tailor such mixed surfaces, comprised chemically disparate polymers covalently grafted to a silica surface. A combination of X-ray photoelectron spectroscopy, synchrotron hard (GISAXS) and soft resonant X-ray techniques (RSoXS), as well as Infrared Atomic Force Microscopy (AFM-IR) was used to provide evidence for responsiveness towards external stimuli. The choice of selective solvents for either of the two species resulted in reversible microphase segregation and can provide a direct pathway towards switchable surface properties.

10:12AM R54.00010: The TUFF Method: Stretching Free-Standing Ultra-Thin Glassy Polymer Films*  
REED BAY (Presenter), ALFRED CROSBY, Polymer Science and Engineering, University of Massachusetts Amherst — TUTTUT (The Uniaxial Tensile Tester for Ultra-Thin films) is a recently developed method for quantifying the complete uniaxial stress-strain relationship for ultra-thin polymer films. The key to TUTTUT is the use of liquids to help support ultra-thin, often fragile, films. Although this method has provided new insights into mechanical properties and deformation mechanisms for dimensionally-confined polymer systems, for some polymers the presence of a liquid may influence the ultra-thin properties. Here, we introduce a new method, TUFF (Tensile tester for Ultra-thin Freestanding Films) to directly measure the uniaxial stress-strain response of freestanding polymer thin films. Using polystyrene thin films, with thickness 20nm-100nm, we observe and quantify large strain deformation mechanisms, as well as yield stress and elastic moduli, and compare these results to TUTTUT measurements. These results provide new fundamental insights into how the surface interactions can alter polymer behavior in thin confined polymer films.

*NSF DMR-1608614

10:24AM R54.00011: Unveiling the Elasticity of Confined Multilayer Hybrid Materials*  
ZUYUAN WANG (Presenter), KONRAD ROLLE, Max Planck Institute for Polymer Research, THERESA SCHILLING, Department of Inorganic Chemistry I, University of Bayreuth, MARKUS RETSCH, Department of Chemistry, University of Bayreuth, JOSEF BREU, Department of Inorganic Chemistry I, University of Bayreuth, GEORGE FYTAS, Max Planck Institute for Polymer Research — The superior elasticity and processing easiness of polymers render them promising as an interfacial filler material. With the progress in hybrid materials fabrication and manufacturing precision, the thickness of interfacial polymer layers has gone down to the nanometer range that can feature strong confinement. A critical question of scientific and applied importance is how the confined polymer layers affect the effective mechanical properties of the hybrid material. In this contribution, we utilize Brillouin light scattering experiments and a continuum-mechanics based model to examine the anisotropic elastic properties of confined hybrid materials composed of alternating polyvinylpyrrolidone and hectorite nanolayers. The clear resolution of the direction-dependent quasi-longitudinal, quasi-transverse, and pure-transverse phonon modes from the Brillouin scattering experiments leads to the full elastic properties of these highly anisotropic samples. We find that as the polymer layer thickness increases from about 1 to 3 nm, the material's Young's moduli in the directions parallel and perpendicular to the layers drop by nearly 50%, implying the crucial role of polymer confinement on the sample's mechanical properties.

*ERC AdG (SmartPhon No. 694977)
Tensile elastic modulus of free-standing single-layer and bilayer polymer films* PAK MAN YIU (Presenter), HAILIN YUAN, Department of Physics, Hong Kong University of Science and Technology, QIAO GU, PING GAO, Department of Chemical and Biological Engineering, Hong Kong University of Science and Technology, OPHELIA TSUI, Department of Physics, Hong Kong University of Science and Technology — Studies have shown that the elastic modulus, $E$, of polymer films may vary with the film thickness, $h$, when $h$ is tens of nanometers. For polystyrene (PS) supported by a polydimethylsiloxane (PDMS) substrate, $E$ had been found to decrease with decreasing $h$ below ~60 nm. For free-standing PS films, however, $E$ was found to be constant with $h$ for $h < ~80$ nm. In this experiment, we conducted uniaxial tensile tests on free-standing PS films (with a molecular weight, MW, of 1,049 kg/mol and $h = 40$ to 150 nm) and bilayer films of PS-PDMS (with various MW from 151 to 1,049 kg/mol and $h = 12$ to 150 nm). The measured elastic modulus of the films agreed with published value of bulk PS, showing insignificant dependences on $h$ or MW.

Surface and Interfacial Tension of Graft Polymer Melts* MICHAEL JACOBS (Presenter), The University of Akron, BRANDON PUGNET, Department of Physics, Lafayette College, HEYI LIANG, ANDREY DOBRYNIN, The University of Akron — Understanding surface properties of polymer melts is crucial for designing new polymeric coatings, adhesives, and composites. Here, we study the effect of molecular architecture on surface and interfacial tension of graft and linear polymer melts by molecular dynamics simulations. In particular, we elucidate the effect of the degree of polymerization of the side chains $n_{sc}$ and their grafting density $1/n_g$ on the surface tension of the graft polymer/vacuum interface, and the interfacial tension of the interface between graft and linear polymer melts. For the case of the graft polymer/vacuum interface, our simulations confirm that the surface tension is a linear function of the fraction of the backbone ends $f_{be}$ and side-chain ends $f_{se}$. This dependence of the surface tension highlights the entropic origin of the surface tension corrections associated with the redistribution of the grafting points and ends at the interface. However, the interfacial tension between graft and linear polymer melts does not show any significant dependence on the molecular structure of the graft polymers, thus pointing out the dominance of the enthalpic contribution to the interfacial tension.

*We acknowledge support of the Research Grants Council of Hong Kong through the Project 16302917.

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Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R55 DPOLY: Polymer Crystallization II: Packing Assembly, Chip Calorimetry and Simulations 8CEC 254B - Claudio De Rosa, University of Naples Federico II Rufina Alamo, Florida A&M and Florida State University - Tag(s): Focus

Isodimorphic biodegradable copolyesters: Structure and crystallization behavior* [Invited] ALEJANDRO J. MULLER (Presenter), POLYMAT and University of the Basque Country UPV/EHU, Spain — Random copolymers with crystallizable components can crystallize in three modes: (a) comonomer exclusion, in which the comonomer is excluded from the crystal lattice of the other component, (b) isomorphism (i.e., strict molecular requirements should be met), in which a single crystalline phase is observed for all compositions, because of comonomer inclusion, and (c) isodimorphism, where two crystalline phases are formed depending on the composition, and both phases allow comonomer inclusion. In the present invited lecture, the detailed structure, morphology, nucleation and crystallization behavior of isodimorphic biodegradable copolyesters will be presented as a function of their comonomer ratio. This information is very significant as it allows tailoring the properties of random copolymers as well as their applications. The materials exhibit a pseudo-eutectic type phase behavior. To the left and to the right of the pseudo-eutectic a single phase is formed, rich in the corresponding parent comonomer. However, near the pseudo-eutectic point, two crystalline phases can be formed. In this way, double crystalline materials with interesting spherulitic superstructures that contain both types of lamellar thickness can be generated. The applications of these materials are potentially very interesting as superstructures with different sensitivities to biodegradation could be prepared and their lifetime can be tailored from their structural characteristics.

References:

*RISE Project, H2020-MSCA-RISE-2017-778092: BIODEST.
MINECO Project: MAT2017-83014-C2-1-P*.
8:36AM R55.00002: Packing Selection of a Helical Semicrystalline Polymer in Solution and Melt-Grown Crystals*
TOSHIKAZU MIYOSHI (Presenter), The University of Akron — Correlation between packing and chain-folding structures of semicrystalline polymers has not been clearly addressed in existing literature. We investigate kinetics effects on chain packing as well as chain-folding structure of a helical chiral polymer in solution- and melt-grown crystals. We will provide a novel concept of intramolecular and intermolecular packing to understand kinetics effects on packing selection in the melt and solution-grown crystals.

*NSF DMR 1708999

8:48AM R55.00003: Semicrystalline polyethylene measurement by Polarized Resonant Soft X-ray Scattering  
DEAN DELONGCHAMP (Presenter), ELIOT H GANN, CHAD RAY SNYDER, National Institute of Standards and Technology — Orientation and conformation in nanoscale amorphous regions often dominates the properties of soft materials such as composites and semicrystalline polymers. In polyethylene (PE), interlamellar amorphous tie chains have been shown to substantially reduce the rate of slow crack growth, which is important for long service life in infrastructure elements such as potable water pipes. I will describe polarized resonant soft X-ray scattering (P-RSoXS) measurements of semicrystalline polyethylenes. The P-RSoXS of PE is highly anisotropic with respect to electric field vector and orientation of the amorphous interlamellar chains is a significant contributor. Real space models reproduce salient features of the P-RSoXS pattern including trends in anisotropy with energy, trends in anisotropy with q, and a clear long period peak. Prospects for correlating interlamellar orientation measurements by P-RSoXS with tie chain population and crack growth will be discussed.

9:00AM R55.00004: Polymorphism in nanolayered comb-like and linear precision polymers*  
VARUN DANKE (Presenter), GAURAV KUMAR GUPTA, MARIO BEINER, Polymeric Material Design, Business Unit Polymer Applications, Fraunhofer Institute for Microstructure of Materials and Systems IMWS — Comb-like polymers with rigid backbones and flexible alkyl side chains are a class of functional materials which often exhibit long range ordered states wherein main and side chains form an alternating layered arrangement on length scales of 1-3 nm. Similarly, linear precision polymers synthesized by ADMET polymerization, incorporating ring-like units placed at regular intervals along a polyethylene backbone also typically show nanolayered structures[1]. Here we present results of a comparative study using X-ray scattering and calorimetry highlighting similarities and differences in structure formation in these two material classes. Of special interest is the competition of the individual packing tendencies of rings and methylene sub-units that drive polymorphic behavior which is a commonly encountered phenomenon in such nanolayered systems. The role of substrates and interfaces on their crystallization behavior is also briefly discussed.


*Financial support within the framework of Sonderforschungsbereich SFB TRR 102 ‘Polymers under multiple constraints’ (projects A03 and B14) is highly appreciated.

9:12AM R55.00005: Unusual crystallization kinetics of long-spaced polyacetals  
XIAOSHI ZHANG (Presenter), SIDNEY CAMERON, RUFINA ALAMO, FAMU-FSU College of Engineering, Florida State University, XIAOBIN ZUO, X-ray Science Division, Argonne National Laboratory, PATRICK ORTMANN, STEFAN MECKING, Department of Chemistry, University of Konstanz — The overall crystallization kinetics of the major polymorphs of a series of polyethylenes with acetal groups precisely placed on each and every 12th, 18th, 19th and 23rd backbone carbon (PA-12, PA-18, PA-19, and PA-23) have been studied by DSC and FSC with parallel studies using FTIR, real-time X-ray and POM. The crystallization kinetics is unusual because multiple minima of isothermal crystallization rates are observed at polymorphic transition temperature regions, which is reminiscent of previous observations of crystallization minima in precision polyethylenes with halogen. The inversion is mainly associated with a confinement effect that the kinetically favored Form I makes on the growth of the more stable Form II. Besides the effect on growth, data of induction time for crystallization indicates that the presence of Form I also retards the nucleation of Form II.
9:24AM R55.00006: Homogeneous crystal nucleation in polymers: New insights from fast scanning calorimetry

EVGENY ZHURAVLEV, Institute of Physics, University of Rostock, RENE ANDROSCH, IWE TFN, Martin Luther University Halle-Wittenberg, RUSLAN ANDRIANOV, Institute of Chemistry, Kazan Federal University, CHRISTOPH SCHICK (Presenter), Institute of Physics, University of Rostock — Crystallization commonly starts from a (sub)nanoscale nucleus which eventually grows to a crystal. Classical nucleation theory (CNT) provides a qualitative description of these processes. Homogeneous nucleation, to become dominant over heterogeneous nucleation, requires deep undercooling of the polymer melt. At cooling rates of several thousand K/s such states can be reached and the kinetics of homogeneous nucleation becomes accessible. Fast scanning calorimetry (FSC), in combination with polarized optical (POM) and atomic force (AFM) microscopy, provides a tool to study homogeneous nucleation and even the thermodynamic stability of the formed nuclei as a function of nucleation temperature and time.


9:36AM R55.00007: Using chip-based calorimetry to monitor crystallization during polymer processing

KENNETH KEARN (Presenter), THOMAS R FIELTZ, RAJEN M PATEL, SHRIKANT DHODAPKAR, TRAVIS MCINTIRE, JIN WANG, CHRISTOPHER M THURBER, ROBBYN PRANGE, Dow Chemical Company — Polymer processing often involves rapid changes in temperature and strain, which significantly modify the properties and thus performance. Advancements in chip-based calorimetric techniques overcome temperature scanning rate and instrument response limitations of conventional differential scanning calorimeters, enabling off-line probing of commercially relevant process conditions. In this talk we will describe how we have used commercial, chip-based calorimetric instrumentation to monitor crystallization under process conditions. Using a chip-based calorimeter we can monitor the crystallization of semi-crystalline polyolefins as they move through the pelletization step of the manufacturing process. Mapping time-dependent crystallization covering up to 1000 seconds was possible. Blown film processing, which undergoes cooling at rates approaching 100 °C/s, could be mimicked using the chip calorimeters. By coupling this data to at-line monitoring schemes, strain-induced crystallization can be deduced.

9:48AM R55.00008: Visualization of Polymer Crystallization by a Combination of Atomic Force Microscopy with Fast Scanning Calorimetry

RUI ZHANG (Presenter), EVGENY ZHURAVLEV, CHRISTOPH SCHICK, Institute of Physics, University of Rostock — Abstract: The chip-sensor of fast scanning calorimetry (FSC) is directly mounted on the scanner of an atomic force microscope (AFM). By combining AFM with FSC (AFM-FSC) this way, AFM can illustrate the crystal structures on the nanoscale, as well as, FSC can treat the sample at any annealing temperature without unexpected crystallization during heating or cooling at scanning rates up to 1,000,000 K/s. First results on crystals' morphologies, spherulites' growth rates and the influence of crystal nuclei by Tammann's two stage method are shown.

Keywords: Fast Scanning Calorimetry, Atomic Force Microscopy, Morphology, Crystal Growth, Tammann's method

10:00AM R55.00009: Slip-link modeling of a crystallizing entangled polymer melt

MARAT ANDREEV (Presenter), GREGORY C RUTLEDGE, Massachusetts Institute of Technology — Modeling of polymer processing is a subject of continuing industrial and theoretical interest. Many industrial polymer melts are entangled and undergo crystallization during processing. Experimental data for the rheology of crystallizing entangled polymers are available in a number of published studies on this topic. In particular, the 'inverse quench' technique allows one to stop crystallization in effect, and to measure the dynamic modulus over a wide range of frequencies. Meanwhile, over the past few years, slip-link models have been demonstrated to be very capable for describing the rheology of entangled melts. In this work, we present a modification of the slip-link model to capture the rheology of an entangled melt during the early stages of crystallization. The model captures the emergence of a secondary, low-frequency plateau observed in the linear regime. The advantage of this approach is the capability to predict the effect of on-going crystallization during non-linear deformation.
10:12AM R55.00010: Monte Carlo simulations of stress-induced polymer crystallization*  WENBING HU (Presenter), JIPING WANG, School of Chemistry and Chemical Engineering, Nanjing University — We developed the previous approach of dynamic Monte Carlo simulations of bulk lattice polymers for strain-induced crystallization [1-3] by incorporating the stress relaxation, and investigated the competition between strain rate and stress relaxation rate. The results reproduce the basic experimental observations and promise a molecular-level understanding of stress-induced polymer crystallization via our new approach.

References:

*The financial support from National Natural Science Foundation of China (Grant No. 21734005) was appreciated.

10:24AM R55.00011: Monte Carlo Simulation of Stress-Induced Polymer Crystallization during Cold Drawing*  JIPING WANG (Presenter), YIHUAN YU, WENBING HU, Nanjing University — Jiping Wang, Yihuan Yu, Wenbing Hu*

Polymers are stretched with stress relaxation in the common industrial processing such as fiber spinning, plastic molding, film stretching and film blowing. Recently we develop a new simulation method which could reproduce the typical stress relaxation behaviors of polymers. Based on this model we investigated polymer crystallization during the drawing process from high to low temperatures. The high temperature results reproduced our previous observations on strain-induced polymer crystallization [1-3]. Since we took the conformational energy barrier and the monomer adhesive barrier into consideration, the low temperature results revealed the stress-induced fragmentation in company with crystallization. This work could help us to understand the semi-crystalline structures in the cold drawing process of polymer materials.

References:
[1] Nie, YJ.; Gao, HH.; Yu, MH.; Hu, ZM.; Reiter, G.; Hu, WB. Polymer. 2013, 54: 3402-3407.

Keywords:
Crystallization, Polymer Processing, Monte Carlo Simulation, Cold Drawing

*Natural Science Foundation of China

10:36AM R55.00012: Polymer Crystallization during shear flow*  GO MATSUBA (Presenter), Grad. Sch. of Organic Materials Engineering, Yamagata University — We evaluated the effect of molecular weight on the formation of a shish–kebab morphology on a wide spatial scale. Here we examined blended polyethylene with 97 wt% deuterated polyethylene and 3 wt% protonated polyethylene comprising molecules with a range of molecular weights. Measurements were conducted with various X-ray and neutron scattering techniques. The nanometer-scale analysis revealed that the crystal lattice is also independent of the molecular weight. Moreover, small-angle X-ray and neutron scattering measurements did not reveal any influence of molecular weight. On the other hands, strong streak-like neutron scattering was observed perpendicular to the drawing direction. The multicore-shell cylinder model was used to evaluate the parameters of the shish structure: the radius of the core cylinders increased with the molecular weight while the number of core cylinders decreased with the molecular weight. On the other hand, the micron-scale analysis using ultra-small-angle X-ray and neutron scattering measurements revealed that the micrometer-scale fibril structure is independent of the molecular weight.

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10:48AM R55.00013: Modeling the melting of a semicrystalline polymer*  
KIRAN IYER (Presenter), MARZBED MARGOSSIAN, MURUGAPPAN MUTHUKUMAR, University of Massachusetts Amherst — The melt state of a semicrystalline polymer is known to have several dependencies on process variables such as melt temperature and annealing time; it is by itself a rich system, possibly consisting of several topological constraints like entanglements. All of these contribute towards the mechanism of melting, resulting in several intriguing observations in experiments. In this work, we study the melting of a pre-formed polymer crystal by use of coarse-grained parallel tempering Langevin dynamics simulations, guided by experimental findings of the melting of a single polyethylene crystal. By investigating the melting of a single crystal, we determine the kinetics of the process. We also determine the kinetics of an aggregate formed by multiple polymer chains, and find that the kinetics is dependent on the polymer chains being able to cross an entropic barrier.

*NSF Grant No. DMR-1713696

Thursday, March 7, 2019 8:00 AM - 10:24 AM

Session R56 GSNP GSOFT: Discrete Structures: Geometry, Mechanics, Graphics, and Computation II  
BCEC 255 - Christian Santangelo, University of Massachusetts Amherst

8:00AM R56.00001: Geometric defects, weak forces, and self-similar buckling in non-Euclidean elastic sheets*  
KENNETH YAMAMOTO (Presenter), SHANKAR VENKATARAMANI, University of Arizona — Non-Euclidean elastic sheets (like lettuce, flowers, and sea slugs) exhibit extreme properties including an inherent floppiness, which we argue is governed by and may, in turn, be quantified by non-smooth geometric defects. The presence and interaction of these localized defects in hyperbolic sheets may be modelled and explored with rough solutions via discrete differential geometry (DDG) based on taking a singular limit that assumes a no-stretching constraint. Non-smooth geometric defects are identified by a skeleton of intersecting asymptotic curves which, along with geometric data along the curves, enables constructing complex morphologies with intricate wrinkling shapes. By computing various energies on discretized elements, numerical simulations using this novel DDG framework reveal the significant impact of non-smooth geometric defects on elastic energy as well as the non-negligible role of weak forces, i.e., effects other than stretching or bending, and associated scaling laws. Ultimately, these modeling techniques have the potential to explain real-world sheets and enable the control/design of thin soft structures.

*Work was supported by the Michael Tabor Scholarship from the Program in Applied Mathematics at the University of Arizona and the Simons Foundation.

8:12AM R56.00002: Discrete PolyCube Surface Flows  
PAUL ZHANG (Presenter), Computer Science, MIT, JOSH VEKHTER, University of Texas System, JUSTIN SOLOMON, Computer Science, MIT, ETIENNE VOUGA, University of Texas System — Discrete flows have been of particular interest to researchers in discrete differential geometry, computational geometry, and computer graphics, due to their connection to the Plateau problem in mathematics, mechanical behavior of various shells and membranes, and their application to shape science problems such as surface fairing, parameterization, collision modeling, registration, and interpolation. We study a new flow, formulated as a variational problem on certain bundles of quotient spaces of rotations over the surface, and describe algorithms to discretize and simulate it. The flow has the following property: stationary surfaces of the flow are polycubes, polyhedra whose facets meet only at right angles. Spheres flow to cubes, and more generally, surface features sharpen or flatten. Moreover the flow is intrinsic to the surface itself, and does not require a choice of preferred planes or directions in the ambient space. This flow has potential applications in crystallography, as well as simplification, discretization, and hexahedralization of shapes.

8:24AM R56.00003: Spatial and Network Effects in Distributed System Design*  
ANDREI A. KLISHIN (Presenter), Physics, University of Michigan, DAVID J. SINGER, Naval Architecture and Marine Engineering, University of Michigan, GREG VAN ANDERS, Physics, Engineering Physics, and Astronomy, Queen's University — Designing a modern complex system requires keeping track of the interplay of the system's logical topology, spatial arrangement, and functionality. Existing frameworks mostly focus on how one of these aspects influences others in a single direction, rather than keeping track of the mutually deterministic nature of design elements. We demonstrate how to determine mutual influences of topology and spatial constraints on each other for a whole ensemble of possible system arrangements. We cast this problem in the modern graphical language of tensor networks, which facilitates computation and allows for extracting a variety of ensemble observables. We demonstrate the power of the approach on a model system routing problem from Naval Engineering, however the method is easily generalizable to other problems.

*U.S. Office of Naval Research Grant no. N00014-17-1-2491.
Physics-inspired optimization for quadratic unconstrained problems using a digital annealer

MALIHEH ARAMON, GILI ROSENBERG, ELISABETTA VALIANTE, 1QB Information Technologies Inc., TOSHIYUKI MIYAZAWA, HIROTAKA TAMURA, Fujitsu Laboratories Ltd., HELMUT KATZGRABER (Presenter), Microsoft Quantum — The Fujitsu Digital Annealer is designed to solve fully connected quadratic unconstrained binary optimization (QUBO) problems. It is implemented on application-specific CMOS hardware and currently solves problems of up to 1024 variables using a parallel-trial algorithm based on simulated annealing. We compare the performance of the Digital Annealer to simulated annealing and parallel tempering Monte Carlo with isoenergetic cluster moves on different spin-glass problems. Our results show that the Digital Annealer currently exhibits a time-to-solution speedup of roughly two orders of magnitude for fully connected spin-glass problems, over the single-core implementations of simulated annealing and parallel tempering Monte Carlo used in this study. This, however, is not the case for sparse two-dimensional problems. We also benchmarked an early implementation of the Parallel Tempering Digital Annealer. Our results suggest an improved scaling over the other algorithms for fully-connected problems of average difficulty with bimodal disorder. The use of specialized hardware paired with fast algorithms thus allows for a more detailed study of statistical physics Hamiltonians in the near future.

Deployable and Mechanical Properties of An Origami Spring Structure*

SOPHIE USHERWOOD (Presenter), CONGRAN JIN, SHICHENG HUANG, Dartmouth College, XIAOHE LIU, Brown University, ZI CHEN, Dartmouth College — Origami has recently been studied intensively by physicists, mathematicians, and engineers due to its deployability, versatility and low cost in potential engineering applications. Examples include self-deployable solar arrays in space and self-folded origami inspired robots. To understand deployable properties of an origami structure, models of an origami “spring” were investigated. Origami spring structures may be useful in robotics and structural designs as their length can vary, while maintaining structural rigidity. Mathematical methods based on the geometry of these spring structures are used to predict ideal maximum height, formulate a relationship between the angle of rotation and the spring height, and to obtain a Poisson’s ratio of the spring structure. We show that the Poisson’s ratio is not constant and is scalable with respect to different geometric parameters. Elastic modulus of the spring structures are also predicted using models based on Hooke’s law and the stationary principle. By studying origami spring models, we discovered interesting and potentially practical engineering designing insights that are embedded in this smart structure.

*NSF of China (51322201 and U1632115) and STC of Shanghai (14JC1400200), Society in Science–Branco Weiss fellowship.

Discrete Geometric Simulation of Elastic Ribbons*

WEICHENG HUANG (Presenter), Department of Mechanical and Aerospace Engineering, University of California, Los Angeles, XILAI ZHANG, Department of Electrical and Computer Engineering, University of California, Los Angeles, MOHAMMAD KHALID JAWED, Department of Mechanical and Aerospace Engineering, University of California, Los Angeles — We report a discrete differential geometry based numerical simulation for elastic ribbons. Ribbon is a mechanical structure whose three dimensions are very different: length >> width >> thickness. In our framework, we use the elastic energy form, with two essential geometric constraints, of a one-dimensional model of the ribbon [Dias and Audoly, J. Elast. 2015]. As non-zero natural curvature in both in-plane (geodesic curvature) and out-of-plane directions have been considered, this model allows a unified treatment of various types of ribbons, e.g. annular and rectangular. This continuous model is discretized into a mass-spring system in a manner similar to well established Discrete Elastic Rods algorithm for simulation of elastic rods. A system of discrete equations of motions are developed that can be solved implicitly using Newton’s method. In parallel with simulations, we perform experiments with several test cases, e.g. large deformation of elastic ribbons under gravity, coupling of twisting and bending in rectangular ribbons, shape of Mobius strips, and buckling in annular ribbons. Quantitative comparison between experiments and simulations validates the correctness of our numerical method.

*We acknowledge support from HSSEAS, University of California, Los Angeles.
Numerical Simulations for Physics-based Training of Robots for Manipulation of Flexible Rods*

LONGHUI QIN (Presenter), YAYUN DU, WEICHENG HUANG, MOHAMMAD KHALID JAWED, Department of Mechanical & Aerospace Engineering, University of California, Los Angeles — Robotic manipulation of flexible ropes has wide ranging application from advanced manufacturing to robot-assisted surgery. We report a physics-based scheme to deploy elastic ropes along a prescribed trajectory with a collaborative robot. A numerical simulation tool, based on the Discrete Elastic Rods method, is developed for the modeling of elastic rods including contact and friction. Given the stochastic nature of the friction between the rope and the ground, avoiding friction is a key to repeatability of experiments with the robot. Exploiting the robustness and efficiency of the computational framework, we generate training data in the numerical simulator. This data is used to plan the optimal path for the robotic arm such that friction is minimized during deployment of ropes on a given trajectory. Compared with physics-blind methods that require empirical training by humans for every single rope, our proposed scheme remains valid for any elastic rope regardless of the geometric and material properties. Moreover, vast amount of data can be produced from the simulator in a few hours on a contemporary CPU to train a general neural network with high accuracy.

*We acknowledge support from Henry Samueli School of Engineering and Applied Science, University of California, Los Angeles.

A Discrete Geometric Approach to Simulation of Soft Multi-limbed Robots

MOHAMMAD KHALID JAWED, University of California, Los Angeles, XIAONAN HUANG (Presenter), CARMEL MAJIDI, Carnegie Mellon University — Because they are primarily composed of mechanically compliant and deformable materials, soft limbed robots can navigate through unstructured terrain and confined spaces without dependency on highly articulated motion and sensing. However, design and control requires a painstaking trial and error process owing to the absence of an accurate and efficient simulation and modeling tools. Here, we present a numerical simulation tool for limbed soft robots inspired by a discrete differential geometry-based computational framework that can run faster than real-time on a single thread of a contemporary desktop processor. The simulation incorporates an implicit method to account for the elasticity of the structure, contact with an uneven surface, and Coulombic friction between the soft robot limbs and ground. To validate the simulation, we build a novel, shape memory alloy driven star-shaped soft robot comprised of seven compliant limbs that can cyclically change shape through electrical Joule heating and passive cooling. Our experiments and simulations show reasonable quantitative agreement and indicate the potential role of this discrete geometric approach as a computational framework in predictive simulations for soft robot design and control.

Topological Characterization of Meta-stable States in Weakly Non-linear Diffusion Processes on Networks

NIMA DEHMAMY (Presenter), ALBERT-LASZLO BARABASI, Northeastern University — Complex networks are ubiquitous. Many dynamical processes on networks, including spreading processes such as SIR and SIS, are generally weakly non-linear and the core of the process consists of a diffusion process. However, while the diffusion may have a trivial fixed point where the probability distributions over all nodes becomes uniform or proportional to their degree, the nonlinearity generally results in the trivial fixed point becoming unstable, yielding non-trivial outcomes. Especially in real networks with modular and other internal structures, characterizing these outcomes requires numerical simulations. Here we report discovering a deep connection between these solutions and symmetry groups. In particular, we consider a multi-dimensional weakly non-linear dynamical process on a network and show that it is equivalent to a force-directed layout problem. We then show how the topology of the embedding space and its symmetry group can be used to characterize the low-energy solutions, which turn out to be topological in nature. Often the trivial fixed-point of the dynamics, where the field over all nodes collapses to zero, is unstable due to constraints arising from non-linear interactions among nodes, resulting in topological low-energy states becoming the dominant.
**9:48AM R56.00010:** Connecting discrete to the continuum: continuum-level simulation of shear-banding in metallic glasses on transforming grids with Lees-Edwards boundary conditions*  
NICHOLAS BOFFI (Presenter), CHRISTOPHER RYCroFT, Harvard University — We simulate a three-dimensional continuum-level elasto-plastic model of a bulk metallic glass based on the shear transformation zone (STZ) theory of amorphous plasticity. The simulation utilizes a new projection method valid in the quasi-static limit based on a mathematical correspondence between the Navier-Stokes equations for incompressible fluid flow and the equations of quasi-static hypoelastoplasticity. We emphasize a variation of the method based on a coordinate transformation that permits the use of Lees-Edwards boundary conditions at the continuum scale, enabling direct comparisons between continuum and discrete simulation. We consider several interesting numerical examples, including simple and pure shear boundary conditions imposed in the transformed frame.

*Funding provided by the Department of Energy Computational Science Graduate Fellowship & National Science Foundation Grant No. DMR-1409560.

**10:00AM R56.00011:** Maxwell Force Shaping of Dielectric Liquid Films on Curved Conducting Substrates  
CHENGZHE ZHOU (Presenter), SANDRA TROIAN, MC 128-95, CALTECH, Pasadena, CA 91125 — The dynamical behavior of thin dielectric films on curved substrates is critically important to a range of processes fundamental to the coating industry, micro-lithography and biological flows. Substrate curvature can strongly affect film shape and stability, especially when the local film thickness couples to an external field. For thin dielectric films on planar domains, accurate solutions can be obtained by exploiting the gradient flow structure of the governing equation and appealing to the Helmholtz minimum dissipation principle. Here we show how this minimization principle can be extended to include thin films on curved substrates wherein the local film thickness is *actively coupled* to an external electric field and whose response is only mitigated by capillary forces. Accurate approximate solutions are obtained by invoking a variational principle and restricting trial solutions to polynomial functions in the direction normal to the substrate. We demonstrate this approach for a thin dielectric film coating a cylindrical conductor using a boundary/finite element method. We find that this solution method offers keen physical insight into allowable film configurations not accessible to planar geometries.

**10:12AM R56.00012:** Cross-Influence of Thermodynamic Driving Forces in Confined Environment  
YU QIAO (Presenter), MENG WANG, University of California, San Diego — The second law of thermodynamics dictates that under a certain condition, the cross-influences of thermodynamic driving forces (tdf) must be balanced. For a galvanic cell, it is equivalent to the well-known Nernst equation; for a double-layer supercapacitor, it is consistent with the classic Gouy-Chapman model. In our recent experiment on confined large pivalate ions in carbon nanopores, however, it was measured that the cross-influences of the electromotive force and the chemical potential were different from each other by an order of magnitude. We attribute this remarkable phenomenon to the confinement effect of the electrode inner surfaces, which forbids the formation of diffuse layer. We argue that in general, in a low-dimensional environment, in the large dimension(s), the laws of classic statistical physics can be applied; but in the small dimension(s) wherein two tdf interact, the governing equations can be distinct. With this unique mechanism, the second law of thermodynamics may break down, in a dissimilar manner to “Maxwell’s demon”. The concept of unbalanced cross-influence of tdf is further examined through a theoretical analysis on a model system comprising of randomly moving elastic particles restricted in a two-dimensional transition zone in a gravitational field.

**Thursday, March 7, 2019 8:00 AM - 11:00 AM**

**Session R57 GSNP DBIO: Noise-driven Dynamics in Far-from-equilibrium Systems II**  
- Stephen Teitsworth, Duke University
8:00AM R57.00001: Enhancing noise-induced escape in systems with distributed delays* IRA SCHWARTZ (Presenter), Nonlinear System Dynamics Section, United States Naval Research Laboratory, YULIYA N. KYRYCHKO, Department of Mathematics, University of Sussex — Many real world dynamical systems exhibit complex behavior often induced by intrinsic time delays, as well as influenced by random perturbations. An important problem, therefore, is to understand how random disturbances are organized such that the dynamics escape from a stable attractor and exhibit new behavior. Although the noise amplitudes are small, the result is a large fluctuation out of the basin of attraction. Here we study the influence of noise-induced large fluctuations on dynamical systems, where the time delay is not taken as a constant but is rather chosen from a given distribution. We use a variational approach to calculate the escape rates out of the basin of attraction for a general kernel of the delay distribution, as well as general nonlinearity. We illustrate the theory by taking two particular examples of the distribution kernel, namely, the uniform and bi-modal kernels, and analyze how the width of the distribution affects the switching rates. Our results show that the switching is affected not only by the mean time delay but also by the width of the delay distribution. Specifically, if the distribution width is increased, this leads to an increase in the switching times.

*Research supported by ONR and NRL Base Research Program.

8:12AM R57.00002: A study of rare-event extinction phenomena in three species cyclic predation games.* SHANNNON SERRAO (Presenter), Center for Soft Matter and Biological Physics, Virginia Tech, DARRA LABAVIC, Laboratoire de Physique des Lasers, Atomes et Molécules, Université Lille 1 Sciences et Technologies, HILDEGARD MEYER-ORTMANNS, Physics and Earth Sciences, Jacobs University Bremen gGmbH — In the modified May-Leonard model with cyclically competing three species, we compute the statistics of rare-event two species extinction process from a long lived metastable three-species coexistence state due to large fluctuations. We employ a master equation based eikonal quasi-stationary approximation of the metastable state effectively reducing the problem to the classical dynamics evolution of a Hamiltonian in six degrees of freedom. We then solve the evolution of this system by applying the Iterative Action Minimization Method(IAMM) and compute the action along the optimal path across the transcritical bifurcation. Our results are compared with action computed from the generating function based Hamiltonian of the said (3,1) game. The results obtained are validated for regions across the transcritical bifurcation in the system and investigated for different values of the system size parameter $V$.

*DFG, German Research Foundation

8:24AM R57.00003: Scaling laws governing stochastic death of individual cells and the extinction of populations. SRVIDYA IYER-BISWAS (Presenter), KUNAAL JOSHI, Purdue University — In this talk I will discuss the scaling laws governing stochastic death of individual cells and the extinction of populations, bridge the timescales of single-cell and population dynamics under conditions when there is significant mortality, and make connections to ongoing experiments on *C. Crescentus* cells.

8:36AM R57.00004: Intergenerational dynamics of individual cells reveal rules governing stochastic cell-size homeostasis KUNAAL JOSHI (Presenter), SRVIDYA IYER-BISWAS, Department of Physics and Astronomy, Purdue University — In this talk I will first establish that cell size homeostasis is maintained under appropriate growth conditions, using multigenerational data from our experiments on individual *C. Crescentus* cells. I will then discuss how our data on intergenerational dynamics of cell size, cell shape and cell division times, obtained under several growth conditions, reveal the rules governing stochastic cell-size homeostasis.

8:48AM R57.00005: Kinetic inversion of repressors and activators in gene expression regulation. ZHIYUE LU (Presenter), CHUDONG WU, AARON DINNER, University of Chicago — In gene expression regulation, repressors and activators compete to bind with the gene's regulatory element, and the chance of activators binding with the regulatory element dictates the activation level of the gene. In a thermal equilibrium regime, this chance of binding is well determined by the concentrations of activators and repressors as well as their binding free energies to the regulatory element -- a high level of repressor will result in a low chance of activator binding. However, inspired by the experimental observations of cooperativity between activators and repressors, we propose a non-equilibrium dynamics model to describe the gene regulatory dynamics when the concentration of the repressor changes rapidly over time. We demonstrate a minimal Markov model where a rapidly changing level of repressor significantly increases the level of activation beyond predicted by equilibrium theory and effectively enhance the activator. Our model introduced an internal degree of freedom of the regulatory element, and its kinetic barrier allows the system to harnesses the chemical work done by the rapidly changing concentration of the repressor and use it to boost the level of gene activation beyond the equilibrium prediction.
9:00AM R57.00006: A partial differential equation for the mean first-return-time phase of a stochastic oscillator

BENJAMIN LINDNER (Presenter), Humboldt University of Berlin, ALEXANDER CAO, PETER J. THOMAS, Mathematics, Case Western Reserve University — Phase reduction of limit cycle dynamics provides a low-dimensional representation of high-dimensional oscillator dynamics. For a deterministic dynamical system with a stable limit cycle, the change to a phase variable is well established. In contrast, for stochastic limit cycle systems, a phase reduction can be defined in several nonequivalent ways (e.g. Schwabedal and Pikovsky Phys. Rev. Lett. 110, 205102 (2013), Lindner and Thomas Phys. Rev. Lett. 113, 254101 (2014)). Schwabedal and Pikovsky introduced a phase for stochastic oscillators based on a foliation of the basin of attraction, with the property that the mean transit time around the cycle from each leaf to itself is uniform and developed a numerical procedure to estimate the corresponding isochrons. For robustly oscillating planar systems driven by white Gaussian noise, we establish a partial differential equation with a mixture of reflecting and jump boundary conditions that governs this phase function. We solve this equation numerically for several examples of noisy oscillators. In addition, we obtain an explicit expression for the isochron function, for the rotationally symmetric case, and compare this analytical result with oscillators that have been studied numerically in the literature.

9:12AM R57.00007: Fitness landscapes as predictor of noise-driven self-organized pattern formation on surfaces

ZG�N YAVUZ, ONUR TOKEL, FATIH ILDAY, SERIM ILDAY (Presenter), Bilkent University — Pattern formation far from equilibrium often exhibits a richness that is quite distinct from near-equilibrium dynamics. Perhaps the most visible consequence is the formation of different patterns in addition to the one favored at or near equilibrium. Can these, then, be controlled, and selected, externally? Here, we adopt the concept of "fitness landscapes" from evolutionary biology to show how nonlocal feedback gain of tailored defects controls and steers the evolution of nanopatterns using Nonlinear Laser Lithography (Iliday, Nat. Photon., 2013), an optical method that forms feedback-regulated patterns with nanometer uniformity. Through numerical simulations and experimental demonstration, we show that stimulated symmetry breaking can direct these nanopatterns to all possible 2D Bravais lattices.

9:24AM R57.00008: Wavenumber Selection in Pattern Forming Systems

SALONI SAXENA (Presenter), JOHN MICHAEL KOSTERLITZ, Brown University — Pattern forming systems are characterized by the emergence of a band of stable spatially periodic states as a control parameter is varied. Wavenumber selection refers to the evolution of such systems to one of these states at long times, irrespective of initial conditions. Numerical studies of pattern forming phenomena indicate that the presence of noise is a mechanism for wavenumber selection at long times. We investigate this for the noisy Stabilized Kuramoto Sivashinsky (SKS) equation. Computational difficulties restricted earlier numerical simulations of this equation to small system sizes and a narrow range of control parameters[1]. Our aim now is two-fold: to determine whether wavenumber selection occurs for larger system sizes and to do so for a broader range of control parameter values. With the use of spectral methods of integration, we have been able to simulate larger system sizes and obtain a crude probability distribution of final states. We present our results for various system sizes and demonstrate a possible connection to large deviation theory[2]. The drawbacks of our approach and possible improvements are also discussed.


9:36AM R57.00009: Crossover between parabolic and hyperbolic scaling, oscillatory modes and resonances near flocking*

CAROLINA TRENADO (Presenter), LUIS BONILLA, Carlos III University of Madrid — A stability and bifurcation analysis of a kinetic equation indicates that the flocking bifurcation of the two-dimensional Vicsek model exhibits an interplay between parabolic and hyperbolic behavior. For box sizes under a certain large value, flocking appears continuously from a uniform disordered state at a critical value of the noise. Bifurcation equations contain two time scales and, due to mass conservation, comprise a scalar equation for the density disturbance from the homogeneous state and a vector equation for a current density. At the shorter scale, they are a hyperbolic system in which time and space scale in the same way. The equations are diffusive at the longer time scale. The bifurcating solution depends on the angle and is uniform in space as in the normal form of the usual pitchfork bifurcation. We show that linearization about the latter solution is described by a Klein-Gordon equation in the hyperbolic time scale. Then there are persistent oscillations with many incommensurate frequencies about the bifurcating solution that may resonate with a periodic forcing of the alignment rule. These predictions are confirmed by direct numerical simulations of the Vicsek model.

*Spain Ministerio de Economia y Competitividad grant MTM2017-84446-C2-2-R.
**9:48AM R57.00010: Spin lattices of walking droplets**

PEDRO SAENZ (Presenter), Massachusetts Institute of Technology, GIUSEPPE PUCCI, Institut de Physique de Rennes, SAM E TURTON, ALEXIS GOUJON, RODOLFO R ROSALES, JORN DUNKEL, JOHN BUSH, Massachusetts Institute of Technology — In this talk, we will introduce a hydrodynamic analog system that allows us to investigate simultaneously the wave-mediated self-propulsion and interactions of effective spin degrees of freedom in inertial and rotating frames. Millimetric liquid droplets can walk across the surface of a vibrating fluid bath, self-propelled through a resonant interaction with their own guiding wave fields. A walking droplet, or `walker', may be trapped by a submerged circular well at the bottom of the fluid bath, leading to a clockwise or counter-clockwise angular motion centered at the well. When a collection of such wells is arranged in a 1D or 2D lattice geometry, a thin fluid layer between wells enables wave-mediated interactions between neighboring walkers. Through experiments and mathematical modeling, we demonstrate the spontaneous emergence of coherent droplet rotation dynamics for different types of lattices. For sufficiently strong pair-coupling, wave interactions between neighboring droplets may induce local spin flips leading to ferromagnetic or antiferromagnetic order. Transitions between these two forms of order can be controlled by tuning the lattice parameters or by imposing a Coriolis force mimicking an external magnetic field.

*NSF CMMI-1333242, DMS-1614043, and CMMI-1727565.

**10:00AM R57.00011: Observation of Stochastic Resonance Induced by Dichotomous Noise in a Liquid Crystal Light Valve with Optical Feedback**

YOSHITOMO GOTO (Presenter), Department of Materials Science and Production Engineering, Oita University, TOMOYUKI NAGAYA, Division of Natural Sciences, Oita University, HIROSHI ORIHARA, Division of Applied Physics, Hokkaido University — Noise-induced phenomena are widely observed in nature and are of great interest in the field of nonlinear dynamics. Stochastic resonance (SR), which is one of the most well-known noise-induced phenomena, has been discussed intensively [1], [2]. SR is a phenomenon in which the response of a nonlinear bistable system to a weak signal is enhanced by the addition of noise. In the present study, we focus on a liquid crystal light valve (LCLV) with optical feedback as one of the bistable systems. In the LCLV with optical feedback, the average orientation of the LC molecules, so-called director, shows bistability in some conditions [3], [4]. In this report, we discuss SR in LCLV with optical feedback system induced by the dichotomous noise (DN), characterized by an autocorrelation time.


*This work was supported in part by JSPS KAKENHI Grant Number JP15K13553, JP18H01374.

**10:12AM R57.00012: Boundary Effects in Stochastic Cyclic Competition Models on a Two-Dimensional Lattice**

M. LAZARUS ARNAU (Presenter), SHANNON SERRAO, UWE CLAUS TAUBER, Virginia Tech — We study noise-induced and stabilized spatial patterns in two distinct stochastic population model variants for cyclic competition of three species, namely the Rock-Paper-Scissors (RPS) and the May-Leonard (ML) models. In two dimensions, it is well established that the ML model can display (quasi-)stable spiral structures, in contrast to simple species clustering in the RPS system. Our ultimate goal is to develop local control schemes which allow us to affect the formation of these spatio-temporal patterns. To this end, we have employed MC simulations to investigate how changing the microscopic rules in a subsection of a two-dimensional lattice influences the macroscopic behavior in the rest of the lattice. Specifically, we implement the ML reaction scheme on a torus, except on a ring-shaped patch, which is set to follow the cyclic Lotka-Volterra predation rules of the RPS model. At the RPS-ML interface we observe a marked disruption of the usual spiral patterns in the form of plane waves emanating from the RPS region. Also, we report a distinct decrease in local population density near the interface in comparison to the bulk of the ML region.

*Research was sponsored by the U.S. Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.
Measurement and feedback are integral components for efficient functioning of physical systems in the microscopic as well as macroscopic world. We will analyze and quantify the thermodynamic costs of performing bit level measurements and energetics of feedback action. The thermodynamic system of interest studied is a Brownian particle in a bi-stable well, which is often used as a model for a single bit memory in the study of erasure of information. Landauer states that the minimum amount of heat dissipation for erasing a memory bit is $k_B T \ln 2$, which provides the Landauer limit. Recent experiments demonstrate that the erasure can be achieved with energetics close to the Landauer's bound. The protocols in prior art are open-loop, where the information on the state of the memory is not employed in the erasure protocol. Here, we quantify the energetics of erasure protocols with feedback; experimentally as well as via Monte Carlo simulations. Results indicate that the deficit between the heat dissipation in the feedback based erasure protocol and the $k_B T \ln 2$ can be accounted for quantitatively by the measurement and feedback mechanisms. Non-conservative bounds are obtained on the deficit.

*The research was supported by the National Science Foundation under the grant NSF ECCS 1809194.

We present a model of a Brownian asymmetric simple exclusion process (BASEP) with overdamped Brownian dynamics that resembles properties of the asymmetric simple exclusion process (ASEP) on a lattice [1]. In this BASEP, particles of size $\sigma$ with hardcore interaction are driven by a constant drag force through a one-dimensional cosine potential with period $\lambda$. The character of the non-equilibrium steady states in the BASEP is strikingly different from that in the ASEP. Compared to the particle current in a system of non-interacting particles, we observe an enhancement for small $\sigma/\lambda$ ratios, caused by a barrier reduction effect arising from multi-occupation of potential wells. Larger $\sigma/\lambda$ ratios lead to a suppression of the current because of blocking effects. Surprisingly, an exchange-symmetry effect causes the current-density relation to be identical to that of non-interacting particles for commensurable lengths $\sigma=\lambda$. A current-density relation similar to the ASEP is obtained only for a limited parameter regime. The rich behavior of the current-density relation leads to phase diagrams of NESS in open systems with up to five different phases. The topology of these phase diagrams changes with varying $\sigma/\lambda$ ratio.


In biological systems, a key concept of interest is the energy required to induce changes in the state of a system. The modern approach to this problem is to identify the energy cost of such control with entropy dissipation. For systems with deterministic control, the lower bounds on entropy dissipation are well known. However such analyses tend to ignore the cost associated with the method of control which becomes crucial at the biological scale. Here we extend such analyses to take into account the entropy cost of exerting control on a system when the control itself is stochastic in nature and subject to fluctuations. Using the formalism of stochastic thermodynamics, we find an intriguing non-trivial unification of previous results for a realizable controlled non-equilibrium steady state system driven at a finite rate around a loop in thermodynamic space. In particular we show that for a model system, the lower dissipation bound is almost the sum of two previously found bounds. Despite this, our result suggests that even for an infinitely long control protocol, it is still impossible to reach the adiabatic limit for stochastic systems.
8:00AM R58.00001: Influence of Elastic Modulus of a Soft Elastomer on Adhesion to Rough Surfaces  SIDDHESH DALVI (Presenter), Department of Polymer Science, The University of Akron, ABHIJEET GUJRATI, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, ALI N DHINOJWALA, Department of Polymer Science, The University of Akron, TEVIS JACOBS, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, LARS PASTEWKA, Department for Microsystems Engineering, University of Freiburg — In the field of adhesion science, it is of practical importance to understand how roughness affects adhesion. This is of direct relevance in designing adhesives for applications in the areas of microelectronics, biomedical devices, and composites. The main idea is to have the adhesives conform to the roughness and approach close enough for van der Waals (or other electrostatic) interactions to be effective. The first complete mathematical formulation for roughness was put forward by Greenwood and Williamson using a single-length-scale model describing the surfaces as hemispherical asperities with a Gaussian distribution of heights. Bo Persson has proposed a multi-scale model to calculate the adhesion energy as a function of modulus and roughness, as described using the power spectral density of topography. Here we have performed contact and fracture mechanics experiments for smooth cross-linked polydimethylsiloxane with varying elastic modulus on polycrystalline diamond surfaces with varying roughness, which have been characterized to obtain accurate multi-scale power spectral densities. We will present the comparison between the predicted adhesion energies calculated using Persson's theory and the experimental adhesion energy measured during approach and separation.

8:12AM R58.00002: Gluing polymer interfaces with nanoparticles: insights from molecular dynamics  NICOLA MOLINARI, BORIS KOZINSKY, Harvard University, STEFANO ANGIOLETTI-UBERTI (Presenter), Department of Materials, Imperial College London — In recent years, nanoparticles have been shown to have the potential to answer the centuries-old question of how to mechanically strengthen an interface between soft materials. A deeper understanding of the mechanism and parameters resulting in the mechanical reinforcement, or lack thereof, would help rationalize experimental findings and, ultimately, guide the design of adhesive solutions. Building on our previous work on polymer in bad solvent conditions [DOI: 10.1021/acs.nanolett.8b00586], we investigate the trends, and the fundamental drivers of, the mechanical properties of polymer interfaces glued with spherical nanoparticles. Using a coarse-grained model, we simulate polymer network structures with different degrees of swelling. The interface between two networks is filled with nanoparticles, and the overall system is then uni-axially strained to construct the stress-strain curve for a given set of parameters. The results from this investigation help disentangling the contributions to the strengthening of the interface and can be used as a guide to experimental design of nanoparticles-based adhesives.

8:24AM R58.00003: Ultra-soft textured substrates*  MARTIN COUX (Presenter), JOHN KOLINSKI, Ecole Polytechnique Fédérale de Lausanne — Droplets deposited on soft elastomers or gels with elastic moduli ~ 1 – 10 kPa induce a micro-scale elastic deformation at the contact line. This significantly modifies the wetting properties of the solid - for example, a droplet deposited on an inclined soft surface will slide downward driven by its weight at velocities orders of magnitude less than a droplet on a similarly inclined rigid solid. Here, we confine the contact between water and a soft silicone gel to micrometric patches by texturing the solid, inducing superhydrophobicity for materials with elastic moduli as low as 3 kPa. The coupling between surface texture and surface compliance strongly influences the behavior of the droplet at both macro- and micro- scales, leading to a giant speed up during descent, and potentially affecting the stability of the Cassie state.

*This work was supported by the Piaget Scientific Award.

8:36AM R58.00004: Hydrogel menisci: Shape and interaction  ANUPAM PANDEY (Presenter), CHARLOTTE NAWIJN, JACCO SNOEIJER, University of Twente — The interface of a soft hydrogel is easily deformed when it is in contact with particles, droplets or cells. Here we compute the intricate shapes of hydrogel menisci due to the indentation of point particles. The analysis is based on a free energy formulation, by which we also assess the interaction laws between neighboring particles on hydrogel interfaces, similar to the “Cheerios effect”. It is shown how the meniscus formed around the particles results from a competition between surface tension, elasticity and hydrostatic pressure inside the gel. We provide a detailed overview of the various scaling laws, which are governed by a characteristic shear modulus $G^* = \sqrt{\gamma \rho g}$ that is based on surface tension $\gamma$ and gravity $\rho g$. Materials with shear modulus larger than $G^*$ exhibit a solid-like response while softer materials are more liquid-like.
8:48AM R58.00005: Equilibration time, swelling, and the tangential contact-line force on a partially immersed gel thread

SHIH-YUAN CHEN (Presenter), AARON R BARDALL, MICHAEL SHEARER, KAREN DANIELS, North Carolina State University — When a liquid contacts a sufficiently soft material, the surface tension of the liquid deforms the substrate at the contact line, forming a ridge. The height of this ridge is on the order of \( y/E \), known as the elastocapillary length. The precise stress boundary condition at the contact line has a significant effect on this mechanism, but is as yet unresolved. A complicating factor is that liquids also interact with gels by swelling and/or contamination from the uncrosslinked oil in the gel. Hence, it is crucial to distinguish these different mechanisms when conducting an elastocapillary experiment. In our talk, we present experiments with a poly(vinyl siloxane) gel thread partially immersed in liquids of different wettability and swellability. We show that when making stress-strain measurements via fluorescent bead microscopy, the positions of the beads only equilibrate after 12 to 24 hrs. This timescale is incompatible with the use of ethanol as the immersion fluid, since it swells the PVS thread; we find that using FC-40 allows the thread to reach equilibrium without swelling. Once these two effects are resolved, the evidence for a tangential force at the contact line is weak.

*National Science Foundation DMR-1608097

9:00AM R58.00006: Using droplet shapes to study the surface tension of soft gels

KATRINA SMITH-MANNSCHOTT (Presenter), QIN XU, ERIC DUFRESNE, ROBERT STYLE, ETH Zurich — Surface tension is a phenomenon typically associated with liquids, rather than with solids. However, interest in interfaces of soft solids has revealed the importance of surface tension, for instance in controlling small-scale adhesion behavior. Here, we aim to develop a new technique to investigate the surface tension of soft gels through the analysis of droplets on a stretched substrate. In particular, we find that small droplets on a stretched surface elongate along the stretch direction. We will show how this is consistent with the presence of strongly strain-dependent surface stresses.

*SNSF Grant 200021-172827

9:12AM R58.00007: Adhesion-Based Measurements of Strain-Dependent Surface Stress in Soft Solids

JEREMY THALLER (Presenter), MINWOO KANG, KATHARINE JENSEN, Williams College — Surface stress, or surface tension, is a fundamental material property of interfaces. However, our understanding of solid surface tension and how it changes with deformation remains limited because it is difficult to measure in traditional stiff materials. Soft materials, including gels, provide a unique opportunity to measure these fundamental properties because they can be stretched elastically to very large strains. In this work, we use an adhesion-based approach to measure the solid surface stress of compliant materials as a function of applied strain. This approach is applicable to a wide range of soft materials.

9:24AM R58.00008: Interfacially Driven Plastic Deformation of Soft Solids

CHRISTOPHER O’BRYAN (Presenter), THOMAS ANGELINI, University of Florida — Capillary forces acting on the surface of a solid result in elastic deformation on the scale of the elastocapillary length. While these elastic deformations may be negligible in stiff materials, they can dominate the behavior of soft solids, including rubbers, hydrogels, and biological tissues. In the extreme case, capillary forces may exceed the material's yield stress, resulting in plastic deformation near the contact line. Although this elastocapillary effect has been theorized, experimental exploration into this phenomenon have remained limited. Understanding the role of interfacial forces on the deformation of soft surfaces is necessary as new methods for manufacturing soft materials with low moduli and yield stresses are developed. Here, we investigate interfacial instabilities of 3D printed microbeams, using jammed granular microgels swollen in aqueous and organic solvents as both sacrificial support materials and as printed inks. By leveraging the highly tunable material properties of these microgel systems and the structural control offered by 3D printing, we systematically explore a range of yield stresses and beam widths to understand how elastocapillary effects can drive mechanical instabilities and material failure in soft solids.

9:36AM R58.00009: Poking a peach: Is testing for ripeness confounded by the skin

DOMINIC VELLA (Presenter), FINN BOX, University of Oxford, MOKHTAR ADDA-BEDIA, ENS Lyon — To test whether soft fruit is ripe, one often pokes with a finger. However, the flesh of the fruit itself is significantly softer than when the skin remains intact. In this talk we will address the question of when the indentation stiffness of a soft material coated by a thin, but significantly stiffer, material is affected by the presence of the coating. We demonstrate a substrate-dominated regime and a mixed regime (in which both coating and substrate are important) and show that the size of the indenter is a key parameter separating the two.

*ERC StG 637334
9:48AM R58.00010: Direct observations of dewetting relaxation at the interface of soft gels [Invited]  QIN XU (Presenter), ETH Zurich, LAWRENCE WILEN, Yale University, ROBERT STYLE, ERIC DUFRESNE, ETH Zurich — Wetting of liquid droplets on soft gels (E~3kPa) deforms gel interface significantly: a wetting ridge grows under the balance between liquid surface tension and solid surface stress near contact line. Using interference microscopy and fast camera imaging, we directly observe the recovery of gel surface from this wetting-induced deformation after removing liquid droplet. We show experimentally that surface relaxation of soft gels cannot be simply modelled by their viscoelastic rheology. Instead, the relaxation behaviour is a consequence of interplay between different restoring stresses near the interface, including solid capillarity and elasticity, and resisting stresses from the bulk, such as osmotic pressure across the network and local viscous stresses. By measuring scaling of wetting shapes under relaxation, we can determine which stress dominates the dissipation. Our results further extend the current understanding of elastocapillarity with the effect of bulk porosity, and bring new insight into the study of wetting dynamics on soft materials.

10:24AM R58.00011: Surface waves and wakes on soft solids  ROBERT HAUSSMAN (Presenter), ADITI CHAKRABARTI, LAKSHMINARAYANAN MAHADEVAN, Harvard University — Understanding the response of soft matter surfaces to dynamical disturbances is critical for a variety of applications, such as ultrasound and needleless injections. Motivated by this, here we explore the dynamical response of a very large, very soft solid due to impulsive and moving pressure disturbances on its surface. In particular, we describe the conditions under which Kelvin wake-like patterns should appear and derive perturbative corrections due to soft elasticity about the well-known inviscid limit, and describe the results of experiments to probe this limit.

10:36AM R58.00012: Measuring the dispersion relation of capillary waves using differential dynamic microscopy*  JING WANG (Presenter), RYAN J. MCGORTY, Department of Physics and Biophysics, University of San Diego — With a recently-developed method for measuring capillary wave dynamics at the interface of fluids we examine non-equilibrium interfacial fluctuations. We use a colloidal-polymer mixture that separates into colloid-rich and colloid-poor fluid phases with an ultra-low surface tension and capillary velocities on the order of a micron per second. We use differential dynamic microscopy (DDM) to measure the two-dimensional dispersion relation of capillary waves at spatial frequencies spanning over an order of magnitude. Using temperature-responsive colloidal particles (pNIPAM) to tune the phase diagram we investigate the interfacial fluctuations between non-equilibrium phases.

*American Chemical Society Petroleum Research Fund (57326-UNI10)

10:48AM R58.00013: How suction cups fail  CHON U CHAN (Presenter), MICHELLE WALSH, L MAHADEVAN, Paulson School of Engineering and Applied Sciences, Harvard University — Suction cups occur in nature and technology, and are widely used in a range of situations across many length scales. They often cannot afford to fail owing to catastrophic consequences associated with examples such as lifting large glass sheets, and in manipulating delicate tissues and organisms. But how do they fail? We report an experimental study that captures the failure dynamics of soft suction cups that involves an interplay of elastic deformation, viscous lubrication flows and interfacial instabilities over time scales that range from milliseconds to hours. Our study allows us to propose a design to prolong the holding time till failure.

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R59 GSOFT: Actuation in Soft Matter I BCEC 257B - Tag(s): Focus

8:00AM R59.00001: Actuation in soft matter [Invited]  ROBERT SHEPARD (Presenter), Cornell University — It has recently been shown that elastic materials may be architected to display remarkable functionality when harnessing mechanical instabilities. These so called mechanical-metamaterials are however often passive elastic structures, which undergo deformations when prompted by external loading. Different modes of actuation have been proposed, such as pressure controlled grabbing fingers in soft-robotics, swelling in shape-morphing gels, electrostatics in dielectric elastomers or temperature in liquid cristal polymers or shape memory alloys. How can these different solution be integrated in future manufactured devices? We are seeking contributions studying the fundamental and practical aspects of the integration of actuation in the design of soft materials. Particularly, we are interested in the (1) the mechanisms of amplification of an input via the architecture of the materials and (2) the programability of a complex response using a simple mode of actuation. This session would be in the core of recent GSOFT topics as illustrated in the previous editions of the March meeting, eg Soft Interfaces Mechanics, Robophysics, Extreme Mechanical Instabilities, Origami and kirigami of metamaterials.
Sequential actuation of deformable actuators, producing a complex preprogrammed response with just a single and simple input. Through a combination of experiments and numerical simulations we demonstrate that the transition waves propagating in a system comprising several bistable dome-shaped membranes that enclose fluid filled cavities can be exploited to trigger the sequential actuation of deformable actuators, producing a complex preprogrammed response with just a single and simple input.

*Prof. K. Bertoldi acknowledges support from the National Science Foundation under Grant No. DMR-1420570

Mechanically programmable sequential actuation of fluid-driven soft actuators

LUUK VAN LAAKE (Presenter), JOHANNES OVERVELDE, AMOLF — Fluid-driven actuators show great promise for robotics operating alongside human beings, for handling delicate and irregularly shaped objects, and for medical implants such as artificial muscles and even potentially heart prostheses. While soft actuators can be produced from materials that exhibit mechanical compliance close to that of human tissue, control of these actuators typically requires rigid elements such as electronic sensors, valves, and wires that may cause stress concentrations limiting the lifetime of the system. To circumvent this issue, we aim to replace the electronics by other modes of control using only soft elements that are embedded in the fluid that drives the soft actuators. Specifically, we focus on elastic hysteretic valves that allow us to program complex actuation patterns. We analyze the dynamic behavior using the electronic-hydraulic analogy and show that these circuits can deliver complex flows (e.g. pulsatile) to individual actuators, while fluidic power to the system is provided by a continuous fixed flow. We furthermore show that we can change the behavior of the soft system by varying the initial conditions, such that we can produce a soft robot that can be mechanically programmed to move using multiple gaits, without the need for electronics.

Walking Sheets: Locomotion in chemo-mechanically driven, non-Euclidean elastic plates

PEARSON MILLER (Presenter), Physics, Massachusetts Institute of Technology, JÖRN DUNKEL, Mathematics, Massachusetts Inst of Tech-MIT — Spatio-temporally varying chemical patterns are an essential mechanism for coordinating force generation in biological systems. Inspired by this, the use of active materials driven by self-oscillating reaction-diffusion equations is increasingly being explored for engineering applications. This talk describes recent investigations into the locomotion of chemically-driven, deformable surfaces from the perspective of non-Euclidean elastic plate theory. Through a combination of numerical and analytical results, we examine the geometric and mechanical characteristics which optimize gait velocity in an elastic sheet driven along a frictional surface. Further, locomotion on non-uniform terrain is considered, in particular the conditions in which external geometry can inhibit or promote robust motion. Overall, we develop insights into how best to utilize incompatible geometry in the design of soft robotics and other applications.

Untethered Soft Machines and Robots by Printing Ferromagnetic Domains in Soft Materials

YOONHO KIM (Presenter), HYUNWOO YUK, Soft Active Materials Lab, Department of Mechanical Engineering, Massachusetts Institute of Technology, RUIKE ZHAO, Department of Mechanical & Aerospace Engineering, The Ohio State University, SHAWN A. CHESTER, Department of Mechanical and Industrial Engineering, New Jersey Institute of Technology, XUANHE ZHAO, Soft Active Materials Lab, Department of Mechanical Engineering, Massachusetts Institute of Technology — Soft active materials capable of transforming into programmed shapes in a remotely controllable manner can bring promising applications in diverse fields such as soft robotics and biomedicine. Several types of shape-programmable soft matter have been proposed but often limited to simple geometries and thus with limited functionalities. We introduce a method of printing ferromagnetic domains in soft materials to realize highly responsive and fully programmable soft active materials that quickly transform into multiple desired shapes in applied magnetic fields. We also discuss the mechanics of our printed magnetic soft materials and the model-based simulation, which enable us to design complex structures with multiple modes of programmed actuation while guiding the material design for optimal actuation performance. Combined with the flexibility in design and fabrication, the fast and dynamic response of our printed soft machines and robots provides a range of potential applications, especially in biomedical areas where remote actuation of such untethered devices can be useful. To open this new avenue, we present a set of demonstrations that exemplify the concept of untethered soft machines and robots in biomedical applications such as magnetically steered catheters and guidewires.
9:24AM R59.00006: Energy Release Through Volume Snapping in Soft Inflatable Actuators* BENJAMIN GORISSEN (Presenter), DAVID MELANCON, NICK VASIOS, MEHDI TORBATI, KATIA BERTOLDI, SEAS, Harvard University — Traditionally, the actuation speed of soft inflatable actuators is limited by the influx of fluid, resulting in slow moving soft robots. To overcome this limitation, we have developed a bistable elastic actuator with an isochoric snap-through. As no external fluid input is needed to pass through this instability, the resulting actuator deformation happens quasi-instantaneous and is characterized by energy release. Besides optimizing the actuator's design for energy release, we also demonstrate its ability to be reset to the initial, undeformed state, enabling cyclic energy release.

*This research was supported by the Fund for Scientific Research-Flanders (FWO).

9:36AM R59.00007: Soft Robot Actuated by Electrostatic Force CONGRAN JIN (Presenter), Thayer School of Engineering, Dartmouth College, JINHUA ZHANG, XI'AN JIAOTONG UNIVERSITY, IAN TRASE, SHICHENG HUANG, ZHE XU, LIN DONG, JOHN X.J. ZHANG, ZI CHEN, Thayer School of Engineering, Dartmouth College — Conventional robots are rigid, powerful and robust, and hence they have been serving as trustworthy tools to assist humans in a variety of activities. However, due to their rigid body, they lack flexibility to cope with situations where space is confined, terrain is complex, or the environment is constantly changing. To solve these problems, researchers have focused on developing soft robots that can adapt to different environments. Nevertheless, most of the current locomotive actuation methods and materials have limited applications due to either large size, heavy weight, low speed, or complicated fabrication. We have designed, prototyped, and tested a thin-film-based electrostatic soft actuator that overcomes many of these drawbacks. A robotic bug based on this electrostatic actuator was designed and showed its (1) climbing ability through ascending inclines up to 30°, (2) flexibility through shape-recovery after crushing, (3) adaptability through walking on both rough and smooth surfaces and (4) maneuverability by precisely steering into a designated space. The development of such light weight flexible soft robotics will enable tasks such as surveillance, search-and-rescue, and detection that are challenging if not impossible for traditional robots in a cost-effective manner.

9:48AM R59.00008: Artificial Muscle by Tailoring Compliance in Magneto-kirigami Lattice YI YANG (Presenter), DOUGLAS PETER HOLMES, Mechanical Engineering, Boston University — The emerging research in soft robotics and micro-robotics has sparked new opportunities for developing artificial muscles of variable length scales and in various working environments. The essential challenge lies in controlling the deformability and compliance of its structural component. In this presentation, we demonstrate a novel approach to precisely control the compliance and deformability via perturbing the elastic energy state of metastable kirigami lattices. Each metastable kirigami lattice has two stable configurations corresponding to two distinct local energy minima. Switching between these two minima leads to either stiffening or softening in lattice structures, which when cycled between these states produces an artificial muscle. Through a combination of experiments and mechanical modeling, we interpreted the stiffening or softening mechanism and characterized the performance of the designed artificial muscle. Since the underlying physics of the metastable kirigami lattice is scale invariant, this kirigami architecture may path a new way to design and fabricate low cost, lightweight artificial muscle at multiple scales.

10:00AM R59.00009: Elastomeric focusing enables portable microvalves* NATE CIRA (Presenter), Harvard University — A continuing challenge in material science is creating active materials in which shape changes or displacements can be generated electrically or thermally. Here we borrow principles from hydraulics, in particular that confined geometries can be used to focus expansion into large displacements, to create solid materials with amplified shape changes. Specifically, we confined an elastomeric poly(dimethylsiloxane) sheet between two more rigid layers and caused focused expansion into embossed channels by local resistive heating, resulting in a 10x greater relative displacement than the unconfined geometry. We used this effect to create electrically controlled microfluidic valves that open and close in less than 100 ms, can cycle >10,000 times, and operate with as little as 20 mW of power. We investigate this mechanism and establish design rules by varying dimensions, configurations, and materials. We show the generality of elastomeric focusing by creating additional devices where local heating and expansion are generated either wirelessly through inductive coupling or optically with a laser, allowing arbitrary and dynamic positioning of a microfluidic valve along the channels.

*This work was supported by NSF GRFP, Siebel Scholar, TomKat, and NIH CTSA grants.
ANDREW GILLMAN, UES, Inc, GREGORY WILSON, University of Texas A & M, KAZUKO FUCHI, University of Dayton Research Institute, DARREN HARTL, University of Texas A & M, ALEXANDER PANKONIEN, PHILIP BUSKOHL (Presenter), Air Force Research Laboratory — The integration of soft actuating materials within origami-based mechanisms is a novel method to amplify the actuated motion and tune the compliance of the system for low stiffness applications. Origami structures provide natural flexibility given the extreme geometric difference between thickness and length, and the energetically preferred bending deformation mode can naturally be used as a form of actuation. However, origami fold patterns with specific actuation motions and mechanical loading scenarios are needed to expand the library of fold-based actuation strategies. In this study, an optimization framework is utilized to predict actuator topologies with different symmetry groups of input and output conditions with respect to the boundary conditions. Utilizing the patterns discovered through the optimization, the multistability of the actuator is further characterized through computational tracking of the bifurcating equilibrium branches and through empirical demonstration with actuator prototypes. This survey of origami mechanisms, comparison of actuation efficiency, and characterization of multistability provides a new set of origami actuators for future integration with soft actuating materials.

JI-HWAN KANG (Presenter), CHRISTIAN SANTANGELO, RYAN HAYWARD, University of Massachusetts Amherst — Self-folding of responsive polymer networks represents a powerful tool to form arbitrary 3D shapes from an initially flat 2D sheet. For example, our groups have previously developed trilayer polymer films that reversibly fold into complex origami designs due to swelling of a temperature-responsive hydrogel mid-layer. However, the configuration space of even very simple origami designs features multiple branches bifurcating from the flat state, meaning that self-folding structures can easily become trapped in an undesired state. Here, we evaluate two methods to avoid such misfolding. First, as suggested by Tachi and Hull (J. Mech. Robot. 2017), we design a set of driving forces that renders the flat state a local minimum along undesired geometrically allowed branches. While we find the approach to be effective for a single degree-6 vertex, this approach is inherently limited to a highly restricted set of crease patterns. Second, we seek to locally program the buckling direction of each vertex by incorporating an orthogonally-addressable (pH-sensitive) element that pre-biases the structure along the desired branch. As this approach should be applicable for generic crease patterns of high complexity, it represents an important step in the design of robustly self-folding structures.

MARY ELIZABETH LEE (Presenter), CHRISTIAN SANTANGELO, Physics, University of Massachusetts, Amherst — Self-folding origami, flat sheets that use mechanical instabilities to fold into three-dimensional structures, have been actuated using swelling polymer gels, surface tension, and more. A universal problem with these structures is that there can be multiple fold configurations for one origami pattern, resulting in the possibility that the structure folds into a configuration other than the one desired. Using an energy model for the structures, we show that the configuration space of a generic origami structure takes the form of nested cones, and that the number of conical branches increases with the number of internal vertices. We will use this geometry to investigate misfolding, with a focus on origami with 5 external vertices.

This work is funded by NSF grant DMR-1822638.

Thursday, March 7, 2019 8:00 AM - 10:24 AM

Session R60 FIP: Condensed Matter/Materials Science Solutions to Environmental Problems BCEC 258A - Abhishek Kumar, NIST - Tag(s): Invited
8:00AM R60.00001: Perovskites for Energy Harvesting* [invited] MARINA LEITE (Presenter), University of Maryland, College Park — The extraordinary performance of perovskite solar cells (> 20%) is still hampered by their dynamic optical and electrical responses, which often lead to degradation. The individual and combined effects of water, oxygen, temperature, bias, and light must be controlled for their future commercialization. To unravel the contribution of each parameter on materials’ properties and devices’ performance, we combine advanced scanning probe methods. We investigate a series of hybrid perovskites, including MAPbI3, MAPbBr3, CsxFA1−xPb(lyBr1−y)3, and triple cation Cs-mixed. Using environmental PL microscopy we elucidate a humidity-induced PL hysteresis, strongly dependent on the Cs/Br ratio. Through Kelvin-probe force microscopy we elucidate the dynamic open-circuit voltage response as a function of chemical composition and illumination treatments. We propose a machine learning (ML) paradigm to identify the influence of each aforementioned parameter on perovskite’s stability and device performance. Our functional microscopy platform, combined with ML, can be leveraged to assess Pb-free perovskites.

*This work has been supported by NSF-EPMD (award #16-10833), the Ovshinsky Sustainable Energy Fellowship from APS, and SPRINT FAPESP-UMD.

8:36AM R60.00002: John Wheatley Award Talk: Multifunctional Materials for Emerging Technologies [invited] FEDERICO ROSEI (Presenter), INRS-EMT — As the age of fossil fuels is coming to an end, now more than ever there is the need for more efficient and sustainable renewable energy technologies. This presentation will give an overview on recent developments in solar technologies that aim to address the energy challenge. In particular, nanostructured materials synthesized via the bottom–up approach present an opportunity for future generation low cost manufacturing of devices. We demonstrate various multifunctional materials, namely materials that exhibit more than one functionality, and structure/property relationships in such systems, including new strategies for the synthesis of multifunctional nanoscale materials to be used for applications in photovoltaics, solar hydrogen production, luminescent solar concentrators and other emerging optoelectronic technologies. [1-22].

References

9:12AM R60.00003: Nanomanufacturing: An enabler for environmental technologies [invited] JAMES LIDDLE (Presenter), National Institute of Standards and Technology — From clean water to clean energy, many environmental technologies rely upon nanoscale phenomena, and consequently on our ability to control and manipulate material structure, composition, and function at that scale. While we have achieved unprecedented control over matter using the tools of integrated circuit manufacturing, the volumes and price points required to meet the demands of environmental technologies mean that the semiconductor manufacturing toolset cannot be used. I will describe the economic landscape relevant to nanomanufacturing in the context of environmental technologies and a selection of those nanostructuring methods that may meet the boundary conditions of scale and cost.

9:48AM R60.00004: Advances in molecular and polymeric photovoltaic devices and the challenges to their commercialization [invited] JAYANT KUMAR (Presenter), University of Massachusetts, Lowell — TBD

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R61 GSOFT DFD: Steerable Colloids I BCEC 258B - Naomi Oppenheimer, Simons Foundation - Tag(s): Focus
8:00AM R61.00001: Chiral electrophoresis: a new steering wheel* [invited] THOMAS A WITTEN (Presenter), James Franck Institute, University of Chicago — Even rigid colloidal objects in conventional fluids in general respond chirally to external gradients such as electric fields. They twist around the gradient direction in a sense dictated by the object. Do real objects have enough chiral response to make a difference? Any chiral response requires either a chiral (non-inversion-symmetric) shape or a chiral charge distribution. But no shape can give chiral electrophoresis if it is uniformly charged. Nor can a sphere respond chirally even with the most chiral charge distribution. Here we demonstrate a new approach for calculating chiral responses of asymmetric objects. It represents the sheath of electrically-driven flow over the object as a superposition of stokeslet sources. Insights from this approach show how symmetric shapes can show strongly chiral response. We illustrate using a cube-shaped object. Chiral response is a handle by which a dispersion can be manipulated in powerful ways using time-varying electric fields.

*Supported by the James Franck Institute and by the University of Chicago Materials Research Science and Engineering Center, which is funded by the National Science Foundation under award number DMR-1420709.

8:36AM R61.00002: Orientation of spheroidal colloids near a charged surface* YOAV TSORI (Presenter), Ben-Gurion University of the Negev — We look at an uncharged spheroidal colloid in a water near a charged flat surface. We solve the nonlinear Poisson-Boltzmann equation outside of the colloid for various tilt angles θ with respect to the surface. The colloid's size is assumed to be comparable to the Debye's length and hence field gradients are essential. The Maxwell stress tensor, including a contribution from the ideal gas of ions, can be integrated along the colloid's surface to give the total force and torque on the colloid. The calculation is for a static colloid but if it were to move translation and rotations would be coupled via the tilt angle. From the torque we calculate the effective angular potential u(θ). The colloid tends to align in the direction perpendicular to the surface (parallel to the field, θ=0) if it is far enough from it. Surprisingly, we find that at short separations or large voltages the colloid will align parallel to the surface (θ=90 degs). Interestingly, colloid orientation parallel to the surface is promoted at a finite value of the eccentricity. Lastly, and this needs to be yet verified, the nonuniform forces on the surface of the colloid seem to amount to a net translational force along the surface although the system is invariant in this direction.

*Israel Science Foundation Grant No. 56/14

8:48AM R61.00003: The Electrohydrodynamic Magnus Effect: Coupling between Electrophoresis and Quincke Rotation Propels Colloids Orthogonal to a Driving Electric Field ZACHARY SHERMAN (Presenter), JAMES W SWAN, Massachusetts Institute of Technology — Colloids dispersed in electrolytes polarize the surrounding ion cloud when exposed to an electric field. For sufficiently strong fields, an instability occurs that causes spherical colloids to break symmetry and spontaneously rotate about an axis orthogonal to the applied field, a phenomenon named Quincke rotation. If the colloids also have a net charge, the electrophoretic motion couples to Quincke rotation and propels particles in a direction orthogonal to both the driving field and the axis of rotation, an electrohydrodynamic analogue to the Magnus effect. The orthogonal Magnus velocity is of a comparable magnitude to the electrophoretic velocity. Typically, motion orthogonal to the field requires anisotropy in particle shape, dielectric properties, or geometry of boundaries. Here, the electrohydrodynamic Magnus effect occurs for bulk, isotropic spherical particles, with the Quincke rotation instability providing broken symmetry driving orthogonal motion. The direction of the Magnus velocity is not changed by flipping the sign of the field, so net orthogonal motion persists in AC electric fields. This orthogonal motion acts as a type of “self-propulsion”, and colloids with an electrohydrodynamic Magnus velocity can be used to create a new type of active matter.
Recent work shows that colloidal dimers with asymmetric geometric or interfacial properties can propel due to the unbalanced electrohydrodynamic (EHD) flow around the particles, offering a new avenue to engineer active particles. In this work, we present experimental studies on the active motion behaviors of boomerang-shaped colloidal particles driven by the EHD flow. We show that by breaking the symmetry of particle shapes, the boomerang particles exhibit several different modes of active motions which can be either translation and/or rotation, and these modes of motions can be fine-tuned or switched by the frequency and initial phase of the electrical fields.

*Funding Acknowledgement: NSF CMMI-1663394 and CBET 1454095

We experimentally create different potential energy landscapes using extended laser light fields, ranging from periodic patterns (laser fringes) to random patterns (speckle patterns). The dynamics of colloidal particles in these potential energy landscapes are followed by video microscopy. Diffusive as well as sub- and super-diffusive behavior can be observed with the extent of the different regimes depending on the specific situation, such as the shape and modulation amplitude of the potential but also the composition of particle mixtures and the particle concentrations. We will review our findings from different experimental conditions and compare the experimentally observed behavior to simulation and theoretical results.

We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, Project No. EG 269/6-1).

Light can be a powerful tool to mechanically manipulate matter, as evidenced by concepts such as optical tweezers and optical traps utilized across biology, colloidal science, microfluidics, and elsewhere. Advances in nanofabrication have enabled the ability to engineer the phase front of light as well as structure the shape of the target object for more advanced mechanical manipulation. We show how the combination of phase-space topology and particle asymmetry can provide a powerful degree of freedom in designing nanoparticles for optimal external manipulation. In particular, we find counterintuitive dynamics where optically asymmetric particles become stable nanoscale motors even in a light field with zero angular momentum. Here, the wavelength of the incident light can be used to externally control the number, orientation, and the stability of the equilibrium states. Finally, we discuss how structural complexity on the nano-scale can enable rich dynamics of optical manipulation of objects much larger than a wavelength in size.

This work was funded by a FY2015 postdoctoral standard fellowship from the Japanese Society for the Promotion of Science (JSPS).
While complex fluids are traditionally studied by imposing bulk forces on a macroscopic samples, here we explore the response of a colloidal dispersion to a local, microscopic driving; a microscale version of rheometry. In particular, we examine the response of a two dimensional layer of Brownian particles to a flow field induced by a circular motion of a probe particle driven by optical tweezers. We observe that particles migrate from high to low strain rate regions and form strong gradients in the density profiles. This non-homogeneity in the density profile is localized and the emerging length scale is set by the competition between the Brownian and shear forces. We further demonstrate that our measurements are quantitatively described, over a large range of strain rates and particle densities, by a phenomenological two phase fluid constitutive model previously discussed in the literature.


*NSF, DMR-1455086.
problems with lower overheads and mitigating some of these difficulties directly. The answer. In this talk I will discuss some of these challenges and recent advances in both the algorithms for simulating these previous methods with no modifications could simply prohibit more qubits from giving a better or more interesting number of utilized qubits for such applications is significantly smaller than a post-supremacy device, and direct application most promising applications for near-term quantum computers. However, even in an optimistic mindset, it is clear that regions. These nano-hydrogels show great promise for application in enhanced oil recovery. Increases up to 80% resulting in significant changes in the flow paths and diversion of the flow towards unexplored hydrogels swell up to 6 times. Hence, by injection of a small amount of the suspension, the resistance of the medium injection of the nano-hydrogels. After injection of the suspension of nano-hydrogels, the shells degrade and nano-phase is created by the leakage of CO2 through the permeable PDMS walls. Mathematical models for early stage particle sorting applications. The behavior of the systems is highly robust and controllable and thus allows it to be used to a wide range of particle focusing and the traveling pulse will be compared with the experimental observations.

10:36AM R61.00012: Spontaneous pulse generation in a steady channel flow of a colloidal suspension*  
SUIN SHIM (Presenter), HOWARD A STONE, Princeton University — We present experiments demonstrating the spontaneous generation and traveling of a colloidal pulse in a steady channel flow. When deionized (DI) water with suspended positively-charged particles flows steadily through a single channel, a pulse of particles is generated, which then flows through the channel at a slower speed than the mean flow velocity. With detailed experimental investigations and quantified results, we rationalize our observations by considering CO2 driven diffusiophoresis. The concentration gradient of ions in the liquid phase is created by the leakage of CO2 through the permeable PDMS walls. Mathematical models for early stage particle focusing and the traveling pulse will be compared with the experimental observations.

*We acknowledge the NSF for support via grant CBET - 1702693.

10:48AM R61.00013: Programmable nano-hydrogels for flow control in porous media  
LIYUAN ZHANG (Presenter), SHIMA PARSA MOGHADDAM, DAVID A WEITZ, Harvard University — We study the effect of injection of programmable nano-hydrogels on the dynamic of the flow through the 3D micromodel porous medium. We develop a core-shell nano-hydrogel with programmable swelling behavior. Using confocal microscopy, we visualize flow in a 3Dmicromodel before and after injection of the nano-hydrogels. After injection of the suspension of nano-hydrogels, the shells degrade and nano-hydrogels swell up to 6 times. Hence, by injection of a small amount of the suspension, the resistance of the medium increases up to 80% resulting in significant changes in the flow paths and diversion of the flow towards unexplored regions. These nano-hydrogels show great promise for application in enhanced oil recovery.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R62 DQI: Noisy Intermediate-Scale Quantum Computers  
BCEC 258C - David McKay, IBM T J Watson Res Ctr - Tag(s): Invited

8:00AM R62.00001: Quantum Computing in the NISQ era and beyond  
JOHN PRESKILL (Presenter), Caltech — Noisy Intermediate-Scale Quantum (NISQ) technology will be available in the near future. Quantum computers with 50-100 qubits may be able to perform tasks which surpass the capabilities of today's classical digital computers, but noise in quantum gates will limit the size of quantum circuits that can be executed reliably. NISQ devices will be useful tools for exploring many-body quantum physics, and may have other useful applications, but the 100-qubit quantum computer will not change the world right away --- we should regard it as a significant step toward the more powerful quantum technologies of the future. Quantum technologists should continue to strive for more accurate quantum gates and, eventually, fully fault-tolerant quantum computing.

8:36AM R62.00002: Advances in quantum simulation on the path towards post-supremacy, pre-fault-tolerant applications  
JARROD MCCLEAN (Presenter), Al Quantum, Google LLC — Quantum simulation looks to be one of those most promising applications for near-term quantum computers. However, even in an optimistic mindset, it is clear that utilizing a post-supremacy device for near-term applications will present a number of challenges. To date, the maximum number of utilized qubits for such applications is significantly smaller than a post-supremacy device, and direct application of previous methods with no modifications could simply prohibit more qubits from giving a better or more interesting answer. In this talk I will discuss some of these challenges and recent advances in both the algorithms for simulating these problems with lower overheads and mitigating some of these difficulties directly.
9:12AM R62.00003: Simple tricks to squeeze more out of your noisy quantum device* [Invited] KRISTAN TEMME (Presenter), IBM Research — Near-term applications of early quantum devices rely on accurate estimates of expectation values to become relevant. Decoherence and gate errors lead to wrong estimates. This problem was, at least in theory, remedied with the advent of quantum error correction. However, the overhead that is needed to implement a fully fault-tolerant gate set with current codes and current devices seems prohibitively large. In turn, steady progress is made in improving the quality of the quantum hardware and we believe that we can build machines in the near term that cannot be emulated by a conventional computer. We discuss simple techniques that increase the quality of short-depth quantum simulations. In light of these advances, it becomes interesting to ask what these noisy devices can be used for. In this talk we will present our advances in the search for quantum algorithms for noisy quantum computers that may be relevant to problems in quantum simulation and quantum machine learning.

*IBM Frontiers Institute

9:48AM R62.00004: Photonic quantum networks* [Invited] IAN A WALMSLEY (Presenter), Physics, Imperial College London — Hybrid light-matter networks offer the promise for delivering robust quantum information processing technologies, from sensor arrays to quantum simulators. Recent developments in new quantum light sources, reconfigurable and modular circuit design and fabrication, novel waveguide-based detectors and low-noise photonic memories have all contributed in progress towards a resilient, scalable photonic quantum network. Purely photonic quantum simulators have been demonstrated, and better understanding of the role of imperfections in degrading the performance of such devices has been made, although concrete limits are known in only a few cases. Meanwhile progress in hybrid networks indicates that scalable performance should be possible, albeit only when a number of engineering challenges have been met.

*This work was funded by the UK Engineering and Physical Sciences Research Council (project EP/K034480/1 and the Networked Quantum Information Technology Hub), the Fondation Wiener Anspach, the John Templeton Foundation (Grant 60469), and the European Commission (H2020-FETPROACT-2014 grant QUCHIP; ERC Advanced Grant MOQUACINO).

10:24AM R62.00005: Scaling Ion-trap Quantum Computing [Invited] THOMAS MONZ (Presenter), Experimental Physics, University of Innsbruck — Scalability is tied to the notion of being able to take individual components, combine an increasing number of these components, and be able to predict the performance of the larger system from its constituents. Verifying scalability is thus tied to routines that allow us to both investigate the performance of building blocks as well as larger systems. In this presentation I will present recent work on investigating the performance of the Innsbruck-based ion-trap quantum computer as the quantum register size increases, provide an ongoing project to extend quantum error correction capabilities including loss and outline changes to the apparatus to push towards a 20-qubit quantum processor with parallel processing capabilities.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R63 DBIO DPOLY: Physics of Proteins and Nucleic Acids I: Structures, Dynamics, Interactions, and Energetics BCEC 259A - Huan-Xiang Zhou, Florida State University - Tag(s): Focus
GAVIN KING (Presenter), Physics and Astro., Joint w/ Biochemistry, University of Missouri-Columbia — How are proteins transported across membranes? The general secretory (Sec) system of *E. coli* exports precursor proteins via a translocase comprising the peripheral ATPase SecA and the translocon, SecYEG. Structural changes of active translocases underlie the translocation process. Yet, the mechanistic details of this complex and dynamic system have proven challenging to study. The atomic force microscope (AFM) is well suited for imaging membrane proteins in near-native conditions and can achieve molecular-scale (~10 Å) lateral resolution coupled with ~1 Å vertical resolution (i.e., normal to the bilayer surface). We imaged individual components of the Sec system as well as active translocases at work in lipid bilayers. In this talk I will review our single molecule results in the context of conventional models in the field, which are based on bulk assays. In addition to imaging, AFM can be used in force spectroscopy mode, providing access to energy landscapes. Our group has applied precision AFM-based force spectroscopy techniques to study a peptide-lipid interaction underlying Sec system activity. Together with analytical modeling and simulations, the results represent a step towards a more detailed understanding of the protein export process in *E. coli*, and more generally, of the stochastic kinetic pathways driving peptide-lipid interactions.

*This work was supported by the National Science Foundation (CAREER award number 1054832) and a Burroughs Wellcome Fund Career Award at the Scientific Interface.

SOLANGE FLATT, Institute of Physics, École Polytechnique Fédérale de Lausanne, LE YAN, Kavli Institute of Theoretical Physics, CAROLINA BRITO, Instituto de Física, Universidade Federal do Rio Grande do Sul, MATTHIEU WYART, Institute of Physics, École Polytechnique Fédérale de Lausanne — Allostery is responsible for the activity regulation of many proteins essential for life. We will discuss a minimal model examining the effect of global motions and long-range interactions on protein functions that involve molecular information processing.

RICCARDO RAVASIO (Presenter), SOLANGE FLATT, Institute of Physics, École Polytechnique Fédérale de Lausanne, LE YAN, Kavli Institute of Theoretical Physics., University of California Santa Barbara, STEFANO ZAMUNER, Institute of Physics, École Polytechnique Fédérale de Lausanne, CAROLINA BRITO, Instituto de Física, Universidade Federal do Rio Grande do Sul, MATTHIEU WYART, Institute of Physics, École Polytechnique Fédérale de Lausanne — Allostery is responsible for the activity regulation of many proteins essential for life. Many efforts on understanding this long-range communication have been made, but the physical picture of allosteric mechanics is not yet clear. Recent progress employing in-silico evolutions studied mechanical networks of harmonic springs with allosteric behaviors. These networks are found to share common principles for the long-range communication to occur. Specifically, the stiffness of the allosteric response scales with the system size with a nontrivial power law. In this work, we test these principles in real systems, using a large set of X-ray structural data of allosteric proteins. Overall, we find that the functional allosteric response of each protein is related to a “mechanism”, a soft and extended mode with strong strain. By extending the theory of allosteric materials to include nonlinearities, we identify two scalings of stiffness setting a regime where the allosteric cooperative binding is optimal. A new scaling exponent appears, in addition to the one from the linear theory. The stiffness from the X-ray structural data falls in this predicted range, suggesting that proteins actually work at optimal cooperativity.
9:12AM R63.00005: Finding the Optimal Folding Routes of self-entangled Proteins via Coarse-Grained Molecular Dynamics*  
CLAUDIO PEREGO (Presenter), Polymer Theory Department, Max Planck Institute for Polymer Research, Mainz (Germany), RAFFAELLO POTESTIO, Physics Department, University of Trento, Trento (Italy) — Among the known protein motifs, several structures exhibit a self-entangled backbone topology. Understanding how polypeptides can efficiently and reproducibly attain such topologies is a crucial biophysical challenge, which might shed new light on our general understanding of protein folding.

In this work we present a molecular dynamics methodology for the study of the possible folding pathways travelled by self-entangled proteins. The method is based on a Coarse-Grained, minimalistic representation of the polypeptide chain, driven by a structure-based angular potential. The heterogeneity of the potentials acting among residues is optimized by means of an evolutionary strategy, aimed at maximizing the folding probability of the model.

The purpose of our approach is two-fold. On the one hand we aim at constructing a simple protein model, capable of attaining the entangled structure in a reproducible and efficient way. On the other hand we mimic an evolutionary mechanism that might have selected a specific folding pathway among the possible routes.

Applying the method to relevant test cases we retrieve indications on the optimal folding pathways of self-entangled proteins, and useful guidelines for simulations via more detailed molecular models.

*EU MSC No 796969

9:24AM R63.00006: Molecular mechanisms for protein-denaturation in urea and guanidinium chloride mixtures*  
PRITAM GANGULY (Presenter), JOAN-EMMA SHEA, University of California, Santa Barbara — Using replica-exchange molecular dynamics simulations, we have studied the thermodynamic stability and the conformational changes of two synthetic mini-proteins, Trp-cage and Trp-zip1, in pure and mixed denaturant solutions of guanidinium chloride (GdmCl) and urea. We have found that urea, which denatures proteins through favorable preferential interactions with protein sidechains and backbone, is more effective in destabilizing and elongating alpha-helical secondary structures of proteins than beta-hairpin structures. Contrarily, GdmCl, which denatures proteins by inhibiting salt-bridge formations between charged amino acids, is more effective in destabilizing beta-hairpin structures than alpha-helical structures. The extent of GdmCl-induced protein-denaturation is not determined by protein-GdmCl preferential interactions. In mixed denaturant conditions, our results indicate that GdmCl may however enhance the overall denaturing effects of urea by promoting protein-urea preferential interactions when full-length proteins are considered, but it may also potentially lead to local compaction of smaller segments of proteins, partially counteracting urea-induced extension of the protein segments.

*NSF Grants MCB-1716956, TG-MCA05S027, NIH Grant R01-GM118560-01A

9:36AM R63.00007: Large-scale, automated prediction of protein-ligand binding structures  
ZHIWEI MA (Presenter), XIANJIN XU, RUI DUAN, XIAOQIN ZOU, University of Missouri — Molecular docking is a useful and important approach for the prediction of protein-ligand structures and for structure-based drug design. The growing number of protein-ligand complex structures, particularly the structures of proteins co-bound with different ligands, in the Protein Data Bank helps us tackle two major challenges in molecular docking studies: the protein flexibility and the energy scoring function. Here, we introduced a systematic strategy by using the information embedded in the known protein-ligand complex structures to improve binding mode predictions. We also developed and integrated several methods for large-scale binding mode prediction, and systematically tested these methods on the weekly Continuous Evaluation of Ligand Pose Prediction (CELPP) competition, an automated workflow to process and evaluate the challenge of ligand pose prediction. Up to October 26, 2018, the quantitative analysis of our docking results for over 3000 targets released by CELPP revealed that our methods improve the success rates of ligand pose prediction.

*NSF Grants MCB-1716956, TG-MCA05S027, NIH Grant R01-GM118560-01A
Inferring protein dynamics through experiment and simulation: collective modes from atomic trajectories  LAUREN MCGOUGH (Presenter), RAMA RANGANATHAN, Center for Physics of Evolving Systems and Department of Biochemistry and Molecular Biology, University of Chicago — Proteins are evolved molecular machines that carry out the essential chemical reactions necessary for life. Like machines designed by humans, proteins execute their functions through an orderly set of motions and fluctuations - their “reaction coordinate”. However, proteins are also marginally stable, with the expectation that functional dynamics are embedded in small subspace of a high dimensional pattern of overall motions. Here, we aim to discover the embedded functional dynamics using experiment and simulation.

One approach to studying intramolecular fluctuations is computational simulation of atomic trajectories. Recent advances in experimental protein dynamics open up the ability to test, validate, and possibly improve the process of molecular simulation through direct comparisons between prediction and data. We describe two such comparative analyses using data from X-ray diffraction studies reporting electric field-stimulated excited state motions and evolutionarily conserved room-temperature conformational fluctuations. The goal is then to use both simulation and experiment to infer the effective variables describing functional, collective motions in proteins. This work initiates a path towards understanding the physics of protein function and evolution.

Temperature dependent studies of proteins and their hydration shell properties using megahertz-to-terahertz dielectric spectroscopy*  ALI CHARKHESHT (Presenter), DJAMILA LOU, BEN SINDLE, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — The low-frequency collective vibrational modes in proteins and the protein–water interface playing an important role in biochemical reactions and biological energy transport strongly depend on the temperature and conditions of the environment. However, capturing a precise picture of collective vibrational dynamics under temperature variations is challenging due to the strong absorption of water. For this reason, we have employed a highly sensitive dielectric megahertz-to-terahertz frequency-domain system to probe the vibrational dynamics of proteins in aqueous solutions from 50 MHz to 2 THz. With this approach, we have performed an exclusive temperature dependent study on myoglobin and lysozyme in water by means of complex dielectric analysis. We have focused on protein collective vibrational processes and atypical surrounding water molecules to outline comprehensive images of aqueous solutions. The results help us to clarify protein dynamics and protein-water interfaces in temperature dependent environment that determine biochemical functions and reactivity of proteins.

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Protein Structural Fluctuations at Criticality in the Temperature-pressure-crowding Folding Phase Diagram*  ANDREI G GASIC (Presenter), CALEB M DAUGHERTY, MARGARET CHEUNG, Department of Physics, University of Houston; Center for Theoretical Biological Physics, Rice University — In the cell, proteins perform complex biological functions through large-scale motion, which are induced by slight environmental perturbations. This characteristic of having high susceptibility is similar to a physical system near a critical point. Indeed, recent experimental and computational findings demonstrate that protein folding transitions in the temperature (T), pressure (P), and crowding volume-fraction (φc) phase diagram point toward signatures of criticality, where distinct folding phases merge. Here, using coarse-grained molecular dynamics simulations, we theoretically show that at the critical regime, fluctuations exhibit high susceptibility and long-range correlations up to the size of the protein. Meaning that near criticality, the dynamics of each residue is influenced by each other residue even across the entire protein. We investigate the structural origin and the effect of macromolecular crowding on this critical behavior. Furthermore, this study leads us one step closer to developing universal principles of protein folding and function in vivo.

*This work is funded by the National Science Foundation through MCB:1412532, PHY:1427654, and ACI:1531814. AGG is supported by a training fellowship on the Houston Area Biophysics Program (T32 GM008280).

Neighbourhood preference based energy function and its applications in structure prediction and protein evolution*  SIYUAN LIU, XILUN XIANG, school of software engineering, university of science and technology of China, HAIGUANG LIU (Presenter), complex systems division, beijing computational science research center — Based on the statistics from known structures in the protein data bank, a statistical energy function is derived to reflect the amino acid neighbourhood preferences. The neighbourhood of one amino acid is defined by its contacting residues, and the energy function is determined by the neighboring residue types and relative positions. A scoring function, Nepre, has been implemented and its performance was tested with several decoy sets. The results show that the Nepre program can be applied in model ranking to improve the success rate in structure predictions. We also applied this empirical energy function in the understanding of protein evolution and the designability of protein structures.

*National Natural Science Foundation of China (grant No. 11575021; grant No. U1530401; grant No. U1430237)

*Authors gratefully acknowledge financial support by the Air Force Office of Scientific Research under award number FA9550-18-1-0263 and National Science Foundation (CHE-1665157)
10:36AM R63.00012: Protein Structure Prediction with MELD x MD* JAMES ROBERTSON (Presenter), Stony Brook University, ALBERTO PEREZ, Stony Brook University (currently University of Florida), KEN DILL, Stony Brook University — Predicting protein structures from their amino acid sequences is a major challenge, especially with atomistic molecular dynamics (MD) simulations. The two major limitations to MD are poor sampling due to high computational cost and inaccurate force fields. Bioinformatics-based methods are an alternative approach to structure prediction that rely on databases of structures or structural fragments, as in threading. Threading has been very successful in predicting protein structures, but about 15% of proteins are not amenable to threading, the so-called nonthreadables. The nonthreadables provide a test set for MELD x MD, which does not rely on bioinformatics databases. We show that MELD x MD accurately predicts 20/41 nonthreadables and give high Boltzmann populations for successful predictions. We also discuss MELD x MD structure prediction on a larger set of proteins, particularly how the method is limited by sampling and force fields, but also how MELD x MD can overcome these limitations.

*NIH K12-GM-102778 & GM125813. NSF Blue Waters (ACI-0725070 and ACI-1238993) PRAC "Petascale integrative approaches to protein structure prediction". The Laufer Center.

10:48AM R63.00013: Dynamic Allosteric Residue Coupling (darc) Spots Shed Light on Functional Changes from Sequence Variation PAUL CAMPITELLI (Presenter), Center for Biological Physics, Arizona State University, LISKIN SWINT-KRUSE, Department of Biochemistry and Molecular Biology, The University of Kansas Medical Center, BANU OZKAN, Center for Biological Physics, Arizona State University — Defining the functional impact of protein sequence variation presents a major challenge in biology and genomics and the importance has grown dramatically as unprecedented advances in sequencing complete exomes have yielded tens of thousands of non-synonymous single nucleotide variants (nSNVs) on the human proteome. Currently there are no consistent methods to capture the mechanisms of functional changes as a result of sequence variations, particularly at non-conserved positions and in the absence of large structural changes. We present the dynamic flexibility index (dfi), a measure of residue-specific flexibility and the dynamic coupling index (dci), a technique determining coupling strength between amino acids. We apply our approach to the lactose repressor protein LacI, where substitutions at non-conserved position V52 produce progressive effects on function. dfi captures changes in flexibility in the DNA binding domain and is correlated with binding affinity. We also use dci to identify important dynamic allosteric residue coupling (darc) spots, distally located to the DNA binding domain. darc spot dfi correlates strongly with changes in repression rate as well as DNA binding affinity and shows conformational dynamics at distal sites plays an important role in LacI function.

Thursday, March 7, 2019 8:00 AM - 10:36 AM

Session R64 DBIO: Physics of Intracellular Transport BCEC 259B - Jing Xu, Univ of California - Merced - Tag(s): Focus

8:00AM R64.00001: The complexity of microtubule-based motility* [invited] MICHAEL VERSHININ (Presenter), University of Utah, JUN ALLARD, STEVEN GROSS, UC Irvine, JAMES KEENER, JARED BERGMAN, University of Utah, MATTHEW BOVYN, UC Irvine, OLAOLU OSUNBAYO, West Physics, CHRIS MILES, New York University, BABU J.N. REDDY, UC Irvine, MANASA GUDHETI, Bruker, FLORENCE DOVAL, ABHIMANYU SHARMA, University of Utah — The tug of war between multiple molecular motors driving the same cargo can take many forms and result in many observable motility phenotypes. I will discuss some of the relevant cases, from movement across microtubule intersections to a minimal tug of war system on a single microtubule. I will show that the overall range of behaviors is remarkably large and in particular that cargos can remain in a tug of war state for extremely long times and that this has significant implications for both cargo routing in cells and for our ability to tell tug of war processes from other pathways to immotility such as diffusion. Finally, I will discuss viable approaches for identifying tug of war in biological systems.

*NSF ENG/CMMI #1563280
suggest the use of crowding as a control parameter to study kinesin's mechanochemical cycle. The importance of motor-motor interactions in cargo transport, explain the long observed variability of cargo velocity, and results from the individuals' increased sensitivity to hindering load in a crowded medium. Our results highlight the teams of motors, while having no effect on single motor velocity. We find that this emergent property of kinesin teams results from the individuals' increased sensitivity to hindering load in a crowded medium. Our results highlight the importance of motor-motor interactions in cargo transport, explain the long observed variability of cargo velocity, and suggest the use of crowding as a control parameter to study kinesin's mechanochemical cycle.

*This work was supported in part by the National Science Foundation grant PHY-1505020 to GTS

9:12AM R64.00003: Intracellular transport is accelerated in early apoptotic cells*  HUI LI (Presenter), CAS Key Lab of Soft Matter Physics, Institute of Physics, Chinese Academy of Sciences — Apoptosis is a process of programmed cell death with dramatic changes in cell morphology and organization, during which signaling molecules are transported within the cells between different organelles. However, how the intracellular transport changes in cells undergoing apoptosis remains unknown. Here, we study the dynamics of intracellular transport by using single-particle tracking method, and find that both the directed motion and diffusive motion of endocytic vesicles are accelerated in early apoptotic cells. With careful elimination of the other factors involving in the intracellular transport, the reason for the acceleration is attributed to be the elevation of ATP concentration. More importantly, we show that the accelerated intracellular transport is critical for apoptosis. Apoptosis is delayed when the dynamics of intracellular transport is regulated back to the normal level. Our results demonstrate the important role of transport dynamics in apoptosis and shed light on the apoptosis mechanism from a physical perspective.

*This project was supported by National Natural Science Foundation of China (Grant No. 11674383)

9:24AM R64.00004: Doppler Spectroscopy of Intracellular Motion in Revived Flash-Frozen Cancer Tissues  ZHEN HUA (Presenter), ZHE LI, JOHN TUREK, MICHEAL CHILDRESS, DAVID NOLTE, Purdue University — Biodynamic imaging is a high-content optical imaging technology based on Doppler spectroscopy and digital holography that uses dynamic speckle as high-content image contrast to probe living tissue. The multimode mixing of Doppler signals produces a fluctuation spectrum that is a function of the acquisition time relative to the persistence time of intracellular transport and hence provides a measure of cellular activity. Creating Doppler spectrograms of tumor tissues responding to anticancer agents usually relies on patient enrollment in IRB-approved trials, which is slow and inefficient. However, if flash-frozen biopsies could be revived and measured, then a large reservoir of tissue-banked samples could become available for phenotypic library building. We have performed biodynamic imaging measurements of flash-frozen canine B-cell cancer tissue and compared the drug-response spectrograms to results from fresh tissues from the same dogs. By compensating for tissue trauma in the frozen sample, we demonstrate a high accuracy for patient clustering between the fresh and frozen samples when correlating with clinical outcomes, identifying resistance or sensitivity to their prescribed chemotherapy.

9:36AM R64.00005: A model of diffusion through a potential captures the effect of competition on the efficiency and speed of nucleocytoplasmic transport  TIANTIAN ZHENG (Presenter), ANTON ZILMAN, University of Toronto — The nuclear pore complex (NPC) facilitates the selective transport of materials between the nucleus and cytoplasm in eukaryotic cells. Typically, many cargo are simultaneously present within the NPC during transport, and it is not fully understood how the NPC can function efficiently despite the crowding in the channel. In this study, we simulate transport through an NPC-like channel with coarse-grained cargoes and NPC-associated intrinsically disordered proteins (FG nucleoporins). From the results of this simulation, we show that cargo densities and trajectories along the direction of transport can be captured by a model of 1-dimensional diffusion through a potential, which is an effective potential arising through the interactions between cargoes and NPC components, and is modified by the non-equilibrium density profiles of cargoes inside the channel. With this framework, we are able to account qualitatively for previously unexplained experimental data which show that an increased number of cargo results in both increased efficiency and speed of transport. Our model therefore provides an explanation for why crowding does not necessarily affect the functioning of the NPC in a negative way, which can explain how the NPC can achieve both high specificity and high throughput.
9:48AM R64.00006: A Semi-Analytical Model to Investigate Cargo Transport by Bi-Directional Molecular Motor Ensemble*  
RACHIT SHRIVASTAVA (Presenter), SHREYAS BHABAN, JAMES MELBOURNE, SIVARAMAN RAJAGANAPATHY, MURTI SALAPAKA, Department of Electrical and Computer Engineering, University of Minnesota, Twin Cities — Deciphering mechanism of transportation of organelles by molecular motors is crucial to understand the genesis of neurodegenerative diseases. We model the ensemble behavior of motors using a semi-analytical approach. This approach uses an individual motor's model to predict their ensemble behavior. The process of cargo transportation is modeled as Markov process with molecular motor arrangements being as its state which satisfies Markov property. Exact probabilities distribution functions of the relative configurations of motor is determined in order decipher the cargo transportation process. When only unidirectional motors are carrying a cargo, this approach has revealed insights such as relative configurations approaching a unique steady state distribution, enforcing the robustness of the motor-cargo assembly. Also it has been observed that as the load on the cargo increases, motors tend to cluster together. We attempt to extend this analysis to ensembles with bidirectional motors such as both kinesin and dynein. This will aid to suggest new hypothesis about motor behavior and drive the design and realization of new experiments. Finally, we attempt to determine the factors responsible for deciding the “tug-of-war” vs coordinated movement.

*Funded by: Cyber Physical Society(NSF)

10:00AM R64.00007: Two-Species Active Transport along Cylindrical Biofilaments is Limited by Emergent Topological Hindrance  
PATRICK WILKE (Presenter), EMANUEL REITHMANN, ERWIN FREY, Physics, Ludwig Maximilian University of Munich — Motivated by recent experimental studies that have addressed the stepping behavior of kinesins, we investigate a lattice gas model for simultaneous transport of two species of active particles on a cylinder. The species are distinguished by their different gaits: While the first species moves straight ahead, the second follows a helical path. We show that the collective properties of such systems critically differ from those of one-species transport. This is most evident in a jamming transition far below full occupation, as well as in nonequilibrium pattern formation. The altered behavior arises because—unlike the case in single-species transport—any given position may be targeted by two particles from different directions at the same time. However, a particle can leave a given position only in one direction. This simple change in connectivity significantly amplifies the impact of steric interactions and thus becomes a key determinant of mixed species transport. We computationally characterize this type of hindrance and develop a comprehensive theory for collective two-species transport along a cylinder. Our observations show high robustness against model extensions that account for additional biomolecular features which suggests relevance also in a biological context.

10:12AM R64.00008: Simulation of membrane-bound cargo transport by teams of kinesin motors*  
NIRANJAN SARPANGALA (Presenter), AJAY GOPINATHAN, Physics, University of California, Merced — In eukaryotic cells, membrane-bound cargoes are transported by teams of molecular motors. Motors on such cargoes diffuse on the lipid membrane. How the fluidity of the membrane affects transport characteristics is still not well understood. Here we develop a stochastic dynamical simulation of kinesin-based cargo transport along microtubules that explicitly considers the Langevin dynamics of motors on the surface of cargo. We study how the number of bound motors, run length, the velocity of cargo and binding rates are influenced by parameters like the diffusion coefficient of motors on cargo surface, ATP concentration, and the cargo size. We show that the distribution of free motors on microtubule-bound cargo surface depends on these parameters and affects the rebinding of cargo to microtubule after its detachment, thus affecting overall transport. Our work suggests that the consideration of motor diffusivity should be important in the cellular context.

*We acknowledge support from National Science Foundation NSF grant DMS-1616926, NSF-CREST:Center for Cellular and Bio-molecular Machines at UC Merced (NSF-HRD-1547848) and computing time on the Multi-Environment Computer for Exploration and Discovery (MERCED) cluster at UC Merced, (National Science Foundation Grant No. ACI-1429783).
subjected to a simple exclusion process. We consider the analytical solution of velocity (V) of a collection of N processive and non-processive motors stepping along one and multiple microtubule filaments in stochastic simulations using Monte Carlo methods. The motor dynamics follow biased random walks along and switching between multiple filaments. In this case, the applied load is shared between the leading motors on each filament. We also show the simulation results of F-V relations of non-processive motors stepping along and switching between multiple filaments. In this case, the applied load is shared between the leading motors on each filament.

*Royal Thai government funded Ph.D. studentship.

**Thursday, March 7, 2019 8:00 AM - 10:48 AM**

**Session R65 DBIO: Biomaterials: Structure, Function, Design IV**

**8:00AM R65.00001: Biomimetic Mineralization via Polymer-Induced Liquid Precursors** [Invited] LAURIE GOWER (Presenter), Materials Science & Engineering, University of Florida — The hallmark of biomineralization is the ability of organisms to form non-equilibrium crystal morphologies. Our group has been using in vitro model systems to examine the physicochemical mechanisms that might be involved in biomineralization, with emphasis on the role that biopolymers play. We have discovered that many of the long-standing enigmatic biomineral features can be reproduced in the beaker using a non-classical crystallization process we call the Polymer-Induced Liquid-Precursor (PILP) process. This process entails adding charged polymers to supersaturated salt solutions which then sequester ions/clusters/phases to induce phase separation of a hydrated amorphous mineral precursor. Interaction of these PILP colloids with various organic templates and matrices leads to a variety of non-equilibrium morphologies and composite textures, many of which emulate those seen in biominerals. We argue that a PILP type process may lie at the foundation of biomineralizing systems ranging from invertebrate exoskeletons to vertebrate bones and teeth. This argument is based on the diversity of features that can be emulated, and their distinct mineralogical signatures of formation mechanism, such as incorporation of high magnesium into calcite, transition bars and shrinkage patterns, and remnant colloidal textures within single-crystalline composites. Through this enhanced understanding of biomineralization processes, we are now developing biomimetic processing methods that enable the fabrication of hard-tissue biomaterials which emulate bone.

*This work was supported by the Office of the Assistance Secretary of Defense for Health Affairs, through the Peer Reviewed Medical Research Program under Award No. W81XWH-17-1-0100. Opinions, interpretations, conclusions and recommendations are those of the author and are not necessarily endorsed by the Department of Defense. Some material is based upon work supported by the National Science Foundation under Grant No. DMR-1309657.

**8:36AM R65.00002: Cell contraction induces long-ranged stress stiffening in the extracellular matrix** YULONG HAN (Presenter), Massachusetts Institute of Technology, PIERRE RONCERAY, Princeton Center for Theoretical Science, Princeton University, CHASE P. BROEDERSZ, Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, MING GUO, Massachusetts Institute of Technology — Animal cells in tissues are supported by biopolymer matrices, which typically exhibit highly nonlinear mechanical properties. While the linear elasticity of the matrix can significantly impact cell mechanics and functionality, it remains largely unknown how cells, in turn, affect the nonlinear mechanics of their surrounding matrix. Here, we show that living contractile cells are able to generate a massive stiffness gradient in three distinct 3D extracellular matrix model systems: collagen, fibrin, and Matrigel. We decipher this remarkable behavior by introducing nonlinear stress inference microscopy (NSIM), a technique to infer stress fields in a 3D matrix from nonlinear microrheology measurements with optical tweezers. Using NSIM and simulations, we reveal large long-ranged cell-generated stresses capable of buckling filaments in the matrix. These stresses give rise to the large spatial extent of the observed cell-induced matrix stiffness gradient, which can provide a mechanism for mechanical communication between cells.

*This work was supported by National Cancer Institute Grant 1U01CA202123 (to M.G.) and a Massachusetts Institute of Technology International Science and Technology Initiatives—Germany seed fund (to M.G. and C.P.B.).
Contaminated Water*  9:12AM R65.00005: Modeling and Design of Adsorption Based Filters and the Bio-remediation of Heavy Metal Contaminated Water*   CHRIS MCCARTHY (Presenter), Mathematics, BMCC City University of New York — I will discuss kinetic models of adsorption, as well as our mathematical models of such filters. These mathematical models have been developed in support of our interdisciplinary lab group and can be used in filter design. Our group conducts research into bio-remediation of heavy metal contaminated water via filtration. The filters are constructed out of biomass, such as spent tea leaves. The spent tea leaves are available in large quantities as a result of the industrial production of tea beverages. The heavy metals bond with the surfaces of the tea leaves (adsorption). I will compare the models’ predictions to data obtained from computer simulations and experimentally by our lab group.

*+CUNY Collaborative Incentive Research Grant (Round 12); CUNY Research Scholars Program; BMCC Faculty Development Grant.

Mucus and mucin biopolymer environments reduce the efficacy of polymyxin and fluoroquinolone antibiotics*  9:24AM R65.00006: Mucus and mucin biopolymer environments reduce the efficacy of polymyxin and fluoroquinolone antibiotics*   TAHOURA SAMAD (Presenter), JULIA Y CO, JACOB WITTEN, KATHARINA RIBBECK, Massachusetts Institute of Technology — Mucus, a biopolymer hydrogel that covers all wet epithelia, is one of the primary arenas for microbes in the body, including the microbiome and pathogenic microbes that can cause serious infections. Mucus has the potential to bind small molecules and influence bacterial physiology, two factors that might affect the efficacy of antibiotics. Despite this, the impact of mucus on antibiotic efficacy has not been thoroughly characterized. We investigated the efficacy of polymyxin and fluoroquinolone antibiotics against the opportunistic pathogen Pseudomonas aeruginosa in native mucus and purified mucin biopolymer environments. We found that mucus reduces the efficacy of polymyxin and fluoroquinolone antibiotics against P. aeruginosa. MUC5AC, MUC2, and MUC5B mucin biopolymers, the gel-forming components of mucus, are primary contributors to this reduced efficacy. Our findings highlight that inclusion of the biomaterial environmental context is an important consideration when evaluating antimicrobial efficacy in vitro.

*This work was supported by the National Institutes of Health (R01-EB017755) and the National Science Foundation (PHY-1454673, DMR-14-19807), National Science Foundation Graduate Research Fellowship (1122374), the Siebel Scholarship and the MIT Collamore-Rogers Fellowship.
9:36AM R65.00007: Morphological change of the phospholipid vesicle induced by actin polymerization of the artificial photosynthetic protocellular system. KEEL YONG LEE, John A. Paulson School of Engineering and Applied Sciences, Harvard University, SUNGJIN PARK, Emory University, A SETIAWATI, SUNGWOO JUNG, HUONG NGUYEN, Chemistry, Sogang University, KEVIN PARKER, John A. Paulson School of Engineering and Applied Sciences, Harvard University, KWAN HWAN JUNG, Sogang University, Kwan Shin (Presenter), Chemistry, Sogang University — We designed, built, and tested a light-harvesting encapsulated artificial organelle system that provides both a sustainable energy source and a means of controlling intracellular reactions. With the reconstitution into lipid vesicles, an ATP synthase and two photoconverters (plant-derived photosystem II [PSII] and bacteria-derived proteorhodopsin [PR]) enabled orchestration of ATP synthesis. Independent activation of the two photoconverters, which respond to different light wavelengths, allowed dynamic regulation of ATP synthesis. The resulting system was able to simulate a ubiquitous process in cells—cytoskeleton formation through ATP-dependent actin polymerization in a giant vesicle. Optical stimulation initiated ATP synthesis and induced ATP-dependent actin polymerization, leading to growth of three-dimensional actin filaments. Cytoskeleton formation and manipulation successfully induced morphological change of the outer membrane of the protocellular system by tuning the attraction–repulsion interactions between actin filaments and phospholipids.

9:48AM R65.00008: Dual-gel Dual-porosity 3D ECM Mimics for Studying flow-induced mechanotransduction* ALIMOHAMMAD ANBARI (Presenter), City College of New York, HUNG-TA CHIEN, Texas A&M, CHUN-WEI CHI, SIHONG WANG, JING FAN, City College of New York — Interstitial flow in the Extracellular Matrix (ECM) has been postulated to play a key role in regulating behaviors of cells. Among the cellular behaviors, cell migration is hypothesized to be influenced by interstitial flow via two mechanisms: autologous chemotaxis and integrin-mediated focal adhesion activation. It is commonly accepted that the effectiveness of the former depends on interstitial fluid velocity and the effectiveness of the latter depends on the flow-induced force on a cell, which relates to both interstitial fluid velocity and matrix permeability. The two mechanisms have never been rigorously verified using the traditional single hydrogel-based models due to the inevitable correlation between matrix permeability and stiffness. In this work, we developed a dual-gel dual-porosity 3D ECM mimics to address this challenge. With the new model, one can individually control the interstitial flow and matrix permeability without affecting the primary matrix stiffness. We also conduct preliminary studies on the efficiency of our model in studying the effect of interstitial flow on cancer cell migration.

*Acknowledgment is made to the donors of the American Chemical Society Petroleum Research Fund for partial support of this research.

10:00AM R65.00009: Targeted photothermal lysing of E. Coli via a geometrically-modified Au-binding M13 virus ZAIRA ALIBAY (Presenter), TAM-TRIET NGO-DUC, Materials Science and Engineering Program, University of California, Riverside, JOSHUA M PLANK, Department of Electrical and Computer Engineering, University of California, Riverside, JOSEPH CHEENEY, Materials Science and Engineering Program, University of California, Riverside, ELAINE D. HABERER, Department of Electrical and Computer Engineering, University of California, Riverside — Increasing antibiotic resistance (ABR) in bacteria is a continuing public threat to human health. Antibody functionalized nanoparticles (NPs) in conjunction with photothermal lysis have been successful in targeting and eradicating these pathogens. Yet, synthesis of antibodies is an expensive and time-consuming process. Alternative approaches capable of selectively delivering photothermally-active NPs to ABR bacteria are essential. In our work, a geometrically-modified, Au-binding M13 bacteriophage offers a novel solution to this challenge. Rod-shaped and spherically-shaped viral templates were created via chloroform interaction with the filamentous bacteriophage. Decorated with Au NPs, both of these scaffolds were capable of targeting E.Coli bacteria via attachment of exposed minor coat protein to the pathogen. Bactericidal studies of rods and spheroids were executed under a range of 532 nm laser irradiation conditions: power (0 - 60 mW) and time (0 - 20 min). Using geometrically-modified M13 scaffolds up to 65% of E.Coli were killed within 20 min. Through genetic modification of the minor coat protein the bactericide effects of these templates could be extended to target other pathogens. These findings advance efforts to engineer versatile and low-cost strategies to tackle ABR.
10:12AM R65.00010: Gold Binding by Design: A Combined Theoretical/Experimental Study of Biohybrid Systems
MARGARET HURLEY (Presenter), MEAGAN C. SMALL, US Army Research Laboratory - APG, MD, DEBORAH A. SARKES, HONG DONG, JUSTIN P. JAHNKE, DIMITRA N. STRATIS-CULLUM, US Army Research Laboratory - ALC, MD — Biomolecular-inorganic hybrid materials have many potential applications in medicine, electronics, and nanotechnology. It is therefore of great interest to design peptides that have predictable and controllable binding to inorganic surfaces, requiring a detailed understanding of biotic/abiotic interactions. Computational models have provided key insight into the underlying intermolecular interactions in such systems. However, owing to limited computational resources, these studies are often performed using periodic models where care must be taken to understand the effects of model size and periodicity, as well as any possible additional limitations in the method. Here we perform DFT calculations exploring the binding interactions between amino acid residues and the Au(111) surface. Results are presented in the context of experimental results from bacterial display studies of engineered E. coli binding to gold surfaces with applications including development of viable E. coli/AuNP hybrid systems and microbial fuel cells.

10:24AM R65.00011: A Comparative Study on Interspecies Blood Rheology*
JEFFREY HORNER (Presenter), ANTONY N BERIS, NORMAN J. WAGNER, DONNA WOULFE, University of Delaware — Blood is a complex suspension of red blood cells (RBCs), white blood cells, and platelets in an aqueous plasma phase with several dissolved proteins. Despite a consistent makeup, with minor changes in constituent sizes and volume fractions, blood from different species exhibits significantly different rheological signatures. Blood from some species including horse, pig, and human exhibit a yield stress at low shear rates, while blood from other species including cow, sheep, and guinea pig exhibit no yield stress. This is attributed to the presence or absence of microstructural RBC aggregates at low shear rates. Moreover, blood samples across all species may exhibit unique transient behavior which enables insight into how blood evolved to the specific organism. In this work, we present new steady and transient rheological data on blood from several species. We show that a previously developed thixotropy model can be used to model blood rheology across species and discuss the similarities and differences. This study improves the understanding of how blood changes across species, which is important for drug clinical testing and elucidates the connection between physiology and blood rheology.

*This work is supported by the National Science Foundation, award number CBET 1510837.

10:36AM R65.00012: Early onset of kinetic roughening due to finite step width in hematin crystallization*
KATY OLAFSON, JEFFREY RIMER, PETER VEKILOV (Presenter), University of Houston — Crystallization is an example of a highly non-equilibrium process, in which the flows of mass and energy are governed by dynamic structures comprising a two-dimensional interface between adjacent three-dimensional semi-spaces. During crystal growth, the structure of its interface with the growth medium dictates the molecular mechanism of solute incorporation, the response of the growth dynamics to temperature and composition gradients, the action of impurities and dopants, and, ultimately, the crystal perfection. Interfaces that are smooth at equilibrium may become rough during growth at elevated supersaturation. We observed a smooth to rough transition during the growth of hematin crystals from a biomimetic mixed organic-aqueous solvent. Hematin crystallization is the main pathway employed by malaria parasites to sequester toxic hematin, released during hemoglobin digestion; its inhibition is considered the most successful target for antimalarial drugs. We show that the transition occurs at a supersaturation significantly lower than that predicted by published criteria.

*This work was supported by NIH (Grant 1R21AI126215-01), NSF (DMR-1710354), NASA (NNX14AD68G and NNX14AE79G), and The Welch Foundation (Grant E-1794).

Thursday, March 7, 2019 8:00 AM - 10:48 AM

Session R66 DBIO GSNP GSOFT: Pattern Formation and Oscillations in Biology BCEC 261 - David Lubensky, Univ of Michigan - Ann Arbor - Tag(s): Focus
**8:00AM R66.00001: Mitotic traveling waves in the Drosophila embryo** [Invited] STEFANO DI TALIA (Presenter), Cell Biology, Duke University Medical Center — Early embryogenesis of most metazoans is characterized by rapid and synchronous cleavage divisions. While diffusion is too slow for synchronization of mitosis across large spatial scales, traveling waves represent a possible process of synchronization. I will discuss our recent work dissecting the molecular and physical mechanisms for the generation of traveling waves of activity of Cdk1, the master regulator of the cell cycle. I will show that the *in vivo* dynamics of Cdk1 are captured by a transiently bistable reaction-diffusion model, where time-dependent reaction terms account for the growing level of cyclins and Cdk1 activation across the cell cycle. I will discuss two distinct regimes. The first one is observed in mutants of the mitotic switch. There, waves are triggered by the classical mechanism of a stable state invading a metastable one. Conversely, waves in wild type reflect a transient phase that preserves the Cdk1 spatial gradients while the overall level of Cdk1 activity is swept upward by the time-dependent reaction terms. This unique mechanism generates a wave-like spreading (sweep-waves) that differs from bistable waves for its dependence on dynamic parameters and its faster speed. I will also discuss how the integration of biochemical and mechanical processes is required for the early establishment of synchronization of the cell cycle.

*NIH grant R01-GM122936

**8:36AM R66.00002: Tuning the Xenopus mitotic oscillator in artificial cells** [Invited] QIONG YANG (Presenter), Biophysics and Physics, University of Michigan Ann Arbor — We study biological oscillations and self-organization phenomena in both artificially constructed mitotic cells and live zebrafish embryos. We focus on how the network structures of biological clocks are linked to their functions, such as tunability and robustness, and how individuals coordinate through biochemical and mechanical signals to generate collective spatiotemporal patterns. To pin down the physical mechanisms that give rise to these complex phenomena, we integrate modeling, time-lapse fluorescence microscopy, microfluidics, and systems and synthetic biology approaches.

Although central architectures drive robust oscillations, networks containing the same core vary drastically in their potential to oscillate. We computationally generate an atlas of oscillators and found that, while certain core topologies are essential for robust oscillations, local structures substantially modulate the degree of robustness. Strikingly, two key local structures, incoherent inputs and coherent inputs, can modify a core topology to promote and attenuate its robustness, additively (Cell Systems 2017). Experimentally, we developed an artificial cell-cycle system to mimic the real mitotic oscillations in microfluidic droplets (eLife 2018). The artificial cells can perform self-sustained oscillations for 40 cycles over multiple days. The oscillation period and number of cycles can be reliably tuned by the amount of clock regulators or droplet sizes. Such innate flexibility makes it key to studying clock functions of tunability and stochasticity at the single-cell level. With nanofabrication and long-term time-lapse fluorescence microscopy, this system enables a high-throughput, single-cell analysis of clock dynamics and functions. We now combine this platform with mathematical modeling to elucidate the topology-function relation of biological clocks.

*This work was supported by grants from NSF (Early CAREER and MCB #1817909), NIH (MIRA #GM119688), and a Sloan Research Fellowship.

**9:12AM R66.00003: Identifying How Single Cells Modulate Population-Wide Pattern Formation** [Invited] ALLYSON SGRO (Presenter), Departments of Biomedical Engineering and Physics and the Biological Design Center, Boston University — One of the key outstanding challenges in understanding multicellular pattern formation is identifying what single cells tune within themselves to change population-wide patterns. A major driver of multicellular patterns is oscillations in single-cell signaling networks, but it is unknown what features single cells naturally modulate in these oscillations to change global patterns. An ideal system for addressing this challenge exists in the social amoeba, *Dictyostelium discoideum*. *Dictyostelium* uses travelling waves of chemoattractant molecules between cells to drive aggregation into a multicellular state when starving. These waves originate within single cells that release this molecule to the environment, and the single-cell signaling network phenomena that drive the creation of these waves are well-characterized. However, it is still unknown what parameters a single cell naturally controls to change the observed population pattern. Using new experimental data in conjunction with an existing phenomenological model, I explore what parameters single cells can modulate to control signaling oscillations and pattern formation.

*This work was supported by a Burroughs Wellcome Fund Career Award at the Scientific Interface to A.E.S.*
9:24AM R66.00004: Single-Mode Turbulence in Pattern-Forming Protein Systems* JONAS DENK (Presenter), JACOB HALATEK, FRIDTJOF BRAUNS, KORBINIAN PÖPPEL, ERWIN FREY, Ludwig Maximilian University of Munich — Protein pattern formation often relies on proteins that cycle between a cytosolic bulk and a membrane at which they undergo molecular interactions. On a flat membrane, this cycling can lead to intriguing protein patterns including spiral waves as well as more irregular dynamics such as chemical turbulence. While theoretical approaches have been able to reproduce various experimentally observed protein patterns, the underlying mechanisms for pattern selection remain poorly understood. Motivated by the bacterial Min protein system, we present a spatially reduced reaction-diffusion model to study pattern selection in protein systems with bulk-membrane coupling. Remarkably, we find that already a single-mode instability can lead to turbulent dynamics at the onset of pattern formation. Further away from this onset, we observe a transition from turbulent to coherent patterns, which can be explained on the basis of diffusively coupled local equilibria. Our study yields insights into a novel route to chaos for a widespread class of mass-conserving reaction-diffusion systems with bulk-boundary coupling.

*This research was supported by the Deutsche Forschungsgemeinschaft via Project B02 within SFB 1032 and the German Excellence Initiatives via the 'NanoSystems Initiative Munich'.

9:36AM R66.00005: Directed and Spiral Wave Propagation in Communities with Correlated Heterogeneity XIAOLING ZHAI (Presenter), Purdue University, JOSEPH LARKIN, GUROL SUEL, University of California, San Diego, ANDREW MUGLER, Purdue University — Directed signal propagation in cellular communities is an important and ubiquitous phenomenon. However, heterogeneity in these communities may pose a challenge to directed propagation. Additionally, spatial correlations in the heterogeneity may alter the dynamic behavior. In general, the relationship between correlated heterogeneity and wave propagation is poorly understood. Here we use a FitzHugh Nagumo-type model to investigate wave propagation in a two-dimensional heterogeneous community. Our model predicts three dynamic regimes in which waves either propagate directly, die out, or spiral indefinitely. In some parameter regimes, correlations in the heterogeneity enhance directionality and suppress spiraling, as expected. In contrast, in other regimes, correlations promote spiraling, a surprising feature that we explain by demonstrating that these spirals form by a second, distinct mechanism. Finally, we characterize the dependence of the spiral period on the degree of heterogeneity and connect our results to percolation theory. Our work reveals that the spatial structure of cell-to-cell heterogeneity can have important consequences for directed signal propagation in cellular communities, and provides predictions that can be tested in experiments.

9:48AM R66.00006: Coexistence and coupling of Min protein patterns in heterogeneous systems JACOB HALATEK (Presenter), Biological Computation Group, Microsoft Research, Cambridge, FRIDTJOF BRAUNS, Physics, Ludwig-Maximilians Universitaet Muenchen, GRZEGORZ PAWLIK, Kavli Institute of Nanoscience, TU Delft, LAESCHKIR HASSAN, Physics, Ludwig-Maximilians Universitaet Muenchen, CEES DEKKER, Kavli Institute of Nanoscience, TU Delft, ERWIN FREY, Physics, Ludwig-Maximilians Universitaet Muenchen — In the past two decades, the Min protein system has been established as paradigmatic model system for self-organized protein pattern formation. Much of this success is owed to the advances made in the reconstitution of Min protein patterns in vitro, which allowed precise control over experimental conditions and thereby the pattern forming phenomena. However, up until recently a theoretical description for in vitro Min protein patterns has been missing. Lately, we proposed a novel theoretical framework for pattern formation in mass-conserved reaction-diffusion systems [1]. One of the key predictions are transitions between chaotic, standing, and travelling wave patterns induced by variations in the system geometry or protein numbers. Here, we present the first experimental confirmation of these predictions. An extension of the theoretical framework enables us to forecast the entire time evolution of patterns and their dynamic transitions in systems with heterogeneous geometry or kinetic parameters. Strikingly, the theory predicts the coexistence of patterns in large heterogeneous systems, which we confirm experimentally.

10:00AM R66.00007: Rectified adaptation - a variance sensor for processing time-varying inputs* KABIR HUSAIN, JACKSON D O’BRIEN, WEERAPAT PITTAYAKANCHIT, PARTHIV PATEL, SAVAS TAY, ARVIND MURUGAN (Presenter), University of Chicago — The role of chemical identity and spatial distribution of biomolecules in pattern formation and cell fate decision making has long been appreciated. However, recent experiments have revealed that the temporal dynamics of molecular concentrations also plays an important role and can affect gene regulation, cell fate decisions and accelerate pattern formation. We identify a general phenomenological behavior - "rectified adaptation" - that plays a critical role in processing oscillatory, pulsatile and fluctuating temporal signals in these diverse biological contexts. Like conventional adaptation, rectified adaptation describes a transient response to step changes in an input signal but the response to step ups and step downs is strongly asymmetric. We show how simple implementations of rectified adaptation can sense the variance of an input signal on specific timescales, helping make decisions in immune response and in embryonic patterning.

*AM thanks the Simons Foundation for support. KH thanks the James S. McDonnell Foundation for support.

10:12AM R66.00008: Critical dynamics in bursts of δ and θ-rhythms across the sleep-wake cycle FABRIZIO LOMBARDI (Presenter), Boston University, MANUEL GOMEZ-EXTREMERÁ, PEDRO BERNAOLA-GALVAN, University of Malaga, THOMAS E SCAMMELL, Harvard Medical School, PLAMEN CH IVANOV, Boston University — Solid evidences indicate that different cortical rhythms characterize distinct phases (sleep stages) of the sleep-wake cycle. Sleep stages are not stable, and sleep periods exhibit numerous transitions among different stages, including short awakenings/arousals. Nature and dynamics of such transitions, as well as origin and functions of arousals, remain elusive. Recently, it has been shown that brief awakenings/arousals do not have a characteristic duration and consistently follow a power-law distributions across different species. Since arousals can be viewed as 'active' states of the brain that interrupt the 'inactive' phase represented by sleep periods, such a scale-free statistics has been interpreted as a fingerprint of criticality in sleep dynamics, suggesting that arousals are an integral part of sleep regulation. In this talk, I will present recent results on the dynamics of relevant cortical rhythms across the sleep-wake cycle that seem to support such a hypothesis. I will show that wake-related θ- and sleep-related δ-bursts exhibit a robust scale invariant temporal organization closely reminiscent of other non-equilibrium phenomena, and discuss their dynamics and coupling in relation to the neuronal circuitry responsible for wake and sleep control in rats.

10:24AM R66.00009: Phase space geometry of reaction--diffusion systems FRIDTJOF BRAUNS (Presenter), JACOB HALATEK, ERWIN FREY, Ludwig Maximilian University of Munich — Self-organized pattern formation — typically studied in terms of spatially extended dynamical systems — is as ubiquitous in nature as it is difficult to deal with conceptually and mathematically. We build on the phase space geometric methods of Nonlinear Dynamics, using geometric structures like nullclines and fixed points, to develop a comprehensive theory for two-component mass-conserving reaction–diffusion systems — a paradigmatic model class for pattern formation, e.g. intracellular polarization. A dissection of space into (notional) compartments enables us to characterize the spatio-temporal dynamics based on the ODE phase space of local reactions. Diffusive coupling leads to mass redistribution between the compartments which, in turn, changes the local phase space properties.

We show that all aspects of pattern formation, from linear instability and excitability to the bifurcations of stationary patterns, can be extracted from the geometric features of the line of chemical equilibria in phase space. Furthermore, our analysis points towards a deep connection between the far from equilibrium reaction–diffusion dynamics to phase separation of binary mixtures near equilibrium, and thus offers a new perspective on phase separation far from equilibrium.
Emergence of traveling waves in linear arrays of electromechanical oscillators

YONG DOU (Presenter), SHASHANK PANDEY, Chemical Engineering, Columbia University, CHARLES CARTIER, OLIVIA MILLER, Chemical Engineering, Pennsylvania State University, KYLE J. M. BISHOP, Chemical Engineering, Columbia University — Traveling waves of mechanical actuation provide a versatile strategy for locomotion and transport in both natural and engineered systems across many scales. These rhythmic motor patterns are often orchestrated by systems of coupled oscillators such as beating cilia or firing neurons. Here, we show that similar motions can be realized in linear arrays of electromechanical oscillators that move and interact via electrostatic forces. Conductive spheres oscillate between biased electrodes through cycles of contact charging and electrostatic actuation. The combination of repulsive interactions among the particles and spatial gradients in their natural frequencies lead to phase locked states characterized by gradients in the oscillation phase. The frequency and wavelength of these traveling waves can be specified independently by varying the applied voltage and the electrode separation. We demonstrate how traveling wave synchronization can enable the directed transport of material cargo. Our results suggest that simple energy inputs can power complex patterns of mechanical actuation with potential opportunities for soft robotics and colloidal machines.

This work was supported by the CBES, an EFRC funded by the U.S. Department of Energy, Office of Science, under Award DE-SC0000989.

Thursday, March 7, 2019 8:00 AM - 11:00 AM

Session R67 DBIO: Physics of Neural Systems II BCEC 050 - Vijay Singh, University of Pennsylvania

Progress on functional connectivity measurement and modeling in C. elegans

FRANCESCO RANDI (Presenter), ANUJ K SHARMA, ANDREW M LEIFER, Department of Physics, Princeton University — Advances in microscopy and optogenetics now permit “functional connectivity” experiments in which some neurons are optogenetically stimulated while the responses of other neurons in the network are simultaneously measured, ideally giving access to the strengths and the dynamical properties of the interactions between neurons. Currently, the nematode C. elegans is an ideal candidate in which to perform such experiments, because of its small nervous system, the known anatomical connectivity map between the neurons, and the graded nature of their activity. I will present progress on such measurements on the whole brain of the worm. Additionally, how should a mathematical description of C. elegans’ neural network be structured so as to be able to best incorporate such measurements of functional connectivity? I will introduce a framework for the description of the neural activity in C. elegans based on Green's functions, which can be directly related to the quantities measured in the above experiments.

This work was supported in part by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030)

Bridging severed nerves in a mouse using Carbon Nanotubes (CNTs): Identifying artifact vs. neural signals suggests transmission was partially restored

VINEET MATHUR (Presenter), Chemistry, University of California Berkeley, ZACHARIAH HENNIGHAUSEN, SWASTIK KAR, Physics, Northeastern University — Stimulation and recording of neural tissue are hallmarks of investigation of neural activity, especially the detection of action potentials. In this context, accurate analysis of curve-shapes holds significant value in distinguishing between neural activity compared to background noise and instrument artifacts. We report the remarkable observation that when probed using an electric field stimulation technique (EFS) in an in-vitro setting, control experiments that contain no neural tissue reproducibly produce curves in-distinguishable from experiments containing sources of neuronal activity. We additionally provide a physical model to explain the origin and behavior of such false-positive signals in relation to the buffer and neural circuits in the system. Lastly, we present data and analysis on in-vivo experiments using a mouse and carbon nanotubes (CNTs). Our experiments detected a previously unreported dominant secondary pulse delayed over 16ms after the artifact signal. Comparing the intact, severed, and bridged (with CNTs) spinal cord suggests transmission of neural signals was partially restored.

Swastik Kar graciously acknowledges financial support from NSF ECCS 1351424.
8:24AM R67.00003: Nonlinear synchronization of neuronal firing on a random graph: Application to breathing rhythm formation in the preBötzinger complex. VALENTIN SLEPUKHIN (Presenter), ALEXANDER JACOB LEVINE, Physics and Astronomy, Univ of California - Los Angeles, JACK L FELDMAN, SUFYAN ASHHAD, Neurobiology, Univ of California - Los Angeles — The preBötzinger complex is a network of a few thousands of neurons that produces the rhythmic signal controlling mammalian breathing (inspiration). In vitro experiments demonstrated that the activation of small group of neurons in this network results in a “burstlet” of neuronal firing that propagates through the network after some delay (Kam et al., 2013). We consider a simple model burstlet dynamics based on the nonlinear synchronization of imprecise neuronal oscillators interacting on a random graph. The numerical simulations based on this model reproduce features observed in the experiment, such as (i) the probability of systemic synchronization in response to a given number of stimulated neurons, and (ii) the time lag between stimulation and systemic synchronization as a function of the number of stimulated neurons. We conclude by discussing how the topology of the neuronal connectivity affects the robustness of the emergent rhythm dynamics of the network in response to local damage (cell death).

8:36AM R67.00004: Modularity as an order parameter for speech reception FENGDAN YE (Presenter), COLIN NOE, SIMON FISCHER-BAUM, MICHAEL DEEM, Rice University — Recent work in cognitive neuroscience has focused on analyzing the brain as a network, rather than as a collection of independent regions. Prior studies taking this approach have found that individual differences in the degree of modularity of the brain network relate in a complexity-dependent way to performance on cognitive tasks. In the current study, we study the effect of modularity in the context of speech perception. We calculate modularity of whole brain EEG data collected during a lexically biasing phoneme categorization task from 20 subjects, and correlate modular activity of the brain with subjects' responses to audio stimuli with varying ambiguity. We find that modularity is correlated with how quickly and decisively a subject switches from one category of phoneme to another. This correlation is also mediated by lexical bias and place of articulation in each pair of phonemes. The results presented here provide a framework for linking measures of whole brain organization from network neuroscience to cognitive processing.

8:48AM R67.00005: Global synchronization due to cluster size heterogeneity in balanced neural networks ABHIJIT CHAKRABORTY (Presenter), GREG MORRISON, Department of Physics, University of Houston — Synchronized brain rhythms have been associated with various cognitive functions as well as neurological disorders, and comprehending how the network connectivities give rise to these behaviors is essential for a better understanding of the importance of network topology on functional brain dynamics. Previous studies have shown that cortical networks with clustered connections give rise to correlated dynamics in individual clusters. However, this same model applied to a network with highly heterogeneous cluster sizes leads to a clear breakdown of the balanced state. In this talk, using a formal definition of the balance matrix, we show why the balance condition breaks and propose a solution to restore balance in the heterogeneous networks. In doing so, we also observe that global synchronization in firing dynamics appears due to cluster size heterogeneity. This modified balance matrix applied to a homogeneous network results in the disappearance of the synchronization. Diversity in cluster sizes has not previously been shown to produce such a global effect in a network of excitatory and inhibitory leaky integrate and fire neurons, and may have important implications in real world cortical networks.

9:00AM R67.00006: Statistical properties of the optimal sensitivity matrix for compressed sensing with nonlinear sensors* SHANSHAN QIN (Presenter), QIANYI LI, CHAO TANG, Peking University, YUHAI TU, IBM Thomas J. Watson Research Center — Natural odors are typically sparse mixtures of a few types of odorants each with a wide range of concentrations. How to encode a large number of sparse odor mixtures with a relatively small number of nonlinear olfactory receptor neurons (ORNs) — the nonlinear compressed sensing problem — remains a puzzle. Here, by using an information theory approach, we study the optimal coding strategies that enable ORNs to best represent olfactory information. Our results show that the optimal odor-receptor sensitivity matrix is sparse and the nonzero sensitivities follow roughly a log-normal distribution, both of which are consistent with existing experiments. We also show that odor-evoked inhibition increases coding capacity, providing a plausible explanation for experimental observation in the fly olfactory system. Furthermore, we show that the optimal sensitivity matrix can enhance accuracy of the downstream decoding tasks. Our results may shed light on understanding the peripheral olfactory sensory system and improving performance of artificial neural networks.

*The work was supported by the Chinese Ministry of Science and Technology (Grant No. 2015CB910300) and the National Natural Science Foundation of China (Grant No. 91430217) and the NIH grant (R01-GM081747).
GORDON BERMAN, Emory University — Social behavior is an important aspect of life for humans and many other animals. Oxytocin, a neurotransmitter often associated with social behavior, is involved in pair bonding. Further, our results suggest the role of model neurons driven by oscillatory input. Our results show that changes in the input to the network and in the excitability of the neurons play an important role in bond formation. Furthermore, our results suggest the role of the phase-amplitude-coupling (PAC) between mPFC drive to NAcc is pivotal for the formation of a bond in Microtus ochrogaster. Key brain areas in this process are the medial prefrontal cortex (mPFC) and the nucleus accumbens (NAcc). It was shown that the phase-amplitude-coupling (PAC) between mPFC drive to NAcc is pivotal for the formation of a bond in voles. Experimental measurements from NAcc suggest non-trivial relations between the input to the network and the resulting PAC features. Using simulations and analytical methods we study the emerging coupling in networks of model neurons driven by oscillatory input. Our results show that changes in the input to the network and in the excitability of the neurons play an important role in the bond formation process. Furthermore, our results suggest the role of oxytocin, a neurotransmitter often associated with social behavior, in pair bonding is to modulate the excitability of certain neurons.

9:24AM R67.00008: Chaotic itinerancy in reservoir computing* HIROMICHI SUETANI (Presenter), Faculty of Science and Technology, Oita University — Recently, the paradigm of reservoir computing (RC) has attracted attention as a new way of recurrent neural network (RNN) training [1]. Especially, Sussillo and Abbott proposed a version of RC, called FORCE-learning[2] and they showed how chaotic activity in a RNN is useful for generating various temporal patterns. In this study, we construct a machine based on the FORCE-learning scheme for generating a set of temporal patterns that are selectable by the combination of trigger pulses through multiple channels. We show that this machine can be actually realized, depending on the adequate choice of parameters of the reservoir. When the machine shows optimal performances, it also shows intermittent transitions among several typical patterns without any trigger inputs, i.e., spontaneous mode, which reminds us chaotic itinerancy [3]. We characterize this pliability of chaos in terms of the large deviation fluctuations of Lyapunov exponents and visualize the itinerant dynamics using the manifold learning such as t-SNE.


*This study is supported by MEXT/JSPS KAKENHI Grant Number 16H01617, 16K00059 and 18H05136.

9:36AM R67.00009: The role of neural excitability and coupling in the formation of social bonds ITAI PINKOVIEZKY (Presenter), AHMED ROMAN, Emory University, ELIZABETH AMADEI, Neuroinformatik u. Neuronale Syst, ETH, ROBERT C LIU, GORDON BERMAN, Emory University — Social behavior is an important aspect of life for humans and many other animals. Yet, our understanding of the biological mechanisms giving rise to it is limited. Although extensive research has been done on the neural basis of social impairment, few studies have attempted to explain the formation of positive behaviors. Here, we report results on the mechanisms responsible for a positive social behavior, pair bonding in prairie voles (Microtus ochrogaster). Key brain areas in this process are the medial prefrontal cortex (mPFC) and the nucleus accumbens (NAcc). It was shown that the phase-amplitude-coupling (PAC) between mPFC drive to NAcc is pivotal for the formation of a bond in voles pair. Experimental measurements from NAcc suggest non-trivial relations between the input to the network and the resulting PAC features. Using simulations and analytical methods we study the emerging coupling in networks of model neurons driven by oscillatory input. Our results show that changes in the input to the network and in the excitability of the neurons play an important role in the bond formation process. Furthermore, our results suggest the role of oxytocin, a neurotransmitter often associated with social behavior, in pair bonding is to modulate the excitability of certain neurons.

9:48AM R67.00010: Precise Spatial Memory in Local Random Networks* JOSEPH NATALE (Presenter), H G E HENTSCHEL, ILYA NEMENMAN, Emory University — Self-sustained, elevated neuronal activity persisting on time scales of ten seconds or longer is vital for working memory. The most prevalent models for persistent activity, known as attractor networks, have come under criticism for their severe reliance on fine-tuning of synaptic architectures. While alternative frameworks exist, many of these invoke fine-tuning implicitly. Here we elaborate a model with local learning rules, and can be derived from principled objective functions. We test these algorithms on data generated from several alternating autoregressive-moving-average (ARMA) models and find very good performance in detecting changes in the generating process within just dozens of samples from the transition point. We compare this to similar methods from control theory that are not directly interpretable as neural models.


*This work was supported in part by grants JSMF/ 220020321 and NSF/IOS/1208126; NIH #1 R01 EB022872 and NIH # NS084844.
10:00AM R67.00011: A physical model for pattern completion of highly overlapping patterns for Human Episodic Memory  
ZAHRA GHASEMI ESFAHANI (Presenter), MARC HOWARD, Boston University — Patterns of neural activity in the hippocampus change very slowly, perhaps in a scale-invariant manner. 
Episodic memory is a consequence of retrieval of a pattern of activity corresponding to a specific event in the past. The physics of attractor networks have been extensively studied. However, it is well known that attractor networks have a small capacity when storing the correlated patterns. This coupled with the strong overlap in patterns of neural activity in the hippocampus makes attractor networks ill-suited to describe human episodic memory. 
Using a concise description of hippocampal time cells, we develop a formal model for pattern completion of hippocampal representations. The model overcomes pattern similarity by relying on the coupling between different temporal scales. Because the model uses the recency of the desired memory as part of the retrieval process, it can be understood as an ‘`address-addressable`` memory. In this sense, time serves as a scaffolding to organize different experiences. We study the capacity and dynamics of this model for memory retrieval and compare to properties of human episodic memory.

10:12AM R67.00012: Novel strategies for holographic optical activation of neurons*  
SAMIRA AGHAYEE (Presenter), PATRICK KANOLD, WOLFGANG LOSERT, University of Maryland, College Park — In-vivo two photon imaging of neuronal activity in the higher sensory cortical layers has revealed that the spatial arrangements of neurons involved in processing sensory stimuli is complex. Recent advances in optogenetics have allowed for optical manipulation of neurons, and holographic microscopy has enabled us to selectively target neurons for activation. Here we introduce the use of extended holographic patterns with high planar selectivity for photo activation of neurons. Our approach takes advantage of a lens function to reduce off-target speckles. We find that in addition to reducing speckles, our approach also generates target patterns with a higher degree of uniformity. We demonstrate the feasibility of this method for in vivo studies of the auditory cortex.

*Supported by BRAIN initiative grant U01NS090569 (PK, WL) and University of Maryland Seed Support.

10:24AM R67.00013: Wiring economy constrains olfactory glomerulus placement in fly larva  
GUANGWEI SI (Presenter), MATTHEW E BERCK, YU FENG, ARAVINTHAN SAMUEL, Harvard University — Olfactory sensory neurons expressing the same receptor converge their axons to a common locus called a glomerulus. The glomeruli placement are largely stereotyped. A plausible theory to explain the placement is the wiring economy principle, where neuronal placement is an optimal solution to minimizing the wiring cost given a synaptic connectivity pattern. Recently, the complete wiring diagram of a glomerular olfactory system, the insect antennal lobe, has been reconstructed using serial section electron microscopy and the fly larva. The reconstruction provides a detailed map of glomerulus placement as well as the underlying synaptic connectivity. Interneuron synaptic connectivity patterns within the antennal lobe are strikingly and consistently heterogeneous in their glomerular innervations. We developed a coarse-grained model to describe the glomeruli placement and calculate the wiring cost to generate this synaptic connectivity. The wiring cost of observed glomerular position is significantly smaller than random glomerular arrangements. We also searched for the theoretical minimal wiring cost, which compares well with the observed glomerular arrangement. Wiring economy provides an explanation in terms of physical optimization for the organization of an olfactory system.

10:36AM R67.00014: Generation of scale-invariant sequential activity in recurrent neural circuits*  
YUE LIU (Presenter), MARC W HOWARD, Department of Physics and Center for Systems Neuroscience, Boston University — Sequential neural activity has been observed in many parts of the brain. Sequential activity can be generated by recurrent neural networks, which have been extensively studied (White and Sompolinsky, 1996, Goldman, 2009, Rajan et al., 2016, Chaudhuri et al., 2016).
Inspired by Weber-Fechner law in the sensory domain and scalar timing in psychophysics, we study the requirements for scale-invariant sequences in linear recurrent neural networks. It is found that 1) the eigenvalues of the connectivity matrix must be geometrically spaced, and 2) the eigenvectors have to have a translation-invariant structure composed of the same motif.
Together the relationship between the eigenvectors and eigenvalues can be thought of a logarithmic mapping from a ratio scale to an interval scale (Luce, 1959). Geometrically spaced network eigenvalues can generically emerge from multiplicative cellular processes (Amir et al., 2012). We are now seeking to extend these results to nonlinear recurrent networks.

*ONR MURI N00014-16-1-2832
NIBIB R01EB022864
Exploring the energy landscape of C. elegans neural activities

XIAOWEN CHEN (Presenter), FRANCESCO RANDI, ANDREW M LEIFER, WILLIAM BIALEK, Princeton University — Recent advances in experimental techniques and application of the maximum entropy principle have allowed us to build models for joint probability distribution of activity in groups of up to 50 neurons in *Caenorhabditis elegans*, a nematode with 302 neurons. These models, which are equivalent to the Boltzmann distribution for a family of Potts glasses, successfully predict the static observables of the network. The energy landscape defined by these models exhibits curious signatures of collective behavior, including a large number of energy minima, as in models for memory, and a clustering of energy barriers that is reminiscent of the dynamical transitions in disordered systems. While these models describe the distribution of network states at a single time, the observed neural dynamics are not consistent with a simple Brownian-like motion on the energy landscape. In particular, the real dynamics exhibit much longer correlation times than predicted from the heights of energy barriers alone. We will show progress towards understanding how the nematode actually explores the energy landscape of its neural network.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S01 DCMP: Fractional Quantum Hall Effect: Novel States and Excitations

Lucia Steinke, Texas A&M University

11:15 AM S01.00001: Zero modes, Bosonization and Topological Quantum Order: Composite Fermions in Second Quantization  
LI CHEN (Presenter), Florida State University, SUMANTA BANDYOPADHYAY, Washington University, St. Louis, KUN YANG, Florida State University, ALEXANDER SEIDEL, Washington University, St. Louis — We develop recursion relations, in particle number, for all (unprojected) Jain composite fermion (CF) wavefunctions. These recursions generalize a similar recursion originally written down by Read for Laughlin states, in mixed first-second quantized notation. In contrast, our approach is purely second-quantized, giving rise to an algebraic, `pure guiding center'' definition of CF states that de-emphasizes first quantized many-body wave functions. Key to the construction is a second-quantized representation of the flux attachment operator that maps any given fermion state to its CF counterpart. An algebra of generators of edge excitations is identified. In particular, in those cases where a well-studied parent Hamiltonian exists, its properties can be entirely understood in the present framework, and the identification of edge state generators can be understood as an instance of `microscopic bosonization'. The intimate connection of Read's original recursion with `non-local order parameters'' generalizes to the present situation, and we are able to give explicit second quantized formulas for non-local order parameters associated with CF states.

11:27 AM S01.00002: Variational principle for an incompressible fluid with Hall viscosity and gapless surface modes*  
GUSTAVO M MONTEIRO (Presenter), UNICAMP-Univ de Campinas, ALEXANDRE ABANOV, Stony Brook University — Hydrodynamics is a powerful tool to study strongly interacting systems, including for example the fractional quantum Hall effect (FQHE). The main features of the quantum Hall hydrodynamics are the incompressibility of the electron flow, due to the gap separation between the FQH ground state and the excited states, and the relation between the density of the fluid and its vorticity. Motivated by this example, we focus in this work on the variational and Hamiltonian formulations of incompressible two-dimensional fluid dynamics with free surface and nonvanishing Hall viscosity. We show that within the variational principle the Hall viscosity contribution corresponds to a purely geometric boundary term. This term modifies effective boundary conditions on the free surface. The modified boundary conditions have a interpretation describing an additional pressure at the free surface proportional to the angular velocity of the surface itself. These boundary conditions are believed to be universal since the proposed hydrodynamic action is fully determined by the symmetries of the system. The extension of this variational principle to compressible flows will be also considered in this talk.

*G.M. was supported by FAPESP. A.G.A. acknowledges NSF DMR-1606591 and US DOE DESC-0017662.
11:39AM S01.00003: Geometric quench in the fractional quantum Hall effect: exact solution in quantum Hall matrix models and comparison with bimetric theory* MATTHEW LAPA (Presenter), Physics, University of Chicago, ANDREY GROMOV, Physics, University of California, Berkeley, TAYLOR HUGHES, Physics, University of Illinois at Urbana-Champaign — We investigate the recently introduced geometric quench protocol for fractional quantum Hall (FQH) states within the framework of exactly solvable quantum Hall matrix models. In the geometric quench protocol a FQH state is subjected to a sudden change in the ambient geometry, which introduces anisotropy into the system. We formulate this quench in the matrix models and then we solve exactly for the post-quench dynamics of the system and the quantum fidelity (Loschmidt echo) of the post-quench state. Next, we explain how to define a spin-2 collective variable \( g_{ab}(t) \) in the matrix models, and we show that for a weak quench (small anisotropy) the dynamics of \( g_{ab}(t) \) agrees with the dynamics of the intrinsic metric governed by the recently discussed bimetric theory of FQH states. We also find a modification of the bimetric theory such that the predictions of the modified bimetric theory agree with those of the matrix model for arbitrarily strong quenches.

*Kadanoff Center for Theoretical Physics and Materials Research Science and Engineering Center at University of Chicago, U.S. National Science Foundation DMR 1420709 and DMR 1351895-CAR, U.S. Department of Energy DE-AC02-05CH11231, Institute for Condensed Matter Theory at University of Illinois at Urbana-Champaign.

11:51AM S01.00004: Interlayer fractional quantum Hall effect in a coupled graphene double-layer XIAOMENG LIU, ZEYU HAO (Presenter), Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, BERTRAND I. HALPERIN, PHILIP KIM, Harvard University — In two-dimensional (2D) electron systems under strong magnetic fields, interactions can cause fractional quantum Hall (FQH) effects. Bringing two 2D conductors to proximity, a new set of correlated states can emerge due to interactions between electrons in the same and opposite layers. Here we report interlayer correlated FQH states in a system of two parallel graphene layers separated by a thin insulator. Current flow in one layer generates different quantized Hall signals in the two layers. This result is interpreted by composite fermion (CF) theory with different intralayer and interlayer Chern-Simons gauge-field coupling. We observe FQH states corresponding to integer values of CF Landau level (LL) filling in both layers, as well as “semi-quantized” states, where a full CF LL couples to a continuously varying partially filled CF LL. Remarkably, we also recognize a quantized state between two coupled half-filled CF LLs, attributable to an interlayer CF exciton condensate.

12:03PM S01.00005: Microwave photo-excited transport in the GaAs/AlGaAs 2DES* ANNIKA KRIISA, Georgia State University, CHRISTIAN REICHL, WERNER WEGSCHEIDER, ETH-Zurich, RAMESH MANI (Presenter), Georgia State University — Collective bulk plasmon excitations of a two dimensional electronic system (2DES) evolve into magnetoplasmons in the presence of a perpendicular magnetic field, with a low frequency cutoff determined by the dispersion relation \( \omega_{MP} = (\omega_C^2 + \omega_P^2)^{1/2} \), where the plasmon frequency \( \omega_P = (ne^2 / 2\varepsilon_{eff}\varepsilon_{om^*})k \), with \( k \) the plasmon wave vector, and \( \omega_C \) the cyclotron resonance frequency. Studies of narrow Hall bar type GaAs/AlGaAs specimens of width, \( w \), have long ago suggested that localization of the plasmon within the boundaries of the sample can lead to the wave vector selection \( k = n\pi/w \) and the observation of the corresponding resonance in magnetotransport under photoexcitation. The observation of zero-resistance states and associated radiation induced magnetoresistance oscillations under microwave/mm-wave/terahertz photoexcitation has brought new interest in the role of the magnetoplasmon, if any, in the ultra high mobility GaAs/AlGaAs 2DES and its interaction with this photo-excited transport phenomena mentioned above. In this study, we re-examine through experiment the role of the magnetoplasmon in the GaAs/AlGaAs magnetotransport and report the results.


12:15PM S01.00006: Microwave-induced resistance oscillations in a tunable-density GaAs quantum well* XIAOJUN FU (Presenter), MICHAEL ZUDOV, University of Minnesota, QI QIAN, JOHN WATSON, MICHAEL MANFRA, Purdue University — We report on microwave-induced resistance oscillations (MIRO) in a tunable-density 30 nm-wide GaAs/AlGaAs quantum. When the second subband becomes populated, we observe that the MIRO amplitude significantly decreases compared to the single-subband regime, the effective mass increases, while the quantum lifetime shows little change. We also find that the MIRO prefactor, which depends on the disorder characteristics and the inelastic relaxation, first decreases and then grows with the carrier density, behaving much the same as the carrier mobility. These findings will be compared to theoretical expectations.

*The work at Minnesota (Purdue) was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. ER 46640-SC0002567 (DE-SC0006671).
Pairing and Pair Tunneling of Electrons at the Edge of a GaAs Quantum Dot Two-Dimensional Electronic System  

AHMET DEMIR, NEAL STALEY, Massachusetts Institute of Technology, K. W. BALDWIN, KENNETH WEST, LOREN PFEIFFER, Princeton University, RAYMOND ASHOORI (Presenter), Massachusetts Institute of Technology — We have large (diameter ~0.8 μm) ultra-clean quantum dots that act as mini-2D electron systems and studied their single electron addition spectra at ~45 mK using capacitive sensing. Single electrons tunnel from an n+ GaAs electrode across an AlGaAs tunnel barrier into an otherwise electrically floating quantum dot. We measured the magnetic field dependence of electron addition energies from a completely empty dot, up to dot occupancies of ~2000 electrons. Here, we report the observation in the addition spectra of individually localized states, incompressible Landau gaps, and isolated tunneling to edge states. We see electron additions to the edge states between filling factors ν = 1 and ν = 2 with single flux quantum (h/e) periodicity in magnetic field. Remarkably, between filling factors ν = 2 and ν = 5, we observe the pairing of electron additions to states at the edges of the quantum dots with a corresponding 2e charge tunneling and with (h/2e) periodicity in magnetic field. These results are consistent with interferometry work from the group of Heiblum[1] showing an unexpected h/2e periodicity around the same filling factors, and they suggest that the same correlated electron physics is creates a novel pair tunneling effect.


Study of spin splitting of Shubnikov de Hass oscillations under microwave photoexcitation in the GaAs/AlGaAs 2DES*  

THARANGA NANAYAKKARA (Presenter), RASANGA SAMARAWEERA, BINUKA GUNAWARDANA, C. RASADI MUNASINGHE, U. KUSHAN WIJEWARDENA, SAJITH WITHANAGE, ANNIKA KRIISA, RAMESH MANI, Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia 30303, USA, CHRISTIAN REICHL, WERNER WEGSCHEIDER, ETH Zürich, CH-8093 Zürich, Switzerland, Laboratorium für Festkörperphysik — We perform magneto transport measurements on GaAs/AlGaAs 2D electron system to understand the influence of the microwave photoexcitation on the spin splitting of the Shubnikov-de Haas oscillations at liquid helium temperatures. The aim of the study is to determine the magnitude of the electron heating under microwave photo-excitation by examining observable spin splitting- and variation thereof under photoexcitation- at high filling factors. Thus, we apply a Lifshitz-Kosevevich type formula to describe the magneto transport data and report here the relevant results.


*This work was supported by the NSF under Grant No. ECCS-1710302, and by the Army Research Office under Grants No. W911NF-14-2-0076 and No. W911NF-15-1-0433.

Collective excitations in the Moore-Read phase: view from superspace*  

ANDREY GROMOV (Presenter), UC Berkeley, SHINSEI RYU, EMIL J MARTINEC, University of Chicago — We present a microscopic theory of the neutral collective modes supported by the Moore-Read fractional quantum Hall state. The theory is formulated in terms of the trial states describing the Girvin-MacDonald-Platzman (GMP) mode and its fermionic counterpart, known as the “Neutral Fermion” mode. To access both modes simultaneously the Moore-Read state is first lifted to the superspace. These modes are created by the same operator which acts in the superspace. The Grassman variables are auxilliary and are integrated over in the end.

* -Kadano Center fellowship

-University of Chicago Materials Research Science and Engineering Center, which is funded by the National Science Foundation under award number DMR-1420709.

-Quantum Materials program at LBNL, funded by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

One-plaquette Chern number: Many-body Chern number without integration*  

KOJI KUDO (Presenter), University of Tsukuba, HARUKI WATANABE, University of Tokyo, TOSHIKAZE KARIYADO, National Institute for Materials Science, YASUHIRO HATSUGAI, University of Tsukuba — The Niu-Thouless-Wu formula defines the many-body version of the Chern number that characterizes the quantized Hall conductance in the presence of disorders or interactions. In this talk, we provide numerical evidence that the integration by twisted angles in the Niu-Thouless-Wu formula is unnecessary if the system size and the excitation gap are sufficiently large. The Berry curvature itself is effectively quantized and the error decays exponentially with the system size. The lack of integration reduces the computational cost, which is advantageous in the interacting many-body problems for a sufficiently large system size. We also discuss the accuracy of the effective quantization in the vicinity of quantum phase transitions.

* The work is supported by JSPS KAKENHI Grant Numbers JP17H06138 (KK, TK, YH), JP16K13845 (KK, YH), JP17K17678 (HW) and JP17K14358 (TK).
1:15PM S01.00011: Search for exact local Hamiltonians for general fractional quantum Hall states

SREEJITH GANESH JAYA (Presenter), Physics, Indian Institute of Science Education and Research Pune, MIKAEL FREMLING, Institute of theoretical physics, Utrecht University, GUN SANG JEON, EWAH Womans University, JAINENDRA JAIN, Physics, Penn State — We report on our systematic attempts at finding local interactions for which the lowest-Landau-level projected composite-fermion wave functions are the unique zero energy ground states. We study in detail the simplest non-trivial system beyond the Laughlin states, namely bosons at filling factor 2/3 and identify local constraints among clusters of particles in the ground state. By explicit calculation, we show that no Hamiltonian up to (and including) four particle interactions produces this state as the exact ground state, and speculate that this remains true even when interaction terms involving greater number of particles are included. Surprisingly, we can identify an interaction, which imposes an energetic penalty for a specific entangled configuration of four particles with relative angular momentum of 6, that produces a unique zero energy solution (as we have confirmed for up to 12 particles). This state is not identical to the projected CF state, but have high overlaps with the CF state and the same root partition, quasiparticle and neutral excitation spectrum as the CF state. On the quasihole side, the quantum numbers of the low energy states agree with the CF state but these states are not separated from the others by a clearly identifiable gap.

1:27PM S01.00012: Prediction of a new non-Abelian state at ν = 1/4 in Wide Quantum Wells

WILLIAM FAUGNO (Presenter), Pennsylvania State University, AJIT COIMBATORE BALRAM, Niels Bohr Institute, MAISSAM BARKESHLI, Physics, University of Maryland, JAINENDRA JAIN, Pennsylvania State University — For zero width systems, the ground state at filling factor 1/4 is described by the fully polarized composite fermion Fermi sea. However, fractional quantum Hall effect (FQHE) has been observed at 1/4 in wide quantum well samples [1]. We consider several single-component candidate states, and conclude that the non-Abelian “22111-parton” state is the most likely candidate. Our calculated phase diagram as a function of the quantum well width and the density is in very good agreement with experiments. We suggest further experiments that can confirm the nature of the 1/4 state and, in particular, distinguish it from other candidate states. We also consider a bilayer system at total filling 3/4 as a function of the interlayer separation and predict that it does not support any incompressible FQHE state.


**Supported by DOE under Grant no. DE-SC0005042

1:39PM S01.00013: Stripe Pairing Order in the 5/2-filling Fractional Quantum Hall State

LUIZ SANTOS (Presenter), Emory University, YUXUAN WANG, University of Florida, EDUARDO HECTOR FRADKIN, University of Illinois at Urbana-Champaign — The nu=5/2 fractional quantum Hall (FQH) state can be effectively described by a paired state of composite fermions with a chiral p-wave order parameter. Motivated by recent works showing an instability of this FQH state towards a phase with broken rotation symmetry, we study the properties of a p-wave pair density wave (PDW) state. We show that the domain walls (DWs) of the PDW order parameter support a pair of counter-propagating Majorana modes whose properties depend on the competition between the Fermi energy and the strength of the PDW order parameter. At weak coupling, the hybridization of DWs generically gives rise to a Majorana Fermi surface (MFS) that is protected by inversion and particle-hole symmetries. A uniform p-wave component gaps the MFS causing the system to enter a striped non-Abelian state with a chiral edge Majorana. At strong coupling, on the other hand, the system is described by a gapped phase without chiral Majorana edge states, which we identify with an striped Abelian paired state. The striped paired FQH state is therefore a fertile arena to study transitions between different topological orders tunneled by the strength of the PDW order parameter.

*Gordon and Betty Moore Foundation Grant No. GBMF4305; NSF grants No. DMR-1725401 and PHY-1607611.

1:51PM S01.00014: Composite fermions mass in an anisotropic two-dimensional electron system

KEVIN VILLEGAS ROSALES (Presenter), EDWIN CHUNG, HAO DENG, KENNETH WEST, K. W. BALDWIN, LOREN PFEIFFER, MANSOUR SHAYEGAN, Princeton University — Recent advances in molecular beam epitaxy capabilities have established a new record in the quality of AlAs two-dimensional electron systems (2DESs). This breakthrough allows us to study the temperature dependence of fractional quantum Hall states up to ν = 7/15 and 7/13 in the extreme quantum limit. We report on the energy gaps and Shubnikov-de Haas mass (mCF) of composite fermions in samples with density n = 1.04 x 10^11 cm^-2 and quantum well widths of 35 and 50 nm. The measured mCF are 0.68 and 1.2 (in units of free electron mass) for the 35 and 50 nm wide quantum well near ν = 1/2, respectively. We contrast our results with the previously reported energy gaps and mCF of 2DESs in GaAs and ZnO, and the 2D hole system in GaAs. Our experiments on AlAs 2DESs demonstrate the important role of electron layer thickness in determining the energy gaps and mCF.
Parton states as unique ground states of frustration free quantum Hall Hamiltonians with Fibonacci anyon excitations

MOSTAFA TANHAYI AHARI (Presenter), Indiana University Bloomington, SUMANTA BANDYOPADHYAY, ZOHAR NUSSINOV, ALEXANDER SEIDEL, Physics, Washington University in St.Louis, GERARDO ORTIZ, Indiana University Bloomington — We develop a general formalism to systematically derive frustration-free fractional quantum Hall (FQH) Hamiltonians in the presence of Landau level (LL) mixing. Their ground state correlations organize according to entangled Pauli principles, encoding the fluid’s DNA and, dictating the fractional nature of the statistics of their topological excitations. As we will show, the densest ground state - conjectured to be an incompressible quantum liquid - can be uniquely associated to a certain (closed-shell) parton state. Using S-duality, we show that for the case of 4 LLs, excitations of a filling fraction 2/3 liquid admit non-Abelian statistics and correspond to Fibonacci anyons.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S02 DMP GMAG: Topological Materials -- Magnetic Materials

11:15AM S02.00001: Theoretical study of topological materials for spintronics

WEI JIANG (Presenter), TONY LOW, Electrical and Computer Engineering, University of Minnesota — Enabling highly efficient current-induced magnetization switching is critical to future spintronic applications, and many proposals relies on topological effects for the conversion of charge current to spin current. Recently, the intrinsic spin-Hall effect (SHE) in the topological materials has been intensely studied and was proposed to play a more important role in the field, because of their extremely large spin Berry curvature. Here, we carried out theoretical studies of different topological materials ranging from topological insulator, Dirac/Weyl semimetal, to topological superconductor, and calculated their intrinsic spin-Hall conductivity (SHC). The figure of merit for charge-to-spin conversion is defined as the SHC over the density of state, based on which we propose a family of topological materials for the spintronics devices.

11:27AM S02.00002: Structural and Physical Properties of Magnetic EuMnSb2 Single Crystals

SILU HUANG (Presenter), XIN GUI, WEIWEI XIE, RONGYING JIN, Louisiana State University — Layered EuMnPn2 (Pn = Sb, Bi) has generated immense interest because of the interplay between complex magnetism (Eu and Mn forming two magnetic sublattices) and topological properties. We have successfully grown EuMnSb2 single crystals, which form the tetragonal structure (space group P4/nmm) containing Sb square net. Both in-plane (ρab) and c-axis (ρc) resistivities show semiconductor-like behavior with an anomaly at TN ~ 20 K. Magnetization measurements indicate that there is an antiferromagnetic (AFM) transition at TN. Upon the application of the magnetic field along the c axis, the in-plane magnetoresistance (MRab) changes sign from positive at T > TN to negative at T < TN, while MRc reveals the opposite trend. This indicates that magnetic interactions are different between the ab plane and c direction. Further discussion will be presented.

11:39AM S02.00003: Crossover of Quantum Anomalous Hall to Topological Hall Effects in Magnetic Topological Insulator Sandwich Heterostructures

JUE JIANG (Presenter), DI XIAO, FEI WANG, JAEOH SHIN, JIANXIAO ZHANG, Department of Physics, Pennsylvania State University, DOMENICO ANDREOLI, Department of Physics, University of New Hampshire, RUN XIAO, YIFAN ZHAO, MORTEZA KAYYALHA, LING ZHANG, Department of Physics, Pennsylvania State University, JIADONG ZANG, Department of Physics, University of New Hampshire, CHAO-XING LIU, NITIN SAMARTH, CUI-ZU CHANG, MOSES H. W. CHAN, Department of Physics, Pennsylvania State University — Electronic band structures with non-trivial topology in momentum space and magnetic spin textures in real space have attracted enormous attention in the past decade since they harbor elegant physics relevant to the Berry curvature. The quantum anomalous Hall (QAH) effect, which is induced by the Berry curvature in the momentum space, supports dissipation-free chiral edge states. The topological Hall (TH) effect is a transport signature of the chiral spin textures that are a consequence of Berry curvature but in real-space. Both QAH and TH effects have been separately reported in magnetically doped TI materials and thus it is natural to ask if both phenomena can coexist in a single sample. Here, by inserting a TI layer between two magnetic TI layers to form a sandwich heterostructure, we observed the crossover from the QAH to TH effects through tuning electrostatic gate voltage. Our theoretical modeling suggests that the inserted TI layer decouples the two magnetic TI layers. As a consequence, the strong Dzyaloshinskii-Moriya interaction in each magnetic TI layer can give rise to chiral spin textures and lead to the TH effect. Our study provides us a new understanding of the interplay between the momentum-space and real-space Berry curvatures in magneto-transport phenomena.

**This work is supported by NSF through Grant Number DMR-1504226**
11:51AM S02.00004: Quantum anomalous Hall effect at the interface between magnetic and topological crystalline insulators*  JINWOONG KIM (Presenter), DAVID VANDERBILT, Rutgers University, New Brunswick — By employing tight-binding and first-principles calculations, we investigate the possible appearance of the quantum anomalous Hall (QAH) effect at the interface between topological crystalline insulators (SnTe, SnSe) and magnetic insulators (EuO, EuS, EuSe). For a surface Dirac cone associated with a band inversion in the bulk, a mass gap acquisition via an effective Zeeman field is a subject of broad interest because of the potential for exotic thin-film states such as the QAH and axionic phases. A number of studies have demonstrated the appearance of such states by using diverse interfacial and magnetic-element-doped systems in agreement with predictions. Although achieving a large mass gap is critical for further investigations and room temperature devices, the microscopic mechanisms determining the size of the mass gap have not been clearly addressed. In this study, we enumerate several combinations of topological crystalline insulators and magnetic insulators in a search for an optimal electronic structure, where a large mass gap is isolated inside a bulk insulating gap. The underlying mechanisms and their dependence on factors such as magnetization orientation will be discussed.

*This work was supported by the National Science Foundation under Grant No. DMR-1408838.

12:03PM S02.00005: Local magnetism in a correlated Kagome magnet with massive Dirac Fermions*  YANGMU LI (Presenter), CMPMS, Brookhaven National Laboratory, QI WANG, Physics Department, Renmin University of China, RYAN DESAUTELS, Neutron Scattering Division, Oak Ridge National Laboratory, QIANHENG DU, CMPMS, Brookhaven National Laboratory, WEIJUN REN, ZHIDONG ZHANG, Institute of Metal Research, Chinese Academy of Sciences, CEDOMIR PETROVIC, CMPMS, Brookhaven National Laboratory, LISA DEBEER-SCHMITT, Neutron Scattering Division, Oak Ridge National Laboratory, IGOR ZALIZNYAK, WEIGUO YIN, CMPMS, Brookhaven National Laboratory, HECHANG LEI, Physics Department, Renmin University of China, JOHN TRANQUADA, CMPMS, Brookhaven National Laboratory — Recent photoemission and scanning tunneling experiments revealed that Fe₃Sn₂, a strongly-correlated Kagome magnet, features massive Dirac fermions and an intrinsic electronic nematicity [1, 2]. DFT calculations show that the Dirac mass depends significantly on the local magnetic moment. The electronic nematicity also relates to local magnetism through the spin-orbital coupling. Here, we present our small-angle neutron scattering and angle-resolved charge transport results in combination with DFT calculations to characterize the complex role of local magnetism in Fe₃Sn₂.


*Work at BNL was supported by Office of BES, U.S. DOE under Contract No. DE-SC0012704. Research conducted at ORNL's SNS was sponsored by the SUFD, Office of BES, U.S. DOE.

12:15PM S02.00006: Anomalous Hall Effect in Intrinsic Antiferromagnetic Topological Insulator MnBi₂Te₄*  SENG HUAT LEE (Presenter), 2D Crystal Consortium, Materials Research Institute, The Pennsylvania State University, YANGLIN ZHU, Department of Physics and Engineering Physics, Tulane University, YU WANG, ZHIQIANG MAO, Department of Physics, The Pennsylvania State University — MnBi₂Te₄ has recently been predicted to be an intrinsic antiferromagnetic topological insulator (AFMTI)¹. This material is also predicted to show ferromagnetism if its dimensionality is reduced to 2D and support other topological states, including type-II magnetic Weyl semimetal state under magnetic fields and Majorana fermions at the interface with a superconductor. Its surface states and magnetic phase transition have been experimentally observed in both bulk² and thin-film samples³. The material provides an excellent platform to study various exotic physics as well as the realization of the quantum anomalous Hall effect at higher temperatures. Here, we report the synthesis of high-quality bulk single crystals of MnBi₂Te₄ by melt-growth technique. Magnetic-transport measurements on bulk samples demonstrated the first observation of the anomalous Hall effect.


*The authors acknowledge funding by NSF through the Penn State 2D Crystal Consortium—Materials Innovation Platform (2DCC-MIP) under NSF cooperative agreement DMR-1539916. Y. Z. is supported by the US DOE under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents.
12:27PM S02.00007: Antiferromagnetic topological insulator MnBi$_2$Te$_4^*$  
MIKHAIL OTROKOV (Presenter), IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain, IGOR P RUSINOV, Saint Petersburg State University, 198504 Saint Petersburg, Russia, MARIA BLANCO-REY, Departamento de Fisica de Materiales, UPV/EHU, 20080 Donostia-San Sebastian, Basque Country, Spain, MARTIN HOFFMANN, Institut fur Theoretische Physik, Johannes Kepler Universitat, A 4040 Linz, Austria, ALEXANDRA YU VYAZOVSKAYA, Tomsk State University, 634050 Tomsk, Russia, SERGEY V EREMEEV, YURY M KOROTEEV, Institute of Strength Physics and Materials Science, Russian Academy of Sciences, 634021 Tomsk, Russia, ARTHUR ERNST, Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany, PEDRO M ECHENIQUE, Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastian, Basque Country, Spain, ANDRES ARNAU, Centro de Fisica de Materiales (CFM-MPC), Centro Mixto CSIC-UPV/EHU, 20018 Donostia-San Sebastian, Basque Country, Spain, EVGUENI CHULKOV, Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastian, Basque Country, Spain — Using ab initio and Monte Carlo calculations we predict the van der Waals layered compound MnBi$_2$Te$_4$ to be antiferromagnetic (AFM) topological insulator [1], which is further confirmed experimentally [1]. MnBi$_2$Te$_4$ appears to be invariant with respect to the combination of the time-reversal and primitive-lattice translation symmetries, giving rise to the Z$_2$ topological classification of AFM insulators, and Z$_2$=1 for MnBi$_2$Te$_4$. Its (0001) surface, breaking the combined symmetry, shows a giant gap in the topological surface state thus representing a promising platform for the quantized magnetoelectric effect observation. In the 2D limit, MnBi$_2$Te$_4$ shows a unique set of thickness-dependent magnetic and topological transitions, which drive it through FM and (un)compensated AFM phases, as well as quantum anomalous Hall (QAH) and intrinsic zero plateau QAH states [2].


*The supports by the Spanish Ministerio de Economia y Competitividad (FIS2016-75862-P), Academic D.I. Mendeleev Fund Program of Tomsk State University (8.1.01.2018), Saint Petersburg State University grant for scientific investigations (15.61.202.2015), and Fundamental Research Program of the State Academies of Sciences for 2013-2020 are acknowledged.

12:39PM S02.00008: Large anomalous Hall effect in topological insulators with a proximitized ferromagnetic insulator*  
MASATAKA MOGI (Presenter), Applied Physics, University of Tokyo, TARO NAKAJIMA, RIKEN CEMS, VICTOR UKLEEV, PSI, ATSUSHI TSUKAZAKI, IMR Tohoku University, RYUTARO YOSHIMI, MINORU KAWAMURA, KEI TAKAHASHI, RIKEN CEMS, TAKAYASU HANASHIMA, KAZUHISA KAKURAI, CROSS, TAKA-HISA ARIMA, GSFS, University of Tokyo, MASASHI KAWASAKI, University of Tokyo, YOSHINORI TOKURA, RIKEN CEMS — Ferromagnetism in topological insulators could lead to exotic quantum phenomena such as quantum anomalous Hall effect. A predominant requirement for such phenomena is the formation of an exchange gap at the Dirac surface states, being realized not only by magnetic doping but also by proximitizing ferromagnetic insulators. Here, we report on the effective gap formation driven by proximity coupling via detection of large anomalous Hall conductivity in heterostructures consisting of ferromagnetic insulator Cr$_2$Ge$_2$Te$_6$ and topological insulator (Bi,Sb)$_2$Te$_3$. While no discernible magnetization in the (Bi,Sb)$_2$Te$_3$ layer is probed by spin-polarized neutron reflectometry, the emergence of large anomalous Hall effect implies that the wavefunction of the Dirac surface state gains an exchange field by penetrating into the Cr$_2$Ge$_2$Te$_6$ by approximately 2-3 nm, finally activating a large Berry curvature. The presently verified mechanism of strong ferromagnetic proximity effect paves a way to enrich the proximity coupling phenomena in versatile topological quantum materials.

*This research was supported by JST CREST (no. JPMJCR16F1) and JSPS through a research fellowship for young scientists (no. 17J03179).
12:51PM S02.00009: Anisotropic magnetotransport and planar Hall effect in the quantum anomalous Hall regime

MICHELLE TOMCZYK (Presenter), DI XIAO, CUI-ZU CHANG, ANTHONY R. RICHARDELLA, CHAO-XING LIU, NITIN SAMARTH, Pennsylvania State University — Perturbations to the metallic surface states of topological insulators (TIs) through interactions with magnetism or superconductivity can result in novel phenomena. For example, magnetically-doped TIs realize the theoretically-predicted quantum anomalous Hall (QAH) insulator, in which the surface states are gapped while current is carried in quantized chiral edge states even in zero magnetic field. Understanding the transition between the QAH insulator and dissipative metallic conduction regimes is of fundamental importance. We study this transition by measuring electrical transport while rotating an external magnetic field in different planes relative to the surface. Using scaling plots of the Hall and longitudinal conductance, we find an equivalency in the phase transition created by either rotating the field in the perpendicular plane or by increasing the temperature. Additionally, the angle-dependent in-plane transverse magnetoresistance, the planar Hall effect, exhibits anomalous behavior when perturbed by a small out-of-plane magnetic field. We interpret these observations in terms of the interplay between magnetization, dissipation-free chiral edge states, and dissipative surface states.

*We acknowledge support from the Eberly Research Fellows Program, ONR, and NSF-MIP/2DCC.

1:03PM S02.00010: Berry Phase Engineering in Magnetic Topological Insulator Heterostructures

FEI WANG (Presenter), YIFAN ZHAO, DI XIAO, Department of Physics, The Pennsylvania State University, WENBO WANG, Department of Physics and Astronomy, Rutgers University, JUE JIANG, LING ZHANG, Department of Physics, The Pennsylvania State University, WEIWEI ZHAO, School of Materials Science and Engineering, Harbin Institute of Technology, CHAO-XING LIU, Department of Physics, The Pennsylvania State University, WEIDA WU, Department of Physics and Astronomy, Rutgers University, MOSES H. W. CHAN, NITIN SAMARTH, CUI-ZU CHANG, Department of Physics, The Pennsylvania State University — The Berry phase, both in momentum-space and real-space, plays a key role in nontrivial transport phenomena such as the anomalous Hall (AH) and topological Hall (TH) effects. The AH effect is induced by Berry curvature in momentum space. The TH effect is a transport hallmark of chiral magnetic textures that are a consequence of Berry curvature in real space. In order to engineer the Berry phase, we have fabricated magnetic TI films and heterostructures and systematically studied their magneto-transport properties. We found that the sign of the AH effect in a magnetic TI film can be reversed through proximity to an undoped TI layer. By fabricating magnetic/nonmagnetic/magnetic TI sandwich heterostructures, we realized a square-shaped “hump” feature in the Hall traces, which is usually known as the TH effect. Combining transport measurements with magnetic force microscopy, we demonstrated that the TH effect-like “hump” feature observed here is not due to chiral magnetic textures but from the superposition of two AH effects with opposite signs. Our study provides a new route to engineer the Berry curvatures in magnetic TI heterostructures and facilitate the understanding of the interplay between the AH and TH effects.

*This work is supported by the ARO, DOE, and NSF 2DCC-MIP.

1:15PM S02.00011: Magneto-transport and Magnetism in Antiferromagnetic GdSbTe

TSUNG-CHI WU (Presenter), AKHILESH SINGH, MING-CHIN CHEN, Institute of Physics, Academia Sinica, RAMAN SANKAR, FANGCHENG CHOU, Center for Condensed Matter Sciences, National Taiwan University, WEI-LI LEE, Institute of Physics, Academia Sinica — The crystal structure of GdSbTe belongs to the PbFCl-type family that is known for exhibiting a possible topological nodal-line phase. The spin-7/2 Gd$^{3+}$ ions form a square lattice in the ab plane with large moments. Recently, a Dirac-like state was observed in GdSbTe by ARPES measurement [1]. Magnetization and specific heat measurements also revealed an antiferromagnetic (AFM) transition with a Néel temperature of around 12 K [2], making it a suitable system to study the interplay between AFM and topological states. Here, we report the angular dependence of the magneto-transport properties in GdSbTe. Several features in magnetoresistance (MR) measurements were uncovered while sweeping an in-plane magnetic field, including abrupt increases of MR occurs at 2 T and 6 T and an unusual hysteretic giant magnetoresistance (GMR)-like behavior at higher magnetic fields. We remark that those features are absent when the magnetic field is applied perpendicular to the ab-plane direction. The magneto-transport and magnetization measurements up to a magnetic field of 14 T will be presented and compared to several metallic spin systems.

1:27PM S02.00012: Magneto-Transport Study of Magnetic/Nonmagnetic Topological Insulator Heterostructures*
DI XIAO (Presenter), FEI WANG, RUN XIAO, LING ZHANG, Physics, The Pennsylvania State University, HAIZHOU LU, Physics, Southern University of Science and Technology, CHAO-XING LIU, MOSES H. W. CHAN, CUI-ZU CHANG, NITIN SAMARTH, Physics, The Pennsylvania State University — Breaking time-reversal symmetry in a topological insulator (TI) by a magnetic perturbation can give rise to a variety of exotic quantum phenomena such as quantum anomalous Hall effect. Since the surface states of TIs have a spin helical massless Dirac structure, undoped TI films usually show weak antilocalization (WAL) quantum corrections to diffusive transport, characterized by a positive magnetoresistance (MR). Here, we fabricate magnetically doped TI films on pristine TI films with different thicknesses to form magnetic/nonmagnetic TI heterostructures and systematically study their magneto-transport properties. When the thickness of the TI layer is ≤ 2QL, the MR shows a typical butterfly shape due to domain wall scattering. However, when the thickness of the TI layer is ≥ 3QL, the MR is suppressed, similar to the WAL cusp, but near the magnetization reversal regime. We speculate that this “dip” in MR near the coercive field is a result of the coexistence of the gapless surface state of the TI layer and the ferromagnetic order in the magnetic TI layer. Our study provides new insights into magneto-transport phenomena in the presence of a superposition of gapped and gapless surface states.

*This work is supported by 2DCC-MIP, DOE, ONR, and the Alfred P. Sloan Research Fellowship.

1:39PM S02.00013: HoBi: The Effect of Magnetism on Extreme Magnetoresistance*
HUNG-YU YANG (Presenter), Department of Physics, Boston College, JONATHAN GAUDET, Department of Physics and Astronomy, McMaster University, ADAM ACZEL, Oak Ridge National Laboratory, DAVID E GRAF, National High Magnetic Field Lab, PETER BLAHA, Institute of Materials Chemistry, Vienna University of Technology, BRUCE GAULIN, Department of Physics and Astronomy, McMaster University, FAZEL FALLAH TAFTI, Department of Physics, Boston College — Since the discovery of extreme magnetoresistance (XMR) in the topological semimetal WTe2, this phenomenon, featuring extremely high and non-saturating MR, has been found in many topological materials. In some cases, it is shown that XMR does not necessarily connect to topology and can be explained by electron-hole compensation unambiguously [1]. Although we have better understood the role of topology in XMR, the effect of magnetism on XMR remains elusive. Previous studies showed the power-law field dependence of XMR holds in both non-magnetic and magnetic XMR materials and is robust against magnetism. In this work [2], we focus on HoBi in the rare-earth monopnictide material family, which has an antiferromagnetic ground state with huge moments. We find an exact correspondence between the phase diagrams mapped by magnetization and transport measurements. Interestingly, we also find the XMR of HoBi is significantly affected by its magnetic order with ordering vector (1/6,1/6,1/6), in strong contrast to its family members like CeSb. The interplay between magnetism and transport makes HoBi a great platform to understand XMR in magnetic semimetals with trivial or non-trivial topology.

References:

*NSF-1708929

1:51PM S02.00014: Neutron scattering study on a topological antiferromagnet
WEILIANG YAO (Presenter), Peking University, YANGMU LI, Brookhaven National Laboratory, KAZUKI IIDA, Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS), TAKASHI OHHARA, Japan Atomic Energy Research Agency, AKIKO NAKAO, Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS), BARRY L. WINN, Oak Ridge National Laboratory, JOHN TRANQUADA, IGOR ZALIZNYAK, Brookhaven National Laboratory, CHENYUAN LI, Peking University, CHEN FANG, Institute of Physics, Chinese Academy of Sciences, YUAN LI, Peking University — As analogue of Dirac fermions in topological semimetals, magnon Dirac points have recently been proposed [1] and observed [2,3] in a three-dimensional antiferromagnet, Cu3TeO6. Motivated by the expected presence of Dzyaloshinskii-Moriya interactions in this system [1], we have performed a detailed magnetic neutron diffraction measurement on a single crystal, aiming to detect possible non-collinear spin arrangements in the magnetically ordered state. The result in turn allows for an estimate of the sizes of the topological nodal lines that are represented by the Dirac points in the U(1)-symmetric approximation. Furthermore, we have attempted the first inelastic neutron scattering experiment in search of the putative topological magnon surface states [1,2].

2:03PM S02.00015: Sign Reversal of the Anomalous Hall Effect in Magnetically Doped Topological Insulator Thin Films* YIFAN ZHAO (Presenter), LING ZHANG, FEI WANG, JUE JIANG, MOSES H. W. CHAN, CUI-ZU CHANG, Department of Physics, Pennsylvania State University — Inducing magnetic orders in a topological insulator (TI) to break its time reversal symmetry has revealed many exotic topological quantum phenomena such as quantum anomalous Hall (QAH) effect. The QAH effect has been experimentally realized in the thin films of Cr- and/or V-doped (Bi,Sb)2Te3. The V-doped Sb2Te3 is one of two parent systems for the QAH state. Recently, we fabricated the V-doped Sb2Te3 films with varying V doping concentration and systematically studied their magneto-transport properties. We observed the sign reversal of the anomalous Hall (AH) effect in the V-doped Sb2Te3 films with increasing the V doping concentration. For low doping level, the sign of the AH effect is negative; When the V doping level reaches ~ 3% of Sb, the AH effect starts to show positive sign, consistent with that of the V-doped QAH samples. The observation of the sign reversal of the AH effect in the V-doped Sb2Te3 films opens a new route to understand the interplay between the topological states and magnetism in magnetic doped TI films and facilitates the exploration of the underlying mechanism of the V-doped QAH system.

*This work is supported by the ARO Young Investigator Program Award (W911NF1810198), the U.S. DOE Award # DE-SC0019064 and the Alfred P. Sloan Research Fellowship.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S03 DCMP: Topological Phases and Their Excitations BCEC 107B - Kunal Tiwari, Univ of Texas, Arlington

11:15AM S03.00001: Growth of a predicted two-dimensional topological insulator based on InBi-Si(111)-√7×√7 CHIA-HSIU HSU, ZHI-QUAN HUANG, Physics, National Sun Yat-sen University, CHO-YING LIN, Physics, National Tsing Hua University, GENNEVIEVE M. MACAM, Physics, National Sun Yat-sen University, YU-ZHANG HUANG, DENG-SUNG LIN, Physics, National Tsing Hua University, TAI-CHANG CHIANG, Physics, University of Illinois, HSIN LIN, Physics, Academia Sinica, FENG-CHUAN CHUANG (Presenter), Physics, National Sun Yat-sen University, LI HUANG, Physics, Southern University of Science and Technology — Using combined scanning tunneling microscopy (STM) measurements and first-principles electronic structure calculations, we extensively studied the atomic and electronic properties of a √7-InBi overlayer on Si(111). We propose and demonstrate an effective experimental process to successfully form a large well-ordered √7 surface by depositing Bi atoms on the In-Si(111)-4×1 substrate. The STM images exhibit a honeycomb pattern. After performing an exhaustive computational search, we identified the atomic structures of the surface at In and Bi coverages of 6/7 and 3/7 monolayers, respectively. We discovered a trimer model with a lower energy than the previously proposed model. The simulated STM images of trimer models confirm the presence of the honeycomb pattern in accord with our experimental STM images. Most importantly, we found that the surface is robust, preserving the topologically nontrivial phase. Our edge state calculations verify that the InBi overlayer on Si(111) is indeed a two-dimensional topological insulator (TI). Moreover, hybrid functional calculations result in band gaps up to 70 meV, which is high enough for room-temperature experiments. Our findings lay the foundation for the materials realization of 2D TIs by growing an InBi overlayer on a Si(111) substrate.

11:27AM S03.00002: Topological Phase Transition from a Quantum Spin Hall Insulator to a Chern Insulator* ZHONGDONG HAN (Presenter), Peking University, TINGXIN LI, Cornell University, GERARD SULLIVAN, Teledyne Scientific and Imaging, RUI-RUI DU, Rice University — The effect of magnetic field on electronic transport in InAs/GaSb quantum spin Hall systems is investigated. As theoretical works [1-3] indicate, the system will undergo an insulator-metal-insulator phase transition at a critical magnetic field where the lowest Landau Levels (LLs) of electron and hole cross. Here we observe a distinct bulk conductance peak emerging around 12T in InAs/GaSb double layer systems. Both its temperature dependence and abruptly increasing signal fluctuation is consistent with a metallic phase arising from the topological phase transition between a QSHI phase and a Chern insulator phase. In the meanwhile the response of helical edge state is also systematically studied and the results will be presented.


*Work at PKU was supported by NBRPC-2014CB92090; work at Rice was supported by NSF DMR-1508644.
11:39AM S03.00003: Shift insulators: rotation-protected two-dimensional topological crystalline insulators*
SHANG LIU (Presenter), ASHVIN VISHWANATH, ESLAM KHALAF, Harvard University — We study a two-dimensional tight-binding model of a topological crystalline insulator protected by rotation symmetry. The model is built by stacking two Chern insulators with opposite Chern numbers which transform under conjugate representations of the rotation group, e.g. $p_x$ orbitals. Despite its apparent similarity to the Kane-Mele model, it does not host stable gapless surface states. Nevertheless the model exhibits topological responses including the appearance of quantized fractional charge bound to rotational defects (disclinations) and the pumping of angular momentum in response to threading an elementary magnetic flux, which are described by a mutual Chern-Simons coupling between the electromagnetic gauge field and an effective gauge field corresponding to the rotation symmetry. We show that although the filled bands of the model do not admit a symmetric Wannier representation, this obstruction is removed on addition of appropriate atomic orbitals, which implies ‘fragile’ topology. As a result, the response of the model can be derived by representing it as a superposition of atomic orbitals with positive and negative integer coefficients.


*AV was supported by a Simons Investigator award and by NSF-DMR 1411343.

11:51AM S03.00004: Scanning tunneling microscopy and spectroscopy on strong spin-orbit coupling chalcogenides*
SHEKHAR DAS (Presenter), ANSHU SIROHI, Department of Physical Sciences, Indian Institute of Science Education and Research Mohali, GAURAV KUMAR GUPTA, Department of Physics, IISc Bangalore, SUMAN KAMBOJ, AASTHA VASDEV, SIRSHENDU GAYEN, Department of Physical Sciences, Indian Institute of Science Education and Research Mohali, PRASENJIT GUPTASARMA, Department of Physics, University of Wisconsin, Milwaukee, TAMMOY DAS, Department of Physics, IISc Bangalore, GOUTAM SHEET, Department of Physical Sciences, Indian Institute of Science Education and Research Mohali — A large number of A$_2$B$_3$ type chalcogenides with strong spin-orbit coupling like Bi$_2$Se$_3$, Bi$_2$Te$_3$, and Sb$_2$Te$_3$ etc. are topological insulators (TI) whereas Sb$_2$Se$_3$ is an exception in this group. In this talk, I will show, as the TI Bi$_2$Se$_3$, Sb$_2$Se$_3$ displays generation of highly spin-polarized current by point contact Andreev reflection spectroscopy. However, unlike in Bi$_2$Se$_3$, in case of Sb$_2$Se$_3$, a prominent quasiparticle interference (QPI) pattern could be observed in STM conductance mapping which contradicts the above experiment. According to the band structure calculation, there are two trivial surface states available and among them, one shows large splitting due to Rashba type spin-orbit coupling. In addition, we observe a large negative and anisotropic magnetoresistance in Sb$_2$Se$_3$. Experimental data reveal Sb$_2$Se$_3$ to be a trivial band insulator under ambient conditions with high spin-polarization due to Rashba type spin-orbit coupling.

*Indian Institute of Science Education and Research Mohali

12:03PM S03.00005: A new topological crystalline insulator state in the TaAs$_2$materials class
BAOKAI WANG (Presenter), Physics, Northeastern University, Boston, Massachusetts 02115, USA, BARUN GHOSH, Physics, Indian Institute of Technology Kanpur,Kanpur 208016, India, WEI-CHI CHIU, Physics, Northeastern University, Boston, Massachusetts 02115, USA, BAHADUR SINGH, Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA /SUZU-NUS Collaborative Center and International Collaborative Laboratory of 2D Materials for Optoelectronic Science & Technology, Engineering Technology Research Center for 2D, AMIT AGARWAL, Physics, Indian Institute of Technology Kanpur,Kanpur 208016, India, HSIN LIN, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan, ARUN BANSIL, Physics, Northeastern University, Boston, Massachusetts 02115, USA — Crystalline symmetries drive a variety of topological crystalline insulator (TCI) phases in materials. Here, based on first-principles calculations combined with associated symmetry analysis, we identify a new rotational-symmetry protected TCI state in the TaAs$_2$ family of compounds. The low-energy band structure consists of two bulk nodal lines in the absence of spin-orbit coupling (SOC) effects. Turning on the SOC opens a continuous band gap in the spectrum and drives the system into a $C_3$ symmetry protected TCI state. On the (010) surface, we show the presence of rotational-symmetry-protected nontrivial Dirac cone states within a local bulk energy gap of 300 meV. Our results indicate that the TaAs$_2$ materials family provides an ideal setting for exploring unique physics associated with the rotational-symmetry protected TCIs.
12:15PM S03.00006: Conductance Oscillations in Gated Topological Insulator Heterostructures*  EKLAVYA THAREJA (Presenter), ILYA VEKHTER, MAHMOUD ASMAR, Louisiana State University — Recent theoretical studies have shown that the properties of the surface state of 3D Topological Insulators (TIs) may be different from the topological interface states in a heterostructure containing TIs [1]. Directly accessing these interface states is, however, challenging. We propose that a transport measurement on a gated double junction sandwich device yields critical information about the topological interface states. We show that the conductance oscillations as a function of the gating potential can be used to extract the Fermi velocity and other parameters characterizing their dispersion. Crucially, these results are only weakly dependent on the boundary conditions at the lateral sandwich junctions. We discuss relevance of our results to proposed applications of TIs in functional devices.


*Supported in part by NSF via DMR Grant 1410741

12:27PM S03.00007: Tunable skyrmion-skyrmion interactions on the surface of a three dimensional topological insulator*  KUNAL TIWARI (Presenter), JULIETTE LAVOIE, WILLIAM COISH, TAMI PEREG-BARNEA, Department of Physics, McGill University — The surface of a three-dimensional topological insulator is characterized by a gapless two-dimensional Dirac cone dispersion. In a magnetic topological insulator, this surface dispersion is gapped by a Zeeman term proportional to the local magnetization. Magnetic skyrmions—stable, low energy excitations in chiral planar magnetic systems—lead to sign changes in this Zeeman term and, consequently, topologically protected bound states. It has been shown previously [1] that magnetic skyrmions on the surface of a topological insulator may result in a discrete set of localized orbitals—skyrmion bound states. We study the skyrmion-skyrmion interaction mediated by the hybridization of these orbitals. In particular, we consider the effective interaction between a pair of skyrmions in the presence of their hybridized orbitals. We show that the skyrmions form a bound state for high chemical potential. For low chemical potential their interaction is strictly repulsive. For intermediate chemical potential, both the bound and the unbound configurations locally minimize the free energy. We support our phenomenological theory with numerical calculations.


*CIFAR, INTRIQ, FRQNT, NSERC

12:39PM S03.00008: Strain-driven topological phase transitions and tunable topological states in the Bi2Se3 family.*  HUGO ARAMBERRI (Presenter), M. CARMEN MUÑOZ, Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC — Strain allows for a controlled manipulation of the topological order and Dirac states in three-dimensional Bi-chalcogenide topological insulators. Based on ab-initio density functional methods, we predict a universal phase diagram for the Bi2Se3 family. Under elastic strain these compounds present metallic, topological and trivial insulating phases. Furthermore, by strain engineering we built realistic topological homojunctions (THs) in Bi2Se3. We show how the topological interface states arising in such THs can be reversibly tuned along with their electron doping, spatial localization and mutual interaction. A TH contains the simplest topological interface, and hence constitutes the ‘Hydrogen atom’ of topological states of matter. Our findings show a route to tune the topological states within the field of straintronics.


*We acknowledge support by the Spanish Ministerio de Ciencia, Innovación y Universidades through Grant MINECO/FEDER No. MAT2015-66888-C3-1R.
**12:51PM S03.00009: Closing the surface bandgap in thin Bi$_2$Se$_3$/graphene heterostructures**  

JIMIN CHAE (Presenter), Department of Physics, Yonsei University, SEOUNG-HUN KANG, Korea Institute for Advanced Study, SANG HAN PARK, Pohang Accelerator Laboratory, HANBUM PARK, KWANGSIK JEONG, TAE-HYEON KIM, SEOK-BO HONG, KEUN SU KIM, Department of Physics, Yonsei University, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung-Hee University, JWONG WON KIM, Division of Industrial Metrology, Korea Research Institute of Standards and Science, MANN-HO CHO, Department of Physics, Yonsei University — Topological insulator (TI), a band insulator with topologically protected edge states, is one of the most interesting materials in the field of condensed matter. For application, suppression of the bulk effect is crucial, but in ultrathin TI materials, with thicknesses less than 3 QL, the surface band has a finite bandgap because of the hybridization between the top and bottom surface states. Here, we studied the gapless top surface Dirac state of strained 3 QL Bi$_2$Se$_3$/graphene heterostructures. A strain caused by the graphene layer reduces the bandgap of surface states, and the band bending resulting from the charge transfer at the Bi$_2$Se$_3$/graphene interface induces localization of surface states to each top and bottom layer to suppress the overlap of the two surface states. In addition, we verified the independent transport channel of the top surface Dirac state in Bi$_2$Se$_3$/graphene heterostructures by measuring the magneto-conductance. Our findings suggest that the strain and the proximity effect in TI/non-TI heterostructures may be feasible ways to engineer the topological surface states beyond the physical and topological thickness limit.

*This work was supported by the National Research Foundation of Korea grant (Grant No. 2018R1A2A1A05023214)

**1:03PM S03.00010: Surface states of topological crystalline insulators**  

ESLAM KHALAF (Presenter), SHANG LIU, Department of Physics, Harvard University, HOI CHUN PO, Department of Physics, Massachusetts institute of Technology, HARUKI WATANABE, Department of Applied Physics, University of Tokyo, ASHVIN VISHWANATH, Department of Physics, Harvard University — We study topological crystalline insulator (TCI) phases hosting anomalous surface states. These include traditional surface states with two-dimensional Dirac dispersion as well as one-dimensional hinge modes characteristic of higher-order phases. Both of these can be captured by analyzing a general surface theory with multiple flavors of Dirac fermions and identifying global symmetry obstructions to achieving a fully gapped surface. This method is used to obtain a full classification of TCIs protected by time-reversal symmetry in the presence of strong spin-orbit coupling in the 230 space groups as well as TCIs protected by inversion in the ten different Altland-Zirnbauer symmetry classes. Furthermore, we establish a correspondence between the existence of surface states in a TCI and the existence of a stable (rather than fragile) obstruction to finding a basis of symmetric localized Wannier functions. Finally, we discuss possible extension of the results to magnetic space groups.

**1:15PM S03.00011: THz spectroscopy of ultralow carrier density topological insulator thin films**  

DIPANJAN CHAUDHURI (Presenter), Johns Hopkins University, MARYAM SALEHI, Rutgers, the State University of New Jersey, MINTU MONDAL, Johns Hopkins University, JISOO MOON, DEEPTI JAIN, SEONGSHIK OH, Rutgers, the State University of New Jersey, PETER ARMITAGE, Johns Hopkins University — Sb$_2$Te$_3$ is one of the earliest known examples of a 3D topological insulator with a single Dirac cone on the surface. Pure Sb$_2$Te$_3$ is generally p-doped with the Fermi level embedded in the bulk valence band which makes it challenging to study surface state dynamics through transport and optical measurements. Only recently, bulk insulating Sb$_2$Te$_3$ thin films have been grown using molecular beam epitaxy via chemical doping and buffer layer engineering. In addition, the carrier densities in these films are exceptionally low, nearly an order of magnitude lower than the best results obtained in Bi$_2$Se$_3$. Here we report the magneto-optical response of regular and bulk insulating (p-type and n-type) Sb$_2$Te$_3$ films at THz frequencies using time-domain polarimetry. While undoped, bulk conducting samples exhibit usual semiclassical behaviour, the bulk insulating samples show unusual optical properties and quantized response in presence of magnetic fields.
and temperature ($T$) using high-quality Bi$_{2-x}$Sb$_x$Te$_{3-y}$Sey single crystal thin films. Integrals of the Berry curvature. In this presentation, we consider what happens to the glide-Z$_2$ invariant, when the combination of the glide-Z$_2$ invariant and the Chern number. From the irreducible representations at high-symmetric points in this case, we can only know possible combinations of the glide-Z$_2$ invariant and the Chern number. Moreover, we show that in both cases the Z$_4$ strong topological invariant for inversion symmetric systems is directly related to the glide-Z$_2$ invariant and the Chern number. Finally, we also investigate topological invariants for glide-symmetric systems with nonprimitive lattice with and without inversion symmetry.

Thursday, March 7, 2019 11:15 AM - 2:15 PM
11:15AM S04.00001: Entropy changes and caloric effects driven by charge transfer: Application to YbInCu₄*
NILSON DE OLIVEIRA (Presenter), Instituto de Física, Universidade do Estado do Rio de Janeiro, AMÓS TROPER, Centro Brasileiro de Pesquisas Físicas — In this work, we propose a new physical mechanism based on charge transfer to produce large entropy and caloric effects even in non magnetic solid materials. In order to carry out the calculations, we use a two subband model in which a strongly correlated narrow band is coupled with a wide conduction electrons band. In the model, the charge transfer is controlled by the energy bandwidth and the hybridization parameter. The entropy and the caloric functions are calculated using the standard relations [1].
We apply the model to YbInCu₄ which exhibits an itinerant behavior at low temperature and a local magnetic moment profile at temperatures larger than the valence temperature $T_V$ around 42 K [2]. Our theoretical results, show that YbInCu₄ presents a large entropy change around 42 K due to the charge transfer from the 4f band to the electron sea. Besides, the isothermal entropy change upon pressure variation exhibits sizeable values in a wide temperature range. This outstanding result, which needs experimental data to be confirmed, can be very important for solid state refrigerators tecnology.


*We acknowledge financial support from CNPq and FAPERJ

11:27AM S04.00002: High field magnetostriction and magnetization of uranium monoantimonide single crystals*
XIAOXIN DING (Presenter), KESHAV SHRESTHA, DANIEL ANTONIO, Idaho National Laboratory, FRANZISKA WEICKERT, NHMFL, FSU, MARCELO JAIME, NEIL HARRISON, MYRON B SALAMON, Los Alamos National Laboratory, TOMASZ DURAKIEWICZ, National Science Foundation, JAMES L SMITH, Los Alamos National Laboratory, KRZYSZTOF GOFRYK, Idaho National Laboratory — Uranium monoantimonide (USb) crystallizes in the cubic NaCl-type crystal structure and is known to order antiferromagnetically with a triple-k magnetic structure, with a wave vector $(1,0,0)$, below $T_N$ = 213 K. In addition, the extent of hybridization that occurs between the uranium's 5f electrons with conduction electrons and its role for magnetism is not fully understood. During the talk we will present results of our recent magnetization and magnetostriction measurements of high-quality single crystals of USb at pulsed magnetic fields up to 65 T. The magnetization measurements help us to reveal the energy scales that are important in USb. In addition, the magnetostriction measurements performed in wide temperature range provides better microscopic understanding of the spin-lattice coupling and its strength in this material. We will discuss implications of these results.

*Work supported by DOE's Early Career Research Program (K.G., K.S. and D.A.). High field measurements have been performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation Cooperative Agreement No. DMR-1157490 and DMR-1644779 and the State of Florida.

11:39AM S04.00003: Pressure-Driven 5f Localized-Itinerant Transition and Valence Fluctuation in Californium
LI HUANG (Presenter), HAIYAN LU, Institute of Materials, China Academy of Engineering Physics — A combination of the density functional theory and the single-site dynamical mean-field theory is employed to study the pressure dependence of electronic structure for cubic phase californium. We predict that its 5f electrons could undergo an orbital-selective localized-itinerant transition under moderate pressure. The volume contraction causes remarkable charge redistribution and valence fluctuation behaviors, which are the driving forces of the divalent-trivalent transition. Additionally, we find that the angular momentum coupling mechanism is hardly affected by pressure. The 5f orbital occupancy is well described by the intermediate coupling scheme.
11:51AM S04.00004: Effective Coulomb interaction in actinides from linear response approach* RUIZHI QIU (Presenter), BINGYUN AO, LI HUANG, Institute of Materials, China Academy of Engineering Physics — The effective on-site Coulomb interaction (Hubbard $U$) between $5f$ electrons in actinide metals (Th-Cf) is calculated with the framework of density-functional theory (DFT) using linear response approach. The $U$ values seldom rely on the exchange-correlation functional, spin-orbital coupling, and magnetic states, but depend on the lattice volume and actinide element. Along the actinide series, the Coulomb parameter $U$ of α-phase first decreases slowly, followed by a jump in the vicinity of Pu and then a monotonous increase. For light actinides, the lattice volume has a sizeable influence on $U$ while the localization of $5f$ electrons is almost constant. But for transplutonium metals, $U$ is almost independent of the lattice volume but the electronic localization increases rapidly. The calculated lattice parameters from DFT+$U$ with the Coulomb parameters as input are in better agreement with the experimental values than those from DFT within local density approximation or Perdew-Burke-Ernzerhof approximation for solids (PBEsol). In particular, the agreement between PBEsol+$U$ and experiment is remarkable.

*We would like to acknowledge the financial support from the Science Challenge Project of China (Grant No. TZ2016004), NSFC (Grant No. 21771167), and the CAEP project (Grant No. TCGH0708).

12:03PM S04.00005: Unifying DFT+$U$ approach for plutonium modeling BORIS DORADO, BERNARD AMADON, MARC TORRENT (Presenter), FRANCOIS BOTTIN, JOHANN BOUCHET, CEA, DAM, DIF — The theoretical description of the plutonium phase diagram still represents a major challenge to modern electronic structure methods. For the δ phase, a comprehensive knowledge has gradually been building up and the correct description of spectroscopic, magnetic, structural properties could be obtained using the DMFT approach. Effective Coulomb interactions in Pu were calculated very recently with DMFT and were found to be around 1 eV, which is much smaller than the "commonly accepted value" of 4 eV. It was also shown that the Hunds exchange, together with the spin-orbit coupling, yields an improved description of all phases, thus opening the way to a unifying theory of Pu.

In the present study, we investigate the influence of these weaker electron correlations on the ground state properties of the α, δ and ε phases of Pu, calculated with DFT+$U$ (GGA), which is a static approximation of the DMFT. We first show that the GGA+$U$+SOC and DMFT approaches yield similar structural properties. This allows us to use the "more simple" DFT+$U$ approximation instead of the "expensive" DMFT to perform ab initio molecular dynamics calculations and extract temperature-dependent phonon spectra. GGA+$U$+SOC approximation allows for an improved description of all phases of Pu at high temperature.

12:15PM S04.00006: Crystal structure and thermal stability of uranium nitride* XIAOFANG WANG (Presenter), RUILONG YANG, QIFA PAN, YIN HU, KEZHAO LIU, Institute of Materials, China Academy of Engineering Physics — Uranium nitrides are among the most promising fuels for Generation IV nuclear reactors, but until now, very little has been known about their thermal stability properties under nonequilibrium conditions. In this work, thermal decomposition of nitrogen-rich uranium nitride (denoted as UN$_{2-x}$) under ultrahigh-vacuum (UHV) conditions was investigated by thermal desorption spectroscopy (TDS). It has been shown that the nitrogen TDS spectrum consists of two peaks at about 723 and 1038 K. The X-ray diffraction, scanning electron microscopy, and X-ray photoelectron microscopy results indicate that UN$_{2-x}$ (UN$_2$ phase) decomposed into the α-U$_2$N$_3$ phase in the first step and the α-U$_2$N$_3$ phase decomposed into the UN phase in the second step. Further studies are needed to fully understand the thermal decomposition kinetics of the UN$_{2-x}$ film, and work is in progress.

*The work was supported by NSAF (Grant U1630250)

12:27PM S04.00007: Plutonium in high magnetic fields.* MARK WARTENBE (Presenter), PAUL H TOBASH, MST-16, Los Alamos National Laboratory, NEIL HARRISON, JOHN SINGLETON, MPA-MAG, Los Alamos National Laboratory, LAUREL WINTER, JESSICA HEBERT, MST-16, Los Alamos National Laboratory — High magnetic field studies of plutonium have been limited up until now. The complex behavior of plutonium's 5f electrons are thought to be responsible for the elements unusual behavior, making it possibly the strangest element in the periodic table. Here we review data from a new set of various experiments involving high magnetic field and extremes of temperature. High magnetic fields are especially effective in probing electronic states and is the highlighted method of this study. We present the data in the context of gaining in site into the 5f electrons physics of the material.

*LANL LDRD Program
Nuclear graphite, is a synthetic graphite typically manufactured by isostatic pressure moulding. It is used in the core structural components of the UK’s nuclear reactors. This material contains many interesting atomic and mesoscale features. Recent TEM imaging shows that in-plane boundaries between misaligned basal planes within the graphite crystallites occur. Our previous work describes this “crazy paving” structure, which consists of nearly perfect slabs of graphite laminae, with nearly parallel c-axis. These slabs range in size from 100-1000 nm, with a thickness of ~30 nm.

Dynamical MD simulations are performed using a recent ReaxFF potential fitting, as well as, the AIREBO potential model. A geometric relaxation method is used to construct these graphite “crazy paving” structures. The optimised structures show that the lowest energy interfaces comprise of 5, 6 and 7 carbon atom rings, with formation energies in the region of 0.5-1.0 eV.

The mechanical properties of these structures are investigated by performing MD simulations of nano-indentation and scratching. The simulated indenter tips are controlled by spring constraints, instead of a rigid moving surface, in order to more closely model the experimental procedure.

*EDF energy funded lectureship.

Graphite has been used for neutron moderation from the beginning of the nuclear reactor era. While research activities have abated over the years, there is renewed interest in graphite motivated by its use in Very High Temperature Reactors (VHTRs) and Molten Salt Reactors (MSRs). Retention of the activated fission products is paramount during normal operating and accident conditions, and a mechanistic understanding of the bonding and diffusion properties of fission products is imperative for predicting the release rates and designing appropriate barriers.

While the simulation, via Density Functional Theory, of the diffusion and adsorption of a number of elements on graphene has received some attention, to the best of our knowledge little work has been conducted on the bonding and diffusion properties of many elements in bulk graphite. We have performed high-accuracy DFT simulations of nuclear fission products on graphene and in bulk graphite using LDA, GGA and van der Waals exchange-correlation functionals. The bonding, structural and diffusive properties have been extracted. These simulations form a basis for the understanding of the diffusion and retention of such products in nuclear graphite.

*We would like to acknowledge the support of EPSRC grant number EP/R005745/1.

The family of actinide compounds \( AX \), where \( A = \text{actinides} \) and \( X = \text{N, P, As, Sb, S, Se, and Te} \) have drawn great interest in research of actinide compounds because of their simple structure and rich magnetic properties. Recent study of \( \text{UO}_2 \) and \( \text{UN} \) revealed the effectiveness in probing the magneto-structural coupling in actinides by high magnetic field magnetostriction. Uranium monosulfide (US) crystalizes in simple cubic rock salt structure and exhibits the highest ferromagnetic transition temperature in uranium monochalcogenides (\( T_C = 177 \text{ K} \)) with easy axis along [111] direction. At the magnetic phase transition the crystal structure undergoes a rhombohedral distortion along one of the [111] directions with a large magnetic anisotropy. This might imply that strong magneto-elastic interactions play important role in this material. In this talk, our recent measurements of the magnetostriction and magnetic torque of uranium monosulfide single crystals will be presented.

*This work is supported by DOE’s Early Career Research Program. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation Cooperative Agreement No. DMR-1157490 and DMR-1644779 and the State of Florida.
1:15PM S04.00011: Extreme Fermi surface smearing in a maximally disordered concentrated solid solution*  
STEPHEN DUGDALE (Presenter), HANNAH ROBARTS, THOMAS E MILLICHAMP, DANIEL A LAGOS, JUDE LAVEROCK, HH Wills Physics Laboratory, University of Bristol, United Kingdom, DAVID BILLINGTON, SPring-8, Japan Synchrotron Radiation Institute, Japan, JONATHAN DUFFY, DANIEL O’NEILL, Department of Physics, University of Warwick, United Kingdom, SEAN GIBLIN, School of Physics and Astronomy, Cardiff University, United Kingdom, JONATHAN TAYLOR, DMSC, European Spallation Source, Denmark, GRAZYNA KONTRYM-SZNAJD, MALGORZATA SAMSEL-CZEKALA, Institute of Low Temperature and Structure Research, Polish Academy of Science, Poland, HONGBIN BEI, SAI MU, GERMAN SAMOLOYUK, GEORGE MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — The impact of extreme chemical disorder on the Fermi surface of the equiatomic alloy Ni0.25Fe0.25Co0.25Cr0.25 was probed by high-resolution X-ray Compton scattering. Such experiments probe the Fermi surface via the occupied momentum states, meaning that such measurements are ideally suited to revealing the electronic structure of such disordered alloys. The smearing of the Fermi surface is rather strong, reaching up to 40% of 2π/a, but nevertheless a Fermi surface can be clearly identified in the experimental data and the extent of the smearing and its variation on and across different sheets has been investigated. By connecting this smearing with the coherence length of the quasiparticle states, estimates of the electronic mean-free-path and residual resistivity have been made. It is found that the mean-free-paths are in the range 0.7 - 0.9 nm.

*The Compton scattering experiment was performed with the approval of the Japan Synchrotron Radiation Research Institute (JASRI, proposal no. 2016A1323). H.R. and D.A.L. gratefully acknowledge the financial support of the UK EPSRC (EP/L015544/1), and the National Secretariat of Higher Education, Science, Technology and Innovation of Ecuador (SENESCYT), respectively.

1:27PM S04.00012: Ballistic effects in squares and crosses of the ultra-pure delafossite PtCoO2*  
PHILIPPA MCGUINNESS (Presenter), ELINA ZHAKINA, VERONIKA SUNKO, MARKUS KOENIG, SEUNGHYUN KHIM, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids — The delafossite PtCoO2 is a layered oxide material with a single-band, hexagonal Fermi surface. This metal is extremely conductive, with a room temperature resistivity of 1.8 μOhmcm and a low-temperature mean free path of 5 μm [1]. Using focused ion beam microstructuring, we have created PtCoO2 square and cross devices which demonstrate strong ballistic behavior when their dimensions are similar to this mesoscopic length scale. These ballistic signals, in a weaker form, persist to structure sizes of at least 50 μm. Novel magnetoresistance effects, not observed in materials with circular Fermi surfaces, are also present within these devices, suggesting an influence of the hexagonal Fermi surface on ballistic transport.


*Max Planck Society, EPSRC studentships (grant number EP/L015110/1)

1:39PM S04.00013: Optical properties of the delafossite PdCoO2*  
CHRISTOPHER HOMES (Presenter), CMPMS, Brookhaven National Laboratory, Upton, New York, USA, SEUNGHYUN KHIM, ANDREW P. MACKENZIE, Chemical Physics of Solids, Max Planck Institute, Dresden, Germany — The delafossite PdCoO2 is remarkable for its extremely low in-plane residual resistivity at low temperature [1]. The in-plane optical properties have been determined over a wide frequency range at a variety of temperatures. At 295 K the reflectance of this material is extremely high (>99%) before encountering a sharp plasma edge at ~ 6000 cm⁻¹, above which it decreases rapidly. The real part of the optical conductivity reveals that the free-carrier (intraband) response falls well below the interband excitations, allowing the plasma frequency to be determined from the f-sum rule, ω_p ~ 33500 cm⁻¹; this value is in good agreement with first principle results. The Drude model for the optical properties of a metal may be used to estimate the free-carrier scattering rate, 1/τ ~ 80 cm⁻¹ at 5 K, which is well above the transport estimate of 1/τ < 0.2 cm⁻¹; this suggests that the scattering rate is strongly renormalized with frequency, and that the optical value is an average of these scattering rates. Structure is observed in the region of the expected infrared-active modes; however, the location and strength of these features suggests that some are not simple vibrations.


*Supported by DOE-BES under DE-SC0012704.
1:51PM S04.00014: Controlled introduction of defects to delafossite metals by electron irradiation* VERONIKA SUNKO, PHILIPPA MCGUINNESS, ELINA ZHAKINA, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, MARCIN KONCZYKOWSKI, JÉRÉMIE LEFEVRE, Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau, France, JÖRG SICHELSCHMIDT, ANDREW MACKENZIE (Presenter), Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — The delafossite metals PdCoO$_2$ and PtCoO$_2$ are among the highest conductivity materials known. At room temperature the mean free path is at least twice as long as those of silver or copper, and at low temperature mean free paths of tens of microns are observed in as-grown single crystals, enabling searches for unusual regimes of ballistic and hydrodynamic electrical transport. In parallel with that class of experiments, we wish to understand the microscopic mechanisms for the existence of these extraordinary mean free paths. Somewhat paradoxically, one route to obtaining more insight is to deliberately introduce point defects and study their effect on the electrical transport properties. We report on a systematic study in which both bulk single crystals and focused ion beam sculpted mesostructures are irradiated with 0.8 - 2.5 MeV electrons and their transport properties studied both in- and ex-situ.

*Max Planck Society, EMIR Network and UK EPSRC through grant EP/L015110/1

2:03PM S04.00015: Local Analysis of Disorder Driven Insulator-to-Metal Transition in the 2D Mott-Hubbard Model. JOSEPH SZABO (Presenter), KYUNGMIN LEE, NANDINI TRIVEDI, Ohio State University, JARED O’NEAL, Mathematics and Computer Science Division, Argonne National Laboratory — We show that increasing the number of disordered sites drives an insulator-to-metal transition in 2D Mott-Hubbard insulator. In our numerical approach we treat the spatial disorder exactly and use real-space Hartree-Fock mean-field decomposition for electron-electron interactions. These numerical methods provide insight into the localization physics as it relates to the interplay between disorder and interactions. Our results reveal an asymmetric closing of the Mott-gap and formation of a pseudogap in the density of states arising from inhomogeneous disorder potential mediated screening of the Hubbard interaction. Global lattice transport properties exhibit a transition from an insulating, gapped optical conductivity to an ungapped, metallic phase. A local picture consisting of magnetic order, compressibility, and charge mobility evolves toward a paramagnetic, metallic state with increasing disorder number due to correlations with regions of greater effective disorder. We present these local measurements to explain and provide avenues to characterize disorder induced transitions in ongoing experimental efforts.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S05 DMP: Topological Superconductivity: Nanowires BCEC 108 - Anushya Chandran, Boston University - Tag(s): Focus

11:15AM S05.00001: Surface superconductivity in gold – a material platform for Majorana bound states* [Invited] PENG WEI (Presenter), University of California, Riverside, SUJIT MANNA, Physics, Massachusetts Institute of Technology, MARIUS EICH, Solid State Physics Laboratory, ETH Zurich, PATRICK LEE, Physics, Massachusetts Institute of Technology, JAGADEESH MOODERA, Department of Physics, Plasma Science and Fusion Center, and Francis Bitter Magnet Lab, Massachusetts Institute of Technology — Proximity effect in multilayer heterostructures allows the creation of new quasiparticles with mixed physical characters. In particular, it may lead to the emergence of Majorana bound states (MBS) by mixing superconductivity, ferromagnetism, and spin-orbit coupling at material interfaces. Inducing superconductivity and magnetic exchange interactions in well-defined Shockley surface states (SS) of high quality ultrathin Au(111) layers has been predicted as an excellent platform for MBS [1]. In this talk, I will first present our device based heterostructure platform for creating and investigating such hybrid superconducting states in Au(111) [2]. By means of electron tunneling spectroscopy, I will demonstrate signatures of superconductivity induced in the two-dimensional SS of Au(111) thin film, as well as the behavior of such superconducting state under a planar Zeeman field. Unlike conventional proximity effects, the induced superconductivity in SS that are physically separated from a bulk superconductor may be governed by indirect quasiparticle scattering processes, which would further allow the manipulations of SS for MBS. Our results on planar tunneling devices made of scalable nanowires fabricated from such Au(111) heterostructures will be discussed.


*The work is supported by John Templeton Foundation Grant No. 39944, ONR Grant N00014-16-1-2657 and NSF (DMR 1700137). Peng Wei acknowledges the funding support from UCR.
11:51AM S05.00002: Backbones of a Topological Qubit – High Quality Selective-Area Grown InSb Nanowire Networks using MBE* GUANZHONG WANG (Presenter), PAVEL ASEEV, LUCA BINCI, AMRITA SINGH, LIEUWE STEK, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, FRENK BOEKHOUT, Netherlands Organisation for Applied Scientific Research (TNO), SENJA RAMAKERS, JIE SHEN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, JOHN WATSON, LEO P KOUWENHOVEN, GIJS DE LANGE, PHILIPPE CAROFF, Microsoft Quantum Delft — Nanowires (NW) made from III-V semiconductors are arguably the most mature platform for studying topological superconductivity and realizing Majorana bound states. So far progress on this front has been restricted to single NWs grown with conventional vapor-liquid-solid method. Although this growth mechanism is capable of producing free-standing NW crosses and hashtags, realization of more complex networks calls for an in-plane strategy to achieve new lithographically defined structures. Here, we implement such in-plane synthesis of InSb NW networks by selective area growth (SAG) using molecular-beam epitaxy (MBE). We perform structural and transport characterization to assess the crystal quality and electronic properties. The high quality of electron transport in InSb NWs and crosses are verified by both classical mobility and quantum transport measurements, with Hall mobility reaching 17,000 cm²/(V*s) and well-defined quantum point contact conductance plateaus at finite magnetic field. We also demonstrate phase coherent transport by studying Aharonov-Bohm interference in loops and induced superconductivity in an Al-covered sample. These results combined make InSb SAG a promising material platform for realizing a topological qubit.

*We acknowledge Microsoft for funding support.

12:03PM S05.00003: Demonstration of Majorana Fermion Pairs in Superconducting gold Surface States* SUJIT MANNA (Presenter), Massachusetts Institute of Technology, PENG WEI, Physics and Astronomy, UCR, YINGMING XIE, KAM TUEN LAW, Physics, HKUST, PATRICK LEE, JAGADEESH MOODERA, Massachusetts Institute of Technology — We present strong evidence for the emergence of Majorana bound states (MBS) in gold nanowires with proximitized superconductivity, as theoretically predicted. The interplay between superconductivity, spin-orbit coupling (SOC) and Zeeman field laid the foundation to realize MBS. We have experimentally achieved novel heterostructures, achieving these three interactions, and developed a unique method to fabricate such heterostructures into scalable nanowires. Using high-resolution scanning tunneling microscopy (STM) under in-plane magnetic field, we show that MBS appears in pairs at the opposite edges of a magnetic nanostructure on Au nanowire at 350 mK. Such spatially resolved pair of bound states, confirmed by further theoretical modeling, provides strong support for the observation of MBS in Au nanowire systems. It opens up the possibility for realizing MBS manipulations in stable and scalable metallic thin-film nanostructures, where strong SOC ensures much more robust MBS compared to other analogous semiconductor-based schemes.

1. A. C. Potter & P. A. Lee PRL 105, 227003 (2010); PRB 85, 094516 (2012)

*Supported by John Templeton Foundation Grant No. 39944, ONR Grant N00014-16-1-2657 and NSF (DMR 1700137)

12:15PM S05.00004: From Spintronics to Majorana Bound States* IGOR ZUTIC (Presenter), TONG ZHOU, Department of Physics, University at Buffalo, NARAYAN MOHANTA, Wayne State University, JONG E HAN, Department of Physics, University at Buffalo, ALEX MATOS ABIAGUE, Wayne State University — Magnetic textures, widely used to store information, can also provide synthetic spin-orbit coupling and confinement, supporting the creation of topologically nontrivial states, such as skyrmions and Majorana bound states (MBS) [1,2]. By a careful design of an array of magnetic nanopillars (MNPs), based on finite-element simulations, the resulting magnetic textures modify a proximity-induced superconductivity in the nearby 2D electron gas to form effective topological wires with MBS emerging at their ends [3]. Using spin-transfer torque, common to spintronics, to control magnetic textures [4], these topological wires can be reconfigured to implement fusion and braiding of MBS [2]. We show that a generalized topological condition for MBS formation [2] can also guide the understanding of the MBS evolution in realistic MNP arrays [3].


12:27PM S05.00005: Interacting Shiba States on Proximitized Superconducting Surface of Bi

YUWEN HU (Presenter), HAO DING, MALLIKA RANDERIA, ALI YAZDANI, Princeton University — Magnetic atoms on the surface of a superconductor induce in-gap Shiba states that can be hybridized to create a topological superconducting phase when placed in one-dimensional chains, with Majorana zero modes localized at their ends [1,2]. We have performed measurements of magnetic adatoms deposited on the surface of epitaxially grown Bi(110) thin films on a superconducting Nb(110) surface using a dilution refrigerator scanning tunneling microscope (STM). Our spectroscopic measurements show the Bi surface to exhibit a hard superconducting gap of 1.6 meV and the presence of Shiba states near magnetic adatoms. Using atomic manipulation techniques with the STM, we have built dimers of magnetic atoms with varying distance and geometry and detected the hybridization of individual in-gap states into “Shiba molecules”. We will report on these results and our efforts to build chains of magnetic atoms on the surface of superconducting Bi. The strong spin-orbit coupling and the large induced superconducting gap by the Nb substrate make this Bi surface an attractive platform for creation of atomic chains that host Majorana zero modes.


*We acknowledge funding from ONR, Moore foundation, NSF-DMR, and NSF-MRSEC.

12:39PM S05.00006: De-localized states in three-terminal InSb nanowire devices

PENG YU (Presenter), JUN CHEN, University of Pittsburgh, MOIRA HOCEVAR, Institut Néel CNRS, GHADA BADAwy, SASA GAZIBEGovic, ROY OP HET VELD, Eindhoven University of Technology, SEBASTIEN PLISSARD, LAAS CNRS, ERIK P. A. M. BAKKERS, Eindhoven University of Technology, SERGEY M FROLOV, University of Pittsburgh — Majorana bound states (MBS) has been predicted to emerge in 1D nanowire with induced superconductivity, spin-orbital coupling and external magnetic field. Although zero bias peak (ZBP) has been observed in different systems for years, no tunneling spectroscopy has verified the existence of the two Majorana bound states that should appear at the boundaries of the topological regime. We fabricated three-terminal devices with 400nm long superconducting contact in the middle and de-localized states have been observed from two sides measured simultaneously. On the contrary of the regime where the ZBP usually be observed in two terminal devices, those de-localized states appear in more open regime with more subbands available. Ongoing measurements will be dedicated to answer whether ZBP could appear in that regime and be observed from two sides.

12:51PM S05.00007: Flux-induced Majorana modes in full-shell nanowires

SAULIUS VAITIEKENAS (Presenter), MINGTANG DENG, PETER KROGSTRUP, CHARLES M MARCUS, Center for Quantum Devices and Microsoft Quantum Lab-- Copenhagen, Niels Bohr Institute, University of Copenhagen — We demonstrate a novel means of creating Majorana zero modes using magnetic flux applied to a full superconducting shell surrounding a semiconducting nanowire core, unifying approaches based on proximitized nanowires and vortices in topological superconductors. In the destructive Little-Parks regime, reentrant regions of superconductivity are associated with an integer number of phase windings in the shell. Tunneling into the core reveals a hard induced gap near zero applied flux, corresponding to zero phase winding, and a gapped region with a discrete zero-energy state for flux around $\Phi_0 = \hbar/2e$, corresponding to $2\pi$ phase winding. Coulomb peak spacing in full-shell islands around one applied flux shows exponentially decreasing deviation from $1e$ periodicity with device length, consistent with the picture of Majorana modes located at the ends of the wire.

https://arxiv.org/abs/1809.05513

*Research was supported by Microsoft, the Danish National Research Foundation, and the European Commission. M.T.D.--acknowledges support from State Key Laboratory of High Performance Computing, China.
1:03PM S05.00008: Advanced hybrid InSb/Al nanowires devices for topological parity readout (Part 2)* SEBASTIAN HEEDT (Presenter), Delft University of Technology, MARINA QUINTERO PEREZ, Microsoft Station Q at Delft University of Technology, FRANCESCO BORSOI, Delft University of Technology, ALEXANDRA FURSINA, Microsoft Station Q at Delft University of Technology, NICK VAN LOO, JIE SHEN, CHIEN-AN WANG, Delft University of Technology, KEVIN VAN HOOGDALEM, Microsoft Station Q at Delft University of Technology, BADAWY GHADA, SASA GAZIBEGOVIC, ERIK P. A. M. BAKKERS, Eindhoven University of Technology, LEO P KOUWENHOVEN, Microsoft Station Q at Delft University of Technology — Majorana bound states (MBS) are expected to enable topological qubits that encode quantum information with particularly long coherence times. The qubit state is stored non-locally in the fermion parity of multiple pairs of MBS hosted on a semiconducting-superconducting charge island. Interferometric readout of these qubits requires phase-coherent loops that comprise high-mobility InSb nanowires and Al to enable proximity-induced superconductivity in the semiconductor. Here, we introduce a fundamentally new approach for the realization of these hybrid devices based on a novel technique for the selective deposition of the Al thin films. We combine this technique with atomic hydrogen cleaning of the nanowires to remove native oxide prior to the Al deposition. The induced superconductivity in the nanowires is demonstrated via voltage-bias spectroscopy and by probing the critical currents in InSb Josephson junctions. Moreover, Cooper pair tunneling is studied in mesoscopic InSb/Al islands and parity transitions are investigated as a function of the applied magnetic field. Finally, advanced circuits are introduced that allow to study basic elements of the prospective topological qubit.

*European Research Council, Dutch Organization for Scientific Research, and Microsoft Corp. Station Q

1:15PM S05.00009: Quantum-Transport in Semiconductor Nanowire Josephson Junctions PRAVEEN SRIRAM (Presenter), SANDESH S KALANTRE, Electrical Engineering, Indian Institute of Technology Bombay, KAVEH GHARAVI, JONATHAN D BAUGH, Institute for Quantum Computing, University of Waterloo, BHASKARAN MURALIDHARAN, Electrical Engineering, Indian Institute of Technology Bombay — Semiconductor nanowire-superconductor hybrid systems provide a promising platform for hosting unpaired Majorana fermions and thus realizing fault-tolerant topological qubits. In this study, we employ the Non-Equilibrium Green’s Function (NEGF) Formalism to model quantum transport in normal (N)-superconductor(S) junctions. We analyze Josephson junctions based on semiconductor nanowires and derive the Andreev bound state spectrum and current-phase relations. Recently, [1], and [2] have reported oscillations in the critical supercurrent with an axial magnetic field. Our simulations indicate that this phenomenon arises from the interference of orbital angular momentum modes of the cylindrical nanowire. We add disorder and study its effect on the critical current oscillations, with an aim to gain a thoroughgoing understanding of the experiments.

References

1:27PM S05.00010: Hysteresis from Nonlinear Dynamics of Majorana Zero Modes in Topological Josephson Junctions JIA-JIN FENG, School of Physics, Sun Yat-sen University, ZHAO HUANG, Department of Physics, The University of Houston, ZHI WANG (Presenter), School of Physics, Sun Yat-sen University, QIAN NIU, Department of Physics, The University of Texas at Austin — We reveal that topological Josephson junctions provide a natural platform for the interplay between the Josephson effect and the Landau-Zener effect through a two-level system formed by coupled Majorana modes. We build a quantum resistively shunted (RSJ) junction model by modifying the standard textbook RSJ model to take account of the two-level system from the Majorana modes at the junction. We show that the dynamics of the two-level system is governed by a nonlinear Schroedinger equation and solve the equations analytically via a mapping to a classical dynamical problem. This nonlinear dynamics leads to hysteresis in the I-V characteristics, which can give a quantitative explanation to recent experiments. We also predict coexistence of two interference patterns with periods h/e and h/2e in topological superconducting quantum interference devices.
1:39PM S05.00011: Current-Controlled Majorana Bound States in Hybrid Semiconductor-Superconductor Nanowires Deposited on Magnetic Stripe Domains*  
NARAYAN MOHANTA (Presenter), Department of Physics and Astronomy, Wayne State University, TONG ZHOU, JONG E HAN, Department of Physics, State University of New York at Buffalo, ANDREW D KENT, JAVAD SHABANI, Department of Physics, New York University, IGOR ZUTIC, Department of Physics, State University of New York at Buffalo, ALEX MATOS ABIAGUE, Department of Physics and Astronomy, Wayne State University — The fringing fields created by magnetic stripes formed in magnetic films [1] generate inhomogeneous magnetic textures on length scales as large as 2 microns. A hybrid semiconductor-superconductor nanowire deposited on the top of a magnetic film in the stripe phase experiences a large synthetic spin-orbit coupling resulting from the fringing fields [2] of the striped domains. We show that such a system can support the formation of Majorana bound states (MBS) localized at the ends of the wire. We investigate the transition to the topological superconducting phase as a function of the stripes size and orientation, which can be tuned by applying a charge current through the magnetic film. This produces changes in the fringing magnetic texture acting on the nanowire and eventually leads to a topological phase transition with the corresponding emergence or destruction of MBS [2]. The proposed platform is promising for electrically tuning MBS in a non-invasive way and without the need for external magnetic fields.


*Work supported by DARPA TEE and U. S. ONR N000141712793 (N. M., I. Z., and A. M-A.).

1:51PM S05.00012: Quantized zero bias conductance plateaus in hybrid nanowire topological quantum information processing platforms without non-Abelian Majorana zero modes*  
CHRISTOPHER MOORE (Presenter), CHUANCHANG ZENG, Clemson University, TUDOR DAN STANESCU, Department of Physics and Astronomy, West Virginia University, SUMANTA TEWARI, Clemson University — Braiding operations in topological quantum computations inherently rely on the spatial separation between Majorana bound states (MBSs), as a result a method of distinguishing between these quasi-Majorana states and true Majorana zero modes (MZMs), localized at the ends of a semiconductor-superconductor (SM-SC) nanowire, is essential in the creation of a topological quantum bit. Here we show that recently observed, 2e^2/h-quantized zero-bias conductance plateaus, may arise in SM-SC nanowires due to the presence of quasi-Majorana states, for which the constituent MBSs are specially separated on the order of the Majorana decay length. Because these quasi-Majoranas form rather generically within the topologically trivial regime, our results establish that the observation of 2e^2/h-quantized zero-bias conductance plateaus does not represent sufficient evidence of the existence of non-Abelian MZMs localized at the opposite ends of a wire. Thus, we conclude that localized charge tunneling measurements, so far considered the primary probe for the existence of MZMs, have exhausted their potential to reveal useful information in distinguishing MZMs from low energy Andreev bound states within SM-SC hybrid structures.

*ARO Grant No. W911NF-16-1-0182

2:03PM S05.00013: Onset of the 4π-periodic Josephson effect and dissipative response at the Majorana phase transition in a semiconducting nanowire junction*  
CHAITANYA MURTHY (Presenter), Physics, UCSB, BERNARD VAN HECK, Microsoft Station Q, UCSB, LEONID GLAZMAN, Physics, Yale University, CHETAN NAYAK, Microsoft Station Q, UCSB — We study the appearance of the 4π-periodicity of the Josephson energy in a single-channel semiconducting nanowire junction much shorter than the coherence length. We compute analytically the Josephson energy of the junction as a function of magnetic field, taking into account the contributions of both discrete and continuous spectrum. We show that, in the limit of perfect transmission, the spectrum of the junction is gapless for a finite range of phase difference and a finite range of magnetic fields on the topological side of the transition. We also study the finite-frequency admittance of the junction, paying particular attention to the critical regime. We show that the expected critical behavior near the phase transition only appears in the current-current correlation function at sub-leading order in the ratio of the induced superconducting gap to the spin-orbit energy, a fact that can be understood within the critical theory of a helical, neutral Majorana mode.

*This work was supported by the Microsoft Corporation

Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S06 DCMP: Quantum Criticality: Theory BCEC 109A - Zhen Bi, Massachusetts Institute of Technology
11:15AM S06.00001: Instabilities of 2d quantum critical metals in the $N_f \to 0$ limit

Petter Säterskog (Presenter), Nordic Institute for Theoretical Physics — We study a Fermi surface coupled to fluctuations of one or more critical order parameters in 1+2 dimensions. The limit of vanishing fermion flavor number gives a controlled way of studying this strongly coupled theory. In this talk I show results for charge, spin and pairing susceptibilities and find that the critical fluctuations may induce charge/spin density wave order or pairing depending on the types of critical order parameter fluctuations and their interplay.

*This work was support by the grant "Exact Results in Gauge and String Theories" from the Knut and Alice Wallenberg foundation.

11:27AM S06.00002: Itinerant Quantum Critical Point with Fermion Pockets and Hot Spots

Zihong Liu (Presenter), Gaopei Pan, Chinese Academy of Sciences, Xiao Yan Xu, Department of Physics, Hong Kong University of Science and Technology, Kai Sun, Department of Physics, University of Michigan, Zi Yang Meng, Chinese Academy of Sciences — Combining determinantal quantum Monte Carlo (DQMC) and elective momentum ultra-size quantum Monte Carlo (EQMC) methods, we systematically investigated the itinerant quantum critical point on a 2D square lattice with antiferromagnetic spin fluctuations at wavevector $Q = (\pi, \pi)$. System sizes of $60 \times 60 \times 320$ ($L \times L \times L_t$) are comfortably accessed, and the quantum critical scaling behaviors are revealed with unprecedented high precision. We found that the antiferromagnetic spin fluctuations introduce effective interactions among fermions and the fermions in return render the bare bosonic critical point into a new universality, different from the bare Ising universality class and the Hertz-Mills-Moriya RPA prediction. At the quantum critical point, a finite anomalous dimension $\eta \sim 0.125$ is observed in the bosonic propagator, and fermions at hot spots evolve into a non-Fermi-liquid. In the antiferromagnetically ordered metallic phase, fermion pockets are formed as energy gap opens up at the hot spots.

11:39AM S06.00003: Emergent O(4) Symmetry and Conserved Current Continuum at a Deconfined Quantum Critical Point in Shastry-Sutherland Model

Jong Yeon Lee (Presenter), Harvard University, Yizhuang You, Physics, University of California, San Diego, Ashvin Vishwanath, Harvard University — In this work, we investigate a possibility of deconfined quantum phase transition in the two dimensional Shastry-Sutherland spin model. Using the level-crossing technique for correlation length spectrum in the infinite DMRG simulation, we demonstrate the evidence for a deconfinement and emergent O(4) symmetry at the phase transition between the plaquette valence bond solid and Neel order. Such a phase transition has been observed in the recent experiment, and we propose experimental signatures for this deconfined quantum criticality that can be measured in both phonon and magnon spectra.

11:51AM S06.00004: Quantum criticality in Ising chains with random hyperuniform couplings

Philip Crowley (Presenter), Christopher Laumann, Boston University, Sarang Gopalakrishnan, CUNY College of Staten Island; The Graduate Center, CUNY — In critical Ising chains, independent random disorder localises almost all excitations, and drives the system to an infinite randomness critical point. However, correlations in the disorder can change the universality, and even make the disorder irrelevant.

We show this in the critical hyperuniform random Ising chain, where increasing hyperuniformity yields a line of Griffiths-free infinite-randomness critical points with continuously varying exponents, this line terminates at the Ising class “critical Ising insulator”.

12:03PM S06.00005: Deconfined quantum criticality from the $QED_3$-Gross-Neveu-Yukawa model: the $1/N$ expansion revisited

Rufus Boyack (Presenter), Ahmed Rayyan, Joseph Maciejko, Physics, University of Alberta — Quantum phase transitions involving dynamical gauge fields are an important class of transitions beyond the standard Landau-Ginzburg-Wilson paradigm. Two subcategories are those where (i) the gauge field deconfines only at the critical point itself, and (ii) the gauge field deconfines in one of the phases separated by the critical point. The latter subcategory is exemplified by the $QED_3$-Gross-Neveu-Yukawa (GNY) model in which there has been great interest recently due to a conjecture relating its critical point to the Néel-to-valence-bond-solid (VBS) deconfined critical point in the first subcategory. Motivated by this, we use the $1/N$ expansion to study the $QED_3$-GNY model in fixed three spacetime dimensions, with $N$ flavors of two-component Dirac fermions. We find new contributions to critical exponents arising from Aslamazov-Larkin diagrams missed by previous epsilon- and $1/N$-expansion studies in arbitrary dimensions. For the specific case of $N = 2$, when the duality is conjectured to hold, we find that the bosonic anomalous dimension and adjoint fermion bilinear scaling dimension are in reasonable agreement with numerical studies of the Néel-to-VBS transition.
12:15PM S06.00006: Dynamical spin susceptibility of a Fermi liquid without conservation law  
PRACHI SHARMA (Presenter), DMITRII MASLOV, University of Florida — Galilean invariance along with the conservation of charge and total spin guarantees that the corresponding susceptibilities vanish at an infinitely long wavelength (q=0) and finite frequency. But the susceptibility of nematic fluctuations or that of spin fluctuations in the presence of spin-orbit interaction (SOI) is not protected by any conservation laws and hence leads to finite spectral weight outside the particle-hole continuum even at q=0 and finite \( \omega \) [1,2]. Finite width of the chiral spin modes for a Fermi liquid (FL) with Rashba SOI was studied at q=0 by Maiti and Maslov [3]. Here, we study the effect of residual interaction on the chiral spin modes of a FL with weak Rashba SOI for a model of dynamic screened Coulomb potential at finite q by going beyond the random phase approximation (RPA). We also study the interplay between the plasmon and chiral spin modes due to their coupling for the non-RPA corrections.


12:27PM S06.00007: Critical strange metal from fluctuating gauge fields in a solvable random model*  
AAVISHKAR PATEL (Presenter), SUBIR SACHDEV, Harvard University — Building upon techniques employed in the construction of the Sachdev-Ye-Kitaev model, which is a solvable (0+ 1)-dimensional model of a non-Fermi liquid, we develop a solvable infinite-ranged random-hopping model of fermions coupled to fluctuating U (1) gauge fields. In a specific large-N limit, our model realizes a gapless non-Fermi-liquid phase, which combines the effects of hopping and interaction terms. We derive the thermodynamic properties of the non-Fermi-liquid phase realized by this model and the charge transport properties of an infinite-dimensional version with spatial structure. We also describe a Higgs transition from this non-Fermi-liquid "strange metal" phase to a weakly-interacting "pseudogap" phase with a relatively reduced low-energy fermion density of states, and gapped gauge field fluctuations.

*This research was supported by the NSF under Grant DMR-1664842. A. A. P. was supported by a Harvard-GSAS Merit Fellowship. Research at Perimeter Institute is supported by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Research and Innovation. S. S. also acknowledges support from Cenovus Energy at Perimeter Institute.

12:39PM S06.00008: Fermion-induced quantum critical points in a generalized SU(N) fermion model  
BOHAI LI (Presenter), Tsinghua University, ZIXIANG LI, University of California, Berkeley, HONG YAO, Tsinghua University — The non-Landau quantum criticality dubbed as "fermion-induced quantum critical point" (FIQCP) was proposed in Ref. [1], where it was shown for 2D SU(N) Dirac fermions with Na2. Here we investigate the nature of quantum phase transition for case of N=1. Our sign-problem-free Majorana quantum Monte Carlo simulations show that, by introducing longer-range interactions, our model exhibits transitions among Dirac semimetals, CDW, and Kekule-VBS phases. This can further provide support for the critical value of N for the occurrence of FIQCP predicted by previous RG studies.

[1] Zi-Xiang Li, Yi-Fan Jiang, Shao-Kai Jian, and Hong Yao, Fermion-induced quantum critical points, Nature Communications 8, 314 (2017).

12:51PM S06.00009: Incommensurate 2k_F charge density wave quantum critical points in two-dimensional metals*  
MATTHIAS PUNK (Presenter), JOHANNES HALBINGER, DIMITRI PIMENOV, Ludwig Maximilian University of Munich — We study two-dimensional metals in the vicinity of a quantum critical point, where incommensurate 2k_F charge density wave (CDW) order develops. Starting from a model of two antipodal hot spots at the Fermi surface which are connected by a 2k_F wavevector, we perform a controlled, perturbative renormalization group analysis in the spirit of earlier work by Dalidovich and Lee [1]. We show that the charge density wave transition is indeed continuous and described by a non-Fermi liquid fixed point with a dynamically nested Fermi surface. Our results are potentially relevant to understand the onset of incommensurate CDW order in Cu_xTaS_2 and NbSe_2 at high pressure.


*Nanosystems Initiative Munich, German Excellence Initiative
1:03PM S06.00010: Quantum criticality of a quantum nonlinear sigma model with Kondo coupling: a renormalization group study  
CHIA-CHUAN LIU (Presenter), QIMIAO SI, Rice University — Quantum criticality has been an active research topic in condensed matter physics, with a lot of effort being made into the heavy fermion material in which local moments are coupled with itinerant electrons through Kondo coupling [1]. From a theoretical perspective, the interplay between different kinds of degrees of freedom makes it challenging to develop a unified framework to study the quantum criticality of such systems [2]. Here we approach the problem from the magnetically ordered side, using a quantum non-linear sigma model with an additional coupling to itinerant fermions [3]. By treating the renormalization of the bosonic and fermionic degrees of freedom on an equal footing, we analyze the effect of the Kondo coupling on the criticality. Our results shed new light on the global phase diagram of the heavy fermion systems.

References:

1:15PM S06.00011: Incoherent metal in the quantum critical region of SU(2) symmetric model*  
PETER CHA (Presenter), Cornell University, OLIVIER PARCOLLET, ANTOINE GEORGES, CCQ, Flatiron Institute, Simons Foundation, EUN-AH KIM, Cornell University — Incoherent metals have recently garnered much interest in their relation to quantum criticality, high-temperature superconductivity, quantum chaos, and holography. In this context, considerable recent interest has been devoted to the SYK model and its variants, as a paradigmatic model for metallic behaviour without quasiparticles.

With the aim at exploring the robustness of this physics beyond the large-N limit, we consider an SU(2) symmetric spin-1/2 model with disordered magnetic exchange and repulsive Hubbard local interaction, in the framework of dynamical mean-field theory. In the insulating regime, we recover the spin-glass and local moment phases of the spin-1/2 disordered Heisenberg Hamiltonian, while deep in the metallic regime we find Fermi liquid behaviour. We discuss the effect of the disordered spin coupling on the metal-insulator transition, and the presence of a quantum-critical non-Fermi liquid in the phase diagram.

*This work was supported by the NSF Materials Innovation Platform grant DMR-1539918.

1:27PM S06.00012: Deconfined Quantum Critical Points in 3+1D*  
ZHENG BI (Presenter), SENTHIL TODADRI, Massachusetts Institute of Technology — Continuous quantum phase transitions that are beyond the conventional paradigm of fluctuations of a symmetry breaking order parameter are challenging for theory. These phase transitions often involve emergent deconfined gauge fields at the critical points as demonstrated in 2+1D. Examples include phase transitions in quantum magnetism as well as those between Symmetry Protected Topological phases. In this work, we present several examples of Deconfined Quantum Critical Points between Symmetry Protected Topological phases in 3+1D for both bosonic and fermionic systems. These critical theories can be formulated as non-abelian gauge theories either in their Infra-Red free regime, or in the conformal window when they flow to the Banks-Zaks fixed points. We will talk about several interesting quantum critical phenomena. We describe situations in which the same phase transition allows for multiple universality classes controlled by distinct fixed points. We exhibit the possibility - which we dub “unnecessary quantum critical points” - of stable generic continuous phase transitions within the same phase.

*ST was supported by NSF grant DMR-1608505 and Simons Investigator Award from the Simons Foundation. ZB acknowledges support from the Pappalardo fellowship at MIT.

1:39PM S06.00013: Quantum-critical conductivity of the Dirac fluid in graphene  
TAIRU LYU (Presenter), PATRICK R GALLAGHER, CHANSAN YANG, FENG WANG, University of California, Berkeley — Graphene near charge neutrality is expected to behave like a quantum-critical, relativistic plasma—the “Dirac fluid”—in which massless electrons and holes rapidly collide at a rate proportional to temperature. We measure the frequency-dependent optical conductivity of clean micron-scale graphene encapsulated in hexagonal Boron Nitride at electron temperatures between 77 and 300 K using on-chip terahertz spectroscopy. At charge neutrality, we observe the quantum-critical scattering rate characteristic of the Dirac fluid. At higher doping, we uncover two distinct current-carrying modes with zero and nonzero total momenta, a manifestation of relativistic hydrodynamics. Our work reveals the quantum criticality and unusual dynamic excitations near charge neutrality in graphene.
Emergent Spacetime Supersymmetry at Superconducting Quantum Criticality of a single Dirac Cone

ZIXIANG LI, Tsinghua University, ABOLHASSAN VAEZI, CHRISTIAN MENDL, Stanford University, HONG YAO (Presenter), Tsinghua University — No definitive evidence of spacetime supersymmetry (SUSY) that transmutes fermions into bosons and vice versa has been revealed in nature so far. Moreover, whether spacetime SUSY in 2+1 and higher dimensions can emerge in generic lattice microscopic models remains open. Here, we introduce a lattice realization of a single Dirac fermion in 2+1 dimensions with attractive interactions that preserves both time-reversal and chiral symmetries. By performing sign-problem-free determinant quantum Monte Carlo simulations, we show that the interacting single Dirac fermion in 2+1 dimensions features a superconducting quantum critical point (QCP). More remarkably, we demonstrate that the N=2 spacetime SUSY in 2+1D emerges at the superconducting QCP by showing that the fermions and bosons have identical anomalous dimensions 1/3, a hallmark of the emergent SUSY [1]. We further show some experimental signatures which may be measured to test such emergent SUSY in candidate systems such as the surface Dirac cone of 3D topological insulators.


Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S07 DCMP: Metal/Insulator and Superconductor/Insulator BCEC 109B - Nandini Trivedi, Ohio State University

11:15AM S07.00001: Spin and charge dynamics of an interacting gas of small (bi)polarons across the mobility edge
GAYAN HETTIARACHCHI (Presenter), Rutgers University, YOSHIFUMI NISHIDA, YUSUKE MASAKI, Osaka University, MOHD NAZLAN MOHD MUHID, HALIMATON HAMDAN, University of Technology Malaysia — We performed electron spin resonance (ESR) and optical studies on a model system that is used to investigate the discontinuous metal-insulator transition in a deformable lattice. The ESR signal below the mobility edge has no correlation to the conductivity and arises purely from a minority of magnetic polarons. Above the percolation threshold of the system and below the mobility edge, the intensity of the ESR signal shows a decrease suggesting that small polarons form paired states, i.e., small bipolarons, with increasing interactions. The conducting transition is marked by the appearance of an asymmetric ESR line shape simultaneously with a decrease in the small bipolaron optical absorption band. The delocalized states result from a partial dissociation of the small bipolarons. Immediately above the mobility edge, competing phases of delocalized (extended) states, small polarons, and small bipolarons coexist. Based on the experimental results, we propose a phase diagram that adds to the theoretical studies and highlight that the polaron density and local interactions are important parameters that determine the balance among competing states in a many-polaron system.

11:27AM S07.00002: Renormalization group analysis of superconductor-insulator transition with disorder
CHAO-JUNG LEE (Presenter), Caltech, MICHAEL C MULLIGAN, Physics and Astronomy, Univ of California - Riverside — A recent experiment [1] indicates the magnetic field-tuned superconductor-insulator transition (SIT) in thin films can exhibit particle-vortex self-dual electrical conductivity. With the aim of understanding this quantum critical behavior, we consider a manifestly self-dual theory consisting of a Dirac fermion coupled to a Chern-Simons gauge field [2] in the presence of quenched disorder. We derive renormalization group fixed points of this theory in the presence of disorder and gauge fluctuations, which are controlled in an expansion in the number of fermion flavors. We then discuss the quantum critical conductivity of these fixed points. This formalism can also be used to understand quantum Hall plateau transitions.


11:39AM S07.00003: New microscopic paradigms in the doped Fermi-Hubbard model
FABIAN GRUSDT (Presenter), ANNABELLE BOHRDT, MICHAEL KNAP, Physics Department, Technical University of Munich, EUGENE DEMLER, Physics Department, Harvard University — The interplay of mobile dopants with anti-ferromagnetic spin correlations is at the heart of high-temperature superconductivity. Here we present a microscopic trial wavefunction describing individual dopants as spinon-chargon composites. We derive the correlations of the charges with their spin environment and reveal short-range hidden string order, which manifests in genuine higher-order correlations developing around the dopants and can be directly observed in state-of-the-art quantum simulations. Our microscopic model explains the observations of string patterns and the dressing cloud of magnetic polarons in recent measurements performed with ultracold atoms in optical lattices. Our approach can be applied at finite doping and paves the way for a microscopic description of the exotic metallic phases in strongly correlated cuprate compounds.
11:51 AM S07.00004: Magnetism and correlation effects in titanium phosphate at high pressure  
JOHAN JÖNSSON (Presenter), MARCUS EKHOLM, IGOR ABRIKOSOV, Linköping University — Titanium phosphate exhibits interesting properties as pressure and temperature is varied e.g., the spin-Peierls transition. We have investigated the influence of magnetism and electron correlation on this behaviour upon compression.

At ambient pressure TiPO₄ forms the orthorhombic structure called phase I, with TiO₆ octahedra forming chains along the c-axis. As pressure is increased these chains begin to dimerise, leading to the incommensurate phase II, further increases of pressure locks the dimerisation in the chains, forming the commensurate and dimerised phase III. Even higher pressures leads to two new phases, IV and V, that show a noticeable increase in density.[1]

The chains in phase III exhibit a behaviour similar to what has been observed in VO₂, as a function of temperature. This suggests that TiPO₄ may be useful to investigate the correlation effects in VO₂ at room temperature but at high pressure.

At high pressure phase III undergoes a transition from a Mott insulating state into a metallic one. This Mott transition triggers another phase transition revealing two new, Mott insulating, phases, one non-magnetic and dynamically stabilised and another antiferromagnetic with strong local magnetic moments.


12:03 PM S07.00005: Quantum electrodynamics of a superconductor-insulator quantum phase transition I: theory  
VLADIMIR MANUCHARYAN (Presenter), ROMAN KUZMIN, RAY MENCIA, NICHOLAS GRABON, NITISH JITENDRASKUMAR MEHTA, YEN-HSIANG LIN, University of Maryland, College Park — We report on our experimental probing of the superconductor-insulator quantum phase transition (QPT) in a 1D Josephson chain in the high-frequency and short-wavelength limit [1]. By contrast, traditional experiments focus on finding a universal scaling of resistance with temperature and other system parameters. The quantum BKT transition resisted this approach for two decades. In part I, we overview the possible issues with the DC transport measurements and describe the advantages of viewing a QPT from the high-energy side. In part II, we show the results of our microwave spectroscopy of long chains of Al/AIOx/Al tunnel junctions. First, we find that an insulating chain can carry AC currents (in a GHz-band) as a near-perfect superconductor. Second, deviations from perfect superconductivity can be resolved. These deviations appear as frequency-dependent linewidths of the collective modes and as a scattering of their frequencies. Both effects arise from interactions and constitute the high-frequency footprint of the insulating phase near the critical point. Our new approach can help bridge theory with the experiments in chains, thin films, nanowires, and cold atom realizations of 1D systems.


12:15 PM S07.00006: Quantum electrodynamics of a superconductor-insulator quantum phase transition II: experiment  
NICHOLAS GRABON (Presenter), ROMAN KUZMIN, RAY MENCIA, NITISH JITENDRASKUMAR MEHTA, YEN-HSIANG LIN, VLADIMIR MANUCHARYAN, University of Maryland, College Park — We report on our experimental probing of the superconductor-insulator quantum phase transition (QPT) in a 1D Josephson chain in the high-frequency and short-wavelength limit [1]. By contrast, traditional experiments focus on finding a universal scaling of resistance with temperature and other system parameters. The quantum BKT transition resisted this approach for two decades. In part I, we overview the possible issues with the DC transport measurements and describe the advantages of viewing a QPT from the high-energy side. In part II, we show the results of our microwave spectroscopy of long chains of Al/AIOx/Al tunnel junctions. First, we find that an insulating chain can carry AC currents (in a GHz-band) as a near-perfect superconductor. Second, deviations from perfect superconductivity can be resolved. These deviations appear as frequency-dependent linewidths of the collective modes and as a scattering of their frequencies. Both effects arise from interactions and constitute the high-frequency footprint of the insulating phase near the critical point. Our new approach can help bridge theory with the experiments in chains, thin films, nanowires, and cold atom realizations of 1D systems.

12:27PM S07.00007: Structural investigation of the insulator-metal transition in NiS$_2-x$Sex compounds
SUNGKYUN CHOI (Presenter), Department of Physics and Astronomy, Rutgers University, GARAM HAN, HWANBEOM CHO, BYUNGMIN SOHN, JE-GUEU PARK, CHANGYOUNG KIM, Department of Physics and Astronomy, Seoul National University (SNU) —
We report [1] on a combined measurement of high-resolution x-ray diffraction on powder and Raman scattering on single crystalline NiS$_2-x$Sex samples that exhibit the insulator-metal (IM) transition [2] with Se doping. Via x-rays, an abrupt change in the bond length between Ni and S (Se) ions was observed at the transition temperature, in sharp contrast to the almost constant bond length between chalcogen ions. Raman scattering, a complementary technique with the unique sensitivity to the vibrations of chalcogen bonds, revealed no anomalies in the phonon spectrum, consistent with the x-ray diffraction results. This indicates the important role of the interaction between Ni and S (Se) in the IM transition. The potential implication of this interpretation is discussed in terms of current theoretical models.


12:39PM S07.00008: Quasi-periodic metal-insulator phase separation in strain engineered La$_{0.66}$Sr$_{0.33}$MnO$_3$ thin films
XINZHONG CHEN (Presenter), Stony Brook University, LIN LI, XIAODONG FAN, USTC, ZHIJING NIU, MENGKUN LIU, Stony Brook University, CHANGGAN ZENG, USTC — We report the electronic phase separation in the prototypical double exchange ferromagnet La$_{0.66}$Sr$_{0.33}$MnO$_3$ (LSMO) thin films grown on LaAlO$_3$ (LAO) substrate. We discovered a peculiar mesoscale stripe pattern that only occurs at specific film thickness, using the scattering-type scanning near-field optical microscope (s-SNOM) at the mid-infrared (mid-IR) frequencies. These novel quasi-periodic mesoscale metal-insulator-metal stripes are contributed to a subtle and delicate balance between the epitaxial strain and surface twin structure of the LAO substrate. Our work strongly suggests the possibility to control the metallicity via interface and strain engineering in strontium doped manganites.

12:51PM S07.00009: Observation of a new collective mode involved in the Verwey transition in magnetite
CARINA BELVIN (Presenter), EDOARDO BALDINI, OZGE I OZEL, Massachusetts Institute of Technology, JOSÉ LORENZANA, Institute for Complex Systems, Italy and University of Rome “La Sapienza”, NUH GEDIK, Massachusetts Institute of Technology — Magnetite (Fe$_3$O$_4$), the oldest known magnetic material, is a strongly correlated transition metal oxide that exhibits complex electronic and structural properties. Below the Verwey transition, the low-temperature insulating phase displays rich features, including the coexistence of charge and orbital orders whose detailed nature is still under debate. Using pump-probe spectroscopy, we photoexcite the system out of equilibrium with a tailored femtosecond laser pulse and examine the evolution of the coherent oscillations due to the system's collective modes in the time domain. We observe signatures of a new mode that undergoes a dramatic softening as a function of laser fluence. We discuss the implication of this collective mode on the understanding of the Verwey transition.

1:03PM S07.00010: Electron localization in 2D extended Hubbard model
HANNA TERLETSKA (Presenter), Middle Tennessee State University, JOSEPH PAKI, SERGEI ISAKOV, University of Michigan, THOMAS MAIER, Oak Ridge National Lab, EMANUEL C GULL, University of Michigan — We use the Dynamical Cluster Approximation to study the finite temperature phase transitions in 2D extended Hubbard model. We find that non-local electron-electron interactions screen the local Hubbard interactions, stabilizing the Mott metal-insulator transition in 2D extended Hubbard model. We also investigate the effect of the temperature and non-local interactions on the competition between antiferromagnetism and charge order. We show that non-local correlations are important, and hence the non-local methods are needed for proper analysis of the phase transitions in this model.
1:15PM S07.00011: Amplitude (Higgs) mode at the superfluid-Mott glass transition*  
JACK CREWSE (Presenter), THOMAS VOJTA, Missouri University of Science and Technology —  
We investigate the amplitude (Higgs) mode of a diluted quantum rotor model in two and three space dimensions close to their respective superfluid-Mott glass quantum phase transitions [1,2]. After mapping the Hamiltonians onto appropriate classical XY models, the systems are simulated by means of large-scale Monte Carlo simulations. The scalar susceptibility of clean, undiluted systems exhibit sharp spectral peaks associated with the amplitude mode that show the expected scaling behavior close to the critical point. However, the diluted systems do not exhibit such sharp peaks. Instead, the scalar susceptibility is dominated by broad, non-critical peaks which obscure any potential amplitude mode. To understand the fate of the amplitude mode in diluted systems we study the localization behavior of the mode by calculating dispersion relations near the critical point, for varying dilution strengths. We also calculate conductivity as an indirect measure of the amplitude modes existence in diluted systems.  

*This work was supported in part by the NSF under grants No. DMR-1506152 and DMR-1828489.

1:27PM S07.00012: Resistive Switching as Nonequilibrium Phase Transition*  
JONG E HAN (Presenter), JIAJUN LI, University at Buffalo, The State University of New York, CAMILLE ARON, Department of Physics, Ecole Normale Superieure, CNRS, Paris, France, GABRIEL KOTLIAR, Department of Physics, Rutgers University — We investigate the quantum mechanical origin of resistive phase transitions in solids driven by a constant electric field in the vicinity of a metal-insulator transition [1]. We perform a nonequilibrium mean-field analysis of a driven-dissipative symmetry-broken insulator, which we solve analytically for the most part. We find that the insulator-to-metal transition (IMT) and the metal-to-insulator transition (MIT) proceed by two distinct electronic mechanisms: Landau-Zener processes and the destabilization of the metallic state by Joule heating, respectively. Our analytic approach enables us to formulate testable predictions on the nonanalytic behavior of I-V relation near the insulator-to-metal transition. Building on these successes, we propose an effective Ginzburg-Landau theory which paves the way to incorporating spatial fluctuations and to bringing the theory closer to a realistic description of the resistive switchings in correlated materials.  

*We acknowledge financial support form National Science Foundation with Grant No. DMR-1733071.

1:39PM S07.00013: Interplay between superconducting and magnetic fluctuations in the doped 2D Hubbard model*  
ANNA KAUCH (Presenter), FELIX HORBINGER, Institute of Solid State Physics, TU Wien, GANG LI, School of Physical Science and Technology, ShanghaiTech University, KARSTEN HELD, Institute of Solid State Physics, TU Wien — The importance of antiferromagnetism for d-wave type superconductivity has already been established within various theoretical methods [1]. In this work we focus on the doped regime, where the magnetic fluctuations become incommensurate [2]. The solution of the Hubbard model by parquet equations gives us the unique opportunity to treat fluctuations in all channels on equal footing. Using the victory parquet equations solver [3] we compute two-particle quantities in the 2D Hubbard model on square lattice in the parquet (PA) and dynamical vertex (DΓA) approximations [4][5]. In the parquet flavour of DΓA, the fully irreducible vertex is assumed to be local and it is obtained from dynamical mean-field theory (DMFT). The analysis of the particle-particle vertex as well as of the leading eigenvalues of the Bethe-Salpeter equations allow us to identify the dominant fluctuations and the symmetry of the pairing.  

*Fonds zur Förderung der wissenschaftlichen Forschung (FWF) project P 30997
1:51PM S07.00014: Effect of Spin-Selective Disorder on the Hubbard model. RAJESH NARAYANAN (Presenter), MADHUPARNA KARMAKAR, SHASHIKANT SINGH KUNWAR, Indian Institute of Technology Madras, PRABUDDHA CHAKRABORTY, Chennai Centre, Indian Statistical Institute — We use a combination of Monte-Carlo techniques to study the effect of spin-selective disorder for both the repulsive and attractive Hubbard models. For the repulsive Hubbard model with spin-selective disorder, by using a determinant quantum Monte-Carlo scheme we show evidence for the existence of a metal-insulator transition for fillings away from half-fillings. We show that the metal-insulator transition is accompanied with a net-polarization of the fermionic fluid and a consequent saturation behavior in the susceptibility. For the case of the attractive Hubbard model at half-filling in the presence of spin-selective disorder, we use a real space based Monte-Carlo scheme to completely elucidate the ground state phase diagram. In particular, we compare and contrast the behavior at weak and strong disorder: In the limit of weak disorder gapless superconductivity obtains whereas in the limit of strong disorder a spin-selective Anderson transition is realized. The effect of thermal fluctuations on the phase diagram is also studied within this approach.

2:03PM S07.00015: Percolative transport in the metal-insulator phase coexistence region of Mott organics* YUTING TAN (Presenter), VLADIMIR DOBROSAVLJEVIC, Department of Physics and NHMFL, Florida State University — The Mott metal-insulator transition of the organic triangular-lattice system $k$–$(ET)_2Cu_2(CN)_3$ has recently been re-examined through low temperature DC [1] transport experiments. These results, displaying striking non-monotonous temperature dependence for a family of resistivity curves, have been previously interpreted in terms of the "continuous" (spinon-based) scenario for the transition. Here we theoretically re-examine the transport properties in this regime, and show that an alternative viewpoint [2], based in the dynamical mean-field theory (DMFT) and a percolation picture [3], naturally explains all the observed anomalies. According to this scenario, the transition assumes first-order character at low temperature, leading to percolative transport in the coexistence regime, which we study theoretically, reproducing the experimental trends.


*This work was supported by the NSF Grant No. DMR-1822258, and the National High Magnetic Field Laboratory through the NSF Cooperative Agreement No. DMR-1167490.

Thursday, March 7, 2019 11:15 AM - 1:39 PM

Session S08 DCMP: Superconductivity in EM fields BCEC 150 - Catalin Martin, Ramapo College

11:15AM S08.00001: Debye mechanism of giant microwave absorption in superconductors* MICHAEL SMITH (Presenter), ANTON V ANDREEV, BORIS SPIVAK, University of Washington — We present a theory of microwave absorption in conventional superconductors and show that in the presence of a superfluid velocity $V_s$ the microwave absorption coefficient can be orders of magnitude larger than at $V_s = 0$. The reason for this is that the $V_s$-dependent contribution is proportional to the inelastic scattering time rather than the elastic scattering time. The mechanism responsible for this larger contribution is similar to the Debye mechanism for microwave absorption in molecules. Further, the $V_s$ dependence of the absorption coefficient is non-analytical, and measurement of this contribution to the absorption coefficient will give direct information about the inelastic scattering time in superconductors which in general has been difficult to directly measure. In the absence of the superfluid velocity we identify a new mechanism of non-linear conductivity with anomalously low threshold.

*This work was supported by the U.S. Department of Energy Office of Science, Basic Energy Sciences under Award No. DE-FG02-07ER46452.
11:27AM S08.00002: A nonlinear THz study of strong light-matter coupling between plasmonic metamaterials and a superconducting Josephson Plasmon in $\text{La}_2\text{xSr}_x\text{CuO}_4$.* JACOB SCHALCH (Presenter), University of California, San Diego, CHUNXU CHEN, XIAOGUANG ZHAO, department of mechanical engineering, boston university, DIMITRI BASOV, department of physics, columbia university, MICHAEL FOGLER, University of California, San Diego, XIN ZHANG, department of mechanical engineering, boston university, RICHARD DOUGLAS AVERITT, University of California, San Diego — The Josephson plasma resonance (JPR) in layered high temperature superconducting cuprates provides a useful probe of the superconducting condensate, as well as an avenue to couple incident electromagnetic fields to the condensate. We enhance this light-matter coupling by applying interchangeable metamaterial tapes to a c-axis single crystal of $\text{La}_2\text{xSr}_x\text{CuO}_4$ and perform linear THz time domain spectroscopy in reflection in order to identify anti-crossing behavior characteristic of strong coupling. We then drive the hybrid superconducting metamaterial system with large single cycle THz fields in excess of 100kV/cm in order to explore emergent nonlinear behavior of the coupled system. This work informs future possibilities of utilizing strong coupling effects in conjunction with large transient fields to achieve coherent control of a superconducting condensate and an avenue towards light enhanced superconductivity.

*Research supported by DOE-BES under DE-SC0018218.

11:39AM S08.00003: Cavity Quantum Enhancement of Superconductivity* JONATHAN CURTIS (Presenter), ZACHARY RAINES, ANDREW ALLOCCA, MOHAMMAD HAFEZI, VICTOR GALITSKI, University of Maryland, College Park — Standard superconductors are known to exhibit a number of fascinating and potentially useful phenomena when driven away from thermal equilibrium by coherent classical electromagnetic radiation. These non-equilibrium effects can often lead to an enhancement in the strength of the superconducting gap and its manifestations. We aim to understand what happens when the classical electromagnetic field is replaced by a fluctuating quantum electromagnetic field, as may be found in a microwave cavity resonator. We show that in the lossy regime non-equilibrium cavity photons can rid the superconductor of deleterious quasiparticles, thereby enhancing the superconducting gap strength. This proposed quantum enhancement of superconductivity opens the door to the study of more exotic phenomena which may arise when superconductors are subjected to cavity quantum electrodynamic environments.

*This work was supported by NSF DMR-1613029 and US-ARO (contract No. W911NF1310172) (Z.R.), the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE1322106 (J.C.), DOE-BES (DESC0001911) and the Simons Foundation (A.A. and V.G.), and AFOSR FA9550-16-1-0323, ARO W911NF15-1-0397, and NSF Physics Frontier Center at the Joint Quantum Institute (M.H.).

11:51AM S08.00004: Modulating Superconductivity with Metamaterial Plasmonic Structures – Theory TYLER DODGE (Presenter), XUEYUAN WU, MARK SCHILLER, MICHAEL J NAUGHTON, KRZYSZTOF KEMPA, Department of Physics, Boston College — In 1972, Kirzhnits et al. reformulated the BCS superconductivity theory in terms of a dielectric response function1. The conclusion of this theory was that the strength of the Cooper pairings can be controlled by the dielectric environment. A demonstration of this effect was recently given in a metamaterial composite made of Al nanoparticles2, designed to have suppressed dielectric function at the Eliashberg function maximum, leading to threefold increase of superconductivity critical temperature. In this work, we have studied theoretically, two-dimensional Babinet metamaterials made of Pb, properly designed to have the Cooper pairing strength systematically controlled (enhanced or suppressed). This work, has been coupled to the parallel effort to determine these effects theoretically.


12:03PM S08.00005: Modulating Superconductivity with Metamaterial Plasmonic Structures – Experiment. MARK SCHILLER (Presenter), TYLER DODGE, XUEYUAN WU, KRZYSZTOF KEMPA, MICHAEL J NAUGHTON, Physics, Boston College — In 1972, Kirzhnits et al. reformulated the BCS superconductivity theory in terms of a dielectric response function,1 concluding that the strength of Cooper pairing can be controlled by the dielectric environment. A demonstration of this effect was recently given in a metamaterial composite made of Al nanoparticles2, designed to have suppressed dielectric function at the Eliashberg function maximum, leading to threefold increase of superconductivity critical temperature. We report fabrication and experimental measurements of thin film Babinet metamaterials made of Pb, designed to have the Cooper pairing strength systematically controlled (enhanced or suppressed). This work is coupled to a parallel effort to determine these effects theoretically.

12:15PM S08.00006: Strong Plasmonic Enhancement of Photoelectric Quantum Efficiency of Nb using In Nano islands  SHOKOUFEH ASALZADEH (Presenter), JOHN ZASADZINSKI, MARK WARREN, LINDA KLAMP SPENTZOURIS, NOAH SAMUELSON, Illinois Institute of Technology — The development of superconducting photocathodes is presented which explores thin film coatings to enhance the quantum efficiency (QE) of superconducting Nb above its bulk value of < 10^-6. Deposition of a 10nm layer of Mg (work function = 3.6 eV) onto Nb after UHV anneal increases QE by a factor of 10. Deposition of ultra-thin islands of In (4 nm) on top of Nb/Nb oxide or Nb/Mg/Mg oxide leads to overall enhancements of QE by up to 400 times. We attribute this latter enhancement to plasmonic effects where the stored EM fields in the In islands couple to Nb electrons

12:27PM S08.00007: Theory of coherent plasmon in one dimensional insulators* JAY SAU (Presenter), University of Maryland, College Park — Recent microwave reflection measurements of Josephson junction ladders have suggested the presence of nearly coherent collective charge oscillations deep in the insulating phase. Here we develop a qualitative understanding of such coherent charge modes by studying the local dynamical charge susceptibility of the insulating phase of the Sine-Gordon model. By considering parameters near the non-interacting Fermion limit where the charge operator dominantly couples to soliton-antisoliton bound states of the Sine-Gordon model, we find that the local charge susceptibility shows an array of sharp peaks in frequency representing coherent plasma oscillations on top of an incoherent background. The strength of the coherent peaks relative to the incoherent background increases as a powerlaw in frequency whose exponents depend on system parameters. The charge susceptibility also clearly shows the insulating gap. We then compare the controlled results in the high frequency limit to phase-slip-induced decay of plasmons in the Josephson junction ladder.

*This work was supported by NSF-DMR-1555135 (CAREER), JQI-NSF-PFC (PHY1430094).

12:39PM S08.00008: Application of metamaterial nano-engineering for increasing the superconducting critical temperature* MICHAEL OSOFSKY (Presenter), United States Naval Research Laboratory, VERA SMOLYANINOVA, Department of Physics Astronomy and Geosciences, Towson University, JOSEPH PRESTIGIACOMO, United States Naval Research Laboratory, PETER ROSEN, MATTHEW DICKSON, BRIAN WOODFIELD, Chemistry and Biochemistry Dept., Brigham Young University, Brigham Young University, JEFFREY W LYNN, NICHOLAS BUTCH, HEATHER CHEN-MAYER, NIST Center for Neutron Research, National Institute of Standards and Technology, IGOR SMOLYANINOV, Department of Electrical and Computer Engineering, University of Maryland — In previous work, we demonstrated that the metamaterial approach to dielectric response engineering increases the critical temperature of a composite superconductor-dielectric system in the epsilon near zero (ENZ) and hyperbolic regimes. To create such metamaterial superconductors three approaches were implemented: 1) mixtures of tin and barium titanate nanoparticles of varying composition and tin and strontium titanate nanoparticles, 2) composite Al_2O_3-coated aluminium nanoparticles, and 3) thin Al/Al_2O_3 heterostructures that form a hyperbolic metamaterial superconductor. IR reflectivity measurements confirmed the predicted metamaterial modification of the dielectric function thus demonstrating the efficacy of the metamaterial approach to T_c engineering. In this talk, we present specific heat data on samples of the composite Al_2O_3-coated aluminium nanoparticle superconductors showing that the normal state density of states (DOS) is similar to that of pure aluminum, thus precluding the DOS from being responsible for the observed enhanced T_c. We will also discuss other features in the specific heat results that are consistent with results of neutron scattering experiments.

*This work was supported in part by DARPA W911NF1710348 and ONR N00014-18-1-2681 grants.

12:51PM S08.00009: Observation of plasmon-phonons in a metamaterial superconductor using inelastic neutron scattering* VERA SMOLYANINOVA (Presenter), Towson University, JEFFREY W LYNN, NICHOLAS BUTCH, HEATHER CHEN-MAYER, NIST, JOSEPH PRESTIGIACOMO, MICHAEL OSOFSKY, NRL, IGOR SMOLYANINOV, Saitenna LLC — Recent experiments have demonstrated that the metamaterial approach is capable of drastically increasing the critical temperature, T_c, of composite metal-dielectric epsilon near zero (ENZ) metamaterial superconductors. For example, a tripling of the critical temperature was observed in bulk Al-Al_2O_3 ENZ core-shell metamaterials. A theoretical model based on the Maxwell-Garnett effective medium approximation provides a microscopic explanation of this effect in terms of electron-electron pairing mediated by a hybrid plasmon-phonon excitation in the composite metal-dielectric metamaterial. We report the first observation of a hybrid plasmon-phonon excitation in Al-Al_2O_3 ENZ core-shell metamaterials using inelastic neutron scattering. These results provide strong support for this novel mechanism of superconductivity in ENZ metamaterials and provide an explanation for the 50 year old mystery of enhanced T_c in granular aluminum thin films.

*This work was supported in part by DARPA W911NF1710348 and ONR N00014-18-1-2681 grants.
1:03PM S08.00010: Interference experiments with superconducting microwave beam splitter*  IULIIA ZOTOVA (Presenter), Moscow Institute of Physics and Technology, YU ZHOU, RUI WANG, Tokyo University of Science, OLEG ASTAFIEV, Moscow Institute of Physics and Technology, JAW-SHEN TSAI, Tokyo University of Science — Superconducting quantum circuit is one of the most promising way for realization of quantum systems. Quite interesting effects in superconducting quantum systems can be observed involving single photons interference[1]. To conduct these type of experiments, different devices like single-photon sources and an element for entanglement generation are required. The most natural realization for such element is a beam splitter [2]. In microwave range, it is convenient to use a hybrid beam splitter [1]. It is natural to use a beam splitter on-chip for less insertion losses. In the talk, the investigation of this kind of beam splitter with proposed interference experiments will be reported.


*We would like to acknowledge the support of JST CREST, ImPACT and NEDO IoP project.

1:15PM S08.00011: Transient optical response of correlated electrons*  ANKIT KUMAR (Presenter), ALEXANDER KEMPER, North Carolina State University — Recent discoveries of non-equilibrium higher order harmonic response of the superconducting condensate in cuprates, enhancement of the transient superconductivity in organic superconductor K$_2$C$_60$ and signature of the Higgs mode in BCS superconductor has attracted much attention. To understand the underlying physics behind such collective response of correlated electrons to electromagnetic field requires an understanding of response functions in the time domain. In our work, we calculate transient optical conductivity using a non-equilibrium Green's function method. We study a phonon mediated superconducting state. In the equilibrium state, we observe the normal superconducting gap in the real part of conductivity, and the $1/\omega$ divergence in the imaginary part. In a pump driven non-equilibrium state we observe suppression and the oscillatory recovery of the order parameter - the Higgs amplitude mode. We use different quantities – probe current, phonon-valley, coherence peak and the gap edge – to study the Higgs mode and the transient superconducting state. Our calculation helps in the understanding of transient superconducting state and provide a general framework to analyze the transient response of correlated electrons.

*This work is supported by NSF DMR-1752713.

1:27PM S08.00012: Manifestation of vibronic dynamics in infrared spectra of Mott insulating fullerides  NAOYA IWAHARA (Presenter), KU Leuven, YUKI MATSUDA, KATSUMI TANIGAKI, Tohoku University, LIVIU F CHIBOTARU, KU Leuven — In order to probe the nature of Jahn-Teller dynamics in alkali-doped fullerides, the fine structure and temperature evolution of infrared spectra have been intensively used last years [1,2]. At the same time, theoretical framework to adequately extract the information on the complicated vibronic dynamics from infrared spectra is still lacking. In this work, the first-principles theory of the infrared spectra of dynamical Jahn-Teller system is developed and applied to the Mott-insulating Cs$_3$C$_60$ [3]. With the calculated coupling parameters for Jahn-Teller and infrared active vibrational modes, the manifestation of the dynamical Jahn-Teller effect in infrared spectra is elucidated. In particular, the temperature evolution of the infrared line shape is explained. The transformation of the latter into Fano resonance type in metallic fulleride [2] is discussed on the basis of obtained results.


Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S09 DCMP: Nanoparticles and Nanoplatelets: Structural and Optoelectronic Properties and Phenomena  BCEC 151A - Chen-Yen Lai, Los Alamos National Laboratory
Second harmonic generation from nanoparticles of noncentrosymmetric geometry

RAKSHA SINGLA (Presenter), W LUIS MOCHAN, Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México — The nonlinear polarization resulting in generation of second harmonic (SH) radiation from centrosymmetrical (CS) media mostly takes place at the surface where the inversion symmetry is lost. This local disruption of symmetry disappears globally for a symmetrical particle, suppressing its total SH polarization. In this work, we explore SHG from particles of CS materials with non-CS geometry. We choose an isolated cylindrical particle with a deformed circular cross-section in the presence of an external field with a long wavelength. Assuming a small deformation parameter, a perturbative scheme is employed to analytically solve the linear and quadratic field equations, employing the dipolium model [1] to calculate the SH bulk and surface polarization. We report the SH dipolar and quadrupolar hyperpolarizability tensors, their spectra, the radiation patterns, and the conversion efficiency.


Quantum Dot Supercrystals: Assembly and properties

EMANUELE MARINO (Presenter), Institute of Physics, University of Amsterdam, TOM KODGER, Physical Chemistry and Soft Matter, Wageningen University, PETER SCHALL, Institute of Physics, University of Amsterdam — The assembly of semiconductor nanoparticles, quantum dots (QD), into dense crystalline nanostructures holds great promise for future optoelectronic devices. Emulsion-templated assembly has recently been shown to provide three-dimensional quantum-dot supercrystals of excellent crystal quality. We combine emulsion-templated assembly with in situ small-angle X-ray scattering to obtain direct insight into the nanoscale interactions underlying the nucleation, growth and densification of quantum dot supercrystals. We show that while hard-sphere behaviour governs their initial nucleation, at later stages the ligands play a crucial role in balancing steric repulsion against attractive van der Waals attraction. We also elucidate the optoelectronic properties of these supercrystals. We show that the supercrystals exhibit Mie resonances that can lead to absorption efficiencies larger than one, beneficial for photovoltaic applications. Ultrafast spectroscopy reveals energy transfer processes due to quantum-dot coupling in these supercrystals.

Electronic, Optical and Transport Properties of PbS Nanocrystal Superlattices

YUN LIU (Presenter), NOLAN PEARD, JEFFREY C GROSSMAN, Massachusetts Institute of Technology — Optoelectronic devices made from colloidal quantum dots (CQDs) often take advantage of the combination of tunable quantum confined optical and electronic properties and carrier mobilities of strongly coupled systems. For lattices of connected CQDs, of interest is the interplay between confinement effects and band-like behavior. In this work, first-principles calculations are applied to investigate the electronic, optical and transport properties of PbS CQD superlattices. Our results show that even in the regime of strong necking between CQDs, quantum confinement can be preserved. In the bandlike regime, computed carrier mobilities for simple cubic and 2D square lattices fused along the (100) facets are 2-4 orders of magnitude larger than those of superlattices fused along (110) and (111) facets. The relative magnitude of the electron and hole mobilities strongly depends on the crystal and electronic structures. We also find that the carrier mobilities of CQD solids increases as the size of the quantum dot increases due to the stronger coupling between neighboring CQDs. Our results illustrate the importance of understanding the effects of crystal structure and connectivity of CQD films.

The authors acknowledge the funding from Tata GridEdge Program at MIT.
measurements reveal that significant diffusional mixing occurs starting at a temperature between 300 and 400° C and involves core/shell nanoparticles to a homogeneous Cu-Ni alloy as a function of both the temperature and the time. These ex-situ x-ray diffraction measurements have been used to follow the conversion of the as-prepared core/shell nanoparticles to a homogeneous Cu-Ni alloy occurring at a temperature of 600° C. We believe that the nanoscale core-shell HMM paves a way to enlarge the development of applications, such as highly optoelectronic conversion efficiency of solar cells, great power extraction of light emitting diodes and wide spectra photodetectors.

*This work was financially supported by the "Advanced Research Center for Green Materials Science and Technology" from The Featured Area Research Center Program within the framework of the Higher Education Sprout Project by the Ministry of Education (107L9006) and the Ministry of Science and Technology in Taiwan (MOST 107-3017-F-002-001).

11:51AM S09.00004: Nanoscale Core-Shell Hyperbolic Metamaterial for Ultralow Threshold Laser Action* HUNG-I LIN (Presenter), KANCHAN YADAV, KUN-CHING SHEN, GOLAM HAIDER, YIT-TSONG CHEN, YANG-FANG CHEN, National Taiwan University — We develop the nanoscale core-shell hyperbolic metamaterial (HMM) possessing a remarkably coupling effect in between the multishell components, which is due to the formation of higher density of states and longer time of collective oscillations of the electrons than the plasmonic-based pure metal nanoparticles. Subsequently, a giant localized electromagnetic wave of surface plasmon resonance is formed at the surface causing the pronounced out-coupling effect. The nanoscale core-shell HMM confines the energy well without being decayed, reducing the propagation loss and then achieving the stimulated emission (e.g., random lasing action by dye molecule) with an ultralow lasing threshold (~30 μJ/cm²). We believe that the nanoscale core-shell HMM paves a way to enlarge the development of applications, such as highly optoelectronic conversion efficiency of solar cells, great power extraction of light emitting diodes and wide spectra photodetectors.

12:03PM S09.00005: Hot-electron generation and energy transfer in plasmonic metastructures with hot spots: Quantum and Classical mechanisms ALEXANDRE GOVOROV (Presenter), LUCAS VAZQUEZ BESTEIRO, ZHIMING M WANG, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China — Generation of energetic (hot) electrons is an intrinsic property of any plasmonic nanostructure under illumination. Simultaneously, a striking advantage of metal nanocrystals over semiconductors lies in their very large absorption cross sections. Therefore, metal nanostructures with strong and tailored plasmonic resonances are very attractive for photocatalytic applications, which often involve excited electrons. However, the central questions in the problem of plasmonic hot electrons are quantifying the number of optically excited energetic electrons in a nanocrystal and finding out how to extract such electrons. Here we develop a theory describing the generation rates and the energy distributions of hot electrons in nanocrystals with various geometries. Hot-electron generation [1] together with non-radiative plasmonic transfer [2] represent efficient mechanisms to transport and localize optical and photo-chemical energies.


12:15PM S09.00006: Solid-state diffusion in Cu core/Ni shell nanoparticles* JIE REN, ROBERT E SCHMIDT, KLAUS H THEOPOLD, KARL UNRUH (Presenter), University of Delaware — Cu core/Ni shell nanoparticles with nominal Cu/Ni atomic ratios of 2/1, 1/1, 1/2, and 1/3 have been prepared in a microwave reactor by the sequential reduction of Cu acetate (at 100° C) and Ni acetate (at 175° C) in ethylene glycol using sodium hypophosphite as the reducing agent. The measured room temperature lattice parameters of the as-prepared samples are slightly smaller/larger than the corresponding bulk Cu and Ni lattice parameters indicating a small amount of diffusional mixing at the Cu/Ni interface during sample preparation. Ex-situ vacuum annealing experiments followed by room temperature x-ray diffraction measurements and in-situ high temperature x-ray diffraction measurements have been used to follow the conversion of the as-prepared core/shell nanoparticles to a homogeneous Cu-Ni alloy as a function of both the temperature and the time. These measurements reveal that significant diffusional mixing occurs starting at a temperature between 300 and 400° C and complete mixing with the formation of a homogeneous Cu-Ni alloy occurs at a temperature of 600° C.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR140076.

12:27PM S09.00007: Growth and Shape Stability of Bi-metallic Nano-particles SONDAN DURUKANOGLU (Presenter), School of Engineering and Natural Sciences, Kadir Has University, EFE ILKER, PSL Research University, MINE KONUK, Piri Reis University, MELIHAT MADRAN, Sabanci University — Controlling the morphology of non-noble bi-metallic nano-crystals has become the focus of several studies as these nano-structures can provide a great opportunity to improve their performance and activity in catalytic reactions. Although much of the focus has been on the overall macroscopic description of synthesis processes, it is still a great challenge to identify the leading factors in a typical crystal growth process at atomic-scale. Here we report results of atomic scale calculations on shape evolution and stability of grown bi-metallic Cu-Ni nano-particles using molecular static and dynamic simulations. Our growth simulations on bare Cu and Ni nano-cubes reveals that single-atom diffusion characteristics play an important role in utilizing the particle with specific morphology and architecture.
12:39PM S09.00008: Interface Modification in Type-II ZnCdSe/(Zn)CdTe QDs for High Efficiency Intermediate Band Solar Cells* VASILIOS DELIGIANNAKIS (Presenter), SIDDHARTH DHOMKAR, MARCEL CLARO, City College of New York, IGOR KUSKOVSKY, Queens College, MARIA TAMARGO, City College of New York — Intermediate band solar cells have been proposed as being able to overcome the Shockley-Queisser limit for single junction solar cells.1 Our group has been devolving a II-VI based material system using type-II submonlayer quantum dots (QDs) composed of (Zn)CdTe embedded in a ZnCdSe host. These materials, when lattice matched to InP closely match the theoretically predicted requirements. However, do to the dissimilar group VI elements and Cd desorption that occurs during the formation of the quantum dots a highly strained interfacial layer is formed.2 A new growth process is proposed to avoid formation of a strain-inducing ZnSe interfacial layer. We show that the new growth sequence allows for improved control of the interfacial composition and simplifies the fabrication of the intermediate band solar cell device structure based on these QDs, since additional strain balancing schemes are no longer required to grow stress-free structures.


*This work is supported by NSF Grant number CBET Award# 1512017 and CREST Center IDEALS HRD-1547830.

12:51PM S09.00009: Observation of optical referigeration on CdSe/CdS quantum dots MUCHUAN HUA (Presenter), RICARDO SANTIAGO DECCA, Indiana University - Purdue University Indianapolis — Optical refrigeration on CdSe/CdS (core/shell) quantum dots (QDs) was observed for the first time. From the observed temperature drop and the experimental conditions, the effective cooling power in our experiment was estimated to be ~10^{-14} W per dot. Experiments were done with samples (colloidal QDs suspension) synthesized in our lab following the method recently developed at Peng's group (DOI: 10.1021/jacs.6b02909), which can effectively eliminate the excitonic non-radiative decay path inside the QDs. The cooling effect comes from the significant up-conversion of the mean emission energy (typical up-conversion of the mean emission energy is >25 meV) observed in the photoluminescence spectra of our samples under sub-band excitation (excitation energy is much lower than the energy band gap of the QDs). Details of the experiments and the observation will be discussed in the presentation.

1:03PM S09.00010: Confined excitons in CdSe/CdMnS and CdSe/ZnMnS nanoplatelets ARMAN NAJAFI (Presenter), PEIYAO ZHANG, TENZIN NORDEN, ARINJOY BHATTACHARYA, Department of Physics, University at Buffalo SUNY, Buffalo, NY, JAMES PIENTKA, Department of Physics, St. Bonaventure University, St. Bonaventure, NY, SUSHANT SHENDRE, SAVAS DELIKANLI, HILMI VOLKAN DEMIR, LUMINOUS! Centre of Excellence for Semiconductor Lighting and Displays, School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore, ATHOS PETROU, Department of Physics, University at Buffalo SUNY, Buffalo, NY — We have used absorption and PL spectroscopies to study the magneto-optical properties of colloidal CdSe/CdMnS and CdSe/ZnMnS core-shell nanoplatelets. We observe three absorption features tentatively attributed to the e_{1}h_{1}, e_{1}l_{1}, and e_{2}h_{2} confined excitons. In the presence of a magnetic field B applied normal to the substrate surface, the PL from e_{1}h_{1} becomes circularly polarized as \( \alpha_{+} \), indicating the presence of exchange interaction between the carrier spins and the spins of the Mn^{2+} ions. The circular polarization initially increases with B and saturates at 4T. At a fixed B the circular polarization decreases with increasing temperature and vanishes around 50K. The circular polarization peak, unlike previously studied samples [1], coincides with the e_{1}h_{1} exciton. This is attributed to the smaller thickness (2ML) of the CdSe core compared to the previously studied samples (5ML). We also measured the e_{1}h_{1} exciton magnetic splitting from the magneto-transmission spectra. Saturation splittings up to 5 meV have been observed.

First-Principles Calculations of Nanoplatelet Heterostructures: Surface Ligands and Strain

SERGIO MAZZOTTI (Presenter), Optical Materials Engineering Laboratory, Department of Mechanical and Process Engineering, ETH Zurich, ARIN R GREENWOOD, Institute for Molecular Engineering, University of Chicago, DAVID J NORRIS, Optical Materials Engineering Laboratory, Department of Mechanical and Process Engineering, ETH Zurich, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Nanoplatelets (NPLs) – highly anisotropic, quasi-two-dimensional semiconductor nanostructures – exhibit optoelectronic properties that are governed by their precisely tunable thickness of a few atomic layers. However, the atomistic structure of NPLs is not completely known and is expected to depend on the passivating ligands. Here we determine the structure of both CdSe-core and CdSe/CdS-core/shell NPLs, using Density Functional Theory (DFT) and the Qbox code[1]. For both core and core/shell NPLs with different thicknesses and ligands, we determined the equilibrium positions and the in-plane strain. We found that NPL thickness, different ligands and the presence of a shell are all factors affecting the axial atomistic structure and they are responsible for inducing an in-plane strain field, which in many studies has been neglected. We show that, compared to CdSe NPL of the same thickness, the lattice constants of the core-shell NPLs expand in the axial direction, in agreement with recent experiments[2]. We rationalize our first principles findings by a continuum elastic model including surface-stress terms that account for the surface passivation of NPLs.


*Supported by DOE grant No. DE-FG02-06ER46262.

First Principles Calculations of Nanoplatelet Heterostructures: Optoelectronic Properties

ARIN R GREENWOOD (Presenter), Institute for Molecular Engineering, University of Chicago, SERGIO MAZZOTTI, Optical Materials Engineering Laboratory, Department of Mechanical and Process Engineering, ETH Zurich, ABHIJIT HAZARIKA, IGOR COROPCEANU, DMITRI TALAPIN, Department of Chemistry and James Franck Institute, University of Chicago, GIULIA GALLI, Institute for Molecular Engineering and Materials Science Division, University of Chicago and Argonne National Laboratory — Two-dimensional, atomically precise core-shell nanoplatelets (NPLs) have recently been synthesized with no sample inhomogeneity, leading to remarkable photoluminescence quantum efficiencies and tunable electronic properties dependent on NPL thickness [1]. Here we use Density Functional Theory and the Qbox code [2] to investigate the unique optoelectronic properties of CdS/CdSe core-shell NPLs. We show that, compared to a pure CdSe NPL of the same thickness, the band gap and dielectric constant of the core-shell NPLs decrease consistent with experimental results, corresponding to a larger exciton binding energy by approximately 30%. We attribute our findings to an expansion of the lattice constant of the core-shell NPLs in the axial direction, leading to a strain-induced modification of the electronic properties of the system. In contrast to nanoparticles, where the optoelectronic properties are governed by quantum confinement, we find that the properties of NPLs depend on a subtle interplay between quantum confinement and strain induced in the NPLs by the heterostructured interfaces.


*Supported by DOE grant No. DE-FG02-06ER46262.
1:39PM S09.00013: Low-temperature photoluminescence spectroscopy of single core/shell nanoplatelets  
LINTAO PENG (Presenter), Center for Nanoscale Materials, Argonne National Laboratory, IGOR COROPECEANU, DMITRI TALAPIN,  
Department of Chemistry and James Franck Institute, University of Chicago, XUEDAN MA, Center for Nanoscale Materials, Argonne National Laboratory — With promising applications in lasing, light-emitting diodes, as well as quantum photonics, semiconducting nanoplatelets (NPLs) with atomically controlled thickness and giant oscillator strength has attracted considerable interest in the past few years. Our previous studies\(^1\) have revealed that with excitons in NPLs being strongly confined in the thickness direction, an increase in their lateral size and a weakening in the in-plane confinement has complex effects on their photon emission statistics and carrier dynamics. These properties are unique to NPLs due to their quasi-two-dimensional structures.

While room temperature studies of single NPLs provide valuable information, the spectrum is broadened by carrier-phonon interactions, making the assignment of optical transitions and the related electronic structures challenging. Here, we perform single NPL spectroscopic measurements at cryogenic temperatures. Spectral linewidth and diffusion are investigated systematically. In addition, we observe rich spectral fine structures from the NPLs. These results will shed new light on the intrinsic electronic structures of the NPLs, and help understand the origin of the much debated side emission peak observed in ensemble measurements.
\(^1\) X. Ma et al. ACS Nano, 2017, 11, 9119 – 9127

1:51PM S09.00014: Tuning the Photophysical Properties of Colloidal Two-Dimensional Nanoplatelets*  
QUNFEI ZHOU (Presenter), Materials Research Center, Northwestern University, YEONGSU CHO, Department of Chemistry, University of Chicago, SHENYUAN YANG, Institute of Semiconductors, Chinese Academy of Sciences, EMILY A WEISS, Department of Chemistry, Northwestern University, TIMOTHY BERKELBACH, Department of Chemistry, University of Chicago, PIERRE DARANCET, Center for Nanoscale Materials, Argonne National Laboratory — Two-dimensional colloidal semiconductor nanoplatelets (NPLs) are promising optoelectronic materials with outstanding photophysical properties, such as large optical cross-sections and high photoluminescence quantum yield.

Using first-principles density functional theory calculations, we demonstrate strong tunability of NPL band edge energies through surface passivation by common organic molecules. We develop a simple quantitative electrostatic theory describing this effect through dipole-dipole interactions mediated by platelet-ligand interactions and ligand-dependent dielectric function. Finally, using parameter-free self-energies and an effective mass model of the excitons, we show that the band-edge tunability of NPLs together with the strong dependence of the optical bandgap of NPL on thickness can lead to favorable, and controlled tunability of photochemical and optoelectronic properties.

* Funded by NSF through Northwestern MRSEC grant DMR-1720139. Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02- 06CH11357.

Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S10 DMP: Fe-based Superconductors -- Nematicity II  
BCEC 151B - Qing-Ping Ding, Ames Laboratory - 
Tag(s): Focus

11:15AM S10.00001: Interplay between nematicity and superconductivity in iron-based superconductors* [Invited]  
JIAN KANG (Presenter), Florida State University — The iron-based high-T\(_c\) superconductors exhibit several remarkable features, including the multi-orbital character and the ubiquity of the nematic phase. One consequence of the multi-orbital Fermi surface is that the spin-fluctuation mediated pairing interactions are sensitive to the orbital spectral weight at the Fermi surface, leading to several different possible gap structures, such as nodeless s\(_±\), nodal s\(_±\), and d-wave. Focused on the orbital order induced in the nematic phase, I will discuss how the nematic order can manipulate the properties of SC. Our calculation shows that not only \(T_c\) is enhanced, but more importantly, the gap structure becomes a mixture of nearly degenerate s and d-wave states by increasing the external strain. This mixture of s and d wave pairing channels has been recently found in the superconducting phase of the bulk FeSe, when SC occurs deeply inside the nematic phase.

* JK was supported by the National High Magnetic Field Laboratory through NSF Grant No. DMR-1157490 and the State of Florida.
11:51AM S10.00002: Probing nematic fluctuations in iron-based superconductors with pair distribution function analysis*  
BENJAMIN FRANDSEN (Presenter), Brigham Young University, KEITH TADDEI, Oak Ridge National Laboratory, DANIEL BUGARIS, Argonne National Laboratory, RYAN STADEL, Northern Illinois University, MING YI, Rice University, QISI WANG, JUN ZHAO, Fudan University, RAYMOND OSBORN, STEPHAN ROSENKRANZ, Argonne National Laboratory, OMAR CHMAISSEM, Northern Illinois University, ROBERT J BIRGENEAU, University of California, Berkeley — The origin and implications of nematicity in iron-based superconductors remain among the most pressing questions in the field. Recent efforts to address this topic have focused not only on the nematic phase itself, but also on the nematic fluctuations that exist outside the region of static nematicity. Pair distribution function (PDF) analysis of x-ray and neutron total scattering data is a proven method of studying local, short-range structural correlations that deviate from the average structure, such as the orthorhombic distortions associated with nematic fluctuations in the high-temperature tetragonal phase of iron-based superconductors. Focusing primarily on the representative hole-doped system (Sr,Na)Fe2As2, we present PDF analysis that reveals a remarkably large region of nanometer-scale local orthorhombic distortions in temperature-composition space, reaching up to approximately 500 K for the parent compound and extending to doping levels beyond the C2 dome near optimal superconductivity. These results offer a rich and detailed view of nematic fluctuations in iron-based superconductors and should be helpful in guiding future experimental and theoretical work.

*Support came primarily from the U.S. Department of Energy under Contract No. DE-AC02-05-CH11231.

12:03PM S10.00003: Spin correlations and B2g nematicity in extremely hole doped iron pnictides  
RONG YU (Presenter), Department of Physics, Renmin University of China, QIMIAO SI, Rice University — There is growing experimental evidence for B2g nematic correlations in the extremely hole doped iron pnictide compounds AFe2As2 (A=K,Rb,Cs). In this work, we construct a general Ginzburg-Landau theory for the nematic transitions driven by incommensurate spin correlations. We find various nematic orders depending on the nature of the incommensurate spin correlations, and demonstrate a unified description of the nematicity in both the parent and doped iron pnictides. For the extremely hole doped iron pnictides, our analysis provides a mechanism for a B2g nematic order developing from the pertinent incommensurate spin fluctuations. We further study an extended bilinear-biquadratic Heisenberg model, which provides additional evidence for the proposed mechanism.

12:15PM S10.00004: Doping-dependent nematic susceptibility and strain-tunable Tc in FeTe1-xSex*  
QIANNI JIANG (Presenter), Physics, University of Washington, YUE SHI, Materials Science & Engineering, University of Washington, JJUN-HAW CHU, Physics, University of Washington — In comparison to the end member FeSe, the role of nematicity in the FeTe1-xSex family is less explored. Using the elastoresistivity technique, we measured the nematic susceptibility of FeTe1-xSex over a wide range of doping, and revealed the presence of strong B2g nematic fluctuations despite the absence of static nematic order. We also studied the effects of anisotropic strain on the superconducting transition temperature, providing insight into the interplay between nematic fluctuations and the superconductivity.

*NSF MRSEC at UW DMR1719797 and The Gordon and Betty Moore Foundation’s EPiQS Initiative Grant GBMF6759

12:27PM S10.00005: Anisotropy in Superconducting CsCa2Fe4As4F2 Single Crystals*  
ZHICHE NG WANG (Presenter), YI LIU, SI-QI WU, YE-TING SHAO, Zhejiang University, ZHI REN, Institute of Natural Science, Westlake University, GUANG-HAN CAO, Zhejiang University — CsCa2Fe4As4F2 is a typical example of 12442-type iron-based superconductors. The novel materialsuperconducts at 29.5 K without extrinsic chemical doping. It contains double Fe2As2 layers that are separated by insulating CaF2 layers. The structural feature may lead to the weak interlayer coupling and strong anisotropy. In this work we successfully synthesized high quality CsCa2Fe4As4F2 single crystals with CsAs flux. Measurements of X-ray diffraction, anisotropic magnetotransport and magnetization were carried out to characterize the single crystals. The anisotropic superconducting upper Hc2 (T), lower critical field Hc1 (T), the anisotropy parameter γ (T) and other related parameters were obtained. The results indicate that CsCa2Fe4As4F2 is one of most anisotropic iron-based superconductors.

*This work was supported by the National Key Research and Development Program of China (Grant No. 2017YFA0303002).
12:39PM S10.00006: Unusual nematic behavior of heavily hole-doped AFe$_2$As$_2$* VLADISLAV BORISOV (Presenter), Institute of Theoretical Physics, Goethe University Frankfurt, Frankfurt am Main, Germany., RAFAEL M FERNANDES, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA., ROSER VALENTI, Institute of Theoretical Physics, Goethe University Frankfurt, Frankfurt am Main, Germany. — We investigate via density functional theory calculations the recently reported unusual nematic behavior of heavily hole-doped pnictides AFe$_2$As$_2$ (A = Rb, Cs) [1,2]. In contrast to the B$_{2g}$ nematic order of the parent 122 compounds, characterized by unequal Fe-Fe bonds, in the former systems nematic order is observed in the B$_{1g}$ channel, characterized by unequal Fe-As-Fe bonds. We attribute this behavior to the evolution of the magnetic ground state along the compound series Sr$_{1-x}$Rb$_x$Fe$_2$As$_2$, from single stripes for small $x$ to double stripes for large $x$. Our simulations using the reduced Stoner theory show that fluctuations of Fe moments are essential for the stability of the double-stripe configuration. We discuss the relationship between these magnetic orderings and the nature of nematicity in terms of vestigial orders [3].

References

*VB and RV acknowledge the financial support by the German Research Foundation (DFG) and the computer time by the Center for Supercomputing (CSC) in Frankfurt. RMF is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.

12:51PM S10.00007: Nematic fluctuations at nonzero q in FeSe vs. Ba(Fe1-xCox)2As2* ADRIAN MERRITT (Presenter), University of Colorado, Boulder, FRANK WEBER, JOHN-PAUL CASTELLAN, Karlsruhe Institute of Technology, ALFRED Q R BARON, DAI SUKE Ishikawa, RIKEN, SPring-8, AYMAN SAID, AHMET ALATAS, Argonne Nati Lab, TRAVIS WILLIAMS, Oak Ridge Nati Lab, RAFAEL M FERNANDES, University of Minnesota, JOERG SCHMALIAN, Karlsruhe Institute of Technology, DMITRY REZNIK, University of Colorado, Boulder — FeSe and Ba(Fe1-xCox)2As2 (Ba122) have several shared phase transitions such as the tetragonal-to-orthorhombic structural transition associated with nematic electronic order as well as a superconducting transition. There are also important differences, including magnetic order found in the Ba122 but not the FeSe compounds. Our recent inelastic X-ray and neutron scattering measurements of TA phonons in these compounds focused on anomalies in their dispersion. These anomalies reflect nematic fluctuations at nonzero q. We obtained nematic correlation length as a function of temperature from fits to these anomalous dispersions and found that it is similar in FeSe and Ba(Fe0.96Co0.04)2As2: compounds whose structural transition temperatures are close. In addition, we measured TA phonon dispersions and linewidths in optimally-doped Ba122 in detail. I will discuss the implications of the observed phenomena, focusing on the relation between nematic correlation length and the structural transitions, magnetic order, and superconductivity.

*DOE, Office of Basic Energy Sciences, Office of Science, Contract No. DE-SC0006939 (AM & DR)
HFIR, Oak Ridge National Laboratory, USA
Advanced Photon Source, Argonne National Laboratory, USA
RIKEN, SPring-8, Japan
ORPHEE, Laboratoire Leon Brillouin, France

1:03PM S10.00008: Nematic fluctuations in Ba(Fe1-xTMx)2As2 (TM = Cr, Mn, V and Cu): Why superconductivity cannot be achieved by these dopants YANHONG GU (Presenter), HUIQIAN LUO, SHILIANG LI, National Laboratory for Superconductivity, Institute of Physics, Chinese Academy of Sciences — We have systematically studied nematic susceptibilities in nonsuperconducting Ba(Fe1-xTMx)2As2 (TM = Cr, Mn, V and Cu) single crystals by measuring the uniaxial pressure dependence of the resistivity along the Fe-As-Fe direction. The nematic susceptibilities in all samples show the Curie-Weiss-like behavior at high temperatures, where the nematic Curie constant $A_n$ can be derived. In Cr, Mn and V doped samples, $A_n$ decreases with the doping level, suggesting the suppression of nematic fluctuations by these dopants. In Ba(Fe1-xCu$_x$)$_2$As$_2$, detailed neutron-diffraction measurements reveal that the collinear antiferromagnetic order persists up to $x = 0.08$ but becomes short-range above $x > 0.04$. Moreover, the nematic susceptibilities in the $x >0.04$ samples are significantly suppressed at low temperatures although $A_n$ obtained by fitting the high-temperature data increases with increasing $x$. Compared with those systems that clearly exhibit superconductivity, such as Co, Ni, K or P doped samples, our results suggest that the reason that no superconductivity is found by doping Cr, Mn, V and Cu in BaFe$_2$As$_2$ may be correlated with the suppression of nematic fluctuations.
Effect of controlled point-like disorder induced by 2.5 MeV electron irradiation on nematic resistivity anisotropy of hole-doped (Ba,K)Fe$_2$As$_2$*  

MAKARIY TANATAR (Presenter), Ames Laboratory US DOE, Ames, Iowa, ERIK TIMMONS, Department of Physics and Astronomy, Iowa State University, Ames, Iowa, KYUIL CHO, YONG LIU, THOMAS ANTONY LOGRASSO, RUSLAN PROZOROV, Ames Laboratory US DOE, Ames, Iowa, MARCIN KONCZYKOWSKI, OLIVIER CAVANI, Laboratoire des Solides Irradiés, École Polytechnique, F-91128 Palaiseau, France — In iron-based superconductors in-plane anisotropy of electrical resistivity in strain-detwinned samples strongly depends on residual resistivity [1]. The mechanism of the electronic transport responsible for sign change of in-plane resistivity anisotropy in hole-doped (Ba,K)Fe$_2$As$_2$ [2] attracts notable interest, since contributions from both elastic scattering due to impurities/defects and inelastic scattering on magnetic excitations and phonons can be anisotropic. We use irradiation with relativistic 2.5 MeV electrons at low temperatures to change residual resistivity and study the contribution of elastic scattering into anisotropic electronic transport. The modification of detwinning technique enabled measurements of the same samples before and after irradiation.


*Nematic Glassy Behavior Probed by NMR under Strain in Iron Pnictide Superconductors  

TANAT KISSIKOV (Presenter), University of California, Davis, MAKARIY TANATAR, PAUL CANFIELD, Ames Laboratory, ERICA CARLSON, Purdue University, KARIN ANDREA DAHMEN, University of Illinois at Urbana-Champaign, NICHOLAS CURRO, University of California, Davis — NMR studies of Ba(M$_x$Fe$_{1-x}$)$_2$As$_2$ (M = Co, Cu) have uncovered inhomogeneous glassy dynamics via stretched exponential relaxation and wipeout of the NMR signal. These signatures emerge below approximately 100-150 K, depending on the doping level, and reach a maximum onset temperature around the nematic quantum critical point. Here we present NMR data under uniaxial strain in Ba(CoxFe1-x)2As2 (x=0.08) at the nematic quantum critical point. The relaxation behavior reveals inhomogeneous relaxation that is strongly temperature-dependent and hysteric with strain. The stretching exponent, which probes the degree of inhomogeneity, remains unchanged under strain. These results suggest that the inhomogeneous relaxation observed by NMR reflects a nematic glass, in which large random strain fields are present and frustrate long-range nematic order.
1:51PM S10.00012: Persistent correlation between superconductivity and antiferromagnetic fluctuations near a nematic quantum critical point in FeSe$_{1-x}$S$_x$ seen by $^{77}$Se NMR*  PAUL WIECKI (Presenter), Karlsruhe Institute of Technology, KHUSBOO RANA, MOUMITA NANDI, Iowa State University, ANNA BOEHMER, Karlsruhe Institute of Technology, SERGEY BUDKO, PAUL CANFIELD, YUJI FURUKAWA, Iowa State University — In the iron-based superconductors, the superconducting pairing interaction is believed to involve antiferromagnetic spin fluctuations. However, fluctuations of the nematic degrees of freedom are also present in these materials and may also be involved in the pairing. A role for electronic nematic fluctuations in achieving high-temperature superconductivity has been suggested by the ubiquitous observation of critical nematic fluctuations near optimal doping in several of the key families. In this context, the FeSe$_{1-x}$S$_x$ system offers an opportunity to study an isolated nematic critical point, as the nematic order of pure FeSe is suppressed by S doping without the appearance of magnetic order. I will present $^{77}$Se NMR measurements which demonstrate that low-energy magnetic fluctuations are well correlated with the superconducting transition temperature $T_c$ in FeSe$_{1-x}$S$_x$, similar to pure FeSe under pressure. These findings confirm that magnetic fluctuations alone are the primary driver of superconductivity, even in the presence of critical nematic fluctuations.


*This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S11 DCMP: Group IV- and III-V-Based Low-Dimensional Semiconductor Heterostructures

11:15AM S11.00001: Band engineering of semiconductor artificial graphene and exploration of flat band physics(*)*  LINGJIE DU (Presenter), Department of Applied Physics and Applied Mathematics, Columbia University, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, SAEED FALLAHI, GEOFFREY GARDNER, Department of Physics and Astronomy, Purdue University, MICHAEL MANFRA, Department of Physics and Astronomy, School of Materials Engineering and School of Electrical and Computer Engineering, Purdue University, VITTORIO PELLEGRINI, Istituto Italiano di Tecnologia, SHALOM WIND, Department of Applied Physics and Applied Mathematics, Columbia University, ARON PINCZUK, Department of Applied Physics and Applied Mathematics and Department of Physics, Columbia University — Semiconductor artificial graphene (AG) has been realized on 2D electron systems in GaAs quantum wells subjected to a lateral potential modulation with honeycomb symmetry [1, 2]. Tunability of the AG band structure is a key property of the artificial systems. Here, we present effective band engineering of semiconductor AG with multiple control knobs that offer flexible and effective exclusive tunability of electron properties. Using the cutting-edge fabrication technology, we fabricated small-period triangular antidot lattices with different honeycomb lattice periods (35 nm to 45 nm) and various AG potentials. The M-point gap, which reveals key characteristics of the AG band structure, was measured by intersubband excitations using resonant inelastic light scattering (RILS) at low temperature. We found that the M-point gap could be tuned from 0.5 meV to 1.2 meV, with the band dispersion near the M point evolving from the Dirac-like case to flat band. Emerging flat-band physics in such tunable system will be discussed. [1] S. Wang, et al. Nature Nanotech. 13, 29 (2018). [2] L. Du, et al., Nature Commun. 9, 3299 (2018).

*(*) Supported by Awards DOE_BES DE-SC0010695, and NSF-DMR-1306976
11:27AM S11.00002: Fabricating shallow 2D systems in GaAs/AlGaAs heterostructures towards the creation of Artificial Graphene  
YONATAN ASHLEA ALAVA (Presenter), OLEH KLOCHAN, QINGWEN WANG, School of Physics, University of New South Wales, ANDREAS D. WIECK, ARNE LUDWIG, JULIAN RITZMANN, Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, ALEX R HAMILTON, School of Physics, University of New South Wales — Patterning ordinary GaAs/AlGaAs heterostructures with a triangular nano-array of quantum anti-dots has been shown to yield Artificial Graphene. The lattice spacing of the patterned quantum anti-dot array must be in the order of 100 nm to enable the observation of Dirac physics. This implies that the GaAs/AlGaAs interface has to be considerably shallower than 100 nm to enable strong modulation of the 2D carriers with surface gates. Fabricating low disorder shallow 2D systems is experimentally challenging due to the close proximity to the surface and the thin barrier to the surface gate, determined by the AlGaAs layer. This thinner barrier increases leakage between the gate and the 2D system, and increases scattering at the interface, damaging the mobility of the 2D carriers.

Here we present results on the fabrication of 2D systems in accumulation mode heterostructures as shallow as 35 nm. We use aluminium gates grown in-situ in the MBE chamber, to avoid exposing the GaAs surface to air. Surprisingly, we find that the 2D mobility with an ‘in situ’ gate is lower than with an ‘ex situ’ gate. We investigate the density dependence of the mobility to identify the underlying scattering mechanisms behind this observation.

11:39AM S11.00003: A novel route to achieve two dimensional (2D) carrier confinement in a wedge-shaped polar semiconductor structure  
SWARUP DEB (Presenter), SUBHABRATA DHAR, Physics, Indian Institute of Technology Bombay — A novel route to achieve two dimensional (2D) carrier confinement in a wedge-shaped polar semiconductor has been demonstrated theoretically. Tapering of the wall along the direction of the spontaneous polarization leads to the development of charges of equal polarity on the two inclined facets of the wall. Negative/positive polarization charges on the facets can push the electrons/holes inward for an n-/p-type material leading to the formation of 2D electron/hole gas at the central plane and depletion regions at the outer edges of the wall. Schrodinger and Poisson equations are solved self-consistently to obtain the potential and charge density distribution in n-type GaN nanowalls, tapered along c-axis by different angles. Carrier mobility in this 2D carrier gas is estimated to be significantly higher than that of bulk. A recent experimental finding indeed shows a very high electron mobility in wedge-shaped GaN nanowall networks. Properties of high mobility and the vertical orientation of the 2D confinement can be exploited in fabricating highly conducting transparent interconnects and high mobility field effect transistors, which can lead to a large-scale integration of 2D devices in future.


11:51AM S11.00004: Classical elements in the magnetoconductance of two-dimensional Lorentz gases*  
BEATE HORN-COSFELD (Presenter), JAKOB SCHLUCK, Condensed Matter Physics, Heinrich-Heine University Düsseldorf, NIMA HAMIDI SIBONI, JÜRGEN HORBACH, Institute of Theoretical Physics II, Heinrich-Heine University Düsseldorf, THOMAS HEINZEL, Condensed Matter Physics, Heinrich-Heine University Düsseldorf — Electrons moving through an array of identically shaped obstacles at random positions form a Lorentz gas. [1] In two-dimensional systems, strong deviations of the magnetoresistance from the Boltzmann model are observed experimentally and in numerical simulations, which have a classical origin. At low magnetic fields, memory effects [2] cause subdiffusive transport, which generates a strong positive magnetococonductivity, while weak localization is absent. At intermediate magnetic fields, the transport develops a superdiffusive character, which is visible as a pronounced maximum in the magnetoconductance at sufficiently large obstacle densities. [3] In dilute two-dimensional Lorentz gases, the interplay between the Lorentz obstacles and the residual background disorder causes strong corrections to the behavior of a clean Lorentz gas.

12:03PM S11.00005: Temperature dependence of transverse magnetic focusing in high-mobility GaAs/AlGaAs*
ADBHUT GUPTA (Presenter), JEAN HEREMANS, Virginia Tech, SAEED FALLAHI, MICHAEL MANFRA, Purdue University — The temperature dependence of the ballistic and mesoscopic transport phenomenon of transverse magnetic focusing (TMF) is investigated in a two-dimensional electron system in a high-mobility GaAs/AlGaAs heterostructure at low temperatures 0.4 K < T < 20 K (electron mean free path ~ 80 μm at 4.2 K). Measurements use in-line configurations with distance between the injector and collector of L = 7 μm, and bent TMF configurations with L = 5 μm horizontal and 2 μm vertical. In both configurations, the TMF amplitude (non-local resistance $R_f$) shows a monotonic decrease as T is increased from 4 K to 20 K, according to $R_f \sim 1/T^2$. The dependence on T is analyzed by fitting $R_f$ according to different scattering mechanisms, with $R_f \sim 1/T^2$ indicating a dominant role for inelastic electron-electron interactions. In the particular temperature range, electron-electron interactions point to the importance of momentum exchange between the ballistic beam and the surrounding carrier fluid, and hence to the existence of a hydrodynamic transport regime, which has recently received increasing attention. The experiments suggest that in addition to ballistic aspects, TMF presents hydrodynamic aspects as well.

*DOE DE-FG02-08ER46532

12:15PM S11.00006: Studies on the nonlinear optical properties of two-step GaAs/Ga$_{1-x}$Al$_x$As quantum well
JUAN CARLOS MARTINEZ OROZCO (Presenter), Unidad Académica de Física, Universidad Autónoma de Zacatecas, F. UNGAN, Faculty of Technology, Department of Optical Engineering, Cumhuriyet University, K. A. RODRÍGUEZ-MAGDALENO, Unidad Académica de Física, Universidad Autónoma de Zacatecas, A. DEL RÍO-DE SANTIAGO, Unidad Académica de Ingeniería, Universidad Autónoma de Zacatecas — The numerical computation for the absorption coefficient and the relative refactive index change, considering the third order correction nonlinear optical properties, is reported. This study was performed for an interesting symmetric two-step GaAs/Ga$_{1-x}$Al$_x$As quantum well subjected to a constant electric field applied along the growth direction z of strength $F$, an in-plane constant magnetic field of magnitude $B$ and considering also the intense laser field effect. The optical properties study is performed by using the well-studied compact matrix formalism expression for the nonlinear optical properties of interest. In the case of the intense laser field effect on the system, when this is irradiated, we implemented the so-called laser-dressed potential deformation characterized by the laser-dressing parameter $\alpha_0$. In general we find that the structural parameters as the step-potential of the central barrier width, permit to control the resonant peak and the amplitude in an important way, the system becomes more sensible to electric than to magnetic field, and finally the intense, non-resonant, laser field can strongly change the optical properties.

12:27PM S11.00007: Carrier Lifetime Analysis in a Transistor Laser by Using Non-Equilibrium Green's Function Method with Effective Bond-Orbital Model*
FU-CHEN HSIAO (Presenter), University of Illinois at Urbana-Champaign, YIA-CHUNG CHANG, Research Center for Applied Sciences, Academia Sinica, JOHN DALLESASSE, University of Illinois at Urbana-Champaign — Carrier injection and recombination in a single quantum well AlGaAs/InGaP/GaAs/InGaAs transistor laser (TL) is examined theoretically with the non-equilibrium Green's function (NEGF) method. The multi-band effects are incorporated in the NEGF method by applying effective bond-orbital model (EBOM). Carrier-phonon scattering are taken into account within the deformation-potential approximation. The squared momentum matrix elements, scattering rate, and the density of states for the quantum well in a TL are presented. In addition, the simulated I-V characteristics as well as the frequency response of the TL is shown and compared with the experimental data. In the end, the carrier recombination in the quantum well as well as the base region are discussed based on the results calculated by the present model.

*This work is based in part upon work supported by the National Science Foundation under Grant Number ECCS 16-40196 and the Semiconductor Research Corporation under Grant Number NERC 2016-NE-2697-A.
Acoustic Nanostructures for Charge Carrier Confinement in GaAs/AlGaAs Multiple Quantum Wells

KEVIN VALLEJO (Presenter), CHRISTOPHER F SCHUCK, KATHRYN E SAUTTER, Micron School of Materials Science and Engineering, Boise State University, TRENT GARRETT, Physics, Boise State University, ARIEL E WELTNER, Micron School of Materials Science and Engineering, Boise State University, BAOLAI LIANG, California NanoSystems Institute, University of California, Los Angeles, ZILONG HUA, DAVID H HURLEY, Idaho National Laboratory, PAUL J SIMMONDS, Micron School of Materials Science and Engineering, Boise State University — Quantum confinement of charge carriers in semiconductors is at the heart of next generation technologies for energy conversion, encryption and computation. We use picosecond-duration surface acoustic phonon pulses to produce lateral 2D and 3D carrier confinement in polar III-V semiconductor quantum wells. Shear strain and dilatation generated by the phonon pulses vary with depth below the sample surface, locally deforming the valence and conduction bands to produce lateral confinement in the plane of a quantum well that is externally controllable. We grew a GaAs/AlGaAs heterostructure containing three quantum wells, 5, 7, and 10 nm wide, at depths of 14, 49, and 112 nm beneath the sample surface respectively, to coincide with different piezoelectric field strengths. We verify carrier confinement and transport using metallic gratings on the surface of the sample to generate and detect surface acoustic phonons. These gratings modulate light absorption on length scales below the optical diffraction limit. Our approach enables a spectrally selective scheme for generating surface acoustic phonons 20 – 200 nm in wavelength. Length scales at the lower end of this range are associated with quantum confinement.

*This work is supported by the US DOE under award LDRD #17P11-030FP

The Effect of Nanostructure on Near-Infrared Absorption in M-Plane AlGaN/(In)GaN Heterostructures

TRANG NGUYEN (Presenter), MOHAMMADALI SHIRAZI-HOSSEINI-DOKHT, YANG CAO, Physics and Astronomy, Purdue University, ALEXANDER SENICHEV, Birck Nano Technology Center, Purdue University, BRANDON DZUBA, Physics and Astronomy, Purdue University, ROSA DIAZ, GEOFFREY GARDNER, Birck Nano Technology Center, Purdue University, OANA MALIS, MICHAEL MANFRA, Physics and Astronomy, Purdue University — Near infrared intersubband (ISB) absorption of nonpolar AlxGa1-xN/(In)GaN is studied due to its broad potential applications into optoelectronic devices. Above 60% Al-composition, m-plane AlGaN alloy becomes kinetically unstable during the plasma-assisted molecular beam epitaxy growth generating unique nanostructures. The nanostructures are imaged with energy dispersive x-ray spectroscopy and scanning transmission electron microscopy. They consist of platforms of higher than expected Al-composition and islands of lower Al-composition AlGaN. We discuss the consequences of these nanostructures on ISB absorption energy and linewidth. We are also investigating strain-balanced AlxGa1-xN/InGaN (x<0.6) as an alternative to AlxGa1-xN/GaN (x>0.6).

*We acknowledge support from the National Science Foundation. MS-HD was supported in part by NSF award DMR-1610893. TN, YC, and OM acknowledge partial support from NSF grant ECCS-1253720. AS and BD was supported from NSF award ECCS-1607173.

Influence of QD Morphology on Photoluminescence in GaSb/GaAs Multilayers

CHRISTIAN GREENHILL (Presenter), ERIC ZECH, ALEXANDER CHANG, Materials Science & Engineering, University of Michigan - Ann Arbor, STEPHEN CLARK, GANESH BALAKRISHNAN, Electrical and Computer Engineering, University of New Mexico - Albuquerque, RACHEL GOLDMAN, Materials Science & Engineering, University of Michigan - Ann Arbor — Due to the predicted composition and strain dependence of type I versus type II band offsets, GaSb/GaAs quantum dots (QDs) are promising for a variety of optoelectronic applications. For GaSb/GaAs multilayers, atomic structures ranging from QDs, quantum rings and clusters have been observed, with photoluminescence (PL) energies ranging from 0.9 to 1.3eV. However, the association of these emission energies with specific nanostructure morphologies remains elusive. We investigate the structural and optical properties of GaSb/GaAs multilayers, with and without 3D nanostructures, using cross-sectional transmission electron microscopy, atom probe tomography (APT), and PL. In both cases, we find PL energies at 1.33eV and 1.49eV, which are attributed to 2D GaSb/As layers and the GaAs matrix, respectively. For the case with 3D nanostuctures, both individual QDs and circular arrangements of QDs, termed QD-rings, are observed. For both cases, Sb-rich cores are apparent, with xSb up to 0.40 (individual QDs) and 0.25 (QD-rings). Thus, we attribute 1.08 eV and 1.2 eV emissions to the individual QDs and QD-rings, respectively. Local measurements of the electronic states using scanning tunneling microscopy will also be presented.

*We gratefully acknowledge support of the NSF, DGE 1256260.
1:15PM S11.00011: Lattice-matched In$_{0.17}$Al$_{0.83}$N/GaN heterostructures for near-infrared intersubband absorption

ALEXANDER SENICHEV (Presenter), TRANG NGUYEN, ROSA DIAZ, BRANDON DZUBA, MOHAMMADALI SHIRAZI-HOSSEINI-DOKHT, YANG CAO, MICHAEL MANFRA, OANA MALIS, Purdue University — Lattice-matched In$_{0.17}$Al$_{0.83}$N/GaN heterostructures are promising platforms for near-infrared optoelectronic devices based on intersubband transitions. Previously, strong near-infrared intersubband absorption (ISBA) was demonstrated in InAlN/GaN superlattices. But, reducing compositional inhomogeneity of InAlN barriers and effective doping of these heterostructures that affect ISBA properties presented open challenges. Here, we demonstrate that InAlN/GaN structures with saturated indium composition of 0.17 can be grown by plasma-assisted molecular beam epitaxy over a wide range of growth conditions and constructed the growth diagram for lattice-matched InAlN layers. Our results indicate that the studied growth conditions alone are not sufficient to eliminate the indium segregation and additional mechanisms are involved. The impact of an indium adlayer and a thin AlN nucleation layer on compositional inhomogeneity of InAlN barriers is discussed. We report the impact of different Si doping profiles and doping levels on structural quality and hence ISBA properties of lattice-matched InAlN/GaN superlattices.

*AS and BD were supported from NSF award ECCS-1607173. TN, YC, and OM acknowledge partial support from NSF grant ECCS-1253720. MS-HD was supported in part by NSF award DMR-1610893.

1:27PM S11.00012: Integrated III-V/Si Visible and IR Nanowire Photodetectors

ARJUN SHETTY (Presenter), EDUARDO BARRERA, FRANCOIS SFIGAKIS, Institute for Quantum Computing, University of Waterloo, MITCHELL ROBSON, NEBILE ISIK, CURTIS GOOSNEY, RAY LAPIERRE, Department of Engineering Physics, McMaster University, JONATHAN D BAUGH, Institute for Quantum Computing, University of Waterloo — Self-assembled nanowires can support optical resonant modes and act as very effective waveguides that concentrate and absorb light over only a few microns of nanowire length, enabling highly efficient photodetection. The resonant absorption shows wavelength selectivity that can be tuned continuously across the visible and IR wavelengths by adjusting the nanowire diameter during molecular beam epitaxy growth on silicon wafers. Thus, ordered arrays of III-V semiconductor nanowires, integrated with standard Si technology, could provide low-cost, high-performance multi-spectral photodetectors.

We realized photodetectors from ordered arrays of InAs (~120 nm diameter) and GaAs (~300 nm diameter) nanowires grown on Si(111) substrates. The nanowires grow out of holes etched into a thin oxide layer down to the Si layer. These holes are lithographically patterned and allow control of the nanowire diameter, pitch and array size, the latter being adjustable down to a single nanowire. The nanowires show a wavelength-dependent response, with a peak centered at ~450 nm for InAs and ~750 nm for GaAs.

1. Rahman et. al., Nanotechnology 26(2015)295202

*We thank NSERC, the Canada First Research Excellence Fund, the Quantum NanoFab facility, and the Centre for Emerging Device Technologies at McMaster.

1:39PM S11.00013: White-light Emitted InGaN Nanorods Grown on Pyramided Si Substrate

CHUN-YEH LIN (Presenter), CHUNG-LIN WU, SHU-JU TSAI, SHENG-SHONG WONG, NIEN-TING TSAI, National Cheng Kung University — In this study, white-light emitted InGaN nanorods were grown on pyramided Si substrate by plasma-assisted molecular beam epitaxy system (PA-MBE) with fixed In/Ga flux ratio. Due to the textured morphology of pyramided Si substrate, using energy-dispersive X-ray spectroscopy (EDS), we demonstrate that the impingement flux ratios of Ga/In and N-plasma varied with different facets of Si pyramids, which results in different light emission ranges on different facets and mixed into white light emission. By conducting spatial resolved catholuminescence spectroscopy (CL), we have resolved that each facet emits different CL spectrum. This finding could assist the design of nanorods-embedded light emitted devices that can be grown more efficient and compact in structure.
1:51PM S11.00014: Tensile-Strained Ge Quantum Dots on (111) and (110) Surfaces*  KATHRYN SAUTTER (Presenter), CHRISTOPHER SCHUCK, TRENT GARRETT, ARIEL E WELTNER, KEVIN VALLEJO, PAULJ SIMMONDS, Boise State University — Si and Ge are ubiquitous in electronics, but their indirect bandgaps make them unsuitable for light emitting devices. Theory shows that placing Ge under tensile strain will allow us to engineer its electronic band structure. Tensile strains of 2–4% should transform Ge either into a direct band gap semiconductor or a semimetal, with applications from infrared emitters to low-loss tunnel junctions. Researchers have therefore tried various ingenious methods to create tensile-strained Ge, but these attempts typically generate strain-induced defects and do not result in viable optoelectronic materials. Our approach to this problem is to create Ge quantum dots (QDs) that self-assemble as a result of biaxial tensile strains on low-index surfaces. We have previously demonstrated defect-free, tensile GaAs(111) QDs. Given the similar lattice constants of GaAs and Ge, we follow the same approach to produce self-assembled Ge QDs at 3.7% tensile strain, which we anticipate should lead to optically active Ge with a reduced bandgap. We will discuss our control of Ge QD properties with growth parameters, and discuss possible reasons for some of the structural and optical phenomena we observed.

*This work is supported by the Air Force Office of Scientific Research under award #FA9550-16-1-0278.

2:03PM S11.00015: Light Emission from Direct Bandgap Hexagonal Silicon Germanium*  ELHAM FADALY (Presenter), ALAIN DIJKSTRA, Applied Physics, Eindhoven University of Technology, JENS RENÈ SUCKERT, Faculty of Physics and Astronomy, Friedrich-Schiller-Universität Jena, MARCEL VERHEIJEN, SEBASTIAN KOELLING, Applied Physics, Eindhoven University of Technology, JONATHAN FINLEY, Physics, Technische Universität München, SILVANA BOTTI, Faculty of Physics and Astronomy, Friedrich-Schiller-Universität Jena, JOS HAVERKORT, ERIK P. A. M. BAKKERS, Applied Physics, Eindhoven University of Technology — Efficient light emission from Si and Ge has been a holy grail due to their indirect bandgap nature. Recently, Ge-rich alloys, with a hexagonal structure have been theoretically predicted to exhibit a direct band gap nature. Density functional theory (DFT) calculations predict a 0.3 eV bandgap for hex-Ge, which can be tuned up to 0.9 eV by alloying with Si. Yet, the fundamental bottleneck is that Ge and its alloys crystallize naturally in the cubic structure which is optically inactive due to its indirect bandgap nature. We have realized hex- SiGe by utilizing wurtzite GaAs nanowire cores as a template to transfer the crystal structure to the SiGe shells in a core-shell geometry. We demonstrate photoluminescence of hex-Ge at 3.5 µm at low temperatures and up to room temperature. In addition, we validate the tunability of the wavelength between 1.8 µm and 3.5 µm via alloying Ge with up to 30% Si. These results reveal the potential of this new material system for SiGe based light emitting devices.

References

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Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S12 DCMP: Adatom and Proximity Driven Electronic Interactions in Graphene

BCEC 153A - Jianhao Chen, Peking University

11:15AM S12.00001: Strained-induced Landau levels in momentum space  ÉTIENNE LANTAGNE-HURTUBISE (Presenter), PASCAL NIGGE, AMY QU, ERIK MÅRSELL, University of British Columbia, STEFAN LINK, Max Planck Institute for Solid State Research, GARY TOM, CHRISTOPHER GUTIERREZ, University of British Columbia, ULRICH STARKE, Max Planck Institute for Solid State Research, DOUGLAS ANDREW BONN, SARAH A. BURKE, ANDREA DAMASCELLI, MARCEL FRANZ, University of British Columbia — It is well known that certain strain patterns in graphene couple to the low-energy Dirac fermions as pseudo-magnetic fields -- i.e. magnetic fields that preserve time-reversal symmetry. This can lead to the formation of quantized Landau levels in the absence of magnetic fields, as first predicted by [Guinea et al., Nat. Phys. 6, 30 (2010)] and subsequently identified in local STM measurements [Levy et al., Science 329, 544 (2010)]. Here we extend this body of work by considering momentum-resolved signatures of large-scale, strain-induced pseudo-magnetic fields in graphene. Our theoretical modeling supports the first observation of Landau levels in ARPES. The corresponding pseudo-magnetic field of 41 T is attributed to strain generated by shallow triangular nanoprisms on our SiC substrates, over which graphene grows without grain boundaries, as revealed by AFM and STM measurements. Our work demonstrates the feasibility of generating strain-induced quantum phases in 2D Dirac materials on a wafer-scale size.
11:27AM S12.00002: Emergence of Kondo Resonance in Graphene Intercalated with Cerium

JINWOONG HWANG (Presenter), Pusan National University, KYOO KIM, Max Planck-POSTECH/Hsinchuen Center for Complex Phase Materials, HYEJIN RYU, Lawrence Berkeley National Laboratory, JINGUL KIM, Pohang University of Science and Technology, JI-EUN LEE, Pusan National University, SOORAN KIM, Pohang University of Science and Technology, MINHEE KANG, Pusan National University, BYUNG IL MIN, Pohang University of Science and Technology, ALESSANDRA LANZARA, UC Berkeley, JINWOOK CHUNG, Pohang University of Science and Technology, SUNG-KWAN MO, JONATHAN DENLINGER, Lawrence Berkeley National Laboratory, BYEONG-GYU PARK, Pohang Accelerator Laboratory, CHOOINGYU HWANG, Pusan National University — The interaction of a magnetic impurity with surrounding electrons has been a core problem in modern physics to understand fundamentals of many-body effects and its relation to magnetism. In particular, antiferromagnetic screening of the local magnetic moment by conduction electrons leads to the formation of a new resonant-type many-body ground state, so-called Kondo resonance. Here we report the realization of the Kondo resonance in a prototypical two-dimensional system, graphene, induced by the presence of cerium with the localized spin of a 4f-electron. The combination of two complementary techniques, angle-resolved photoemission spectroscopy and dynamic mean-field theory, reveals the development of new spectral weight near Fermi energy at lower temperature that is hybridized with the graphene π-band. The observed T-dependence provides not only a direct evidence of the formation of the many-body ground state in graphene, but also novel insight how Kondo physics emerges in the sea of two-dimensional Dirac electrons.

11:39AM S12.00003: Gate Modulated Interaction Between Quantum Dots in a Graphene/hBN Heterostructure

EBERTH QUEZADA (Presenter), FREDERIC JOUCKEN, ZHEHAO GE, JOHN L DAVENPORT, University of California, Santa Cruz, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, JAIRO VELASCO JR., University of California, Santa Cruz — Understanding interactions between atoms is fundamental in condensed matter systems. In heterostructures of graphene and hexagonal boron nitride (hBN) we are able to create tailor-made quantum dots in a background of Dirac fermions. Recent studies have explored the nature of single quantum dots and how their behavior is influenced by the application of a perpendicular magnetic field. However, no efforts have been made towards understanding the interaction between a pair of Dirac fermion quantum dots. We will discuss and present spatially-resolved scanning tunneling spectroscopy studies performed on a pair of quantum dots. We will also show how their behaviour is influenced by changes in their shape, size, and separation attained through the modulation of an electrostatic backgate.

11:51AM S12.00004: Proximity-induced Ising spin orbit coupling in bilayer graphene/WSe2 van der Waals heterostructures

XIAOMENG CUI (Presenter), JOSHUA ISLAND, University of California, Santa Barbara, JUN KHOO, CYPRIAN LEWANDOWSKI, MIT, HAOXIN ZHOU, ERIC SPANTON, University of California, Santa Barbara, DANIEL A RHODES, JAMES HONE, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, LEONID LEVITOV, MIT, MICHAEL ZALETEL, University of California, Berkeley, ANDREA YOUNG, University of California, Santa Barbara — Interlayer proximity effects at van der Waals interfaces provide a tool for engineering electronic phases that do not occur in isolated two-dimensional materials. A longstanding goal is proximity induced spin orbit coupling (SOC) in graphene. While previous experimental efforts have reported signatures of SOC in graphene-transition metal dichalcogenide (TMD) heterostructures, these studies have primarily relied on indirect charge and spin transport measurements preventing definitive resolution of the strength, nature, or origin of the induced SOC. Here we report on the direct observation of proximity induced SOC in bilayer graphene in contact with tungsten selenide (WSe2). Using spin- and layer-resolved broken symmetry Landau levels as a probe of layer specific proximity-induced SOC, we observe rearrangement of these levels consistent with an Ising (valley-Zeeman) type SOC with a strength of ≈2 meV. Our observations pave the way toward new engineered topological phases in van der Waals heterostructures.

12:03PM S12.00005: Strain engineering of a pseudo gauge field superlattice in a suspended graphene nanoribbon studied by scanning probe microscopy

RIJU BANERJEE (Presenter), Pennsylvania State University, VIET-HUNG NGUYEN, Université catholique de Louvain, LAVISH PABBI, TOMOTAROH GRANZIER-NAKAJIMA, Pennsylvania State University, AURELIEN LHERBIER, Université catholique de Louvain, ANNA BINION, MAURICIO TERRONES, Pennsylvania State University, JEAN-CHRISTOPHE CHARLIER, Université catholique de Louvain, ERIC HUDSON, Pennsylvania State University — Engineering exotic electronic states in novel materials, which are unrealizable in traditional systems, has been the focus of intense research over the past decade. Unlike present electronics, which rely on controlling the flow of charges primarily by electric fields, strain, for example, can control electrons by generating pseudo gauge fields in 2D materials. In this talk, we report strain engineering of pseudo electric and magnetic superlattices in suspended graphene nanoribbons by extreme (>10%) strain and study the local electronic density of states by scanning tunneling microscopy. These measurements reveal Landau levels in the presence of highly non-uniform pseudo-magnetic fields. DFT and tight binding calculations imply the existence of counterpropagating snake states along the edges of the nanoribbons reminiscent of topological materials.

*NSF Grant: 1229138
12:15PM S12.00006: Charge density wave induced proximity spin-orbit coupling effects in graphene on 1T-TaS₂*
KAROL SZALOWSKI, University of Lodz, MARTIN GMITRA (Presenter), P. J. Safarik University —
Graphene on transition-metal dichalcogenides (TMDCs) exhibits proximity spin-orbit effects opening new venues for optospintronics [1], and provides route for exploring robust helical edge states [2, 3]. 1T-TaS₂ is a layered TMDC showing metal-insulator transition and the sequence of different charge density wave (CDW) transformations [4]. We present our first-principles results for the electronic band structures of graphene on 1T-TaS₂ in normal state and for periodic lattice distorted David star pattern providing commensurate CDW phase. We discuss the orbital and spin-orbital proximity effects with phenomenological symmetry-based Hamiltonian that we use to fit the first-principles data. The extracted spin-orbit coupling parameters are of the order of meV. A fascinating finding is that induced proximity effects in graphene on 1T-TaS₂ are significantly influenced by the presence of the commensurate CDW in 1T-TaS₂.


*The work is supported by the 2015/19/B/ST3/03142, MSVVaS SR 90/CVTISR/2018, and VVGS-2018-887.

12:27PM S12.00007: Synthetic topological phases in bilayer graphene via van der Waals proximity induced spin orbit coupling  JOSHUA ISLAND (Presenter), XIAOMENG CUI, University of California, Santa Barbara, JUN KHOO, CYPRIAN LEWANDOWSKI, Massachusetts Institute of Technology, HAOXIN ZHOU, ERIC SPANTON, University of California, Santa Barbara, DANIEL A RHODES, JAMES HONE, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, LEONID LEVITOV, Massachusetts Institute of Technology, MICHAEL ZALETEL, University of California, Berkeley, ANDREA YOUNG, University of California, Santa Barbara — Spin orbit coupling (SOC) forms the basis of time reversal invariant topological insulators. While graphene provided the first theoretical model for a topological insulator, the small intrinsic SOC in carbon make such phases unobservable. Here we engineer a synthetic topological insulator-like phase in bilayer graphene via proximity induced SOC from WSe2 in a van der Waals heterostructure. At zero magnetic field, we observe a new incompressible phase at charge neutrality due to proximity induced Ising-type SOC, having equal and opposite magnitude on each layer. Transport measurements show enhanced conductance within this new phase, which is rapidly suppressed by an in-plane magnetic field, consistent with modeling that suggests the new phase hosts spin filtered edge states and has a nearly quantized spin Hall conductance. Interestingly, spin is approximately conserved in this system despite large Rashba spin orbit coupling, whose effects are strongly suppressed in the spin-filtered edge states. Remarkably, electric field can be used to tune the system between the quantum spin Hall phase and a trivial insulator, permitting reconfigurable topological edge state circuits.

12:39PM S12.00008: Topological phases in intercalated epitaxial graphene* CAI-ZHUANG WANG (Presenter), MINSUNG KIM, KAI-MING HO, Ames Laboratory — Intercalation is one of the effective methods to functionally manipulate the electronic structure of epitaxial graphene. Here, using first-principles density functional theory calculations, we design 2D topological insulators in epitaxial graphene via intercalation. We find that the electronic band structure near the Fermi energy shows Dirac-cone type or quadratic band dispersion depending on the type of intercalants, and topologically nontrivial band gap opens due to the considerable strength of the spin-orbit coupling. Our results indicate that the intercalation is a promising way to realize topological phases in graphene, and could be important in future nano device applications of graphene.

*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. The research was performed at Ames Laboratory, which is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358.
Effect of High gate-voltage application on the molecular adsorption on Graphene*  KAZUYUKI TAKAI (Presenter), TAICHI UMEHARA, YASUSHI ISHIGURO, Hosei University — The electronic properties of graphene are well tuned by guest chemical species due to its 2D nature. We have clarified that the charge transfer between molecules and graphene proceeds by an electrochemical process based on the fact that the kinetics of the charge transfer decreases with down and up shift of the Fermi energy of graphene for electrons and holes, respectively. In this study, the electrochemical potential is widely varied by graphene FET in order to induce various electrochemical reactions for the charge transfer phenomena. In the case of the hole doping by oxygen adsorption on graphene, the lower gate-voltage, the slower hole doping reactions as we reported [1] and finally no charge doping occurs at enough higher gate-voltage around -80 V. Interestingly, further lowering of the gate-voltage results in the electron doping by the oxygen adsorption on graphene. Even in this condition, the doping kinetics are accelerated by the presence of water molecule. This suggests that different electrochemical reactions are responsible for the charge transfer by oxygen adsorption on graphene between the higher gate-voltage region and lower voltage region.


*This work was supported by JSPS KAKENHI Grant No. 16K05758 and 26107532

Graphene-Bi (111) interface: atomic structure and electronic properties*  IVAN NAUMOV (Presenter), PRATIBHA DEV, Physics and Astronomy, Howard University — Interfacial interactions are widely used to engineer desired electronic properties. In this context, the interface between graphene and nanostructured bismuth is especially interesting since both the materials exhibit unique properties associated respectively with the Dirac cones and quantum spin-Hall states along the edges and hinges. In this work, using first-principles calculations, we study the interfacial interaction between graphene and Bi (111) surfaces. Since the actual structure of graphene on Bi (111) can be incommensurate, we investigated a large number of crystal approximants to the incommensurate interface and found the most stable one. Despite hybridization between graphene and substrate orbitals, the graphene-derived Dirac cones are preserved, although shifted with respect to the Fermi level due to the n-doping of graphene. We also find that a small gap opens up at the original Dirac points in these cones due to interface-induced spin–orbit coupling within graphene. At the same time, the bands near the gamma point are mostly Bi-derived and resemble the corresponding surface states in pure Bi. Using the obtained results, we discuss possible applications of graphene/Bi interfaces in future electronic devices.

*This research was supported by W. M. Keck Foundation.

Comparative Mapping of the Local Potential of Graphene/hBN Systems Using Scanned Probe Techniques  WYATT BEHN (Presenter), VICTOR W BRAR, ZACH KREBS, KEENAN SMITH, GREGORY HOLDMAN, University of Wisconsin - Madison — Mapping the local electrostatic potential of 2D materials is an important step in understanding how defects and strain affect local electrostatic structure. Potential mapping can also reveal the strength of el-el interactions in a material, and – when performed under transport conditions – can directly probe the nature of electronic flow. Specifically, probing the local potential gradient of a current-driven graphene sheet could provide insight into how electronic transport shifts between ballistic and diffusive regimes. We present preliminary results comparing three scanned probe methods for mapping electrostatic potential of a graphene sheet: Kelvin probe force microscopy (KPFM), scanning tunneling potentiometry (STP), and scanning tunneling spectroscopy (STS). We discuss the comparative advantages of each technique, describing how each method performs when measuring a graphene/hBN system with current applied in situ.

Concomitant enhancement of electron-phonon coupling and electron-electron interaction in graphene decorated with ytterbium  MINHEE KANG (Presenter), JINWOONG HWANG, JEUN LEE, Pusan National University, ALEXEI V FEDOROV, Lawrence Berkeley Natl Lab, CHOONGYU HWANG, Pusan National University — The presence of foreign atoms induces exotic many-body physics in a condensed matter system. Especially, a two-dimensional system is very sensitive to such an external perturbation to lead metal-insulator transition, Kondo effect, strongly enhanced electron-phonon coupling, etc. Here we report that the presence of Yb results in the enhancement of not only electron-phonon coupling, but also electron-electron interaction in graphene. When the band structure of graphene with Yb exhibits the characteristics of electron-phonon coupling that is not clearly observed in as-grown graphene, the slope of the energy-momentum dispersion was also found to decrease by the presence of Yb using angle-resolved photoemission spectroscopy. Within the Fermi liquid theory, the decreased slope indicates enhanced electron-electron interaction, suggesting possibility interplay between electron-phonon coupling and electron-electron interaction in graphene decorated with foreign atoms.
1:39PM S12.00013: Nanoscale distribution of strains and defects in graphene transferred onto polymethylmethacrylate

DMITRY VOYLOV (Presenter), Mechanical Engineering, Tufts University, IVAN VLASSIOUK, Energy & Transportation Science Division, Oak Ridge National Laboratory, NICK LAVRIK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, ALEX KISLIUK, ALEXEI P SOKOLOV, Chemical Sciences Division, Oak Ridge National Laboratory — Graphene has attracted a wide interest over the last decade and deeper understanding of formation of defects and strains controlling its properties is one of the major goals. One of the commonly used methods for transferring graphene on a substrate of interest utilizes polymethylmethacrylate (PMMA) as a temporary support. While several studies demonstrated that the length scale of strain can be as small as a few nm for graphene on SiO₂ substrates [1], the strain coherence length and distribution of defects on a nanoscale for graphene laying on PMMA remains poorly understood. Here we present tip-enhanced Raman Spectroscopy (TERS) study of single layer graphene on top of PMMA. Our results provide a clear experimental evidence that the locations of defects correlate with topological features of PMMA, which on the other hand replicates topological structure of copper foil. We found that the strain is anisotropically distributed with a length scale varies from tens hundred nm.


* This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science & Engineering Division for partial financial support. DV. thanks the NSF CBET 1428919.

1:51PM S12.00014: Deposition of single-molecule magnets on graphene quantum dots.

LUKE ST. MARIE (Presenter), Physics, Georgetown University, JAKUB HRUBY, CEITEC, JAMES HUNT, Physics, Georgetown University, PETR NEUGEBAUER, IVAN NEMEC, CEITEC, A EL FATIMY, Physics, Georgetown University, RACHAEL MYERS-WARD, DAVID KURT GASKILL, US Naval Research Laboratory, MATTIAS KRUSKOPF, YANFEI YANG, RANDOLPH E ELMQUIST, National Institute of Standards and Technology, PAOLA BARBARA, Physics, Georgetown University — Gapless graphene is a single-atom-thick material that yields ultra-broadband photodetectors for applications that require high sensitivity. These applications include spectroscopy of single molecule magnets (SMMs), metal-ion complexes that exhibit quantum behavior at low temperatures and have great potential as components for quantum computing and molecular spintronics. By grafting small amounts of SMMs directly to the surface of a graphene quantum dot, we can utilize the high sensitivity of a graphene hot-electron bolometer to perform spectroscopy on the SMMs. We have investigated various methods of grafting transition-metal-based SMMs to the graphene and characterizing the deposited molecules.

* This work was supported by the US Office of Naval Research (N00014-16-1-2674) and the NSF (ECCS-1610953).

Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S13 DMP GMAG: 2D Materials (General): Transport and Optical Phenomena -- Magnetism

BCEC 153B - TeYu Chien - Tag(s): Focus

11:15AM S13.00001: Magneto-optical properties of bilayer transition metal dichalcogenides

MUHAMMAD ZUBAIR (Presenter), Physics, Concordia University, MUHAMMAD TAHIR, Colorado State Univ, PANAGIOTIS VASILOPOULOS, Physics, Concordia University — In transition metal dichalcogenides (TMDCs) the spin-orbit interaction affects differently the conduction and valence band energies as functions of the wave vector k and the band gap is usually large except in few TMDCs that are metallic without band gaps. Consequently, when a perpendicular magnetic field B is applied, the conduction and valence band Landau levels are also different and this leads to a splitting of the interband optical absorption lines in both the absence and presence of an external electric field Ez. When B and Ez are present, the peaks in the imaginary part of the Hall conductivity give two distinct contributions of opposite sign to the interband spectrum. The real part of the right- and left-handed interband conductivity, however, retains its two-peak structure but the peaks are shifted in energy and amplitude with respect to each other in contrast with graphene.

*M.Z. and P.V. acknowledge the support of the Canadian NSERC Grant No. OGP0121756 and Concordia University Graduate Fellowship. The work of M.T. was supported by Colorado State University.
Magneto-Raman Spectroscopy of Layered Transition-Metal Dichalcogenides

JEFFREY SIMPSON (Presenter), Towson University, HEATHER M. HILL, SUGATA CHOWDHURY, FRANCESCA TAVAZZA, ANGELA HIGHT WALKER, NIST — Raman spectroscopy offers a non-contact, non-destructive, and high-throughput optical technique to probe the fundamental physics of two-dimensional (2D) layered materials. We discuss our unique magneto-Raman capability, which affords measurement of Raman spectra with simultaneous variation of temperature (4K to 400K), laser excitation wavelength (tunability from UV to near-IR), and magnetic field (up to 9 T). Coupling to a triple-grating spectrometer provides measurement of low-frequency phonons. Recent results on novel 2D materials will be presented to highlight instrumentation capabilities, including metallic TaSe2, which exhibits transitions between commensurate and incommensurate charge-density wave (CDW) phases, and related, layered materials. The dependence of the observed Raman-active phonons in TaSe2 on temperature and magnetic field will be presented and compared with earlier results on MoS2 and calculations using density functional theory. Specifically, we observe the appearance of low-frequency, zone-folded modes in the CDW state. The phase, amplitude, and previously unanalyzed zone-folding modes are assigned to specific phonons observed in experimental spectra and DFT. Uniquely, the calculations show Ta-rich stripes emerge in the commensurate CDW phase.

Magnetoplasmons in the pseudospin S=1 \(\alpha\)-T3 lattice

ANTONIOS BALASSIS (Presenter), Physics, Fordham University, DIPENDRA DAHAL, Graduate Center, CUNY, GODFREY GUMBS, Hunter College, CUNY — We calculate the dynamical polarizability and the dispersion relation for magnetoplasmons for the \(\alpha\)-T3 model at zero temperature at integer filling. In the absence of magnetic field, the low energy spectrum described by a Dirac-Weyl Hamiltonian consists of a pair of Dirac cones and a dispersionless (flat) band in the K and K' valleys. We use the Peierls substitution to generate the Landau level spectrum for this structure with pseudospin \(S = 1\) which is characterized by a parameter \(\alpha\) for measuring the coupling strength between an additional atom at the center of the honeycomb graphene lattice and the A and B atoms of graphene. We present results for a doped layer for various \(\alpha\) and magnetic fields in the random-phase approximation. These modes may be observed with the aid of inelastic light-scattering experiments.

Negative Magnetoresistance from Berry Curvature and Orbital Magnetic Moment

HAILONG ZHOU (Presenter), CONG XIAO, QIAN NIU, University of Texas at Austin — Longitudinal negative magnetoresistance has attracted tremendous amount of attention since the emergence of three-dimensional topological materials, e.g. Weyl semimetals, due to the effect of chiral anomaly in these systems. In contrast to the extensively studied longitudinal negative magnetoresistance, transverse magnetoresistance in topological systems has been somewhat overlooked. We formulate transverse magnetoresistance for topological systems with non-zero Berry curvature based on semiclassical Boltzmann theory. Model calculation based on gapped two-dimensional valley systems shows explicitly that magnetoresistance is negative in large range of magnetic field, stemming from Berry curvature and orbital magnetic moment.

Electrical and Magneto Transport Properties in Weyl Semimetal MoTe2

LEI WANG (Presenter), Materials Characterization Core, Yale University West Campus, JOSHUA PONDICK, JOHN WOODS, PENGZI LIU, MILAD YARALI, SAJAD YAZDANI, Energy Sciences Institute, Yale University West Campus, MIN LI, Materials Characterization Core, Yale University West Campus, JUDY CHA, Energy Sciences Institute, Yale University West Campus — Molybdenum ditelluride MoTe2, a type II Weyl semimetal, has attracted intense interest due to novel properties such as large magnetoresistance, quantum spin Hall effect and massless carriers. Here we report on electrical and magneto transport studies of exfoliated multilayer MoTe2. Weak antilocalization is observed at low magnetic fields due to strong spin-orbit coupling. We also investigate layer dependent magnetoresistance at various temperatures. A back-gate voltage is applied to change the carrier density and Fermi level. It is shown such electronic properties can be effectively tuned by gate voltage.
12:15PM S13.00006: Magnetotransport in monolayer 2H-MoTe2*  

DANIEL RHODES (Presenter), Columbia Nano Initiative, Columbia University, AUGUSTO GHIOTTO, Department of Physics, Columbia University, ABHINANDAN ANTONY, BUMHO KIM, JAMES HONE, Department of Mechanical Engineering, Columbia University — Monolayer transition metal dichalcogenides (TMD) have been investigated for a variety of interesting aspects: valley Hall effect, biexcitons, and 2-D superconductivity. In magnetotransport, monolayer TMDs break inversion symmetry and as a result have degenerate K/K’ bands which are spin-split. In MoS2, this spin-splitting between the lower and upper K/K’ bands in the conduction band is around 15 meV, 5x larger than expected, and similar results have been extracted from monolayer WSe2. In both cases, neither system can be investigated via electrical transport in both the n- and p-type carrier regime due to the large bandgap and issues with contacts. Monolayer, 2H-MoTe2 however, has a much smaller bandgap of 1.1 eV. Though there has been much work done on electrical characterization in MS2 and MSe2 (M = Mo or W), there has been almost no work done on 2H-MoTe2 as the monolayer is air sensitive and more difficult to contact than like 2-D air sensitive materials such as InSe or black phosphorus. In this study we report the magnetotransport of monolayer 2H-MoTe2 in the ultra-clean limit.

*We would like to acknowledge the support of the National Science Foundation MRSEC program through Columbia in the Center for Precision Assembly of Superstratic and Superatomic Solids (DMR-1420634).

12:27PM S13.00007: Theory of magnetotransport for a cavity-embedded two-dimensional electron gas

NICOLA BARTOLO (Presenter), CRISTIANO CIUTI, Laboratoire MPQ, Université Paris Diderot - Paris 7 — We present a theory pointing out the crucial role of virtual polariton excitations in controlling the dc charge transport properties of cavity-embedded systems. Specifically, we consider the linear magnetotransport of a cavity-embedded two-dimensional electron gas (2DEG) in the regime where no real photons are injected or created in the resonator [1]. Our theory shows that, for a cavity photon mode with in-plane linear polarization, the dc bulk magnetoresistivity of the 2DEG is anisotropic. For high filling factors of the Landau levels, we predict a profound modification in the envelope of the Shubnikov-de Haas oscillations, with the resistivity being increased or reduced depending on the system parameters (an effect observed in recent experiments [2]). In the limit of low magnetic fields and in the ultrastrong light-matter coupling regime, the resistivity along the cavity-mode polarization direction is enhanced.


12:39PM S13.00008: Coordinate-shift induced electron transport in strong magnetic field*

JINGJING FENG (Presenter), University of Texas at Austin, YANG GAO, Department of Physics, Carnegie Mellon University, QIAN NIU, University of Texas at Austin — In a strong magnetic field, electrons primarily execute cyclotron motion, with transverse transport in an electric field from the drifting of cyclotron orbits. We present a classical-Boltzmann theory of longitudinal transport in terms of coordinate shifts of such orbits upon scattering with impurities. During the electron-impurity scattering, the guiding centers suddenly shift their positions, which accumulatively contribute to a longitudinal current. Along with coordinate shifts, the cyclotron orbit radius are also changed, accounting for energy dissipation in the electric field. The resulting longitudinal conductivity is in agreement with the Drude phenomenological theory even beyond the weak scattering limit.

*Welch Foundation

12:51PM S13.00009: Investigation on the Non-trivial Photoluminescence in 2D Antiferromagnetic Layers*

XINGZHI WANG (Presenter), JUN CAO, HIKARI KITADAI, WEIJUN LUO, XI LING, Department of Chemistry, Boston University — Two-dimensional (2D) magnetic systems have attracted intense attention due to potentially applications in low-dimensional spintronic and magnetic devices. Recently, we observe a non-trivial photoluminescence in metal phosphorus chalcogenides, which are 2D antiferromagnetic materials. Multiple photoluminescence peaks are observed and some of them show a strong dependence on the excitation-wavelength and temperature in both the bulk and few-layer cases, which are different from the emission in conventional 2D semiconductors. A rational model based on the special electronic structures and transitions of the materials is proposed to explain this phenomenon. Our studies reveal the intrinsic electronic and magnetic properties in 2D crystals, and suggest the potential functionalities and applications of 2D magnetic layers.

*This work is supported by Boston University. We acknowledges the membership of the photonics center at Boston University.
Spin filter and spin-polarized electric current in silicene nanoribbons induced by point defects

LUIS ROSALES (Presenter), CESAR D. NUÑEZ, PEDRO ORELLANA, Departamento de Fisica, Universidad Tecnica federico Santa Maria, FRANCISCO DOMÍNGUEZ-ADAME, Departamento de Fisica de Materiales, Universidad Complutense de Madrid, RUDOLF ROEMER, 2Department of Physics, University of Warwick — Half-metals, in which one spin channel is conductive but the other one is insulating or semiconducting, is the key ingredient to achieve spin-polarized currents. Hybrid structures of 2D materials and ferromagnetic insulators, like EuO, provide a route to induce half-metallicity and pave the way for spintronic applications. The ferromagnetic insulator induces a proximity exchange interaction between the spins in the material that results in a spin modulation of the structures. In this context, in this work we address the effects of a random distribution of adatoms on the electron transport properties of silicene nanoribbons. The tunnel coupling between adatoms and silicon atoms induces an electronic Fano effect that makes the conductance vanish when the Fermi level matches the resonant energy induced by the adatoms. The resonant energy is independent of the random distribution of adatoms, provided that they do not cluster. When the nanoribbon is in close proximity to a ferromagnetic insulator, the resonant energy depends on the electron spin and consequently the electric current can be highly spin polarized. Our results expand the base of available materials to designing a tunable source of polarized electrons for spintronics.

*Authors thanks Fondecyt 1180914 and USM PIL2517.

Anisotropic spin relaxation in graphene/hBN heterostructures

KLAUS ZOLLNER (Presenter), Institute for Theoretical Physics, University of Regensburg, MARTIN GMITRA, Institute of Physics, P. j. Safarik University in Kosice, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg — Measurements show a large and tunable anisotropy in the spin relaxation of hBN encapsulated bilayer graphene1,2, similar to what is observed in graphene/TMDC heterostructures3. Combining systematic first principles calculations for graphene/hBN heterostructures with a minimal tight-binding model, we extract spin-orbit coupling parameters of graphene in the µeV range. The extracted model parameters depend on (i) interlayer distances, (ii) stacking configurations, and (iii) an external electric field, resulting in a rich parameter space. Based on the Dyakonov-Perel formalism we calculate spin relaxation times for graphene, in the nanosecond range, in agreement with recent experimental measurements. A very important finding is that the spin relaxation anisotropy is maximum close to the charge neutrality point, decreasing with the doping level. In addition, we also show that the anisotropy can be tuned by means of an external electric field, via the precise control of the Rashba SOC.

1 Xu et al., PRL 121, 127703 (2018)
2 Leutenantsmeyer et al., PRL 121, 127702 (2018)
3 Cummings et al., PRL 119, 206601 (2017)

*This work is supported by the DFG SPP 1666.

Bilayer silicene in a magnetic field: spin localization and its effect on the integer and fractional Hall conductivity

THI NGA DO (Presenter), Dept. of Physics, National Cheng Kung University, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College of the City University of New York, POHSIN SHIH, Dept. of Physics, National Cheng Kung University, DANHONG HUANG, US Air Force Research Laboratory — The Hall conductivity of many condensed matter systems presents step structure when a uniform perpendicular magnetic field is applied. We report the emergence of fractions of the Hall conductivity due to the grouping in pairs of an electron with a bilayer silicene sublattice site due to strong spin-orbit coupling. The collective behavior of this pairing causes the conductivity to exhibit steps of \( e^2/h \) or \( 4/5 \ e^2/h \) high for the low-lying spectrum, depending on the dominating sublattices of Landau levels. This coexistence of integer and fractional Quantum Hall States arises from the interplay of lattice geometry, atomic interaction, spin-orbit coupling, and external magnetic field. We also report the significant effect of an external electric field on the evolution of integer and fractional quantum Hall effects.

*This material is based upon work supported by the Air Force Office of Scientific Research (AFOSR) under award number FA2386-18-1-0120. We acknowledge the support from the DoD Lab-University Collaborative Initiative (LUCI) Program and the Air Force Research Laboratory (AFRL) through Grant No. 12530960.
1:39PM S13.00013: Fano Resonance in Two-Dimensional Magnetic Semiconductor CrPS₄  
PINGFAN GU (Presenter), School of Physics, Peking University, QINGHAI TAN, Institute of Semiconductors, Chinese Academy of Sciences, ZILING LI, YI WAN, XIAOHAN YAO, School of Physics, Peking University, JUN ZHANG, Institute of Semiconductors, Chinese Academy of Sciences, YU YE, School of Physics, Peking University — The two-dimensional (2D) magnetic materials have attracted extensive research interests, not only because of their novel physical properties induced by quantum confinement, but also for their promise for spintronic devices. Chromium thiophosphate (CrPS₄) is a promising ternary antiferromagnetic semiconductor with a Neel temperature of 36 K. We synthesized CrPS₄ single crystals by chemical vapor transport method and performed spectroscopy study at different temperature. The spectra at low temperature showed an asymmetric Fano-resonance shape, which can be explained by coupling between a discrete state and continuum state. This is the first observation of Fano resonance in 2D magnetic materials in near infrared spectrum region. Moreover, we also studied Fano resonance of layered CrPS₄ on dependence of magnetic field, excitation power, laser polarization, etc. Our findings may provide insight of the electronic transition of CrPS₄, which is related to its intrinsic magnetic properties.

1:51PM S13.00014: Si-doped Defect in Monolayer Graphene: Magnetic Quantization*  
POHSIN SHIH (Presenter), THI NGA DO, BOR-LUEN HUANG, Dept. of Physics, National Cheng Kung University, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College of the City University of New York, DANHONG HUANG, US Air Force Research Laboratory, MING-FA LIN, Dept. of Physics, National Cheng Kung University — We explore the rich and unique magnetic quantization of Si-doped graphene defect systems for various concentrations and configurations using the generalized tight-binding model. This model takes into account simultaneously the non-uniform bond lengths, site energies and hopping integrals, as well as a uniform perpendicular magnetic field. The magnetic quantized Landau levels (LLs) could be classified into four different groups based on the probability distributions and oscillation modes. The magneto-optical selection rules, reflecting the main characteristics of LLs, cover Δn = |n⁺−n⁻| = 0 and 1. These rules for inter-LL excitations arise from the non-equivalence or equivalence of the and sublattices in a supercell. The spectral intensity can be controlled by oscillator strength using a canonical momentum as well as by density of states using concentration and distribution of doped Si atoms.

*This material is based upon work supported by the Air Force Office of Scientific Research (AFOSR) under award number FA2386-18-1-0120. We acknowledges the support from the AFOSR and from the DoD Lab-University Collaborative Initiative (LUCI) Program and the support from the Air Force Research Laboratory (AFRL) through Grant \#12530960.

Thursday, March 7, 2019 11:15 AM - 1:39 PM

Session S14 DMP: 2D Materials (Metals, Superconductors, and Correlated Materials) -- Twisted Graphene II  
BCEC 153C - Roland Koch - Tag(s): Focus

11:15AM S14.00001: Electronic compressibility of magic-angle graphene superlattices  
SPENCER TOMARKEN (Presenter), YUAN CAO, AHMET DEMIR, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, NIMS, PABLO JARILLO-HERRERO, RAYMOND ASHOORI, Massachusetts Institute of Technology — Recent calculations and measurements have revealed that the superlattice formed by twisting and stacking two monolayers of graphene at particular small twist angles (dubbed ‘magic angles’) relative to their crystallographic axes can form an electronic system with substantially reduced Fermi velocity compared to monolayer graphene. Moreover, exotic insulating [1] and superconducting phases [2] near fractional filling of the moiré miniband have been observed in initial transport and capacitance measurements, drawing comparisons to the high-Tc cuprates and other superconducting platforms with analogous phase diagrams. Here we report the first thermodynamic compressibility measurements of magic angle twisted bilayer graphene in the low frequency limit. We find strongly incompressible features at quarter- and half-filling of the electron-doped regime, whereas we find substantially weaker features at the equivalent hole-doped densities. We extract the thermodynamic gaps at fractional filling and compare our results to recent transport studies.

11:27 AM S14.00002: Multicomponent Superfluidity and Screening in Biased Electron-Hole Double Bilayer Graphene with Realistic Bands. ANDREA PERALI, Fisica, University of Camerino — Superfluidity has recently been reported in double electron-hole bilayer graphene. The multiband nature of the bilayers is expected to be very important because the band gaps between conduction and valence bands are small. Here we report on a detailed mean-field study that takes into account the effects of multichannel electron-hole pairing, including Josephson-like pair transfer between bands; screening from both intraband and interband excitations; and effects of the non-parabolic band dispersion that accompanies the variable band gaps in bilayer graphene. From the self-consistent calculation based on the random phase approximation in superfluid state, we obtain a density range for superfluidity consistent with the density range reported in the recent experiments. We find for non-zero gaps, that the boost of the density of states from the flattening of the bands strengthens the superfluidity. We also find that the superfluidity modifies the intraband screening in a fundamentally different way from the interband screening. Surprisingly, the net effect of the screening is to restrict the superfluid pairing entirely to the conduction band - even for very small band gaps. This makes the system behave almost analogously to a one-band superfluid.

11:39 AM S14.00003: Symmetry, maximally localized Wannier states, and low energy model for the twisted bilayer graphene narrow bands* JIAN KANG (Presenter), OSKAR VAFEK, Florida State University — We build symmetry adapted maximally localized Wannier states, and construct the low energy tight binding model for the four narrow bands of the twisted bilayer graphene. We do so when the twist angle is commensurate, near the "magic" value, and the narrow bands are separated from the rest of the bands by energy gaps. On each layer and sublattice, every Wannier state has three peaks near the triangular Moire lattice sites. However, each Wannier state is localized and centered around a site of the honeycomb lattice that is dual to the triangular Moire lattice. Space group and the time reversal symmetries are realized locally. The corresponding tight binding model provides a starting point for studying the correlated many-body phases.

* J. K. was supported by the National High Magnetic Field Laboratory through NSF Grant No. DMR-1157490 and the State of Florida. O. V. was supported by NSF DMR1506756.

11:51 AM S14.00004: Maximally Localized Wannier Orbitals and the Extended Hubbard Model for Twisted Bilayer Graphene* MIKITO KOSHINO (Presenter), Osaka University, FANQUI YUAN, MIT, TAKASHI KORETSUNE, Tohoku University, MASAYUKI OCHI, KAZUHIKO KUROKI, Osaka University, LIANG FU, MIT — We develop an effective extended Hubbard model to describe the low-energy electronic properties of the twisted bilayer graphene. By using the Bloch states in the effective continuum model and with the aid of the maximally localized algorithm, we construct the Wannier orbitals and obtain an effective tight-binding model on the emergent honeycomb lattice. We find that the Wannier state takes a peculiar three-peak form in which the amplitude maxima are located at the triangle corners surrounding the center. We estimate the direct Coulomb interaction and the exchange interaction between the Wannier states. At the filling of two electrons per supercell, we find an unexpected coincidence in the direct Coulomb energy between a charge-ordered state and a homogeneous state, which could possibly lead to an unconventional many-body state.

*M. K. acknowledges the financial support of JSPS KAKENHI Grant No. JP17K05496. N. F. Q. Y. and L. F. are supported by the DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0010526. L. F. is partly supported by the David and Lucile Packard Foundation. T. K. is supported by JSPS KAKENHI Grant No. JP18K03442 and JST PRESTO Grant No. JPMJPR15NS. K. K. is supported by JSPS KAKENHI Grant No. JP18H01860.

12:03 PM S14.00005: Collisionless transport close to a fermionic quantum critical point in Dirac materials VLADIMIR JURICIC (Presenter), NORDITA, the Nordic Institute for Theoretical Physics, Stockholm University and KTH, Stockholm, Sweden, BITAN ROY, Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — Quantum transport close to a critical point is a fundamental, but enigmatic problem due to fluctuations, persisting at all length scales. In this talk, we discuss the scaling of optical conductivity (OC) in the collisionless regime ($\omega \gg T$) in the vicinity of a relativistic Gross-Neveu-Yukawa quantum critical point, separating two-dimensional ($d=2$) massless Dirac fermions from a fully gapped insulator or superconductor. In particular, we show that close to such a critical point a universal suppression of both the inter-band OC and the Drude peak (while maintaining its delta function profile) inside the critical regime occurs due to strongly coupled gapless fermionic and bosonic excitations [1]. We carry out the computation to the leading order in $1/N_F$ and $\varepsilon$-expansions, where $N_F$ counts fermion flavor number and $\varepsilon=3-d$. Correction to the OC at such a non-Gaussian critical point due to the long-range Coulomb interaction and generalizations of these scenarios to a strongly interacting three-dimensional Dirac or Weyl liquid are also presented.

importance. In many novel superconductors of interest, fluctuations of the phase of the SC order parameter determines the highest valence band, thus reinforcing our microscopic approach to the superconductivity of twisted bilayer graphene. To the superconducting phase, and whose onset typically takes place for a Hubbard repulsion below the bandwidth of the shape close to the magic angle. We also consider the competition with charge and spin-density-wave instabilities, adjacent in a channel with odd parity under the exchange of the two mirror patches of the Fermi line, which develop a universal belonging to different K valleys. The highly anisotropic screening of the Coulomb interaction induces an effective attraction electronic spectrum. This leads to extended saddle points and energy contours with almost perfect nesting between states first magic angle is approached, we find two consecutive transitions between different topologies in the highest valence band of the twisted bilayers, driven by the doubling and subsequent strong coupling of van Hove singularities in the graphene near the "magic angle". The non-local interaction terms are novel and their form can be traced to the topologically non-trivial nature of the narrow bands. In the strong coupling limit and at the filling of two electrons/holes per moire unit cell, the ground state can be found exactly; it is SU(4) ferromagnetic with exactly one electron/hole on each honeycomb lattice site. The kinetic terms break the SU(4) symmetry and select the ground state in which the two valleys with opposite spins are equally mixed. Although such an insulating state is not quite a spin singlet, the magnetic moment per particle vanishes in the thermodynamic limit and therefore its Zeeman coupling to an external magnetic field also vanishes at linear order. We also find gapped extended excited states with a gap that decreases in an external magnetic field. Finally, we propose that an insulating stripe ferromagnetic phase could be the ground state for the filling of one electron/hole per unit cell, with a gap that does not decrease in an external magnetic field.

\*NSF DMR1506756
NSF DMR-1157490

**12:27PM S14.00007: Strong coupling phases of partially filled twisted bilayer graphene narrow bands**

OSKAR VAFEK (Presenter), JIAN KANG, Florida State University — We identify the many-body insulating states favored by the Coulomb interactions projected onto the microscopically constructed Wannier basis of the four narrow bands of the twisted bilayer graphene near the "magic angle". The non-local interaction terms are novel and their form can be traced to the topologically non-trivial nature of the narrow bands. In the strong coupling limit and at the filling of two electrons/holes per moire unit cell, the ground state can be found exactly: it is SU(4) ferromagnetic with exactly one electron/hole on each honeycomb lattice site. The kinetic terms break the SU(4) symmetry and select the ground state in which the two valleys with opposite spins are equally mixed. Although such an insulating state is not quite a spin singlet, the magnetic moment per particle vanishes in the thermodynamic limit and therefore its Zeeman coupling to an external magnetic field also vanishes at linear order. We also find gapped extended excited states with a gap that decreases in an external magnetic field. Finally, we propose that an insulating stripe ferromagnetic phase could be the ground state for the filling of one electron/hole per unit cell, with a gap that does not decrease in an external magnetic field.

**12:39PM S14.00008: Gate-Tunable Mott Insulator in Trilayer Graphene-Boron Nitride Moiré Superlattice**

GUORUI CHEN (Presenter), LILI JIANG, Physics, UC Berkeley, SHUANG WU, Electrical Engineering and Computer Sciences, UC Berkeley, BOSAI LV, HONGYUAN LI, Physics, Shanghai Jiaotong University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ZHIWEN SHI, Physics, Shanghai Jiaotong University, YUANBO ZHANG, Fudan University, FENG WANG, Physics, UC Berkeley — Mott insulator plays a central role in strongly correlated physics, where the repulsive Coulomb interaction dominates over the electron kinetic energy and leads to insulating states with one electron occupying each unit cell. A tunable Mott insulator, where the competition between the Coulomb interaction and the kinetic energy can be varied in situ, can provide an invaluable model system for the study of Mott physics. Here we report the realization of such a tunable Mott insulator in the ABC trilayer graphene (TLG) and hexagonal boron nitride (hBN) heterostructure with a Moiré superlattice. The Moiré superlattice in TLG/hBN heterostructures leads to narrow electronic minibands that are gate-tunable. The Mott insulator states emerge at 1/4 and 1/2 fillings, corresponding to one electron and two electrons per site, respectively. Moreover, the Mott states in the ABC TLG/hBN heterostructure exhibit unprecedented tunability: the Mott gap can be modulated in situ by a vertical electrical field, and at the meantime the electron doping can be gate-tuned to fill the band from one Mott insulating state to another. Our observation opens up tremendous opportunities to explore novel strongly correlated phenomena in two-dimensional Moiré superlattice heterostructures.

**12:51PM S14.00009: Kohn-Luttinger Superconductivity in Twisted Bilayer Graphene**

JOSE GONZALEZ (Presenter), Instituto de Estructura de la Materia, CSIC, Spain, STAUBER TOBIAS, Instituto de Ciencia de Materiales de Madrid, CSIC, Spain — We propose that the superconductivity observed in twisted bilayer graphene can be explained as the consequence of a Kohn-Luttinger instability, which leads to an effective attraction between electrons with originally repulsive interaction. As the first magic angle is approached, we find two consecutive transitions between different topologies in the highest valence band of the twisted bilayers, driven by the doubling and subsequent strong coupling of van Hove singularities in the electronic spectrum. This leads to extended saddle points and energy contours with almost perfect nesting between states belonging to different K valleys. The highly anisotropic screening of the Coulomb interaction induces an effective attraction in a channel with odd parity under the exchange of the two mirror patches of the Fermi line, which develop a universal shape close to the magic angle. We also consider the competition with charge and spin-density-wave instabilities, adjacent to the superconducting phase, and whose onset typically takes place for a Hubbard repulsion below the bandwidth of the highest valence band, thus reinforcing our microscopic approach to the superconductivity of twisted bilayer graphene.
1:03PM S14.00010: Magnetotransport properties in twisted bilayer graphene at magic angle*  EVAN LAKSONO (Presenter), Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, ALEXANDER REAVES, MANRAAJ SINGH, Yale-NUS College, XINGYU GU, JIA NING LEAW, NIMISHA RAGHUVANSHI, SHAFFIQUE ADAM, Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore — Recent experimental works on magic-angle twisted bilayer graphene have pointed to the existence of insulating and superconducting phases when the flat bands are half-filled. Among the mysteries in the experiments is the observed Landau fan diagram which shows a reduction in degeneracy close to the charge neutrality point compared to that at larger twist angle. These features are a remarkable departure from theoretical expectations. In this work, we use our recently developed theory for the non-interacting band structures [1, 2] to understand the behaviors of twisted bilayer graphene under the influence of magnetic field, and offer the possible scenarios that lead to the unconventional features in the magnetotransport at charge neutrality and at half-filling.

References:

*This research is funded by Singapore Ministry of Education AcRF Tier 2 (MOE2017-T2-2-140).

1:15PM S14.00011: Strong Correlations and d+id Superconductivity in Twisted Bilayer Graphene*  JOHANNES LISCHNER (Presenter), Imperial College London, DANTE KENNES, CHRISTOPH KARRASCH, Freie Universitaet Berlin — We compute the phase diagram of twisted bilayer graphene near the magic angle where the occurrence of flat bands enhances the effects of electron-electron interactions and thus unleashes strongly-correlated phenomena. Most importantly, we find a crossover between d+id superconductivity and Mott insulating behavior near half-filling of the lowest electron band when the temperature is increased. This is consistent with recent experiments. Our results are obtained using unbiased many-body renormalization group techniques combined with a mean-field analysis of the effective couplings.

*DMK and CK acknowledge support by the Deutsche Forschungsgemeinschaft through the Emmy Noether program (KA 3360/2-1)

1:27PM S14.00012: Topological and strong correlation physics in orbital-active honeycomb lattice materials -- applications to twisted bilayer graphene, bismuthene, transition-metal oxide film, etc  CONGJUN WU (Presenter), Department of Physics, University of California, San Diego, CA 92093, USA, SHENGLONG XU, Condensed Matter Theory Center and Department of Physics, University of Maryland, College Park, Maryland 20742, USA — We apply the symmetry principle to analyze the physical properties of orbital-active honeycomb systems which include a large class of materials (e.g. the twisted-bilayer graphene, transition-metal-oxide layer, bismuthene, stanene, metal-organic framework, and quantum dot array). Their orbital degree of freedom transforms as a two-dimensional irreducible representation of the lattice symmetry group, which results in band structures consisting of both the dispersionless flat bands and orbital-active Dirac bands. The flat bands amplify strong correlation effect to yield Wigner crystal and flat-band ferromagnetism. The active-orbital degree of freedom boosts the topological gap of the Dirac bands to the order of atomic scale spin-orbit coupling, i.e. at the scale of 1eV, as observed experimentally in bismuthene. In the Mott-insulating states, the orbital exchange becomes heavily frustrated as described by a novel 120 degree model whose classic ground states are mapped to all possible loop configurations covering the lattice, and quantum fluctuations select the closest packed loop configuration. The orbital degree of freedom also facilitate an f-wave superconductivity in which the gap nodal lines are determined by the orbital symmetry independent of the concrete pairing interactions.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S15 DMP: 2D Materials (Semiconductors) -- Emerging Materials I  BCEC 154 - Kristie Koski, University of California, Davis - Tag(s): Focus
11:15AM S15.00001: An Orbitally-Derived Single Atom Magnetic Memory  BRIAN KIRALY (Presenter), Scanning Probe Microscopy, Radboud University, ALEXANDER N. RUĐENKO, School of Physics and Technology, Wuhan University, WERNER M. J. VAN WEERDENDURG, DANIEL WEGNER, Scanning Probe Microscopy, Radboud University, MIKHAIL KATSNELSON, Theory of Condensed Matter, Radboud University, ALEXANDER A. KHAJETOORIANS, Scanning Probe Microscopy, Radboud University — Single atoms at the surfaces of solids have demonstrated rich electronic, chemical, and magnetic properties. In this direction, we show that we can manipulate the valency of a single cobalt atom on a crystalline black phosphorus surface. Using the local electric field generated from an STM tip, individual cobalt atoms residing at the same hollow site can be reversibly switched between two stable states, which correspond to the different valencies. Consistency between experimentally observed charge densities and density functional theory calculations reveal distinct high and low total magnetic moments for each state. We investigate the stability of each configuration, as well as compare the experimentally measured impurity states with DFT calculations. Finally, we probe the switching dynamics to determine the underlying mechanism and energy scale of the switching. This system opens up the horizon to explore complex memory based on both the orbital and spin degrees of freedom.

11:27AM S15.00002: Anisotropic Quantum Transport in Black Phosphorus Two-dimensional Hole Gas  FANGYUAN YANG, ZUOCHENG ZHANG, Fudan University, NAI ZHOU WANG, University of Science and Technology of China, SHUAIFEI GUO (Presenter), Fudan University, HAO WANG, Southern University of Science and Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, XIN WAN, Zhejiang University, XIANGHUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Fudan University — High-mobility two-dimensional (2D) electron system in black phosphorus van der Waals heterostructures has provided a new platform for studying electron-electron interaction in 2D. In particular, the large anisotropy distinguishes black phosphorus from other high-mobility two-dimensional (2D) electron systems. Here, we observed that new anisotropic states emerge at fractional filling factors for spin-split Landau levels $N > 4$. The new states manifest as resistance maxima or minima when current flows in different directions. Our results indicate the formation of charge-density-wave stripe phase in black phosphorus 2D hole gas that is surprisingly robust against thermal fluctuation and impurity scattering.

11:39AM S15.00003: "Resonant Tunneling in Black Phosphorus Homojunction"  YASIR HASSAN (Presenter), SAINT, Sungkyunkwan University Suwon Korea, PAWAN KUMAR SRIVASTAVA, School of Mechanical Engineering, Sungkyunkwan University Suwon Korea, BUDHI SINGH, Inter University Accelerator Center, New Delhi, India, CHANGUU LEE, School of Mechanical Engineering, Sungkyunkwan University Suwon Korea — Most common resonant tunnel devices (RTDs) consist of a quantum well formed between double barrier structures. Here for the first time, we demonstrate the RTD in a homojunction. By taking highly anisotropic nature of black-phosphorous (BP) into account, we have fabricated RTDs by sandwiching a thin (4-7 nm)-BP layer between two thick (40-72 nm)-BP flakes. We have observed that RTD could be realized in a BP homojunction by careful alignment of BP flakes. Moreover, a formation of a quantum well at the junction derives from the work function tunability of BP with flake thickness. Work function difference of thick-BP and sandwiched thin-BP layers results in band bending near the junction creating a quantum well. Under certain bias conditions, an electron can tunnel from one side to other through bound states in the quantum well. Such RT has been manifested by observation of negative differential resistance (NDR) in the current-voltage characteristics. The observed NDR peak in the current-voltage characteristics shifts to a higher voltage with decreasing quantum well thickness. Temperature-dependent current-transport reveals that momentum conservation for resonant tunneling is satisfied with acoustic/optical phonon scattering of electrons in the quantum well.

11:51AM S15.00004: Strain Tuning of the Electronic Structures of Few-Layer Black Phosphorus  SHENYANG HUANG (Presenter), GUOWEI ZHANG, FENG-REN FAN, FANJIE WANG, QIAOXIA XING, CHONG WANG, HUA WU, HUGEN YAN, Fudan University — Black phosphorus (BP) is a Van Der Waals material consisted of puckered atomic layers coupled together by the weak Van Der Waals force. Although Van Der Waals force is weak, it plays an important role in their bandstructure evolution. In this work, we tune the bandstructures of few-layer (2-10 layer) black phosphorus by applying in-plane biaxial strain. A large tunability has been observed for all of the few-layer BP samples. Careful examination reveals that the strain effect has layer dependence and transition order dependence, which can be accounted by the interlayer coupling effect. Meanwhile, Raman studies for the strained BP have been performed as well, which corroborate our observations.
**12:03PM S15.00005: Layer-Dependent Ultrafast Carrier and Coherent Phonon Dynamics in Black Phosphorus**

XIANCHONG MIAO (Presenter), MINBIAO JI, Fudan University — Black phosphorus is a layered semiconducting material, demonstrating strong layer-dependent optical and electronic properties. Probing the photophysical properties on ultrafast time scales is of central importance in understanding many-body interactions and nonequilibrium quasiparticle dynamics. Here, we applied temporally, spectrally, and spatially resolved pump–probe microscopy to study the transient optical responses of mechanically exfoliated few-layer black phosphorus, with layer numbers ranging from 2 to 9. We have observed layer-dependent resonant transient absorption spectra with both photobleaching and red-shifted photoinduced absorption features, which could be attributed to band gap renormalization of higher subband transitions. Surprisingly, coherent phonon oscillations with unprecedented intensities were observed when the probe photons were in resonance with the optical transitions, which correspond to the low-frequency layer-breathing mode. Our results reveal strong Coulomb interactions and electron–phonon couplings in photoexcited black phosphorus, providing important insights into the ultrafast optical, nanomechanical, and optoelectronic properties of this novel two-dimensional material.

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**12:15PM S15.00006: Prolonged photo-carriers generated in Black Phosphorus**

MUNISA NURMAMAT (Presenter), Department of Physics Science, Graduate School of Science, Hiroshima University, Japan, YUKIAKI ISHIDA, Institute for Solid State Physics, the University of Tokyo, Japan, RYOHEI YORI, KAZUKI SUMIDA, SIYUAN ZHU, Department of Physics Science, Graduate School of Science, Hiroshima University, Japan, MASASHI NAKATAKE, Aichi Synchrotron Radiation Center, Aichi Science & Technology Foundation, Japan, YOSHIFUMIUEDA, MASAKI TANIGUCHI, Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan, SHIK SHIN, Institute for Solid State Physics, the University of Tokyo, Japan, YUICHI AKAHAMA, Graduate School of Material Science, University of Hyogo, Japan, AKIO KIMURA, Department of Physics Science, Graduate School of Science, Hiroshima University, Japan — Transient electron-hole pairs generated in semiconductors can exhibit unconventional excitonic condensation. By optical pumping, photoexcited carriers facing across the band gap form excitons due to the Coulomb interaction between electrons and holes. As being a direct band gap and highly anisotropic semiconductor, black phosphorus (BP) can be expected to form excitons due to the nonequilibrium electron and hole populations after optical pumping. However, the electrons excited in the conduction band and their carrier dynamics which can offer hints on e-h pair condensation have not yet been clarified.

Here we employ time-resolved ARPES to explore the dynamics of photo-generated carriers in BP. The electronic structure above the Fermi level has been clearly observed, where a massive-and-anisotropic Dirac-type dispersions are confirmed. Importantly, we have directly observe that the photo-carriers generated across the direct band gap have the life time exceeding 400 ps. Such a long duration can be attributed to the stabilized e-h pairs between conduction and valence bands and confirms that the BP is a suitable platform for excitonic condensations.

**12:27PM S15.00007: Strain-engineered p-type to n-type transition in mono-, bi- and tri-layer phosphorene**

ANASS SIBARI (Presenter), ZINEB KERRAMI, Physics, Mohammed V University - Rabat, ABDEIKADER KARA, Physics, University of Central Florida, OMAR MOUNKACHI, Physics, Mohammed V University - Rabat, MOHAMMED HAMEDOUN, ABDELILAH BENYOUSSEF, MASciR Foundation, MOHAMMED BENAÏSSA, Physics, Mohammed V University - Rabat — Using density functional theory, a detailed computational study is performed to explore the structural and electronic properties of a phosphorene monolayer, bilayer and trilayer under a uniaxial strain along the armchair (b axis) and zigzag (a axis) directions. In the case of a monolayer phosphorene, it is found that strain along the armchair direction slightly affects the a lattice parameter and the puckering height (Δ). Along the zigzag direction, however, variation of the a lattice parameter is compensated by both the a and b lattice parameters while the parameter Δ remains unaffected. In terms of electronic properties, strain along the armchair and zigzag directions changes the nature of the Γ point in the bandgap from a direct to an indirect electronic transition as a function of the strain value. In the strain range from -14% to +6%, all phosphorene structures behave like most semiconductors under strain. However, size and strain combined effect significantly affects the Fermi energy position. Around 0% strain, all phosphorene structures are of p-type, while they switch to an n-type semiconductor in the range of strain values from +2% up to +14%. This p-type to n-type transition may have a major technological impact in fields where mono- and hetero-junctions are needed.
12:39PM S15.00008: Probing topology through optical response in group V monolayers*  
GAOFENG XU (Presenter), TONG ZHOU, University at Buffalo, The State University of New York, BENEDIKT SCHARF, University of Würzburg, IGOR ZUTIC, University at Buffalo, The State University of New York — Experiments on Bi monolayers on a SiC substrate reveal an interplay between a huge topologically nontrivial gap ~0.8 eV and strong spin-orbit coupling (SOC), leading to striking transport properties such as a robust quantum spin Hall effect (QSHE)[1]. With a suitable choice of substrates it is also possible to remove valley degeneracy and realize multiple Hall effects in a single materials system [2]. In contrast to transport properties, much less is known about how an optical response could yield topological signatures in these group V monolayers. By combining first-principles calculations for different substrates and a careful inclusion of strong SOC and Coulomb interaction in effective models for these monolayers on various substrates, we show that the changes in optical response reveal topological properties inherent to these systems. We explain how these findings offer new opportunities for proximitized materials [3]. [1] F. Reis, et al., Science 357, 287-290 (2017); F. Dominguez, et al., Phys. Rev. B 98, 161407(R) (2018). [2] T. Zhou, et al., npj Quant. Mater. 3, 39 (2018). [3] I. Zutic, et al., Materials Today (2018).

*U. S. DOE, Office of Science BES

12:51PM S15.00009: Multiple Hall Effects in Functionalized Bismuth Monolayers*  
TONG ZHOU (Presenter), Department of Physics, University at Buffalo, JIAYONG ZHANG, School of Mathematics and Physics, Suzhou University of Science and Technology, HUA JIANG, School of Physical Science and Technology, Soochow University, IGOR ZUTIC, Department of Physics, University at Buffalo, ZHONGQIN YANG, Department of Physics, Fudan University — Advances in (quantum) spin and anomalous Hall effect, as well as (anomalous) valley Hall effect suggest the electronic degrees of freedom (spin, charge, and valley) can be used as different information carriers [1,2]. The realization of multiple Hall effects in a single 2D material provides a fascinating opportunity to manipulate the implementation of such information [3]. Motivated by the experiments [4], we combine a tight-binding model with first-principles calculations to reveal that with a large nontrivial gap, quantum spin Hall effects (QSHEs) and valley Hall effects appear simultaneously in the functionalized bismuth monolayers [5]. A staggered exchange field is introduced to realize the spin-valley polarized QSHEs. With gate control, QSHE and anomalous charge, spin, valley Hall effects can be observed in the single system [5]. These predicted multiple Hall effects could enable applications of the functionalized bismuth monolayers in electronics, spintronics, and valleytronics.


1:03PM S15.00010: Properties and Device Prospects of Emerging Two-Dimensional Materials* [Invited]  
HAN WANG (Presenter), Ming Hsieh Department of Electrical Engineering, University of Southern California — In this talk, I will discuss our recent research in studying the electronic, optical and ferroelectric properties of emerging low-dimensional materials, and in developing them for electronic and photonic device applications. The first part of the talk will focus on discussing the basic properties of emerging 2D materials such as black phosphorus and its applications in mid-infrared optoelectronics. Our recent research on the ferroelectric monolayer materials will also be presented. In the second part of the talk, I will discuss our work on applying advanced 4-dimensional imaging technique to study the carrier transport in low dimensional materials and in studying optical phenomenon. I will conclude with remarks on promising future research directions of low-dimensional material properties and devices, and how the emerging materials may benefit future generations of electronics and photonics technology in sensing, imaging and communications.

*This work is supported by Army Research Office (Grant no. W911NF1810268), National Science Foundation (Grant no. ECCS-1653870) and Air Force Office of Scientific Research (Grant no. FA9550-15-1-0514).
1:39PM S15.00011: Electronic structures and unusually robust bandgap in an ultrahigh-mobility layered oxide semiconductor, Bi$_2$O$_2$Se

CHENG CHEN (Presenter), MEIXIAO WANG, shanghaiTech University, JINXIONG WU, peking university, HUIXIA FU, Weizmann Institute of Science, HAIFENG YANG, ZHEN TIAN, shanghaiTech University, TENG TU, peking university, HAN PENG, University of Oxford, YAN SUN, Max Planck Institute, XIANG XU, tsinghua university, JUAN JIANG, shanghaiTech University, NIELS SCHROTER, YIWEI LI, DING PEI, University of Oxford, SHUAI LIU, shanghaiTech University, SANDY ADHITIA EKAHANA, University of Oxford, HONGTAO YUAN, Nanjing University, JIAMIN XUE, GANG LI, shanghaiTech University, JINFENG JIA, shanghai jiao tong university, ZHONGKAI LIU, ShanghaiTech University, BINGHAI YAN, Weizmann Institute of Science, NIELS SCHRÖTER, YIWEI LI, DING PEI, University of Oxford, SHUAI LIU, shanghaiTech University, SANDY ADHITIA EKAHANA, University of Oxford, HONGTAO YUAN, Nanjing University, JIAMIN XUE, GANG LI, shanghaiTech University.

Semiconductors are essential materials that affect our everyday life in the modern world. Two-dimensional semiconductors with high mobility and moderate bandgap are particularly attractive today because of their potential application in fast, low-power, and ultrasmall/thin electronic devices. We investigate the electronic structures of a new layered air-stable oxide semiconductor, Bi$_2$O$_2$Se, with ultrahigh mobility (~2.8 × 10$^5$ cm$^2$/V.s at 2.0 K) and moderate bandgap (~0.8 eV). Combining angle-resolved photoemission spectroscopy and scanning tunneling microscopy, we mapped out the complete band structures of Bi$_2$O$_2$Se with key parameters (for example, effective mass, Fermi velocity, and bandgap). The unusual spatial uniformity of the bandgap without undesired in-gap states on the sample surface with up to ~50% defects makes Bi$_2$O$_2$Se an ideal semiconductor for future electronic applications. In addition, the structural compatibility between Bi$_2$O$_2$Se and interesting perovskite oxides further makes heterostructures between Bi$_2$O$_2$Se and these oxides possible platforms for realizing novel physical phenomena.

1:51PM S15.00012: Stable holey two-dimensional C$_2$N structures with tunable electronic structure*

RAPHAEL LOBATO (Presenter), JENAINA RIBEIRO SOARES, Departamento de Física, Universidade Federal de Lavras — We investigate the phonon stability of several bulk C$_2$N holey two-dimensional crystals (C$_2$N-h2D), a recently synthesized carbon nitride layered material, by using first-principles calculations. Among the polytypes addressed, only one does not display phonon instabilities. The electronic structure evolution of dynamically stable C$_2$N-h2D from monolayer to bilayer and to bulk is unveiled. The direct band gap at Γ can be decreased by 34% from monolayer to bulk, offering opportunities in optoelectronics. The effective masses of both carriers become smaller as the number of layers increases, and their anisotropy along in-plane directions displayed in the monolayer is reduced, which suggest that the carrier mobility may be tuned as well. These effects are then explained according to the interaction of the orbitals in neighboring layers.

*The authors thank the Foundation for Research Support of Minas Gerais (Grant No. CEX-APQ-01865-17), and the National Council for Scientific and Technological Development (Grant No. 310813/2017-4).

2:03PM S15.00013: Chlorine termination of Silicene on Silver (111)

JENNIFER DEMELL (Presenter), MICHAEL DREYER, ROBERT E BUTERA, Laboratory for Physical Sciences — Silicene is the 2D form of silicon, which grows readily on silver (111) as single layers or even bi-layers, showing several surface reconstructions in scanning tunneling microscopy images. Discrete Fourier transform calculations of halide-terminated single and multi-layers predict superconducting as well as topological behavior. In fact, a previous study [1] found possible superconductivity in plain silicene/silver, which – so far – we have been unable to confirm. We successfully grew silicene on silver (111) crystals and imaged them using scanning tunneling microscopy/spectroscopy at 4.2 K. The topographic and spectroscopic results on chlorine-terminated surfaces will be presented.


Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S16 DMP: Transport in Nanostructures -- 2D Materials and Their Heterostructures BCEC 155 - Shixiong Zhang, Indiana University Bloomington - Tag(s): Focus
11:15AM S16.00001: Electron transport in III-VI and IV-VI mono-chalcogenide nanostructures* [invited] XUAN GAO (Presenter), Case Western Reserve University — One focal point in recent studies of 2D semiconductors beyond transition metal dichalcogenides (e.g. MoS2) is non-transition metal based III-VI and IV-VI monochalcogenides. In this talk, I will highlight our transport studies of monochalcogenide InSe, SnS and SnSe for future 2D semiconductor applications. First, few and multilayer InSe nanoflakes are demonstrated to be promising 2D semiconductor nanostructures with high electron mobility and gate tunable Rashba spin-orbit coupling for high-performance n-type transistor and spintronic devices. Then I will discuss the gate and doping control of nanostructured IV-VI monochalcogenide SnS and SnSe's electrical and thermoelectric transport properties. In particular, the impact of SnS and SnSe's intrinsic p-type nature in the device behavior will be addressed. References: Nano Letters 15, 3815 (2015); Nano Letters 18, 4403 (2018); Nanoscale 8, 19050 (2016); Jour of Appl Phys, 123, 115109 (2018).

* The author acknowledges NSF CAREER Award (grant number DMR-1151534) for funding support.

11:51AM S16.00002: Inducing transport-anisotropy in graphene with 1D superlattices YUTAO LI (Presenter), SCOTT A DIETRICH, CARLOS FORSYTHE, SHAOWEN CHEN, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science (Japan), JAMES HONE, CORY DEAN, Columbia University — Graphene devices subjected to one-dimensional periodic superlattice potential have been studied extensively over the last decade. Previous experimental studies on such systems interpreted their data in fundamentally different ways: either based on commensurate effects such as Fabry-Perot interference, or a band structure based picture. Here we exploit our recently developed technique of dielectric superlattices to pattern graphene with a 1D superlattice, with periodicity as low as as low as 55nm. We observe strong anisotropy in electrical transport features along directions parallel versus perpendicular to the SL basis vector. For transport parallel to the SL basis vector, we see features consistent with Fabry-Perot interference at zero magnetic field, and Hofstadter butterfly-like features at high field that suggest band structure modifications. Possible interplay between commensurability effects and band structure modifications in such systems are discussed.

12:03PM S16.00003: Commensurate Lattice Vector Dependent Thermal Conductivity of Twisted Bilayer Graphene* CHENYANG LI (Presenter), BISHWAJIT DEBNATH, ROGER LAKE, University of California, Riverside — The in-plane thermal conductivity, as well as phonon dispersion of twisted bilayer graphene (TBG), are investigated as a function of temperature and rotation angle using both nonequilibrium molecular dynamics (NEMD) and density functional theory (DFT) combined with the phonon Boltzmann transport equation. The central result from the NEMD calculations is that the thermal conductivity decreases approximately linearly with the increasing lattice constant of the commensurate TBG unit cell. Comparisons of the phonon dispersions from both the DFT and NEMD calculations show that misorientation has the negligible effect on the low-energy phonon frequencies and velocities. However, the larger periodicity of TBG reduces the Brillouin zone size to the extent that the zone edge acoustic phonons are thermally populated allowing Umklapp scattering to reduce their lifetimes. This explanation is supported by DFT calculations of phonon-phonon lifetimes.

*This work was supported by the National Science Foundation under Award NSF EFRI-1433395. The ab initio simulations used the Extreme Science and Engineering Discovery Environment (XSEDE), supported by the National Science Foundation (NSF) grant No. ACI-1548562 and allocation ID TG-DMR130081.

12:15PM S16.00004: Anomalous Hall effect in strain-engineered graphene systems SHENG-CHIN HO (Presenter), CHING-HAO CHANG, YI-CHIANG HEISH, SHUN-TSUNG LO, THI-HAI-YEN VU, TSE-MING CHEN, Department of Physics, National Cheng Kung University — The pseudo-magnetic field in graphene is of significant interest because it provides a means to modify the band structures and consequently the electronic properties through mechanical deformations or, more precisely, by engineering the strain1,2. Here, we report the observation of a non-vanishing Hall conductivity in a strain-engineered graphene system in the absence of an external magnetic field.

**12:27PM S16.00005: Probing spin fluctuations in graphene nanoribbons with STM tunnelling spectroscopy**
RICARDO ORTIZ CANO (Presenter), University of Alicante, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory — We address the question of how scanning electron tunnelling spectroscopy can be used to probe spin excitations that emerge in localized states in atomically precise graphene ribbons. We consider both sequential and cotunnelling regimes, and discuss how the dI/dV curves provide information about the fluctuating local moments that are expected to occur in zigzag edges and other zero modes that occur in graphene ribbons. We model the graphene nanoribbons with a Hubbard model and we obtain the relevant electronic states by numerical diagonalization in a reduced active space. We conclude that inelastic electron tunnelling spectroscopy provides an image, with atomic scale resolution, of the spectral function of the low energy spin excitations in nanographene, and should provide unambiguous evidence of the emergence of local moments in this class of systems.

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2) "Generalitat Valenciana" and "Fondo Social Europeo" for the Ph.D. fellowship (ACIF/2018/198)
3) Fundação para a Ciência e a Tecnologia (FCT) for financial support via projects P2020-PTDC/FIS-NAN/3668/2014 and PTDC/FIS-NAN/4662/2014
4) FCT-UT Austin project UTAP-EXPL/NTec/0046/2017

**12:39PM S16.00006: High efficiency thermoelectricity with indirect excitons in a transition-metal dichalcogenide nanostructure**
CHUNJING JIA (Presenter), KAI WU, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory — High thermoelectric efficiency requires a large Seebeck coefficient and electric conductivity while maintaining low thermal conductivity. Recent development of modern synthesis techniques in nanomaterials provides new approaches to conquer such limits and usher the study of the thermoelectric effect into a new era. We propose to use indirect excitons (IEs) in two-dimensional TMDC nanostructures as a highly efficient thermoelectric device. We develop the exciton transport theory and numerically simulate the thermoelectric transport coefficients based on materials-specific parameters obtained from ab initio density functional theory calculations and experiments. Our numerical simulation shows that the excitons in bilayer TMDCs can dramatically enhance the figure of merit and the power factor an order of magnitude compared with those of separated TMDC monolayers. These enhancements are general consequences of increasing the Seebeck coefficient and electric conductivity of IEs simultaneously, thus demonstrating robustness for enhancing the thermoelectric effect.

**12:51PM S16.00007: Spin Hall effect for polaritons in a TMDC monolayer embedded in a microcavity**
OLEG Berman (Presenter), ROMAN KEZERASHVILI, Physics Department, New York City College of Technology, City University of New York, New York, USA, YURIII LOZOVIK, Laboratory of Nanophysics, Institute of Spectroscopy, Troitsk, Russia — The spin Hall effect (SHE) for polaritons in a transition metal dichalcogenides (TMDC) monolayer embedded in a microcavity is predicted. We demonstrate that two counterpropagating laser beams incident on a TMDC monolayer can deflect a polariton flow due to generation the effective gauge vector and scalar potentials. The components of polariton conductivity tensor for a weakly-interacting Bose gas of polaritons in the presence of Bose-Einstein condensation (BEC) and superfluidity and for non-interacting polaritons without BEC are obtained. We propose to study the superfluidity of microcavity polaritons by experimental measurement of components of a total conductivity tensor as functions of the effective gauge magnetic field at different temperatures. It is shown that the concentrations of the normal and superfluid components and the Kosterlitz-Thouless temperature of occurrence of superfluidity can be determined by experimental measurement the components of the total conductivity tensor. The possible experimental observation of the SHE for microcavity polaritons is proposed, which provides the signature of the superfluidity of microcavity polaritons.

*The work was supported by U.S. Department of Defense under Grant No. W911NF1810433.*
Quantum scattering in two-dimensional nanostructures using a novel method of sources and absorbers

SATHWIK BHARADWAJ (Presenter), Department of Physics, Worcester Polytechnic Institute, Worcester, MA 01609, L RAMDAS RAM-MOHAN, Department of Physics, Electrical and Computer Engineering and, mechanical engineering, Worcester Polytechnic Institute, Worcester, MA 01609 — There have been several attempts in the literature to provide a variational approach to solve quantum scattering problems. However, the asymptotic boundary conditions (BCs) used in such methods do not take crucial evanescent modes into account, making them unsuitable for applications in meso- and nano-scale devices. Further, widely used atomistic models are computationally expensive for any device scale applications. We develop a method based on sources and absorbers to study quantum scattering in two-dimensional systems. The Cauchy BCs that are essential in the action integral formulation of scattering are reduced to simpler Dirichlet BCs by introducing totally absorbing “stealth regions.” Solutions decay within the stealth regions, thereby vanishing at the finite boundaries. A Green's function source is constructed to provide incident plane waves in the active scattering regime. This method overcomes the limitations of the currently prevalent approaches to provide a complete non-asymptotic variational description for scattering in confined as well as open domain quantum systems. We also discuss the applications of our method in simulating nanoscale rectifiers and enhancement of the thermoelectric power in quantum waveguides with embedded defects.

Strong exciton-plasmon coupling in two-dimensional transition metal dichalcogenides

AARON ROSE (Presenter), JEREMY R DUNKLIN, HANYU ZHANG, Chemistry & Nanoscience Center, National Renewable Energy Laboratory, JUAN M. MERLO, MICHAEL J NAUGHTON, Physics, Boston College, JAO VAN DE LAGEMAAT, Chemistry & Nanoscience Center, National Renewable Energy Laboratory — Two-dimensional transition metal dichalcogenides (2-D TMDs) show promise as photocatalytic materials for water splitting due to their strong light-matter interactions and favorable band gaps and band alignments. Incorporation of plasmonics into these systems is expected to enhance performance due to a variety of effects including large exciton-plasmon coupling.

Here, we show that strong exciton-plasmon coupling is possible in many 2-D TMD systems as evidenced by Rabi splitting in modeled photonic dispersion of thin films of 2-D TMDs coupled to tunable surface plasmons. The results show coupling in every metal-TMD combination between the metals Au, Al, Ag, and Cu and the 2-D TMDs MoS2, MoSe2, WS2, and WSe2. Finally, we discuss current experimental progress on such systems.

Phonon-Dislocation Interaction Mediated Thermal Transport in Polycrystalline MoS2

CHANGPENG LIN (Presenter), Shenzhen Geim Graphene Center (SGC), Tsinghua–Berkeley Shenzhen Institute (TBSI), Tsinghua University, XIAOBIN CHEN, School of Science, Harbin Institute of Technology, Shenzhen, XIAOLONG ZOU, Shenzhen Geim Graphene Center (SGC), Tsinghua–Berkeley Shenzhen Institute (TBSI), Tsinghua University — Phonon-dislocation interaction plays an important role in minimizing the lattice thermal conductivity in thermoelectric materials historically. Here, we implemented a systematic study of heat transport in polycrystalline MoS2 by molecular dynamics simulation and atomic Green’ s function method. Simulation results indicate that thermal boundary conductance of diverse grain boundary in MoS2 scales quasi-linearly to grain boundary energy. The existence of grain boundary strongly scatters the phonons with frequency larger than 3 THz, below which transmission function remains almost unchanged. Furthermore, the breakdown of classical Casimir model is observed by directly comparing to the thermal conductivity results obtained from realistic polycrystalline MoS2 with different grain size, and the detailed phonon dynamics should be taken into account to accurately describe the phonon scattering at grain boundary. Our findings will provide crucial guidelines for designing efficient thermoelectrics by phonon-dislocation interaction.

This work was supported by the Development and Reform Commission of Shenzhen Municipality under the "Low Dimensional Materials and Devices Discipline", the Youth 1000-Talent Program of China, and the Tsinghua-Berkeley Shenzhen Institute (TBSI).
1:39PM S16.00011: Frequency-Domain Magneto-Optical Kerr Effect for thermal property measurements of anisotropic 2-dimensional materials  SIMONE PISANA (Presenter), Department of Electrical Engineering and Computer Science, York University, Toronto, ON, Canada, MIZANUR RAHMAN, Department of Physics and Astronomy, York University, Toronto, ON, Canada, MOHAMMADREZA SHAHZADEH, Department of Electrical Engineering and Computer Science, York University, Toronto, ON, Canada — The rapidly increasing number of 2-dimensional materials that have been isolated or synthesized provides an enormous opportunity to realize new device functionalities. Whereas optical and electrical characterization has been more readily applicable to these new materials, quantitative thermal characterization is more challenging due to the difficulties with localizing heat flow. Optical pump-probe techniques that are well-established for the study of bulk materials or thin-films have limited sensitivity to lateral heat transport, and the characterization of the thermal anisotropy that is common in 2-dimensional materials is therefore challenging. Here we present a new method to quantify the thermal properties based on the magneto-optical Kerr effect that yields enhanced sensitivity to in-plane heat transport. Using a magnetic material as transducer for heat transport allows the use of semi-transparent layers that are very thin, increasing the in-plane thermal gradients. We apply this approach to measure the thermal properties of a range of 2-dimensional materials which are of interest for device applications, including single layer graphene and h-BN, multilayer h-BN and MoS₂, and bulk MoSe₂.

1:51PM S16.00012: Quantum Dragon Solutions for the Tight Binding Model of 2D Ribbon Nanodevices. GODFRED INKOOK (Presenter), MARK NOVOTNY, Mississippi State University, TOMAS NOVOTNY, Mathematics and Physics., Charles University — We present quantum dragon solutions for electron transport for the tight binding model with strong disorder in nanoribbons based on 2D hexagonal, rectangular, and square-octagonal graphs. When the nanodevice is connected between two thin semi-infinite leads, the Landauer formula gives the electrical conductance, \( G \). The electron transmission probability, \( T(E) \) from the solution of the time-independent Schrödinger equation, yields \( G = \frac{2e^2}{h} T(E) \). In the presence of uncorrelated randomness, \( T(E) \ll 1 \) for most electron energies, \( E \). Recently, the theoretical discovery of a large class of nanostructures called quantum dragons has been published [1]. Quantum dragon nanodevices have strong, correlated randomness but have \( T(E) = 1 \) for all \( E \) of electrons which propagate through the leads. Here, we show that both uniform leads and dimerized leads coupled to hexagonal, rectangular, and square-octagonal graphs with different boundary conditions can have the quantum dragon property [2]. We discuss how added disorder affects \( T(E) \) near a quantum dragon solution, and discuss experiments relevant to quantum dragon nanodevices.


Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S17 DCOMP: Matter in Extreme Environments: Theoretical Methods and Applications III BCEC 156A - Shuai Zhang, Lawrence Livermore National Laboratory

11:15AM S17.00001: Many-body molecular dynamics force fields for chemistry at extreme conditions* LAURENCE FRIED (Presenter), REBECCA LINDSEY, CONG HUY PHAM, NIR GOLDMAN, Lawrence Livermore Natl Lab — Molecular materials at high pressures and temperatures, such as those produced by a shock wave or detonation, often undergo rapid chemical reactions. There has been significant progress in understanding chemical processes at extreme conditions through simulations based on Kohn-Sham density function theory (DFT). DFT simulations, however, are typically limited in size to less than 1000 atoms and in time to less than 100 ps. We have developed a reactive molecular dynamics force field, called ChIMES, that retains much of the accuracy of density functional theory, while allowing application to much larger systems and longer time scales. The ChIMES approach has been recently extended to treat 4 body interactions and charge fluctuations. We find that these additions significantly enhance the accuracy of the force field, but require more sophisticated calibration methods to maintain accuracy and stability for a wide range of conditions. Effective calibration methods will be presented based on techniques adapted from the machine learning community. Applications to liquid carbon, H₂O, and N₂H will be discussed.

*This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
11:27AM S17.00002: Modeling High Strain Rate Plasticity in BCC Lead* ROBERT RUDD (Presenter), LIN YANG, ANDREW KRYGIER, PHILIP D POWELL, HYE-SOOK PARK, Lawrence Livermore Natl Lab, PETER GRAHAM, AWE — High-energy lasers have enabled the determination of constitutive properties of metals at very high pressures and strain rates. Here we consider the strength (flow stress) of lead in the high-pressure body-centered cubic (bcc) phase. There were two models of high-strain-rate lead strength available previously. Both models were constructed using data from the low-pressure, face-centered cubic phase of lead. Plasticity in bcc and fcc crystals can be very different. Experiments conducted at the National Ignition Facility have used ramp-compression to drive Rayleigh-Taylor instability and measured the ripple growth to infer lead strength in the bcc phase. We have developed an Improved Steinberg-Guinan model for bcc lead strength [1] using ab initio calculations of the shear modulus at pressure. We compare the predictions of the model with those from the two previous models and results from experiment. We also discuss the effect of alloying.

*This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.

11:39AM S17.00003: Role of “soft” wall confinement in the particle dynamics of supercritical fluids* KANKA GHOSH (Presenter), KRISHNAMURTHY C.V, Department of Physics, Indian Institute of Technology Madras, India — Supercritical fluids (SCF), having a heterogeneous phase behavior (“liquid-like” and “gas-like”) across the Frenkel line (FL) [1], seem to be a promising candidate for the study of the effect of wall softness on the particle dynamics. Recently, structural features of SCF have been found to vary significantly as the walls became “softer”[2].

Molecular dynamics simulations are carried out to understand the effect of softness of the walls on the particle dynamics of a supercritical fluid using mean-squared displacement (MSD) and the velocity autocorrelation function (VACF). Walls are systematically made “softer” by lowering the stiffness coefficient of the springs attached to each of the wall particles. The existence of non-diffusive modes, and the effect of wall softness on it, is investigated through the vibrational density of states (DoS). We discuss the contrasting trends observed in self-diffusion parallel to the walls, on the either side of the FL, as a function of the wall-stiffness. The effect of the “softness” of the walls to support or disrupt collective motion will also be discussed.


*Department of Science and Technology(DST), INSPIRE Fellowship.

11:51AM S17.00004: Maximum initial growth-rate of strong-shock-driven Richtmyer-Meshkov instability* AKLANT K BHOWMICK (Presenter), ARUN PANDIAN, Carnegie Mellon University, ROBERT F STELLINGWERF, Stellingwerf Consulting, SNEZHANA ABARZHI, Univ of Western Australia — We focus on the classical problem of the dependence on the initial conditions of the initial growth-rate of strong shock driven Richtmyer-Meshkov instability (RMI) by developing a novel empirical model and by employing rigorous theories and Smoothed Particle Hydrodynamics simulations to describe the simulation data with statistical confidence in a broad parameter regime. For the given values of the shock strength, fluid density ratio, and wavelength of the initial perturbation of the fluid interface, we find the maximum value of the RMI initial growth-rate, the corresponding amplitude scale of the initial perturbation, and the maximum fraction of interfacial energy. This amplitude scale is independent of the shock strength and density ratio and is characteristic quantity of RMI dynamics. We discover the exponential decay of the ratio of the initial and linear growth-rates of RMI with the initial perturbation amplitude that excellently agrees with available data.

*National Science Foundation (USA)
12:03PM S17.00005: Water and hydrocarbon desorption from rapidly-heated metal oxide surfaces  JASON P KOSKI (Presenter), KEVIN LEUNG, AIDAN THOMPSON, J MATTHEW D LANE, Sandia National Labs — Understanding and controlling water and hydrocarbon desorption from steel surfaces under vacuum are crucial for high-voltage pulsed power applications. Ohmic heating in Sandia's Z-machine conductors can drive temperature rises of 1000 K over nanoseconds, leading to plasma formation and current loss. We apply reactive and non-reactive classical molecular dynamics (MD) and grand canonical Monte Carlo (GCMC) methods to study the thermodynamics and kinetics of fast desorption from hematite Fe2O3 surfaces. MD simulations are conducted using thermodynamically consistent coverages deduced from GCMC. For water, the resulting time- and temperature-dependent desorption profiles on the Fe2O3 (0001) and (1-102) surfaces show cooperative behavior. Results are in reasonable agreement with simple Temkin isotherm model estimates. Similar reduced models will be discussed for hydrocarbons desorption. The effect of external electric field on desorption profiles will also be discussed.


12:15PM S17.00006: Sweeping wave impact on tantalum plate* DUAN ZHANG (Presenter), CURT A BRONKHORST, Los Alamos National Laboratory — The tensile plasticity (TEPLA) model is extended to study sweeping wave impact, where the material undergoing large deformation, pore growth, and failure. We start with the ensemble phase averaging method to derive averaged equations for inhomogeneous material. For a given time and spatial position, it only averages over the material configurations in which the given spacetime is occupied by the specified material. The averaging method leads to the decomposition of the velocity gradient into intrinsic part representing the gradient experienced by the solid material and the plastic part caused by deformations related to slipping planes, void growth, and sliding on the crack surfaces.

To compute large plastic deformation, while accurately tracking the material history Dual Domain Material Point (DDMP) method is employed. The DDMP method uses both Eulerian and Lagrangian descriptions. We use the Eulerian capability to compute the large deformation of the solid caused by a sweeping shock wave and the Lagrangian capability to track history dependent plastic pore growth. Numerical results are compared to an experiment to show the needed improvements on both the physical models and numerical techniques.

* Work performed under the auspices of the United States Department of Energy.

12:27PM S17.00007: Effects of alloying elements on defect production and evolution in Fe-based alloys  YAXUAN ZHANG (Presenter), CURT A BRONKHORST, Los Alamos National Lab, XIAN-MING BAI, Material Science and Engineering, Virginia Polytechnic Institute and State University — Fe-based alloys are important structural and cladding materials for current and future nuclear reactors. Radiation-induced defect production and subsequent defect evolution play important roles in microstructural evolution in these alloys. In this work, the effects of alloying elements on defect production and evolution in Fe-based alloys have been investigated using molecular dynamics simulations. Primary damage simulations have been conducted for pure Fe and Fe-based alloys, including Fe-Cr, Fe-Cu, and Fe-W. It is found that Cr or Cu do not affect the total number of produced Frenkel pairs, while oversized W increases the total number of Frenkel pairs. In addition, Cr interstitials are over-produced while Cu and W interstitials are under-produced comparing to their solute concentrations. Both dislocation loops and C-15 clusters have been found in these alloys but their population is affected by the alloying elements. Interstitial cluster evolution is studied in these alloys. It is found that Cr and W suppress the growth of dislocation loops. Finally, the defect energetics are calculated to interpret these simulation results.

12:39PM S17.00008: Dynamic recrystallization in adiabatic shear banding: an entropic, effective-temperature model  CHARLES K LIEOU (Presenter), HASHEM MOURAD, CURT A BRONKHORST, Los Alamos National Laboratory — Dynamic recrystallization (DRX) is often observed in conjunction with adiabatic shear banding (ASB) in polycrystalline materials. The recrystallized nanograins in the shear band have few dislocations compared to the material outside of the shear band. We reformulate the recently developed Langer-Bouchbinder-Lookman (LBL) continuum theory of polycrystalline plasticity and include the creation of grain boundaries. While the shear-banding instability emerges because thermal heating is faster than heat dissipation, recrystallization is interpreted as an entropic effect arising from the competition between dislocation creation and grain boundary formation. We show that our theory closely matches recent experimental results in sheared ultrafine-grained titanium and in compressed AISI 316L stainless steel. The theory thus provides a thermodynamically consistent way to systematically describe the formation of shear bands and recrystallized grains therein.
12:51PM S17.00009: Crack deflection-penetration at a nanoscale interface of graphene/hBN heterostructure
TOUSIF AHMED (Presenter), MD Z HOSSAIN, Mechanical Engineering, University of Delaware — We investigate crack deflection-penetration behavior at an interface of two elastically dissimilar 2D nanomaterial taking an interface between graphene and hexagonal boron nitride (hBN) as an example test case. Growth of an edge crack from graphene towards hBN and similar growth of crack from hBN towards graphene are considered in two separate cases. Crack deflection-penetration (DP) criterion for continuum study is redefined in terms of cohesive energies of individual solids in this MD study. In case of graphene/hBN heterostructure, crack typically prefers to penetrate either material over deflection when it reaches the interface. Ratios of cohesive energies of interface and material ahead of the crack are 0.67 (when crack in graphene) and 1.0 (when crack in hBN). As these ratios lie in the crack penetration zone of the DP criterion, crack penetration is the only logical choice. However, in some cases slight deflection has been observed. This phenomenon occurs when crack bifurcates into several branches and the mother crack interacts with defects formed at the interface due to lattice constant mismatch. This initial study indicates that at nanoscale crack growth, DP criterion developed for continuum studies cannot be directly applied due to the role of crystallography itself.

1:03PM S17.00010: Assessing the Impact of Strength Model Parameters on Simulated Cerium Flyer Plate Behavior*
JOANNE BUDZIEN (Presenter), Los Alamos National Laboratory — Cerium flyer plate experiments were simulated using the LANL Lagrangian hydrodynamics code FLAG and results were compared to experimental results. The range of experiments examined includes shocking through the cerium γ-α phase transition. Several sets of parameters for the Preston-Tonks-Wallace strength model have been produced through fits to experimental Hopkinson bar data. We will present simulation results showing the effect of varying the strength parameter sets including simulations with no strength. This process may aid in differentiating the various parameter sets by testing them under conditions different from the calibration experiments.

*Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396.

1:15PM S17.00011: Update on the Development of a Multiscale Friction Model
MARVIN ZOCHER (Presenter), MARK KENAMOND, JAMES EDWARD HAMMERBERG, Los Alamos National Laboratory — Two sets of experiments designed to produce dry sliding of metal-on-metal resulting in normal pressures up to tens of GPa and sliding velocities up to hundreds of meters per second are simulated numerically for the purpose of evaluating a new multiscale friction model. These experiments involve the impact of a cylindrical copper flyer onto a composite cylindrical target composed of an aluminum inner core and a stainless steel circumferential confinement. The primary diagnostic in these experiments is a measurement of free-surface velocity. Numerical simulations are conducted using the Los Alamos finite volume continuum mechanics code FLAG. The primary metric of evaluation is a comparison of predicted free-surface velocities to those measured. The importance of accounting for friction in the simulation of these experiments is clearly demonstrated. It is shown that the FLAG implementation of the new multiscale friction model provides capabilities that are essential in the modeling of dry sliding friction.

1:27PM S17.00012: Uncertainty Quantification of Velocimetry-Based Load Current Inferences for 100 ns Multi-Mega-Amp Pulsed Power Experiments
ANDREW PORWITZKY (Presenter), JUSTIN BROWN, CHRISTOPHER JENNINGS, Sandia National Laboratories — Accurate determination of the electric current delivered to the load region is critical to the success of various multi-mega-amp pulsed power experiments. Magnetic inductance (B-dot) probes often fail over ten mega-amps, and when successful can only infer current centimeters from the load region, before major current loss mechanisms kick in. This has prompted interest in velocimetry-based load current inferences. The present work is part of a systematic uncertainty quantification effort. Here we apply Bayesian statistics to a series of synthetic experiments. Tens of thousands of multiphysics simulations were run with perturbed drive currents to determine correlations between input current and output surface velocity (our experimental measurable). We find that for very short pulses (100 ns rise time) relevant to cylindrical platforms significant uncertainties, not typical of planar dynamic materials experiments, can be introduced around peak current if the velocimetry measurement is not well matched to the current pulse. All regions of enhanced uncertainty are explained physically, and compensating strategies are developed in order to increase confidence and certainty in load current inferences.
1:39PM S17.00013: Numerical modeling of the phase transition kinetics for the sub-microsecond solidification of water under dynamic compression*  DANE STERBENTZ (Presenter), University of California, Davis, PHILIP MYINT, Lawrence Livermore National Lab, JEAN-PIERRE DELPLANQUE, University of California, Davis, JONATHAN BELOF, Lawrence Livermore National Lab — Several landmark experimental studies on the solidification of liquid water to the high-pressure ice VII phase under multiple-shock and ramp dynamic compression have been carried out over the past two decades, yet modeling this rapid phase transition has proven challenging. The application of classical nucleation theory (CNT)-based approaches to rapid phase transition kinetics occurring under extreme temperatures and pressures presents a variety of new opportunities for predictive computational modeling. This work attempts to model the liquid water-ice VII phase transformation using a numerical discretization scheme to solve the Zel'dovich-Frenkel partial differential equation, an underlying CNT-based kinetic equation describing the statistical time-dependent behavior of solid cluster formation. One major result of this research is that the Zel'dovich-Frenkel equation is able to accurately determine—the duration of the induction time prior to the onset of the phase transformation.  

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. We thank A. Arsenlis, D.P. McNabb, and B. Wallin for funding and project support.

1:51PM S17.00014: Li-ion battery material under high pressure: amorphization and enhanced conductivity of Li$_4$Ti$_5$O$_12$*  LIN WANG (Presenter), High Pressure Science and Technology Advanced Research — Li$_4$Ti$_5$O$_12$ (LTO), a “zero-strain” anode material for lithium-ion batteries, exhibits excellent cycling performance. However, its poor conductivity highly limits its applications. Here, the structural stability and conductivity of LTO were studied using in situ high-pressure measurements and first-principles calculations. LTO underwent a pressure-induced amorphization (PIA) at 26.9 GPa. The impedance spectroscopy revealed that the conductivity of LTO improved significantly after amorphization compared with its starting phase. Furthermore, our calculations demonstrated that the different compressibility of the LiO$_6$ and TiO$_6$ octahedra in the structure was crucial for the pressure-induced amorphization. The amorphous phase promotes Li$^+$ diffusion and enhances its ionic conductivity by providing defects for ion migration. Our results not only provide an insight into the pressure depended structural properties of a spinel-like material but also facilitate exploration of the interplay between pressure-induced amorphization and conductivity.  

*This work was mainly supported by Science Foundation of China (Grant No. 11874076), National Science Associated Funding (NSAF, Grant No. U1530402), and Science Challenging Program (Grant No. JCKY2016212A501).

Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S18 DCOMP: Electronic Structure Methods I  BCEC 156B - Jianwei Sun, Temple University - Tag(s): Focus

11:15AM S18.00001: van der Waals density functional with corrected long-range behavior*  TIMO THONHAUSER (Presenter), Department of Physics, Wake Forest University, KRISTIAN BERLAND, Department of Physics, University of Oslo, DEBAJIT CHAKRABORTY, Department of Physics, Wake Forest University — A new van der Waals density functional, i.e. vdw-DF3, has been developed by maintaining an accurate balance between short- and long-range contributions to the non-local correlation in the original vdw-DF scheme. We stay entirely true to the original design criteria of vdw-DF, adhering to the exact same physical constraints. But, we take advantage of some freedom in defining the plasmon-dispersion model ω$_Q$ which allows us to significantly improve the asymptotic behavior and the resulting calculated C$_6$ coefficients, overcoming the problem of unreliable C$_6$ coefficients from previous vdw-DF functionals. Our functional predicts very well the binding energies (<5% error) and separation for molecular dimers of commonly used reference datasets (such as S22, A24, X40, S66 etc.); performance in solids, layered structures, and noble gas dimers is also good.  

*This work has been funded by NSF grant No. DMR-1712425.
**11:27 AM S18.00002: A fitted van der Waals density functional with accurate short and long-range interactions**

DEBAJIT CHAKRABORTY (Presenter), Department of Physics, Wake Forest University, KRISTIAN BERLAND, Department of Physics, University of Oslo, TIMO THONHAUSER, Department of Physics, Wake Forest University — A fitting scheme has been developed to create a new van der Waals density functional, called vdW-DF-fit. The original vdW-DF kernel, as well as the plasmon dispersion model, are numerically modified and fitted to minimize the binding energy and separation errors with respect to experimental/RPA/high-level quantum chemistry results of a list of commonly used reference datasets (S22, A24, X40, S66 etc.). We are also pursuing automated fitting schemes using machine-learning techniques. This is work in progress and we are reporting first, promising results.

*This work has been funded by NSF grant No. DMR-1712425

**11:39 AM S18.00003: A Generalized Gradient Approximation with Local Parameters.** ANGEL ALBAVERA MATA (Presenter), Departamento de Química, Centro de Investigación y de Estudios Avanzados, KARLA BOTELLO MANCILLA, Escuela Superior de Ingeniería Química e Industrias Extractivas, Instituto Politécnico Nacional, DANIEL MEJIA-RODRIGUEZ, Quantum Theory Project, Department of Physics, University of Florida, SAM B TRICKEY, Quantum Theory Project, Department of Physics and Department of Chemistry, University of Florida, JOSE L GAZQUEZ, Departamento de Química, Universidad Autónoma Metropolitana, ALBERTO VELA, Departamento de Química, Centro de Investigación y de Estudios Avanzados — The dependence of typical generalized gradient approximations (GGA) for exchange-correlation (XC) on fixed, global parameters makes them incapable of providing good accuracy in predicting, simultaneously, molecular and solid properties. This drawback has motivated recent interest in constructing more flexible GGAs incorporating XC parameters that depend on the density, bounding their values to those for the high- and low-density regimes. In this work we explore a scheme to couple X and C functionals through the density-dependence of the gradient expansion coefficient derived beyond the random phase approximation [1,2] employed in different C functionals [3-5]. We discuss the implications of such local dependence of the gradient coefficient and show results of these GGAs for various properties involving test sets of atoms, molecules, and solids.


**11:51 AM S18.00004: Neural-Network Implementation of Transferable Kohn-Sham Exchange-Correlation Functionals**

RYO NAGAI (Presenter), Institute of Solid State Physics, University of Tokyo, RYOSUKE AKASHI, SHU SASAKI, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo, OSAMU SUGINO, Institute of Solid State Physics, University of Tokyo — The accuracy of Kohn-Sham density functional theory [1] depends crucially on its approximated exchange-correlation functional. Structures of conventional density functionals depend on, however, combination of a number of physical constraints, making thereby the construction technically demanding and systematic improvement of their accuracy difficult. In order to overcome this difficulties, we present a new strategy free from the use of complicated physical constraints: representing the functional structure with Neural-network (NN), which is an extremely flexible function with a large number of parameters.

We demonstrate two types of NN-based functional. (i)Non-local functionals, which is made to reproduce the exact exchange-correlation potential of 1D model systems consisting of two electrons applied with various external potentials [2], (ii)Semi-local functionals, which is made to reproduce densities provided by an accurate quantum chemical calculation of only a few molecules [3]. We show potentials of the NN-based functionals for high accuracy and out-of-training transferability.


Theory will be presented, and only passing familiarity is assumed. The uniform electron gas in three and two dimensions is treated exactly by popular Kohn-Sham density functional approximations. However, no general-purpose semi-local functional can find the correct behavior of a 3D electron gas undergoing extreme compression in one dimension. In this talk, I will present our recent work [1] applying the SCAN functional to this perennial problem. While the exact exchange-correlation energy per electron tends to a finite 2D limit, the local density and generalized gradient dimension. In this talk, I will present our recent work [1] applying the SCAN functional to this perennial problem. While the exact exchange-correlation energy per electron tends to a finite 2D limit, the local density and generalized gradient approximations to it diverge to minus infinity. SCAN tends to a finite limit that is however an order of magnitude too negative. These errors at high compression are in one sense harmless, since the noninteracting kinetic energy, treated exactly in Kohn-Sham density functional theory, overwhelms them. Relevant background in Kohn-Sham density functional theory will be presented, and only passing familiarity is assumed.


*Supported by:

Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Grant No. DE-SC0012575.

Army Research Laboratory, Grant No. W911NF-16-2-0189.

We discuss two sets of response functionals for estimating the local, non-negative kinetic energy density of initially free electrons that are perturbed by a static external potential. We begin with first- and second-order functionals of the perturbing potential, which are directly analogous to known response functionals for the electron density and the integrated kinetic energy. We provide reciprocal-space formulations of these functionals that complement previously known real-space expressions. We then present alternate first- and second-order response functionals that operate on the induced electron density and do not depend explicitly on the applied potential. The structure of these latter functionals will help guide the design of the more sophisticated kinetic energy functionals that enable orbital-free density functional theory simulations of materials. We examine the performance of the response functionals, in density-functional form, when applied to electron densities generated from local pseudopotential calculations for Li, Al, and Si solids.

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12:51PM S18.00009: Koopmans compliance: a functional theory for spectral properties  ANDREA FERRETTI (Presenter), Nanoscience Institute, S3 Center, National Research Council, NICOLA COLONNA, NGOC LINH NGUYEN, NICOLA MARZARI, THEOS, Ecole Polytechnique Federale de Lausanne — Energy functionals which depend explicitly on each individual orbital density, rather than the total charge density, appear naturally when applying self-interaction corrections to density-functional theory. Rather than a limitation, we argue that this is a powerful feature, and show how it is possible to interpret the orbital-dependency of densities and potentials as an effective frequency dependency. Such a frame is naturally amenable to describe electronic spectroscopies [1], and is free from e.g. the constraint of having derivative discontinuities in the exact formulation. Excellent agreement is achieved for ionization potentials and affinities, fundamental gaps, and deeper orbital levels (photoemission) for both molecules and solids [2-4]. We believe that a functional theory for the spectral density is therefore emerging, able to address at the same time total energies and spectral properties.


1:03PM S18.00010: The Self-Consistent Field in Kohn-Sham Density Functional Theory: A Review of Methods and Algorithms* NICK WOODS (Presenter), MICHAEL C PAYNE, Department of Physics, University of Cambridge, PHIL HASNIP, Department of Physics, University of York — Software that computes the electronic structure of a material by searching for an infimum of the Kohn-Sham energy functional - achieving self-consistency - requires the use of an algorithm that iterates an initial estimate of the particle density toward the self-consistent particle density. We present a review of methods and algorithms that solve this problem in the context of plane-wave, pseudopotential density functional theory. This review involves first identifying features intrinsic to the Kohn-Sham framework that produce sources of numerical difficulty for self-consistency algorithms. A test suite of over fifty Kohn-Sham inputs is then designed in order to exploit these difficulties and target weaknesses in contemporary algorithms. In order to utilise this test suite, a sample of methods from literature are then implemented in the plane-wave, pseudopotential density functional theory code, CASTEP. These methods are then benchmarked on the test suite, and a novel set of analysis tools allow us to determine the effectiveness of each method. We believe this study will not only elucidate the current state of the literature, but also assist future method development by providing a systematic work-flow for presenting new methods and assessing their effectiveness.

*EP/L015552/1

1:15PM S18.00011: Obtaining Stationary States in Density Functional Theory Using Imaginary Time Propagation* CEDRIC FLAMANT (Presenter), GRIGORY KOLESOV, Harvard University, EFSTRATIOS MANOUSAKIS, Florida State University, EFTHIMIOS KAXIRAS, Harvard University — Density functional theory (DFT) is widely successful for determining electronic and structural properties of materials and molecules. In order to perform a DFT calculation, the Kohn-Sham nonlinear equations must be solved self-consistently, a task usually achieved using self-consistent field (SCF) loops. However, for large systems SCF can occasionally struggle to find the ground state. Using time-dependent DFT in imaginary time, a given starting state can be purified into its lowest-energy component with reliable monotonic convergence. With appropriate constraints, it is also possible to obtain excited states with imaginary time propagation (ITP). We compare and analyze the performance of ITP and SCF in a few difficult systems, and present a few excited state calculations performed with the method.

*This work was supported by the Army Research Office MURI Award No. W911NF-14-0247. We used computational resources on Odyssey cluster at Harvard University and XSEDE (NSF Grant No. ACI-1053575).
1:27PM S18.00012: Path-integral imaginary-time TDDFT simulation of the hydrogen-bonded systems*  
GRIGORY KOLESOV (Presenter), Harvard University, EFSTRATIOS MANOUSAKIS, Department of Physics and National High Magnetic Field Laboratory, Florida State University, EFTHIMIOS KAXIRAS, Harvard University — We have recently developed a new imaginary-time time-dependent density-functional theory (iTDDFT)-based approach for computing the ground-state electron-ionic structure of atomistic systems[1]. In this method the ionic degrees of freedom are treated in the path-integral formalism, whereas electronic degrees of freedom are treated with iTDDFT. Our method, given an exact functional of the electronic density, is in principle exact in the zero-temperature limit. With approximate functionals it offers a practical path to direct \textit{ab initio} simulation of molecular and condensed matter systems going beyond the Born-Oppenheimer approximation. In this work we apply our method to study properties of hydrogen-bonded and tautomeric molecules: hydrogen sulfide, formic acid and terephthalic acid dimers. We compare the results of our simulations to known experimental and theoretical results.


*This work was supported by the Army Research Office MURI Award No. W911NF-14-0247. We used computational resources on Odyssey cluster at Harvard University and XSEDE (NSF Grant No. ACI-1053575).

1:39PM S18.00013: Benchmarking the structure selection performance of the SCAN functional relative to PBE and PBE+D3*  
JULIA YANG (Presenter), Materials Science and Engineering, University of California, Berkeley, DANIIL KITCHAEV, Materials, University of California, Santa Barbara, GERBRAND CEDER, Materials Science and Engineering, University of California, Berkeley — The ability of first-principles computational methods to reproduce ground-state crystal structure is key to their application in the study of structural phase transitions and the discovery of new materials. In assessing the reliability of structure selection made on the basis of density-functional theory, it is critical to understand the impact of various errors on structure stabilization arising from the choice of density functional. Here, we evaluate the SCAN functional performance in structure selection relative to widely-used PBE and PBE+D3 functionals and build on recent reports that the SCAN functional significantly improves crystal structure selection across a wide range of main group compounds [1]. We demonstrate that the origin of this improvement is to a large extent the inclusion of van der Waals interactions.


*J.Y. acknowledges support from the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program.

1:51PM S18.00014: From one to three, exploring the rungs of Jacob’s ladder in magnetic alloys*  
MATTHIEU VERSTRAETE (Presenter), University of Liege, ALDO H ROMERO, Physics and Astronomy, West Virginia University — Magnetic systems represent an important challenge for electronic structure methods, in particular Density Functional Theory (DFT). We benchmark different exchange correlation (xc) functionals with respect to each other, and with respect to available experimental data, on two families of binary iron alloys. We climb three rungs in Jacob’s ladder of DFT (i) the local density approximation, (ii) the industry standard approximations due to Perdew, Burke and Ernzerhof, and PBEsol, and finally (iii) the meta-GGA functional SCAN. More than 400 structures in ferromagnetic and antiferromagnetic configurations were considered. We compare the Convex Hull, magnetic moment, structure, and formation energy. None of the functionals work in all conditions: the GGAs and mGGA give a fair crystal structure, but SCAN strongly overestimates the formation energy (wrt PBE and experiment). Magnetic moments are better predicted by PBE as well. Our results show that magnetic and strongly correlated materials are a tough litmus test for DFT, and that they represent the next frontier towards a truly universal xc functional.


*NSF ACI-1053575 & TACC, FNRS 2.5020.11, Walloon Region 1117545  
DMREF-NSF 1434897, NSF OAC-1740111, DOE DE-SC0016176, CfWB ARC 15/19-09

Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S19 DMP: Computational Materials Design and Discovery -- Data-Driven Electronic Structure BCEC 156C - Alexander Urban - Tag(s): Focus
11:15 AM S19.00001: Data-driven design of electronic band structure for materials [Invited]  ERIC ISAACS (Presenter), Northwestern University — Designing a material with a desired electronic band structure is an outstanding challenge in materials physics. In this talk, I will describe an approach using materials database screening with materials attributes based on the constituent elements, nominal electron count, atomic coordination environment, and thermodynamics. Using the over half a million real and hypothetical inorganic crystals of the Open Quantum Materials Database, this approach is applied to two disparate band structure design problems. In the first, we seek a “pudding-mold” band structure containing both flat and dispersive components, which leads to large thermoelectric power factor. One of the identified compounds, BaPdS_2, exhibits ultralow lattice thermal conductivity in addition to the pudding-mold band structure, leading to remarkable thermoelectric figure-of-merit approaching 3. In the second, we search for materials with a single correlated d band at low energy, an important yet rare property of the cuprates, to search for possible superconductors and benchmarks for the one-band Hubbard model. Several Cu compounds, including bromide, oxide, selenate, and pyrophosphate chemistries, achieve the desired electronic structure and exhibit properties such as Mott insulating behavior and antiferromagnetism.

11:51 AM S19.00002: Discovery of Novel Dielectric Materials With Large Energy Bandgaps Using Statistical Optimization*  ABHIJITH GOPAKUMAR (Presenter), CHRISTOPHER WOLVERTON, Northwestern University — We present results from a feedback-based materials design work-flow to find novel materials with optimized dielectric properties. The objective is to improve the performance of electrical devices that depend on charge bearing capacity, which directly depends on dielectric constants and band-gap energies of the compounds. A data-set containing data of dielectric tensors for 1864 materials was extracted from MaterialsProject.org¹ to train the statistical deep-learning models. The set of thermodynamically stable materials from OQMD.org² was used as the search-space to discover novel materials with large values for dielectric constants and bandgap energy. A reliable neural network model was built over the small training data and combined it with statistical optimization strategies. Dielectric properties of predicted materials were computed using Density Functional Perturbation Theory and fed back into subsequent generations of neural network models. Each design cycle in this approach successfully picked up new promising materials from the large search-space, including mixed anion compounds with very large bandgap and dielectric constants - a highly optimized scenario for industrial applications.


*Samsung GRO 2017

12:03 PM S19.00003: Designing Materials with High Refractive Index and Wide Band Gap: A First-Principles High-Throughput Study*  FRANCESCO NACCARATO (Presenter), Faculty of Science, Technology and Communication, University of Luxembourg, FRANCESCO RICCI, Institute of Condensed Matter and Nanoscience, Université Catholique de Louvain, JIN SUNITIVICH, Department of Materials Science and Engineering, Cornell University, GEOFFROY HAUTIER, Institute of Condensed Matter and Nanoscience, Université Catholique de Louvain, LUDGER WIRTZ, Faculty of Science, Technology and Communication, University of Luxembourg, GIAN-MARCO RIGNANESE, Institute of Condensed Matter and Nanoscience, Université Catholique de Louvain — Materials combining both a high refractive index and a wide band gap are of great interest for optoelectronic and sensor applications. However, these two properties are typically described by an inverse correlation with high refractive index appearing in small gap materials and vice-versa. Here, we conduct a first-principles high-throughput study on more than 4000 semiconductors (with a special focus on oxides). Our data confirm the general inverse trend between refractive index and band gap but interesting outliers are also identified. It turns out that the negative effect of a large band gap on the refractive index can be counterbalanced by the presence of weakly dispersive states for transitions between the top of the valence band and the bottom of the conduction band. Focusing on oxides, we use our data to investigate how the chemistry influences this inverse relationship and rationalize why certain classes of materials would perform better. Our findings can be used to search for new compounds in many optical applications both in the linear and non-linear regime (waveguides, optical modulators, laser, frequency converter, etc.).

*EJD-FunMat project
12:15PM S19.00004: Rational Design and Discovery of Novel High Temperature Superconductors* ONYEDINACHI IRONKWE (Presenter), HTSC Design & Search Division, RTSD Technologies, San Diego, CA — Rational design of high temperature superconductors, (HTSCs), with predicted stoichiometry and transition temperature, Tc, is a major challenge in superconductivity. We presented in previous APS meetings (2015, 2016, 2017 and 2018), our computational design model called Material Specific Characterization Dataset (MSCD) Framework, and also design algorithms, and generalized periodic system (GPS), for superconductors. Over the past year, we have put to experimental test, our designs of oxide, oxy-sulfide and oxy-chloride systems predicted by MSCD Framework to be HTSCs. At this March 2019 meeting, we present the experimental results of this great challenge and announce the discovery, at ambient pressure of new classes of HTSCs without copper.

*This research is funded by Dr. M.J. Schaffer and RTSD Technologies, San Diego, CA

12:27PM S19.00005: Building and browsing ab initio computational databases in quest of materials with exceptional opto-electronic properties [Invited] GEOFFROY HAUTIER (Presenter), Universite catholique de Louvain — Essential materials properties can now be assessed through ab initio methods. When coupled with the exponential rise in computational power, this predictive power provides an opportunity for large-scale computational searches for new materials. We can now screen thousands of materials by their computed properties even before the experiments. This computational paradigm allows experimentalists to focus on the most promising candidates, and enable researchers to efficiently and rapidly explores new chemical spaces.

In this talk, I will present the challenges and opportunities in materials discovery offered by high-throughput ab initio computing in searching for materials with exceptional optical and electronic properties. Examples from the fields of transparent conducting oxides and electrides will be especially highlighted. As high-throughput computing generates large amounts of data, I will finish my talk by giving an update on the new properties recently added to the Materials Project (http://www.materialproject.org), including electronic transport but also phonon and vibrational properties.

1:03PM S19.00006: Classification models for high-throughput electronic band structures using feature extraction BRADLEY MAGNETTA (Presenter), VIDVUDS OZOLINS, Yale Univ — Applying machine learning techniques to aid materials engineering has become possible due to the existence of large databases of materials data. While models can be built using only scalar data, these databases also provide higher-dimensional data, such as high-throughput electronic band structures, which contain important information for many applications. For instance, the efficiency of thermoelectric materials is known to benefit from certain features in the band structure. We demonstrate how feature extraction techniques can be used to build classification models for band structures and show how these models can be used to aid materials innovation.

1:15PM S19.00007: Fully-automated construction of Maximally Localized Wannier Functions: High-Throughput calculations of material properties* VALERIO VITALE (Presenter), Cavendish Laboratory, Department of Physics, University of Cambridge, GIOVANNI PIZZI, ANTIMO MARRAZZO, Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne, JONATHAN YATES, Department of Materials, University of Oxford, NICOLA MARZARI, Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne, ARASH A MOSTOFI, Departments of Materials and Physics, and the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London — Maximally localized Wannier functions (MLWFs) are increasingly used in the computation of advanced properties of materials from first principles and as a localized basis for accurate beyond-DFT methods [1].

Conventionally, MLWFs are obtained by performing a multi-objective non-convex optimization [1]. In the case of MLWFs that represent so-called "entangled bands", e.g. for metals, the MLWFs may depend on the trial orbitals used to initiate the optimization. Consequently, automatic generation of MLWFs within high-throughput workflows is hindered by the need for user intervention in the selection of the initial guess.

A recently developed approach, the "selected columns of density matrix" (SCDM) algorithm [2] for obtaining localized Wannier functions does not require any initial guess and, by introducing only two parameters, is also applicable to the case of entangled bands.

We have implemented SCDM in a fully-integrated framework that combines the AiiDA workflow management platform, Quantum ESPRESSO and Wannier90 to achieve user-intervention-free construction of MLWFs. This work paves the way for high-throughput computation of advanced materials properties with Wannier functions.

Refs.
1 Rev. Mod. Phys. 84 1419 (2012)

*European Union grant No. 676531
1:27PM S19.00008: Universal $d=1$ flatband generator from compact localized states*

WULAYIMU MAIMAITI (Presenter), SERGEJ FLACH, ALEXEI ANDREANOV, Center for Theoretical Physics of Complex Systems, Institute for Basic Science — The band structure of some translationally invariant lattice Hamiltonians contains strictly dispersionless flatbands (FB). These are induced by destructive interference, and typically host compact localized eigenstates (CLS) which occupy a finite number $U$ of unit cells. FBs are important due to macroscopic degeneracy and consequently due to their high sensitivity and strong response to different types of weak perturbations. We use a recently introduced classification of FB networks based on CLS properties, and extend the FB Hamiltonian generator introduced in Phys. Rev. B 95, 115135 (2017) to an arbitrary number $v$ of bands in the band structure, and arbitrary size $U$ of a CLS. The FB Hamiltonian is a solution to equations that we identify with an inverse eigenvalue problem. These can be solved only numerically in general. By imposing additional constraints, e.g. a chiral symmetry, we are able to find analytical solutions to the inverse eigenvalue problem.

*This work was supported by the Institute for Basic Science in Korea (IBS-R024-D1).

1:39PM S19.00009: Coupling of lattice distortions to bands near the Fermi level in ABC compounds from first principles*

KONRAD GENSER (Presenter), Rutgers University, New Brunswick, CYRUS DREYER, Stony Brook University, JASON KAWASAKI, Univ of Wisconsin, Madison, KARIN RABE, Rutgers University, New Brunswick — ABC intermetallic compounds exhibit a rich variety of crystal structures and electronic properties. In this work, we use first-principles calculations to elucidate the coupling of lattice distortions to the electronic bands near the Fermi level in a family of hexagonal P6mm and P63mc ABC compounds, where A is a rare earth, B is a transition metal and C is a main group element. In particular, we have shown that in certain compounds in this family, a polar distortion that buckles the honeycomb layers can open a gap at the Fermi level. In addition, we show that epitaxial strain couples to the bands near the Fermi level directly, as well indirectly through polarization-strain coupling. These results have a number of implications for the targeted design of functional properties in these class of materials, which have been previously proposed as novel candidate ferroelectrics and piezoelectrics.

*This work was supported by NSF-DMREF 1623946 and ONR N00014-17-1-2770

1:51PM S19.00010: Material design of indium-based compounds: possible candidates for charge, valence and bond disproportionation and superconductivity

CHANG-JONG KANG (Presenter), GABRIEL KOTLIAR, Rutgers University, New Brunswick — We design and investigate the physical properties of new indium compounds AInX$_3$ (A = alkali metals, X = F or Cl). We find nine new indium-based materials in their ground state and are thermodynamically stable but are not reported in Inorganic Crystal Structure Database (ICSD). We also discuss several metastable structures. This new series of materials display multiple valences, charge and bond disproportionation, and dimerization. The most common valence of In is 3+. We also find two rare alternatives, one has In$^{2+}$ with In-In dimerization and the other shows valence disproportionation to In$^{1+}$ and In$^{3+}$ with bond disproportionation. We study the possibility of superconductivity in these new In compounds and find that CsInF$_3$ has a transition temperature of about 24 K with sufficient hole doping and pressure.

Thursday, March 7, 2019 11:15 AM - 1:51 PM

Session S20 DMP: Hybrid Perovskites -- Photovoltaics

BCEC 157A - Joseph Berry, National Renewable Energy Laboratory - Tag(s): Focus
We demonstrate that at the intrinsic limit, the mobility of charge-carriers is predominantly governed by interaction of carriers with optical vibrations of the lead halide lattice (Fröhlich interaction). In the absence of trap-mediated charge recombination, band-to-band recombination will dominate losses near the Shockley-Queisser limit. We show that in methylammonium lead triiodide perovskite, such processes can be fully explained as the inverse of absorption, and exhibit a dynamic that is heavily influenced by photon reabsorption inside the material. Finally, we demonstrate that in the absence of degradation, perovskite solar cells can exhibit appreciably higher energy-conversion efficiencies under solar concentration, where they exceed the Shockley-Queisser limit and exhibit elevated open-circuit voltages.


*This work has been supported by the EPSRC.

Unraveling the role of low-frequency phonon modes in carrier relaxation and regeneration in lead-halide perovskites

EE MIN CHIA (Presenter), Nanyang Technological University — Carrier-phonon scattering, a ubiquitous effect in all condensed matter systems, has been discussed in the halide perovskites in the context of placing an upper limit to the carrier mobility. Using time-resolved terahertz spectroscopy on a formamidinium-based perovskite system, we will show that phonons play a much larger role than thought previously. The combination of phonon emission during carrier relaxation, phonon-assisted exciton dissociation, and free-carrier screening, ensure a large and long-lived carrier population in the material. Our work reveals the delicate interplay among carriers, phonons and excitons, that affect the photo-physical properties of the halide perovskites, that ultimately determines the photovoltaic performance of halide perovskite-based solar cells.

*(1) Singapore Ministry of Education AcRF Tier 2 (MOE2015-T2-2-065 and MOE2016-T2-1-054)
(2) Theoretical and Computational Science (TaCS) Center, Thailand Research Fund (MRG6080264)
(3) Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE) an Energy Frontier Research Center funded by US DOE
(4) Alliance for Sustainable Energy, LLC for the US DOE under Contract No. DE-AC36-08GO28308.
(5) ONR and ARO
(6) NTU Biophysics Center
(7) Center for Integrated Nanotechnologies, a US DOE BES user facility.

Electron and Hole Mobilities in Organic-Inorganic Hybrid Perovskites

YAXIN ZHAI (Presenter), MATTHEW C BEARD, National Renewable Energy Laboratory — One of the fundamental semiconducting properties, charge-carrier mobilities have been widely studied in the organic-inorganic hybrid perovskites. However, the reported values of mobilities ranges widely from 0.4 to 600cm²(V s)⁻¹ and most of the experimental methods cannot distinguish the electron and hole mobilities. Other than photoluminescence quenching (PLQ) methods that requires the presence of an extractor layer, here we report an optical method to determine the electron and hole mobilities individually in organic-inorganic hybrid perovskite films and single crystals.

*We gratefully acknowledge support from the Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE) an Energy Frontier Research Center funded by the Office of Basic Energy Sciences, Office of Science within the U.S. Department of Energy through contract number DE-AC36-08GO28308.
12:15PM S20.00004: Direct Measurement of the Carrier Diffusion in CH$_3$NH$_3$PbI$_3$ Hybrid Thin Films and How It Compares with Other Inorganic Thin Film Materials* JOSE CASTANEDA (Presenter), FAN ZHANG, University of North Carolina at Charlotte, WUQIANG WU, JINSONG HUANG, University of North Carolina at Chapel Hill, YONG ZHANG, University of North Carolina at Charlotte — Large charge carrier diffusion lengths are believed to be one of the critical reasons for the high efficiencies demonstrated with organic-inorganic perovskite solar cells, as large diffusion lengths are often viewed as a necessity to maximize collection efficiencies of photovoltaic devices. Using energy selective PL imaging, diffusion lengths for carriers with different kinetic energies can be measured directly under focused laser excitation [1]. In this work, we directly measured the carrier diffusion length of surface passivated polycrystalline CH$_3$NH$_3$PbI$_3$ thin films under CW 532 nm excitation as a function of power density, which was found to be on the order of ~1 µm in approximately 7 – 40 W/cm$^2$ or 70 – 400 sun illumination density. Further comparisons were then made to other prominent thin film materials such as CdTe and GaAs, which tend to exhibit significantly longer diffusion lengths when as double-heterostructures. The carrier diffusion length in CH$_3$NH$_3$PbI$_3$ is also found to increase systematically with reducing kinetic energy, suggesting that carriers are localized due to disordering and not properly thermalized along with the existence of energy transfer among different emitting sites. [1] Zhang et al., J. Lumin. 185, 200 (2017).

*UNC/ROI

12:27PM S20.00005: Long Exciton Diffusion Length in Single Crystal Halide Perovskites* LUKE MCCLINTOCK (Presenter), RUI XIAO, CLINTON GIBSON, YASEN HOU, University of California, Davis, SONG JIN, Chemistry, University of Wisconsin-Madison, LIANG TAN, Lawrence Berkeley National Laboratory, DONG YU, University of California, Davis — Hybrid inorganic-organic halide perovskites have garnered an incredible amount of attention over the last few years, thanks to power conversion efficiencies climbing from 3% to now 22.7% in less than a decade. The majority of published work thus far has focused on creating higher quality thin films, while the underlying carrier transport processes are not well understood. By studying single crystal methylammonium lead iodide (MAPbI$_3$) samples, we avoid the issues caused by thin film grain boundaries and shed light on the inherent carrier transport mechanisms of this revolutionary material. We determined the carrier diffusion lengths via scanning photocurrent microscopy (SPCM). We observed excitonic behavior through electric field independent photocurrent distributions as well as a measured exciton diffusion length that increased abruptly below the phase transition temperature from the room temperature tetragonal phase to the low temperature orthorhombic phase. The low temperature phase diffusion reached up to 100 µm at 80 K. We attributed the long exciton diffusion length to the reduced carrier scattering because of the suppressed ion rotation in the orthorhombic phase.

*U.S. National Science Foundation Grant DMR-1710737 and the UC Laboratory Fees research program

12:39PM S20.00006: Comparative photovoltaics studies of prominent PV materials, organometal halide perovskite, CdTe, and GaAs with direct comparison of carrier recombination through power dependent photoluminescence* FAN ZHANG (Presenter), JOSE CASTANEDA, University of North Carolina at Charlotte, WUQIANG WU, JINSONG HUANG, The University of North Carolina at Chapel Hill, YONG ZHANG, University of North Carolina at Charlotte — Comparative Photovoltaics refers to the study of material properties of different PV materials by making direct and meaningful comparison to reveal their relative strength and weakness. Although the hybrid perovskite based solar cell has reached up to 23.3% energy conversion efficiency, it remains unclear what the enabling factors are for the impressive performance, in particular how it differs from the better-known PV materials CdTe and GaAs. Power dependent PL measurements show that perovskite samples tend to have stronger PL than the inorganic counterparts in the very low excitation density region (e.g., 0.1 – 1 sun), indicating that Shockley-Read-Hall (SRH) recombination is relatively less effective in the perovskite. PL lineshape analysis suggests that carriers in the perovskite are not in thermal equilibrium due to structural disordering, which in turn suppresses the nonradiative recombination. Both relatively low effective point defect density and moderate crystalline disordering in the perovskite contribute to the low nonradiative recombination loss, thus, high cell efficiency.

*UNC/ROI
The energy level alignment that occurs at the interfaces in planar-hetero structured perovskite photovoltaic devices strongly influences the charge transport across the interface and thus plays a role in overall device performance. To directly observe the energy level alignment requires pristine homogeneous surfaces that are free of contamination. Coevaporation has been employed to grow perovskite films. The method involves thermally evaporating the perovskite precursors such as PbI₂ and CH₃NH₃I, and some early reports have shown that the perovskite film formation and stoichiometry are problematic at ultralow coverages. Using photoemission spectroscopy, we investigated the perovskite precursors PbI₂ and MAI on gold and highly oriented pyrolytic graphite (HOPG) surfaces. Results show that the nature of the surface and the deposition conditions can strongly influence the film formation. Excessive iodine observed in the initial evaporation stages appears to be substrate dependent, and this may influence the overall energy level alignment.

The present work focuses on halide-related defects, the main contributors to ionic conductivity [2]. We use first principles density functional theory calculations to simulate the migration of halide vacancies in CsPbBr₃ perovskite. The well-established nudged elastic band method [3] is used to compute minimum-energy pathways and energy barriers of halide-related defects. We systematically study the change of migration activation energies upon moving from the surface into the bulk. Our results show that ions migrate more easily in soft lattices showing a pronounced dependence on surface proximity, depending on the availability and size of interstitial sites.


Organic-inorganic hybrid perovskites have been intensively studied in recent years as a very promising next-generation photovoltaic technology. Surface and interfacial engineering have been a focus for performance improvement. The microstructure-property relationship, particularly at the surface, has yet to be resolved. Here we investigated the intrinsic structural and electrical properties of single perovskite layers. The associated microstructure, which depends on the depth inside the layer, changes from a layer of randomly oriented grains at the surface to grains with a preferential orientation in the bulk with a post treatment. This structural change leads to a uniform bandgap for the entire system and an efficient hole accumulation at the surface that is concentrated at the grain boundaries. The established relationship between the surface and bulk, and the switch in the role of the grain boundaries between ideal charge transport highways and non-ideal defect locations enrich the understanding of the working mechanism of the devices, opening a pathway to increased efficiencies.

Raman spectroscopy as a probe of local strain in perovskite solar cells

Vibrational frequencies are shifted due to strain in a material and we want to enable use of this phenomenon to map local stress-strain behavior within a perovskite material via Raman spectroscopy, as is done in crystalline silicon and other materials [D. A. Strubbe et al., Phys. Rev. B 92, 241202(R) (2015)]. We study vibrational properties of different phases of methylammonium lead iodide (CH₃NH₃PbI₃) structures and calculate the slope of the shift of each mode for applied strains along different crystal directions to provide a calibration curve for measuring local strain. Our study also gives insight into the interaction between strain, structural changes and vibrational modes which may help to understand the degradation that plagues these materials.
Direct Optical Characterization of Subgrain Boundaries and Carrier Diffusion Rates in Perovskites

WENHAO LI (Presenter), SRINIVAS YADAVALLI, JUAN LIZARAZO FERRO, NITIN PADTURE, RASHID ZIA, Brown University — Perovskite solar cells (PSCs) have attracted considerable attention in recent years due to their rapidly increasing power conversion efficiency (PCE), which currently exceeds 23%. An important feature in organic–inorganic halide perovskites (OIHPs) that limits PCE is their defect densities. Here we report an optical spectroscopy method for identifying subgrain special boundaries that introduce defects and limit carrier diffusion. These subgrain boundaries do not exhibit clear surface morphology features that can be recognized by scanning electron microscopy (SEM) or atomic force microscopy (AFM). Such special boundaries may explain why PSC performance has not scaled with apparent grain size. Furthermore, in order to quantitatively study the role of defects, we establish a method to estimate defect density by directly studying the spatial and temporal distribution of carriers in OIHP thin films.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S21 DMP: Nanostructures and Metamaterials -- Functional Systems

11:15AM S21.00001: Plasmonic Aerosols: a novel phase of plasmonic matter*  JAKE FONTANA (Presenter), United States Naval Research Laboratory, JEFFREY GELDMEIER, PAUL JOHNS, ASEE-NRL Postdoctoral Fellow, NICHOLAS J. GREYBUSH, NRC-NRL Postdoctoral Fellow, JAWAD NACIRI, United States Naval Research Laboratory — The field of plasmonics has given rise to many innovative optical materials over the years, however these plasmonic materials are limited to only a few phases of matter, either as 2D solids or dilute liquids. Here, we introduce a novel phase of plasmonic matter by aerosolizing gold nanorods into the gas phase from liquid suspensions and simultaneously measure their optical spectra. We show by controlling the aspect ratio of the nanorods that the aerosol absorption peaks are tunable from visible to mid-wave infrared wavelengths. We find for large aspect ratio nanorods extraordinary sensitivity to changes in the refractive index of the host gas (~4,000 nm per refractive index unit). Utilizing this sensitivity dependence, we demonstrate the feasibility to use these plasmonic aerosols as environmental sensors.

*This material is based upon work supported by the Office of Naval Research under (N0001418WX00122) & (N0001417WX00884)

11:27AM S21.00002: Controlling light using dynamic plasmonic pixels*  NICHOLAS J. GREYBUSH (Presenter), NRC-NRL Postdoctoral Fellow, KRISTIN M. CHARIPAR, NICHOLAS CHARIPAR, United States Naval Research Laboratory, PAUL JOHNS, JEFFREY GELDMEIER, ASEE-NRL Postdoctoral Fellow, JAWAD NACIRI, JAKE FONTANA, United States Naval Research Laboratory — With the end of Moore's law, information needs to move from electron- to photon-based systems, if computational processing power is going to continue to increase. To enable this paradigm shift, optical elements are needed to dynamically control the propagation of light. Here we demonstrate the spatial, spectral and temporal control of light using electric field aligned plasmonic nanorods. We show these suspensions are color tunable from visible to infrared wavelengths, with microsecond switching times, and can be spatially tuned using lithographically defined electrodes. These suspensions may lead to novel dynamic plasmonic pixel devices for optical display, filter and spatial light modulators applications.

*This material is based in part upon work supported by the Office of Naval Research under (N0001418WX00122) & (N0001417WX00884)
11:39AM S21.00003: Finite-thickness effects in plasmonic films with periodic cylindrical anisotropy*  IGOR BONDAREV (Presenter), Math & Physics, North Carolina Central University, USA — Using the earlier developed Lagrange formalism[1], the plasma frequency and the dielectric response function are derived for finite-thickness plasmonic films formed by periodic parallel arrays of metallic cylinders embedded in a host dielectric matrix[2]. The plasma frequency of the system is shown to have the unidirectional square-root-of-momentum and quasilinear momentum spatial dispersion for the thick and ultrathin films, respectively. This spatial dispersion and the unidirectional dielectric response nonlocality associated with it can be adjusted by the film material composition, the film thickness, the cylinder length, the cylinder-radius-to-film-thickness ratio, and by an appropriate choice of substrates and superstrates of the film. The theory developed is discussed in application to the finite-thickness periodically aligned carbon nanotube film system as a potential candidate for the new generation of flexible multifunctional metasurfaces[3], for which the importance of the nondispersive interband plasmon modes of individual nanotubes is stressed in the ultrathin film regime. -- [1]I.V.Bondarev & V.M.Shalaev, Opt. Mater. Expr. 7, 3731 (2017); [2]I.V.Bondarev, arXiv1810.07303; [3]A.L.Falk, et al, Phys. Rev. Lett. 118, 257401 (2017).
*US NSF DMR-1830874

11:51AM S21.00004: Realization of A Novel Fibonacci Metasurface and K-space Imaging of Interference Pattern of Surface Plasmon Polariton*  CHUN YUAN WANG (Presenter), Department of Physics, The University of Texas at Austin, Austin, Texas, 78712, USA., SHANGJR GWO, Department of Physics, National Tsing-Hua University, Hsinchu 30013, Taiwan, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin, Austin, Texas, 78712, USA. — Metasurface is an artificial surface structure which are composed of, in general, period structure of metal or dielectric material to enable a spatially varying electromagnetic response, molding optical wavefronts or modulating surface plasmon polaritons (SPPs) [1, 2]. A Fibonacci sequence is defined mathematically as \( \{S_n\} \) where \( S_{n+1} = S_n, S_{n-1} \). If one creates a real space structure following the Fibonacci sequence, then the structure would not be periodic yet containing a long range order, in a manner similar to a quasicrystal whose structure is ordered but not periodic [3]. In this work, we fabricated Fibonacci sequence nanogrooves on epitaxial silver film via focus ion beam. Based on the angle-resolved reflectance mapping, we show multiple scattering of in-plane lattice-SPPs resulting from the hierarchial Fourier components of the Fibonacci sequence. It opens a way to understand coherent scattering in an ordered yet non-periodic structure.

References.

*We acknowledge funding from the AOARD FA-2386-18-1-4097 in US and MOST 105-2112-M-007-011-MY3 in Taiwan.

12:03PM S21.00005: A generative model for the inverse design of metamaterials  ZHAOCHENG LIU (Presenter), WENSHAN CAI, Georgia Institute of Technology — The advent of metamaterials in recent years has ushered in a revolutionary means to manipulate the behavior of light on the nanoscale, and thereby enabling diverse applications in optical imaging, beam steering, light modulation, dispersion engineering, holography, and many more. However, the design of such structures, to date, has relied on the expertise of an optical scientist to guide a progression of electromagnetic simulations that iteratively solve Maxwell’s equations until locally optimized solution can be attained. Here, we develop a framework leveraging a deep generative model to identify the photonic structures in arbitrary topology from a geometric dataset given target optical response. Furthermore, if black-box optimization methods are incorporated, the framework is able to automate the inverse design and generate patterns of photonic structure with few interventions of human. The evaluation shows that over 95% average accuracy can be achieved in less than 5 seconds for all the unit patterns of the nanostructure tested. Our work introduces a generic approach for the design of photonic and optical structures in response to the near-field and far-field requirements, with broad applications in large-scale photonic design requiring trial-and-error practices.
Divacancy spin defects coupled to photonic crystal cavities in 4H-SiC

ALEXANDER CROOK

(Presenter), CHRISTOPHER P ANDERSON, KEVIN MIAO, ALEXANDRE BOURASSA, HOPE LEE, University of Chicago, DAVID BRACHER, XINGYU ZHANG, Harvard University, HIROSHI ABE, TAKESHI OHSHIMA, National Institutes for Quantum and Radiological Science and Technology (QST), EVELYN L HU, Harvard University, DAVID AWSCHALOM, University of Chicago — Silicon carbide (SiC) has recently been developed as a platform for optically addressable spin defects in the form of the neutral divacancy, most notably in the 4H polytype [1-3]. Here we present progress in the fabrication and characterization of 4H-SiC photonic crystal cavities coupled to neutral divacancies. We use a combination of nanolithographic techniques and a dopant-selective photoelectrochemical etch to produce suspended cavities. For divacancies in the cavity mode, the Purcell effect enhances near-infrared optical emission from the defect. This results in increased photon count rates due to reduced excited state lifetimes, and for cavity wavelengths matched with the defect, the Purcell enhancement increases emission into the zero-phonon line. This enhancement has applications for the scalability of long-distance entanglement schemes that require the interference of indistinguishable photons from spatially separated defects.


*This work is supported by AFOSR, ARO, NDSEG, NSF, and UChicago MRSEC.

Photothermal Effect and Circular Dichroism in Chiral Plasmonic Metamaterials and Bolometers

LAROUSSE KHOSRAVI KHORASHAD (Presenter), XIANG-TIAN KONG, ALEXANDER O. GOVOROV, Department of Physics and Astronomy, Ohio University, USA — Chiral nanostructures have already shown their promising chiro-optical properties in many areas of plasmonic science and photonics. Simultaneously, plasmonic nanostructures are suitable tools to efficiently enhance light absorption and increase temperature as a result of the light-matter interaction. In this project, we couple chirality and a strong plasmonic photothermal effect to present a new type of chiral spectroscopy. We utilize the idea of chiral planar superabsorber to enhance the chiro-optical effect. Our simulation models show that the hybrid nanostructure introduces high chiral light sensitivity that leads to the polarization-sensitive local temperature distributions and to strong photothermal circular dichroism in a nanostructure. These ideas can be applied for polarization-sensitive photochemistry, plasmonic thermal switches and chiral bolometers [1].


Air-Spaced Triple Band Metamaterial Perfect Absorber

CHUNXU CHEN (Presenter), XIAOGUANG ZHAO, Boston University, JACOB SCHALCH, UC San Diego, SULTAN CAN, GUANGWU DUAN, Boston University, RICHARD DOUGLAS AVERITT, UC San Diego, XIN ZHANG, Boston University — We present a polarization insensitive air spaced triple band metamaterial perfect absorber (MMPA) consisting of a metamaterial layer and metallic ground plane. For our MMPA, the three near unity-absorption peaks can be individually specified by selecting the size of the ring resonators within one metamaterial unit cell – that is, inter-unit cell coupling is negligible. For our MMPA design, the coupling between the metamaterial layer and the ground plane is very strong. As a result, near-field interactions must be taken into account to properly analyze the electromagnetic response (EMR). Interference theory is often used to model the EMR of MMPAs. To account for near-field coupling we incorporate a correction term into our interference model. Our approach is in agreement with full-wave numerical simulations and experimental measurements. These findings demonstrate that a capacitance increase and an inductance decrease due to the coupling between the metamaterial layer and the ground plane are the primary causes for the difference between the standard interference theory and the experimental results.

*Research supported by National Science Foundation under Grant No. ECCS-1810252.

Photonic Forces on Dielectric Metasurfaces for Passive Stabilization of Laser Propelled Spacecraft

JOEL SIEGEL (Presenter), ANTHONY WANG, University of Wisconsin - Madison, SERGEY MENABDE, KAIST, MIKHAIL A. KATS, University of Wisconsin - Madison, MIN SEOK JANG, KAIST, VICTOR W BRAR, University of Wisconsin - Madison — In this talk, we will show that the ability of metasurfaces to create arbitrary reflected/transmitted wavefronts leads to complex – and measurable – optical forces on the metasurface. We will show how these forces manifest on the microscopic scale for individual resonators (the base elements of the metasurface) and on the macroscopic scale. In addition, we will discuss the non-intuitive behavior these forces can exhibit and the challenges that result in controlling these forces. Finally, we will demonstrate the potential value of a metasurface to serve as a ‘laser sail’ for a recently proposed relativistic spacecraft. To this end, photonic forces are used to passively stabilize the metasurface in a high power laser beam.
room temperature also facilitate their application potential. Their robustness for a wide range of parameters and thus can dramatically tune the complex correlation between the spin- and charge-density waves, giving rise to a number of novel phases with distinct unusual magnetic and electronic features. Under the electric field in the ribbon width direction. Such setting imposes strong tendency to charge inhomogeneity and theoretical studies of the electronic and magnetic properties of lightly doped zigzag-edged graphene nanoribbons [1].

The electric field is one of the ideal ways for spintronics device applications due to its precise controllable nature. We report engineering magnetism on graphene nanoribbons by electric field* YUAN ZHOU (Presenter), Department of Physics, Nanjing University, WEIGUO YIN, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, SHUNLI YU, WENCHAO CHEN, Department of Physics, Nanjing University, CHANGDE GONG, Center for statistical and theoretical condensed matter physics, Zhejiang Normal University — Manipulating magnetism by means of the electric field is one of the ideal ways for spintronics device applications due to its precise controllable nature. We report theoretical studies of the electronic and magnetic properties of lightly doped zigzag-edged graphene nanoribbons [1] under the electric field in the ribbon width direction. Such setting imposes strong tendency to charge inhomogeneity and thus can dramatically tune the complex correlation between the spin- and charge-density waves, giving rise to a number of novel phases with distinct unusual magnetic and electronic features. Their robustness for a wide range of parameters and room temperature also facilitate their application potential.


*NSFC 11274276 and 11674158; Ministry of Science and Technology of China 2016YFA0300400; U.S. DOE DE-SC0012704
1:51PM S21.00014: Wafer-scale photolithography of ultra-sensitive nanocantilever force sensors* YING PAN (Presenter), CALDER MILLER, KAI TREPKA, YE TAO, Harvard University — The detection of small forces using singly-clamped cantilevers is a fundamental feature in ultrasensitive versions of scanning probe force microscopy. In these technologies, silicon-based nanomechanical devices continue to be the most widespread high-performance nanomechanical sensors for their availability, ease of fabrication, inherently low mechanical dissipation, and good control of surface-induced mechanical dissipation.

Here, we develop a robust method to batch fabricate extreme-aspect-ratio (10^3), singly-clamped scanningnanowire mechanical resonators from plain bulk silicon wafers using standard photolithography. We discuss the superior performance and additional versatility of the approach beyond what can be achieved using the established silicon-on-oxide (SOI) technology.

*Y. P. acknowledges funding from a Rowland Postdoctoral Fellowship. C. M. and K. T. acknowledge support from the Harvard Physics Department, the Harvard Office of Undergraduate Research and Fellowships, and the Rowland Institute. This work was supported by a Rowland Fellowship to Y. T.. The sample fabrication was carried out at the Center for Nanoscale Systems (CNS) at Harvard University.

2:03PM S21.00015: Resolution of Ultra-thin Piezoresistive Silicon Nanomechanical Resonators for Single Molecules Mass Spectrometry JARVIS LI (Presenter), WARREN FON, MICHAEL ROUKES, Caltech — Nanoelectromechanical-system mass spectrometry (NEMS-MS) measures the mass of single particles, one at a time, through determining the shift in the frequency of a nanomechanical resonator due to adsorption of molecules. This allows rapid identification and stratification of bio-molecules and individual analytes, as an alternative to conventional mass spectrometry. To achieve broad applications in native mass spectrometry, which focuses on large protein complexes over 1MDa, a mass resolution of less than 5kDa is desired. Ultra-thin silicon resonators provide a viable platform to achieve this desired resolution, as well as the ability for scaled up operation. Here we demonstrate optimizations in the mass sensitivity of ultra-thin silicon piezoresistive devices through dimensional scaling and cryogenic operations. We also discuss practical advantages and limits of this device architecture as it relates to single molecule analysis.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S22 DCOMP DMP: Electrons, Phonons, Electron-Phonon Scattering and Phononics VI BCEC 157C - Yan Li, American Physical Society APS - Tag(s): Focus

11:15AM S22.00001: An Ab-Initio Study of the Effect of Impurities on Electron-Phonon Energy Transfer in Niobium* NATHAN SITARAMAN (Presenter), JAMES MANISCALCO, TOMAS ARIAS, MATTHIAS ULF LIEPE, Cornell University — A precise understanding of electron-phonon energy transfer is crucial to the optimization of superconducting radio frequency (SRF) cavities, photocathodes, and other material systems in which electrons are out of thermal equilibrium with phonons. The role played by interstitial impurities is a point of particular interest; SRF scientists have long believed that impurities affect electron-phonon energy transfer in niobium cavities, but it is difficult to distinguish this effect from other impurity-induced effects. An inability to precisely control impurity concentrations and directly measure electron temperature further complicates the problem.

In order to shed light on this rich and important topic, we take an ab-initio approach, using recently developed packages for our in-house density functional theory software JDFTx to explore the dependence of electron-phonon energy transfer on electron and phonon temperatures, and on the concentrations of common impurities such as H, C, N, and O. We perform our calculations using a Wannier representation of the electronic state, which makes possible the dense k-space sampling necessary to study processes at cryogenic temperatures in the large unit cells necessary to study impurities.

*Funded by the Center for Bright Beams.
11:27AM S22.00002: Understanding the chemical enhancement mechanism of graphene-enhanced Raman Spectroscopy (GERS) – A first principles study.  KANCHAN ULMAN (Presenter), SU YING QUEK, National University of Singapore — Surface-enhanced Raman spectroscopy (SERS), involving the enhancement of Raman signals for molecules on metal substrates, is a well-established field that has enabled the detection of trace concentrations of molecules. In recent years, graphene was found to be a candidate substrate for SERS, giving rise to a rapidly expanding field of graphene-enhanced Raman spectroscopy (GERS), and opening doors for other two-dimensional materials to be used for SERS. In conventional SERS, the Raman signal is enhanced by a combination of the dominant electromagnetic enhancement effect, and the smaller chemical enhancement effect, which stems from electron-phonon coupling in the system. The latter chemical enhancement effect is thought to play a dominating role in GERS, thus enabling detailed studies of electron-phonon coupling effects for organic-graphene interfaces. Yet, the details of the chemical enhancement effect in GERS are not well understood. Using first principles calculations, we study the GERS chemical enhancement mechanism using typical probe molecules such as pyridine adsorbed on graphene. We uncover a novel ground state enhancement mechanism that is distinct from the typical ground state charge transfer mechanism in conventional SERS.

11:39AM S22.00003: Kagome modes, a new route to ultralow thermal conductivity?* DAVID VONESHEN (Presenter), ISIS Pulsed Neutron and Muon Source, Science and Technology Facilities Council, MONICA CIOMAGA HATNEAN, Physics Department, University of Warwick, TOBY PERRING, HELEN C WALKER, ISIS Pulsed Neutron and Muon Source, Science and Technology Facilities Council, KEITH REFSON, Physics Department, Royal Holloway University of London, GEETHA BALAKRISHNAN, Physics Department, University of Warwick, JON GOFF, Physics Department, Royal Holloway University of London — From next generation gas turbines to scavenging waste heat from car exhausts, finding new materials with ultra-low thermal conductivity (κ) has the potential to lead to large gains in device efficiency. Crystal structures with inherently low κ are consequently desirable, but candidate materials are rare and often difficult to make. Using first principles calculations and inelastic neutron scattering we have studied the pyrochlore La2Zr2O7 which has been proposed as a next generation thermal barrier. We find that there is a highly anharmonic, approximately flat, vibrational mode associated with the kagome planes. Our results suggest that this mode is responsible for the low thermal conductivity observed in the pyrochlores and that kagome compounds will be a fruitful place to search for other low κ materials.

*STFC (RB1710105)

11:51AM S22.00004: Thermodynamics of Tin Using AFLOW-APL* MATEO RONQUILLO (Presenter), MICHAEL MEHL, United States Naval Academy, COREY OSES, STEFANO CURTAROLO, CORMAC TOHER, Duke University — Tin is one of the more interesting metallic elements, with a 13.2°C phase transition from diamond-like “gray” (α-Sn) to “white” (the eponymous β-Sn). Density Functional Theory (DFT) finds a simple hexagonal phase (sh-Sn, hP1) nearly degenerate with the other phases, although it is never seen. sh-Sn is very close in energy to β-Sn at all volumes, as found by a variety of density functionals. While the simple hexagonal structure is a high pressure phase of Si, there it is not close to the ground-state structure at normal pressures.

To understand this behavior we used the high-throughput AFLOW-APL (AFLOW Harmonic Phonon Library) to find the energy-volume relationship, phonon spectra and free energy for tin in the α-, β-, and sh-phases. Our results showed significant discrepancies between DFT and experiment. We find that DFT predicts the β-Sn phase as the ground state of tin, and a transition from β-Sn to sh-Sn at 200\,K. Both of these results contradict experiment. Our results are thus a cautionary tale about the use of DFT for understanding the behavior of systems with nearly degenerated crystal structures.

* MJ Mehl is funded by the Kinnear Foundation and Duke University. Duke University research is funded by the US Office of Naval Research grant N00014-17-1-2090.
12:03PM S22.00005: Hybridization of Localized Surface Phonon Polaritons via Symmetry Breaking in Dolmen Nanostructures  
SWATHI IYER (Presenter), CHASE ELLIS, ALEXANDER GILES, United States Naval Research Laboratory, DMITRY CHIGRIN, Dept of Physics, Institute of Physics (IA), RWTH Aachen University, Aachen, Germany, RICHARD KASICA, CNST, National Instrumentation Science and Technology (NIST), Maryland, USA, MICHAEL MEEKER, United States Naval Research Laboratory, JOSHUA D CALDWELL, Mechanical Engineering Dept, Vanderbilt University, Nashville, TN, USA, JOSEPH G TISCHLER, United States Naval Research Laboratory —  
Subdiffractional confinement of light coupled with low optical losses mediated through surface phonons polaritons (SPhPs) in polar dielectric materials such as SiC have enabled infrared based nanophotonic applications. By utilizing a nano-Dolmen architecture, we experimentally and theoretically demonstrate hybridization between localized, sub-diffractional SPhP modes via spatial symmetry breaking. The substrate mediated, extended coupling nature of the vertically oriented monopole leads to gap-tunable symmetric and antisymmetric modes with high quality factors (200-250) and field localization in the coupled oscillator. By theoretical modelling we demonstrate monopolar excitation, otherwise excited so far only by off-normal light, through dipolar nearfields via normal incidence by overcoming the selection rules leading to direct and indirect excitation pathways for monopolar activation in the Dolmen system. Further, in contrast to the plasmonic systems, despite strong coupling the bound continuum states in narrow SPhP modes do not exhibit Fano interference. By controlling nanoscale geometry, spacing and excitation, we are able to obtain highly tunable optical responses resulting in strong phonon polariton hybridization and large near-field enhancements in these high-Q resonators.

12:15PM S22.00006: Nonlinear Physics for the Engineering of Phononic Frequency Combs*  
ADARSH GANESAN (Presenter), ASHWIN SESHIA, University of Cambridge — Phononic frequency combs (PFC) represent a new nonlinear phenomenon in the physical domain of micromechanical resonators [1]. The emergence of PFC is mediated by nonlinear modal coupling. Through a series of experiments with micromechanical resonators, various features of PFC have now been identified. These include drive parameters for comb operation, hysteresis for comb spectrum tailoring and evolving spectral envelopes of combs. Potential applications of PFC include high-precision sensing, spread spectrum information processing and other applications in timing and frequency control. However, for the successful realization of such applications, the nonlinear physics of micromechanical resonators underlying the evolution of PFC must be fully elucidated. Specific future directions include developing experimental protocols for engineering frequency combs at low drive power levels; resonant and off-resonant excitation; understanding comb frequency fluctuations; tailoring combs for broadband multi-octave spanning spectra; and modelling sensitivity to system parameters and physical perturbations.  
*Funding from the Cambridge Trusts is gratefully acknowledged.

12:27PM S22.00007: Studying the correlations and solubility of hydrogen in niobium using Density Functional Theory calculations  
ARVIND RAMACHANDRAN (Presenter), School of Sustainable Engineering and the Built Environment, Arizona State University, DR. HOULONG ZHUANG, School for Engineering of Matter, Transport & Energy, Arizona State University, KLAUS S LACKNER, School of Sustainable Engineering and the Built Environment, Arizona State University — In this work, we present a Density Functional Theory (DFT) study of hydrogen correlations and solubility in niobium. Finding the preferred interstitial site for single hydrogen atoms, calculating the pair-wise hydrogen correlations, and the treatment of many hydrogen atoms in a niobium cell are parts of this work. By studying how the pair-wise hydrogen-hydrogen interaction energy varies as a function of their distance, we develop the theoretical counterpart of the empirical Westlake criterion, a rule that states that hydrogen atoms cannot simultaneously occupy pairs of interstitial sites closer than 0.21 nm. Based on this inference, we provide a systematic way of populating many (>3) hydrogens in the niobium lattice. Using the differential binding energies and vibrational frequencies of dissolved hydrogens at varying hydrogen concentrations, we estimate the solubility of hydrogen in niobium. Apart from the conventional way of calculating the entropy of interstitial hydrogens under the harmonic oscillator approximation, this work includes a new approximation that treats the hydrogens as a monatomic ideal gas. The solubility predictions are in good agreement with experimental data.

12:39PM S22.00008: A simple method to determine lattice constants  
CHEN XIAO-FAN (Presenter), Department of Physics, Harbin Institute of Technology — A simple method to determine lattice constants is proposed. The method is based on the relation between electric conductivity and the lattice constants. A way to solve a puzzle in high-temperature superconductivity is also presented.
Purely electronic instabilities versus Peierls instabilities in semi-metallic 1D atomic chains*

MATTEO BARBORINI, SVEN REICHARDT, PIER LUIGI CUDAZZO, Physics and Materials Science Research Unit, University of Luxembourg, MATTEO CALANDRA, Institut des Nanosciences de Paris, Université Pierre et Marie Curie, FRANCESCO MAURI, Dipartimento di Fisica, Università di Roma La Sapienza, LUDGER WIRTZ (Presenter), Physics and Materials Science Research Unit, University of Luxembourg — In 1929 Peierls hypothesized that a semi-metallic linear chain of equally spaced single electron atoms is unstable due to electron-phonon coupling at T=0: periodic lattice distortions along the longitudinal mode of vibration lead to the opening of an electronic band gap, lowering the symmetry of the lattice and stabilizing a semiconducting ground state. The origin of the symmetry breaking and of the formation of a charge density wave (CDW) state, was thus directly linked to the ionic displacement.

Here we study two equidistant semi-metallic linear chains, the (hypothetical) hydrogen chain and the carbon chain (carbyne), by means of accurate ab initio calculations based on quantum Monte Carlo and density functional theory (DFT). For both chains we find that the CDW state is more stable than the metallic phase even without any lattice distortion. This means that the ground state is electronically unstable. In DFT we show that the presence of the electronic instability is directly related to the non-locality of the Hartree-Fock exchange term that appears in the hybrid functionals. These results suggest that in 1D semi-metals there exists a pure electronic instability that opens a gap, leading to a CDW phase which is prior to Peierls distortion.

We acknowledge funding by FNR and ANR.

Magnetoelastic coupling, phonon and magnons in inverse spinel NiFe2O4*

QIANG ZHANG (Presenter), Louisiana State University & Oak Ridge National Laboratory (current affiliation), ROSHAN NEPAL, Physics and astronomy, Louisiana State University, ASHFIA HUQ, ALEXANDER I KOLESNIKOV, STEPHEN NAGLER, Oak Ridge National Laboratory, RONGYING JIN, Physics and astronomy, Louisiana State University — The inverse spinel NiFe2O4 has attracted enormous interest due to the potential applications in several important fields such as electronic devices and catalysis. NiFe2O4 exhibits a cation distribution of (Fe3+)A(Ni2+Fe3+)B04, with Fe3+ occupying the tetrahedral(A) sites forming a diamond lattice, and Ni2+ and Fe3+ sharing the octahedral(B) sites forming a pyrochlore lattice. Powder neutron diffraction reveals the cubic spinel structure persisting down to 5 K. A collinear ferrimagnetic order with antiparallel moments between A and B sites is found below T_N ≈ 860 K with a magnetoelastic coupling at T_N. Magnetization measurements further reveal NiFe2O4 enters a state with the coexistence of a ferrimagnetic order and a spin glass like state below the freezing temperature T_f ≈ 40 K. A few branches of phonons and magnons with a crossing feature are observed via single-crystal inelastic neutron scattering at 100 K (T_f < T < T_N) and 5 K (T < T_f). All these results and magnetic exchange constants will be compared to the well-known magnetite Fe3O4 to reveal the distinct spin, lattice and orbital degrees of freedom.

The work has been supported by the U.S. DOE under EPSCoR Grants No. DESC0012432, DE-SC0016315 and US DOE Basic Energy Sciences Division of Scientific User Facilities.

First-principles calculation of Seebeck coefficient of transition-metal elements

HISAZUMI AKAI (Presenter), University of Tokyo, SONJU KOU, Graduate School of Engineering Science, Osaka University — Calculation of the Seebeck coefficient S of transition metal elements is challenging. The difficulties are that, first, at T=0K, the conductivity of pure metal diverges. Second, the Fermi surfaces of transition metals composed of many different states, For this a formal cancelation of the relaxation time appearing in L_{12} and L_{11} in the expression of S=C(L_{12}/L_{11}) cannot be applied. To overcome the difficulties, we included the effects of electron-phonon scattering in the calculation of S. We exploited the Korringa--Kohn--Rostoker (KKR) Green's function method combined with the coherent potential approximation (CPA, KKR-CPA) and linear response theory. The approach combines three components: linear response theory in the framework of the KKR method; ab-initio phonon calculations; and an alloy analogy applied to the local static phonons using the KKR-CPA. The calculated Cu resistivity and the Seebeck coefficients for various transition-metal elements at finite temperature show reasonably good overall agreements with experiments. The present approach provides us with a framework applicable to a wide range of materials, including pure metals, compounds, ordered and disordered alloys, opening up the possibilities of computational design of useful thermoelectric materials.
1:27PM S22.00012: Nonlinear Anomalous Thermoelectric Current*  
YANG GAO (Presenter), DI XIAO, Carnegie Mellon University — Using the concept of the orbital magnetic quadrupole, we derive a nonlinear anomalous thermoelectric current, i.e. a current quadratic in temperature gradient and perpendicular to its direction. In the system that breaks time reversal, inversion, and one mirror symmetry, but has the combined time reversal and inversion symmetry, the linear anomalous thermoelectric current vanishes but the nonlinear current we obtained does not vanish and hence can be used to probe such system. We demonstrate this nonlinear current in the loop-current model in the pseudogap phase.

*This work is supported by the Department of Energy, Basic Energy Sciences, Grant No.—DE-SC0012509.

1:39PM S22.00013: Nanosecond Shape-driven Localized Surface Plasmon Resonance Switching in Silver Nanoparticles*  
VENKATANARAYANA P SANDIREDDY, Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, KRISHNA KOIRALA, Department of Physics and Astronomy, University of Tennessee, Knoxville, RAMKI KALYANARAMAN (Presenter), Department of Material Science and Engineering, University of Tennessee, Knoxville — The ability to tune the localized surface plasmon resonance (LSPR) in a fast and repeatable manner could form the basis for a hypothetical optical switch. Here we demonstrate a reversible change in the LSPR wavelength of Ag nanoparticles based on nanosecond melting induced shape effects. When Ag nanoparticles are melted by nanosecond laser pulses, the resulting contact angle is determined by the fluid environment during melting. For instance, Ag nanoparticles on quartz substrates melted in air are near hemispherical in shape (with contact angle ~ 96°), while those melted under water and glycerol have larger contact angles of ~127° and ~172° respectively. This shape or contact angle change significantly modifies the intensity and wavelength of the dipolar and quadrupolar plasmonic signals. We have utilized this shape change to switch the plasmonic signals over multiple cycles of irradiation and determined the fatigue limit of LSPR switching between air and glycerol environments. Such shape control and repeatable modification of the plasmonic wavelength could serve as a useful system for biological sensing and optical tuning applications.

*This work is supported by FAPESP (2012/50259-8, 2015/11779-4), INCT/Nanocarbono, Fapemig, CNPq and MackPesquisa. H.B.R. acknowledges FAPESP fellowships (2017/20100-0 and 2018/04926-9). L.S. acknowledges support from FAPESP (2017/00486-1) and computational facilities from SDumont/LNCC supercomputer.

1:51PM S22.00014: Theory of time-resolved resonant inelastic x-ray scattering for studying material dynamics  
YUAN CHEN (Presenter), Department of Applied Physics, Stanford University, YAO WANG, Department of Physics, Harvard University, CHUNJING JIA, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, JAMES FREERICKS, Department of Physics, Georgetown University, ANDRIJ SHVAIKA, Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory — With recent progress in the X-ray beamline and pump-probe instrumentation, time-resolved RIXS (tr-RIXS) promises to detect the nonequilibrium dynamics of collective modes, which play significant roles in quantum materials. Here we present a theory for evaluating the tr-RIXS cross-section. This time-domain theory is based on nonequilibrium linear response and can reproduce the common Kramers-Heisenberg formula at equilibrium. We numerically evaluated tr-RIXS cross-section for some example systems out of equilibrium, including a graphene nanoribbon and the 2D single-band Hubbard model. We show that tr-RIXS can capture the dynamics of multi-particle Floquet excitations in a momentum-resolved way, revealing underlying physics such as Floquet band renormalization, topological edge states, and pump-induced collective excitations.

2:03PM S22.00015: Polarized Raman spectroscopy at the edges of exfoliated GeS and GeSe crystals*  
HENRIQUE BUCKER RIBEIRO (Presenter), MackGraphe, Mackenzie Presbyterian University, SÉRGIO L. L. DE MORAES RAMOS, Centro de Tecnologia em Nanomateriais (CTNano), Universidade Federal de Minas Gerais, LEANDRO SEIXAS ROCHA, CHRISTIANO DE MATOS, MackGraphe, Mackenzie Presbyterian University, MARCOS ASSUNÇÃO PIMENTA, Departamento de Física, Universidade Federal de Minas Gerais — Germanium sulfide (GeS) and germanium selenide (GeSe) are layered crystals which structure bears a strong resemblance to that of black phosphorus (BP). As recently observed and reported, BP exhibits atomic rearrangements at crystal terminations, which lead to the activation of Raman modes that are otherwise forbidden by polarization selection rules. Considering the similarities in the crystalline structure of BP, GeS, and GeSe, the same behavior would be expected at the edges of these crystals. In this work, the Raman modes GeS and GeSe edges were experimentally studied using polarized Raman spectroscopy. We show, at the edges, the appearance of modes that are symmetry-forbidden. By carrying out DFT calculations, we conclude that the anomalous behavior is a consequence of edge atomic rearrangements. Such rearrangements, therefore, appear to be a general feature in lamellar crystals with the crystalline structure of BP.

*This work is supported by FAPESP (projects 2012/50259-8, 2015/11779-4), INCT/Nanocarbono, Fapemig, CNPq and MackPesquisa. H.B.R. acknowledges FAPESP fellowships (2017/20100-0 and 2018/04926-9). L.S. acknowledges support from FAPESP (2017/00486-1) and computational facilities from SDumont/LNCC supercomputer.
Quantitatively accurate numerical modeling of amplitude and phase contrast in broadband near-field infrared spectroscopy

Patrick Mcardle (Presenter), David Lahneman, Muhammad M. Qazilbash, Department of Physics, College of William & Mary, Amlan Biswas, Department of Physics, University of Florida. Proper modeling of near-field infrared spectroscopy data is critical to extracting useful material properties. Current analytical models make underlying assumptions about the probe geometry that makes their use applicable in only limited situations. When strong coupling between probe and sample exists, a more robust solution method must be used. A full-wave numerical method for calculating broadband demodulated near-field amplitude and phase contrast will be presented. Our method captures the probe geometry accurately and is thus essential for obtaining quantitative results free of underlying assumptions and tunable parameters. We will present simulation results on SiO$_2$ and SrTiO$_3$, both of which exhibit surface phonon-polariton modes, and will compare the simulation results to experimental data.

* M.M.Q acknowledges support from NSF DMR-1255156. The simulation work was performed, in part, using computing facilities at the College of William and Mary which are supported by contributions from the National Science Foundation, the Commonwealth of Virginia Equipment Trust Fund, and the Office of Naval Research.

Tunable narrow band sources for anisotropic THz spectroscopy

Deepu George (Presenter), Physics, University at Buffalo, Ian Mcnee, Patrick Tekavec, Vladimir Kozlov, MicroTech Instruments, Peter Schunemann, BAE Systems, Andrea Markelz, Physics, University at Buffalo. THz spectroscopy is well suited for material identification and characterization in many different fields due to unique molecular vibrational signatures in this range. Recently this has been extended to feature identification in large biomolecules like proteins and DNA, using the newly developed time domain Anisotropic Terahertz Microscopy (ATM)[1]. ATM measures polarization dependent changes in THz absorption and thus generates a comprehensive map of the vibrational modes, featuring their frequencies as well as their directions. Despite these advances, proliferation of THz systems is hindered by low dynamic ranges of measuring systems, large footprints and cost. Therefore, development of high power, compact THz sources and their characterization are critical. In this study we investigate the suitability of using quasi CW THz radiation generated by pumping Orientation Patterned Gallium Phosphide with a 1064 nm fiber laser for identifying anisotropic signatures of molecular crystals. THz generation from 0.5 to 4 THz is achieved. Results compared with that obtained using a broadband time domain spectrometer. The results show that new narrow band sources are suitable for high dynamic range THz systems.


Terahertz Coherent Acoustic Phonons in SrRuO$_3$/SrTiO$_3$ Superlattices

Chiyuan Yang (Presenter), Department of Physics, National Taiwan University, Pingchun Wu, Yings-Hao Chu, Department of Materials Science and Engineering, National Chiao Tung University, Kung-Hsuan Lin, Institute of Physics, Academia Sinica. We utilized time-resolved pump-probe spectroscopy to generate and detect coherent acoustic phonons (CAPs) in SrRuO$_3$/SrTiO$_3$ superlattices with frequencies according to the spatial modulation of the heterostructures. Thanks to the pulse laser deposition techniques, precise manipulation of atomic layers enables the fabrication of high-quality heterostructures and generation of CAPs in THz regime. Dynamics of CAPs from hundreds of GHz to 1 THz were investigated. By introducing a control pulse, coherent control of CAPs was also demonstrated. Since many complex oxides with perovskite structures can be deposited on the SrRuO$_3$/SrTiO$_3$ superlattices, our demonstrated technique can be used to study their coherent acoustic properties in THz regime.
11:51AM S23.00004: Near Field Optical-Pump-Terahertz-Probe Experiments on Graphene/InAs Heterostructure
ZHENG YAO, JIAWEI ZHANG (Presenter), SCOTT MILLS, Stony Brook University, XIAOGUANG ZHAO, Boston University, XINZHONG CHEN, RYAN MESCALL, Stony Brook University, VYACHESLAV SEMENENKO, Skolkovo Institute of Science and Technology, HAI HU, Nanophotonics Research Division, National Center for Nanoscience and Technology, THOMAS P CIAVATTI, Stony Brook University, STEPHAN MARCH, SETH BANK, Electrical and Computer Engineering, The University of Texas at Austin, HU TAO, Shanghai Institute of Microsystem and Information Technology, State Key Laboratory of Transducer Technology, VASILI PEREBEINOS, Skolkovo Institute of Science and Technology, XIN ZHANG, Boston University, QING DAI, Nanophotonics Research Division, National Center for Nanoscience and Technology, XU DU, MENGKU LIU, Stony Brook University — We show that graphene is a perfect terahertz reflector in the high q regime with terahertz s-SNOM. We also demonstrate optical pump terahertz near-field probe (n-OPTP) and optical pump terahertz near-field emission (n-OPTE) experiments on graphene/InAs heterostructure. Femtosecond pulse laser is used to both pump samples and to generate terahertz pulses. We show that in the near-field regime a single layer graphene is transparent to near-IR (800 nm) optical excited terahertz emission from InAs but completely “screens” the photo-induced carrier dynamics in InAs probed by a separate THz pulse.

12:03PM S23.00005: Developing Wide-angle Spherical Neutron Polarimetry at Oak Ridge National Laboratory
NICOLAS SILVA (Presenter), TIANHAO WANG, HARISH K AGRAWAL, FANKANG LI, LISA DEEBER-SCHMITT, MASAAKI MATSUDA, JILLIAN RUFF, Neutron Science Directorate, Oak Ridge National Laboratory, ROGER PYNN, Physics, Indiana University Bloomington, XIN TONG, BARRY L. WINN, CHENYANG JIANG, Neutron Science Directorate, Oak Ridge National Laboratory — Spherical Neutron Polarimetry (SNP) analyzes complex magnetic structures through distinguishing contributions from nuclear-magnetic interference and chiral structure in addition to nuclear magnetic scattering separation. This analysis is achieved through determining all components in the polarization transfer process. Currently, wide-angle SNP is being realized at Oak Ridge National Laboratory (ORNL) for multiple beamlines including: the polarized triple-axis spectrometer (HB-1) and general-purpose small angle neutron scattering instrument (CG-2) at the High Flux Isotope Reactor (HFIR), as well as the hybrid spectrometer (HYSPEC) at the Spallation Neutron Source (SNS). The SNP device consists of three units: incoming/outgoing neutron polarization, sample environment and a zero-field chamber. The incoming/outgoing neutron polarization regions use high-Tc superconducting YBCO films and mu-metal to achieve full control of neutron polarization. The sample environment is a dilute refrigerator with a customized tail piece placed into the zero-field chamber. The device is under construction with performance simulations complete and calibration and demonstration experiments scheduled for next year.

TIANHAO WANG (Presenter), CHENYANG JIANG, HASSINA Z BILHEUX, INDU DHIMAN, JEAN-CHRISTOPHE BILHEUX, MORRIS LOWELL CROW, LANDEN MCDONALD, LEE ROBERTSON, Oak Ridge National Laboratory, NIKOLAY KARDJILOV, Institute Applied materials, Helmholtz Zentrum berlin, ROGER PYNN, Department of Physics, Indiana University Bloomington, XIN TONG, China Spallation neutron Source — Polarized Neutron Imaging (PNI) visualizes magnetic field distribution through interactions between the neutron polarization and the magnetic field. The PNI technique creates unique imaging contrast related to magnetic properties in comparison to traditional absorption-based neutron imaging. Furthermore, quantitative PNI provides a nondestructive measurement on internal magnetic structures. At the Oak Ridge National Laboratory, a new PNI capability was implemented on the CG-1D neutron imaging beamline at the High Flux Isotope Reactor (HFIR). The PNI setup at ORNL uses an in-situ optical pumping $^3$He neutron spin filter to provide a non-distorted radiographs with a stable 90% neutron polarization. The polarized beamline operates in either polychromatic or monochromatic mode, with a field of view of 50mm×50mm and 350μm spatial resolution. Based on the new capability, a series of experiments were performed investigating the magnetic field distortion caused by Meissner effect of superconductors. The results of these experiments combined with modeling will be presented. The PNI team at ORNL is now seeking collaborations to utilize the PNI technique at CG-1D.
12:27PM S23.00007: Cross-Section and Measurement Considerations for Polarized Neutron Scattering from NMR Spin-Modulated Systems  MICHAEL KOTLARCHYK (Presenter), GEORGE THURSTON, Rochester Institute of Technology — We present a development of theoretically predicted cross sections, along with potential measurement scenarios, associated with the scattering of polarized thermal neutrons from target nuclei whose spins are modulated using nuclear magnetic resonance (NMR). Specifically, we investigate the modulation of the polarized differential scattering cross sections under the following two scenarios: (i) Measurements that take place during the time-interval between the application of radio-frequency (RF) pulses that repeatedly impart transverse rotations to selected sets of spin-1/2 target nuclei, and (ii) Measurements that take place during continuous RF irradiation of these nuclei. The aim of this work is to provide foundational knowledge and necessary considerations to explore, and ultimately achieve, the design of instrumentation that would provide enhanced scattering signals from selected nuclei in liquids and solutions by leveraging the use of NMR techniques. We discuss our in-progress calculations which are aimed at evaluating signal-to-noise for a prototypical molecular mixture in the context of NMR/neutron scattering protocols such as those outlined in our recent paper (1).


12:39PM S23.00008: Designs of neutron microscopes for high-resolution imaging*  MUHAMMAD ABIR, BORIS KHAYKOVICH (Presenter), Massachusetts Institute of Technology, DANIEL HUSSEY, National Institute of Standards and Technology — We demonstrate designs of two types of neutron microscopes. Like an optical microscope, the neutron microscope consists of a condenser and an image forming optics. Neutrons are focused at the sample by a condenser optic. An image forming optic focuses transmitted neutrons at the detector. The condenser optic is designed to maximize the neutron flux and to obtain desired beam divergence at the sample. The condenser consists of axisymmetric confocal paraboloid and a hyperboloid mirrors, which are concentrically nested. The image-forming optics are designed using two different types of Wolter mirrors, confocal nested ellipsoid and hyperboloid sections. The design of magnification-10 mirrors should achieve the spatial resolution of about 10 μm. Importantly, the resolution of the microscope is determined by the mirrors rather than by the beam collimation as in conventional pinhole imaging, leading to possible dramatic improvements in the signal rate and resolution. Also in contrast with pinhole imaging, in the microscope the samples are placed far from the detector to allow for bulky sample environment.

*The work at MIT was supported by the award 60NANB15D361 from U.S. Department of Commerce, National Institute of Standards and Technology.

12:51PM S23.00009: Portable Mid-IR Spectrometer  TAEYOON JEON (Presenter), AMIRHOSSEIN NATEGHI, AXEL SCHERER, Caltech — We describe a mid-IR spectrometer by combining a commercial thermal imaging camera with a Diesel engine glow-plug and a micromachined hyperspectral filter. Our hyperspectral mid-IR filter consists of two silicon/air mirrors that form an optical cavity. A small angle between the two high-reflectivity mirrors provides us with a gradual variation of the cavity resonance peak and we obtain a position-dependent transmission filter. The linear variation of resonance frequency with position enables the ~40,000 pixels in the thermal bolometer camera to be converted into an optical multichannel spectrometer. Filters are made of multiple layers of silicon and air, and the high refractive index and transparent properties of silicon in the mid-IR region provide a wide free spectral range of up to 10 micrometers. Different wavelengths can be assigned to each pixel in the microbolometer array, enabling rapid spectral acquisition in our compact spectrometer. This allows us to measure the mid-IR spectra of various types of polymers, biomolecules and medications in a compact system. Here we show mid-IR molecular absorption spectra from different materials measured with this spectrometer and compare them to Fourier-Transform Infrared Spectroscopy (FTIR) results.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S24 DAMOP DCMP: Topological States in AMO Systems I  BCEC 159 - Chao-Xing Liu - Tag(s): Focus
11:15AM S24.00001: Topological triply-degenerate points in ultracold atoms and photonic hyperbolic metamaterials* [Invited] CHUANWEI ZHANG (Presenter), University of Texas at Dallas — Topological states of matter provide a fertile ground for discovering new quasiparticles in condensed matter physics, such as Weyl and Dirac fermions, which were originally predicted in high-energy physics and recently observed in solid-state materials. In topological semimetals, Weyl and Dirac points correspond to two- and fourfold degenerate linear band crossing points, hallmarks of relativistic particles with half-integer spins. Remarkably, the recent discovery of triply degenerate points (TDPs) in semimetals has opened an avenue for exploring new types of quasiparticles that have no analog in quantum field theory. Such TDPs possess effective integer spins while preserving Fermi statistics and linear dispersions. In previous studies, the emergence of such protected nodes was often attributed to spin-vector-momentum couplings. In this talk, I will discuss three new types of TDPs that are classified by different monopole charges (C = +/- 2, 1, 0) and induced by the interplay between spin-tensor- and spin-vector-momentum couplings. I will discuss how to realize these new types of TDPs using ultracold atoms in optical lattices and photons in non-Hermitian hyperbolic metamaterials. These proposed atomic and photonic systems may provide highly controllable platforms for exploring and engineering novel quasiparticles without counterparts in quantum field theory.

References:

*This work was supported by ARO, AFOSR, and NSF.

11:51AM S24.00002: A Bose-Einstein Condensate on a Synthetic Hall Cylinder* CHUAN-HSUN LI (Presenter), YANGQIAN YAN, SAYAN CHAUDHURY, DAVID BLASING, QI ZHOU, YONG CHEN, Purdue University — Interplay between matter and fields in physical spaces with nontrivial geometries gives rise to many exotic quantum phenomena. However, their realizations are often impeded by experimental constraints. Here, we realize a Bose-Einstein condensate (BEC) on a synthetic cylindrical surface subject to a net radial synthetic magnetic flux, topologically equivalent to a two-dimensional (2D) Hall ribbon with two edges connected. This cylindrical surface comprises a real spatial dimension and a curved synthetic dimension formed by cyclically-coupled spin states. The BEC on such a Hall cylinder has counterintuitive properties unattainable by its counterparts in 2D planes. We observe Bloch oscillations of the BEC with doubled periodicity of the band structure, analogous to traveling on a Möbius strip, reflecting the BEC’s emergent crystalline order with nonsymmorphic symmetry-protected band crossings. We further demonstrate such topological operations as gapping the band crossings and unzipping the cylinder. Our work opens the door to engineering synthetic curved spaces and observing intriguing quantum phenomena inherent to the topology of spaces.

*Our experiment is supported by NSF grant PHY-1708134. D. B. B. acknowledges Purdue Ph.D. fellowship. Q. Z. acknowledges Purdue startup funds.

12:03PM S24.00003: Topological Phases of Fermions in Kagome Optical Lattices* VITO SCAROLA (Presenter), MENGSU CHEN, HOI-YIN HUI, Physics, Virginia Tech, SUMANTA TEWARI, Physics, Clemson University — Frustration can favor topological states of matter over conventionally ordered states. We use numerical diagonalization and mean field theory to study models of fermionic atoms and molecules placed in kagome optical lattices. We show that just the long range part of dipolar interactions between fermions can drive the creation of a topological Mott insulator. We also study applications of applied synthetic fields using optical flux lattices and laser assisted tunneling. We find that effective magnetic fields lead to topological phases, including the chiral spin liquid, even for atoms interacting with only the contact interaction. Experimental challenges for realizing these topological states with atomic gases in optical lattices are discussed.

*We acknowledge support from AFOSR (FA9550-18-1-0505) and ARO (W911NF-16-1-0182).
We propose a realistic scheme for the full characterization of Floquet topological insulators realized in optical lattices. We construct a family of drives that connects the target Hamiltonian to a topologically trivial reference point for the periodically driven systems that we identify as the high-frequency regime. Our proposal relies on the detection of topological singularities in the Floquet spectrum with respect to the reference point as the drive parameters are varied within a specific drive family. Bypassing the difficulties of adiabatic preparation through a topological transition, we show how the topological charge of individual singularities can be measured using state tomography techniques. We demonstrate our scheme by using two concrete examples of periodically driven systems in two dimensions relevant to experiments. Our proposal paves the way to full experimental characterization of nonequilibrium topological phases in driven systems with the measurement of both regular and anomalous Floquet topological invariants.

Work supported by the DFG-Research Unit 2414, the NSF CAREER grant DMR-1350663, the BSF Grant 2014245, and the College of Arts and Sciences at Indiana University.
Wavefunction localization is a characteristic phenomenon occurring in disordered and quasiperiodic systems as well as with edges states in topological phases. We study the quasiperiodic Aubry-Andre-Harper (AAH) model, known to exhibit a unique localization-delocalization transition in one dimensions, defying standard Anderson localization. Generalizations of the AAH model include next-nearest neighbor (NNN) hopping, or additional incommensurate on-site terms and have so far been studied numerically. For such extended models the appearance of a mobility edge i.e. an energy cut-off dictating which wavefunctions undergo the localization-delocalization transition is expected. To study properties of these models, we employ transfer matrices which are known to characterize localization physics through Lyapunov exponents. We use the symplectic nature of transfer matrices to represent them as points on a torus. Related wavefunctions then form toroidal curves. We obtain distinct toroidal curves for localized, delocalized and critical wavefunctions, thus demonstrating a geometrical characterization of localization physics. Applying the transfer matrix method to the NNN AAH model, we formulate a geometrical picture that captures the emergence of the mobility edge in a visually striking way.

Keywords: 06.01.04 Non-Equilibrium Physics with Cold Atoms and Molecules, Rydberg Gases, and Trapped Ions (DAMOP, DCMP); 06.01.02 Topological States in AMO Systems (DAMOP, DCMP)


1:51PM S24.00012: Geometric phases enable real-world models of classical and quantum dynamics in Hall effects and in three-body molecular dynamics*  
F. J. LIN (Presenter), F. J. Lin Research — Almost sixty years ago, Aharonov and Bohm pointed out that electrons could be affected by vector potentials without an external magnetic field. They described an \textit{ad hoc} phase shift required for wave functions in vector potentials, e.g., representing magnetic fields. The phase shift exemplifies a geometric phase (or Berry's phase). In classical and quantum dynamics, vector potentials producing \textit{coupled} overall rotation lead to geometric phases. Instead of neglecting it, now the coupling is used to create a frame with \textit{decoupled} overall rotation and vanishing classical and quantum geometric phases. A general formulation of classical dynamics describes both the dynamics of topological matter, such as Hall effects, and three-body molecular dynamics. A quantum extension describes the quantum dynamics of topological matter and the three-body molecular dynamics in the Born-Oppenheimer approximation. Real-world models with or without magnetic fields contribute to developing optoelectronic and photonic devices. Real-world models for three-body dynamics contribute to developing optimal molecular reaction dynamics.

*Travel support by a Douglas C. Basil Award from the University of Southern California Emeriti Center is gratefully acknowledged.
Topological phases in 1D bosonic Bogoliubov bands with dynamical instability

TERUMICHI OHASHI (Presenter), SHINGO KOBAYASHI, YUKI KAWAGUCHI, Applied physics, Nagoya University — Topological phases of matter have attracted much attention in solid-state physics, but most of studies treat Hermitian Hamiltonians [1]. Recently, there has been growing interest in non-Hermitian topological phases [2], which exhibit exotic phenomena absent in Hermitian ones [3]. Non-Hermitian Hamiltonian describes an open quantum system in which loss and gain of particles coexist. Here, we note that bosonic Bogoliubov quasiparticles, which are elementary excitations from a Bose-Einstein condensate (BEC), are also described with a non-Hermitian Hamiltonian, where a BEC works as a particle bath. In this sense, topological classification of BECs is an open question. In the case when the non-Hermitian Hamiltonian has real eigenvalues, the topological properties of quasiparticles is discussed [4].

In this talk, we consider more general cases of 1D BECs and find topological invariants in 1D BDI and D classes. As concrete examples, we discuss topological properties in a 1D Kitaev model [4] and in a 1D SSH model.


Thursday, March 7, 2019 11:15 AM - 2:15 PM


11:15AM S25.00001: Microgravity experiments with radiofrequency-dressed Bose-Einstein condensates aboard NASA's Cold Atom Laboratory

NATHAN LUNDBLAD (Presenter), MAXWELL GOLD, XIAOLE JIANG, RYAN CAROLLO, Bates College — Microgravity conditions present opportunities for studying ultracold atomic systems free of gravitational perturbation. One such opportunity is the study of shell- or bubble-like Bose-Einstein condensates, which have not been observed terrestrially due to gravitational effects dominating condensate mean-field energy in typical experimental conditions. We present recent measurements using NASA's Cold Atom Laboratory facility aboard the International Space Station focusing on both preliminary characterization of the CAL atom-chip magnetic trap and on the physics of radiofrequency (rf) dressed magnetic traps in a microgravity environment, and discuss model predictions of bubble-BEC properties in such an environment.

*NASA Fundamental Physics / JPL RSA No. 1597429

11:27AM S25.00002: Proposal for measuring Big G using the NASA Cold Atom Lab aboard the International Space Station

COLSON SAPP (Presenter), Georgia Southern University, CHARLES W CLARK, JQI and NIST, MARK EDWARDS, Georgia Southern University — We propose an atom interferometry (AI) experiment to measure Big G constant in a microgravity environment. Our experiment is assumed to be conducted in NASA's Cold Atom Laboratory currently deployed to the International Space Station. The idea is to carry out an AI sequence many times, first with a source mass present and then with no source mass. The basic AI sequence is to split a Bose-Einstein condensate (BEC) into two pieces using pulsed optical lattice potentials. These pieces fly apart in the presence of an harmonic potential and finally stop after one quarter trap period. The trap is then turned off for a wait time. The pieces acquire a relative velocity difference due to the differential gravitational pull of the source mass. The trap is turned back on and the pieces then recombine and are split again. The result is two clouds left nearly motionless near the trap center creating an interference pattern due to their relative velocity. We have simulated this sequence using the Lagrangian Variational Method (LVM) where the trial wave function is a sum of Gaussian clouds. We show how big G can be extracted from the interference pattern that results and present an approximate error budget for the measurement.

*Work supported by NSF grants 1413768 and 1707776.
11:39AM S25.00003: Measurement induced dynamics and defect stabilization in spinor condensates*  
HILARY HURST (Presenter), I. B. SPIELMAN, Joint Quantum Institute and National Institute of Standards and Technology — Weakly measuring many-body systems and allowing for feedback in real time can simultaneously create and measure new phenomena in quantum systems. We study weak measurement and classical feedback in spinor Bose-Einstein condensates, focusing on the trade-off between usable information obtained from measurement and quantum backaction. As a prototype example, we consider the dynamics of a domain wall in a two-component BEC and show that quantum backaction due to measurement causes two primary effects: domain wall diffusion and overall heating. The system dynamics and signal-to-noise ratio depend on the choice of measurement observable. We describe a feedback protocol to create and stabilize a domain wall in the regime where domain walls are unstable, giving a prototype example of Hamiltonian engineering using measurement and feedback. Finally, we discuss extensions of this idea to higher spin systems.

*This work was partially supported by the Air Force Office of Scientific Research's Quantum Matter MURI, NIST, and NSF (through the Physics Frontier Center at the JQI). HMH acknowledges the support of the NIST/NRC postdoctoral program.

11:51AM S25.00004: Nonthermal fixed points in a one-dimensional antiferromagnetic spinor Bose gas  
KAZUYA FUJIMOTO (Presenter), RYUSUKE HAMAZAKI, MASAHITO UEDA, Department of Physics, University of Tokyo — Recently, a nonthermal fixed point (NFTP) is proposed as a universal thermalization scenario [1], where a system evolving from a nonequilibrium initial state is attracted to the NTFP and shows a universal dynamical scaling law. We theoretically study quench dynamics in a one-dimensional (1D) antiferromagnetic (AF) spinor Bose gas, finding universal thermalization dynamics characterized by a NTFP induced by two types of solitons. One soliton is a magnetic soliton having a locally magnetized part, and the other is an exotic bound state of magnetic solitons, which we refer to as a Flemish string because of the twisted magnetic structure. We numerically find that the stable magnetic solitons can disappear through formation of the Flemish strings, and that the cooperative soliton dynamics through the Flemish string promotes the relaxation. Then, we elucidate the dynamical scaling regarded as a signature of the NTFP in the quench dynamics. Furthermore, studying the experiment for a trapped 1D AF Bose gas [2], we find that the universal thermalization with the NTFP appear if the applied filed is quenched more strongly compared with the experiment.


12:03PM S25.00005: Universal relations and Tan contact matrix for 1D spinor quantum gases*  
SHAH SAAD ALAM (Presenter), HAN PU, Rice University — The Tan contact and associated Tan relations, such as the tail of the momentum distribution, have been previously studied for a few kinds of spinor quantum gases, such as spin-zero/half fermions, bosons, SU(N) symmetric cases or multicomponent gases. Inspired by our previous work on interacting spinor quantum gases with arbitrary spins, we present results of our investigation of the Tan contact matrix and its connection to the large momentum tail for arbitrary spin cases with spin-dependent interactions at arbitrary strengths. We further discuss the connection of the Tan contact matrix to two body density matrices, energetics and other universal relations.

*NSF, Welch Foundation

12:15PM S25.00006: Supercurrent induced by multipoles in nonmagnetic spin-2 Bose-Einstein condensates*  
EMI YUKAWA (Presenter), Center for Emergent Matter Science, RIKEN, MASAHITO UEDA, Department of Physics, University of Tokyo — In spinor Bose-Einstein condensates (BECs), a supercurrent is known to be induced by the magnetic degrees of freedom when the magnitude of the spin vector is finite. On the other hand, when a spinor BEC is nonmagnetic, the supercurrent originating from the magnetic degrees of freedom is absent for a spin-1 BEC; however, it has remained to be clarified if it is essentially zero for any spin degrees of freedom. We show that a supercurrent can be induced by magnetic multipoles for a non-magnetic spin-2 BEC. We analytically derive a superfluid in a nonmagnetic spin-2 BEC that involves components originating from the magnetic degrees of freedom. We also numerically demonstrate that these components can be induced by a spatially dependent magnetic field via the quadratic Zeeman effect.

*This work is supported by JSPS Grant-in-Aid for Scientific Research(B) KAKENHI Grant No. JP18H01145 and JSPS Grant-in-Aid for Scientific Research on Innovative Areas Topological Material Science KAKENHI Grant No. JP15H05855.
12:27PM S25.00007: Internal oscillations of a dark-bright soliton in a harmonic potential* MAJED ALOTAIBI (Presenter), LINCOLN CARR, Colorado Sch of Mines — We investigate the dynamics of a dark-bright soliton in a harmonic potential using a mean-field approach via coupled nonlinear Schrodinger equations appropriate to multi-component Bose-Einstein condensates. We use a modified perturbed dynamical variational Lagrangian approximation, where the perturbation is due to the trap, taken as a Thomas-Fermi profile. The wave function ansatz is taken as the correct hyperbolic tangent and secant solutions in the scalar case for the dark and bright components of the soliton, respectively. We also solve the problem numerically with pseudo-spectral Runge–Kutta methods. We find, analytically and numerically, for weak trapping the internal modes are nearly independent of center of mass motion of the dark-bright soliton. In contrast, in tighter traps the internal modes couple strongly to the center of mass motion, showing that for dark-bright solitons in a harmonic potential the center of mass and relative degrees of freedom are not independent. This result is robust against noise in the initial condition and should, therefore, be experimentally observable.

*National Science Foundation: grant numbers PHY-1520915, OAC-1740130.

12:39PM S25.00008: Collision of Bose-Einstein Condensates* FABIO LINGUA (Presenter), Physics Departement, Clark University, LUCA LEPORI, INFN, Laboratori Nazionali del Gran Sasso, FRANCESCO MINARDI, LENS European Laboratory for Non-Linear Spectroscopy, VITTORIO PENNA, Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino, LUCA SALASNICH, Dipartimento di Fisica e Astronomia Galileo Galilei and CNISM, Università di Padova — We study the collision of two interacting Bose-Einstein Condensates of $^{87}$RB and $^{41}$K in a weak harmonic confinement. The study is performed by means of numerical solution of two coupled Gross Pitaevskii equations. The process is investigated in presence of both attractive and repulsive interaction between the two atomic components, showing various complex phenomena such as the formation of dark and bright solitons, condensate trapping, and coupled oscillations of boson populations.

*We thank Giacomo Lamporesi for useful discussions. FM acknowledges funding from FP7 Cooperation STREP Project EQuaM (Grant n. 323714). LS acknowledges Project BIRD164754 of University of Padova for partial support.

12:51PM S25.00009: Filamentary Dynamics of Dark Solitons, Vortex Rings and Knots* PANAYOTIS KEVREKIDIS (Presenter), University of Massachusetts Amherst — In the present talk, we will revisit some principal excitations in self-repulsive Bose-Einstein condensates, namely dark solitons, vortex rings and knots. For dark solitons, upon introducing them and explaining their existence and stability properties in 1d, we will extend them both in the form of stripes and in that of rings in two-dimensions, presenting an adiabatic-invariant formulation of their stability and excitations. We will explore their filamentary dynamics, as well as the states that emerge from their transverse (snaking) instability. Then, we will consider these structures even in three dimensions, in the form of planar, as well as spherical shell solitons and generalize our adiabatic invariant formulation to the case of vortex rings and their own filamentary dynamics. Finally, time permitting, we will give some glimpses of how some of these dynamical features in 1d and 2d generalize to the case of vortex rings and their own filamentary dynamics.

*This work is supported by NSF-PHY-1602994.

1:03PM S25.00010: Lattice and continuum model for ultra-cold atoms in a crossed-cavity system* POORNIMA SHAKYA (Presenter), AMULYA RATNAKAR, SANKALPA GHOSH, Indian Institute of Technology Delhi — Recent experiments by ETH and MIT groups have reported on the formation of a super-solid, respectively in scalar and spinorial ultra-cold atomic systems, an enigmatic phase of matter that shows superfluidity and solid-like density modulation, simultaneously. In this paper [1], we derive the extended Bose-Hubbard Hamiltonian for a Bose-Einstein condensate loaded in a crossed-cavity set-up. Subsequently, in the continuum limit, we obtain the Gross-Pitaevskii energy functional and the Gross-Pitaevskii equations for the superfluid order parameters for such a super-solid phase and discuss its significance.


*P.S. is supported by UGC Fellowship and S.G. and A.R. both are supported by BRNS (DAE, Govt. of India) Grant no. 21/07/2015-BRNS/35041 (DAE SRC Outstanding Investigator scheme).
1:15PM S25.00011: Production of smooth flow in racetrack BECs at zero and non-zero temperatures

BENJAMIN ELLER (Presenter), DANIEL FOGARTY, Georgia Southern University, CHARLES W CLARK, JQI and NIST, MARK EDWARDS, Georgia Southern University — We have studied the production of smooth, persistent currents in ultracold (bosonic) gas systems that consist of an atomic BEC and a non-condensate cloud. The BEC is assumed to be strongly confined in a horizontal plane by a vertical harmonic trap and, within this plane, subjected to an arbitrary two-dimensional potential. The racetrack potential is made up of two straight parallel channels connected on both ends by semicircular channels of the same width and energy height as the straightaways. The zero-temperature behavior of the system is simulated using the Gross-Pitaevskii equation and at non-zero temperature by the Zaremba-Nikuni-Griffin model. The flow is realized by stirring along the channel with a rectangular barrier. We conducted simulations of stirring racetrack BECs for a range of different racetrack geometries, barrier speeds and maximum energy heights both at zero and non-zero temperatures. We also investigated the mechanism for producing flow in order to be able to predict the amount of flow and its onset using a 1D model. We will present the results of the simulations and also discuss the effect of temperature on the amount of flow produced.

*This work was funded by NSF grant numbers 1413768 and 1707776.

1:27PM S25.00012: Bistability of Bose-Einstein condensates with a local loss term and pinning potentials

MASAYA KUNIMI (Presenter), Kyoto University, IPPEI DANSHITA, Kindai University — Recent technological advances in ultracold atom experiments allow for introducing couplings to environment, namely dissipation, in a well-controlled manner [1,2]. In particular, the experimental group at Technische Universitat Kaiserslauten has reported the observation of unexpected bistability in a Bose-Einstein condensate in the presence of local one-body dissipation created with an electron beam [1]. To clarify the origin of the bistability under the local particle loss, we construct a simple mean-field model that describes the bistability of superfluids. In this work, we will show that exact solutions of the Gross-Pitaevskii equation with a local particle loss term and pinning potentials of the delta function type. We point out that the pinning potentials play an essential role for the bistability. When there are not the pinning potentials, the bistability does not appear [3]. We also discuss the roles of the pinned solitons for the bistability. [1] R. Labouvie, et al., Phys. Rev. Lett. 116, 235302 (2016). [2] T. Tomita et al., Sci. Adv. 3, e17011513 (2017). [3] D. Sels and E. Demler, arXiv:1809.10516 (2018).

1:39PM S25.00013: Dimensional phase transitions from 1D quantum liquids to 3D condensates

SEBASTIAN EGGERT (Presenter), IMKE SCHNEIDER, AXEL PELSTER, POLINA MATVEEVA, DENIS MORATH, University of Kaiserslautern, DOMINIK STRASSEL, Fraunhofer ITWM — We consider weakly coupled strongly interacting quantum chains, such as quantum wires, anisotropic ultracold gases, or quasi-1D spin-chain compounds. It is known that a phase transition from the 1D Luttinger liquid behavior to a 3D ordered states can be qualitatively described by a chain mean field theory to determine the critical temperature, but the quantitative corrections and the range of validity is not well established. We therefore simulate the transition using a fully 3D microscopic model with very large scale quantum Monte Carlo calculations and compare with theoretical prediction including higher order terms in the chain mean field theory. We not only determine the very strong quantitative corrections, but also find a new regime of low density behavior where long range quantum correlations between the chains dominate the behavior, which leads qualitatively different powerlaws as a function of interchain couplings.

1:51PM S25.00014: Robust cat state from kinetic driving of a boson gas

FERNANDO SOLS (Presenter), GREGOR PIEPLOW, CHARLES E. CREFFIELD, Universidad Complutense de Madrid, Madrid, Spain — We investigate the behavior of a one-dimensional Bose-Hubbard gas whose kinetic energy is made to oscillate with zero time-average. The effective dynamics is governed by an atypical many-body Hamiltonian where only even-order hopping processes are allowed. In some parameter range the system has similarities to the Richardson model, which permits a detailed understanding of its key features. The ground state is a cat-like superposition of two macroscopically occupied one-atom states of opposite momentum. Interactions give rise to a reduction (or modified depletion) cloud that is common to both macroscopic options. Symmetry arguments permit a precise identification of the two orthonormal, macroscopically distinguishable many-body states yielding the cat state, each involving a large number of momentum configurations. For a gas between hard walls, the cat correlations are fundamentally robust because the system cannot collapse into a nonzero current state.

*Spain’s MICINN through Grant No. FIS2017-84368-P, Real Colegio Complutense at Harvard, and Harvard-MIT Center for Ultracold Atoms.
Emergence of correlations in the process of thermalization of interacting bosons

FAUSTO BORGONOVI (Presenter), istituto nazionale di fisica nucleare, FELIX IZRAILEV, Istituto de fisica, BUAP, Mexico — The relevance of thermalization to the increase of correlations in the quench dynamics of an isolated system with a finite number of interacting bosons has been studied. Specifically, we analyze how correlations between occupation numbers increase in time resulting in the emergence of the Bose-Einstein distribution. Before saturation, the two-point correlation function increases quadratically in time (as predicted by perturbation theory), while the out-of-time-order correlator (OTOC) increases algebraically with an exponent 2.5 beyond the perturbative region. Our results, that can be confirmed experimentally in traps with interacting bosons, may be also relevant to the problem of black hole scrambling.

*We acknowledge financial support from VIEP-BUAP Grant No. IZF-EXC16-G (FMI) and Iniziativa Specifica INFN-DynSysMath (FB)

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S26 DQI: Superconducting Circuits: Fluxonium and Superinductance Devices BCEC

160B - Vladimir Manucharyan

11:15AM S26.00001: Cavity-less circuit quantum electrodynamics of a fluxonium artificial atom – Design

HAONAN XIONG (Presenter), YEN-HSIANG LIN, University of Maryland, College Park, NATHANAEL COTTET, Ecole Normale Superieure de Lyon, LONG NGUYEN, RAY MENCIA, AARON SOMOROFF, VLADIMIR MANUCHARYAN, University of Maryland, College Park — In circuit quantum electrodynamics (cQED), a high-quality factor cavity plays a central role: it protects a qubit from spontaneous emission and acts as a buffer system enabling a quantum non-demolition (QND) dispersive readout of the qubit state. Here we experiment with a fluxonium artificial atom capacitively connected to a 1D transmission line. We simultaneously achieved a strong coupling of a high-frequency “cycling” transition (0→3 or 1→2) to the traveling waves and a complete suppression of the spontaneous emission of the low-frequency qubit transition (0→1). This allowed implementing the fluorescence “shelving” readout of a highly-coherent and fully controllable qubit. Unlike in conventional cQED, here the cycling dynamics during the readout is confined to a small Hilbert space and can be understood within a simple optical pumping model. Our system realizes a hardware-efficient interface between qubits and photons and hence can be useful in constructing quantum networks. It can also help understanding the processes leading to the loss of QND-ness in cQED at relatively low photon numbers.

11:27AM S26.00002: Cavity-less circuit quantum electrodynamics of a fluxonium artificial atom - Experiment

YEN-HSIANG LIN (Presenter), HAONAN XIONG, University of Maryland, College Park, NATHANAEL COTTET, Ecole Normale Superieure de Lyon, LONG NGUYEN, RAY MENCIA, AARON SOMOROFF, VLADIMIR MANUCHARYAN, University of Maryland, College Park — In circuit quantum electrodynamics (cQED), a high-quality factor cavity plays a central role: it protects a qubit from spontaneous emission and acts as a buffer system enabling a quantum non-demolition (QND) dispersive readout of the qubit state. Here we experiment with a fluxonium artificial atom capacitively connected to a 1D transmission line. We simultaneously achieved a strong coupling of a high-frequency “cycling” transition (0→3 or 1→2) to the traveling waves and a complete suppression of the spontaneous emission of the low-frequency qubit transition (0→1). This allowed implementing the fluorescence “shelving” readout of a highly-coherent and fully controllable qubit. Unlike in conventional cQED, here the cycling dynamics during the readout is confined to a small Hilbert space and can be understood within a simple optical pumping model. Our system realizes a hardware-efficient interface between qubits and photons and hence can be useful in constructing quantum networks. It can also help understanding the processes leading to the loss of QND-ness in cQED at relatively low photon numbers.
11:39AM S26.00003: Single-Shot Readout of Fluxonium Qubits.* KONSTANTIN NESTEROV (Presenter), University of Wisconsin - Madison, IVAN PECHENEZHSKIY, LONG NGUYEN, YEN-HSIANG LIN, AARON SOMOROFF, RAY MENCIA, VLADIMIR MANUCHARYAN, University of Maryland-College Park, MAXIM VAVILOV, University of Wisconsin - Madison — We discuss the possibility of the single-shot readout of fluxonium superconducting qubits [1] based on the preparation of the "bright" and "dark" cavity states. With a proper choice of parameters, the dispersive shift of the cavity (the distance between its dressed and bare resonance frequencies) for the qubit 0 state can be made much smaller than this shift for the qubit 1 state. Thus, the cavity nonlinearity can be made much weaker for the qubit 0 than for the qubit 1 states. This has a potential to improve two types of single-shot qubit readout schemes that are used in the transmon readout, when the cavity nonlinearity is comparable for the two transmon states. First, for the readout based on microwave photon counters [2], one can achieve a higher cavity occupation in its bright state. Second, for the high-power readout [3], the onset of the bright transmission for one of the qubit states can occur at lower power.


*We acknowledge funding from the U.S. Army Research Office (Grant No. W911NF-18-1-0146).

11:51AM S26.00004: Nanowire Superinductance Fluxonium Qubit* THOMAS HAZARD (Presenter), ANDRAS GYENIS, Electrical Engineering, Princeton University, AGUSTIN DI PAOLO, Institut Quantique and Département de Physique, Université de Sherbrooke, ABRAHAM ASFAW, Electrical Engineering, Princeton University, ALEXANDRE BLAIS, Institut Quantique and Département de Physique, Université de Sherbrooke, STEPHEN APLIN LYON, ANDREW HOUCK, Electrical Engineering, Princeton University — We characterize a fluxonium qubit consisting of a Josephson junction inductively shunted with a NbTiN nanowire superinductance. We explain the measured energy spectrum by means of a multimode theory accounting for the distributed nature of the superinductance and the effect of the circuit nonlinearity to all orders in the Josephson potential. Using multiphoton Raman spectroscopy, we address multiple fluxonium transitions, observe multilevel Autler-Townes splitting and measure an excited state lifetime of $T_1 = 20 \mu$s. By measuring $T_1$ at different magnetic flux values, we find a crossover in the lifetime limiting mechanism from capacitive to inductive losses.

*Army Research Office Grant No. W911NF-15-1-0421 and the Princeton Center for Complex Materials DMR-142052

12:03PM S26.00005: Fast qubit reset of a low frequency fluxonium circuit* NATHANAEL COTTET (Presenter), JEREMY STEVENS, BENJAMIN HUARD, Ecole Normale Superieure de Lyon — The improvement of the lifetime and coherence time of superconducting circuits is a critical step towards the development of quantum processing of information. Recent results demonstrated coherence times and lifetimes above 100 microseconds on the first transition of fluxonium circuits biased at half flux quantum. These timescales can be improved tenfold by decreasing the transition frequencies below 500 MHz, without compromising on the gate time. The drawback is that the qubit is thermally excited at thermal equilibrium in a dilution refrigerator. Fast and efficient initialization processes are therefore crucial to follow that road. We present and characterize two initialization schemes on a low frequency fluxonium circuit. First, we use optical pumping to convert circuit excitations into cavity ones in a process similar to the one demonstrated for transmons. Second, using quantum-limited amplifiers, we use single-shot measurements to herald on the initial qubit state.

*This program is funded by the HiPS program of the ARO.

12:15PM S26.00006: Towards a fluxonium-based quantum processor I: non-interacting qubits AARON SOMOROFF (Presenter), LONG NGUYEN, YEN-HSIANG LIN, RAY MENCIA, IVAN PECHENEZHSKIY, University of Maryland, College Park, KONSTANTIN NESTEROV, MAXIM VAVILOV, University of Wisconsin, Madison, VLADIMIR MANUCHARYAN, University of Maryland, College Park — We describe our progress in experimentally realizing a microwave-activated two-qubit gate with capacitively coupled fluxonium qubits. When biased at the flux sweet-spot, the individual qubits have frequencies around 500 MHz and reproducibly reach long coherence times in excess of 100 us (the best device had $T_2 > 300$ us) [1]. A c-Phase gate can be achieved by sending a short 2π-pulse at the frequency near the 1→2 transition of the target qubit [2]. Our work includes characterization of coherence and parameter fluctuations in multi-qubit chips, modeling and experimentally validating the two-qubit interactions, optimizing the joint readout, and benchmarking of the gate operations.

We describe our progress in experimentally realizing a microwave-activated two-qubit gate with capacitively coupled fluxonium qubits. When biased at the flux sweet-spot, the individual qubits have frequencies around 500 MHz and reproducibly reach long coherence times in excess of 100 us (the best device had $T_2 > 300$ us) [1]. A c-Phase gate can be achieved by sending a short 2π-pulse at the frequency near the $1/2$ transition of the target qubit [2]. Our work includes characterization of coherence and parameter fluctuations in multi-qubit chips, modeling and experimentally validating the two-qubit interactions, optimizing the joint readout, and benchmarking of the gate operations.


A promising alternative for the implementation of superinductors, compared to the predominantly used mesoscopic Josephson junction arrays, is granular aluminum (grAl), with a microstructure consisting of pure aluminum grains embedded in an AlOx matrix, effectively forming a self-assembled Josephson junction network [1]. This material offers a large kinetic inductance, while its non-linearity is orders of magnitude smaller than that of Josephson junction arrays [2]. We present a fluxonium qubit employing a granular aluminum superinductor with coherence times $T_1$ up to 23 μs and $T_2^R$ up to 30 μs at the flux bias sweet spot. The measured $T_2^E$ approaches the limit $2 \times T_1$ [3]. These coherence times recommend granular aluminum for increasingly complex protected superconducting quantum circuits, while they also evidence the need to further investigate and mitigate loss mechanisms in high impedance qubits.


*Funding was provided by the Alexander von Humboldt foundation in the framework of a Sofja Kovalevskaja award endowed by the German Federal Ministry of Education and Research.

We present a superconducting fluxonium qubit employing a superinductor with impedance $Z > R_Q$, fabricated from a grAl thin film, in-situ integrated with a conventional Al/AlOx/Al Josephson junction. The measured qubit spectrum is in good agreement with the fluxonium Hamiltonian [3].


*Funding was provided by the Alexander von Humboldt foundation in the framework of a Sofja Kovalevskaja award endowed by the German Federal Ministry of Education and Research.
1:03PM S26.00010: Circuit-QED Studies of Josephson Junction Arrays in the Quantum Regime* HIROKI IKEGAMI (Presenter), Center for Emergent Matter Science (CEMS), RIKEN, COSMIC RAJ, Research Center for Advanced Science and Technology (RCAST), The University of Tokyo, YASUNOBU NAKAMURA, Center for Emergent Matter Science (CEMS), RIKEN — Josephson junction arrays (JJAs) in superconducting circuits offer model systems for studying various many-body phenomena both in the classical and quantum regimes. One of the remarkable phenomena observed in JJAs is the quantum phase transition between superconducting and insulating phases associated with the competition between the Josephson energy and the charging energy. In our previous study, we used a circuit-QED technique to study dynamics of the superconductor-metal transition of a classical JJA at a single photon level and found that the internal loss of the cavity shows a peak at the transition temperature. Here we use the experimental technique to explore JJAs in the quantum regime. We find that the temperature at which a peak appears in the cavity loss decreases when the charging energy becomes more dominant than the Josephson energy, i.e., the quantum effect becomes more significant. In the talk, we will discuss the result in connection with the quantum phase transition between the superconducting and insulating phases.

*This work was partly funded by ImPACT Program of Council for Science, Technology and Innovation and Matsuo Foundation.

1:15PM S26.00011: Implementation of π-periodic Josephson Elements for Topologically Protected Charge-Parity Qubits* YEBIN LIU (Presenter), KENNETH DODGE, MICHAEL ANTHONY SENATORE, Physics, Syracuse University, SHAOJIANG ZHU, FNU NAVEEN, ABIGAIL J SHEARROW, FRANCISCO SCHLENKER, ANDREY KLOTS, LARA FAORO, LEV B IOFFE, ROBERT F MCDERMOTT, Physics, University of Wisconsin-Madison, B.L.T. PLOURDE, Physics, Syracuse University — Superconducting qubits with topological protection against local noise hold the promise of significantly enhanced coherence times and higher gate fidelities than is possible with conventional qubits. We are developing one such protected design — the hybrid charge-parity qubit that combines arrays of high kinetic inductance nanowires and conventional Josephson junctions and involves the individual flux control in each plaquette. For appropriate values of the Josephson energy and charging energy of the junctions and the inductive energy of the nanowires, the arrays can be tuned between a periodicity of 2π and π by varying the external magnetic flux through the array. We describe the fabrication of these arrays and experiments to characterize the periodicity with phase by incorporating the array into an rf SQUID.

*Supported by the U.S. Government under Grant W911NF-18-1-0106

1:27PM S26.00012: Granular aluminum: A source of non-linearity for superconducting quantum circuits PATRICK WINKEL (Presenter), DENNIS RIEGER, LUKAS GRUENHAUPT, Physikalisches Institut, Karlsruhe Institute of Technology, KIRIL BORISOV, Institute of Nanotechnology, Karlsruhe Institute of Technology, NATALIYA MALEEVA, MARTIN SPIECKER, ALEXEY V. USTINOV, WOLFGANG WERNSDORFER, IOAN-MIHAI POP, Physikalisches Institut, Karlsruhe Institute of Technology — Superconducting granular aluminum (grAl) has already proven its applicability as linear inductor in kinetic inductance detectors and Fluxonium qubit designs [1]. Evaporated in an oxygen atmosphere, aluminum self-assembles into crystalline grains separated by amorphous aluminum oxide, resulting in highly inductive and low-loss superconducting grAl films [2]. We model the cQED properties of grAl microwave resonators using an effective array of Josephson junctions, and obtain self-Kerr coefficients that are inversely proportional to the grAl volume and the critical current density [3]. By shunting a small grAl volume with a thin film aluminum capacitor, we enhance the self-Kerr nonlinearity of the resulting LC mode, $K_{11}$, up to values much larger than the spectral linewidth of the fundamental mode, $\kappa$, with $K_{11} \approx 100\kappa$. By driving the resonator with increasingly larger power, we observe up to 30 multi-photon transitions between the levels of the fundamental mode, from which we extract a value of $K_{11}$ in the MHz range.

1:39PM S26.00013: Phase Transitions and Edge States in Fluxonium Qubit Systems A. BARIS OZGULER (Presenter), Department of Physics, University of Wisconsin - Madison, VLADIMIR MANUCHARYAN, Department of Physics, University of Maryland, MARK DYKMAN, Department of Physics and Astronomy, Michigan State University, MAXIM VAVILOV, Department of Physics, University of Wisconsin - Madison — A chain of fluxonium qubits provides the means for simulating quantum many-body phenomena in spin-1/2 magnets. The available controls allow us to map a qubit chain on an Ising chain in a transverse magnetic field with variable parameters. The role of the transverse field is played by the tunnel-induced splitting between the lowest energy states at the half-flux sweet spot [1]. The interaction comes from the inductive qubit coupling between fluxoniums' superinductors and can exceed the level splitting [2]. The magnetic flux detuning from the sweet spot plays the role of the longitudinal field for an Ising spin. In this talk, we discuss the phase diagram of the fluxonium chain. We demonstrate the quantum phase transition with the varying level splitting and the emergence of the edge states. We compare these states to the Majorana states in a fermion chain. We study how the edge state localization length depends on the disorder in the random longitudinal and transverse fields.


1:51PM S26.00014: Intrinsically Error Protected Superconducting Architecture Based on Superinductance* ANDRAS GYENIS (Presenter), THOMAS HAZARD, Department of Electrical Engineering, Princeton University, AGUSTIN DI PAOLO, Institut Quantique and Département de Physique, Université de Sherbrooke, ANDREI VRAJITOAREA, Department of Electrical Engineering, Princeton University, ALEXANDRE BLAIS, Institut Quantique and Département de Physique, Université de Sherbrooke, JENS KOCH, Department of Physics and Astronomy, Northwestern University, ANDREW HOUCK, Department of Electrical Engineering, Princeton University — Significant effort has been recently devoted to develop qubits with hardware-level protection, where the disjoint nature of the qubit wavefunctions offers protection against various relaxation mechanisms. Among the superconducting architectures, the so-called 0-π qubit [PRA 87, 052306 (2013)] is a promising candidate for realizing such a system. Here, we introduce the soft-0-π qubit: a twist on the original 0-π qubit proposal that relaxes some of the constraints on the qubit design parameters. In this talk, we present spectroscopic and time-domain measurements on this device. Our approach exploits an exponentially small overlap between the qubit logical wave functions and flux sweet spots to render the soft-0-π qubit noise-protected.

*Army Research Office Grant W911NF-15-1-0421

2:03PM S26.00015: Characterizing Granular Aluminum in Superconducting Circuits* ALEXANDER PLACE (Presenter), THOMAS HAZARD, ANDRAS GYENIS, ANDREW HOUCK, Princeton University — High kinetic inductance materials are promising candidates for implementing large inductances which are crucial for several proposed qubit designs. These materials also allow for a distributed nonlinear element, opening the door for a new family of qubits. Here, we present a new method to deposit granular aluminum in addition to spectroscopic and time domain measurements of granular aluminum-based superconducting qubits.

*This work is supported by the Army Research Office, Grant W911NF-15-1-0421

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S27 DQI: Landauer-Bennett Award Session: Quantum Error Correction Theory and Experiment III BCEC 160C - Markus Kesselring - Tag(s): Focus
11:15AM S27.00001: Rolf Landauer and Charles H. Bennett Award in Quantum Computing talk: Repeated parity measurement and feedback in a mixed-species trapped ion register [Invited] JONATHAN HOME (Presenter), ETH Zurich — Quantum error correction is essential for realizing the full potential of large-scale quantum information processing devices. Fundamental to its experimental realization is the repetitive detection of errors via projective measurements of quantum correlations among qubits, as well as corrections using conditional feedback. I will describe experiments in which we demonstrate up to 50 sequential measurements of correlations between two beryllium ion microwave qubits using an ancillary optical-frequency qubit in a calcium ion, and implement feedback that allows us to stabilize two-qubit subspaces as well as maximally entangled Bell states [1]. The use of multiple ion species allows us to completely reset the ancilla after measurement and completely mitigate any unwanted effects. Looking towards further scaling, many apparent challenges appear to lie in the use of radio-frequency traps, including power-dissipation and the need to co-align microscopically varying potentials. I will describe how this might be mitigated using micro-fabricated arrays of Penning traps, which would also provide a powerful tool for implementing trapped-ion quantum simulation on a variety of two-dimensional lattices.


11:51AM S27.00002: Optimality of Gottesman-Kitaev-Preskill (GKP) Codes for Bosonic Quantum Error Correction KYUNGJOO NOH (Presenter), Yale Univ, VICTOR ALBERT, Caltech, LIANG JIANG, Yale Univ — Bosonic quantum error correction has recently risen as a hardware-efficient alternative to the conventional multi-qubit-based quantum error correction. We mainly focus on photon loss error, which is a dominant error source in microwave cavity modes. Previously, it was shown that GKP codes outperform many other bosonic quantum error-correcting codes in correcting photon loss errors, despite the fact that GKP codes are not designed to correct loss errors [1]. Here, we explain why GKP codes perform well against photon loss errors by providing a near-optimal decoding scheme and analyzing its performance. Furthermore, we formulate a biconvex optimization to find the best single-mode bosonic error-correcting code for photon loss errors. In particular, we solve the biconvex optimization heuristically by an alternating semi-definite programming method and show that, starting from Haar random initial codes, our numerical optimization yields a hexagonal GKP code as an optimal encoding in a practically relevant regime [2].


12:03PM S27.00003: High-threshold fault-tolerant quantum computation with GKP qubits and realistically noisy devices KOSUKE FUKUI (Presenter), Kyoto University, AKIHISA TOMITA, Hokkaido University, KEISUKE FUJII, Kyoto University — To implement fault-tolerant quantum computation with continuous variables, the Gottesman-Kitaev-Preskill (GKP) qubit has been recognized as an important technological element. We have proposed a method to reduce the required squeezing level to realize large scale quantum computation with the GKP qubits [Phys. Rev. X. 8, 021054 (2018)]. Although our method can reduce the required squeezing level to less than 10 dB, which is within the reach of the current experimental technology, we have assumed that the CZ gate and an efficiency of the homodyne detection are ideal. In this work, we show that the required squeezing level is around 10 dB under the realistic assumption that the CZ gate and homodyne detection degrade the squeezing level of the GKP qubits, developing a method to reduce a noise on the GKP qubit by using postselection and maximum-likelihood methods.

12:15PM S27.00004: Grid states for encoding and stabilizing a logical qubit in superconducting circuits (Part 1)* ALEC EICKBUSCH (Presenter), STEVEN TOUZARD, PHILLIPE CAMPAGNE-IBARCQ, EVAN ZALYS-GELLER, NICHOLAS FRATTINI, VOLODYMYR SIVAK, SHRUTI PURI, MAZYAR MIRRAHIMI, SHYAM SHANKAR, MICHEL H. DEVORET, Yale Univ — Quantum computation requires that systems preserve quantum information in the presence of noise. The impact of this noise can be mitigated by redundantly encoding a quantum bit of information within a space with a large number of dimensions. Stabilization is done by detecting noise-induced transformations of the system state before the encoded information is lost. In 2001, Gottesman Kitaev and Preskill (GKP) proposed to encode a quantum bit in non-local grid states of a harmonic oscillator. Remarkably, GKP codes have the potential to protect quantum information against all known error channels. In this talk, I will review GKP code properties and present a protocol based on a tunable interaction with an ancillary two-level system to create and stabilize GKP grid states using phase-estimation of the harmonic oscillator field.

*Work supported by ARO, AFOSR and YINQE
12:27PM S27.00005: Grid states for encoding and stabilizing a logical qubit in superconducting circuits (Part 2)*
STEVEN TOUZARD (Presenter), ALEC EICKBUSCH, PHILIPPE CAMPAGNE-IBARCO, EVAN ZALYS-GELLER, NICHOLAS FRATTINI, VOLODYMYR SIVAK, SHRUTI PURI, MAZAR MIRRAHMI, SHYAM SHANKAR, MICHEL H. DEVORET, Yale Univ — Protecting quantum information requires encoding a quantum bit of information into a space with a large number of dimensions. To this end, Gottesman Kitaev and Preskill (GKP) proposed to use a single harmonic oscillator as an alternative to an ensemble of many two-level systems. In this scheme, the information is encoded in grid states of the oscillator. The dispersive interaction between the oscillator and an ancillary two-level system is sufficient to create and stabilize these non-local states, provided that the interaction strength is periodically modulated in time. In this talk, I will show how to engineer such a modulated interaction and I will present our experimental progress towards the creation and stabilization of GKP grid states.

*Work supported by ARO, AFOSR and YINQE

12:39PM S27.00006: Continuous symmetries and approximate quantum error correction* PHILIPPE FAIST (Presenter), California Institute of Technology, SEPEHR GHAZI NEZAMI, Stanford University, VICTOR ALBERT, California Institute of Technology, GRANT SALTON, Stanford University, FERNANDO PASTAWSKI, Freie Universitaet Berlin, PATRICK HAYDEN, Stanford University, JOHN PRESKILL, California Institute of Technology — Quantum error correction and symmetries are relevant to many areas of physics, including many-body quantum systems, holographic quantum gravity, and reference-frame error-correction [Hayden et al., arXiv:1709.04471]. Here, we show that any code is fundamentally limited in its ability to approximately error-correct against erasures at known locations if it is covariant with respect to a continuous local symmetry. Our bound vanishes either in the limit of large individual subsystems, or in the limit of a large number of subsystems, and is approximately tight in these regimes. Furthermore, we prove an approximate version of the Eastin-Knill theorem that quantifies a code's ability to correct erasure errors if it admits a universal set of transversal logical gates. The bound is in terms of the local physical subsystem dimension. We provide a collection of example codes illustrating our bounds in different regimes. In the context of the AdS/CFT correspondence, our approach provides insight into how time evolution in the bulk corresponds to time evolution on the boundary without violating the Eastin-Knill theorem, and our five-rotor code can be stacked to form a covariant holographic code.

*Swiss National Science Foundation, NSF, DoE, ARO, DOE, IARPA, and the Simons Foundation

12:51PM S27.00007: Numerically optimized quantum error-correcting codes for a bosonic mode MATTI SILVERI (Presenter), KARI MÄKINEN, University of Oulu — Bosonic quantum error-correcting codes, such as cat and binomial codes, provide good performance against photon loss errors and are experimentally realizable e.g. with superconducting circuits. Motivated by this and aiming to broaden the spectrum of bosonic codes, we have numerically searched for bosonic single-mode codes. The codes are constructed from a finite superposition of Fock states. By utilizing numerical methods, the complex coefficients of the Fock states are chosen so that a code protects against L photon loss errors and minimizes the probability for the L+1:th error to occur. We have found codes that are protected up 9 photon loss errors. We present the structure and analyze the performance of these numerically optimized codes.

1:03PM S27.00008: Single-mode bosonic error correcting codes with rotation symmetry* ARNE GRIMSMO (Presenter), Physics, The University of Sydney, JOSHUA COMBES, School of Mathematics and Physics, The University of Queensland, BEN Q BARAGIOLA, Science, RMIT University — Bosonic mode error correcting codes, or mode codes for short, are error correcting codes where a qubit (or qudit) is encoded into one or multiple bosonic modes, i.e., quantum oscillators with an infinite Hilbert space. In this talk I focus on single-mode codes that obey rotation symmetry in phase space, such as the the well known Cat-, Binomial- and GKP codes. I will introduce a universal scheme for this class of codes based only on simple and experimentally well-motivated interactions. The scheme is fault-tolerant in the sense that small errors are guaranteed to remain small under the considered gates. I will also introduce a fault-tolerant error correction scheme based on cross-Kerr interactions and destructive phase measurement (e.g., heterodyne). Remarkably, the error correction scheme approaches the optimal recovery map for Cat and Binomial codes when the ancilla modes are error free. We numerically compute break-even thresholds under loss and dephasing, both with ideal and faulty ancillas.

*This work is supported by the Australian Research Council (ARC) via Centre of Excellence in Engineered Quantum Systems (EQUIS) Project No. CE170100009.
**1:15PM S27.00009: Simplified mixed-state encoding for quantum computation with continuous-variable systems**

KEVIN MARSHALL, DANIEL JAMES (Presenter), Dept. of Physics, University of Toronto, Toronto, Canada, ALEXANDRU PALER, Institute for Integrated Circuits, Johannes Kepler University, Linz, Austria, HOI-KWAN LAU, Institute for Molecular Engineering, University of Chicago — Recent development of mixed-state encoding (MSE) allows a pure-state logical qubit to be encoded by a continuous-variable system in mixed physical state. Despite interest due to its counter-intuitiveness, the utility of current MSE is limited due to several operational drawbacks, namely probabilistic initialisation, redundant information carrier, and requirement of discrete-variable measurement. In this work, we present a simplified MSE that does not suffer from any of these drawbacks. Specifically, our protocol encodes each qubit by only one mixed-state harmonic oscillator, and the logical basis can be deterministically initialised by displacing a thermal equilibrium state. By using measurement-based quantum computation formalism, logical operations can be performed by only continuous-variable interaction and measurement. Without the necessity of ground state cooling, our proposal could broaden the candidate for quantum computation, and reduce the re-initialisation time of measured qubits. Additionally, the noise tolerance of logical quantum information can be enhanced by treating conventional pure-state encoded qubits as MSE qubits.

**1:27PM S27.00010: Fault-tolerant gates on a logical qubit**

SERGE ROSENBLUM (Presenter), PHILIP REINHOLD, WENLONG MA, LIANG JIANG, LUIGI FRUNZIO, ROBERT J SCHOELKOPF, Yale Univ — A fault-tolerant architecture based on error-corrected qubits requires the implementation of logical gates that do not induce uncorrectable errors. Here, we present a fault-tolerant construction for a gate on a cavity-encoded logical qubit. The scheme uses the multilevel structure of a transmon ancilla, along with RF-tunable transmon-cavity interaction, to apply arbitrary phases to the cavity Fock states. This enables a broad range of gates on a variety of encodings, while protecting the logical qubit against photon loss, as well as ancilla decay and dephasing. Together with the previously demonstrated fault-tolerant syndrome measurements [1], this result further expands the toolbox towards fully fault-tolerant processing of logical qubits.


*This research was supported by the Army Research Office (W911NF-18-1-0212), and the Air Force Office of Scientific Research (FA9550-14-1-0052 and FA9550-15-1-0015).

**1:39PM S27.00011: Optimal condition for a cavity QED-based fault-tolerant quantum computation**

RUI ASAOKA (Presenter), RINA KANAMOTO, Physics, Meiji university, YUUKI TOKUNAGA, NTT SC Labs., TAKAO AOKI, Applied physics, Waseda university — Cavity quantum electrodynamics (QED) has been extensively studied for decades as one of the promising candidates for the realization of quantum computing and quantum network. For example, the controlled phase flip gate between photons assisted by cavity-QED systems was proposed in 2004[1] and demonstrated recently[2]. However, fault-tolerant quantum computing is still difficult because of the infidelity and the losses originated from imperfections of the cavity QED system.

In this work, we theoretically investigate optimal conditions for the cavity-QED-based quantum gate. Controllable experimental parameters are optimized not only to suppress photon loss considered in previous study[3] but also to increase fidelity. As a result, the experimental conditions for achieving the fault-tolerant threshold is much relaxed compared to the previous one. We finally derive the error and loss probability in the optimal condition assuming the typical experimental values of the nanofiber cavity-QED system as a promising candidate for the near future development[4].

1:51PM S27.00012: Simulation of Gaussian channels via teleportation with applications to error correction and secret-key capacities.†  SPYROS TSERKIS (Presenter), JOSEPHINE DIAS, School of Mathematics and Physics, University of Queensland, RICCARDO LAURENZANDA, SAMUEL L BRAUNSTEIN, STEFANO PIRANDOLA, Computer Science, University of York, TIMOTHY RALPH, School of Mathematics and Physics, University of Queensland — Gaussian channels are the typical way to model the decoherence in continuous-variable quantum states. It is known that those channels can be simulated by a teleportation protocol using as a resource state either a maximally entangled state passing through the same channel, i.e., the Choi-state, or a state that is entangled at least as much as the Choi-state. Since the construction of the Choi-state requires infinite mean energy and entanglement, i.e. it is unphysical, we derive instead every physical state able to simulate a given channel through teleportation with finite resources. Finally, we use those states to generalize a previously known error correction protocol by making it able to correct noise coming from thermal loss channels, and we also show how finite-energy resource states are able to provide tight upper bounds to the secret-key capacity of Gaussian channels.

arXiv.1803.03516 (Accepted - PRA)
arXiv.1808.00608 (Under Review - PRA)

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EPSRC via the UK Quantum Communications Hub (EP/M013472/1).

2:03PM S27.00013: Recovering noise-free quantum observables  MATTHEW OTTEN (Presenter), STEPHEN K GRAY, Argonne Natl Lab — We introduce a technique for recovering noise-free observables in noisy quantum systems by combining the results of many slightly different experiments. Our approach is applicable to a variety of quantum systems but we illustrate it with applications to quantum computing and quantum sensing. The approach corresponds to repeating the same quantum evolution many times with known variations on the underlying systems' error properties, e.g. the spontaneous emission and dephasing times, T1 and T2. As opposed to standard quantum error correction methods, which have an overhead in the number of qubits, our method has only an overhead in number of evaluations, allowing the overhead to, in principle, be hidden via parallelization. We show that the effective spontaneous emission, T1, and dephasing, T2, times can be increased using this method in both simulation and experiments on an actual quantum computer. We also show how to correct more complicated entangled states and how Ramsey fringes relevant to quantum sensing can be significantly extended in time. This work was performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, and supported by the U.S. Department of Energy, Oce of Science, under Contract No. DE-AC02-06CH11357.

Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S28 DQI: Quantum Measurement and Sensing III  BCEC 161 - Lucas Sletten, University of Colorado, Boulder - Tag(s): Focus

11:15AM S28.00001: Role of nonclassical correlations in quantum parameter estimation assisted by a local measurement scheme in thermal equilibrium†  AKIRA SONE (Presenter), Nuclear Science and Engineering, Massachusetts Institute of Technology, QUNTAO ZHUANG, Physics, University of California, Berkeley, CHANGHAO LI, YI-XIANG LIU, PAOLA CAPPELLARO, Nuclear Science and Engineering, Massachusetts Institute of Technology — We discuss the role of nonclassical correlations in enhancing estimation sensitivity of parameters characterizing the quantum system in thermal equilibrium, in terms of greedy local measurement scheme, where subsystems are measured sequentially with the local optimal measurements. We introduce a practical discord, called discord for local metrology, to measure the nonclassical correlations induced by local optimal measurement, and we explicitly derive its relation to loss in quantum Fisher information in the high-temperature limit. We also demonstrate that discord for local metrology becomes diagonal discord when the estimated parameter is linearly coupled to the Hamiltonian. Practically, this result in the high-temperature limit could provide a measurement or control strategy to utilize nonclassical correlations to achieve a precise sensing or imaging in room-temperature NMR system or living cells.

†This work was supported in part by the U.S. Army Research Office through Grants No. W911NF-11-1-0400 and W911NF-15-1-0548 and by the NSF PHY0551153. AS acknowledges Thomas G. Stockham Jr. Fellowship. QZ acknowledges the U.S. Department of Energy through Grant No. PH-COMPHEP-KA24 and the Claude E. Shannon Research Assistantship.
**11:27 AM S28.00002: Super-sensitive Metrology using Induced Coherence**

WILLIAM PLICK (Presenter), Physics, University of Dayton, NATHANIEL R MILLER, Physics and Astronomy, Louisiana State University — We theoretically analyze the phase sensitivity of the well-known “Induced-Coherence Interferometer”, including the case where the sensitivity is “boosted” into the sub-shot-noise-limit regime with coherent-light seeding. We find scaling which reaches below the standard quantum limit, even when seeding the spatial mode which does not interact with the sample. This allows bright, super-sensitive phase estimation of an object with different light fields for interaction and detection, with various potential applications, especially in cases where the sample may be sensitive to light or is most interesting in frequency domains outside what is easily detected. It is a hybrid of a linear and non-linear interferometers, and aside from the super-sensitivity, is distinguished from other systems by “preferring” an imbalance in the gains of the two nonlinearities, and non-monotonic behavior of the sensitivity as a function of the gain of the coherence-inducing medium. We use an analysis in terms of general squeezing and show that super-sensitivity occurs only in this case - that is, the effect is not present in the spontaneous-parametric-down-conversion regime, which previous analyses and experiments have focused on.

*University of Dayton Dean's Fellowship

**11:39 AM S28.00003: Oxygenated (113) diamond surface for nitrogen-vacancy quantum sensors with preferential alignment and long coherence time from first principles**

SONG LI (Presenter), JYH-PIN CHOU, JIE WEI, Department of Mechanical Engineering, City University of Hong Kong, MINGLEI SUN, School of Mechanical Engineering, Southeast University, ALICE HU, Department of Mechanical Engineering, City University of Hong Kong, ADAM GALI, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics — Shallow nitrogen-vacancy (NV) center in diamond is promising in quantum sensing applications however its sensitivity has been limited by surface terminators and defects. There is an immediate quest to find suitable diamond surfaces for NV sensors. In this work, the surface terminators of (113) diamond to host shallow NV centers are studied by means of first principles calculations. Results indicate that complete oxygen termination of (113) diamond creates positive electron affinity with no surface states in-gap levels. Combining this with the ~73% preferential alignment of as-grown NV centers in (113) oriented diamond, oxygenated (113) diamond is presently supposed to be the most prospective host for NV quantum sensors.

Kaviani, M. Nano Lett. 2014, 14, 4772-4777

*S. L., J.-P. C., and A. H. acknowledge the funding support from City University of Hong Kong under the project 9610336. A. G. acknowledges the support from the National Research Development and Innovation Office of Hungary (NKFIH) within the Quantum Technology National Excellence Program (project no. 2017-1.2.1-NKP-2017-00001) and EU QuantERA Q-Magine (NKFIH Grant no. 127889).

**11:51 AM S28.00004: Quantum-enhanced rotation measurements – a multiparameter problem**

AARON GOLDBERG (Presenter), DANIEL JAMES, Physics, University of Toronto — Precise rotation measurements have numerous classical and quantum applications. Particular quantum states can be used to dramatically increase sensitivities in estimating rotation angles around a known axis. We present a class of states that offer similar enhanced sensitivities in estimating both the orientation of an unknown rotation axis and the angle rotated about it. We derive a quantum Cramér-Rao bound for simultaneously estimating the three Euler angles of a rotation and discuss states that achieve Heisenberg-limited sensitivities for all three. Our states are “anticoherent” states, for whose identification we provide new geometric insights. This result is immediately useful for shot-noise-limited metrology.

Journal reference: Physical Review A 98 (3), 032113

*The authors acknowledge funding from NSERC.
12:03PM S28.00005: Detecting Macroscopic Indefiniteness of Cat States in Bosonic Interferometers* SHANE KELLY (Presenter), EDDY M.E. TIMMERMANS, Los Alamos Natl Lab, SHAN-WEN TSAI, University of California, Riverside — The paradigm of Schrodinger's cat illustrates how specific superposition states preclude the assignment of definite properties to a macroscopic object (realism). In this work we develop a method to investigate the indefiniteness of cat states using currently available cold atom technology. The method we propose, uses observation of a statistical distribution to demonstrate the macroscopic distinction between dead and alive states and the interferometric sensitivity(Fisher Information) to detect the indefiniteness of the vital status of the cat. We show how these two observations can provide information about the quantum state without full quantum state tomography. We test this method using a cat state proposed by Gordon et. al.(PRA 59 4623), which is dynamically produced from a coherent state. As a control, we consider a set of states produced using the same dynamical procedure acting on an initial thermal distribution. Numerically simulating our proposed method, we show that as the temperature of this initial state is increased, the produced state undergoes a quantum to classical crossover where the indefiniteness of the vital status of the is lost, while the macroscopic distinction between dead and alive states of the cat is maintained.

*NSF DMR-1411345,UC Lab Fee LGF-17- 476883

12:15PM S28.00006: Optimal Estimation of Complex Squeezing in Phase Space* JASMINDE SIDHU (Presenter), PIETER KOK, University of Sheffield — All optical fields fluctuate in both phase and amplitude due to stochastic indeterminacy, which imposes a fundamental shot noise uncertainty to measurements. Squeezed states surpass this precision limit in one quadrature at the expense of a concomitant increased uncertainty to the complementary quadrature. These states are heavily used in continuous variable quantum information processing [1], quantum metrology [2], and optical quantum computing. Full characterisation of the squeezed states used is required to envisage the progression of these applications.

We apply quantum estimation theory to optimally characterise the squeezing parameter ξ. Previous works have been limited to estimates of its magnitude r. However, a complete understanding also requires knowledge of its direction θ. We derive the fundamental precision bounds for both parameters for general Gaussian states. We find that saturating these bounds through simultaneous measurements are prohibited, even asymptotically. Despite this, we show how correlated intensity measurements saturate the individual precision bounds for complete characterisation of squeezed light sources.


*DSTL Quantum 2.0 Technologies Programme.

12:27PM S28.00007: Minimal quantum state representations from denoising auto-encoders* SHIVA LOTFALLAHZADEH BARZILI (Presenter), RAZIEH MOHSENINIA, JUSTIN DRESSEL, Chapman University — As multi-qubit systems increase in size, the state space scales exponentially. This makes accurate state tomography increasingly challenging and places a high demand on computational resources. This problem is compounded by the addition of experimental noise in tomographic measurements. We investigate the use of supervised machine learning, in the form of modified denoising auto-encoders, to simultaneously remove experimental noise while finding minimal latent representations of the quantum state. These representations can be later decoded into more traditional state representations.

*Army Research Office (ARO) grant No. W911NF-18-1-0178

12:39PM S28.00008: An implementation of the generalized coherent-state measurements* CHRISTOPHER JACKSON (Presenter), University of New Mexico — Generalized coherent-states are a beautiful theoretical tool for describing quantum systems with Lie group symmetries. The POVM of projectors onto the continuum of generalized coherent-states is also known to be the optimal measurement for estimating unknown states given multiple copies. However, it has been thought that this POVM is in general not practical to realize. We show how one can in principle realize this POVM by a sequence of isotropic weak measurements.

*This work was supported by the National Science Foundation under grant PHY-1630114.
Detecting Dark Matter with Polar Materials using ab initio calculations. 

SINEAD GRIFFIN (Presenter), Lawrence Berkeley National Laboratory, SIMON KNAPE, IAS, Princeton, TONGYAN LIN, Physics, University of California, San Diego, KATHRYN M ZUREK, Physics, University of California Berkeley — Dark matter (DM) comprises ~25% of the mass-energy density of the universe, yet to date has eluded direct detection. Ultra-light DM has emerged as a promising possibility for DM, and is only now becoming experimentally viable for direct searches. In this work we propose the direct detection of DM with polar materials, considering both the scattering of optical and acoustic phonons by light DM, and the absorption of dark photons by optical phonons. Using Density Functional Theory, we calculate the material-specific matrix elements, and show that DM scattering in an anisotropic crystal has a strong directional dependence. We find that phonon-based detectors have comparable or greater sensitivity to sub-MeV dark matter scattering and sub-eV dark matter absorption than other current proposals.

*Supported by the Office of Science of the DoE under contract DE-AC02-05CH11231.

Long-living coherence in 2D and 3D disordered dipolar-coupled spin systems under strong periodic driving

VIATCHESLAV DOBROVITSKI (Presenter), QuTech and Kavli Institute of Nanoscience, TU Delft, the Netherlands, WALTER HAHN, QuTech, TU Delft, the Netherlands — It has been found recently [1] that a 3D dipolar-coupled network of electronic spins under periodic driving shows long-living coherence and signatures of the time-crystal-like order. Similar behavior has also been observed and studied before [2,3], in the 3D networks of the nuclear spins subjected to the spin-echo pulse trains, and has been used for 70,000-fold improvement in NMR spectroscopy [2]. We numerically simulated these effects in 2D and 3D dipolar-coupled spin systems, directly solving the time-dependent Schrodinger equation. We show that the many-body localization is only marginally related to the appearance of the slowly decaying coherence. We identify the simplest Hamiltonian where the long-living coherence are observed in agreement with experiments, and the relevant parameters for 2D spin systems, to enable application of the long-living coherence in advanced sensing and metrology.


*Work supported by DARPA DRINQS program

Results and model for single-gate ratchet charge pumping

NEIL ZIMMERMAN (Presenter), ROY MURRAY, JUSTIN K PERRON, MICHAEL DAVID STEWART, National Institute of Standards and Technology, MASAYA KATAOKA, STEPHEN GIBLIN, JONATHAN FLETCHER, National Physical Laboratory — Single-gate ratchet pumping is based on a Brownian motor mode, and thus can present subtle behavior. We show experimentally that, in the same devices, we can demonstrate multiple two-gate pumping modes but not the single-gate mode. We propose three mechanisms to explain the lack of plateaus in the single-gate ratchet mode: a large plunger-to-barrier ratio compared to the charging energy (Δptb/EC), nonlinear tunnel barriers, and phase offset leading to nonequilibrium heating. Our analysis shows that each of these could contribute to the lack of plateaus in the 1-gate ratchet pumping, but allow 2-gate pumping methods to work with robust plateaus. We propose several methods to reduce these sources of error, including reducing gate oxide thickness and reducing cross capacitances.

Superparamagnetic reversal of single magnetic nanoparticles near phase transition

NING WANG (Presenter), WENG HANG LEONG, GANG-QIN LIU, XI FENG, CHUFENG LIU, SEN YANG, Department of Physics, The Chinese University of Hong Kong, JOERG WRACHTRUP, Institute of Physics, Research Center SCoPE and IQST, University of Stuttgart, QUAN LI, RENBAO LIU, Department of Physics, The Chinese University of Hong Kong — The magnetic properties of single magnetic nanoparticles, especially the superparamagnetic (SPM) reversal near the phase transition point, are relevant to information storage, biomedicine imaging, and paleology. However, it is challenging to study the SPM reversal of single nanoparticles due to the weak magnetic moment and the sharp temperature dependence of the reversal rate. Here, we utilize nitrogen-vacancy centers in diamond as a quantum probe to study the SPM reversal of individual magnetic particles. Such a configuration enables the verification of the Neel-Arrhenius law and the Stoner-Wohlfarth model at the single-particle level. We observe that the reversal rate changes from 10^{-2} Hz to 10^4 Hz in approximate 10 K temperature range. The SPM reversal rate as a function of temperature indicates that the Neel-Arrhenius law is still valid when the temperature is 1/20 Tc close to the Curie temperature of the magnetic nanoparticle.

*This work was supported by Hong Kong RGC.
OLENDSKI (Presenter), Department of Applied Physics and Astronomy, University of Sharjah — Shannon quantum information entropies $S_{p,γ}$, Fisher informations $I_{p,γ}$, and Onicescu energies $O_{p,γ}$ are calculated in the position (subscript $p$) and momentum (subscript $γ$) spaces for the azimuthally symmetric 2D nanoring that is placed into the combination of the transverse uniform magnetic field $B$ and Aharonov-Bohm (AB) flux $Φ$. Position (momentum) Shannon entropy depends on the field as negative (positive) logarithm of $ω_{\text{eff}} = (ω_c^2 + ω_p^2/4)^{1/2}$, with $ω_c$ being cyclotron frequency, what makes the sum $S_p + S_γ$ a field-independent quantity that increases with the principal $n$ and azimuthal $m$ quantum numbers and satisfies entropic uncertainty relation. Position Fisher information does not depend on $m$, linearly increases with $n$ and varies as $ω_{\text{eff}}$ whereas its Onicescu counterpart changes as $1/ω_{\text{eff}}$. The products $I_{p,γ}$ and $O_{p,γ}$ are both $B$-independent quantities. Dependence of the measures on the thickness of the ring is discussed. It is shown that position Shannon entropy has the same dependence on the AB flux $Φ$ as the energy spectrum. Other analytic and numerical results for all measures are discussed too and their physical meaning is highlighted.

* Supported by SEED Project No. 1702143045-P from the Research Funding Department, Vice Chancellor for Research and Graduate Studies, University of Sharjah

1:51PM S28.00014: Electron spin coherence measurements of high-density silicon vacancy ensembles in silicon carbide  
JOHN ABRAHAM (Presenter), JACOB EPSTEIN, JEREMIAH WATHEN, Applied Physics Laboratory — High density ensembles of defects in solids hold the potential to realize highly correlated states or high sensitivity quantum sensors. To explore the feasibility of this development path for silicon vacancies in silicon carbide, we will present electron spin coherence measurements of neutron irradiated samples of silicon carbide. To date, published measurements of the electron spin coherence time of this system have primarily been with electron or proton irradiated samples where the density of defects is not uniform throughout the sample. Since the density of defects is uniform throughout the sample with neutron irradiation, these measurements will shed light regarding the observed anomalies (Phys. Rev. B 95, 045206 (2017)) in the density dependence of the spin coherence time with silicon vacancy ensembles.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S29 DQI: Semiconducting Spin Qubits, Photonic and Phononic Coupling BCEC 162A -
Xiangyu Ma, University of Delaware - Tag(s): Focus

11:15AM S29.00001: Coupling superconducting qubits to traveling surface acoustic wave phonons*  
ETIENNE DUMUR (Presenter), Institute for Molecular Engineering, University of Chicago, KEVIN SATZINGER, Physics, University of California, Santa Barbara, YOUPENG ZHONG, HUNG-SHEN CHANG, Institute for Molecular Engineering, University of Chicago, GREGORY A PEAIRS, Physics, University of California, Santa Barbara, MING-HAN CHOU, AUDREY BIENFAIT, CHRISTOPHER CONNER, JOEL GREBEL, RHYS G POVEY, ANDREW N CLELAND, Institute for Molecular Engineering, University of Chicago — Surface acoustic wave (SAW) devices are heavily used in classical signal processing applications. SAWs have also been proposed as a method to coherently couple disparate solid-state quantum systems, such as superconducting and semiconducting qubits[1-4]. Recently the quantum control of phonons in a SAW resonator has also been demonstrated[5]. In this talk, we report the experimental development of a device coupling two superconducting qubits through SAW phonons. The transduction of the energy quantum is performed by a unidirectional SAW transducer. We examine the influence of the material properties, coupling strategy, acoustic velocity and design on the performance of the state transfer.


11:27AM S29.00002: Quantum State Transfer Using Surface Acoustic Wave Phonons* AUDREY BIENFAIT (Presenter), Institute for Molecular Engineering, University of Chicago, KEVIN SATZINGER, Department of Physics, University of California, Santa Barbara, YOUPENG ZHONG, HUNG-SHEN CHANG, MING-HAN CHOU, CHRISTOPHER CONNER, ETIENNE DUMUR, JOEL GREBEL, Institute for Molecular Engineering, University of Chicago, GREGORY A PEAIRS, Department of Physics, University of California, Santa Barbara, RHYS G POVEY, ANDREW N CLELAND, Institute for Molecular Engineering, University of Chicago — Heavily used in classical signal processing, surface acoustic waves (SAWs) have also been proposed as a means to couple distant solid-state quantum systems. Several groups have reported the coherent coupling of standing SAWs modes to superconducting qubits, opening the door to the control and detection of quantum phonon states. Here, we explore the coherent coupling of superconducting qubits to propagating SAWs. The experimental device comprises a 2-mm-long SAW resonator coupled to two xmon-style qubits. The resonator operates at 4 GHz and sustains 70 standing SAW modes with a free spectral range of 2 MHz. We demonstrate that each qubit reaches the strong multi-mode regime, where the coupling to one standing mode exceeds the resonator free spectral range. We show that in this regime, each qubit can launch a propagating SAW into the resonator and capture it at a later time, showing that the SAW resonator can act as an acoustic communication channel. We perform quantum state transfer as well as remote entanglement generation between the two qubits using this acoustic channel.


11:39AM S29.00003: Giant Atom Bounded in Continuum* SHANGJIE GUO (Presenter), YIDAN WANG, Joint Quantum Institute, University of Maryland, THOMAS PURDY, National Institute of Standards and Technology, JACOB TAYLOR, Joint Quantum Institute, University of Maryland — Tremendous progress in coupling light to matter has enabled strong coupling of qubits to modes of a photonic or phononic resonator. Here we consider what happens in the phononic case when the qubit is coupled to an electromagnetic antenna that enables supersonic propagation of the qubit oscillations. One can consider this as a giant – many wavelength-long – atom from the perspective of the phonons. We find that even in the absence of phononic resonances, as the atom size is increased, new bound states emerge from the continuum. We find a toy model that captures these effects while being exactly solvable. Compared to a sub-wavelength size atom, the bound states of this non-Markovian giant atom has localized wavefunctions, reduced dissipation, and amplified vacuum Rabi frequencies. This result also agrees with our generalized Levinson's theorem, as the number of bound states always equals the winding number of transmission phase. Application of this approach to surface acoustic wave devices will be considered.

*This research was partially supported by the NSF-funded Physics Frontier Center at the Joint Quantum Institute

11:51AM S29.00004: Solid-state quantum interfaces of spins and photons* METE ATATURE (Presenter), University of Cambridge — Optically active spins in solids offer exciting opportunities as scalable and feasible quantum-optical devices. Numerous material platforms, such as diamond, silicon carbide and semiconductors, are under investigation, where each platform brings advantages along with challenges. For example, diamond nitrogen-vacancy centre is a fantastic host for spins, yet suffers from its optical properties. In contrast, the brightness and the coherence of photons from semiconductor quantum dots remain practically unchallenged today, while the electronic spin coherence is modest owing to the magnetic noise generated by the nuclear spins of the quantum dot. In this talk, I will present an overview of the current progress to overcome such challenges for solid-state spin-photon interfaces in two example platforms: First, I will highlight the diamond group-IV vacancy centres and their promise to combine desirable optical and spin properties. Then, I will finish with the semiconductor quantum dots and their potential to transform their nuclei from nuisance to resource.

*This work was supported by the European Research Council ERC Consolidator Grant PHOENICS No. 617985.
12:27PM S29.00005: Tunable coupling of a double quantum dot spin system to a mechanical resonator*  
SAMUEL CARTER (Presenter), ALLAN S BRACKER, MICHAEL K YAKES, MAXIM ZALALUTDINOV, U.S. Naval Research Laboratory, MJIN KIM, KeyW Corporation, CHUL SOO KIM, U.S. Naval Research Laboratory, BUMSU LEE, NRC Research Associate at the U.S. Naval Research Laboratory, DANIEL G GAMMON, U.S. Naval Research Laboratory — Hybrid systems in which a mechanical resonator is coupled to a microscopic quantum system are of strong practical and fundamental interest. Achieving a large interaction strength is vital for many goals in this field, and the ability to tune this coupling is also valuable. This has been challenging in solid state spin systems, where often the coupling is weak and fixed. Here we use pairs of coupled InAs quantum dots embedded within GaAs cantilevers to achieve high spin-mechanical coupling through strain. One electron is injected into each dot, with the tunnel coupling inducing a splitting between the singlet and triplet spin states. While optically driving motion of the cantilever, we measure the time-dependent shifts of the singlet and triplet transitions and find that the spin splitting can be highly sensitive to the motion-induced strain. This sensitivity depends strongly on the electrical bias of the system and can even be tuned to zero. The results can be explained by the difference in strain experienced by the two QDs, due to their different positions in the cantilever, which results in a change in the exchange interaction.

*This work was supported by the U.S. Office of Naval Research, the Defense Threat Reduction Agency, and the OSD Quantum Sciences and Engineering Program.

12:39PM S29.00006: Coupling a mechanical oscillator to a parametric amplifier*  
DAVID ZOEPFL (Presenter), MATHIEU L. JUAN, CHRISTIAN SCHNEIDER, GERHARD KIRCHMAIR, University of Innsbruck — In our experiment, we inductively couple a mechanical oscillator to a microwave circuit. We place a magnet on the tip of the mechanical resonator, a cantilever, which leads to a position dependent magnetic field. This field is coupled via a SQUID embedded into a microwave resonator: its resonance frequency depends on flux and consequently on the position of the cantilever. In addition to being a flux sensitive element, the SQUID also constitutes a non-linear element. This non-linear system is modelled with the Duffing model, describing our measurement data with good accuracy. The non-linearity also enables us to use the resonator as a parametric amplifier, and boost the system's sensitivity.

By sideband cooling the cantilever – a macroscopic object – we aim to reach the quantum mechanical ground state. In the future we plan to replace the microwave resonator with a qubit, we can exploit strong single-photon single-phonon coupling for example by preparing the cantilever in a non-Gaussian state. In addition, our system can be used as a highly sensitive acceleration sensor.

*Funded by European Union's Horizon 2020 – FET (No. 736943) and Austrian Science Fund FWF – DK-ALM (W1259-N27)

12:51PM S29.00007: Hardware-efficient quantum random access memory using hybrid quantum acoustic systems*  
CONNOR HANN (Presenter), Departments of Applied Physics and Physics, Yale Univ, CHANG-LING ZOU, Key Laboratory of Quantum Information, USTC, YAXING ZHANG, YIWEN CHU, ROBERT SCHOELKOPF, STEVEN GIRVIN, LIANG JIANG, Departments of Applied Physics and Physics, Yale Univ — Hybrid quantum systems where acoustic resonators couple to superconducting qubits are promising quantum information platforms. High quality factors and small mode volumes make acoustic modes ideal quantum memories, while the qubit coupling enables the initialization and manipulation of quantum states. In this talk we consider the practical applications of multi-mode quantum acoustic systems as hardware-efficient quantum processors. Quantum gates between different acoustic modes can be implemented using resonant interactions between the phonons and qubit, but such gates are vulnerable to qubit decoherence. As an alternative, we propose the use of off-resonant interactions that only virtually excite the qubit. This virtual approach overcomes limitations placed by qubit decoherence and attains considerably higher fidelities for long-lived acoustic modes. Given advances in performance, we propose a quantum acoustic implementation of a quantum random access memory (qRAM). We show how information can be routed through the system such that data stored in memory modes can be accessed in superposition according to the state of designated address modes—implementing a qRAM on a single chip.

*Work supported by: ARO, ARL, AFOSR, NSF, Sloan Foundation, and Packard Foundation
1:03PM S29.00008: Toward the preparation of sub-Poissonian states in a low frequency mechanical oscillator

XIZHENG MA (Presenter), JEREMIE VIENNONT, JILA, Univ of Colorado - Boulder, SHLOMI KOTLER, NIST - Boulder, KONRAD LEHNERT, JILA, Univ of Colorado - Boulder — Preparation of non-classical states of motion in a macroscopic object has been an ambition in the field of opto- and elecro-mechanics. We propose a protocol for the preparation of one type of non-classical state, the sub-Poissonian state. We dispersively couple a Cooper-pair box qubit to a 25 MHz aluminum drumhead mechanical oscillator, and enter the phonon number sensitive regime [1]. In this regime, the motion-induced AC Stark shift on the qubit allows us to address phonon populations with a number resolution of 7, and to extract the phonon distribution via the qubit lineshape. Using sideband transitions between the qubit and mechanics, we demonstrate progress towards preparing the mechanical oscillator in a sub-Poissonian state, where the variance in the phonon distribution is less than the mean phonon number.


1:15PM S29.00009: Resolving Phonon Number States with an Acoustic Ramsey Interferometer+

LUCAS SLETTEN (Presenter), BRADLEY MOORES, K. W. LEHNERT, JILA, University of Colorado at Boulder — The rise of quantum control over surface acoustic waves (SAWs) introduced a novel concept: a “giant atom” many wavelengths long. The large size of the atom, formed by a transmon qubit with a piezoelectric transducer, generates fine frequency features in the qubit-phonon interaction strength that are determined by the shape of the transducer. Here, we combine a multi-mode SAW cavity with a qubit whose transducer is spatially engineered to enter the strong dispersive regime. The transducer comprises two halves separated by 38 wavelengths that, in close analogy to Ramsey interferometry, generate narrow frequency fringes in the qubit-phonon coupling. We observe these fringes both as a sharp frequency dependence in the qubit emission of unconfined phonons and as a modulated coupling strength to acoustic cavity modes. This modulation creates frequency regions of strong coupling in close proximity to windows of vanishing coupling, a combination that enables both dispersive operation and a coupling strength that is comparable to the free spectral range. The strong coupling creates a large dispersive shift that exceeds both qubit and acoustic linewidths.

*This material is based upon work supported by the National Science Foundation under Grant No. PHY 1734006.

1:27PM S29.00010: Nonexponential decay of a giant artificial atom

GUSTAV ANDERSSON (Presenter), Microtechnology and Nanoscience MC2, Chalmers University of Technology, BALADITYA SURI, Indian Institute of Science, LINGZHEN GUO, Max Planck Institute for the Physics of Light, THOMAS AREF, PER DELSING, Microtechnology and Nanoscience MC2, Chalmers University of Technology — The interaction between light and atoms has been conventionally studied using small atoms interacting with electromagnetic radiation of wavelengths that are several orders of magnitude larger than the atomic dimensions. In contrast, quantum acoustic experiments allow reaching the giant atom regime, where the coupled field wavelength is orders of magnitude smaller than the atomic dimensions. This is achieved by coupling a superconducting qubit to surface acoustic waves on a piezoelectric substrate at two points with separation on the order of 100 wavelengths. This approach is comparable to controlling the radiation of the atom by attaching an antenna. The slow velocity of sound leads to a significant internal time-delay for the field to propagate across the giant atom, and thus strongly non-Markovian dynamics. We demonstrate signatures of this non-Markovianity in the frequency spectrum as well as time domain relaxation of the giant atom.

1:39PM S29.00011: Strong coupling of a transmon qubit and a phononic crystal cavity array+

PATRICIO ARRANGOIZ-ARRIOLA (Presenter), ALEX EDWARD WOLLACK, MAREK PECHAL, ZHAOYOU WANG, WENTAO JIANG, TIMOTHY MCKENNA, AMIR SAFAVI-NAEINI, Applied Physics, Stanford University — Coupling superconducting circuits to nanomechanical systems opens up new opportunities in quantum acoustics (e.g. QND phonon detection) and the exploration of technologically-relevant devices such as quantum memory elements. In particular, phononic crystal cavities (PCCs), which localize sound at the wavelength scale, show great promise as ultra-compact, long-lived mechanical elements which can be strongly coupled to a superconducting circuit despite being orders of magnitude smaller. Building upon our previous work, we now demonstrate coupling of a transmon qubit to an array of PCCs with mode frequencies in the 2.0-2.4 GHz range. We fabricate the qubit and associated control and readout circuitry on a silicon substrate and the PCCs on a suspended thin film of lithium niobate, effectively forming an array of one-dimensional “phononic wires” with localized resonances at a set of precisely engineered frequencies. The phononic defects sites are coupled to the qubit via superconducting electrodes patterned directly on top of the cavity mirrors. We measure qubit-phonon coupling rates in excess of 10 MHz, putting the system well in the strong coupling regime.

*Work supported by a Packard Fellowship, ONR MURI QOMAND, and Stanford University.
2:03PM S29.00013: Demonstration of the Generalized Kennedy Receiver as a Near Quantum-Optimal Measurement for the Discrimination of Weak Classical Optical States* JONATHAN HABIF (Presenter), ARUNKUMAR JAGANNATHAN, University of Southern California — We describe an experimental testbed demonstrating quantum measurements on a single spatio-temporal, polarization mode, photon-starved classical state of light. The measurements are designed to optimally discriminate between coherent and incoherent optical states at mean photon numbers $n < 2$. A narrow-linewidth, 780 nm laser is used to prepare a coherent state or a thermal state in a single spatio-temporal, polarization mode. Three measurement strategies are implemented for the discrimination problem: photon counting, shot-noise limited coherent detection, and the near-optimal, generalized Kennedy receiver. For each receiver type we present discrimination error probability measurements as a function of the mean photon number of the received optical state.

*AR was funded by EU Marie Sklodowska-Curie Grant No 642688 (SAWtrain). AN was supported by UK Department for Business, Innovation and Skills.

Thursday, March 7, 2019 11:15 AM - 1:15 PM

Session S30 GSNP DBIO: Scaling and Phase Transitions in the Life Sciences - From Proteins to Tropical Forests BCEC 162B - Marek Cieplak, Polish Academy of Sciences - Tag(s): Focus

11:15AM S30.00001: Measuring the multiscale and multi-mass heterogeneity of complex spatial patterns in synthetic and real datasets NEKTARIOS VALOUS (Presenter), Applied Tumor Immunity Clinical Cooperation Unit, National Center for Tumor Diseases, German Cancer Research Center, Im Neuenheimer Feld 460, 69120 Heidelberg, Germany, WEI XIONG, Statistical Physics and Theoretical Biophysics Group, Institute for Theoretical Physics, Heidelberg University, Philosophenweg 16, 69120 Heidelberg, Germany, NIELS HALAMA, INKA ZÖRNING, Department of Medical Oncology, National Center for Tumor Diseases, Heidelberg University Hospital, Im Neuenheimer Feld 460, 69120 Heidelberg, Germany, DENNIS CANTRE, ZI WANG, BART NICOLAI, PIETER VERBOVEN, Division of Mechatronics Biostatistics and Sensors, Department of Biosystems, KU Leuven - University of Leuven, Willem de Croylaan 42, 3001 Heverlee, Belgium, RODRIGO ROJAS MORALEDA, Applied Tumor Immunity Clinical Cooperation Unit, National Center for Tumor Diseases, German Cancer Research Center, Im Neuenheimer Feld 460, 69120 Heidelberg, Germany — Spatial patterns may exhibit scale-dependent changes in structure and are often difficult to characterize. Lacunarity measures how data fill space enabling the parsimonious analyses of patterns. The lacunarity index (monolacunarity) averages the behavior of variable size structures in a binary image. The generalized lacunarity concept (multilacunarity) on the basis of generalized distribution moments is an appealing model that can account for differences in the mass content at different scales. The method was proposed in *Physica A* 388, 4305 (2009). Here, the aim is to provide validation on synthetic images (lacking in the original paper) and to quantify the mesostructural changes in the intercellular air spaces of pome and stone fruit parenchymatous tissue after storage and ripening, respectively. These generalized moments can yield an enhanced measure of the spatial organization of intercellular air spaces which is complementary to the monolacunarity model. Essentially, the multilacunarity morphometric is a multiscale multi-mass measure of spatial heterogeneity that offers insights regarding modifications upon the arrangement of cells and voids. This can further stimulate research interest in analyzing tissue (plant, human) under various metabolic and physiological changes.
11:27AM S30.00002: Percolation in protein cores: a novel approach to protein decoy detection  JOHN TREADO (Presenter), ZHE MEI, ZACHARY LEVINE, LYNNE REGAN, COREY SHANE O’HERN, Yale Univ — Protein cores are regions of densely packed, solvent-excluded residues, and void space inside of cores can often destabilize the structure. Here, we measure the void space in protein cores and find that the void structure is equivalent to that in jammed packings of repulsive residue-shaped particles. A continuum void percolation transition can be defined as when the characteristic void length scale approaches the system size. Using finite-size scaling, we show that the percolation of void space in protein cores belongs to the same universality class as voids in static packings of residue-shaped particles. This result provides a novel approach for evaluating whether computationally designed protein structures will take a desired fold in experiments. Molecular dynamics simulations often generate “decoy” protein structures that have low potential energy, but are not observed experimentally. We argue that decoy protein structures will have a fundamentally different void distribution, i.e. belong to a different universality class than the void distribution in real protein structures. Therefore, by analyzing the universal aspects of connected voids in computationally generated protein structures, we will be able to differentiate experimentally observed structures from protein decoys.

11:39AM S30.00003: Scaling and phase transitions – from proteins to ecology [invited]  JAYANTH BANAVAR (Presenter), University of Oregon — The nature of a phase of matter transcends the microscopic material properties. For example, materials in the liquid phase have certain common properties independent of the chemistry of the constituents: liquids take the shape of the container; they flow; and they can be poured — alcohol, oil and water as well as a Lennard-Jones computer model exhibit similar behaviour when poised in the liquid phase. I will introduce a simple model of a chain molecule with no spurious symmetries and present the results of computer simulations of its ground state phase diagram. Our calculations on relatively short chains (recall proteins are also much shorter than conventional polymers) reveals a hitherto unstudied “phase” that may have a relationship to proteins, the workhorse molecules of living cells. Our findings may be relevant for understanding proteins as well as for the creation of novel bio-inspired nano-machines.

Scaling ideas are most useful, when one is unable to deal with the full complexity of a problem or more importantly, when many of the details are not essential for the type of information that one is seeking. An important example of scaling arises in the field of ecology, when one wishes to understand the threats of losing bio-diversity. I will describe some recent results on the metabolic scaling of individual trees and a forest comprised of many trees. Our scaling framework unifies seemingly distinct trends in a forest and provides a simple yet promising approach to begin to quantitatively understand a bewilderingly complex many-body system with imperfectly known interactions.

Collaborators: Amos Maritan, Tomasso Anfodillo, Marek Cieplak, Achille Giacometti, Trinh Hoang, Andrea Rinaldo, Tatjana Skrbic, Igor Volkov

12:15PM S30.00004: RG-inspired analyses of activity in networks of real neurons*  LEENOY MESHULAM (Presenter), Massachusetts Institute of Technology, JEFFREY L GAUTHIER, CARLOS D BRODY, DAVID W TANK, WILLIAM BIALEK, Princeton University — The renormalization group (RG) allows us to understand how theories of macroscopic dynamics can be simpler and more universal than the underlying microscopic mechanisms. Inspired by these ideas, we develop an approach to coarse-graining complex biological systems in which highly correlated groups of variables play the role of spatial neighborhoods or block spins. We apply this to experiments on the activity of 1000+ neurons in mouse hippocampus, recorded as the animal navigates a virtual environment. We find power-law dependences of several static and dynamic quantities on the coarse-graining scale, over two decades, with exponents that are strikingly reproducible across experiments. In addition, the probability distribution of coarse-grained variables seems to converge on a non-trivial fixed form. We explore how different coarse-graining schemes affect the scaling behaviors, and construct minimal models for the coarse-grained variables. Finally, we investigate how the coding properties of the neurons change as we move along the RG flow.

*Supported in part by the NSF Center for the Physics of Biological Function (PHY-1734030), Center for the Science of Information (CCF-0939370), and grant PHY-1607612; by HHMI; and by the Simons Collaboration on the Global Brain.
**12:27PM S30.00005: Hierarchy Near a Critical Point: From the Ising Model to Gene Networks**

SHUBHAM TRIPATHI (Presenter), MICHAEL DEEM, Rice University — The renormalization group approach involves locally averaging over microscopic variables to obtain coarse-grained variables that describe the macroscopic behavior of the system. We propose that hierarchical clustering corresponds to the same approach. We used the cophenetic correlation coefficient (CCC) to quantify how well the relationships between the components in a system are approximated by a hierarchical construct that captures the macroscopic behavior. Since the behavior of a system near a critical point is dominated by macroscopic variables, we expected the CCC to be higher near such a point. This was verified for the 2D Ising model. We then applied this approach to gene networks with distinct behaviors in different regions of the parameter space, separated by critical surfaces. The CCC was higher near the critical surface for the two gene networks investigated. Further, a higher CCC correlated with higher susceptibility of the networks to perturbations, mirroring the higher susceptibility of physical systems near a critical point. We suggest that the CCC can be a useful quantitative signature of criticality in biological systems.

*This work was supported by the National Science Foundation (PHY-1427654).

**12:39PM S30.00006: Collective sensing by cell populations with feedback-induced long-range correlations**

MICHAEL VENNETTILLI (Presenter), Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA, AMIR EREZ, Department of Molecular Biology, Princeton University, Princeton, NJ 08544, USA, ANDREW MUGLER, Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA — Cells sense their environment with remarkable precision, and recent experiments have shown that this precision can be enhanced by cell-cell communication. However, most theoretical investigations of this effect have assumed linear sensing and communication, whereas it is well known that cells use nonlinear feedback to internally amplify sensed signals. Here, using a minimal stochastic model we investigate the interplay of feedback and communication in determining sensory precision. We find that feedback can induce a critical transition and long-range correlations among cells. We investigate the associated sensing tradeoff: on the one hand, we expect long-range order to enhance communication; on the other hand, fluctuations become large at the critical point, so order may come at the cost of precision. We find that depending on the parameters the system can exist in one of two universal regimes, one which permits an ordered phase and one which does not.

*This work was supported by the Simons Foundation.

**12:51PM S30.00007: Chemotaxis: A New Mechanism for Molecular Transport**

FARZAD MOHAJERANI (Presenter), Chemical Engineering, Pennsylvania State University, AYUSMAN SEN, Chemistry, Pennsylvania State University, DARRELL VELEGOL, Chemical Engineering, Pennsylvania State University — In aqueous environments, molecules bounce around through random Brownian walk. However, the environment is often not uniform and there might be a gradient of an interacting solute. In that case, the probe molecules can show directional motion known as chemotaxis. In contrast to diffusion, the chemotactic motion is directional and can be toward or away from high solute concentration which constitutes positive or negative chemotaxis. We have found that enzyme undergoes directional movement towards high concentration of substrate under different conditions, even when the enzyme is not catalyzing the corresponding reaction [1]. In addition to enzymes, we have shown that chemotaxis can happen in a simpler system comprised of dye and interacting polymer molecules [2]. Despite the very different chemistries of the two chemotaxing species (enzyme and dye), the driving force for molecular chemotaxis appears to be similar: the lowering of chemical potential due to a thermodynamically favorable interaction or binding. Based on this thermodynamic insight, we have proposed a general expression to model the observed molecular chemotaxis.


*NSF CBET-1603716 and Penn State MRSEC (NSF DMR-1420620)*
1:03PM S30.00008: Ising model with memory: results and applications to synchronization in population ecology*
VAHINI REDDY NAREDDY (Presenter), Physics, University of Massachusetts Amherst, JONATHAN MACHTA, Physics, University of Massachusetts Amherst, Santa Fe Institute, KAREN ABBOTT, Biology, Case Western Reserve University, ALAN HASTINGS, Environmental Science and Policy, University of California at Davis, Santa Fe Institute — Synchronized oscillations in spatially extended populations can be modeled by coupled noisy, quadratic maps in the two-cycle regime. These dynamical systems exhibit a phase transition from incoherence to synchrony that is in the equilibrium Ising universality class. However individuals in real populations have phase memory that is not contained in the standard Ising model. In this work we analyze a dynamical Ising model with an additional memory term and investigate the phase transition using analytical and numerical approaches. The effective equilibrium model of this dynamical system undergoes a phase transition in the equilibrium Ising universality class with a critical temperature that increases with the strength of the memory. We present results for this system and discuss connections to coupled map systems and also to agricultural data describing oscillations in pistachio production (masting) where tree level data from an orchard in California reveals Ising critical behavior.

*This work is supported in part by NSF grant 1840221

Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S31 DCP: Wavefunction Methods (ES3) BCEC 203 - James Shepherd - Tag(s): Focus


11:51AM S31.00002: Localized active-space self-consistent field method: a size-extensive, linear-scaling MC-SCF approach for strongly-correlated materials* MATTHEW HERMES (Presenter), LAURA GAGLIARDI, Chemistry, University of Minnesota — The complete active space (CAS) SCF method and its perturbative corrections are the standard computational strategy in the field of quantum chemistry for computing accurate wave functions of strongly-correlated molecular systems. They are, however, not applicable to materials in a condensed phase because they are not size extensive and/or have exponential cost scaling, and common cost-controlling approximations such as restricted or generalized active space (RAS, GAS) do not resolve this difficulty. However, our recently-developed localized active space (LAS) SCF method, which is based on a union of density matrix embedding theory (DMET) and MC-SCF concepts, generates a wave function which, unlike RAS or GAS, is multiplicatively separable between disjoint, real-space-localized active subspaces. LASSCF is therefore both size consistent and size extensive, and in principle, its computational cost is linear scaling with respect to system size. We test this method on various realistic chemical models of strongly-correlated systems and show that LASSCF gives CASSCF-quality results, implying an attractive possibility for computing wave functions of strongly-correlated condensed systems.

*This work was supported by the U.S. DOE, BES, CSGB under Award No. DEFG02-12ER16362.

12:03PM S31.00003: Transitioning High-Accuracy Electronic Structure Methods from Molecules to the Solid State* MALTE LANGE (Presenter), TIMOTHY BERKELBACH, University of Chicago — This presentation discusses ongoing work to transfer trusted computational and theoretical tools that are traditionally used in the molecular regime to the rapidly growing field of solid state physics. Specifically, Equation of Motion Coupled Cluster (EOM-CC) is compared to the current state-of-the-art method, the so-called GW approximation for the GW100 test set. Ongoing challenges to the implementation of periodic EOM-CC including finite size effects, basis set effects, and pseudopotentials to reduce computational complexity will be addressed. Preliminary results indicate that this problem is not trivial and requires consideration of many inputs and extrapolation schemes in order to achieve reliable results. In addition to these computational schemes, a systematic hierarchy of approximations is introduced to quantitatively gauge computational cost and accuracy trade-offs, exploring theoretical errors in addition to computational errors.

*This work was supported by:
Midwest Integrated Center for Computational Materials (MICCoM)
NSF Graduate Research Fellowships Program (GRFP)
Development of electronic structure theory methods for periodic systems has been hampered for decades due to the unaffordable scaling with system size. One of the obstacles is the computation of two-electron repulsion integrals, whose near-field interaction can only be computed exactly or approximated using density fitting (DF). In this work, a massively-parallel implementation of an efficient local DF algorithm is presented in which atomic orbital (AO) products are fitted using only auxiliary AOs on one of the nuclei in that product. We applied this approach on the exact exchange term in Hartree-Fock with periodic boundary conditions (periodic HF) based on linear combinations of Gaussian-type AOs. Our algorithm has shown a significant reduction of computational costs with an accuracy below millihartree per atom, and thus will be beneficial to both hybrid density functional theory and post-HF methods.

References:

*This research was supported by the U.S. National Science Foundation, Award No. 1550456 and 1362655.

When a system has semi-periodic boundary condition, caution is needed to remove the interaction between the overall potential and the charge density in the neighboring boxes. For neutral systems, owing to the locality of one-body potential, a common trick in DFT calculations is to use a finite space of vacuum to mimic the free boundary. When moving to the periodic post-HF methods, the effectiveness of this treatment was yet verified. It was known that the finite-size correction to HF needs to be carefully handled in the periodic coupled cluster methods [1]. When the same treatment was applied to low-dimension systems, numerical uncertainty or slow convergence were observed. We compared the effects of vacuum treatments in periodic-MP2, periodic-CCSD calculations. We observed that the finite-size correction at HF level has different effects on different post-HF methods. In this talk, we will analyze the reasons that cause the numerical issues in semi-periodic post-HF methods. For different periodic post-HF methods, different solutions will be presented.


Doped nanocrystals exhibit infrared absorption and are promising candidates for sensors, solar energy conversion, and optical communications. The infrared absorption appears to undergo a transition from a single-particle to plasmonic absorption as a function of doping density and radius. This transition is not well understood from an experimental or theoretical point of view. This talk will present results from correlated quantum chemistry calculations of a particle-in-a-sphere model for a doped nanocrystal. The transition of the infrared absorption from single-particle to plasmonic is found to also depend on the absolute number of doped electrons. In particular, a single-particle transition can be broken into true single-particle, and Coulombically bound, but collective, excitations. These results highlight the importance of many-body exchange and correlation effects in quantum confined nanostructures.

*This work was supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0058.

Quasiparticle spectra of polyacetylene using coupled-cluster singles and doubles (CCSD)*

Those to periodic systems, however, suffer from large computational cost for k point sampling. We developed interpolation techniques for reducing the cost for obtaining reliable GFs. We apply them to polyacetylene and examine their validity by comparing the original spectral function and the interpolated ones.


*This research was supported by MEXT as “Exploratory Challenge on Post-K computer” (Frontiers of Basic Science: Challenging the Limits).
1:27PM S31.00008: Coupled cluster theory for condensed phase spectroscopy*  ALAN LEWIS (Presenter), TIMOTHY BERKELBACH, James Franck Institute, University of Chicago — We use state-of-the-art equation-of-motion coupled-cluster theory with single and double excitations (EOM-CCSD) to calculate the dynamic structure factor of the uniform electron gas. Our calculations are performed at densities corresponding to the valence electron densities of common metals. We compare our results to those obtained using the random-phase approximation, which is known to provide a reasonable description of the collective plasmon excitation. We find that EOM-CCSD, instead of providing a perturbative improvement on the RPA plasmon, predicts a many-state plasmon resonance, where each contributing state has a double-excitation character of 80 percent or more. This finding amounts to an ab initio treatment of the plasmon linewidth and highlights the strongly correlated nature of lifetime effects in condensed-phase electronic structure theory.

*This work was supported by the Air Force Office of Scientific Research under award number FA9550-18-1-005.

1:39PM S31.00009: Effect of basis set on the outcome of external energy mediated chemical reactions*  SHARMA SRKC YAMIJALA (Presenter), ZULFI ALI, BRYAN M WONG, CEE, University of California, Riverside — Directing the energies of an hot-electron or atom or molecule towards a specific vibrational mode to tune the reaction outcomes is an active area of catalytic research and ab initio molecular dynamics is one of the indispensable tools in understanding the mechanistic details of these reactions. In this work, we show that the predicted thermodynamic and catalytic properties of a reaction using an AIMD simulation highly depends on the quality of the employed basis set. To this end, we have considered the reactants and products of the water-gas shift reaction (viz., CO, CO2, H2, and H2O) and studied their interaction with the ZnO(10-10) surface using DFT and Born Oppenheimer Molecular Dynamics (BOMD) simulations. By merely changing the quality of the basis set from double zeta (commonly used in most calculations of these systems) to triple zeta, we show that the reaction outcome of an H2O molecule colliding with a ZnO surface pre-covered with carbon monoxide gives qualitatively different results. Furthermore, we show that the calculated adsorption energies can vary by as much as 380 meV (which is an order of magnitude larger than room temperature) by merely changing the basis.

*The authors acknowledge the support of the U.S. Army Research Office under grant number W911NF-17-1-0340

1:51PM S31.00010: Electronic Structure of NiO from Gaussian-based Periodic Coupled Cluster Theory  YANG GAO (Presenter), MARIO MOTTA, JAMES MCCLAIN, QIMING SUN, GARNET CHAN, AUSTIN MINNICH, Caltech — Accurate description of ground and excited state properties of strongly correlated materials is a grand challenge in ab initio condensed matter simulation. While typical mean field methods performs poorly for these solids, increase in computational power now allows us to employs time-independent perturbation theory in quantum chemistry to systematically improve towards the exact solution for crystalline materials. Here, we present a numerical study of NiO using a Gaussian-based periodic coupled cluster method with single and double excitations. We compute ground-state properties of the antiferromagnetic phase as well as the quasiparticle band structure using the equation of motion ansatz (EOM-CCSD). We compare our results to other ab-initio methods and experimental data.
11:27AM S33.00002: Role of surface reconstruction and passivation mechanisms on the structural and electronic properties of diamond surfaces  BISHWAJIT DEBNATH, Electrical and Computer Engineering, University of California Riverside, MAHESH NEUPANE (Presenter), A. GLEN BIRDWELL, JAMES WEIL, PANKAJ SHAH, TONY IVANOV, US Army Rsch Lab - Adelphi — Diamond is an insulating material in the bulk form which can exhibit two-dimensional p-type conducting characteristics when its surface is passivated with hydrogen. It is postulated that the formation of a conducting channel at the hydrogenated surface is mainly due to charge transfer between the surface and atmospheric adsorbates. A fundamental understanding of the source of p-type conductivity at the hydrogenated surface is key to the realization of diamond surface field effect transistor (FET). Though there have been many experimental studies in this direction, theoretical studies correlating surface termination and reconstruction to structural and electronic properties have been limited. To address these fundamental questions, we have utilized ab initio density functional theory (DFT) and performed systematic studies of surface reconstruction phenomena in (100) and (110) diamond surfaces. Based on the observed structural and electronic properties, we have made an attempt to establish a correlation between the surface reconstruction and passivation with the electronic properties of the diamond surfaces, such as surface energy, electron affinity, and effective mass.

11:39AM S33.00003: Examining the effects of changing film composition and temperature on the optical properties of GaAsBi epitaxial films*  SAMUEL LENNEY (Presenter), MARGARET STEVENS, KEVIN GROSSKLAUS, THOMAS VANDERVELDE, Tufts University — GaAs_{1-x}Bi_x semiconductor alloys are being considered for a range of new infrared optoelectronic applications. This is because small changes in Bi content can produce large decreases in film bandgap, opening up new lattice parameter and bandgap combinations for devices. However, the optical properties of GaAsBi as a function of changing Bi content have not been thoroughly documented and seldom tested at temperatures relevant for infrared detectors or thermophotovoltaics. In this work we study the optical properties of GaAsBi films of varying Bi composition grown by solid source molecular beam epitaxy (MBE). Optical properties are measured by variable angle spectroscopic ellipsometry over a wavelength range from 300 nm to 32 μm and at temperatures ranging from 77K to 600K. The optical properties of the system are modeled so that the GaAsBi optical constants can be separated from those of the underlying substrate. Characterization of GaAsBi optical properties over a range of Bi compositions and temperatures will provide the necessary data for design of future devices and a better fundamental understanding of the material system.

*This work was supported by United States Office of Naval Research

11:51AM S33.00004: A Computational study of Magnetic Field-controlled Acoustic Coherent Phonon Generation and Propagation in Ferromagnetic GaMnAs*  SUNIL THAPA (Presenter), GARY DONALD SANDERS, University of Florida, BRENDEN A MAGILL, GITI KHODAPARAST, Physics, Virginia Tech, STEPHEN A MCGILL, JADE HOLLEMAN, NHMFL, Florida State University, HIRO MUNEKATA, Institute of Innovative Research, Tokyo Institute of Technology, CHRISTOPHER J STANTON, University of Florida — We present a theoretical study of magnetic field-controlled generation and propagation of coherent longitudinal acoustic phonons (CLAP) generated by ultrafast laser pulses in a Ferromagnetic Ga_{1-x}Mn_xAs (x=0.082) thin film grown on an intrinsic GaAs substrate subjected to an in-plane static magnetic field varying between 2-10T. Electron-phonon deformation potential coupling is considered for the generation of the CLAP at the surface as well as at the interface for a pump energy of 3.1 eV with their propagation being governed by a semi-classical wave equation. The field-induced variation in the bandstructure, dielectric functions, and, hence, the CLAP amplitude are calculated using an 8-band Pidgeon-Brown model including the effects of magnetic, Mn impurities. The calculated differential reflectivity at the probe energy 1.55 eV agrees well with experimental time-resolved differential reflectivity measurements and suggests that a substantial contribution to the signal comes from the interface. The magnetic field dependence of the reflectivity amplitude arises from the Seraphin coefficients.

temperatures between 10 K and 740 K. The interband CPs $E_0$ and $E_0 + \Delta_0$, where $E_0$ is the direct band gap of Ge and $\Delta_0$ is

The dielectric function of Ge has been measured between 0.5 eV and 1.3 eV using spectroscopic ellipsometry at various

Development of electronic and optoelectronic devices.

Knowledge of the behavior of critical points (CPs) of Ge and other semiconductors is valuable for the further

Polytechnicheskaya, St. Petersburg 194021, Russia, NARESH M SHAKYA, Department of Applied Physics, New York University, NYU -

University - Germanium is an indirect bandgap semiconductor having its onset of absorption at 0.8 eV at room

temperature. Knowledge of the behavior of critical points (CPs) of Ge and other semiconductors is valuable for the further
development of electronic and optoelectronic devices.

The dielectric function of Ge has been measured between 0.5 eV and 1.3 eV using spectroscopic ellipsometry at various

temperatures between 10 K and 740 K. The interband CPs $E_0$ and $E_0 + \Delta_0$, where $E_0$ is the direct band gap of Ge and $\Delta_0$ is

the spin-orbit splitting occurring at the center of the Brillouin zone, lie in this energy range and are subject of our

investigations. Applying an analysis in reciprocal space by performing a discrete Fourier transform of the data points and

fitting the resulting Fourier coefficients, the parameters describing the line shape of $E_0$ are found as a function of

temperature. Like for the CPs at higher energies, the authors find a red shift of the $E_0$ and $E_0 + \Delta_0$ energies which can be

fitting the resulting Fourier coefficients, the parameters describing the line shape of $E_0$ are found as a function of

the temperature and external electric field. The exciton energies are very sensitive to the thickness of the quantum wells.

We performed low temperature ER measurements of the RBS samples of different thicknesses by tuning the angle of

incidence of the light for double resonance and observed ER features related to the exciton transitions at excited states

such $x(e_2-h_2), x(e_2-h_1), x(e_2-h_3)$ $x(e_2-l_1)$ and $x(e_1-h_3)$ exciton transitions along with the sharp features of $x(e_1-h_1)$ and

and $x(e_1-l_1)$ ground state exciton transitions. Details about the origin of the ER features related to the transitions will be

presented.

12:15PM S33.00006: Electoreflectance studies of GaAs/AlGaAs multiple quantum well based resonant Bragg

structure at excited states NIKESH MAHARJAN (Presenter), MIM L NAKARMI, Department of Physics, Brooklyn College and The

Graduate Center of the CUNY, Brooklyn, NY 11210, USA, VLADIMIR CHALDYSHEV, Department of Physics, Ioffe Institute, 26

Polytekhnicheskaya, St. Petersburg 194021, Russia, NARESH M SHAKYA, Department of Applied Physics, New York University, NYU -

Tandon School of Engineering, Brooklyn, NY 11201 — Electoreflectance (ER) Spectroscopy was employed to study the optical

properties of GaAs/AlGaAs multiple quantum well (MQW) based resonant Bragg structure (RBS). The sample used in this

experiment consists of 60 periods of quantum well structures with GaAs well and AlGaAs barrier layers grown by

molecular beam expitaxy on a semi-insulating GaAs substrate. The sample structure was designed to achieve a double

resonance condition to coincide the Bragg resonance peak with the exciton transitions at the second quantum state. Bragg

peak can significantly be tuned by changing the angle of incidence of the light. Exciton energies can be tuned by changing

the temperature and external electric field. The exciton energies are very sensitive to the thickness of the quantum wells.

We performed low temperature ER measurements of the RBS samples of different thicknesses by tuning the angle of

incidence of the light for double resonance and observed ER features related to the exciton transitions at excited states

such $x(e_2-h_2), x(e_2-h_1), x(e_2-h_3)$ $x(e_2-l_1)$ and $x(e_1-h_3)$ exciton transitions along with the sharp features of $x(e_1-h_1)$ and

and $x(e_1-l_1)$ ground state exciton transitions. Details about the origin of the ER features related to the transitions will be

presented.

12:27PM S33.00007: Analysis of the Critical Point Parameters of $E_0$ and $E_0 + \Delta_0$ of Bulk Ge CAROLA EMMINGER

(Presenter), NUWANJULA S SAMARASINGHA ARACHCHIGE, FARZIN ABADIZAMAN, STEFAN ZOLLNER, New Mexico State University — Germanium is an indirect bandgap semiconductor having its onset of absorption at 0.8 eV at room

temperature. Knowledge of the behavior of critical points (CPs) of Ge and other semiconductors is valuable for the further
development of electronic and optoelectronic devices.

The dielectric function of Ge has been measured between 0.5 eV and 1.3 eV using spectroscopic ellipsometry at various

temperatures between 10 K and 740 K. The interband CPs $E_0$ and $E_0 + \Delta_0$, where $E_0$ is the direct band gap of Ge and $\Delta_0$ is

the spin-orbit splitting occurring at the center of the Brillouin zone, lie in this energy range and are subject of our

investigations. Applying an analysis in reciprocal space by performing a discrete Fourier transform of the data points and

fitting the resulting Fourier coefficients, the parameters describing the line shape of $E_0$ are found as a function of

temperature. Like for the CPs at higher energies, the authors find a red shift of the $E_0$ and $E_0 + \Delta_0$ energies which can be

described by a Bose-Einstein factor taking into account electron-phonon interactions. The results of the reciprocal-space

analysis are compared to the parameters determined by a parametric semiconductor fit.


TAKAYAMA (Presenter), Department of Physics, The University of Tokyo, CHANGSU KIM, HIDEFUMI AKIYAMA, Institute of Solid

State Physics, The University of Tokyo, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University,

RYO SHIMANO, Cryogenic Research Center and Department of Physics, The University of Tokyo — The exciton-exciton (ex-ex)

interaction has long been investigated from the viewpoint of excitonic nonlinear optics in a variety of semiconductors [1].

Recently, the problem has gained a renewed interest partly triggered by the progress of researches in the field of polariton

Bose-Einstein condensation in a quantum well system embedded in a microcavity. In contrast to intensive theoretical

studies devoted over decades, however, the quantitative evaluation of ex-ex interaction in bulk system has been lacked.

Here we revisited this long-standing issue with near-infrared optical pump optical-probe/terahertz probe spectroscopy

technique. In bulk GaAs at the lattice temperature 5K, we observed a blueshift of exciton absorption peak caused by the

ex-ex interaction when the pump photon energy tuned to 1s-exciton resonance. Combined with the terahertz

spectroscopy, the density dependence of the excitonic blueshift is evaluated, which allows to determine the ex-ex

interaction strength quantitatively. The value coincides well with that predicted from mean-field theory. The dynamics of

the excitonic blueshift will also be discussed with respect to the thermalization of cold exciton gas.

12:51PM S33.00009: Moments analysis of the dielectric function  
ERIC SHIRLEY (Presenter), JOHN VINSON, National Institute of Standards and Technology — For many purposes, the random-phase approximation (RPA) is an adequate approximation for dielectric screening when the latter is required within a calculation. Therefore, an efficient approximation to the RPA is similarly useful in a wide range of situations. In this talk, we will describe a model for the same based on knowledge of several approximate frequency moments of the irreducible polarizability function. These models rely, in part, on the Fourier transform of the two-point, one-electron density matrix. We test our model calculations against numerical density-function theory (DFT) calculations in isolated atoms, the homogeneous electron gas, and a wide variety of metals, semiconductors, and insulators.

1:03PM S33.00010: Electronic Transport Studies of Boron-Doped Diamond-on-Graphene Heterostructures*  
ADRIAN NOSEK (Presenter), Physics, University of California, Riverside, ROBERT BOGDANOWICZ, MATEUSZ FICEK, MICHAL SOBASZEK, LUKASZ GOLUNSKI, Metrology and Optoelectronics, Gdansk University of Technology, JAKUB KARCZEWSKI, Applied Physics and Mathematics, Gdansk University of Technology, ANDRES JARAMILLO-BOTERO, WILLIAM GODDARD, Materials and Process Simulation Center, California Institute of Technology, MARC BOCKRATH, Physics, Ohio State University, TADEUSZ OSSOWSKI, Analytical Chemistry, University of Gdansk — Diamond-on-graphene heterostructures are a promising route for operating novel electronic devices at high temperatures due to their excellent thermal properties. For this purpose, boron-doped diamond thin films were grown in a microwave plasma-assisted chemical vapor deposition (CVD) system on a tantalum substrate which allows us to peel off diamond films [1]. Successive mechanical transfer of the diamond films onto CVD graphene on either Si/SiO₂ or quartz results in our heterostructure devices. We will present current-voltage characteristics as a function of temperature and their tunable gate dependence at specific temperatures. Varying the doping level of boron in the diamond films leads to variations in device behavior. Our latest results will be discussed.


*This work was supported by NATO's Science for Peace and Security Programme.

1:15PM S33.00011: Thermal transport in two-dimensional disordered electron systems at intermediate temperatures*  
WOO-RAM LEE (Presenter), University of Alabama, ALEXANDER FINKELSTEIN, Texas A&M University, KAREN MICHAELI, Weizmann Institute of Science, GEORG SCHWIETE, University of Alabama — Theoretical studies of transport properties of two-dimensional electron gases often focus on two limiting cases: (i) The diffusive regime that occurs at low temperatures where inelastic electron-electron scattering is substantially weaker than scattering by disorder. (ii) The hydrodynamic limit characterized by strong electron-electron scattering which requires relatively high temperatures. The latter has been widely studied in the context of strongly correlated electron systems and graphene. Here, we report a study of electron transport in an intermediate regime where both electron-electron scattering and scattering on impurities are equally important. To address this regime, we first analyzed a simplified kinetic equation which we supplemented by a more detailed analysis of the elastic and inelastic scattering terms. In particular, we derived the thermal conductivity of a degenerate electron system at intermediate temperatures.

*This work is supported by DOE, ISF, NSF, and the College of Arts and Sciences at the University of Alabama.

1:27PM S33.00012: Comprehensive Characterization of Alkaline Earth Metal Halides using First Principles Calculations*  
LU WANG (Presenter), SARIT DHAR, MARCELO KURODA, Auburn University — Alkaline earth metal halides are among the scarce insulators with dielectric constants and band gaps larger than those of SiO₂. Here, we present a study of this class of high K/large band gap materials using first principles calculations with different levels of sophistication. In particular we focus on changes in their electronic and thermal properties as a function of composition and structure. Our results show that the most stable phases of these materials are those with larger band gaps. Determination of their band gaps requires hybrid approaches to overcome well-known limitations of density functional theory. Phonon properties and dielectric response are compared using different exchange-correlation functionals: (i) Localized Density Approximation (LDA), (ii) Generalized Gradient Approximation (GGA) and (iii) Generalized Gradient Approximation including van der Waals forces (GGA+vdW). We find that the dispersive forces correct the mode softening observed in low-frequency phonon modes in the GGA functionals yielding results similar to LDA. The different trends found in these materials class relative to their composition and structure are discussed.

*This work is supported by the Grant ARMY-W911NF-18-2-0160.
1:39PM S33.00013: In-plane field dependence of spin resolved magnetic focusing in 2D hole systems  MATTHEW RENDELL (Presenter), SCOTT LILES, ASHWIN SRINIVASAN, OLEH KLOCHAN, Univ of New South Wales, IAN FARRER, University of Sheffield, DAVID A RITCHIE, University of Cambridge, ALEX R HAMILTON, Univ of New South Wales — The spin orbit interaction allows for all-electrical control of spin. Transverse magnetic focusing provides a method for spatially separating spins so that spin dynamics can be studied. We perform transverse magnetic focusing experiments of heavy holes in highly symmetric (100) GaAs/AlGaAs heterostructures, and observe two clear spin resolved focusing peaks. It is tempting to use the area of the focusing peaks as a measure of the spin polarisation, however we find that the peak area is extremely sensitive to in-plane magnetic fields - as small as 0.1T. Additionally, we find that the peak area is asymmetric when the in-plane field direction is reversed, and this asymmetry is conserved under Onsager time reversal. This suggests that there is an additional non-spin polarisation effect at play, and that care must be taken when using focussing techniques to measure spin.

1:51PM S33.00014: Epitaxial growth of large grain size polycrystalline silicon on SiO2 by reduced pressure chemical vapor deposition  KAIGUI ZHU (Presenter), FANGFANG CHEN, Beihang University, HUICAI ZHONG, Institute of Microelectronics of Chinese Academy of Sciences — Epitaxial growth of polycrystalline silicon (poly-Si) on SiO2 was successfully carried out by reduced pressure chemical vapor deposition (RP-CVD) using SiH4/H2 mixtures. The growth rate and grain size of ploy-Si were significantly improved by increasing the epitaxial temperature. The film deposition rate was 3.1nm/s with the epitaxial temperature at 820°C. The grain size of the poly-Si film could reach as large as 700nm on annealed seed layer. Good quality poly-Si film with large and uniform grain was obtained by direct deposition on SiO2 substrate. The electrical properties of the doped poly-Si film were tested by Hall Effect and four-probe method.

2:03PM S33.00015: Chemistry Perspective to Design Novel Magnetic Semiconductors/Semimetals*  WEIWEI XIE (Presenter), XIN GUI, Chemistry, Louisiana State University, RONGYING JIN, Physics, Louisiana State University — Magnetic semiconductors combine the complementary functions of magnetic and semiconducting materials, providing tremendous potential for the development of new devices for today's information technology. If employed in devices, these materials could lead to a new pathway to control information: by charging carriers not only in traditional electronics but also in spin dimensions. The Zener model was modified by Dietl et al. to explain the origin of ferromagnetism in Mn-doped GaAs and predicted the room-temperature ferromagnetism in other semiconductors and oxides. This remarkable work opened up the era of searching for room-temperature ferromagnetism in semiconductors. It still remains a lot of work to identify plausible targets for new magnetic materials. Previous studies mainly focused on hybrid structures consisting of ferromagnetic and semiconducting multilayers and Mn-doped binary semiconductors. However, only a small handful of intrinsic magnetic semiconductors have thus far been reported. Thus, the design of specifically targeted by synthetic scientists is highly demanded. In this talk, I will describe some empirical design rules and examples that have yielded new magnetic semiconductors/semimetals.

*The research is supported through Beckman Young Investigator (BYI) award.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S34 FIAP: Adventures of Entrepreneurial Physicists or Where You Should Find Your Next Job  BCEC 205A - Matt Kim - Tag(s): Careers, Industrial, Invited, Undergraduate

11:15AM S34.00001: Harnessing the Nanoscale Physics of Living Systems to Transform the Delivery of Healthcare  ANITA GOEL (Presenter), Nanobiosym — TBD

11:51AM S34.00002: Physicists who lead: You don't need your own invention to found a deep-tech startup  OMAR ZAHR (Presenter), Tandem Launch — TBD

12:27PM S34.00003: Physics and Entrepreneurship – Changing the World with your Brain  JESKO VON WINDHAM (Presenter), Duke University — TBD

1:03PM S34.00004: TBD  JOHN FAN (Presenter), Kopin Corporation — TBD

1:39PM S34.00005: Panel Discussion with Speakers on their Wisdom and Future Jobs at Startups  —

Thursday, March 7, 2019 11:15 AM - 2:15 PM
11:15AM S35.00001: Multilayer coaxial superconducting circuits with integrated 3D wiring* [Invited] PETER LEEK (Presenter), University of Oxford — Superconducting circuits are one of the leading candidates for the realization of quantum computers, in particular for near-term applications which may already be reached with circuits consisting of a few hundred qubits, provided they are operated at high fidelity. Until recently, the topology of superconducting circuits has typically been constrained to two dimensions, which becomes increasingly difficult as the number of qubits is scaled up and control and measurement wiring is needed for qubits in the middle of large arrays. It is natural to explore new circuit topologies that incorporate wiring in the third dimension to solve this problem. In this talk I will present an overview of an approach that builds on a coaxially-symmetric circuit QED unit cell with out-of-plane wiring [1] that provides a simple route to scaling to grids of many qubits. In this approach, arrays of qubits and resonators can be fabricated on opposing sides of a substrate and capacitively coupled, while control and readout are achieved via off-chip coaxial wires which run perpendicular to the chip plane and are built into a precision micromachined enclosure that provides a high-quality microwave environment for the circuit.


*We acknowledge financial support from the EPSRC and Oxford Quantum Circuits Ltd.

11:51AM S35.00002: Flux Tunable Superconducting Qubits With 3D Wiring* JEREMY BEJANIN (Presenter), CAROLYN EARNEST, Physics & IQC, University of Waterloo, THOMAS G MCCONKEY, Electrical And Computer Engineering & IQC, University of Waterloo, EVAN PETERS, MATTEO MARIANTONI, Physics & IQC, University of Waterloo — Superconducting qubits have the potential to lead to large-scale quantum computers, where 10^5 or more qubits are arranged in two-dimensional arrays forming quantum processing units (QPUs) on silicon chips. Operating such an array necessarily requires control signals to come from wires in the third dimension, so as to avoid overlapping control lines on the device itself. While various implementations of 3D wiring have been realized in the last few years, none has been used with flux-tunable superconducting qubits, which require a current line to inductively bias the superconducting loop of a SQUID. In this talk, we show and characterize the performance of tunable superconducting Xmon transmon qubits using the quantum socket, for which the control wiring is fully 3D, including the fast flux bias lines used for frequency tuning. We demonstrate one-qubit gates and perform quantum gate tomography to quantify gate fidelity as a function of flux bias for two Xmon transmon qubits.

*This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund (CFREF) and the Discovery and Research Tools and Instruments Grant Programs of the Natural Sciences and Engineering Research Council of Canada (NSERC).

12:03PM S35.00003: Increasing reliability for 3D integrated high-coherence superconducting qubits* BETHANY M NIEDZIELSKI (Presenter), DAVID K KIM, JONILYN L YODER, DANNA ROSENBERG, MOLLIE E. SCHWARTZ, RABINDRA DAS, ALEXANDER MELVILLE, DONNA-RUTH YOST, JUSTIN MALLEK, ALEXANDRA L DAY, STEVEN WEBER, CYRUS F. HIRJIBEHEDIN, WILLIAM D OLIVER, MIT Lincoln Laboratory — As designs for superconducting qubits become more complex, 3D integration of two or more vertically bonded chips can enable increased density and connectivity. Precise control of the spacing between these chips is required to give designers accurate parameters to plan and predict circuit performance. In this talk, we will describe our process for using silicon hard-stop mesas to control chip spacing and tilt, and our integration of these features with our high-coherence superconducting qubit fabrication process.

*This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.
12:15PM S35.00004: 3D-wired coaxial circuit QED I: Extension to multi-qubit devices* SALHA JEBARI (Presenter), JOSEPH RAHAMIM, ANDREW D PATTERSON, PETER A SPRING, TAKAHIRO TSUNODA, SOPHIA SOSNINA, MARTINA ESPOSITO, KITTI RATTER, GIOVANNA TANCREDI, BRIAN VLASTAKIS, PETER LEEK, Condensed Matter Physics, University of Oxford — In order to realise superconducting circuits at a sufficient scale for useful near-term applications, an architecture is required which implements good connectivity between qubits, and allows for selective readout and control of the qubits without introducing detrimental crosstalk or decoherence. Since the number of readout and control lines increases linearly with the number of qubits, scaling up a circuit which is constrained to a 2D surface becomes increasingly difficult. Here we present the extension of our recently demonstrated 3D-wired coaxial circuit QED architecture [1] to 2D arrays of qubits. Qubits and readout LC resonators are fabricated on opposing sides of a substrate and entirely off-chip coaxial wiring is built into the chip enclosure and runs perpendicular to the chip plane. Scaling is simply achieved by the repetition of the unit cell across a 2D plane. We present the performance of multi-qubit circuits based on this architecture, including coherence times and two-qubit gate fidelities.


*We acknowledge financial support from the EPSRC, Oxford Instruments Nanoscience, Oxford Quantum Circuits Ltd, the Oxford Centre for Applied Superconductivity, the Nakajima Foundation and the Masason Foundation.

12:27PM S35.00005: 3D-wired coaxial circuit QED II: Evaluation of crosstalk* JOSEPH RAHAMIM (Presenter), SALHA JEBARI, ANDREW D PATTERSON, PETER A SPRING, TAKAHIRO TSUNODA, SOPHIA SOSNINA, MARTINA ESPOSITO, KITTI RATTER, GIOVANNA TANCREDI, BRIAN VLASTAKIS, PETER LEEK, Condensed Matter Physics, University of Oxford — Evaluating crosstalk in multi-qubit superconducting circuits is becoming increasingly important. Control-wiring crosstalk can cause coherent control errors that become increasingly impractical to correct in larger scale circuits, and measurement crosstalk can induce dephasing. Selective control and coupling is intrinsic to our architecture [1] due to the use of coaxial circuit elements on two planes, mode-matched to out-of-plane 3D wiring. However, in any multi-qubit circuit the electromagnetic fields associated with individual circuit elements and control signals will never be perfectly confined. We present a careful characterisation of resonator and qubit control-line crosstalk, as well as measurement crosstalk due to coupling between neighboring qubits and resonators. We incorporate a detailed understanding of the two-qubit Hamiltonian in order to extract the qubit control-line crosstalk, and utilise measurement-induced dephasing to directly characterize resonator control-line, as well as measurement crosstalk.


*We acknowledge financial support from the EPSRC, Oxford Instruments Nanoscience, Oxford Quantum Circuits Ltd, the Oxford Centre for Applied Superconductivity, the Nakajima Foundation and the Masason Foundation.

12:39PM S35.00006: Superconducting Qubits Integrated with Superconducting Through-Substrate Vias (TSVs): Fabrication* DONNA-RUTH YOST (Presenter), MOLLIE E. SCHWARTZ, DANNA ROSENBERG, JUSTIN MALLEK, RABINDRA DAS, ALEXANDRA L DAY, DAVID K KIM, BETHANY M. NIEDZIELSKI, ALEXANDER MELVILLE, WAYNE WOODS, JONILYN L YODER, ANDREW JAMES KERMAN, WILLIAM D OLIVER, Massachusetts Institute of Technology — Three-dimensional integration (3DI) is a promising approach to provide increased connectivity for complex arrays of superconducting qubits while maintaining qubit performance. In this talk we describe our process flow for fabricating wafers of superconducting through-substrate vias (TSVs) which may be integrated directly into superconducting qubit chips and/or bump bond integrated with high-coherence qubits to carry signals to and from the qubit layer.

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

MOLLIE E. SCHWARTZ (Presenter), DONNA-RUTH YOST, DANNA ROSENBERG, JUSTIN MALLEK, RABINDRA DAS, ALEXANDRA L DAY, DAVID K KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, JONILYN L YODER, ANDREW JAMES KERMAN, WILLIAM D OLIVER, MIT Lincoln Laboratory — Three-dimensional integration (3DI) is an enabling technology for superconducting qubits as circuits become larger, more complex, and more highly-connected. One promising approach to 3DI is the vertical routing of signals through superconducting through-substrate vias (TSVs), which may be integrated directly into a superconducting qubit chip or may carry signals to and from a high-coherence qubit layer via an interposer chip. We discuss recent results demonstrating superconducting qubit control, readout, and integration with high-aspect ratio superconducting TSVs.

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

Multilayer Microwave Integrated Quantum Circuits: Part 1

CHAN U LEI (Presenter), LEV KRAYZMAN, SUHAS GANJAM, Yale University, TERESA L BRECHT, Yale University & HRL, CHRISTOPHER J AXLINE, Yale University & ETH, YIWEN CHU, LUKE BURKHART, LUIGI FRUNZIO, ROBERT J Schoelkopf, Yale University — Recently, superconducting quantum circuits have advanced from circuits containing few qubits to larger-scale ones with several tens of qubits. In order to increase the computational power of these circuits, many more circuit elements need to be integrated without degrading coherence of the individual components. Although the number of lithographic-precision elements in fully-planar (2D) circuits can be scaled up, it is very challenging to maintain interconnects and suppress decoherence induced by crosstalk as the circuits grow. On the other hand, three dimensional (3D) circuits which use conventionally-machined cavities to engineer the electromagnetic environment offer superior coherence but are challenging to scale up. In this talk, we discuss the multilayer microwave integrated quantum circuit (MMIQC), a platform which combines planar circuits with 3D superconducting enclosures to gain scalability while maintaining coherence.

High-quality superconducting bonds are a critical element in constructing multilayer microwave integrated quantum circuits (MMIQCs). In order to provide lithographic precision for 3D enclosures made in wafers, it is necessary to create cavities with a high aspect ratio which places the seam in a region of high current density. In this talk, we describe a model for quantifying the loss associated with the seam, present our progress on indium bonding in microwave circuits, and discuss its application in scalable 3D superconducting quantum circuits.

Development of superconducting connection by flip-chip bonding for a multilayer superconducting quantum annealing machine

KAZUMASA MAKISE (Presenter), MASAHIK MAEZAWA, MITSUO HIDAKA, HIROSHI NAKAGAWA, KATSUYA KIKUCHI, SHIHO KAWABATA, National Institute of Advanced Industrial Science and Technology (AIST) — To realize practical-scale quantum annealing machines, a large number of qubits are required for the quantum processor. However, implementation of high-density qubits-array on a chip is a difficult problem because the size of qubits is limited by the size of wiring layer, Josephson junction and SQUID. To solve this problem, we have proposed an “QUIP” (Qubit-chip, Interposer and Package-substrate) 2.5-dimensional (2.5 D) packaging structure. Therefore, development of the packaging technology of qubits is one of the most important issue for QUIP. In this presentation, we focus on flip-chip bonding (FCB) connection as a 2.5 D mounting method. We design and fabricate circular lead/indium alloy solder bumps with a 10 um diameter and 5 um height on the top chip and Nb/Ti/Au-opposing-contact pads on the base chip to form a daisy chain of over 10000 chip-to-chip interconnects. The electrical transport measurements are performed in a cryocooler using a standard dc four-probe technique. We observe a critical current for the daisy chain devices with 15000 bump array, $I_c \sim 4 \text{ mA}$.

This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO), Japan.
1:39PM S35.00011: Intel Superconducting Qubits, Part 1: Performance improvements towards enabling quantum applications  ROMAN CAUDILLO (Presenter), DAVID MICHALAK, LESTER LAMPERT, ADEL A ELSHERBINI, Components Research, Intel, JAVIER A FALCON, YE SEUL ASHLEY NAM, PRESTON T MYERS, DATD, Intel, SONIKA JOHRI, XIANG CHRIS ZOU, Intel Labs, Intel, JEANETTE MARIE ROBERTS, Components Research, Intel, ALESSANDRO BRUNO, NANDINI MUTHUSUBRAMANIAN, CORNELIS CHRISTIAAN BULTINK, FILIP MALINOWSKI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, NADIA HAIDER, QuTech and TNO, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, JIM CLARKE, Components Research, Intel — Quantum processors based on superconducting materials with flux-tunable transmon qubits present many challenges, including minimizing flux and microwave crosstalk, improving qubit frequency targeting, extending coherence times, and ultimately maximizing gate fidelities. Here we present our fabrication capabilities addressing some of these challenges on die sizes ranging from small laterally wirebonded 2-qubit chips to larger flip-chip, ball-grid-array-bonded 7- and 17-qubit chips. Through improved die processing, including better-controlled materials interfaces, integration of air bridges, and Josephson Junction fabrication optimization, we demonstrate low flux and microwave crosstalk and qubit performance improvements resulting in one- and two-qubit gate fidelities that enable algorithm exploration and execution.

1:51PM S35.00012: Intel Superconducting Qubits, Part 2: Integration on through-silicon-via (TSV) substrates.  DAVID MICHALAK (Presenter), ROMAN CAUDILLO, LESTER LAMPERT, ADEL A ELSHERBINI, Components Research, Intel, JAVIER A FALCON, YE SEUL ASHLEY NAM, PRESTON T MYERS, DATD, Intel, JEANETTE MARIE ROBERTS, Components Research, Intel, ALESSANDRO BRUNO, NANDINI MUTHUSUBRAMANIAN, CORNELIS CHRISTIAAN BULTINK, FILIP MALINOWSKI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, NADIA HAIDER, QuTech and TNO, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, JIM CLARKE, Components Research, Intel — Quantum computing holds the potential for significantly improving computing speed relative to classical computing for selected algorithms and applications. Many researchers using transmons in a circuit QED quantum hardware architecture are producing chips with ever-increasing numbers of qubits. The corresponding increase in chip size shifts the cavity/drum resonant modes into a frequency range where qubits could be adversely affected. One solution is to implement through-silicon-vias (TSVs) and chip/cavity contact pins to supply more ground connections. We present recent microwave modeling and fabrication results on qubit chips containing membrane-covered TSVs. These flip chips are assembled using a ball-grid-array die-package interface for signal I/O.

2:03PM S35.00013: 3D Integration of Superconducting Qubits in a Three-Tiered Quantum Processor*  JUSTIN MALLEK (Presenter), DONNA-RUTH YOST, RABINDRA DAS, DANNA ROSENBERG, VLADIMIR BOLKHOVSKY, GREG CALUSINE, MATTHEW COOK, EVAN GOLDEN, DAVID K KIM, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, MOLLIE E. SCHWARTZ, COREY STULL, SERGEY TOLPYGO, WAYNE WOODS, JONILYN L YODER, WILLIAM D OLIVER, MIT Lincoln Laboratory — Heterogeneous 3D integration is an enabling technology for the construction of a quantum processor with a large number of superconducting qubits and a high degree of qubit interconnectivity. Our approach entails the construction of a three-tiered quantum processor where the high-coherence superconducting qubits are controlled and read-out through superconducting through silicon vias (TSVs) in an interposer which is bump bonded to a superconducting multichip module using indium microbumps. We will discuss our work on the fabrication and integration of the interposer with superconducting TSVs as well as the superconducting multichip module and the electrical data measured from test structures.

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

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S36 GMAG: Quantum Molecular Nanomagnets  BCEC 205C - Enrique Del Barco, Univ of Central Florida -

Tags: Invited
11:15AM S36.00001: Forbidden Transitions in Molecular Nanomagnets* [Invited] JONATHAN FRIEDMAN (Presenter), Department of Physics and Astronomy, Amherst College — Selection rules typically arise from the constraints imposed by conservation laws. In electron-spin resonance spectroscopy, the standard single-photon-transition selection rule $\Delta m = 0, \pm 1$ arises from angular momentum conservation. Such selection rules can be lifted when the magnetic quantum number of the spin system under study is not a good quantum number. In molecular nanomagnets (MNMs), magnetic anisotropy can lead to a preferred (easy) axis of orientation for the molecule's spin, giving rise to an anisotropy barrier between “up” and “down” states. In addition, transverse anisotropy breaks the system's symmetry, leading to state mixing and tunneling between spin states. Thus, tunneling can lead to the observation of forbidden transitions that strongly violate selection rules. I will report studies by my group of two MNMs that exhibit such highly forbidden transitions. In the Ni$_4$ MNM, a spin-4 system, we observe single-photon transitions in which the magnetic moment changes by as much as $\sim 7 \hbar$, nearly reversing the molecule's spin [1]. In addition, we observe direct transitions between tunnel-split states in this MNM, allowing us to precisely determine its transverse anisotropy [2]. In the Cr$_7$Mn MNM, a spin-1 system, there is a large tunnel splitting lifting the zero-field ground-state degeneracy. The two lowest states then have the structure of an atomic-clock transition in which the transition frequency is to first order independent of magnetic field, making the system largely immune to the decohering effects of external-field fluctuations. We find that the decoherence time $T_2$ is enhanced by a factor of three in the vicinity of this clock transition in Cr$_7$Mn.


*Work supported by NSF grants DMR-1310135 and DMR-1708692.

11:51AM S36.00002: Coherent manipulation of three spin qubits in a GdW$_{30}$ single-ion magnet* [Invited] FERNANDO LUIS (Presenter), Instituto de Ciencia de Materiales de Aragón (ICMA), Consejo Superior de Investigaciones Científicas (CSIC), MARK D JENKINS, Kavli Institute of Nanoscience, Delft University of Technology, YAN DUAN, Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, JUAN JOSE GARCÍA-RIPOLL, Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas (CSIC), ALEJANDRO GAITÁ-ARIÑO, CARLOS GIMÉNEZ-SAIZ, Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, PABLO J ALONSO, Instituto de Ciencia de Materiales de Aragón (ICMA), Consejo Superior de Investigaciones Científicas (CSIC), ALBERTO CASTRO, Instituto de Biofísica y Física de Sistemas Complejos (BIFI), Universidad de Zaragoza, DAVID ZUECO, Instituto de Ciencia de Materiales de Aragón (ICMA), Consejo Superior de Investigaciones Científicas (CSIC), EUGENIO CORONADO, Instituto de Ciencia Molecular (ICMol), Universidad de Valencia — Implementing quantum computation with spins faces the challenge of increasing the number of qubits while keeping errors under control. Even the simplest algorithm implies coupling two or more qubits in a controlled manner. However, dipolar interactions are also an important source of decoherence [1]. Here, we explore a way to scale up quantum resources, without introducing additional decoherence, by integrating several electron spin qubits in a single magnetic ion with spin $S > \frac{1}{2}$. This approach is illustrated with a [Gd(H$_2$O)$_5$W$_{30}$O$_{110}$]$^{12-}$ polyyxometalate single-ion magnet [2]. Electron paramagnetic resonance experiments have been performed on molecules diluted in a crystal of the diamagnetic isostructural derivative [Y(H$_2$O)$_5$W$_{30}$O$_{110}$]$^{12-}$. The seven allowed transitions between the $2S+1=8$ spin states have been separately addressed and its spin coherence $T_2$ and spin-lattice relaxation $T_1$ rates measured. Rabi oscillations have been observed for all transitions. The spin states of each Gd$^{3+}$ ion can then be mapped onto the states of three addressable qubits (or, alternatively, of a $d = 8$-level molecular “qudit”), for which the seven allowed transitions form a universal set of operations. Within this scheme, one of the coherent oscillations observed experimentally provides an implementation of a controlled-controlled-NOT (or Toffoli) three-qubit gate. We also propose a way to implement a simple quantum error correction code using this single-ion “processor”. Our findings [3] open prospects for developing more complex and robust quantum computation schemes based on molecular spin qubits.


*Funds were provided by the Spanish MINECO (grants MAT2015-68204-R and Excellence Unit Maria de Maeztu MDM-2015-0538) and the European Union (COST 15128 Molecular Spintronics and QUANTERA SUMO projects)
**12:27PM S36.00003: Multifrequency and Chemical Tuning Studies of V(IV) Quantum Spins**

[Invited] JOSPEH ZADROZNY (Presenter), CHUN-YI LIN, CASSIDY JACKSON, Chemistry, Colorado State Univ. JOHAN VAN TOL, National High Magnetic Field Laboratory — Complexes of the magnetic ion vanadium(IV) are at the frontier of molecular qubit research. Indeed, several recent investigations demonstrate that these ions are capable of spin relaxation times comparable to diamond's nitrogen vacancy centers. In light of these exciting results, significant fundamental knowledge is still needed to further design these ions as qubits. For example, understanding the frequency dependence of V(IV) electron paramagnetic resonance properties underlies many applications, yet EPR studies are largely focused at only one frequency, X-band. Separately, understanding how ligand chemical composition affects spin relaxation times would enable the further improvement of relaxation times. Yet, the majority of research in this area is focused on vanadium ions surrounded by ligands that are composed entirely of carbon, oxygen, and sulfur. In this presentation, results from multi-frequency EPR analyses on families of vanadium(IV) complexes will be presented, with an eye toward the foregoing fundamental insight.

*National Science Foundation (CHE-1836537)

**1:03PM S36.00004: Operating quantum states in single magnetic molecules**

[Invited] WOLFGANG WERNSDORFER (Presenter), PHI-INT, KIT, CLEMENT GODFRIN, FRANCK BALESTRO, Neel, CNRS — The endeavour of quantum electronics is driven by one of the most ambitious technological goals of today’s scientists: the realization of an operational quantum computer. We have started to address this goal by the new research field of molecular quantum spintronics, which combines the concepts of spintronics, molecular electronics and quantum computing. The building blocks are magnetic molecules, i.e. well-defined spin qubits. Various research groups are currently developing low-temperature scanning tunnelling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors) to read and manipulate the spin state and perform basic quantum operations. We will present our recent measurements of geometric phases, the iSWAP quantum gate, the coherence time of a multi-state superposition, and the application to Grover’s algorithm [1-5].


*WW aknowledges the Humboldt foundation and the ERC Advanced Grant: MoQuOS

**1:39PM S36.00005: Magnetic relaxation dynamics in dysprosium complexes**

[Invited] NICHOLAS CHILTON (Presenter), DANIEL RETA, JON KRAGSKOW, DAVID MILLS, University of Manchester, YANZHEN ZHENG, Xi'an Jiaotong University, RICHARD WINPENNY, University of Manchester — Following our discovery of the first dysprosium metallocenium cation, (Dy(Cp3)2)[B(C6F5)4], which is the vanguard of the new generation of high-temperature single-molecule magnets, we have been investigating the magnetic relaxation dynamics of various dysprosium-based single-molecule magnets (SMMs) by experimental and theoretical techniques. Here we present our recent results in unravelling the competing magnetic relaxation processes, and offer some insights into the origin of the previously pervasive quantum tunneling of the magnetization in high-barrier dysprosium(III) SMMs.


*EPSRC, The University of Manchester, The Ramsay Memorial Trust

**Thursday, March 7, 2019 11:15 AM - 1:51 PM**

Session S37 GMAG DCMP DMP: Spin Glasses, Spinels and Other Frustrated Systems BCEC

206A - Adam Aczel, Oak Ridge National Laboratory - Tag(s): Focus

2597 of 3305
11:15AM S37.00001: Role of Anisotropy in Spin Glass 1/f Noise Measurements* DAVID HARRISON (Presenter), E. DAN DALHBERG, University of Minnesota - Twin Cities, RAYMOND ORBACH, University of Texas at Austin — We have measured the 1/f noise in the resistance of the spin glass state of Cu$_{1-x-y}$Mn$_x$Au$_y$ and Ag$_{1-x-y}$Mn$_x$Au$_y$ thin films. The magnitude of 1/f noise shows a relatively abrupt increase as the system is cooled below its spin glass transition temperature. Doping of both the Ag and Cu based alloys with Au, allows us to systematically change the strength of the Dzyaloshinskii-Moriya interaction (DMI), a unidirectional anisotropy believed to give metallic spin glasses a more Ising-like characteristic. Witness films fabricated with the noise samples allow us to make a direct comparison of the temperature dependence of our noise measurements and conventional SQUID magnetometry measurements. We also compare our data with previously published results.

*Work supported by DOE Award Number DE-SC0013599.

11:27AM S37.00002: A statistical approach to rejuvenation and memory in spin glasses* RAYMOND ORBACH (Presenter), University of Texas at Austin — Rejuvenation and memory in spin glasses are approached from a statistical perspective. The analysis is based on temperature chaos being a "rare-event-driven phenomenon." Three regions are identified with increasing magnitudes of negative temperature shifts $\delta T$ ($\delta T > 0$). The first region exhibits reversible dynamics for $\delta T$ sufficiently small. The second is the chaotic regime for larger $\delta T$ where the dynamics re-start, termed "rejuvenation." Only a few spatial regions of size of the order of the spin glass correlaton length go chaotic. The large number of separated correlated regions for correlation lengths much less than the sample thickness or crystalline size (e.g. thin films or bulk samples) suggests that, as the temperature is lowered further, the probability that those regions that went chaotic in the rejuvenation regime would go chaotic again is statistically small. The growth of free energy barriers in these "rare" regions as the temperature is lowered further ($\delta T$ increasing) "freezes" their dynamics. As the temperature is raised back to the rejuvenation regime, their dynamics are "revived" and return to those initially measured. This is the origin of "memory."

*Supported by the U.S. Department of Energy, Office of Science, award DE-SC0013599

11:39AM S37.00003: Heisenberg domain state in thin-film ferromagnet/antiferromagnet bilayers is a magnetic glass* WEIJIE LI (Presenter), SERGEI URAZHDIN, Emory University — Random exchange interaction at the interface between ferromagnetic (F) and antiferromagnetic (AF) films results in the formation of a multidomain state. It was predicted by Malozemoff that for sufficiently thin films, domains become smaller than the domain wall width, forming a "Heisenberg domain state" (HDS) [1]. The nature and properties of HDS remain unexplored. We utilize magnetoelectronic and magneto-optical measurements of relaxation and dynamical characteristics in F/AF bilayers with AF=CoO, NiO, and FeMn to show that HDS is a magnetic glass. Our observations include nearly temperature-independent universal magnetic aging below a certain temperature $T_G$, transitioning to a strong temperature dependence at $T>T_G$. The transition is associated with a qualitative change in the dependence on the magnetic history. Transverse ac susceptibility measurements indicate that the magnetic viscosity varies by 4 orders of magnitude when $T>T_G$ is varied by 20 K, indicative of magnetic freezing consistent with the glass transition. Our results demonstrate that thin-film F/AF bilayers are a readily realizable and experimentally accessible quasi-2d magnetic glass system with controllable characteristics.


*Supported by NSF DMR-1504449
11:51AM S37.00004: Investigation of the Magnetic Ground State of Ni-Mn-Sn-based Shape Memory Alloy: a combined muSR and Powder Neutron Diffraction Study*  SUBHAM MAJUMDAR (Presenter), Indian Association for the Cultivation of Science, JHUMA SANNIGRAHI, D. T. ADROJA, J LORD, DMITRY KHALYAVIN, ADRIAN HILLIER, ISIS Neutron and Muon Source Science and Technology Facilities Council — We performed muon spin relaxation (muSR) and neutron powder diffraction (NPD) measurements as a function of temperature (T) on a metamagnetic shape memory alloy of nominal composition Ni51Mn35Sn14. The initial asymmetry (A0) of the muSR data shows some unusual T variation. A0 falls rapidly below the ferromagnetic (FM) transition at TCA = 320 K, indicating the onset of bulk magnetic order. A0 regains its full asymmetry value below the structural transition at TMS = 290 K suggesting the collapse of the FM order into a fully disordered paramagnetic state. A0 again falls below the second magnetic transition at TCM = 240 K. Interestingly, A0 increases sluggishly below the exchange bias blocking temperature TB = 120 K. This indicates that the system attains a disordered/glassy magnetic phase below TB, which is responsible for the exchange bias and anomaly in the ac susceptibility data. The NPD does not show any magnetic superlattice reflection ruling out the possibility of a long range antiferromagnetic state at low temperatures. The ground state is likely to be comprising of a spin-glass phase in the backdrop of an FM state.

*The work is supported by the India-RAL collaborative project (SR/NM/Z-07/2015).

12:03PM S37.00005: Low-temperature and dynamic magnetism of highly frustrated 5d2 Li4MgOsO6 in comparison with 5d3 Li3Mg2OsO6*  JEREMY CARLO (Presenter), Department of Physics, Villanova University, SHAHAB DERAKHSAN, Department of Chemistry and Biochemistry, California State University - Long Beach, THOMAS GREDIG, Department of Physics, California State University - Long Beach, GRAEME LUKE, Department of Physics, McMaster University, JOHN GREEDAN, Department of Chemistry and Chemical Biology, McMaster University — Geometric magnetic frustration (GMF) has attracted substantial interest due to the exotic physics and rich phase diagrams revealed by the cancellation of normally-dominant magnetic interactions, giving impetus for the search for novel frustrated systems, most often based on antiferromagnetic correlations between magnetic ions decorating triangular or tetrahedral lattices. We report low-temperature magnetic susceptibility and muon spin relaxation results on Li4MgOsO6 and Li3Mg2OsO6, members of the A5BO6 “rock salt ordered” family of frustrated materials. In Li3Mg2OsO6 we find spin freezing below 12K. In Li4MgOsO6, which can crystallize into either orthorhombic Fddd or monoclinic C2/m crystal symmetries depending on synthesis conditions, we find magnetism consistent with glassy-like behavior dominating below 2K, with partial ordering and evidence for dynamics at somewhat higher temperatures.

*JPC acknowledges support from the Research Corporation for Science Advancement (Cottrell College Science Award #23314). SD is grateful for financial support from NSF-DMR-RUI Award #1601811 and the W. M. Keck Foundation for establishment of the Keck Energy Materials Program at CSULB. We thank the TRIUMF CMMS for assistance with muSR experiments.

12:15PM S37.00006: Spin Glass Behavior in Spinel Ni0.8Fe2.2O4*  ROSHAN NEPAL (Presenter), MOHAMMAD SAGHAYEZHIAN, JIANDI ZHANG, RONGYING JIN, Louisiana State University — Spinel oxides (AB2O4) with magnetic A and B ions are known to exhibit complex magnetic behavior that emerge from the competing AA, AB, and BB magnetic interactions. Here, we report the magnetic and thermal properties of single-crystalline Ni0.8Fe2.2O4, which orders ferrimagnetically (Fi) below TF ∼ 860 K, followed by another magnetic transition at TSG ∼ 14 K. The dc magnetization shows a dramatic downturn upon cooling below TSG, whereas both real and imaginary parts of ac susceptibility show frequency dependence. Further quantitative analysis reveals the presence of de Almeida-Thouless (A-T) line, dynamic magnetization behavior, memory effect, and the critical power law dependence of transition temperature to ac frequency, all indicative of a spin glass ground state. The origin of the spin glass state and its implication to other physical properties will be discussed.

*This work is supported by DoE through DE-SC0016315.
Recent experiments have demonstrated a lack of long-range magnetic order in spin-1 diamond lattice compounds such as NiRh$_2$O$_4$ [1]. These compounds can potentially provide a rich playground for exotic quantum states such as a proposed quantum spiral spin liquid [2]. We study the phase diagram of the Heisenberg model with bilinear and biquadratic interactions between nearest and next-nearest neighbors on the diamond lattice to search for ordered and quantum spin liquid states. The phase diagram for this frustrated spin-1 model reveals ground states that lack long-range spin order, including quadrupolar states and valence-bond solids. We use variational Monte Carlo with projected fermionic states to compare energies for different candidate states within a plausible region of the phase diagram corresponding to NiRh$_2$O$_4$.


*Robert A. Welch Foundation Grant C-1818, NSF Grant DMR-1350237

Coexisting zero-field and field induced relaxation channels in spinel spin ice

EDWARD RIORDAN (Presenter), Cardiff University, TOM FENNELL, paul scherrer institute, ELSA LHOTEL, Neel Institute, OKSANA ZAHARKO, paul scherrer institute, VLADIMIR TSURKAN, university of ausburg, SEAN GIBLIN, Cardiff University — Spin ice materials exhibit novel magnetic behaviour because of their atomic interactions and geometric constraints of the crystal lattice. This novel behaviour takes the form of emergent quasi-particles that behave as magnetic monopoles. We have studied the spin ice materials CdEr$_2$Se$_4$ and CdEr$_2$S$_4$ using a bespoke high frequency ac susceptometer capable of measuring at low temperatures (>2K). These ac susceptibility measurements have uncovered novel behaviour when in the presence of applied DC fields, in the form of two coexisting relaxation channels with differing time scales and temperature dependence. Such behaviour has not been so directly observed before. We have further investigated the relaxations by use of DC magnetisation and muon spin rotation techniques.

Spin Jahn-Teller effect in the antiferromagnet CoTi$_2$O$_5$

FRANZ LANG (Presenter), FRANZISKA KIRSCHNER, STEPHEN BLUNDELL, ROGER JOHNSON, DHARMALINGAM PRABHAKARAN, University of Oxford — We have used a combination of neutron powder diffraction and muon spin rotation experiments, complemented with DFT calculations, to solve the magnetic structure of orthorhombic CoTi$_2$O$_5$, which we find adapts a long-range ordered, antiferromagnetic state below 26 K with a moment of 2.72(1)μB per Co$^{2+}$ ion and propagation vector $k=(±1/2,1/2,0)$ [1]. Interestingly, in the experimentally determined crystal structure all the magnetic exchange couplings are completely frustrated by the underlying symmetry. Therefore, we conclude that the magnetic transition must driven by a Spin Jahn-Teller effect, in which the large spin degeneracy is relieved by a distortion of the crystal structure and an associated lowering of the structural symmetry. We investigate this distortion using high resolution x-ray experiments and DFT calculations. Furthermore, we discuss recent experimental studies of FeTi$_2$O$_5$ and the observed similarities to CoTi$_2$O$_5$, which leads us to conlcude that spin-phonon coupling can induce magnetic order in lower symmetry systems than previously reported.


*This work is supported by EPSRC (UK) grant EP/N023803/1. It made use of the STFC ISIS Facility (RAL, UK), the Swiss Muon Source (PSI, Switzerland), and the Univ. of Oxford Advanced Research Computing facility.

Single-Crystal Neutron Scattering Studies of Breathing Pyrochlore Ba$_3$Yb$_2$Zn$_5$O$_{11}$

SACHITH DISSANAYAKE (Presenter), WILLIAM STEINHARDT, ZHENZHONG SHI, STEPHEN J KUHN, Department of Physics, Duke University, NICHOLAS BUTCH, Center for Neutron Research, National Institute of Standards and Technology, MATTHIAS D FRONTZEK, Neutron Scattering Division, Oak Ridge National Laboratory, YIMING QIU, Center for Neutron Research, National Institute of Standards and Technology, DAVID E GRAF, National High Magnetic Field Laboratory and Department of Physics, Florida State University, HONGCHENG LU, CASEY MARJERRISON, SARA HARAVIFARD, Department of Physics, Duke University — Recently a new class of materials called Breathing pyrochlore compounds have attracted much attention. These systems consist of two alternating, opposing tetrahedra expanded and contracted, leading to differing intra- and inter-tetrahedra exchange interactions and the emergence of the Dzyaloshinskii-Moriya interaction due to loss of inversion symmetry. They are predicted to host exotic physics, including quantum spin ice state and the field-tunable Weyl magnon. In this talk we will present our recent magneto-transport and field-dependent diffuse and inelastic neutron scattering results measured on single crystal of the breathing pyrochlore compound Ba$_3$Yb$_2$Zn$_5$O$_{11}$.
1:15PM S37.00011: Powder inelastic neutron scattering of a spin-liquid candidate $\text{Ba}_3\text{ZnRu}_2\text{O}_9^*$

DANIEL PAJEROWSKI (Presenter), LIURUKARA SANJEEWA, MATTHEW BRANDON STONE, ZHENG GAI, Oak Ridge National Laboratory, JOSEPH KOLIS, Clemson University — $\text{Ba}_3\text{ZnRu}_2\text{O}_9$ (BZRO) is a 6-H perovskite compound that contains triangular lattice layers of $\text{Ru}^{5+}$ dimers, and was recently reported to have no signatures of long-range-magnetic-order down to 37 mK and therefore put forward as a spin-liquid candidate.[1] We present inelastic neutron scattering measurements on BZRO powder that show a magnetic feature with a momentum dependence that is similar to the Ru-magnetic-form-factor, a peak energy intensity at 25 meV, and no obvious dispersive character. This magnetic mode is then considered in the context of density functional theory calculations and magnetization measurements. Comparisons are then made to the historical work on the analogous $\text{Ba}_3\text{CaRu}_2\text{O}_9$.[2]


*This research used resources at the Spallation Neutron Source and High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

1:27PM S37.00012: Magnetic excitations of the classical spin-liquid $\text{MgCr}_2\text{O}_4^*$

MARTIN MOURIGAL, XIAOJIAN BAI, Georgia Institute of Technology, JOSEPH PADISON, Cambridge, ELIOT KAPIT, Mines, SEYED KOOPHAYEH, Johns Hopkins, JIAJIA WEN, SLAC, SIAN E DUTTON, Cambridge, COLLIN BROHOLM, Johns Hopkins, JOHN CHALKER, Oxford, ANDREI T SAVICI (Presenter), GARRETT E GRANROTH, ALEXANDER I KOLESNIKOV, ORNL — We report a comprehensive inelastic neutron-scattering study of the frustrated pyrochlore antiferromagnet $\text{MgCr}_2\text{O}_4$ in its cooperative paramagnetic regime. Theoretical modeling yields a microscopic Heisenberg model with exchange interactions up to third-nearest neighbors, which quantitatively explains all the details of the dynamic magnetic response. Our work demonstrates that the magnetic excitations in $\text{MgCr}_2\text{O}_4$ are faithfully represented in the entire Brillouin zone by a theory of magnon excitations propagating in a highly-correlated paramagnetic background. Our results also suggest that $\text{MgCr}_2\text{O}_4$ is proximate to a spiral spin-liquid phase distinct from the Coulomb phase, what has implications for the magneto-structural phase transition observed at low temperature in this material.

*This was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under awards number DE-SC-0018660 and DE-FG02-08ER46544.

1:39PM S37.00013: Possible Random Singlet phase in the $S = 1/2$ magnet $\text{Y}_2\text{CuTiO}_6^*$

AVINASH MAHAJAN (Presenter), SUSANTA KUNDU, Department of Physics, Indian Institute of Technology Bombay, Powai Mumbai 400076, India, JEAN-CHRISTOPHE ORAIN, muSR group, Paul Scherrer Institute, 5232 Villigen, Switzerland, MICHAEL BAENITZ, Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — $\text{Y}_2\text{CuTiO}_6$ contains edge-shared triangular planes where the vertices are occupied by magnetic Cu and nonmagnetic Ti atoms in equal proportion. In spite of the large dilution of the triangular magnetic lattice, the magnetic susceptibility shows a large, AF $\theta_{\text{CW}}$ of about 240 K without any sign of ordering down to 1.8 K. No bifurcation is observed in the ZFC/FC magnetisation data in a low field of 50 Oe, down to 0.5 K. Likewise, the heat capacity shows no anomalies and the magnetic contribution has a power law behaviour at low-temperatures. Our muSR measurements down to 50 mK also do not show any signs of ordering. These observations are typical of potential quantum spin liquid systems. In the present case, however, the magnetic heat capacity $C_m$ depends on the magnetic field $H$. We observed that the data could be scaled such that $H^\gamma C_m/T$ vs $T/H$ follows a universal curve with $\gamma = 0.6$. Such a scaling behaviour has been suggested in systems with random singlet formation. The randomness of exchange coupling in $\text{Y}_2\text{CuTiO}_6$ might be due to the random occupation of Cu and Ti on the vertices of triangles. It is nevertheless surprising that in spite of the large (50%) depletion of the lattice, no spin freezing is observed.

*AVM and SK thank IIT Bombay and DST for support.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S38 GMAG DCMP DMP: Frustrated Square Lattice and Other Low-Dimensional Structures BCEC 206B - Oleg Tchernyshyov, Johns Hopkins University - Tag(s): Focus
Quantum Spin Liquid with Broken Unidirectional Symmetry in a Square Lattice Spin-1 Model

WENJUN HU, Department of Physics and Astronomy, Rice University, SHOUHSHU GONG, Department of Physics and International Research Institute of Multidisciplinary Science, Beihang University, Beijing, HSIN-HUA LAI, HAOYU HU, QIMIAO SI, ANDRIY NEVIDOMSKYY (Presenter), Department of Physics and Astronomy, Rice University — Quantum spin liquids (QSL) are known to arise in strongly frustrated spin systems as a result of competing interactions. Here we consider a spin-1 model on a square lattice, where despite the absence of geometric frustration, competition between the nearest neighbor Heisenberg ($J_1$) and biquadratic ($K_1$) interactions results in a QSL around the $J_1 = K_1$ point, as evidenced by our density matrix renormalization group (DMRG) studies. At that point, the model has an emergent SU(3) symmetry and calculations based on $N=3$ flavor-wave theory indicate the presence of large quantum fluctuations that destabilize the nearby antiferromagnetic and quadrupolar orders. What emerges is a QSL with no long-range order in spin or quadrupolar channels, which nevertheless has fluctuations peaked at the wavevector $(\pi, 2\pi/3)$ and spontaneously breaks the $C_4$ rotational symmetry of the square lattice [1]. We demonstrate, by studying an anisotropic model, that this lattice-nematic spin liquid is distinct from the limit of weakly coupled Haldane chains. Instead, analysis of the spectral gaps and entanglement entropy is consistent with the QSL being either gapless or having a very small gap.


Characterization of quantum spin liquids and their spinon band structures via functional renormalization

JOHANNES REUTHER (Presenter), MAX HERING, JONAS SONNENSchein, Physics Department, Freie Universitaet Berlin, YASIR IQBAL, Department of Physics, Indian Institute of Technology Madras — We combine the pseudofermion functional renormalization group (PFFRG) method with a self-consistent Fock-like mean-field scheme to calculate low-energy effective theories for emergent spinon excitations in spin-1/2 quantum spin liquids. Using effective spin interactions from PFFRG as an input for the Fock equation and allowing for the most general types of free spinon ansatze as classified by the projective symmetry group (PSG) method, we are able to systematically determine spinon band structures for spin-liquid candidate systems beyond mean-field theory. We apply this approach to the antiferromagnetic J1-J2 Heisenberg model on the square lattice and to the antiferromagnetic nearest-neighbor Heisenberg model on the kagome lattice. For the J1-J2 model, we find that in the regime of maximal frustration a SU(2) pi-flux state with Dirac spinons yields the largest mean-field amplitudes. For the kagome model, we identify a gapless Z2 spin liquid with a small circular spinon Fermi surface and approximate Dirac-cones at low but finite energies.

Critical Level Crossings and Gapless Spin Liquid in the Square-Lattice Spin-1/2 J1-J2 Heisenberg Antiferromagnet

LING WANG (Presenter), Beijing Computational Science Research Center, ANDERS W SANDVIK, Physics Department, Boston University — We use the density matrix renormalization group method to calculate several energy eigenvalues of the frustrated $S=1/2$ square-lattice J1-J2 Heisenberg model on $2L \times L$ cylinders with $L \leq 10$. We identify excited-level crossings versus the coupling ratio $g=J2/J1$ and study their drifts with the system size $L$. The lowest singlet-triplet and singlet-quintuplet crossings converge rapidly (with corrections $\propto L^{-2}$) to different $g$ values, and we argue that these correspond to ground-state transitions between the Neel antiferromagnet and a gapless spin liquid, at $gc1=0.46$, and between the spin liquid and a valence-bond solid at $gc2=0.52$. Previous studies of order parameters were not able to positively discriminate between an extended spin liquid phase and a critical point. We expect level-crossing analysis to be a generically powerful tool in density matrix renormalization group studies of quantum phase transitions.

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*L.W. is supported by the National Key Research and Development program of China (Grant No. 2016YFA0300603), and the National Natural Science Foundation of China (Grants No. NSFC-11734002 and No. NSFC-11474016). A. W. S. was supported by the NSF under Grants No. DMR-1410126 and No. DMR-1710170, and by a Simons Investigator Grant.
11:51AM S38.00004: Observation of topological phenomena induced by frustration and quantum fluctuations in a programmable lattice of 1,800 qubits  [Invited] ISIL OZFIDAN (Presenter), ANDREW KING, D-Wave Systems, JUAN CARRASQUILLA, Vector Institute, JACK RAYMOND, MOHAMMAD AMIN, D-Wave Systems — The celebrated work of Berezinskii, Kosterlitz and Thouless in the 1970s [1] revealed exotic phases of matter governed by topological properties of low-dimensional materials such as thin films of superfluids and superconductors. Key to this phenomenon is the appearance and interaction of vortices and antivortices in an angular degree of freedom—typified by the classical XY model—due to thermal fluctuations. In the 2D Ising model this angular degree of freedom is absent in the classical case, but with the addition of a transverse field it can emerge from the interplay between frustration and quantum fluctuations. Consequently a Kosterlitz-Thouless (KT) phase transition has been predicted in the quantum system by theory and simulation [2]. Here we demonstrate a large-scale quantum simulation of this phenomenon in a network of 1,800 in situ programmable superconducting flux qubits arranged in a fully-frustrated square-octagonal lattice [3]. Essential to the critical behavior, we observe the emergence of a complex order parameter with continuous rotational symmetry, and the onset of quasi-long-range order as the system approaches a critical temperature. We use a simple but previously undemonstrated approach to statistical estimation with an annealing-based quantum processor, performing Monte Carlo sampling in a chain of reverse quantum annealing protocols. Observations are consistent with classical simulations across a range of Hamiltonian parameters. We anticipate that our approach of using a quantum processor as a programmable magnetic lattice will find widespread use in the simulation and development of exotic materials.


12:27PM S38.00005: Thermodynamics of a frustrated quantum magnet on a square lattice* VIVEK BHARTIYA (Presenter), KIRILL POVAROV, ZEWU YAN, ANDREY ZHELUDEV, Department of Physics, ETH Zurich — We report the magnetic and calorimetric measurements in single crystal samples of the square lattice $J_1 - J_2$ quantum antiferromagnet BaCdVO(PO4)2 [1]. An investigation of the scaling of magnetization reveals a “dimensionality reduction” indicative of a strong degree of geometric frustration. Below a characteristic temperature less than 150 mK we observe the emergence of a new strongly fluctuating quantum phase close to full magnetic saturation. It is separated from the magnetically ordered state by 1-st and 2-nd order phase transitions, depending on the orientation of the applied magnetic field. We suggest that the new phase may indeed be the theoretically predicted spin nematic state.

*This work was supported by Swiss National Science Foundation, Division II.

12:39PM S38.00006: Improving the full update and probing frustrated J1-J2 spin-1/2 model on a square lattice JURAJ HASIK (Presenter), FEDERICO BECCA, International School for Advanced Studies — The optimization of infinite projected entangled-pair state (iPEPS) ansatz represents the main challenge in obtaining accurate ground states of lattice models. In this work, we propose a simple modification of the full-update algorithm [1] and benchmark it on a frustrated $J_1-J_2$ spin-1/2 Heisenberg model on a square lattice. Using an improved full-update, we obtain extremely accurate ground-state energies but, most importantly, also values of the magnetization that are comparable with previous results from more complex variational optimization [2,3]. Moreover, we show that the recent scaling technique based on the correlation length [4,5] leads to a considerable improvement in analysis of the phase diagram.

12:51PM S38.00007: Accuracy of Restricted Boltzmann Machine wavefunctions for frustrated spin systems
FRANCESCO FERRARI (Presenter), SISSA-ISAS, International School for Advanced Studies, Trieste (Italy), JUAN CARRASQUILLA, Vector Institute for Artificial Intelligence, Toronto (Canada), FEDERICO BECCA, SISSA-ISAS, International School for Advanced Studies, Trieste (Italy) — Artificial neural networks (ANNs) constitute a powerful tool to approximate multi-variable functions in a plethora of different contexts. In the quest for an efficient representation of the ground state wavefunction of many-body quantum systems, ANNs have recently emerged as a flexible framework to construct variational ansätze [1]. We investigate the accuracy of Restricted Boltzmann Machine (RBM) networks as many-body Jastrow factors for the study of spin systems. In particular, we apply the RBM factor on top of a Gutzwiller-projected fermionic wavefunction [2], in order to construct a variational ansatz for the ground state of the spin-1/2 J1-J2 Heisenberg model in two dimensions. In the magnetically ordered phase (J2=0), Monte Carlo results show that the RBM correlator yields a significant improvement of the variational energy [2]. On the other hand, when competing interactions are turned on and the system becomes highly frustrated, the energy gain due to the RBM becomes remarkably less pronounced.


1:03PM S38.00008: Magnetic superstructures inside the ⅓ and ½ magnetization plateaux in Ba2CoTeO6 revealed by magnetostriction and magnetocaloric effect measurements* DAGMA WEICKERT (Presenter), National High Magnetic Field Laboratory, Florida State University, CAROLINA CORVALAN-MOYA, CONICET, NCNEA-UNTREF, MYRON B SALAMON, University of Texas at Dallas, CHAO DONG, KOICHI KINDO, YOSHIMITSU KOHAMA, ISSP, Tokyo University, NOBUYUKI KURITA, HIDEKAZU TANAKA, Tokyo Tech — Ba2CoTeO6 is composed of two nearly decoupled magnetic spin-systems stacked as alternating 2D layers along the crystallographic c-direction in the trigonal crystal structure. Subsystem A is a S = ½ triangular Heisenberg antiferromagnet that orders at TA = 3K. System B is a J1-J2 honeycomb Ising antiferromagnet with ordering temperature TB = 12K. Both underlying spin-models are interesting due to geometrical frustration (A) and bond frustration (B) causing magnetic plateaux upon the application of magnetic fields H. We present a combination of magnetostriction and magnetocaloric effect (MCE) measurements in high pulsed and static magnetic fields to map out the phase diagram for H ll and perp. to the A and B layers. We observe distinct anomalies in the sample length ΔL/L as a function of field and temperature indicating phase transitions as well as signatures in the MCE measurement indicating a change of entropy. These anomalies are accompanied by significant hysteresis in decreasing compared to increasing magnetic fields.

*A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490 and DMR-1644779, the US Department of Energy, and the State of Florida.

1:15PM S38.00009: Spin structure and dynamics of Pb2VO(PO4)2* SIMON BETTLER (Presenter), FLORIAN LANDOLT, ÖMER M. AKSOY, ZEWU YAN, Laboratorium für Festkörperphysik, ETH Zurich, CH-8093 Zurich, ERIC RESSOUCHE, Univ. Grenoble Alpes, CEA, INAC-MEM, F-38000 Grenoble, SERGEI ZYVAGIN, ALEXEY PONOMARYOV, Dresden High Magnet Field Lab HLD, Helmholtz Zentrum Dresden Rossendorf, KETTY BEAUVOIS, Univ. Grenoble Alpes, CEA, INAC-MEM, F-38000 Grenoble, YIMING QIU, NIST Centre for Neutron Research, National Institute of Standards and Technology, STEPHANE RAYMOND, Univ. Grenoble Alpes, CEA, INAC-MEM, F-38000 Grenoble, SEVERIAN GVASALIYA, ANDREY ZHELUDEV, Laboratorium für Festkörperphysik, ETH Zurich, CH-8093 Zurich — Pb2VO(PO4)2 is one of few quantum magnets proposed to realize the frustrated spin-1/2 square lattice with ferromagnetic nearest-neighbor exchange. We have determined the magnetic structure and excitation spectrum of Pb2VO(PO4)2 by means of single crystal neutron diffraction and neutron spectroscopy going beyond previous limited powder sample studies. The spin dynamics show qualitative differences – which were independently confirmed by ESR – from what is expected for an ideal square lattice. These are attributed to having as many as three nearest neighbor and two next-nearest neighbor. We discuss the implications for closely related materials proposed to realize a frustrated square lattice.

*This work was supported by the Swiss National Science Foundation, Division 2 Access to MACS was provided by the Center for High Resolution Neutron Scattering, a partnership between the National Institute of Standards and Technology and the National Science Foundation under Agreement No. DMR-1508249.
1:27PM S38.00010: Magnetisation process in the rare earth tetraborides, NdB₄ and HoB₄
OLEG PETRENKO (Presenter), University of Warwick, DANIEL BRUNT, National Physics Laboratory, UK, NAVID QURESHI, Institut Laue-Langevin, France, GEETHA BALAKRISHNAN, DANIEL MAYOH, MARTIN LEES, University of Warwick — We report a study into the field-induced magnetisation of the two frustrated rare earth tetraborides, HoB₄ and NdB₄. NdB₄ shows a fractional magnetisation plateau occurring at $M/M_{\text{sat}} \approx 1/5$ before saturating in a field of 33 kOe. On cooling down to 0.5 K the temperature dependent susceptibility of NdB₄ shows an unconventional transition where the system returns to the zero field antiferromagnetic state from a higher-temperature ferrimagnetic state. We are able to reconstruct the magnetic phase diagram of NdB₄ from the magnetisation, susceptibility and resistivity measurements for both $H//c$ and $H\perp c$. For HoB₄, the most interesting behaviour is found at the lowest temperature of 0.5 K, where the field dependent magnetisation demonstrates a new fractional 1/2-magnetisation plateau. Further insight into the relations between the exchange interactions and single ion effects is gained through high-field magnetisation measurements in both HoB₄ and NdB₄.

1:39PM S38.00011: Evolution of the spin-flop antiferromagnetic transition and the emergence of frustration in saw-tooth lattice Mn₂SiS₄₋ₓSex (x = 0 - 4) chalcogenides
HARIHARAN NHALIL, Department of Chemistry and Biochemistry, University of Oklahoma, RAJU BARAL, ADRIAN COSIO, BETHUEL O KHAMALA, SRINIVASA RAO SINGAMANENI, University of Texas, El Paso, MAGDALENA FITTA, Department of Magnetic Materials and Nanostructures, 3The Henryk Niewodniczanski Institute of Nuclear Physics -PAN, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas, El Paso, DANIEL ANTONIO, KRZYSZTOF GOFRYK, Idaho National Laboratory, BAYRAMMURAD SAPAROV, Department of Chemistry and Biochemistry, University of Oklahoma, HARIKRISHNAN NAIR (Presenter), University of Texas, El Paso — The olivine $A_2BX_4$ structure takes $Pnma$ symmetry where the $A$ site forms the triangle-based one dimensional saw-tooth chain structure and are known for optoelectronics, thermoelectric and magnetic applications. We studied the olivines, Mn₂SiS₄₋ₓSex (0 < x < 4), using magnetization, specific heat, thermal conductivity and ab initio density functional theory (DFT) calculations and tracked the evolution of spin-flop transition and frustration. It is seen that the antiferromagnetic transition temperature $T_N$ shows a linear decrease from 86 K for Mn₂SiS₄ towards 66 K for Mn₂SiSe₄ as $x$ varied; whereas the critical field for spin-flop varied non-linearly. The magnetic phase transitions characterized using specific heat reveal very low magnetic entropy evolved at the $T_N$, suggesting the underlying frustrated nature of the Mn²⁺ ions in the saw-tooth like triangular arrangement. A semiconducting-like thermal conductivity is revealed by the olivines where the DFT calculations show a small energy gap (~0.5 eV) between the valence and conduction bands. Our results are explained based on the emergence of frustration in the triangular units of the saw-tooth Mn lattice.

*UTEP is acknowledged for the faculty start-up grant.

1:51PM S38.00012: Quantum disordered state in the $J_{\text{eff}}=1/2$ triangular lattice antiferromagnet NaYbO₂
MITCHELL BORDELON (Presenter), Materials, University of California Santa Barbara, ERIC KENNEY, Physics, Boston College, LORENZO POSTHUMA, Chemistry, University of California Santa Barbara, MARZIEH KAVAND, YUANQI LYU, MARK STEPHEN SHERWIN, Physics, University of California Santa Barbara, CRAIG BROWN, NIST Center for Neutron Research, MICHAEL JOHN GRAF, Physics, Boston College, LEON BALENTS, Physics, University of California Santa Barbara, STEPHEN WILSON, Materials, University of California Santa Barbara — There has been a great deal of interest in realizing unconventional quantum disordered magnetic ground states in frustrated antiferromagnets driven by strong fluctuations in the small spin limit. Experimentally, real materials often preclude this limit due to symmetry-breaking structural or magnetic processes or innate chemical disorder that lifts ground state degeneracies. NaYbO₂ ($R-3m$) contains geometrically-frustrated triangular layers of $J_{\text{eff}}=1/2$ Yb³⁺ ions with ideal chemical order, a robust lattice geometry to 330 mK and lacks conventional signs of magnetic ordering under zero-field conditions to 50 mK. Under a moderate applied field, NaYbO₂ enters an antiferromagnetic phase below 1 K. This material stands as an appealing candidate to realize a dynamically-disordered quantum ground state driven by highly-anisotropic, spin-orbit entangled Yb ions whose transition into a nearby field-driven magnetically-ordered phase can be probed experimentally and theoretically.

*DOE, Office of Science, Basic Energy Sciences under Award DE-SC0017752
Competing paramagnetic phases and itinerant magnetic frustration in SrCo$_2$As$_2$*  

BING LI (Presenter), BENJAMIN UELAND, WAGEESHA T JAYASEKARA, Ames Laboratory, Iowa State University, DOUGLAS L ABERNATHY, Oak Ridge National Laboratory, SANGEETHA N. S., DAVID C JOHNSTON, QING-PING DING, YUJI FURUKAWA, PETER P. ORTH, ANDREAS KREYSSIG, ALAN IRA GOLDMAN, ROBERT MCQUEENEY, Ames Laboratory, Iowa State University — Cobalt arsenides with a layered square lattice tend to be itinerant ferromagnets. However, using inelastic neutron scattering we find in SrCo$_2$As$_2$ stripe-type antiferromagnetic (AF) spin fluctuations, though no long-range AF order is observed down to 50 mK. The stripe phase competes with the itinerant ferromagnetism and wins below 115 K, resulting in the development of AF spin fluctuations concomitant with a suppression of the uniform magnetic susceptibility. Comparison of our experimental data to exact diagonalization and classical Monte Carlo simulations of a frustrated local-moment J$_1$-$J_2$ model suggests that itinerancy enhances frustration. We conclude that SrCo$_2$As$_2$ is a candidate for frustrated itinerant magnetism and harbors unique frustrated magnetism on the boundary between itinerant ferromagnetic and stripe AF instabilities.

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Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S39 GMAG DMP: Magnetic Memories and Computing  

Research Center - Tag(s): Focus

11:15AM S39.00001: Ultrafast p-bits using synthetic antiferromagnets*  

JAN KAISER (Presenter), KEREM Y CAMSARI, SUPRIYO DATTA, PRAMEY UPADHYAYA, Purdue University — Various applications ranging from cryptography to stochastic computing need random number generators (RNGs) which can be implemented in hardware using magnetic tunnel junctions (MTJs) with low barrier unstable ferromagnets (LBMs). It has been shown that with proper design such ferromagnets can show random fluctuations at GHz speeds. In this talk using stochastic LLG simulations, we will show that synthetic antiferromagnets (SAFs) built out of LBMs can fluctuate with even higher speeds. Using full SPICE simulations, we show that MTJs using SAFs can be combined with standard transistors to provide a fast tunable RNG or p-bit which can speed up numerous applications.

*This work was supported in part by the Center for Probabilistic Spin Logic for Low-Energy Boolean and Non-Boolean Computing (CAPSL), one of the Nanoelectronic Computing Research (nCORE) Centers as task 2759.005, a Semiconductor Research Corporation (SRC) program sponsored by the NSF through ECCS 1739635.

11:27AM S39.00002: Physical meaning of the full width half maximum of switching time distribution in ferromagnetic nano-structure  

JUNG-HWAN MOON, Advanced Technology Development Team, Semiconductor R&D Center, Samsung Electronics Co. Ltd., TAE YOUNG LEE, New Memory Device and Process Integration Group, SK Hynix, CHUN-YEOL YOU (Presenter), Department of Emerging Materials Science, DGIST — Generally, line width or full width half maximum of physically measurable quantity. For example, the line with of RLC is related with quality factor of the circuit, and one of ferromagnetic resonance is related with damping constant of the ferromagnetic materials. The switching time of the ferromagnetic nano-structure has been actively studied because of its importance in the physics and device applications. And the switching behavior itself is well described by Fokker Planck Equation (FPE) [1]. Recently, we found that the full width of half maximum (FWHM) of switching time distribution is closely related with the damping constant [2]. We solved FPE with high barrier approximation, we obtained the FWHM is inversely proportional to the external applied field, and the damping constant can be obtained from the slope. Surprisingly enough, the obtained relation is quite similar to the equation for the damping constant and line width of the ferromagnetic resonance, while its underlying physics are totally different.

MD ALI AZAM (Presenter), DHIRITIMAN BHATTACHARYA, Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, CAROLINE ANNE ROSS, Department of Materials Science and Engineering, Massachusetts Institute of Technology, DAMIEN QUERLIOZ, Centre de Nanosciences et de Nanotechnologies, University of Paris-Sud, JAYASIMHA ATULASIMHA, Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University — We present micromagnetic simulation of voltage-controlled spintronic neuron and synapse by utilizing domain wall (DW) motion in the free layer of a Magnetic Tunnel Junction (MTJ). The free layer is a soft ferromagnet (CoFeB) exchange coupled to a magnetostrictive Rare Earth Iron Garnet (REIG) racetrack with perpendicular magnetic anisotropy (PMA) deposited on a heavy metal layer. The whole stack is fabricated on a piezoelectric substrate. Chiral domain walls can be introduced in the free layer due to PMA and Dzyaloshinskii-Moriya Interaction (DMI) [1, 2], translated with spin orbit torque by applying a current pulse to the heavy metal layer and arrested at specific location along the racetrack domain by tuning the bulk PMA of the magnetic layer using a highly localized voltage-generated strain from the piezoelectric layer. Micromagnetic simulations with realistic defects and thermal noise will be presented for an energy efficient neuron and non-volatile programmable synapse using this device.

References:

* M. A. A, D.B and J.A acknowledge NSF CAREER grant CCF-1253370.

PANAGIOTIS CH. FILIPPOU, IBM Almaden Research Center, JAЕWOO JEONG, New Memory Technology Lab, Samsung Electronics, YARI FERRANTE (Presenter), SEE-HUN YANG, TEYA TOPURIA, MAHESH G. SAMANT, IBM Almaden Research Center, STUART S P PARKIN, Max Plank Institute for Microstructure Physics — The task of improving the performances of next-generation spin-transfer torque magnetoresistive random access memory (STT-MRAM) requires the use of new magnetic materials with high perpendicular magnetic anisotropy (PMA) and low magnetic moment within the magnetic tunnel junction, i.e. MRAM storage element. Heusler alloys are a large family of compounds with tunable magnetic properties. Some of these have a tetragonal structure with its elongated axis perpendicular to the film plane and thus they may display PMA due to their structure broken symmetry. However, so far, PMA has been observed only for 50Å-thick films, i.e. too thick for technological applications. In this talk we demonstrate that X3Z (X=Mn; Z=Ge,Sn,Sb) tetragonal Heusler films, as thin as only 1 unit cell, can be developed by using a novel chemical templating technique. We show this can be achieved by growing the Heusler films, even at room temperature, onto atomically-ordered X’Z’ (X’=Co; Z’=Al,Ga,Ge,Sn) underlayers that promote chemical ordering within the Heusler films. Excellent PMA with square hysteresis is found in Mn3Z layers that are only 1-2 unit cells thick. The possibility of preparing ultrathin Heusler films with PMA makes possible their technological application for a wide range of spintronic devices.

JAMES VOORHEIS (Presenter), VASYL S TYBERKEVYCH, Oakland University — Neuromorphic signal processing is one of the most promising post-Von Neumann computational paradigms [1]. Recently, it was proposed that antiferromagnetic (AFM) spin Hall oscillators, operating in a sub-critical regime, can function as ultra-fast artificial neurons [2, 3]. One of the characteristic features of AFM neurons is the inertial nature of their dynamics: a sufficiently large input spike may induce not one, but several output spikes. Here, we show that this feature can be used for effective encoding and decoding of information from conventional binary to neuromorphic format. The neuromorphic encoder has several inputs, which represent information in parallel binary format, and one output neuron, which produces a train of several spikes. The number of spikes produced by the output neuron equals the input binary code. The decoder reverses this operation, splitting one multi-train input into several binary outputs. The proposed neuromorphic encoder/decoder can be used as an interface between neuromorphic and conventional circuits.

12:15PM S39.00006: Voltage controlled memory device based on fixed magnetic skyrmions*  DHRITIMAN BHATTACHARYA (Presenter), Virginia Commonwealth University, SEYED ARMIN RAZAVI, HAO WU, KANG L. WANG, University of California, Los Angeles, JAYASIMHA ATULASIMHA, Virginia Commonwealth University — Manipulating static magnetic skyrmions with voltage control of magnetic anisotropy (VCMA) can be utilized to design energy efficient memory devices with reduced device footprint. Using micromagnetic simulation, we demonstrate such devices. With application of a sequential positive and negative voltage pulse, two skyrmionic (core-up and core-down) and two ferromagnetic (up and down) states can be achieved [1]. Further, starting from a ferromagnetic state, a voltage pulse that reduces PMA can induce reversal via skyrmion breathing [2]. As a proof of concept experiment, we demonstrate such VCMA induced manipulation of magnetic skyrmions in an antiferromagnet/ferromagnet/oxide heterostructure film. We observed annihilation of skyrmions while increasing PMA and formation of more skyrmions by reducing PMA. This reversible creation and annihilation of skyrmions could potentially lead to novel skyrmion based memory devices.


*D.B and J.A acknowledge NSF CAREER grant CCF-1253370, VCU Quest Commercialization Grant and Virginia Microelectronics Seed Grant. S. A. R., H. W., and K. W. acknowledge NSF (ECCS 1611570) and NSF-TANMS.

12:27PM S39.00007: YIG-based microwave magnonic circuits at millikelvin temperatures*  ALEXY KARENOWSKA (Presenter), SANDOKO KOSEN, ARJAN F. VAN LOO, University of Oxford — The experimental exploration of microwave magnonic systems at millikelvin temperatures has attracted significant recent interest. Work in this area is motivated both by the desire to better understand the behaviour and physics of these systems at very low temperatures, and their potential application in solid-state quantum information processing. In this talk, we explore recent experimental results from a range of investigations into the low-temperature properties of yttrium iron garnet (YIG) -based magnonic systems [1-4]. We discuss related technical and materials considerations relevant to successful quantum magnonic experiments, and offer a perspective on future work in this area


*The authors acknowledge EPSRC grant EP/K032690/1 and SK is grateful for the support of LPDP Indonesia.

12:39PM S39.00008: Broadband communication and information processing with edge spin waves*  FARKHAD ALIEV (Presenter), ANTONIO LARA, DIEGO CASO, CESAR GONZALEZ-RUANO, Autonomous University of Madrid, KONSTANTIN GUSLIENKO, , Universidad del País Vasco and Ikerbasque, the Basque Foundation for Science, JOSE LUIS PRIETO, Universidad Politecnica de Madrid — Spin waves, being usually reflected by domain walls, could also be channeled along them. Here we discuss quasi one-dimensional spin waves in Permalloy dots of different geometries and in different magnetic states. Recent studies allowed observation of spin waves along domain walls in rectangular, circular [1] and triangular dos in the ground or metastable states. Triangular dots could also present edge pinned inhomogeneous magnetic states, depending on the direction of the external magnetic field. These edge domain walls yield the interesting, and potentially applicable to real devices property of broadband spin waves confinement to the edges of the structure [2,3] with capabilities to be redirected at angles exceeding 100 degrees. We also show how these waves could be generalized for arbitrary shapes and propose few devices (such as edge spin wave interferometers, controllers or splitters) where edge spin waves could be implemented. [1] F. G. Aliev, et al., Phys. Rev. B84, 144406 (2011); [2] A. Lara, V. Metlushko, F. G. Aliev, J. Appl. Phys. 114, 213905 (2013); [3] A. Lara, J. Robledo, K.Y. Guslienko, F. G. Aliev, Scientific Reports, 7: 5597 (2017).

the drive frequency matches with $f_0$. These novel phenomena can be used to realize coupled oscillatory nanomagnets faster, analogous to temperature annealing. We further demonstrate the phenomenon of stochastic resonance in our underlayer. Depending on the polarity and strength of the feedback, the magnetization fluctuation becomes slower or unstable nanomagnets with weak perpendicular anisotropy made from Ta/CoFeB/MgO stack. The magnetization of such nanomagnets shows random telegraphic fluctuation with a mean that is tunable by the giant spin Hall effect (GSHE) current generated in the Ta underlayer. These nanomagnets form stochastic oscillators with a natural frequency $f_0$, given by $f_0 = (t_{up} + t_{dn})^{-1}$, where $t_{up}$ and $t_{dn}$ are the average dwell time of the magnetization in the “up” and “down” state. We demonstrate tuning of $f_0$ of individual nanomagnets by electrical feedback of the magnetization state to the GSHE underlayer. Depending on the polarity of the feedback, the magnetization fluctuation becomes slower or faster, analogous to temperature annealing. We further demonstrate the phenomenon of stochastic resonance in our nanomagnets, where the magnetization follows a weak external periodic drive through the GSHE underlayer only when the drive frequency matches with $f_0$. These novel phenomena can be used to realize coupled oscillatory nanomagnet networks with dynamic connectivity, which alleviates the full connectivity requirement in a network of $N$ oscillators from $N^2$ weighted connections to $N$ homogenous connections.

1:15PM S39.00011: Electrical annealing and stochastic resonance in superparamagnets for oscillatory networks with dynamic connectivity PUNYASHLOKA DEBASHIS (Presenter), PRAMEY UPADHYAYA, ZHIHONG CHEN, Electrical and Computer Engineering, Purdue University — In this work, we report electrical annealing and stochastic resonance in thermally unstable nanomagnets with weak perpendicular anisotropy made from Ta/CoFeB/MgO stack. The magnetization of such nanomagnets shows random telegraphic fluctuation with a mean that is tunable by the giant spin Hall effect (GSHE) current generated in the Ta underlayer. These nanomagnets form stochastic oscillators with a natural frequency $f_0$, given by $f_0 = (t_{up} + t_{dn})^{-1}$, where $t_{up}$ and $t_{dn}$ are the average dwell time of the magnetization in the “up” and “down” state. We demonstrate tuning of $f_0$ of individual nanomagnets by electrical feedback of the magnetization state to the GSHE underlayer. Depending on the polarity and strength of the feedback, the magnetization fluctuation becomes slower or faster, analogous to temperature annealing. We further demonstrate the phenomenon of stochastic resonance in our nanomagnets, where the magnetization follows a weak external periodic drive through the GSHE underlayer only when the drive frequency matches with $f_0$. These novel phenomena can be used to realize coupled oscillatory nanomagnet networks with dynamic connectivity, which alleviates the full connectivity requirement in a network of $N$ oscillators from $N^2$ weighted connections to $N$ homogenous connections.

1:27PM S39.00012: Fabrication and programming of nanomagnet arrays for nanoscale magnetic field synthesis Tzu-Ming Lu (Presenter), Ezra Bußmann, Sandia National Laboratories — Nanoscale magnetic field synthesis finds applications in band structure engineering, nano-particle manipulation, and local spin resonance. In the presence of a 1D spatially rotating magnetic field, the band structure of a 1D electron system without spin-orbit coupling can be engineered such that an effective spin-orbit (SO) gap appears in the energy dispersion. Inside the effective SO gap the spin degeneracy is removed. We present our results on fabricating nanomagnet arrays using two magnetic materials with distinct coercivities, programming the nanomagnet arrays using a global external magnetic field, and characterizing the magnetization configuration using magnetic force microscopy.

*This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories, and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. DOE’s National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.
1:39PM S39.00013: Magnetic tunnel junction synapses for neuromorphic computing  
BENJAMIN MADON (Presenter), M A MUEED, NOEL ARELLANO, BRIAN HUGHES, IBM Research, Almaden, San Jose, California 95120, United States, MATTHIEU GRELIER, ANGELO COUTO, ESPCI, Paris, 75005, France, ERIC BILLAUD, Ecole polytechnique, Palaiseau, 91128, France, SPENCER MATONIS, University of Connecticut, Storrs, Connecticut, 06269, United States, AAKASH PUSHP, IBM Research, Almaden, San Jose, California 95120, United States — Deep learning algorithms are now widely used. However, the amount of computation power they require to run on conventional CMOS electronics remains high. Consequently, there is an important need for specialized fast and energy-efficient processors tailored for deep learning. We believe that magnetic tunnel junctions in a crossbar array potentially have all the required characteristics of an ideal synapse: high resistance (kOhms), gigahertz speed and symmetric and bi-directional partial switching behavior.

Following up on the pioneering work of Lequeux et al. [1], we have studied different device geometries and material sets. Here we demonstrate nanodevices with resistances on the order of several kiloohms in which several intermediate resistance steps were obtained and their controlled partial switching behavior were achieved using nanosecond pulses.


1:51PM S39.00014: Magnetoelectric device read-out schemes based on electric resistivity measurements in heavy metal Hall bar structures*

ATHER MAHMOOD (Presenter), WILL ECHTENKAMP, JUNLEI WANG, CHRISTIAN BINEK, University of Nebraska - Lincoln — Controlling magnetism by electrical means is a key challenge in the field of spintronics and essential for energy efficient devices in computing. Previously suggested magnetoelectric MRAMs suffer from detrimental effects associated with the magnetization reversal of a ferromagnetic layer. Eliminating a ferromagnet reduces the energy-delay product by eliminating the need to reverse a ferromagnet and us the intrinsically high switching speed of antiferromagnets (AFM). We study the electrically-controlled boundary magnetization of the AFM magnetoelectric (ME) chromia in thin films using Pt as a sensing layer. We provide evidence that the main contribution to the anomalous Hall effect (AHE)-signal in chromia/heavy metal (HM) devices originates from spin Hall magnetoresistance and not from the proximity induced magnetization in the HM. To accomplish this, we investigate the temperature, magnetic field, and Pt-thickness dependence of the transverse and longitudinal resistivity. Our results promise a pathway to optimize AHE readout, overcoming energy-delay constraints accompanying magnetization reversal in ferromagnets.

*This work was supported through MRSEC DMR-1420645, by E2CDA a joint initiative between NSF and SRC, by NRI & the Nebraska Center for Materials and Nanoscience.

2:03PM S39.00015: Anderson localization in transition metal oxides and its application in neuromorphic circuitry*

CHRISTOPHER SINGH (Presenter), Binghamton University, KEITH T BUTLER, ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, WEI-CHENG LEE, Binghamton University — It has become increasingly clear that the performance of modern computing architectures is reaching a quantum mechanical road-block, and that neuromorphic computing, a brain inspired computing model, is a very promising paradigm in going beyond the von Neumann computing architecture. At the very core of this technology, is the ability to induce fast, reversible metal-insulator transitions. We propose that Anderson localization in select transition metal oxides can be exploited to design a new generation of memristors. Utilizing toy models as well as first principles descriptions of niobium and vanadium oxide structures, we show that disordering the system can be leveraged to engineer the metal insulator switching, a key physical mechanism in the construction of modern day neuromorphic circuits. Furthermore, we demonstrate that a simple metric of eigenstate localization, the Gini vector, can be an efficient way to capture the localization properties in a first-principles tight binding model.

*This work is supported by the Air Force Office of Scientific Research under award number FA9550-18-10024.
11:15AM S40.00001: Emergent electronic phases in Ruddlesden-Popper chromium oxide perovskites*
RICCARDO COMIN (Presenter), ZHIHAI ZHU, JONATHAN PELLICIARI, JIARUI LI, Massachusetts Institute of Technology, CHRISTIE NELSON, Brookhaven National Laboratory — Chromium-based compounds realize a multitude of electronic and magnetic phases: half-metals (CrO$_2$), ferromagnetic insulators (CrI$_3$, YCrO$_3$), antiferromagnetic insulators (Cr$_2$Se$_3$, CrSe$_2$, Cr$_2$O$_3$ and LaCrO$_3$), or antiferromagnetic metals (Cr and SrCrO$_3$). These compounds, whose magnetic transitions are often near room temperature, represent a far less charted platform for emergent quantum matter compared to their other 3$d$ transition metal siblings.

Low-dimensional perovskites of tetravalent chromium deserve particular attention as they uniquely realize a strongly-correlated electron system with $d^2$ electronic configuration and active spin and orbital degrees of freedom. Antiferromagnetism is ubiquitous in these systems, but recent theoretical studies indicate the presence of proximate electronic phases, including orbital order and superconductivity. These materials cannot be easily stabilized in bulk form and in the Cr$^{4+}$ oxidation state (with spin $S=1$) but could host interesting new phenomena enabled by the strong interplay of spin, charge, and orbital degrees of freedom.

To explore these scientific opportunities, we have grown thin films of various members of the Ruddlesden-Popper series of chromium oxide perovskites: SrCrO$_3$, Sr$_2$CrO$_4$, and Sr$_4$Cr$_3$O$_{10}$. In this talk, I will report on the synthesis and characterization of their transport and magnetic properties, including recent investigations of spin and orbital ordering in the ground state of these materials.

*This work was supported primarily by the MRSEC Program of the National Science Foundation under award number DMR - 1419807.

11:51AM S40.00002: Rh-based Double Perovskites with Unusual Properties: A computer prediction*
TANUSRI SAHA-DASGUPTA (Presenter), Indian Association for the Cultivation of Science, ANITA HALDER, S.N. Bose National Centre for Basic Sciences, PRABUDDHA SANYAL, Indian Institute of Technology, Roorkee — Using a combination of computational tools involving genetic algorithm, denisty functional theory and finite temperature Monte Carlo simulation, we make prediction on yet-to-be synthesized Rh-based double perovskites with novel properties. Interestingly while some of the predicted compounds show half-metallic ferromagnetic behavior, the rest show rare antiferromagnetic metallic properties. This makes this series of compounds a promising class of magnetic materials which need to be synthesized and investigated further.

*The authors acknowledge the computational resources created through funding of Nano-mission of Department of Science and Technology, India.

12:03PM S40.00003: Transition between two metallic ferroelectric orders in multiferroic Ca$_3$Ru$_2$O$_7$, induced by magnetism-mediated orbital re-polarization
ZHETING JIN (Presenter), WEI KU, Tsung-Dao Lee Institute & School of Physics and Astronomy, Shanghai jiao Tong University — For the past decades, the low-temperature phase of Ca$_3$Ru$_2$O$_7$ below the 48K first-order phase transition remains a puzzle with controversial suggestions involving metallic ferroelectric, orbital or magnetic ordering.

Through analysis of experimental lattice structure, density functional theory calculation, and effective model analysis, we propose that the 48K phase transition is a bond formation transition promoted by the magnetism mediated orbital re-polarization. Most interestingly, this transition is accompanied by a switch of two metallic ferroelectric orders from a $xy+y$ symmetry to $xz+z$.

Our study not only resolves a long-standing puzzle of this phase transition in this material, but also demonstrates perhaps the first example of transition between multiple emergent ferroelectric orders in bad metals, resulting from interplay between multiferroic orders.
12:15PM S40.00004: Electronic correlations in early transition metal oxides with oxygen vacancies*  JAIME SOUTO
CASARES (Presenter), NICOLA SPALDIN, CLAUDE EDERER, ETH Zurich — Oxygen vacancies are known to affect profoundly the
properties of the host system, coupling to the already coupled degrees of freedom. Electronically, in early transition metal
oxides, the presence of oxygen vacancies locates electronic states in the gap between the transition metal t_{2g} band and
the oxygen p-band, with occasional occurrences of crossings with the t_{2g}-band. The closeness and influence of the vacancy
band on the correlated electronic bands calls for a beyond-DFT analysis. Constructing an extended t_{2g} correlated subspace
where the oxygen vacancy state is explicitly consider, we have performed dynamical mean-field theory (DMFT) and
constrained random phase approximation (cRPA) calculations for three different lanthanum transition metal oxides with
different t_{2g}-occupations (LaBO_{3}, with B={Ti(d^{1}), V(d^{2}), Cr(d^{3})}) in order to investigate what is the effect of the vacancy on
the Mott insulating phase, and to monitor how the ab-initio effective Coulomb interaction parameters change.

*Work supported by the Swiss National Science Foundation, NCCR MARVEL.

12:27PM S40.00005: An ab-initio DFT+DMFT study of the effect of oxygen vacancies on structural, electronic and
magnetic properties of rare-earth nickelate perovskites (RNIo_{3})*  UTHPALA HERATH (Presenter), West Virginia University,
HYOWON PARK, Physics, University of Illinois at Chicago, ALDO H ROMERO, West Virginia University — The electronic correlations
in materials are responsible for a variety of fascinating phenomena including magnetism, superconductivity, colossal
magneto-resistance and metal-insulator transitions. As shown in previous studies, the ability to manipulate the oxygen
vacancies within these strongly correlated materials gives rise to new degrees of freedom in tuning their properties. We
employ ab-initio density functional theory (DFT) coupled to dynamical mean field theory (DMFT) calculations to
systematically study the influence of oxygen vacancies on structural, electronic and magnetic properties of strongly
correlated rare-earth nickelates, RNIo_{3} (R=rare earth element). The DFT Kohn-Sham orbitals are projected onto maximally
localized Wannier Functions within a hybridization window to provide the correlated subspace for the DMFT problem
which is solved using a continuous time quantum Monte-Carlo (CTQMC) algorithm. Based on our calculated results we
elucidate the role of oxygen vacancies on the material properties also focusing their effects on individual orbitals, which
thus far has not been studied extensively in the case of strongly correlated rare earth nickelate perovskites.

*Work supported by the Canadian Natural Sciences and Engineering Research Council (NSERC), the Natural Sciences and
Engineering Research Council of Canada (NSERC), the University of British Columbia, the Université de Sherbrooke (USHERCO), the
Max-Planck-UBC-UTokyo Center for Quantum Materials, the Newton Research Fellowships, the Department of Physics, University of British
Columbia, and the Quantum Materials Fund.

12:39PM S40.00006: The Electronic Structure and Properties of Negative Charge Transfer Compounds*  ROBERT
GREEN (Presenter), University of British Columbia; University of Saskatchewan, GEORGE ALBERT SAWATZKY, University of British
Columbia — In high oxidation state oxides like the trivalent nickel oxides, tetravalent cobalt and iron oxides as well as the
parent superconductors BaBiO3 and SrBiO3, the cation electron affinity for the formal valence taking oxygen to be 2- can
result be larger than the oxygen ionization potential. This leads to a so-called negative charge transfer energy, where the
cations are more accurately described with reduced valences and the oxygen states are self-doped with holes. As a
consequence, one can have very different electronic structures and x-ray spectra than expected from the formal oxidation
state picture. We demonstrate that with this in mind we can very well explain many of the properties and phases of the
trivalent nickelates and tetravalent ferrates. Utilizing the negative charge transfer approach in cluster exact diagonalization
calculations resolves a 25 year old puzzle concerning core level spectra of nickelates, and reveals interesting orbital
polarization phenomena in strained nickelate and ferrate films.

*This research was supported by NSERC and the Max-Planck-UBC-UTokyo Center for Quantum Materials.

12:51PM S40.00007: Evolution of Antiferromagnetism with Hole Doping in HgBa_{2}Ca_{2}Cu_{3}O_{6}: A Parameter Free
Perspective  CHRISTOPHER LANE (Presenter), Northeastern University, YUBO ZHANG, Tulane University, MATTHEW MATZELLE,
Northeastern University, JOHANNES NOKELAINEN, LUT, JAMES FURNESS, Tulane University, ROBERT MARKIEWICZ, Northeastern
University, BERNARDO BARBIELLINI, LUT / Northeastern Univ, JIANWEI SUN, Tulane University, ARUN BANSIL, Northeastern
University — Since the discovery of the cuprates 33 years ago, connecting their physical properties to their electronic
structure has proven extremely challenging to capture within a uniform theoretical picture. Here, by utilizing the recently
constructed SCAN metaGGA, we show how the charge, spin and lattice degrees of freedom of HgBa_{2}Ca_{2}Cu_{3}O_{6+δ} evolve
with oxygen hole doping. Both the layer and doping dependence of our theoretically predicted antiferromagnetic order
are in good agreement with NMR observations. In particular, a local maximum in the number of holes in the CuO_{2} plane is
found in agreement with near optimal δ=0.16 doping for high-T_{c} superconductivity. Additionally, we find the doped
interstitial oxygens play a consequential role at the Fermi level throughout the phase diagram, indicating the importance
of inter-layer coupling between the CuO_{2} planes and the charge reservoir layer.
1:03PM S40.00008: Antiferromagnetism in a rocksalt high entropy oxide*  JUNJIE ZHANG (Presenter), JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, STUART CALDER, Neutron Scattering Division, Oak Ridge National Laboratory, QIANG ZHENG, ERICH T. VON GEIS, Materials Science and Technology Division, Oak Ridge National Laboratory, DOUGLAS L ABERNATHY, Neutron Scattering Division, Oak Ridge National Laboratory, YANG REN, SAUL H. LAPIDUS, Advanced Photon Source, Argonne National Laboratory, KATHARINE L. PAGE, Neutron Scattering Division, Oak Ridge National Laboratory, HONG ZHENG, Materials Science Division, Argonne National Laboratory, JOHN WILLIAM FREELAND, Advanced Photon Source, Argonne National Laboratory, JOHN D BUDAI, RAPHAEL HERMANN, Materials Science and Technology Division, Oak Ridge National Laboratory — High entropy oxides have attracted much attention because they not only significantly broaden the phases beyond the conventional phase diagram of doping, but also have the potential to exhibit multifunctional physical properties and emergent phenomena including superconductivity and quantum criticality [1-3]. The existence of extreme chemical disorder in these materials is expected to suppress the long range magnetic order. Here, by combining magnetometry, synchrotron x-ray and neutron powder diffraction, we report for the first time that a rocksalt high entropy oxide exhibits long range antiferromagnetic order at ~120 K with q=(½, ½, ½). Inelastic neutron scattering reveals strong magnetic excitations at 100 K that survive up to room temperature. The shear modulus obtained from resonant ultrasound spectroscopy shows an anomaly around the magnetic transition, and surprisingly it hardens with decreasing of temperature without saturation down to 3 K. References: [1] Rost, C. M. et al. Nat. Commun. 6, 8485 (2015). [2] Gao, M. C. et al. Nat. Mater. 18 (2018). [3] Sales, B. C. et al. npj Quantum Mater. 2, 33 (2017).

*JZ and RPH acknowledge support from the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

1:15PM S40.00009: The effect of the Co-O covalency on the spin-state ordering in LaCoO3: A DFT+DMFT study  HYOWON PARK (Presenter), University of Illinois at Chicago, RAVINDRA R NANGUNERI, Brown University — We investigated the effect of the Co-O covalency on the spin-state transition in LaCoO3 using the charge-self-consistent density functional theory plus dynamical mean field theory (DFT+DMFT) method implemented using the maximally localized Wannier functions as basis sets. The strong covalent bonding between Co and O produces the occupancy of the Co d orbital as d7 with one hole in the O ion when computed using DFT+DMFT with the fully localized form of the double counting potential. The effect of the Co-O covalency is studied by changing the double counting potential within DFT+DMFT for both homogeneous and the mixed high/low spin states. The total energy calculation of DFT+DMFT shows that the low-spin state is the lowest in energy for the d occupancy close to 7 while the spin-state ordering (high and low spins) between two Co ions occurs when the d occupancy is below 6.7 as the Co-O covalency is reduced. The valence histogram in DFT+DMFT shows that the charge ordering also occurs for the spin-state ordered LaCoO3 as the higher spin state Co ion has a higher d6 configuration than the low-spin state Co ion does. Both the charge and the energy differences between the homogeneous and the spin-state ordered phases are smaller in DFT+DMFT compared to DFT+U results.

1:27PM S40.00010: Spontaneous non-stoichiometry and ordering of metal vacancies in degenerate transparent conductive oxides*  OLEKSANDR MALYI (Presenter), University of Oslo, MICHAEL T. YEUNG, KENNETH POEPPELMEIER, Northwestern University, CLAS PERSSON, University of Oslo, ALEX ZUNGER, University of Colorado Boulder — The existence of non-stoichiometry in oxides is often thought to be a growth effect rather than a specific electronic instability. We show via DFT calculations that the presence of electrons in the conduction band of insulators can destabilize materials with respect to the spontaneous formation of cation vacancy acceptors. These tendencies result ultimately in the formation of ordered vacancy compounds (OVCS). For Ca-Al-O and Ba-Nb-O, we find that OVCS with different stoichiometries I:m:n are stable under different ranges of elemental chemical potentials, controllable during synthesis. Since each I:m:n OVC depletes the conduction band of electrons by a different amount, the formation of OVCS can be used to reduce plasma absorption, modify interband absorption, and enhance materials stability. This clarifies how non-stoichiometry often seen in oxides is an electronic effect — a high Fermi energy induces the formation of electron-killer acceptors such as cation vacancies. This also provides insights into the stability of the transparent conductive states while pointing out that controllable formation of non-stoichiometric degenerate insulators can be used to design next-generation transparent conductive oxides.

*The work is supported by RCN #251131, DMR-1806939, and DMR-1806912
1:39PM S40.00011: Magnetic percolation transition in diluted hexaferrites* CAMERON LERCH (Presenter), THOMAS VOJTA, Missouri University of Science and Technology — The hexagonal ferrites BaFe₁₂O₁₉, SrFe₁₂O₁₉ and PbFe₁₂O₁₉ are ferrimagnets with Neel temperatures of approximately 720K that also show interesting ferroelectric properties. By randomly substituting Ga ions for the Fe ions, the Neel temperature can be suppressed to zero. Recent experiments [1] have found the phase boundary to vary as \( T_N \sim (1 - x/x_c)^{2/3} \) over a wide x range, with \( x_c \) very close to the percolation threshold of the iron spins. The shape of the phase boundary in the neighborhood of \( x_c \) does not agree with current theoretical predictions for a classical percolation transition. We investigate the shape of the low-temperature phase boundary close to the percolation threshold using large-scale Monte Carlo simulations of a three-dimensional site-diluted Heisenberg model.


*This work was supported in part by the NSF under Grants Nos. DMR-1506152 and DMR-1828489.

1:51PM S40.00012: Variations in the Magneto-optical Properties of CuAl₁₋ₓFeₓO₂ with Fe Concentration MINA AZIZIHA (Presenter), JAMES PATRICK LEWIS, Department of Physics and Astronomy, West Virginia University, SETH A BYARD, Department of Physics, Grove City College, MOHINDAR S SEEHRA, MATTHEW BRUCE JOHNSON, Department of Physics and Astronomy, West Virginia University — CuAlO₂ is among several ternary delafossites in which the electronic bandgap (2.68 eV) is less than the optical bandgap (3.5 eV). Because alloying is expected to allow band engineering in delafossites, we are investigating magneto-optical properties of CuAl₁₋ₓFeₓO₂ for \( x = 0 \) to1. The samples were prepared by solid-state reaction in air. X-ray diffraction of the powder samples shows an expansion of the rhombohedral unit cell with increasing \( x \), in accordance with Vegard’s Law. X-ray photoelectron spectroscopy, and SEM-based energy dispersive (x-ray) spectroscopy were also used to confirm the Fe concentrations. Analysis of the magnetization (\( M \)) vs. temperature data (\( T = 2 \) to 300 K) and magnetic field (up to \( H = 90 \) kOe) verifies Fe³⁺ as the electronic state of Fe and Fe³⁺-Fe³⁺ exchange coupling signifies anti-ferromagnetism for CuAl₁₋ₓFeₓO₂ for \( x = 0 \) to 0.1. The high-resolution M vs. H hysteresis loop measurements done at 300 K and 10 K shows some hysteresis, particularly for the \( x = 0.1 \) sample. However, it is concluded that this hysteresis is due to hematite impurity which is not detectable in the XRD analysis of the samples. In this talk, we will specifically report on magnetic measurements of CuAl₁₋ₓFeₓO₂ for \( x > 0.1 \) and optical absorption studies in the CuAl₁₋ₓFeₓO₂ samples.

2:03PM S40.00013: Anti-doping in Insulators and Semiconductors* QIHANG LIU (Presenter), Department of Physics, Southern University of Science and Technology, Shenzhen, China, GUSTAVO DALPIAN, ALEX ZUNGER, RASEI, University of Colorado, Boulder, US — Ordinary doping by electrons (holes) generally means that the Fermi level shifts towards the conduction band (valence band) and that the conductivity of free electrons (holes) increases. Recently, however, some peculiar doping characteristics were sporadically recorded in different materials without noting the mechanism: electron doping was observed to increase the band gap and thus lead to a decrease in conductivity. This behavior we dub as “anti-doping” was seen in rare-earth nickel oxides SmNiO₃, cobalt oxides SrCoO₂₋₅, Li-ion battery materials and even MgO with metal vacancies. Given the apparent generality of this phenomenon and that it may offer an unconventional way of controlling conductivity, we demystify the physical origin of anti-doping as well as its inverse problem – the “design principles” that would enable intelligent search of materials. We find that electron anti-doping is expected in materials having pre-existing trapped holes and is caused by annihilation of such “hole polarons” via doping.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Grant No. DE-SC0010467.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S41 GMAG DMP: Spin-Transfer and Spin-Orbit Torques

BCEC 209 - Luqiao Liu, Massachusetts Institute of Technology - Tag(s): Focus
First-principles calculation of spin-orbit torques in ferromagnet/heavy-metal bilayers

KIRILL BELASHCHENKO (Presenter), ALEXEY KOVALEV, University of Nebraska - Lincoln, MARK VAN SCHILFGAARDE, King's College London — The spin-orbit torque in Co/Pt, Co/Pd, and Co/Au bilayers is calculated using a first-principles non-equilibrium Green's function formalism with an explicit treatment of disorder. The torque is formally split in the Fermi-sea and Fermi-surface contributions. The Fermi-sea term is important at low temperatures, but the Fermi-surface term dominates at room temperature. In addition to the usual damping-like and field-like terms, the odd torque contains a sizeable planar Hall-like term \( mE \times (z \times m) \), which contributes to damping and has been observed experimentally. While the torques that contribute to damping are largely due to spin-orbit coupling on the heavy-metal atoms, the field-like torque does not require it. The dependence of the torque on the thicknesses of the layers is also examined.


Deterministic spin-orbit torque switching via structural engineering

TIANYUE CHEN, HSIN-I CHAN, WEI-BANG LIAO, CHI-FENG PAI (Presenter), National Taiwan University — Current-induced spin-orbit torque (SOT) can be employed to control magnetization in magnetic random-access memory (MRAM) with perpendicular magnetic anisotropy (PMA), but typically requires an applied in-plane magnetic field. To eliminate the need of this applied field and achieve better on-chip memory designs, we deposit 4d transition metal Mo in a canted way as the SOT source. Although the spin-orbit interaction in Mo is weaker than in 5d metals such as Pt, W, or Ta, deterministic switching can still be achieved. This result suggests that growth configuration can play a more important role than material selection in some cases, which could really impact the engineering of next-generation field-free SOT-MRAM.

*This work was partly supported by the Ministry of Science and Technology of Taiwan under grant No. MOST 105-2112-M-002-007-MY3 and by the Center of Atomic Initiative for New Materials (AI-Mat), National Taiwan University, from the Featured Areas Research Center Program within the framework of the Higher Education Sprout Project by the Ministry of Education (MOE) in Taiwan under grant No. NTU-107L9008.

Spin-Orbit Torque Switching in Asymmetric Structures with Double Non-Magnetic Metal Layers

SEYED ARMIN RAZAVI (Presenter), Electrical and Computer Engineering, University of California, Los Angeles, GUOQIANG YU, Chinese Academy of Sciences, HAO WU, QIMING SHAO, KIN WONG, KANG-LUNG WANG, Electrical and Computer Engineering, University of California, Los Angeles — Spin-orbit torque (SOT) switching of magnetization is a promising emerging technology for non-volatile memory and logic applications. However, deterministic switching with SOTs requires breaking of inversion symmetry, usually provided by an external magnetic field, which is not suitable for applications. It has been shown that structures with lateral asymmetry can eliminate the need for external field and realize field-free SOT switching [1]. In this work we study field-free SOT switching in asymmetric structures with double non-magnetic metal layers, where current-induced out-of-plane effective fields are created. We break the structural symmetry by inserting a wedge-shaped second metallic layer between the ferromagnet and the first heavy metal. We investigate the creation and origin of current-induced out-of-plane effective fields, \( H_{\text{eff}} \), in various material systems (W/IrMn, W/Ta, Pt/IrMn, W/Ti), and we show the realization of field-free SOT switching in these structures. Our work provides a route for practical application of SOT devices and challenges the current understanding of the origins of SOTs in structures with lateral asymmetry.


*This work is supported by NSF Award EEC-1160504, and NSF Grant No. 1611570.
11:51AM S41.00004: Strong Spin-Orbit Torques, Tunable DMI, and Variable Interfacial Spin-Orbit Coupling in Pt-based Spin Hall Metal/Ferromagnet Systems [Invited] LIJUN ZHU (Presenter), Cornell University, KEMAL SOBOTKIEWICH, XIN MA, XIAOQIN (ELAINE) LI, The University of Texas at Austin, DAN RALPH, ROBERT BUHRMAN, Cornell University — Recent work finds that the spin Hall effect in Pt is dominated by the intrinsic Berry phase effect. The internal spin Hall ratio $\theta_{SH}$ should be enhanced by alloying Pt with a component that raises the resistivity $\rho$ but does not materially reduce the spin Hall conductivity $\sigma_{SH}$. This talk will report on an extensive study of two fcc Pt alloys which establishes that for Au$_{1-x}$Pt$_x$(Pd$_{1-x}$Pt$_x$), at the optimal concentration $x \approx 0.25$, anti-damping spin-orbit torque efficiency $\xi_{DL} \approx 0.30$ (0.26) for $\rho = 83$ (57.5) μΩ cm at 4 nm thickness [1,2]. This indicates $\theta_{SH} \geq 0.58$ (0.47) and $\sigma_{SH} \approx 0.7(1) \times 10^6 \, \Omega^{-1} \text{m}^{-1}$; considerably larger than predicted by recent first principles-calculations. Moreover, the DMI at the Pt alloy/FM interface is both strong and tunable by composition over a wide range. These results establish Au$_{1-x}$Pt$_x$ and Pd$_{1-x}$Pt$_x$ as the most energy-efficient spin current generators for spin-torque manipulation of metallic FM systems and for chiral spintronics applications. The effect of interfacial spin-orbit coupling (ISOC) on the spin transparency of the Pt(alloy)/FM interface has also been examined through controlled variation of its strength through thermal annealing, revealing that ISOC at HM/FM interfaces should be minimized via interfacial passivation to maximize $\xi_{DL}$ [3,4].


12:27PM S41.00005: First Principles Study of Spin-Orbit Torque in Pt/Co and Pd/Co Bilayers* FARZAD MAHFOUZI (Presenter), NICHOLAS KIOUSSIS, Physics and Astronomy, California State University, Northridge — Spin-orbit torque (SOT) induced by spin Hall and interfacial effects in heavy metal(HM)/ferromagnetic(FM) bilayers has recently been employed to switch the magnetization direction using in-plane current injection. In this work, using the Keldysh Green’s function approach and first principles electronic structure calculations we determine the Field-Like (FL) and Damping-Like (DL) components of the SOT for the HM/Co (HM = Pt, Pd) bilayers. We investigate the effects of HM and FM thicknesses, strain, oxidation as well as rigid shift of the chemical potential on the SOTs. We compare the HM thickness dependence and also effect of oxigen in the FM with the experimental results where we see an overall good agreement. The dependence of the SOT on the position of the Fermi level suggests that the DL-SOT dominated by the Spin Hall effect of the bulk HM.

*The work is supported by NSF ERC-Translational Applications of Nanoscale Multiferroic Systems (TANMS)- Grant No. 1160504 and by NSF-Partnership in Research and Education in Materials (PREM) Grant No. DMR-1205734.

12:39PM S41.00006: Excitation and Amplification of Propagating Spin Waves by Spin-Orbit Torque* BORIS DIVINSKIY, VLADISLAV DEMIDOV, SERGEY DEMOKRITOV, Physics, University of Muenster, SERGEI URAZHDIN (Presenter), RYAN FREEMAN, Emory University — Spin-orbit torque (SOT) produced by electric current is among the cornerstones of modern nanomagnetism. However, until now SOT could not be utilized for the generation of propagating spin waves for magnonic (spin wave-based) applications.

We experimentally demonstrate a SOT oscillator directly incorporated into a SOT-enhanced magnonic nano-waveguide. The studied nanostructure is based on a Permalloy(Py)/Pt bilayer patterned into a nanowire forming a spin-wave waveguide, with Py thickness reduced in a narrow notched region of the nanowire. SOT produced by dc electrical current in Pt induces coherent magnetization oscillations in the nano-notch region, emitting spin waves into the nanowire. We utilize spectrally- and spatially-resolved microfocus Brillouin Light Scattering (BLS) measurements to demonstrate unidirectional emission of coherent spin waves, controlled by the direction of the static magnetic field, and simultaneous enhancement of their decay length by SOT. The demonstrated system combines all the advantages provided by the SOT, and can be used as a building block for novel integrated spin-orbit magnonic nano-circuits.


*Supported by NSF ECCS-1804198
work we compute the spin-mixing conductance for Co/Bi\textsubscript{2}Se\textsubscript{3}, Co/Pt and Co/W junctions.

Functional theory combined with Floquet-nonequilibrium-Green function formalism [Phys. Rev. B] as the pre-factor of spin current vs. precession cone angle dependence, where we compute spin current using density

well-defined when spin-orbit coupling is present directly at the interface. Nevertheless, an effective one can be extracted

phenomena have been observed recently in heavy metals and topological insulators, where the spin-orbit coupling plays

axial in-plane. We show that magnetic thin films interfaced with CdWO\textsubscript{4} have strong magnetic anisotropy induced by the

substrate with strong spin-orbit coupling whose symmetries can be restricted to a single mirror plane if cleaved with the b-

axis in-plane. We show that magnetic thin films interfaced with CdWO\textsubscript{4} have strong magnetic anisotropy induced by the

low-symmetry crystal structure. This anisotropy is strongly temperature-dependent, exceeding 200 Oe at low

temperatures. In addition, measurements of spin-orbit torque in such bilayers exhibit torque components that are

commensurate with the symmetry of CdWO\textsubscript{4}. This suggests an interfacial torque mechanism in which spin-polarized

electrons flowing within the magnetic layer and scattering from the insulating CdWO\textsubscript{4} can produce a spin-orbit torque

acting back on the magnetic layer.

Demonstration of a micron-scale spin-orbit-torque emitter for coherent magnonics

MICHAEL EVELT, Institute for Applied Physics and Center for Nonlinear Science, University of Muenster, 48149 Muenster, Germany, LUCILE SOUMAH, Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris-Saclay, Palaiseau, France, ANATOLII BRONISLAVOVICH RINKEVICH, Institute of Metal Physics, Ural Division of RAS, Ekaterinburg 620108, Russia, SERGEJ DEMOKRITOV, Institute for Applied Physics and Center for Nonlinear Science, University of Muenster, 48149 Muenster, Germany, JAMAL BEN YOUSSEF, LABSTICC, UMR 6285 CNRS, Universite de Bretagne Occidentale, 29238 Brest, France, GREGOIRE DE LOUBENS, SPEC, CEA-Saclay, CNRS, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, OLIVIER KLEIN, SPINTEC, CEA-Grenoble, CNRS and Université Grenoble Alpes, 38054 Grenoble, France, PAOLO BORTOLOTTI, VINCENT CROS, ABDELMADJID ANANE (Presenter), Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris-Saclay, Palaiseau, France, VLADISLAV DEMIDOV, Institute for Applied Physics and Center for Nonlinear Science, University of Muenster, 48149 Muenster, Germany — Using micro-focus Brillouin light scattering (BLS), we experimentally demonstrate generation of coherent propagating magnons in ultra-thin magnetic-insulator films by spin-orbit torque induced by dc electric current [1]. We show that this challenging task can be accomplished by utilizing magnetic-insulator films with large perpendicular magnetic anisotropy (PMA) possessing ultra-low Gilbert damping ($\gamma = 8 \times 10^{-4}$ for 20 nm thick Bismuth substituted YIG [2]). Fine tuning of the PMA allows to exactly cancel the dipolar field (the effective magnetization $\mathbf{M}_{\text{eff}} = 0$). As a result, the usually observed non-linear shift of the auto-oscillation frequency is suppressed. Hence, the dominant mechanism for self-localization of the auto-oscillations is inhibited. We demonstrate simple and versatile spin-orbit torque devices, which can be used as highly efficient nanoscale sources of coherent propagating magnons for insulator-based spintronic applications.


1:15PM S41.00009: Spin mixing conductance of ferromagnet/topological-insulator and ferromagnet/heavy-metal bilayers with strong interfacial spin-orbit coupling: A first-principles time-dependent quantum transport approach

KAPILDEB DOLUI (Presenter), UTKARSH BAJPAI, BRANISLAV NIKOLIC, University of Delaware — Spin pumping and related phenomena have been observed recently in heavy metals and topological insulators, where the spin-orbit coupling plays an essential role. Conventional spin mixing conductance, which governs the magnitude of pumped spin current, is not well-defined when spin-orbit coupling is present directly at the interface. Nevertheless, an effective one can be extracted as the pre-factor of spin current vs. precession cone angle dependence, where we compute spin current using density functional theory combined with Frouquet-nonequilibrium-Green function formalism [Phys. Rev. B 85, 05446 (2012)]. In this work we compute the spin-mixing conductance for Co/Bi$_2$Se$_3$, Co/Pt and Co/W junctions.

1:27PM S41.00010: Correlation between resonance mode crossing and spin torque switching probability in magnetic tunnel junctions

CHRIS SAFRANSKI (Presenter), JONATHAN SUN, IBM T. J. Watson Research Center — We report on the effect of coupled free- and reference-layer dynamics on switching errors in a spin-torque switched magnetic tunnel junction. Perpendicularly magnetized magnetic tunnel junctions (MTJ) [1-3] are used for this study. The free layer switching speed and probability is related to magnetization dynamics as revealed by spin-torque driven, and thermal fluctuation-driven ferromagnetic resonance (STT- and Thermal-FMR) spectra. We investigate the probability in spin torque driven switching as a function of applied magnetic field, and compare with the STT- and thermal-FMR spectrum in the same field range. A nonmonotonic dependence of the switching probability on field and on bias-voltage is seen, correlating to STT-FMR mode-crossings between the free- and reference-layer spectra-lines. At field values corresponding to the intersections of free- and reference-layer spin wave modes, an increase of errors is observed in switching. Our results show that excitation of the reference layer’s dynamics can affect the MTJ’s net STT-switching probability.

**1:39PM S41.00011: Zero-Threshold Rectification Using Low-Barrier Magnets**

SHEHRIN SAYED (Presenter), EECS, University of California, Berkeley, KEREM Y CAMSARI, RAFATUL FARIA, SUPRIYO DATTA, ECE, Purdue University — Stable magnets with energy barriers (~40-60 kT) have been the center of focus for spintronics. Recently, low energy barrier magnets have attracted growing interest in the community for novel applications e.g. random number generation, stochastic oscillators, probabilistic computers, etc. Using experimentally benchmarked models [1,2], we show that the charge current induced spin voltage measurements, well-established for diverse materials with spin-orbit coupling, could be used for zero-threshold rectification when the stable magnet is replaced with a low barrier magnet either with an in-plane or perpendicular anisotropy. These experiments can be used to characterize such stochastic magnets and extract parameters that determine (i) spin-orbit torque induced magnetization pinning and (ii) the frequency band of rectification. We analytically determine this frequency band from angular momentum conservation principles. The proposed structure could find application as highly sensitive passive rf detectors and as energy harvesters from weak ambient sources where standard technologies may not operate.


*This work was supported by ASCENT, one of six centers in JUMP, a SRC program sponsored by DARPA.

**1:51PM S41.00012: Fermi surface of CrNb$_3$S$_6$: giant spin-orbit effect**

TATSUYA SHISHIDOU (Presenter), MICHAEL WEINERT, University of Wisconsin - Milwaukee — Chiral magnets are of particular interest because of their exotic magnetic and transport properties. In the case of CrNb$_3$S$_6$, the ground-state magnetic configuration is a planar flat spiral with a periodicity of 48nm along the hexagonal c axis. Moderate external fields ($H$) alter the spin texture into the chiral soliton lattice ($H \perp c$) or the chiral conical phase ($H \parallel c$). With increasing $H$, these phases continuously transform into forced ferromagnetic (FM) configurations that appear at $H \sim 0.2$ ($H \perp c$) and 2 Tesla ($H \parallel c$). Using a density functional theory approach, we investigate the FM state of CrNb$_3$S$_6$, paying particular attention to the spin-orbit coupling (SOC) and its effect on the electronic band structure and Fermi surface. Importantly, for some bands near the Fermi level, SOC introduces giant and peculiar first-order changes of the band energies when the magnetization is parallel to the c axis: the band dispersion appears to be shifted in k space. Consequently, the deformed Fermi surface has a highly asymmetric shape that could lead to nonreciprocal transport. Symmetry arguments and detailed analysis of SOC effects will be given.

*This work is supported by the U.S. National Science Foundation, EFMA-1741673.

**2:03PM S41.00013: Observations of large spin mixing conductance in poly(3-methylthiophene) polymer brushes/NiFe heterostructures**

ERIC VETTER (Presenter), North Carolina State University, IAN VONWALD, chemistry, university of north carolina at chapel hill, DALI SUN, North Carolina State University, WEI YOU, chemistry, university of north carolina at chapel hill — Observations of large inverse spin Hall effect (ISHE) in a fullerene (C$_{60}$) thin film – usually only appearing in metals and semiconductors with heavy elements - indicate that spin-orbit coupling in terms of spin Hall angles would be significantly influenced by chemical structure parameters, such as stacking and curvatures. Here, we report studies on the effective spin mixing conductance in ‘spun cast’ poly(3-hexylthiophene) (P3HT) and ‘polymer brush’ poly(3-methylthiophene) (P3MT) thin films using ferromagnetic resonance (FMR) and spin pumping techniques. P3HT and P3MT films were spun cast and self-assembly grown, respectively, onto ITO/glass substrates followed by NiFe. Frequency-dependent FMR and ISHE measurements were carried out on both films as a function of film thickness, from which the effective spin mixing conductances were obtained. We find that the P3MT films exhibit a large increase in the effective spin mixing conductance, in contrast to that in P3HT films. The large spin mixing conductance in the ‘polymer brush’ P3MT thin films is attributed to morphological differences as compared with the spun cast films.

*I.V.W. was supported by the NSF GRFP under Grant No. DGE-1650116. I.V.W. and W.Y. were supported by NSF Grants No. DMR-1610879.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

**Session S42 DMP: Millie Dresselhaus’ Legacy in Nanoscience** BCEC 210A - Daniel Dessau, University of Colorado, Boulder - Tag(s): Invited

**11:15AM S42.00001: Nanoelectronic Tools for Brain Science** [Invited] CHARLES LIEBER (Presenter), Harvard University — TBD

**11:51AM S42.00002: Quantum Transport in 2D Materials and Heterostructures** [Invited] CHUN NING LAU (Presenter), Ohio State University — TBD
10:30AM S42.00003: Millie Dresselhaus and 2D Materials [Invited] ANTONIO HELIO CASTRO NETO (Presenter), National University of Singapore — TBD

1:03PM S42.00004: Millie Dresselhaus the Queen of Carbon: A Role Model, an Inspiration of Young Generations, a Mentor and Colleague [Invited] MAURICIO TERRONES (Presenter), Department of Physics, Pennsylvania State University — I will review the scientific impact Mildred S. Dresselhaus (Millie) had in the Physics of Carbon since her pioneering work on the magneto-optic response of graphite crystals to establish a proper identification of electrons and holes in the Brillouin zone. Undoubtedly, Millie was a major pillar in Carbon Science, and was widely recognized as the “Queen of Carbon”. She contributed to a variety of topics that include: 1) the physical properties of graphite, 2) the electronic structure of graphene and rolled graphene (known as carbon nanotubes), 3) physico-chemical properties of graphite intercalated compounds, 4) fullerenes and derivatives, 5) Li-ion batteries, 6) the fundamentals of Raman spectroscopy in different nano-carbons, 7) enhanced Raman effects caused by two dimensional (2D) materials, etc. Sadly, Millie departed in February 2017, but she left us with an incredible amount of Physics knowledge. She was and will always be an inspiration for women, young and well-established scientists. This talk will summarize her major scientific achievements, as well as some personal experiences with her close collaborators. Millie really enjoyed science and she had a clear admiration for carbon nanomaterials. Working on carbon for more than fifty years, Millie always got engaged in the scientific understanding of novel forms of carbon and provided a forward vision. She is a great loss for Science, but fortunately, she has left us with an incredible amount of scientific knowledge and lessons to learn.

1:39PM S42.00005: Millie Dresselhaus’ Legacy and Recent Advances in Thermoelectrics [Invited] GANG CHEN (Presenter), Massachusetts Institute of Technology — Thermoelectric phenomena such as the Seebeck and the Peltier effects have been exploited for solid-state power generation and cooling, but the efficiency values of thermoelectric devices are limited by the low thermoelectric figure of merit of available materials, which is proportional to the electrical conductivity and the square of the Seebeck coefficient but inversely proportional to the thermal conductivity. These properties of a material in most cases are strongly contradictory to each other, limiting advances in the field. In 1993, Millie Dresselhaus published two pioneering papers on exploiting quantum size effects in 2D and 1D quantum structures to improve thermoelectric figure of merit (PRB, 47, 12727; 47, 16631, 2013). These papers played a significant role in reinvigorating the field of thermoelectrics, stimulating worldwide research in improving existing thermoelectric materials and searching for new ones. Since then, the field has evolved significantly, and new ideas and concepts have emerged and the materials figure of merit has seen significant improvements. This presentation will start with a summary of Millie’s contributions to the field, followed by a critical review of other successful ideas that have emerged, together with some discussion of novel electron and phonon transport physics emerged in advancing materials.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Spin-wave excitations, confinement, and coupling in high-quality organic-based magnetic structures* [Invited] MICHAEL CHILCOTE (Presenter), Ohio State University — The study of coherent magnonic interactions relies implicitly on the ability to excite and exploit long lived spin wave excitations in a magnetic material. Surprisingly, the organic-based ferrimagnet vanadium tetracyanoethylene (V[TCNE]x; x ≈ 2) has recently emerged as a low-loss material and offers a compelling alternative to yttrium iron garnet (YIG). Here, we present the synthesis of a new class of organic-based magnetic nanostructures consisting of nanowires of V[TCNE]x that assemble along the ridges of a grooved substrate. These nanowires exhibit uniaxial magnetic anisotropy with an in-plane easy axis perpendicular to the nanowires, which is in direct contrast to the isotropic in-plane response of typical thin-films. These nanostructures support the excitation of multiple modes, and when these different magnon modes are brought into resonance by varying the orientation of an in-plane magnetic field, we observe anticrossing behavior, indicating strong coherent coupling between the excitations. Furthermore, micromagnetic simulations using real nanowire profiles extracted from cross-sectional scanning electron microscopy faithfully reproduce the experimentally measured spectra without any free parameters, including spin-wave and other higher-order modes. Additionally, we use this data to explore the origin of the induced anisotropy in this materials system and note that these results offer insight into a whole class of organic-based magnetic materials of the form M[Acceptor]x (M = transition metal; x ≈ 2). These results also introduce a new degree of freedom for organic-based magnetism and spintronics, and together with recent demonstration of encapsulation technologies and demonstrated functional microwave devices that exhibit high quality factors across a frequency range, suggest future promising applications in microwave electronics and quantum magnonics.

Signatures of quantum dipole liquid in an organic Mott insulator κ-(BEDT-TTF)Hg(SCN)2Br* [Invited] NATALIA DRICHKO (Presenter), Johns Hopkins University — Mott insulators are commonly pictured with electrons localized on lattice sites. Their low-energy physics involves spins only. Recent theoretical work suggests that in molecular systems a new on-site charge degree of freedom can emerge. On a frustrated lattice with charge-spin coupling it would result in a new quantum spin liquid state. We experimentally demonstrate [1] a presence of this fluctuating charge degree of freedom in a molecule-based Mott insulator κ-(BEDT-TTF)2Hg(SCN)2Br. When electrons localize on a triangular lattice of molecular dimers of this compound at temperatures below 100 K, they form electric dipoles which do not order at low temperatures and fluctuate, resulting in a so-called quantum dipole liquid state. A frequency of dipole fluctuations of 40 cm\(^{-1}\) is detected experimentally in our Raman spectroscopy experiments through an observation of a related collective mode. We show that this spectroscopic response of a quantum dipole liquid is qualitatively different from a response of molecular Mott insulators with no on-site charge degree of freedom. The Raman spectra of the latter show two-magnon excitations at frequencies below 500 cm\(^{-1}\) expected for a S=1/2 antiferromagnet on a triangular lattice with J=250 K. Our results can be a key to understanding of organic triangular lattice spin liquid candidates.

References:

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0019331.

RICHARD GEILHUFE (Presenter), Nordic Institute for Theoretical Physics, Stockholm University, KTH Royal Institute of Technology — We present the organic materials database - OMDB, a freely accessible electronic and magnetic structure database for previously synthesized 3-dimensional organic crystals, available at https://omdb.diracmaterials.org [1]. We discuss the implementation and application of materials informatics tools towards the prediction of novel functional organic materials, with a particular focus on organic Dirac materials [2]. Here we explore mechanisms of protection and formation of Dirac nodes and semimetallicity together with aspects of stability of organic compounds [3, 4]. We finish by outlining applications of organic Dirac materials, e.g., towards dark matter detection [5], as well as by showing other examples beyond Dirac matter where the OMDB was applied recently.


*European Research Council DM-321031, the Knut and Alice Wallenberg Foundation, and the Villum Fonden Grant No. 11744

1:03PM S43.00004: Superconductivity in potassium-doped organic materials

HAI-QING LIN (Presenter), Beijing Computational Science Research Center — Abstract: Recent discoveries demonstrated that organic materials could be candidates for high temperature superconductors. In aromatic hydrocarbons, superconducting transition temperatures were observed up to 33 K, while in potassium-doped p-terphenyl and p-quaterphenyl, there were signatures indicating Tc of 120K. These results clearly indicate that organic materials are potential high temperature superconductors. However, the accurate amount of doped electrons and their positions have not been established experimentally, nor has any consensus reached for its superconducting mechanism. Here, we report the systematic studies of the crystal structures, charge transfer, electronic structures, electron-phonon interactions, magnetism, electronic correlations, and pressure effects in potassium-doped organic materials. Our calculations show that there exists a unified superconducting phase in the same 5-7 K range for all molecules containing benzene rings. Doping two electrons in the near constant density of states at the Fermi level accounts for this unified phase. The materials exhibit multiple superconducting phases and the high density of states at Fermi level upon 2+x-electron doping is responsible. The roles of doping content, electronic correlations, and pressure effect on superconductivity are emphasized.

*H.Q. Lin acknowledges financial support from NSAF U1530401 and computational resources from the Beijing Computational Science Research Center.
Giant Rashba-splitting in 2D organic-inorganic halide perovskites measured by optical modulation spectroscopies* [invited] ZEEV VARDENY (Presenter), University of Utah — Two-dimensional (2D) layered hybrid organic-inorganic halide perovskite semiconductors form natural ‘multiple quantum wells’ that possess strong spin-orbit coupling due to the heavy elements in their building blocks. This may lead to ‘Rashba-splitting’ (RS) close to the extrema in the electron bands. We have employed a plethora of ultrafast transient, electro-absorption magneto-optical spectroscopies, and theoretical calculations for studying the primary (excitons) and long-lived (free-carriers) photoexcitations in thin films of 2D perovskite, namely (C$_6$H$_5$C$_2$H$_4$NH$_3$)$_2$PbI$_4$ [1]. The density functional theory calculation shows the occurrence of RS in the plane perpendicular to the growth direction. From the electroabsorption spectrum [2] and photoinduced absorption spectra from excitons and free-carriers we indeed obtain a giant RS in this compound, with energy splitting of ~40 meV and Rashba parameter of ~1.6 eV Angstrom; which are among the highest RS size parameters reported so far. The influence of the RS on the magneto-optical properties of this compound has been measured by field induced circular dichroism and polarization at high magnetic field up to 25T. We found that the exciton absorption and photoluminescence emission spectra split due to the RS, and show g-values that are considerable shifted from that of the free electron.


*The work was supported by the Department of Energy Office of Science, grant DE-SC0014579. The film growth facility was supported by the Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE) an Energy Frontier Research Center funded by the Office of Basic Energy Sciences, Office of Science within the US Department of Energy program at the University of Utah.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S44 DCMP GMAG: Quantised Transport and Disorder in Kitaev Magnets BCEC 210C -

Tag(s): Invited

11:15AM S44.00001: Vison crystals in an extended Kitaev honeycomb model [invited] GABOR HALASZ (Presenter), Oak Ridge National Laboratory — We introduce an extension of the Kitaev honeycomb model by including four-spin interactions that preserve the local gauge structure and hence the integrability of the original model. The extended model has a rich phase diagram containing five distinct vison crystals, as well as a symmetric π-flux spin liquid with an approximate Fermi surface of Majorana fermions and a sequence of topological Lifshitz transitions. We discuss possible experimental signatures and, in particular, present finite-temperature Monte Carlo calculations of the specific heat and the static vison structure factor. We argue that our extended model emerges naturally from generic perturbations to the Kitaev honeycomb model.

11:51AM S44.00002: Field dependent magnetic excitations and possible topological transitions in α-RuCl₃* [invited] CHRISTIAN BALZ (Presenter), Oak Ridge National Laboratory — It is now well-known that when a magnetic field of approximately 7.5 T is applied in the honeycomb plane, the quantum magnet α-RuCl₃ displays a transition from zigzag magnetic order to a disordered state, believed to be a quantum spin liquid. This is reflected in the magnetic excitation spectrum as a disappearance of spin waves and a strengthening of a scattering continuum centered on the 2D Γ point that is interpreted as a signature of fractionalized excitations. Published measurements by Y. Kasahara et al (Nature 559, 227 (2018)) of the thermal Hall effect suggest a possible topological transition at an even higher field. Here I will discuss new high-resolution measurements of the excitations at fields spanning these two transitions. At the highest fields the broad scattering continuum is altered, and the response is seen to be dominated by a sharp peak at the lower bound, providing a strong indication that a new phase has been entered. The implications of these observations will be discussed in detail.

*The work at ORNL's Spallation Neutron Source and the High Flux Isotope Reactor was supported by the United States Department of Energy (US-DOE), Office of Science - Basic Energy Sciences (BES), Scientific User Facilities Division, managed by UT-Battelle LLC under contract number DEAC05-00OR22725.
12:27PM S44.00003: A spin-orbital-entangled quantum liquid on a honeycomb lattice* [Invited] Hidenori Takagi (Presenter), Max Planck Institute for Solid State Research — In 5d Ir$^{4+}$ oxides, the spin-orbit coupling for 5d electrons is as large as ~0.5 eV and not small as compared with on-site Coulomb $U$. This often gives rise to a spin-orbital Mott state with $J_{\text{eff}}=1/2$ isospins [1]. In the family of insulating 5d Ir$^{4+}$ oxides with a honeycomb-based structure, such as a-, b-, g-Li$_2$IrO$_3$ and Na$_2$IrO$_3$ (and also their 4d analogue a-RuCl$_3$), Ir$^{4+}$ ions are connected by the three orthogonal Ir-O$_2$-Ir plane bonds, which gives rise to a bond-dependent Ising interactions among $J_{\text{eff}}=1/2$ isospins. These compounds were pointed out theoretically to be a materialization of Kitaev model with a topological spin liquid as the ground state [2, 3]. However, a long range magnetic ordering rather than a liquid state was observed in these compounds, likely due to the presence of magnetic interactions other than the Kitaev interactions. We recently visited a new generation of honeycomb iridates H$_3$LiIr$_2$O$_6$, where all the interlayer Li$^+$ ions in a-Li$_2$IrO$_3$ are replaced with H$^+$, and discovered that a quantum spin liquid state is realized in H$_3$LiIr$_2$O$_6$ [4]. H$_3$LiIr$_2$O$_6$ does not show any trace of magnetic ordering down to 0.05 K, despite that an energy scale of magnetic interaction is ~ 100 K. We found at low temperatures below ~5K that the magnetization $M$, the NMR $1/T_1$ and the specific heat $C$ are dominated by the contributions from spin defects and follows a scaling with $B/T$. After subtracting the scaled contribution from the defects, we find only $T^3$-contribution in $C(T)$ within the given resolution, which can be ascribed to the lattice contribution. This suggests the presence of a gap in the magnetic excitations.


*This work was supported by Alexander von Humboldt Foundation and JSPS KAKENHI (17H01140, JP15H05852, JP15K21717).

1:03PM S44.00004: The scale-invariant magnetic anisotropy of RuCl$_3$ [Invited] Kimberly Modic (Presenter), Max Planck Institute for Chemical Physics of Solids, Arkady Shekhter, National High Magnetic Field Laboratory, Brad Ramshaw, Cornell University, Ross McDonald, Los Alamos National Laboratory, Philip Moll, Ecole polytechnique federale de Lausanne — We present a detailed study of the magnetic anisotropy of RuCl$_3$ – a layered honeycomb structure of effective spin-1/2 moments. The strong spin-orbit coupling of ruthenium enhances magnetic frustration, which leads to a zigzag antiferromagnetic (AFM) ground state at 7K – a temperature much lower than the exchange interaction energy scale. With magnetic fields of roughly 10 T, AFM order is suppressed and an unconventional spin state emerges. This state, characterized by an unsaturated magnetization, persists up to magnetic fields of order 100 T. We use a newly-developed technique – resonant torsion magnetometry – to explore the temperature evolution of the magnetic anisotropy in the high-field state of RuCl$_3$. The high sensitivity of this technique allows us to measure a single crystallographic, and hence magnetic, domain. With increasing magnetic field, we observe a single transition associated with the suppression of AFM order. Above this transition, the magnetic anisotropy saturates (unlike the isotropic component of the magnetization), with a saturation field that scales linearly with temperature. Our data shows that the energy scale that determines the magnetic anisotropy is set only by field and temperature. This suggests that the intrinsic energy scale is driven to zero by strong correlations – a signature of a fluid-like spin state that is decoupled from the underlying exchange interactions.

1:39PM S44.00005: Quantization of the thermal Hall conductivity at small Hall angles* [Invited] Mengxing Ye (Presenter), University of Minnesota — Recent experiments have described the measurement of a near-quantized thermal Hall conductance in α-RuCl$_3$ as direct evidence for the propagation of a chiral Majorana mode in this system and consequently as smoking gun evidence for an intermediate chiral spin liquid phase in this system. However, the large experimental longitudinal thermal conductivity, attributed to bulk phonons, begs for an investigation of the spin-lattice coupling, and its role on the quantization of the thermal Hall conductivity. We show that due to the bulk and edge mixing of energy propagation, the temperature gradient of the bulk phonons develops a transverse component which may contribute to a quantized effective thermal Hall conductance. We also discuss the situations where the quantization breaks down and predict notable experiments that test it.


*M.Y. acknowledges the KITP graduate fellowship program, where this work was done.
11:15AM S45.00001: Low loss amorphous Ta2O5 coatings grown by reactive sputtering for dielectric mirrors used for gravitational wave detection* KEERTI SHUKLA (Presenter), Materials Science and Engineering, UC Berkeley, MANEL MOLINA-RUIZ, Physics, UC Berkeley, MATT ABERNATHY, United States Naval Research Laboratory, ALENA ANANYEVA, LIGO Laboratory, California Institute of Technology, RICCARDO BASSIRI, MARTIN FEJER, Applied Physics, Stanford University, ERIC KEITH GUSTAFSON, LIGO Laboratory, California Institute of Technology, XIAO LIU, United States Naval Research Laboratory, ASHOT MARKOSYAN, Edward L. Ginzton Laboratory, Stanford University, THOMAS METCALF, United States Naval Research Laboratory, GABRIELE VAJENTE, LIGO Laboratory, California Institute of Technology, FRANCES HELLMAN, Physics and Materials Science and Engineering, UC Berkeley — The ability of LIGO and others in the gravitational wave community to detect astronomical events relies on the quality of optical mirrors used in interferometers. A lot of effort is devoted to reduce optical absorption and mechanical loss in the layers that make up the mirror coatings. Amorphous tantala is of interest as the high index of refraction layer but contributes the most to overall mechanical loss. The mechanisms that lead to mechanical loss must be understood in order to minimize the losses.

Amorphous tantala 500nm films are deposited using reactive sputtering of a tantalum target where growth temperatures are varied from room temperature to 600C. Thermally activated and tunneling mechanisms both contribute to the overall mechanical loss which can be measured through internal friction techniques. The thermally activated are measured at room temperature using Gentle Nodal Suspension and the tunneling are measured at temperatures below 10K using Double Paddle Oscillators. These results provide a deeper understanding of the energy dissipation in amorphous tantala due to both tunneling and thermally activated loss mechanisms.

*Gordon and Betty Moore Foundation

11:27AM S45.00002: WITHDRAWN ABSTRACT —

11:39AM S45.00003: Understanding the role of carbon in active trap centre formation in porous alumina for ion beam dosimetry SANGITA BHOWMICK (Presenter), SAPTARSHI PAL, DIP DAS, Shiv Nadar University, VIPIN KUMAR SINGH, devi ahilya university, SAIF KHAN, inter university accelarator center, RENE HUEBNER, Electron Microscopy Laboratory, Helmholtz-Zentrum Dresden - Rossendorf (HZDR) Institute of Ion Beam Physics and Materials Research, SUDIPTO ROYBARMAN, devi ahilya university, DINAKAR KANJILAL, inter university accelarator center, ALOKE KANJILAL, Shiv Nadar University — In recent days, due to increased use of hadron therapy for cancer and tumor treatment, precise online dose monitoring is an important issue for safety purpose. Regarding hadron therapy, recently carbon ion beam with high Linear Energy Transfer (LET) is found to be more effective than the photon beams. Among several known TL/OSL oxides phosphors, C-doped alumina (Al2O3) is favorable for radiation dosimetry, especially in medical field due to its tissue equivalent in terms of radiation absorption, simple glow curve, and high sensitivity. A facile approach to improve thermoluminescence sensitivity of electrochemically anodized porous Al2O3 (AAO) is presented by introducing carbon ions for ion beam dosimetry. Initially, ion implantation technique has been carried out for Carbon doping in AAO in controlled manner. HAADF-STEM, EDS mapping, SEM studies reveal the evolution of a porous structure followed by the carbon distribution upto 200nm. However, the evolution of optically active F+ centres with increasing ion fluence has been examined by photoluminescence investigation at room temperature and thermoluminescence (TL) measurement while the chemical nature of such defect centres has been extracted by depth dependent XPS analysis.
11:51AM S45.00004: Interface-engineered hole doping in Sr2IrO4/LaNiO3 heterostructure* FANGDI WEN (Presenter), XIAORAN LIU, Rutgers University, New Brunswick, QINGHUA ZHANG, Beijing National Laboratory for Condensed-Matter Physics and Institute of Physics, Chinese Academy of Sciences, MIKHAIL S KAREEV, BANABIR PAL, Rutgers University, New Brunswick, YANWEI CAO, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, JOHN WILLIAM FREELAND, Advanced Photon Source, Argonne National Laboratory, ALPHA N'DIAYE, PADRAIC SHAFER, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, LIN GU, Beijing National Laboratory for Condensed-Matter Physics and Institute of Physics, Chinese Academy of Sciences, JAK CHAKHALIAN, Rutgers University, New Brunswick — The relativistic Mott insulator Sr2IrO4 is known for the Jeff = 1/2 Mott insulating state which closely resembles the electronic structure of parent compounds of superconducting cuprates. Here, by means of interface engineering of the Sr2IrO4/LaNiO3 heterostructure, the hole-doped phase of Sr2IrO4 has been realized with a markedly higher doping level close to 10%. X-ray absorption studies at Ni L2 edge confirmed that 5d electrons from Ir sites are transferred onto Ni sites leading to the formation of a high spin Ni2+ state. Despite the large amount of doping, Sr2IrO4/LaNiO3 heterostructure shows a non-metallic behavior but a narrower band gap compared to the bulk Sr2IrO4. This implies strong electronic reconstruction at the interfaces. These findings highlight a powerful utility of interfaces to realize emerging electronic states of the Ruddlesden-Popper phases of Ir-based oxides.

*F. W. was supported by the Claud Lovelace Graduate Fellowship. Q. Z. and L. G. were supported by the Strategic Priority Research Program of CAS and NNSF. M. K. and B. P. were supported by the DOE and J. C. acknowledged the support by the Gordon and Betty Moore Foundation EPIQS Initiative. This research used resources of the Advanced Light Source, which is a DOE Office of Science User Facility.

12:03PM S45.00005: Over 100-THz Bandwidth Selective-Difference-Frequency Generation at LaAlO3/SrTiO3 Nanojunctions* LU CHEN (Presenter), ERIN SUTTON, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNGWOO LEE, Department of Materials Science and Engineering, University of Wisconsin-Madison, JIANAN LI, Department of Physics and Astronomy, University of Pittsburgh, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — The ability to combine continuously-tunable narrow-band terahertz (THz) generation that can access both far-infrared and mid-infrared regimes, holds great potential for uncovering the underlying light-matter interactions as well as realizing selective control of rotational or vibrational resonances in nanoscale objects. Here, we report selective difference frequency generation with over 100 THz bandwidth through femtosecond optical pulse shaping. The THz emission is generated at nanoscale junctions at the interface of LaAlO3/SrTiO3 defined by conductive atomic force microscope lithography, with the potential to perform THz spectroscopy on individual nanoparticles or molecules. Numerical simulation of the time-domain signal helps to identify different contributing components for the THz generation. These results transform the LaAlO3/SrTiO3 interface into a promising platform for integrated lab-on-chip devices.

*JL acknowledges support from ONR (N00014-16-1-3152) and a Vannevar Bush Faculty Fellowship, funded by ONR (N00014-15-1-2847). C-BE acknowledges support from AFOSR (FA9550-15-1-0334), NSF DMREF (DMR-1629270), and NSF MRSEC (DMR-1420645) (C-BE). ES acknowledges support from the NSF Graduate Research Fellowship Program (1747452).

12:15PM S45.00006: Morphological anisotropy and mosaicity in epitaxially grown VO2 films* ANATOLY SHABALIN (Presenter), University of California, San Diego, ELIHU ANOUCHI, Department of Physics, Bar-Ilan University, MARTIN HOLT, Center for Nanoscale Materials, Argonne National Laboratory, AMOS SHARONI, Department of Physics, Bar-Ilan University, OLEG SHPYRKO, University of California, San Diego — Epitaxially grown films of VO2 are one of the most promising materials for oxide electronics due to a very convenient temperature and remarkable controllability of the insulator-metal phase transition (IMT) by doping, strain, photo excitations or applying an electric field. Scaling the IMT-based devices down to submicron size is a technological challenge because of the high variability of the resulted functional characteristics from device to device. Our work focuses on the structural and morphological origins of such variations.

We used X-ray nano diffraction mapping to study the evolution of mosaicity, strain and phase coexistence in 70 nm thick VO2 film (r-cut Al2O3) during thermal cycling and annealing. We found high anisotropy in the grain and crack network structure which remarkably resonates with anisotropy of transport properties. We were able to distinguish a persistent morphological pattern due to the film manufacturing from transient features introduced by thermal cycling. Our results manifest the important role of nanomorphology in the performance of VO2-based nanodevices. We suggest that it can also be considered as a new degree of freedom to control functional properties in oxide electronics.

*This work was supported by DOE- Office of Basic Energy Sciences.
Preparation and X-Ray Diffraction Study of Strongly Oriented Thin Films with Potential Magnetoelectric Effect

RADOMIR KUZEL (Presenter), Faculty of Mathematics and Physics, Charles University, JOSEF BURSIK, ROBERT UHRECKY, MIROSLAV SOROKA, Institute of Inorganic Chemistry, Czech Academy of Sciences, JAN PROKLESKA, Faculty of Mathematics and Physics, Charles University — Thin films of M, Y and Z hexagonal ferrites with a potential of magnetoelectric (ME) effect were prepared by chemical solution deposition method and processing parameters were tested and optimized. Several substrates were used, and different substrate/seeding layer/ferrite layer architectures were proposed to get strong preferred grain orientation. The films were studied by X-ray diffraction (XRD), AFM and EBSD. Lattice parameters, out-of-plane and in-plane grain orientations, crystal sizes, microstrains and residual stresses were obtained by different XRD symmetric and asymmetric scans and their combinations.

New Y-ferrite phases were prepared with the composition BaSrZnCoFe_{11}(Me)O_{22} (Me = Al, Ga, In, Sc). For Me = Al, Ga the magnetic structure is of non-collinear ferrimagnetic type with unspecified helical magnetic structure. ME Z-type ferrite Sr_{3}Co_{2}Fe_{24}O_{41} and Ba_{x}Sr_{3-x}Co_{2}Fe_{24}O_{41} thin films were prepared and characterized for the first time. Three present M, S and Z phases showed well out-of-plane and in-plane mutual orientations.

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1:03PM S45.00010: High Temperature Oxidation of Amorphous Zr-B-C-N Thin Films Grown by Electron Beam Evaporation*  
MORTON GREENSLIT (Presenter), MORGEN BENNINGHOFF, ROBERT J LAD, University of Maine — Boron carbonitride films have been shown to yield enhanced hardness and oxidation resistance, making them potentially attractive as protective coatings for high temperature applications. Most previous work has focused on thick films (>1μm) grown by magnetron sputtering. In this study, 200 nm thick ZrBCN films with a range of stoichiometries were grown on r-sapphire substrates at 850°C using e-beam evaporation of ZrC and B sources in a nitrogen plasma. As-deposited films were found to be amorphous by XRD, and the nitrogen content was relatively constant independent of ZrC or B evaporation rates. XPS analysis of the films after air annealing over the range 500-800°C showed that B and N were entirely depleted at the surface, while ZrO2 grains nucleated within the amorphous film matrix. XRD showed the formation of a tetragonal-ZrO2 phase at 600°C that became replaced by a monoclinic-ZrO2 phase at 800°C as the ZrO2 grains grew in size. SEM analysis showed film delamination and cracking during high temperature oxidation to relieve film stress. The oxidation resistance of the 200 nm ZrBCN films is much less than reported for thicker sputtered films, indicating that the oxidation resistance mechanism is strongly dependent on film thickness.

*This work was supported by NSF grant #1309983.

1:15PM S45.00011: Reduction of Stress in Dual Ion Beam Sputtered Ta2O5 and SiO2 Optical Interference Coatings*  
EMMETT RANDEL (Presenter), AARON DAVENPORT, CARMEN SUSANA MENONI, Colorado State Univ — We studied the mechanical and optical properties of tantalum pentoxide (Ta2O5) and silicon dioxide (SiO2) films prepared by dual ion beam sputtering with the goal to realize thin films with a stress below 0.3 GPa. It is shown that the use of a low energy assist beam consisting of oxygen and argon species results in a Ta2O5 film with a stress below 100 MPa and a SiO2 film with a stress below 250 MPa. Using photothermal common path interferometry (PCI), spectrophotometry, and ellipsometry, it is shown that these films are suitable for use in interference coatings.

*DoD HEL JTO and ONR grant No. N00014-17-1-2536

1:27PM S45.00012: Properties of CCTO, a High Dielectric Constant Material*  
PARVEEN KUMAR (Presenter), University of California Merced 95343 USA, D. C. AGRAWAL, IIT Kanpur UP 208016 India — CaCu3Ti4O12 (CCTO) shows an extremely high dielectric constant, which, in contrast to ferroelectrics like BaTiO3, is nearly constant in a broad temperature range. Thus, this material has attracted tremendous attention due to its possible applications, e.g., for enhancing the performance of capacitive electronic elements. We used a simple Sol-Gel technique and established a novel composition of CCTO with high dielectric constant, and fabricated stable and reliable thin films. We have successfully incorporated silver nanoparticle in CCTO thin films. The conducting metal particles dispersed in a dielectric matrix are known to increase the effective dielectric constant of the medium. Based on these novel materials, we developed tunable multilayer capacitor with high dielectric constant.

*This work is done at IIT Kanpur.

1:39PM S45.00013: Influence of Assist Ion Bombardment on Mechanical Loss of Amorphous Tantala Thin Films for Gravitational Wave Interferometers*  
LE YANG (Presenter), EMMETT RANDEL, Colorado State Univ, GABRIELE VAJENTE, ALENA ANANYEVA, ERIC KEITH GUSTAFSON, California Institute of Technology, ASHOT MARKOSYAN, MARTIN FEJER, Stanford University, CARMEN SUSANA MENONI, Colorado State Univ — Thermal noise in high-reflectivity coatings is critical for improving the sensitivity of future gravitational wave detectors. Amorphous tantala (Ta2O5) thin film, used as high-index material, with lower mechanical loss is expected as one solution to further reduce the coating thermal noise. The material is also regarded as promising candidate for use in resistance random access memory as well as optical applications. In this work, amorphous tantala thin films have been deposited by reactive ion beam sputtering with assist Ar⁺ and Xe⁺ ion bombardment to investigate the effect of ion-induced surface diffusion on coating's mechanical and structural properties. The results show that the atomic structure of ion bombarded tantala thin films remain amorphous and their composition is mostly stoichiometric. The mechanical loss of ion-bombardeed tantala coatings shows no significant improvement compared to non-bombardeed samples. The coating loss angle of tantala is insensitive to ion dose or ion mass. An analysis based on surface diffusivity suggests that the ion-assisted surface diffusivity may be insignificantly modified under the current typical deposition conditions.

*This work is supported by the National Science Foundation LIGO program through grant No. 1708010
1:51PM S45.00014: TiO$_2$ doped Ta$_2$O$_5$ coatings grown by biased target ion beam deposition for gravitational wave detectors*  
MARIANA FAZIO (Presenter), Department of Electrical and Computer Engineering and NSF ERC for Extreme Ultraviolet Science and Technology, Colorado State University, Fort Collins, CO, USA, GABRIELE VAJENTE, ALENA ANANYEVA, ERIC KEITH GUSTAFSON, LIGO Laboratory, California Institute of Technology, Pasadena, CA, USA, CARL LÉVESQUE, FRANÇOIS SCHIETTEKATTE, Université de Montréal, Montréal, Quebec, Canada, ASHOT MARKOSYAN, RICCARDO BASSIRI, MARTIN FEJER, Department of Applied Physics, Ginzton Laboratory, Stanford University, Stanford, CA, USA, CARMEN SUSANA MENONI, Department of Electrical and Computer Engineering and NSF ERC for Extreme Ultraviolet Science and Technology, Colorado State University, Fort Collins, CO, USA — Advanced LIGO employs as end masses high reflectance mirrors of alternating layers of SiO$_2$ and Ta$_2$O$_5$ doped with 25% of TiO$_2$. Doping Ta$_2$O$_5$ with 25% TiO$_2$ decreased the mechanical loss which increased the sensitivity of the detector, but the physical reasons of this are still unknown. In this work we studied thin films of Ta$_2$O$_5$ doped with different TiO$_2$ concentrations grown by biased target ion beam deposition to evaluate the effect of doping in the mechanical loss and to search for high index materials with improved performance for the upcoming upgrade of LIGO and future detectors. The deposition system consists of a low energy ion source and metallic targets individually pulsed biased. Control of each target bias allows for mixing Ta$_2$O$_5$ and TiO$_2$, with estimates of the doping obtained by x-ray photoelectron spectroscopy. Extensive characterization shows the films are nearly stoichiometric and dense, with an absorption loss at 1064 nm lower than 20 ppm. Mechanical loss was measured in as deposited coatings and after annealing. For all TiO$_2$ concentrations the mechanical loss is reduced after annealing, reaching a minimum for around 20% TiO$_2$ after annealing at 600 C comparable to state-of-the-art TiO$_2$ doped Ta$_2$O$_5$.

*Work supported by the Center for Coatings Research NSF award No.:1710957.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S46 DMP: Complex Oxide Interfaces & Heterostructures -- Electronic and transport properties  
BCEC 212 - Ryan Comes, Auburn University - Tag(s): Focus

11:15AM S46.00001: Strain-engineered SrSnO$_3$ films with high room-temperature electron mobility*  
TIANQI WANG, ABHINAV PRAKASH (Presenter), Chemical Engineering and Materials Science, University of Minnesota - Twin Cities, YONGQI DONG, University of Science and Technology of China, TRISTAN TRUTTMANN, Chemical Engineering and Materials Science, University of Minnesota - Twin Cities, ASHLEY BUCSEK, RICHARD D JAMES, Aerospace Engineering and Mechanics, University of Minnesota - Twin Cities, DILLON D FONG, Materials Science Division, Argonne National Laboratory, JONG-WOO KIM, PHILIP RYAN, HUA ZHOU, Advanced Photon Source, Argonne National Laboratory, TURAN BIROL, BHARAT JALAN, Chemical Engineering and Materials Science, University of Minnesota - Twin Cities — Bulk SrSnO$_3$ (SSO) exhibits four crystalline polymorphs as a function of temperature. Through comprehensive thin film growth using novel radical-based MBE approach, synchrotron x-ray scattering, electronic transport, and first-principles calculations, we report on the stabilization of different polymorphs of SSO at room temperature (RT), in thin film form. Compressive strain stabilized the high-symmetry tetragonal phase of SSO at RT, which, in bulk, exists only at temperatures between 1062 K and 1295 K. A mobility enhancement of over 300% in the doped tetragonal phase of SSO films compared with the low-temperature orthorhombic polymorph was achieved. We will discuss these results in the context of the role of strain, doping, and disorder on structure and electronic transport of doped SSO films.

*Work supported by AFOSR YIP and NSF DMR
11:27AM S46.00002: Electrostatic gating of MBE-grown SrSnO$_3$ films using ion-gel*  
LAXMAN RAJU THOUTAM  
( Presenter), JIN YUE, ABHINAV PRAKASH, TIANQI WANG, BHARAT JALAN, University of Minnesota — Electrostatic gating using ion-gel is an effective way to dynamically tune electronic phase transitions in solid materials. We report the first experimental findings of reversible electrostatic control of insulator-to-metal transition in La-doped SrSnO$_3$ films grown by the hybrid molecular beam epitaxy method. The low temperature sheet resistance ($R_s$) of the films were modulated over four orders of magnitude at an applied gate voltage of $+4$V. The careful analysis of the temperature dependent transport properties reveal a smooth crossover from strong-localization to weak-localization behavior at 2 K with increased positive gate voltages. We further discuss the nature of quantum corrections that are responsible for the upturn in $R_s$ at low temperatures and its effect on the induced carrier density, on the metallic side of insulator-to-metal transition. The excellent overlap of the measured $R_s$ (at zero gate bias) before and after multiple sequence of $R_s$ vs T measurements at different applied gate biases indicate the true reversible and electrostatic control of the gating process in stannate systems.

*Work supported by UMN NSF MRSEC and AFOSR YIP

11:39AM S46.00003: Wide Range Reversible Transport Modulation and Electron Density Dependence of Mobility in Ion-Gel-Gated BaSnO$_3$ Films*  
HELIN WANG (Presenter), JEFFERY J WALTER, KOUSTAV GANGULY, ABHINAV PRAKASH, BIIQIONG YU, GUICHUAN YU, HAN FU, MARTIN GREVEN, CHRIS LEIGHTON, University of Minnesota — Rapid progress has been made with BSO films since the report of room temperature mobility $>300$ cm$^2$V$^{-1}$s$^{-1}$ in bulk crystals. Questions remain over mobility-limiting mechanisms, however. Here we report doping-dependent electronic transport in epitaxial-BSO-based electric double layer transistors using ion gel electrolytes. Over an exceptional gate voltage window of -3 to $+4$V, at 300 K, electrostatic gating mechanisms dominate, supported by reversible transport response and operando synchrotron X-ray diffraction experiments. This is in stark contrast with many complex oxides and, vitally, is attributed here to the exceptionally small diffusivity of oxygen vacancies in BSO. Wide-range voltage control of resistance is demonstrated in a series of undoped and initially chemically $n$-doped BSO films, including a strong to weak localization crossover. Interfacial electron density ($n$) and mobility ($\mu$) are extracted from two-channel conduction modelling and the $\mu$-n relation is probed from $\sim10^{18}$ cm$^{-3}$ to $>10^{20}$ cm$^{-3}$. Universally, $\mu$ increases rapidly with $n$ before decreasing above $\sim10^{20}$ cm$^{-3}$, potentially due to surface scattering. The highest $\mu$ achieved is 140 cm$^2$V$^{-1}$s$^{-1}$ in La-doped BSO films by increasing $\mu$ with gating by up to 55%.

*Work supported by NSF MRSEC under DMR-1420013.

11:51AM S46.00004: Weak (anti)localization in NdTiO$_3$/SrTiO$_3$ Heterointerfaces*  
XINXIN CAI (Presenter), YILIKAL AYINO, School of Physics and Astronomy, University of Minnesota, JIN YUE, PENG XU, BHARAT JALAN, Department of Chemical Engineering and Materials Science, University of Minnesota, VLAD S PRIBIAG, School of Physics and Astronomy, University of Minnesota — The quasi-two-dimensional interfacial electron gas formed at complex oxide interfaces exhibits a wide range of interesting physical properties including spin-orbit coupling and magnetism. We report magneto-transport studies on NdTiO$_3$/SrTiO$_3$ heterostructures grown by hybrid molecular beam epitaxy. The magneto-transport behavior exhibits a systematic crossover between weak antilocalization and weak localization with changing temperature. The weak-antilocalization analysis of the magnetoresistance provides information about the spin and phase relaxation mechanisms and may indicate the interplay between the interfacial magnetism and spin-orbit coupling.

*This work is supported by the Office of Naval Research and DOE Center for Quantum Materials.
12:03PM S46.00005: Quantised conductance of one-dimensional strongly-correlated electrons in a ZnO heterostructure*  
HANGTIAN HOU, University of Cambridge, YUSUKE KOZUKA, Research Center for Magnetic and Spintronic Materials, National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba 305-0047, Japan, JUN-WEI LIAO, LUKE W SMITH, DEAN KOS, JONATHAN GRIFFITHS, University of Cambridge, JOSEPH FALSON, Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany, ATSUSHI TSUKAZAKI, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, MASASHI KAWASAKI, Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), The University of Tokyo, Tokyo 113-8656, Japan, CHRISTOPHER J FORD (Presenter), University of Cambridge — Oxide heterostructures are versatile platforms with which to research and create novel functional nanostructures. We have developed one-dimensional (1D) quantum-wire devices using quantum point contacts on MgZnO/ZnO heterostructures and observe ballistic electron transport with conductance quantised in units of $2e^2/h$. Using DC-bias and in-plane-field measurements, we find that the $g$-factor is enhanced to around 6.8, more than three times the value in bulk ZnO. We show that the effective mass $m^*$ increases as the electron density decreases, resulting from the strong electron-electron interactions. In this strongly interacting 1D system we study features matching the '0.7' conductance anomalies up to the fifth subband. We demonstrate that high-mobility oxide heterostructures such as this can provide good alternatives to conventional III-V semiconductors in spintronics and quantum computing as they do not have their unavoidable dephasing from nuclear spins. This paves a way for the development of qubits benefiting from the low defects of an undoped heterostructure together with the long spin lifetimes achievable in silicon.

*YK is also at NIMS, Tsukuba and JST, PRESTO, Saitama, Japan. Work was partly supported by JST, PRESTO Grant No. JPMJPR1763 and JST, CREST Grant No. JPMJCR16F1.

12:15PM S46.00006: The formation of small polaron at the conducting LaAlO$_3$/SrTiO$_3$ interface  
WEILONG KONG (Presenter), JUN ZHOU, Department of Physics, National University of Singapore, MING YANG, Institute of Materials Research and Engineering (IMRE), A*STAR (Agency for Science, Technology and Research), YUAN PING FENG, Department of Physics, National University of Singapore — The interplays among various degrees of freedom such as charge, spin, orbital and lattice generate striking physical properties in oxide heterostructures that are not observed in their parent bulk materials. In this study, via first-principles calculations, we show that the excess electrons at the conducting LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface favor the formation of polaron states. These electrons interact strongly with the lowest $d_{xy}$ orbital of the interfacial Ti lattices, forming localized splitting states. Compared with SrTiO$_3$ bulk, the formation of the polaron states is more favorable at LAO/STO interface, which is ascribed to the reduced dimensionality and lattice symmetry. These results suggest that some of the excess electrons are localized and do not contribute to the transport effectively, and also shed light on a new direction to understand various novel properties of the conducting LAO/STO interface.

12:27PM S46.00007: Systematic Study of Superconductivity in Hybrid MBE-grown Sr$_{1-x}$Nd$_x$TiO$_3$ Films*  
JIN YUE (Presenter), Department of Chemical Engineering and Materials Science, University of Minnesota, YILIKAL AYINO, School of Physics and Astronomy, University of Minnesota, LAXMAN RAJU THOUTAM, Department of Chemical Engineering and Materials Science, University of Minnesota, VLAD PRIBIAG, School of Physics and Astronomy, University of Minnesota, BHARAT JALAN, Department of Chemical Engineering and Materials Science, University of Minnesota — Ever since the discovery of superconductivity in n-doped SrTiO$_3$ (STO) ($10^{18}$ – $10^{21}$ cm$^{-3}$), STO has received significant attention. More recently, it has been shown that superconductivity can be stabilized at much lower concentrations ($5.5 \times 10^{17}$ cm$^{-3}$) using oxygen-vacancy doped STO raising many questions on the role of dopants and disorder on superconductivity in STO. To-date, these works have been limited to the bulk STO single crystals. In this talk, we will present the first systematic study of superconductivity in epitaxial n-doped Sr$_{1-x}$Nd$_x$TiO$_3$ films grown using hybrid molecular beam epitaxy. We will also discuss the role of dopants, point disorder, and epitaxial strain on the superconductivity and normal state transport in doped STO films.

*This work is supported by DOE center for quantum materials. Yilikal Ayino and Vlad Pribiag acknowledge UMN MRSEC for millikelvin measurements.
12:39PM S46.00008: Electrical control of phase transitions through ion transfer in oxide superlattices  DI YI (Presenter), Stanford University, YUJIA WANG, Tsinghua University, HONGTAO YUAN, Nanjing University, OLAF M VAN T ERVE, US Naval Research Laboratory, MICHAEL VEIT, PURNIMA BALAKRISHNAN, Stanford University, YONGSEONG CHOI, Argonne National Laboratory, ALPHA N'DIAYE, PADRAIC SHAFER, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, BEREND JONKER, US Naval Research Laboratory, PU YU, Tsinghua University, YURI SUZUKI, Stanford University — Electrical control of phase transitions through ion transfer has been of great interest recently. Ion transfer can have a dramatic influence on a material’s electronic, magnetic and optical properties, and thereby provides a powerful tool for fundamental research and enables many practical applications. However only a few materials have been found to exhibit significant tunability and good reversibility of electrically controlled ion transfer. In this talk, we show that superlattices comprised of the 5d oxide SrIrO3 and 3d oxide La1-xSr2MnO3 exhibit a reversible phase change under ionic liquid gating. Ionic liquid gating modulates the lattice constant by seven percent and modifies the valence of both Mn and Ir cations. The gate voltage induces a reversible transition between a ferromagnetic metallic state and a nonmagnetic insulating state, along with a large modulation of optical transmittance. Secondary ion mass spectrometry indicates that these reversible transitions are mediated by the transfer of hydrogen and oxygen ions in the superlattices. Single layer films of the constituent materials do not exhibit such significant changes in properties. Our study shows that the electrically controlled ion transfer can be engineered by designing materials at the atomic scale.

12:51PM S46.00009: Emergent Phenomena at Mott Insulator/ Band Insulator Interfaces* [Invited] YURI SUZUKI (Presenter), Stanford University — Complex oxide interfaces have been explored extensively in recent years as emergent phenomena, ranging from magnetism, metallicity, superconductivity to spin-orbit coupling, have been generated at these interfaces due to electronic, magnetic, orbital reconstruction etc. Electronic reconstruction at a Mott insulator/ band insulator interface has been predicted to exhibit a wide range of emergent electronic and magnetic behavior. A particularly interesting model system is the LaTiO3/ SrTiO3 interface where electronic reconstruction gives rise to low dimensional metallic behavior accompanied by giant Rashba spin-orbit coupling. We studied ultrathin films of LaTiO3 on SrTiO3 substrates where interface reconstruction dominates the transport behavior. We found evidence for giant Rashba spin splitting in two sets of Shubnikov-de Haas oscillations associated with an inner and outer Fermi surface, Berry phase of π, substantial anisotropic magnetoresistance and a weak anti-localization correction to the magnetoconductivity. Together these results indicate a large Rashba coupling coefficient of 2.0 x 10^{-11} eV-m which is an order of magnitude larger than other complex oxide interfaces. Such a large Rashba coupling suggests that such a Mott/band insulator interface may be an excellent candidate for spin current-based electronics.

*†This work was done in collaboration with Michael Veit, Remi Arras, Brad Ramshaw, Mun Chan and Rossitza Pentcheva and funded by the Vannevar Bush Faculty Fellowship of the Department of Defense under Contract No. N00014-15-1-0045.

1:27PM S46.00010: Controlled epitaxial growth and oxygen excess doping of the Mott insulator LaTiO3* RALPH CLAESSEN, PHILIPP SCHEIDERER, MATTHIAS SCHMITT, JUDITH GABEL, MICHAEL ZAPF, MARTIN STÜBINGER, PHILIPP SCHÜTZ, LENART DUDY, Universität Würzburg, Germany, CHRISTOPH SCHLUETER, TIEN-LIN LEE, Diamond Light Source, UK, MICHAEL SING (Presenter), Universität Würzburg, Germany — Here we demonstrate that thin films of the prototypical Mott insulator LaTiO3 grown by pulsed laser deposition under oxygen atmosphere are readily tuned by excess oxygen doping across the line of the band-filling controlled Mott transition in the electronic phase diagram [1]. The detected insulator to metal transition is characterized by a strong change in resistivity of several orders of magnitude. The use of suitable substrates and capping layers to inhibit oxygen diffusion facilitates full control of the oxygen content and renders the films stable against exposure to ambient conditions. These achievements represent a significant advancement in control and tuning of the electronic properties of LaTiO3+x thin films making it a promising channel material in future Mottronic devices.


*Work supported by Deutsche Forschungsgemeinschaft through SFB 1170 “ToCoTronics”.

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1:39PM S46.00012: Charge Transfer and Built-in Electric Fields Between the Crystalline Oxide SrNbxTi1-xO3-δ and Silicon
ZHENG HUI LIM (Presenter), Department of Physics, University of Texas-Arlington, NICHOLAS F QUACKENBUSCH, Materials Measurement Science Division, National Institute of Standards and Technology, JOSEPH NGAI, Department of Physics, University of Texas-Arlington — Heterojunctions between semiconductors and oxides are fundamental to field-effect devices that have revolutionized information technology. However, their principal functionality remains as capacitors within the metal-insulator-semiconductor (MIS) paradigm. Here we report charge transfer and the formation of built-in electric fields across heterojunctions between single-crystalline SrNbxTi1-xO3-δ and Si(001). A non-monotonic anomaly in the sheet resistance is observed, accompanied by a crossover in sign of the Hall resistance which indicates the formation of a hole gas in the Si and the presence of strong built-in fields. Hard X-ray photoelectron spectroscopy measurements reveal pronounced asymmetric features in both the SrNbxTi1-xO3-δ and Si core-level spectra that we show arise from built-in fields. Analysis of these unprecedent asymmetries enables band-bending to be spatially mapped across the heterojunction. Control of charge transfer and built-in fields opens a pathway to realize hybrid pn-junctions, isotype junctions etc., that elevate the functionality of semiconductor-oxide heterojunctions beyond the MIS paradigm.

2:03PM S46.00013: Direct Measurement of Band Edge Profiles at Epitaxial Oxide/Semiconductor Heterojunctions*
SCOTT CHAMBERS (Presenter), PETR SUSHKO, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, NICHOLAS F QUACKENBUSCH, JOSEPH WOICIK, Materials Measurement Science Division, National Institute of Standards, ZHENG HUI LIM, MATTHEW CHRYSLER, JOSEPH NGAI, Department of Physics, University of Texas at Arlington, TIEN-LIN LEE, Diamond Light Source, JAMES LEBEAU, Department of Materials Science & Engineering, North Carolina State University — Band edge profiles for semiconductor heterojunctions can be approximated using transport data and/or calculated from first principles, assuming an atomistic materials structure. However, direct and accurate experimental measurement has not been possible by traditional means. We have used hard x-ray photoelectron spectroscopy (HAXPES) to extract band edge profiles from core-level spectra by developing an effective algorithm that fits experimental heterostructure spectra to sums of flat-band spectra, measured for pure reference materials, in which the binding energies are exhaustively varied to sample the phase space of physically reasonable potential profiles over all layers within the HAXPES probe depth. We apply this method to heterojunctions of n-SrNb_xTi_1-xO_3 and intrinsic Si(001), prepared by molecular beam epitaxy. Heterojunction formation results in a Si hole gas and a surface depleted dead layer in the SrNb_xTi_1-xO_3. The band edge profiles resulting from the HAXPES fitting reveal both of these features, and match what is expected based on Hall data remarkably well. In this talk, we present highlights of this analysis.

*This work was supported by the U.S. Department of Energy, Office of Science, Division of Materials Sciences and Engineering under Award #10122.
TAKAHIRO CHIBA (Presenter), Fukushima National Institute of Technology, SABURO TAKAHASHI, Advanced Institute for Materials Research (AIMR), Tohoku University — Thermoelectric (TE) conversion from thermal energy into electric energy has been attracting attention as a renewable energy harvesting. The conversion efficiency is evaluated by the dimensionless figure of merit $ZT$ and for practical use $ZT \geq 1$ (conversion efficiency is 10%) is required. Bismuth chalcogenide is not only known as a representative material with high $ZT$ but also has received attention as a topological insulator (TI) phase in recent years. Here we theoretically study the thermoelectric effect on the surface of TIs that are ionically disordered as the consequence of hypothetical doping for systematic control of the Fermi levels. Coulomb type long range potential is introduced as the ionic disorders. Based on Boltzmann transport theory at finite temperature, we calculate the TE coefficient and $ZT$. As a result, we find that $ZT$ can achieve substantially high values even for the thermal phonon. Our theory may help us understand recent TE transport measurements in TI thin films and could make an ionically disordered TI a promising material for TE conversion technology.

SUNGJIN PARK (Presenter), Korea Electrotechnology Research Institute, MIN HO LEE, Institute for Metallic Materials, Leibniz Institute for Solid State and Materials Research, Dresden, BYUNGKI RYU, Korea Electrotechnology Research Institute — PbTe is very noteworthy thermoelectric material working at intermediate temperatures. Most investigations of PbTe were focused on PbTe-based alloys to control band convergence, formation of resonant level, and nanostructuring. However, the intrinsic-defect nature of PbTe is still not well understood yet. The semiconductor type of PbTe-related alloys is known to be determined by Pb concentration with respect to Te concentration. In binary, Pb-rich or Te-rich PbTe typically exhibits n-type or p-type behavior, respectively. Our experiments showed that 10% excess-Pb doping merely changes the lattice parameter (+0.3%). To understand such atomic and electrical behaviors in off-stoichiometric PbTe, we theoretically investigated the formation of intrinsic defects in PbTe by performing first-principle density functional theory calculations. We used PAW method and GGA-PBE, which are implemented in VASP code. The defect formation energies of various charged states were computed on the 128-atom FCC supercell and a 3x3x3 k-point mesh. We suggest that the formation of Pb interstitial or Te vacancy might be responsible for the off-stoichiometry in Pb-rich PbTe, while the formation of Pb vacancy or Te vacancy might be responsible in Te-rich PbTe.

JAVIER FERNANDEZ TRONCOSO (Presenter), PABLO AGUADO-PUENTE, Queen's University Belfast — Lead telluride (PbTe) is a reference high-performance thermoelectric which can exhibit low values of thermal conductivity in the presence of intrinsic defects. Here, we present an optimized Buckingham potential that provides an improved description of this material, especially for the lattice thermal conductivity. The latter is computed using two different methods: Green-Kubo method and direct thermostatting. Comparison with other classical force fields proposed in the literature shows substantial improvement.

Using this potential we studied how intrinsic defects influence the thermal conductivity, paying special attention to vacancies, interstitials and grain boundaries. Our results show that intrinsic point defects and grain boundaries can reduce the lattice conductivity of PbTe by a factor of 4, and converge towards the value of pristine PbTe under typical experimental concentrations of defects in samples. We also determine the thermal resistance of grain boundaries.

This work was supported by a research grant from Science Foundation Ireland (SFI) and the Department for Economy (Northern Ireland).
Desirable dopants for thermoelectrics

JIAWEI ZHOU (Presenter), QICHEN SONG, TE-HUAN LIU, Massachusetts Institute of Technology, JUN MAO, HANGTIAN ZHU, University of Houston, RAN HE, Institut für Metallische Werkstoffe, WUYANG REN, ZIHANG LIU, ZHIFENG REN, University of Houston, GANG CHEN, Massachusetts Institute of Technology — Doping is a common technique to achieve good electrical conduction in semiconductors, and is often used to optimize the performance of thermoelectric materials. While its effect on the electron mobility has been widely appreciated, the understandings still mostly rely on simplified models, which often neglect the chemical details of the dopants. On the other hand, experimental evidence has suggested that dopants with different chemical nature can behave quite differently. The lack of theory to explain such observations, however, has impeded our understanding for controlling dopants, and defects in general, for thermoelectric materials. Recently we have developed a first principles approach to quantitatively evaluate the the effects of dopants on the electron transport. We will discuss how the bonding environment of the atoms - a previously overlooked aspect - can significantly affect the electron transport. The study potentially provides guidelines for finding efficient dopants for thermoelectric materials.

*This work is supported partially by DOE EFRC (Grant No. DE-SC0001299, for fundamental studies on thermoelectrics), and partially by DARPA MATRIX program (Grant No. HR0011-162-0041 for supporting its thermoelectrics programs).

Dopability on Complex Diamond-Like Semiconductors: new candidates for thermoelectric applications

LIDIA GOMES (Presenter), JIAXING QU, University of Illinois at Urbana-Champaign, BRENDEN ORTIZ, ERIC TOBERER, Colorado School of Mines, ELIF ERTEKIN, University of Illinois at Urbana-Champaign — The diamond-like semiconductors (DLS) have recently garnered interest for the potential use as thermoelectric materials. DLS share the diamond structure, forming a chemically rich family of binary, ternary and quaternary compounds. To be a good thermoelectric, however, a material must be sufficiently dopable and the defect chemistry of this group is currently not well characterized.

In this work, we show our recent efforts to investigate the defect physics of these complex materials using first-principles calculations. We focus on a subset within the DLS, formed by ternary and quaternary tellurides. We show that there is a large diversity in the stability phase diagrams in this group and how this impact defect formation energies and the range of achievable carrier concentrations. Most of the ternaries show dopability windows ranging from highly p-type to intrinsic or slightly n-type. In addition, a control of carrier concentrations can be achieved by growth under different thermodynamic environments. We also highlight the importance of the computational approach to an accurate prediction of these quantities, that can be used to guide experimental works.

*We acknowledge the support of the National Center for Supercomputing Applications and the NSF via grants 1729594 and 1729149.

Hierarchical design of nanomaterials for improving the power factor

NEOPHYTOS NEOHYTOS (Presenter), LAURA DE SOUSA OLIVEIRA, VASSILIOS VARGIAMIDIS, University of Warwick — Hierarchically nanostructured thermoelectric materials, where nanoinsertions are inserted at various length scales (grain boundaries, embedded quantum dots, atomistic defects), have shown the potential to provide much larger thermoelectric performance compared to pristine materials. This is to-date being attributed to drastic reductions in the thermal conductivity, but less on power factor improvements. In this work we combine Molecular Dynamics simulations for the thermal conductivity and Non-Equilibrium Green's Function simulations for electronic transport to study thermoelectric transport through materials with hierarchically embedded nanoinsertions, namely superlattice-type barriers with quantum dots and voids in between them. We show that beyond the drastic reductions in thermal conductivity, the nanomaterials can be designed such that the power factor: i) is resilient to the presence of nanoinsertions, and ii) is even improved compared to pristine materials, independently of the density of the distorting nanoinsertions.

*This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 Research and Innovation Programme (Grant Agreement No. 678763).
Utilizing Magnetism and Nanostructures to Enhance Performance of Thermoelectric Materials

[Invited] TAKAO MORI (Presenter), International Center for Materials Nanoarchitectonics (WPI-MANA) and Center for Functional Sensor & Actuator (CFSN), National Institute for Materials Science (NIMS) — New principles and strategies are desired to overcome the traditional tradeoff between thermoelectric (TE) properties, i.e. electrical conductivity \( \sigma \) and thermal conductivity \( \kappa \), and Seebeck coefficient \( \alpha \). We have been trying to develop TE enhancement principles which can be relatively easily implemented and applied to a wide range of materials [1]. Porosity had been considered detrimental for TE materials, with the penalty for \( \sigma \) usually being similar or larger than the \( \kappa \) reduction. Introducing a moderate volume of nano-micropores with size distribution by simple evaporation of a secondary phase, has led to effective phonon selective scattering, and 100% enhancement to figure of merit \( \sigma\alpha^2/\kappa = ZT \approx 1.6 \) in rare earth-free (“empty”) skutterudites [2]. This strategy has also led to ZT enhancement in other materials which will be presented. We have proposed to utilize magnetic interactions between carriers and magnetic moments to enhance the power factor \( \sigma\alpha^2 \) [3]. Unlike magnon drag, TE enhancement via magnetic interaction is not solely dependent on ordering, and is effective at higher temperatures also. Magnetic ion doping for example, has led to TE enhancement for a variety of cases, CuGaTe\(_2\), BiCuSeO, Bi\(_2\)Te\(_3\), SnTe, etc., if effective coupling is created. We have also demonstrated significant enhancement of the Seebeck coefficient via spin fluctuation. CREST project members are acknowledged.


*CREST JPMJCR15Q6 and JSPS KAKENHI JP17H02749,JP16H06441 funding is thanked.

Enhanced Seebeck effect in ion-gated FeSe

SUNAO SHIMIZU (Presenter), RIKEN, SHIOGAI JUNICHI, Tohoku University, NAYUTA TAKEMORI, SHIRO SAKAI, RIKEN, HIROAKI IKEDA, Ritsumeikan University, RYOTARO ARITA, RIKEN, TSUTOMU NOJIMA, ATSUISHI TSUKAZAKI, Tohoku University, YOSHIHIRO IWASA, University of Tokyo — The reduction of the dimensionality leads to the manifestation of quantum phenomena and the development of electronic correlation. Such low dimensional effects often become even more pronounced in nano-scale materials including exfoliated atomic layers and their hetero structures, triggering the emergence of the novel electronic, optical, and magnetic properties. Here we report the thermoelectric effect of FeSe ultrathin films with an electric double layer configuration, which allows us to control not only the carrier density but also the film thickness down to monolayer [J. Shiogai et al., Nature Phys. 12, 42 (2016)]. By utilizing a chemical etching induced by applying a large gate bias, the thickness of thin films is reduced in a layer-by-layer manner. Accompanying the emergence of the high-\( T_c \) superconductivity, the ionic liquid gating on FeSe thin films induces the anomalous enhancement of the Seebeck effect. We will discuss the thickness and the temperature dependence of the thermoelectric properties in FeSe thin films in detail.

*This work was supported by JSPS KAKENHI Grant Numbers JP25000003, JP16H00923 (SATL), JP16H06345, JP17H02928, JP17K19060.

Performance Analysis of nanostructured Peltier coolers

ANIKET SINGHA (Presenter), Electronics and Electrical Communication Engineering, Indian Institute of Technology Kharagpur, BHASKARAN MURALIDHARAN, Electrical Engineering, Indian Institute of Technology Bombay — Employing non-equilibrium quantum transport models [1], we investigate the details and operating conditions of nano-structured Peltier coolers embedded with an energy filtering barrier. Our investigations point out non-trivial aspects of Peltier cooling which include an inevitable trade-off between the cooling power and the coefficient of performance, the coefficient of performance being high at a low voltage bias and subsequently deteriorating with increasing voltage bias. We point out that there is an optimum energy barrier height for nanowire Peltier coolers at which the cooling performance is optimized. However, for bulk Peltier coolers, the cooling performance is enhanced with the height of the energy filtering barrier. Exploring further, we point out that a degradation in cooling performance with respect to bulk is inevitable as a single moded nanowire transitions to a multi-moded one. The results discussed here can provide theoretical insights into optimal design of nano Peltier coolers.

Reference

Doping effects and magnetic instabilities in full-Heusler Fe$_2$YZ$_{1-x}$A$_x$ thermoelectric compounds*  
SÉBASTIEN LEMAL (Presenter), FABIO RICCI, MATTHIEU VERSTRAete, PHILIPPE GHOZEz, University of Liége — Giant thermoelectric power factors have been theoretically predicted on n-doped Fe-based full-Heusler compounds, however, when dealing explicitly with dopants, they may undergo to a magnetic phase transition with a consequent power factor reduction. Using computer experiments, we demonstrate that such transitions is purely related to electronic effects. Exploiting the broader nature of 4$d$ and 5$d$ transition metal orbitals, the appearance of the magnetic instability can be shifted to higher doping regimes, recovering high power factors. The unveiled very large power factors and magnetic fluctuations are fascinatingly very promising respectively for standard thermoelectric and spin-caloritronic device applications.

*F. R. and Ph. G. were supported by the European Funds for Regional Developments (FEDER) and the Walloon Region in the framework of the operational program "Wallonie-2020.EU" (project: Multifunctional thin films/LoCoTED). S. L. and Ph. G. were supported by the ARC project AIMED 15/19-09 785. Calculations have been performed on the Belgian Céci facilities funded by F.R.S-FNRS Belgium (Grant No 2.5020.1) and Tier-1 supercomputer of the Fédération Wallonie-Bruxelles funded by the Walloon Region (Grant No 1117545).

NMR Study of Doped Tetrahedrite Thermoelectric Materials.*  
NADER GHASSEMI (Presenter), Department of Physics and Astronomy, Texas A&M University, XU LU, XIAOYUAN ZHOU, YANCI YAN, Department of Applied Physics, Chongqing University, YEFAN TIAN, JOSEPH HANSBRO ROSS, Department of Physics and Astronomy, Texas A&M University — Tetrahedrite thermoelectric materials with compositions between Cu$_{12}$Sb$_4$S$_{13}$ and Cu$_{10}$Zn$_2$Sb$_4$S$_{13}$ were analyzed from room temperature to 4.2 K by $^{63}$Cu and $^{65}$Cu NMR. Cu$_{12}$Sb$_4$S$_{13}$ is known to have a metal-insulator phase transition at T = 88 K, however, structural details of the transformation are not very well known, particularly in the substituted materials of interest for thermoelectric devices. Cu NMR is very sensitive to changes in local structure, and we found the metal-insulator transition still present for Cu$_{11}$ZnSb$_4$S$_{13}$, but absent in the Zn$_2$ material. However, differences in high-temperature NMR spectra reveal a distinct local structure for Zn$_2$ vs the undoped material. Also, we found NMR evidence for Cu-ion hopping, which disappears in the Zn$_2$ material. Spin-lattice relaxation rates (1/T$_1$) furthermore provide a measure of local anharmonic vibrational motions, through an electric quadrupolar process. Results indicate that the rattling behavior is little changed by Zn substitution up to Zn$_2$, despite the structural differences.

*Robert A. Welch Foundation, Grant No. A-1526 and National Natural Science Foundation of China, Grant No. 51772035.

Influence of the Mobility Ratio and Density of States Width on the Thermoelectric Properties of Polymer Blends*  
ASHKAN ABTAHI (Presenter), Physics ans Astronomy, University of Kentucky, YADONG ZHANG, Chemistry, Georgia Institute of Technology, XUYI LUO, JIANGUO MEI, Chemistry, Purdue University, SETH R. MARDer, Chemistry, Georgia Institute of Technology, KENNETH GRAHAM, Chemistry, University of Kentucky — Conjugated polymers can be used in mechanically flexible and low cost thermoelectric (TE) devices, but their thermoelectric performance must be improved to make them commercially viable. The performance of thermoelectric materials depends on the electrical conductivity, Seebeck coefficient and thermal conductivity. The higher the doping concentration, the more electrically conductive the material becomes, but generally at the cost of a decrease in the Seebeck coefficient. Blending of n-conjugated polymers has been proposed as a method to minimize the tradeoff between electrical conductivity and the Seebeck coefficient. By blending two polymers, the total density of states (D.O.S.) will be manipulated, which may be used to alter the charge transport in the TE material. The major parameters that we expect to impact the power factor in polymer blends are the mobility ratios between the two polymers and the shape of D.O.S. Here, we use a model introduced by Bässler and Arkhipov to theoretically probe how these two parameters impact the thermoelectric performance. We find that a narrower D.O.S. and lower mobility of the added polymer with respect to host polymer can lead to an enhancement in the Power factor of the TE material.

*American Chemical Society Petroleum Research Fund
Porous Structure  SEOUNG-HUN KANG (Presenter), KISUNG CHAE, SEON-MYEONG CHOI, Korea Institute for Advanced Study, DUCK YOUNG KIM, Center for High Pressure Science & Technology Advanced Research, YOUNG-WOO SON, Korea Institute for Advanced Study — Thermoelectric device is a promising next-generation energy solution owing to its capability to transform waste heat into useful electric energy, which can be realized in materials with high electric conductivities and low thermal conductivities. A recently synthesized silicon allotrope of Si24 features highly anisotropic crystal structure with nanometer-sized regular pores. Here, based on first-principles study without any empirical parameter we show that the slightly doped Si24 can provide an order-of-magnitude enhanced thermoelectric figure of merit at room temperature, compared with the cubic diamond phase of silicon. We ascribe the enhancement to the intrinsic nanostructure formed by the nanopore array, which effectively hinders heat conduction while electric conductivity is maintained. This can be a viable option to enhance the thermoelectric figure of merit without further forming an extrinsic nanostructure. In addition, we propose a practical strategy to further diminish the thermal conductivity without affecting electric conductivity by confining rattling guest atoms in the pores.

Thursday, March 7, 2019 11:15 AM - 1:03 PM

Session S48 DFD GSOFT GSNP: Drops II BCEC 251 - Irmgard Bischofberger, Massachusetts Institute of Technology - Tag(s):

Focus

11:15AM S48.00001: Drying of colloidal droplets on hydrophobic surfaces  PAUL LILIN (Presenter), PHILIPPE BOURRIANNE, GUILLAUME SINTES, IRMGARD BISCHOFBERGER, Massachusetts Institute of Technology — The evaporation of drops of colloidal suspensions on hydrophilic substrates leads to a variety of patterns, from the well-known coffee stain effect to radial crack formation. Here, we investigate the drying of aqueous solutions of silica nanoparticles on hydrophobic substrates for a large range of particle volume fractions. As the water evaporates, the particle volume fraction increases leading to a transition from a moving to a pinned contact line. This pinned contact line induces a large stress buildup within the material during the further evaporation process, which eventually gets released through the formation of fractures that shatter the dried drop into a multitude of pieces.

11:27AM S48.00002: Analyzing the Effect of Collision of Droplets on Evaporation Rate  SIAVASH ZAMANI (Presenter), AARON B MORRIS, Mechanical Engineering, Purdue University — Spray drying is a process used by many industries such as food, agricultural and pharmaceutical to convert a liquid feed into powder. Many studies have used CFD to model fluid and powder flow. However, continuum approaches track bulk powder properties resulting in loss of data for individual particles. To improve the accuracy of these models, fundamental research on drying behavior is critical. This work focuses on simulating the initial phase of the process where an atomized droplet behaves as a liquid due to excess moisture content. At this stage, the droplets collide frequently, and particle size distribution changes rapidly. Accurate calculation of the moisture content of the droplet is essential for further analysis on drying kinetics and morphology of particulate form. A computational framework has been developed where the gas phase is modeled as a continuum and individual droplets are tracked in the Lagrangian frame. Using this approach, individual droplets and their characteristic properties are captured, while evaporation effects are accurately accounted for. This works provides high-fidelity data for particle size distribution and moisture content which paves the path toward modeling of the second phase of drying, when liquid droplet has transformed into a wet-particle.

11:39AM S48.00003: Evaporation and Dynamics of Transcritical Dodecane Droplets: A Theoretical Investigation Using a Sharp Interface Method  YUVAL DAGAN (Presenter), Massachusetts Institute of Technology, PING HE, Lamar University, AHMED F GHONIEM, Massachusetts Institute of Technology — Evaporation of droplets injected into a supercritical environment plays an important role in many physical, chemical and high-pressure propulsion applications. In such processes, complex interactions due to coupling of the multiphase flow, heat transfer and multicomponent mass transfer, as well as diffusion processes across the phase interface essentially impact the droplet evaporation and surface tension. This, in turn, may drastically change the droplet's dynamic response as its interface and surface tension diminish. In this study, we use a sharp interface method to investigate the structure and the dynamic response of cold n-Dodecane droplets that are introduced into high-pressure and high temperature (supercritical) environments. The phase-change of single droplets undergoing transcritical evaporation at different conditions are explored, as well as droplet trajectories in a simplified one-dimensional flow model. A non-ideal equation of state is used to compute the fluid properties such as density, fugacity and enthalpy, and to predict phase equilibrium composition. The sharp-interface method provides a new realization for an effective radius of transcritical droplets, and a new phase diagram reveals the complex evolution of droplet during transcritical evaporation.
11:51AM S48.00004: Dynamics and structure in the deposition profile of the coffee-ring effect* NICHOLAS SCHADE (Presenter), University of Chicago, JEROME SEEBECK, Caltech, SIDNEY ROBERT NAGEL, University of Chicago — We investigate the growth dynamics and three dimensional structure of ring stains in evaporating drops of solutions and colloidal suspensions. Drying solutions generally leave behind ring stains. While this “coffee-ring effect” has been widely studied, the microscopic details of how the deposition patterns form have not been completely characterized experimentally. Using fluorescence and laser-confocal microscopy, we measure the growth rate and height profile of the deposit as functions of time, initial particle concentration, and particle size. Starting at the contact line, the particle deposition grows into the interior of the drop. The deposition front accelerates as the drop dries and the front steadily becomes sharper until the thickest part of the deposit has formed. Our experiments with fluorescent microspheres reveal the growth of a film of particles over the entire fluid-air interface. This film contracts and detaches from the contact line during the later stages of evaporation. The final deposits often contain patterns of particles in the interior of the rings resembling fractals. Prior theoretical work does not adequately describe many of the phenomena that we observe.

*NSF MRSEC

12:03PM S48.00005: The underside of a Leidenfrost drop on a bath LAURENT MAQUET, GRASP Lab, University of Liège, BENJAMIN SOBAC (Presenter), TIPs Lab, Université libre de Bruxelles, ALEXIS DUCHESNE, Department of Physics, Technical University of Denmark, HATIM MACRAFI, Thermodynamics of Irreversible Processes, University of Liège, ALEXEY REDNIKOV, TIPs Lab, Université libre de Bruxelles, PIERRE DAUBY, Thermodynamics of Irreversible Processes, University of Liège, PIERRE COLINET, TIPs Lab, Université libre de Bruxelles, STEPHANE DORBOLO, GRASP Lab, University of Liège — The Leidenfrost effect can also be observed on a liquid substrate, i.e., volatile drops may levitate on their own vapor when placed on a hot bath of non-volatile liquid. Compared to the classical Leidenfrost effect on solid substrates, the liquid bath presents three major differences: the substrate is atomically smooth, deformable, and fluid. As a consequence of such fluidity, heat transfer through the bath to the drops is most certainly dominated by convection and not by just conduction as in the solids. Here, we examine experimentally and numerically the flow motion in the bath of silicone oil V20 under the action of a Leidenfrost drop. We highlight the development of a toroidal vortex under the drop. Interestingly, the sense of circulation in this vortex is found to depend on the nature of the liquid that makes the drop. We show that this is due to a shift in a complex and delicate interplay between three mechanisms pulling in different directions: the local cooling of the bath by the drop gives rise to both (i) a buoyancy action and (ii) Marangoni stresses, whereas the vapor escaping from the gap between the drop and the bath exerts (iii) a shear action on the bath surface.

12:15PM S48.00006: Droplet moving on frosted glass* STEPHANE DORBOLO (Presenter), University of Liège — The surface of the frosted glass is very rough. This roughness offers numerous pinning sites for any sessile droplet. In the present case, the angle of contact of a water droplet is about 50°. The advancing angle is rather large (about 70°) and contrasts with the receding angle that is quite zero. This strong hysteresis has a direct consequence on the motion of a droplet when the plate is inclined. The droplet leaves a trace after its passage. The dynamic of the droplet going down the plane is studied and the microflows in the trace are described. Finally, the behavior of oil droplets is compared. As the oil wets the glass, the motion of the sliding droplet superposes to the diffusion process of the oil in the crevices of the frosted surface.

*SD is a FNRS senior research associate. Part of this work has been financially supported by the Interuniversity Attraction Pole Programme (IAP 7/38 MicroMAST) initiated by the Belgian Science Policy Office, by the PDR Wolflow (T.0021.18) and by University of Liège.

12:27PM S48.00007: Experimental and analytical studies on colliding merging of two immiscible drops* CHU-PO HUANG, KUO-LONG PAN (Presenter), Department of Mechanical Engineering, National Taiwan University — Two types of merging between two immiscible drops have been found in their collisions. Depending on the interfacial tensions among the three media of different components, including air and immiscible liquids, at an equilibrium state with negligible impact energy, partial engulfing and complete engulfing between the drops can be identified. With sufficient inertia of relative motion between the drops, it would yield adhesive merging, whereby two drops adhere to each other, or encapsulation, whereby the softer drop totally encapsulates the harder one which has higher surface tension. Based on two dimensionless numbers, a Weber number and an impact parameter, we have identified a regime diagram that indicates the parametric conditions of different regimes, including other types of consequences specifically those show separation following temporary coalescence. While the outcome of interaction between two drops at rest can be analyzed by an approach of free energy, those with significant relative motions need to account for the impact inertia. Via an analysis based on conservation of energy, a model has been established to predict the critical Weber number of transition between two different regimes of merging.

*We thank the support of NTU projects (NTU-CDP-106R7822 & NTU-107L7822).
12:39PM S48.00008: Oscillations of a hydrodynamic crystal lattice  
STUART THOMSON (Presenter), MILES COUCHMAN, JOHN WM BUSH, Massachusetts Institute of Technology — When brought into close proximity, two or more droplets bouncing on a vertically vibrating fluid bath exhibit a rich spectrum of dynamical behaviour. In particular, pairs of droplets have been shown to destabilize into oscillatory, orbiting, and promenading modes, while a collection of multiple droplets can form crystal-like lattices with highly regular structure. In this talk, we present the results of a combined experimental and theoretical study in which we characterize and rationalize the behaviour of a circular chain of bouncing drops, reminiscent of a one-dimensional crystal lattice. As the vibrational forcing is increased, the stationary chain first destabilizes into an oscillatory mode and then into a striking soliton-like disturbance, before “melting” at sufficiently high acceleration of the bath. Similarities with models such as the Toda lattice, used to model crystal vibrations in solid-state physics, are discussed.

12:51PM S48.00009: A hydrodynamic analog of the quantum potential*  
JOHN BUSH (Presenter), MATTHEW DUREY, Massachusetts Institute of Technology, PAUL MILEWSKI, Mathematics, University of Bath — A droplet may walk on a vibrating fluid bath through a resonant interaction with its own wave field. This walking droplet system has become the subject of research in the nascent field of hydrodynamic quantum analogs. We here consider the motion of droplets walking in closed systems, and demonstrate the relation between the histogram of the particle and its mean pilot-wave field. Furthermore, we demonstrate that as the Faraday threshold is approached, the instantaneous wave field converges to its mean. The resulting mean pilot-wave potential thus plays the role of the quantum potential in Bohmian mechanics. Our study highlights the differences between Bohmian mechanics and de Broglie's relatively rich double-solution theory of quantum dynamics.

*JB gratefully acknowledges the support of the NSF through award CMMI-1727565.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S49 DPOLY: Polymers in Reactive Conditions BCEC 252A - Nir Goldman, Lawrence Livermore Natl Lab - Tag(s): Focus

11:15AM S49.00001: Capturing shock-driven dissociation of polymers and foams* [Invited]  
DANA DATTELBAUM (Presenter), JOSHUA COE, Los Alamos National Laboratory — Polymers, and polymer-based composites and foams are used extensively in engineering and defense applications in a range of components including structural bodies and supports, insulating layers, and vibration and shock mitigation parts. In several applications, they may be subjected to impact and shockwave compression. Under these loading conditions, polymers have several features that differ from those of metals, including compression of network volume at low pressures, viscoelastic behaviors, and shock-driven dissociation. A novel equation of state methodology has been developed for describing the shock-driven decomposition of solid and porous polymers at moderate shock input conditions. Examples of the shockwave response of several polymers, and a comparison of historical metals-based equation of state approaches to the new methodology will be presented. Furthermore, this modeling approach has been extended to porous polymer foams, and revealed, through a large series of plate impact experiments, a phenomena we have termed “reactive anomalous compression.” A striking feature of our results is the shift from densification to expansion of shock-driven reaction products as a function of initial porosity. Expansion with increasing shock pressure is most commonly associated either with shock heating due to pore collapse in chemically inert materials such as metals or exothermic decomposition (detonation) of energetic materials. We describe an unexpected admixture of these two effects: shock heating due to pore collapse, but expansion in conjunction with chemical reaction. Lastly, efforts to measure reactive wave structures in shock-dissociated polymers, and new x-ray based diagnostic techniques will be described.

*This work was funded by the U.S. Department of Energy, National Nuclear Security Administration to Los Alamos National Laboratory. The authors acknowledge funding from the Dynamic Materials Properties Campaign and Advanced Simulation and Computing program.
Polymer degradation kinetics and reaction mechanisms are of a great interest for many applications. Reports about chemistry related aging effects found in the literature are, however, rarely correlated to the performance of these materials under dynamic compression conditions. One longstanding question is how much degradation must occur before a polymer-based component is significantly affected? Answering this question requires high-throughput testing under a broad spectrum of aging conditions. In this talk, we describe a path forward using an ultrafast laser compression platform. First, we demonstrate validation results from PDMS-based polymers, reproducing available gas-gun shock Hugoniot data and further, show Hugoniot slope changes with polymer filler and radiation-induced damage. Lastly, we present shock results from a set of CVD deposited Kapton and Parylene films cured at different thermal/humidity aging conditions. Discussion of our main findings and future development plans are presented.

*This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344. LLNL-ABS-760541

12:03PM S49.00003: Predicted pathways for chemical degradation in siloxane polymers*  MATTHEW KROONBLAWD (Presenter), NIR GOLDMAN, JAMES LEWICKI, Lawrence Livermore National Laboratory — Chemical degradation can result in undesirable changes in the performance of functional materials over the service lifetime, but the underlying atomic-scale processes are often subtle to probe with experiments. We use ensembles of quantum molecular dynamics (QMD) simulations to predict the chemical reactions that follow radiation-induced excitations of phenyl groups in a model copolymer of polydimethylsiloxane and polydiphenylsiloxane. Initial benzene-forming proton transfer reactions are predicted to induce subsequent reactions including intrachain cyclization and chain scission reactions. Water is found to play a crucial role in chain scission reactions, which indicates a possible synergistic effect between environmental humidity and radiation that could promote alterations of a larger polymer network. An approach for obtaining probability distributions of reaction intermediates and products by coupling high throughput semiempirical QMD simulations with automated graph-based structure recognition tools is discussed.

*Prepared by LLNL under Contract DE-AC52-07NA27344.

12:15PM S49.00004: Perturbing effects on the structure and properties of physically and chemically crosslinked phenolic resins  WEIWEI ZHAO, SHAW HSU (Presenter), University of Massachusetts Amherst — Crosslinked polymers may consist of physical crosslinks such as hydrogen bonds, or covalent bonds or both. The network of crosslinked phenolic resins involves the both. The formation of each type of crosslinking has not been studied in detail. Their contributions to the physical properties are also unclear. Utilizing a combination of infrared spectroscopy, thermal analysis, low field NMR and a cantilever deflection technique, the relative contributions of two types of crosslinks have been characterized as a function of temperature and moisture. The results show that the increased chemical crosslinks reduced the formation of hydrogen bonds. As expected, the covalent bonds dominate at elevated temperatures. However, the contribution of hydrogen bonds is unexpectedly important at low temperatures. As expected, the hydrogen bonding contribution of crosslinked structures is significantly decreased by the moisture absorbed. However, segmental relaxation behavior measured under different humidity levels depends on not only the two types of crosslinks achieved but also the morphological features affecting the moisture absorption process.

12:27PM S49.00005: Photothermally-driven oxidative degradation of LDPE nanocomposites containing plasmonic nanoparticles*  GABRIEL FIRESTONE (Presenter), Department of Physics, North Carolina State University, HONGLU HUANG, RUSSELL E GORGA, Fiber and Polymer Science, North Carolina State University, LAURA CLARKE, JASON R BOCHINSKI, Department of Physics, North Carolina State University — Novel approaches to control and drive polymer degradation are interesting because of the multiple challenges to remediating plastic waste including minimizing its effect when unconfined in the environment and potentially recovering value from discarded material. Photothermal heating from metal nanoparticles, where light is focused and converted into heat at the nanoscale, can be used to drive chemical reactions, such as oxidative degradation within low density polyethylene (LDPE), and results in a high temperature, high electric field environment in the particles' immediate vicinity within which reactions could be manipulated. It also provides a mechanism to convert sunlight to internal heat. We present an LDPE nanocomposite system incorporating silver nanoparticles and cobalt ions where the cobalt-mediated oxidative process is driven by heat resulting from illumination with blue light. In this configuration, the observed degradation (characterized by FTIR, absorption spectroscopy, electron microscopy and mechanical testing) under photothermal heating is almost identical to that due to heating conventionally, as expected due to the non-local oxidative process. We discuss these results and next steps.

*Support from National Science Foundation CMMI- 1462966
12:39PM S49.00006: Phase field model for reactive blending of a symmetric binary polymer blend* MUKUL TIKEKAR (Presenter), KRIS T DELANEY, DOUGLAS R. TREE, GLENN FREDRICKSON, University of California, Santa Barbara — Reactive blending is a process for forming polymer alloys where mutually reactive homopolymers are mixed together to form compatibilizers in-situ. The dynamics of the problem is replete with rich nonequilibrium physics stemming from reactions between the polymers, spatiotemporal transport, thermodynamics of mixing, and externally imposed processing conditions, and has hence been poorly understood. To study this process, we develop a coarse-grained phase-field model designed to capture all of the above physical effects. We then implement the model using pseudospectral collocation and semi-implicit time stepping to solve for temporal evolution of concentration distributions. In the case of reaction-diffusion dynamics, we find that the reaction typically progresses with the formation of an interfacial, diblock-rich layer. Eventually, the diblock diffuses out of the interface and the homopolymers diffuse in, as the reaction proceeds toward completion. The reaction rates in each stage depend on the incompatibility of the species, the Damkohler number and the initial distribution.

*We acknowledge support from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1720256) and NSF CNS-1725797. We also thank Royal DSM N. V. for support.

12:51PM S49.00007: Integrating Particle and Field-Theoretic Simulations: A Multiscale Approach to Complex Polymeric Solutions NICK SHERCK (Presenter), KRIS T DELANEY, M. SCOTT SHELL, GLENN FREDRICKSON, University of California, Santa Barbara — Our work investigates the phase-behavior of complex polymeric solutions leveraging the strengths of both particle and polymer field-theoretic simulations. Mesostructured polymeric solutions are difficult to simulate using traditional particle-explicit approaches due to the disparate time and length scales, while the predictive capability of field-theoretic simulations is hampered by the need to specify emergent parameters (e.g., chi parameters) with nonobvious connections to molecular architecture. To overcome the weaknesses of both, we discuss an original way to use small-scale, atomistic simulations to parameterize statistical field theory models. Subsequently, field-theoretic simulations can probe behavior at larger length scales in polymeric solutions efficiently while maintaining a connection to the underlying polymer chemistry. This synergistic approach to polymer simulations opens the door to explore-de-novo-a wide variety of polymeric solution phase behavior. In particular, we will show how the above machinery can predict complex inter-colloidal potentials-of-mean force as modulated by the surrounding polymeric solution.

1:03PM S49.00008: Hydration of the polymer block in globular protein-polymer bioconjugates* HELEN YAO (Presenter), BRADLEY DAVID OLSEN, Massachusetts Institute of Technology — Protein-polymer bioconjugates are a type of AB block copolymer where one block is a globular protein. The self-assembly of these systems in solution differ significantly from that of synthetic coil block copolymers. The chemistry of the polymer block and the resulting interactions with the solvent (water) can tune the phase behavior of bioconjugates. Previously, our group has observed that changing the hydrogen bonding of the polymer can shift phase boundaries, create new phases, and change order-disorder transitions. Using small angle neutron scattering (SANS), we have devised a contrast matching method to quantify the hydration number, the number of water molecules associated with a repeat unit, of polymers that can be conjugated to globular proteins. This generalizable method can be applied to polymer solutions above the overlap concentration and does not require any underlying assumptions. The SANS data show that there are differences in the hydration of zwitterionic polymers, hydrogen bond donors, and hydrogen bond acceptors. Moreover, the hydration number correlates with a polymer's tendency to order and the homopolymers diffuse in, as the reaction proceeds toward completion. The reaction rates in each stage depend on the incompatibility of the species, the Damkohler number and the initial distribution.

*This work is funded by DOE Award DE-SC0007106

1:15PM S49.00009: Controlled Crystallization of Small Organic Molecules using Polymers: the Role of Hidden Liquid-Liquid Phase Domain* GAGAN KANGOVI (Presenter), SUNGMIN PARK, SANGWOO LEE, Rensselaer Polytechnic Institute — We investigated the crystallization behaviors of model organic compound pyrene mixed with polystyrene using differential scanning calorimetry. The thermal characterization of the pyrene and polystyrene mixtures provided extensive thermodynamic information regarding the phase states and transition temperatures. Using the glass transition temperatures, the chemical compositions of phase-separated phases are elucidated. Remarkably, the crystallization temperature curve of pyrene of the mixtures shows a clear signature of upper critical solution temperature (UCST) with the composition. We attribute the UCST signature to the hidden liquid-liquid phase domain of pyrene and polystyrene in which the nucleation barrier of crystallization is significantly depressed by the spinodal decomposition of liquid phases. This result suggests that polymer additives can be effectively utilized to control the crystallization behaviors.

*ACS - PRF
1:27PM S49.00010: Dynamics of photoresponsive molecules in glassy solids  KENNETH SALERNO (Presenter), TIMOTHY SIRK, US Army Research Laboratory, JUAN DE PABLO, Institute for Molecular Engineering, University of Chicago — The photoresponse of azobenzene and azobenzene-like molecules undergoing the trans → cis photoisomerization transition has been primarily explored through simulation and experiment in solution or vacuum. The response and behavior of these photoactive molecules in solids, where barriers to rearrangement are significantly higher, is less well characterized. Here we use molecular dynamics simulations to study the behavior of azobenzene and disperse red one during and after photoactivation in glassy samples. Data show that the dynamics of photoactivated molecules and the surrounding solid depends little on the sample temperature or measures of local stability such as density and energy. On the other hand, the height of transition barriers, which depends strongly on intermolecular interactions, cooling rate and temperature, is reflected in the waiting time between photoactivation and a local transition. The timescale for flipping is compared with the timescale for rotational and diffusive motion. The rotation of azobenzene or disperse red one around the long axis of the molecule is correlated with the wait time or barrier to flipping while the translational motion and the rotation of the long-axis itself is less correlated with the flipping wait time.

1:39PM S49.00011: Why do Silicones do that? A Perspective on the Stability and Dynamics Polysiloxane based Polymers*  JAMES LEWICKI (Presenter), Materials Science Division, Lawrence Livermore National Laboratory — Polysiloxane polymers (silicones) are a uniquely widespread class of inorganic polymeric material, which find application in some of the most challenging environments on, or indeed off the planet. Despite their comparative ubiquity, even the most basic aspects of their structure remain something of a mystery to many involved in their use and study at a scientific and technical level. This veil of uncertainty is in part due to the unusual path polysiloxanes took from the laboratory to the commercial sector; initially as a WW2 ace of the aided forces and later a jealously guarded jewel of the giants of the chemical industry. This spy story-esque beginning for silicones meant that silicones popped unexpectedly into public light of day in the mid 1970's and were something of a surprise for both the writers of textbooks and the materials scientists of the time. Polysiloxanes are a physically and chemically unique class of polymeric material. With significantly different electronic configuration to a carbon backboned polymer, the lowest glass transition of any stable polymer, no energy barrier to rotation of the main chain segment, their dynamics stand out over a range of size scales as 'odd'. In the rubbery state, they are best described as statistically pinned liquids rather than solids and exhibit such poor mechanical properties that they must be compounded with a range of additives to even be useable. With all this in mind then, why do silicones end up as the material of choice so many in extreme applications and just how do they behave at the extremes of temperatures, pressure and irradiation? In this paper we aim to discuss some aspects of the response of polysiloxanes under such extremes and attempt to relate their behavior in these regimes to their underlying chemical and network structure.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S50 DPOLY DMP: Organic Electronics III: Organic Transistors and Sensors  BCEC 252B - Xiaodan Gu, University of Southern Mississippi - Tag(s): Focus

11:15AM S50.00001: Y-shape DNA guided Ni ion chain based nanowire transistor development and characterization*  CHIA-CHING CHANG (Presenter), WEN-HUNG WANG, Biological Science and Technology, National Chiao Tung University, WEN-BIN JIAN, YU-CHANG CHEN, Electrophysics, National Chiao Tung University, Hsinchu, Taiwan — Recently studies indicate that DNA template guided Ni ion chain (Ni-DNA) is a conducting nanowire and it possesses multi-states memory effect owing to the Ni ions redox state transition by external bias. By designing the sequences of DNA, Y-shape Ni-DNA molecules have been synthesized and characterized. Furthermore, these unique Ni-DNA molecules were linked with three-terminal nanodevice via self-assembly process. The negative differential resistance behavior of I-V curves can be observed between each two terminals of device. By assigning these three terminals as source, drain and gate terminal and the source-drain currents can be regulated by different gate voltage. This is the first Ni-DNA nanowire based transistor has be developed in the world.

*This study is supported in part by the Ministry of Science and Technology (MOST), Taiwan (ROC) MOST 107-2112-M-009-016-MY3
Impact of self-assembled monolayers on electronic properties of poly(3-hexylthiophene) at the polymer/substrate interface

JILL WENDEROTT (Presenter), University of Michigan, PETER GREEN, National Renewable Energy Laboratory — The impact of self-assembled monolayers (SAMs) on electronic properties of poly(3-hexylthiophene) (P3HT) thin films, of different morphologies, at P3HT/substrate interfaces is reported. The SAMs, trichloro(1H,1H,2H,2H-perfluorooctyl)silane (FTS) and octadecyltrichlorosilane (OTS), modified the surface energy and work function (WF) of indium tin oxide substrates, which influenced charge transfer and band bending behavior of P3HT films at the polymer/substrate interface. This band bending behavior could not be explained solely in terms of substrate WF modification. Investigations of P3HT films fabricated via matrix-assisted pulsed laser evaporation (MAPLE) and spin-casting revealed that the degrees of band bending and breadths of densities of states were associated with changes to electronic structure, strongly affected by the morphological structures of films. The morphological structures of films were influenced by film fabrication method and surface energies of the substrates. The implications of our findings are that the electronic properties of the system are influenced by the WFs and surface energies of SAM-modified substrates and the morphologies of thin P3HT films.1


Enhanced Charge Injection Properties of Organic Field Effect Transistor via Molecular Implantation Doping

YOUNGROK KIM (Presenter), Physics and Astronomy, Seoul National University, SEUNGJUN CHUNG, Korea Institute of Science and Technology, KYUNGJUNE CHO, Physics and Astronomy, Seoul National University, DAVID HARKIN, University of Cambridge, WANG-TAEK HWANG, DAEKYOUNG YOO, JAE-KEUN KIM, WOOCHEOL LEE, Physics and Astronomy, Seoul National University, YOUNGGUL SONG, Electrical and Computer Engineering, Seoul National University, HEEBEOM AHN, Physics and Astronomy, Seoul National University, YONGTAEK HONG, Electrical and Computer Engineering, Seoul National University, HENNING SIRRINGHAUS, University of Cambridge, KEEOON KANG, TAKHEE LEE, Physics and Astronomy, Seoul National University — Organic semiconductors (OSCs) have been widely studied due to their merits such as mechanical flexibility, solution processability, and large-area fabrication. However, because of the Schottky contact at the metal/OSC interfaces, a non-ideal transfer curve feature often appears in the low drain voltage region. Here, we demonstrated a selective contact doping of 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ) by solid-state diffusion in poly 2,5-bis(3-hexadecylthiophen-2-yl) thiophene (PBTTT) to enhance carrier injection in bottom-gate PBTTT organic field effect transistors (OFETs). This doping exhibited a high conductivity with favorable charge transport properties [1]. Furthermore, we investigated the effect of post-doping treatment on diffusion of F4-TCNQ molecules in order to improve the device stability. In addition, the application of the doping technique to the low-voltage operation of PBTTT OFETs with high-k gate dielectrics demonstrated a potential for designing scalable and low-power organic electronic devices by utilizing doping of conjugated polymers.

References
11:51AM S50.00004: Contacts in Organic Field-Effect Transistors [Invited] OANA JURCHESCU (Presenter), Department of Physics and Center for Functional Materials, Wake Forest University — Organic semiconductors are versatile materials for emerging low-cost, lightweight, flexible devices, but their incorporation in consumer applications is delayed by inadequate performance. Inefficient charge injection at the electrode/semiconductor interface represents a significant hurdle in the pursuit of the promised potential of organic semiconductors. Moreover, with increasing the effective mobility of organic semiconductor layer and reducing the channel dimensions, this problem becomes even more prevalent. In this talk, I will focus on describing the origin and characterization of contact effects in organic field-effect transistors and their impact on device performance and accuracy in extraction of charge carrier mobility. Several types of manifestations of contact effects will be presented, as well as their impact on the device characterization. I will discuss methods for reducing contact resistance and will emphasize on a simple strategy consisting of developing high workfunction surface domains at the surface of the injecting electrodes to promote channels of enhanced injection [1]. This led to contact resistances of 200 Ωcm and device charge carrier mobilities of 20 cm²/Vs independent of the applied gate voltage. The proposed approach is efficient for both small molecule and polymeric thin-film transistor devices, and can be generally applied in all common processes and device architectures. In addition to allowing the demonstration of high-mobility transistors with near ideal current-voltage characteristics, the use of this method leads to accurate measurement of the charge carrier mobility, a critical step in a rational material design.


12:27PM S50.00005: Limits to Charge Carrier Motion in High-Performance Organic Semiconductors: Role of Energy Barriers at Grain Boundaries and Interface Traps ILJA VLADIMIROV, MICHAEL KÜHN, THOMAS GESSNER, FALK MAY, BASF SE, RALF WEITZ (Presenter), Ludwig Maximilian University of Munich — Using our recently developed surface-crystallization method [1], we have realized 3 – 10 nm thin, highly-crystalline thin films of a novel perylene diimide and investigated temperature-dependent charge transport. Via a combination of as-measured density-of-states with Kinetic Monte Carlo simulations [2], we present strong hints that it is rather the energetic barriers at grain boundaries than the usually identified energetic traps that limit charge carrier motion below room temperature. We furthermore have observed that above room temperature the charge carrier mobility decreases upon increasing the charge carrier density in the semiconducting film [3]. While the true cause for this suppression is currently unclear, we present evidence that the squeezing of charges closer to the semiconductor/dielectric by the gate dielectric field a subsequent scattering at this interface might cause the drop in mobility. We believe that our combined observations will help to understand the still debated nature of charge transport in high-quality organic semiconductors.


12:39PM S50.00006: Impact of Mixed Phases and Domain Network Tortuosity on Long-Range Charge Transport in Phase-Separated Organic Semiconductor Blends* MICHAEL HEIBER (Presenter), Center for Hierarchical Materials Design, Northwestern University, ANDREW HERZING, Materials Measurement Science Division, National Institute of Standards and Technology, LEE RICHTER, DEAN DELONGCHAMP, Materials Science and Engineering Division, National Institute of Standards and Technology — Quantitative structure-property models for how the molecular-scale and meso-scale structure in polymer blends affect long-range charge transport behavior is needed to refine design rules for a wide variety of organic electronic device applications, such as photovoltaics, field-effect transistors, thermoelectrics, and bioelectronics. In this presentation, we will demonstrate the use of kinetic Monte Carlo simulations with morphologies derived from electron tomography measurements and a simple Ising-based model to probe how the multi-length-scale structure due to disordered interfacial mixed phases and mesoscale domain network tortuosity impact long-range charge transport phenomena. We will specifically quantify how these features impact the electric field and temperature dependence of the charge carrier mobility.

*Financial assistance award 70NANB14H012 from U.S. Department of Commerce, NIST as part of the Center for Hierarchical Materials Design (CHiMaD).
Controlling the Doping Mechanism in Thin Film Transistors Through Design of Polymeric Ionic Liquid Gate Dielectrics

DAKOTA RAWLINGS (Presenter), ELAYNE THOMAS, MICHAEL L. CHABINYC, RACHEL SEGALMAN, University of California, Santa Barbara — Two disparate modes of operation can occur when gating an organic thin film transistor (OTFT) with an electrolyte. Field-effect (FE) doping occurs when the semiconductor is impermeable to ions, whereas electrochemical (EC) doping of the bulk occurs when the active layer is permeable to ions. Here, we present a method to control the mode of charge accumulation in an OTFT with a constant semiconducting layer by gating with polymeric ionic liquids (PILs) of opposite polarity. Ion infiltration into the active layer is driven by attraction between ions and electronic carriers of opposite charge. As a result, tethering either the anion or the cation to a polymer backbone in the dielectric enables a direct comparison between FE and EC doping. Two PILs of opposite polarity have been synthesized and employed as the dielectric in p-type OTFTs. Tethering either the anion or the cation is shown to dictate whether ions infiltrate the active layer. Interfacial FE doping decreases the accumulation layer thickness and increases the carrier concentration as a function of injected charge. The local carrier concentration in the accumulation layer is found to be the main factor effecting the threshold voltage and the conductivity of the devices, despite the difference in doping mechanisms.

Hysteresis and Gate Bias Stress Effects in Organic Electrochemical Transistors based on Room Temperature Ionic Liquids

VIKASH KAPHLE (Presenter), SHIYI LIU, CHANG MIN KEUM, BJORN LÜSSEM, Kent State University — Organic Electrochemical Transistors (OECTs) transduce ionic into electronic signals. The transconductance of OECTs is in the mS range and outperforms other traditional and emerging transistors.[1] Here, we show that the transconductance of OECTs is limited by a voltage dependent contact resistance at the source/drain electrodes.[2] By an optimization of the device geometry and by using a mixture of room temperature ionic liquid (C2MIM EtSo4) and PBS as an electrolyte, we reach a transconductance greater than 2 mS. For later applications of OECTs, the stability of these devices is of utmost importance. We investigate the origin of a hysteresis observed in the transfer characteristic and the origin of gate bias stress effects. We propose that these instabilities are caused by ions moving slowly inside the electrolyte and the semiconductor, leading to a different time constant and hence reversible gate stress bias effects. We discuss several approaches to minimize these instabilities.[3]

References


Chemical Doping Efficiency by Semiconducting Polymer Type in Electrolyte-gated Polymer Transistor

SEUNG HOON OH (Presenter), JIYOUN LEE, Pukyong National University — We report the characterization of chemical doping process with electrolyte-gated polymer transistors (EGT), where classical highly crystallized semiconducting polymer - PBTTT or amorphous donor-acceptor (D-A) type semiconducting copolymer -DPP-2T-TT was used as the active layer and an ion gel comprising a polymer network swollen with an ionic liquid was used as the electrolyte. Gate-bias dependent doping concentration that is extracted from the transfer curves reveals that the chemical doping process in disordered DPP-2T-TT copolymer film is more efficient than that of PBTTT film. These results are somewhat contrary to the general observation that neutral molecule doping such as F4-TCNQ was effectively worked in a thiophene-based highly crystalline polymer rather than a D-A type copolymer. However, optical and structural investigations using UV-vis spectroscopy and grazing incident X-ray diffraction (GIXRD) have shown that the structural factors of the polymer semiconductors have a greater influence than the chemical characteristics between the polymer semiconductors and the ionic species in electrolyte.

*This research was supported by the Basic Science Research Program through NRF funded by the Ministry of Science, ICT & Future Planning of Korea (code no. 2018R1A1A1A05021060)
1:27PM S50.00010: High performance organic field-effect transistors with wire bar-coated semiconducting polymer film

DO YEON KIM (Presenter), JIYOU LEE, Pukyong National University — We fabricated high performance organic field-effect transistors (OFETs) with wire bar-coated semiconducting polymer film as an active layer. For an active layer of the OFETs, we employed cyclopentadiithiophene–benzothiadiazole (CDT–BTZ) donor-acceptor (D-A) type copolymers consisting of CDT as an electron-donating unit and BTZ as an electron-accepting unit. The OFETs with bar-coated CDT–BTZ semiconducting copolymer films shows about five times higher field-effect mobility of 0.51 cm²/Vs than 0.11 cm²/Vs of the OFETs with spin-coated CDT–BTZ film, although the charge carrier mobility of the D-A type semiconducting copolymer is less critical to the degree of alignment of the semiconducting polymer. Overall, the results demonstrate that the wire bar-coating process offers opportunities to enhance the performance of the OFETs.

*This research was supported by the Basic Science Research Program through NRF funded by the Ministry of Science, ICT & Future Planning of Korea (code no. 2018R1A1A105021060)

1:39PM S50.00011: Polymer light emitting field effect transistors with steadily high efficiency over three orders of magnitude of current

BANG-YU HSU (Presenter), Materials Science and Engineering, National Cheng Kung University — To simultaneously achieve efficient and intensified optical output is the most challenging task for polymeric light emitting field effect transistors (PLEFETs). A p-type unipolar PLEFET with high brightness but oversaturated holes will limit recombination efficiency. Instead, an ambipolar PLEFET with high recombination current will decrease on/off ratio. An ideal solution will be the combined advantages of both LEFETs, significant on/off ratio, high current density, and efficient recombination. A bilayer PLEFET can meet the three criteria satisfactorily by applying asymmetric organic/inorganic-hybrid transparent contacts. Hole/electron injections and photon output in a p-type PLEFETs was simultaneously improved. For source-drain current over 3 orders of magnitude from sub-micro ampere to sub-mini ampere, corresponding to 26 to 3747 cd/m², external quantum efficiency (EQE) steadily sustained 0.5%. EQE of the PLEFETs in this work was enhanced remarkably, 0.5% vs. < 0.08% (conventional ones), and on/off ratio remained high at 10³–10⁵. Asymmetric organic/inorganic-hybrid transparent contacts demonstrated a promising strategy for energy-efficient PLEFETs.

*This research is sponsored by the Ministry of Science and Technology, Taiwan, R.O.C. (MOST 107-2112-M-006-003)

1:51PM S50.00012: A Molecularly-Imprinted Electrochemical Sensor to Detect VOCs in the Breath Print of Lung Cancer Patients

SHADI EMAM (Presenter), NIAN XIANG SUN, Electrical Engineering, Northeastern University — Lung cancer is the leading cancer killer in both men and women in the United States. The cost of lung cancer was $13.4 billion in 2015 based on the National Institute of Health report. The majority of living lung cancer patients have been diagnosed within the last five years. VOCs are organic chemicals that form less than 1% of the exhaled breath. The exchange of blood and the air in the alveolar leads to transferring chemicals in the blood, which was formed during metabolism inside the body, to find a way to the exhaled breath. Thus, measurement of VOCs in the breath can provide a window into the biochemical processes of the body. In this paper, a new methodology is proposed to detect hexanal and heptane, which are two chemicals found in the breath print of lung cancer patients. A three-layer sensor was formed through deposition of a thin layer of graphene and Prussian blue onto a silicon substrate. Selective binding of the analyte was facilitated by molecular imprinting polymer. Subsequent polymerization and removal of the analyte yielded a polymer layer on top of the sensor containing molecularly imprinted cavities selective for the target molecule. The sensors were tested over 1-20 parts per billion (ppb) level of concentration while the sensor resistance has been monitored.

2:03PM S50.00013: Low-power photonic organic artificial synapse inspired by dopamine-facilitated synaptic activity

SEONGGIL HAM (Presenter), SANGHYEON CHOI, HAEIN CHO, GUNUK WANG, KU-KIST Graduate School of Converging Science & Technology, Korea university — The ability of the synaptic plasticity in an artificial synapse can offer significant improvement in low-power recognition, and learning capability in a neuromorphic system [1]. Inspired by light-assisted dopamine-facilitated, which achieves rapid learning and adaptation by lowering the threshold of the synaptic plasticity, we fabricate a organolead halide perovskite (OHP)-based photonic synapse in which the synaptic plasticity is modified by both electrical pulses and light illumination. Owing to the accelerated migration of the iodine vacancy inherently existing in the OHP film under light illumination, the OHP synaptic device exhibits light-tunable synaptic functionalities with very low programming inputs (~0.1 V). It is also demonstrated that the threshold of the long-term potentiation decreases and synaptic weight further modulates when light illuminates the device. Notably, under light exposure, the OHP synaptic device achieves rapid pattern recognition with ~81.8% accuracy with a low power consumption (4.82 nW/the initial update for potentiation), which is ~2.6×10³ times lower than when the synaptic weights are updated by only high electrical pulses. References


Thursday, March 7, 2019 11:15 AM - 2:15 PM
11:15AM S51.00001: Nonlinear Elongational Rheology of Unentangled Polystyrene and Poly(p-tert-butyl styrene) Melts [Invited] HIROSHI WATANABE (Presenter), YUMI MATSUMIYA, Kyoto University, YUICHI MASUBUCHI, Nagoya University, QIAN HUANG, OLE HASSAGER, Technical University of Denmark — Nonlinear rheology under uniaxial elongation was examined for unentangled melts of polystyrene (PS27; $M = 27k$, $n_K = 30$) and poly(p-tert-butyl styrene) (PtBS53; $M = 53k$, $n_K = 35$) having nearly the same number $n_K$ of Kuhn segments per chain. For both materials, the steady state elongational viscosity $\eta_E$ exhibited hardening and then softening on an increase of the Weissenberg number $Wi \geq 0.3$ ($Wi = \tau \kappa$, with $\tau$ and $\kappa$ being the longest relaxation time and the Hencky strain rate). For these unentangled melts, the hardening was unequivocally related to the finite extensible nonlinear elasticity (FENE), and the softening, to suppression of the FENE effect due to reduction of the segmental friction $\zeta$ occurring for the highly stretched/oriented chain. Thus, the $\zeta$-reduction, speculatively discussed for entangled melts, was experimentally confirmed for unentangled melts. The softening at high $Wi$ was weaker for PtBS53 than for PS27 despite the similarity of their $n_K$ values, which suggested that the magnitude of $\zeta$-reduction depends on the chemical structure of the chain. Further details of this $\zeta$-reduction, analyzed with the aid of the FENE bead-spring model modified for the $\zeta$-reduction, are discussed in relation to the local motion of the chain necessary for adjusting $\zeta$.

11:51AM S51.00002: Salt-induced polyelectrolyte capsule formation in microfluidics* [Invited] WILLIAM SHARRATT, CARLOS LOPEZ, JOAO CABRAL (Presenter), Imperial College London — Microfluidics provides an exceptional platform for the generation of polymer solution droplets and their subsequent manipulation. We describe the formation of carboxymethyl cellulose (CMC) particles and capsules induced by salt diffusion. Generally used as a sodium salt, NaCMC is an anionic, weak, semiflexible polyelectrolyte, and one of the most widely used polyelectrolyte cellulose derivatives, with applications in the food, pharmaceutical, personal care, cosmetic, and paper industries. We employ SANS, light scattering, and rheology to probe the conformation and dynamics of aqueous NaCMC solutions across a wide range of molecular weight (Mw), degree of substitution, salt (mono, di and trivalent) and polymer concentrations. We then investigate the addition of a series of multivalent salts to induce the gelation and/or precipitation of bulk NaCMC solutions, which is spatiotemporally resolved by SANS and microscopy, establishing salt front propagation kinetics and accompanying conformational changes of the polymer. Equipped with this knowledge, we design and fabricate CMC gel capsules and particles with prescribed dimensions and external shape, microstructure and dissolution profile.

*Funding from Engineering and Physical Sciences Research Council (EPSRC, UK) and Procter & Gamble is gratefully acknowledged.

12:27PM S51.00003: Topological Effects on Movements of Charged Macromolecules in Crowds* [Invited] MURUGAPPAN MUTHUKUMAR (Presenter), University of Massachusetts Amherst — Charged macromolecules dispersed in aqueous media are ubiquitous since life began on Earth and continue to catalyze formulations of modern materials. A fundamental understanding of the rich phenomenology on movements of charged macromolecules in crowded environments continues to be elusive, due to the long-ranged nature of both the topological correlation from chain connectivity and electrostatic correlation from the charges in the system. Strong coupling among these long-ranged interactions results in a variety of rich behavior unparalleled in uncharged systems. We will present recent advances on the collective dynamics of charged macromolecules in solutions and hydrogels. In particular, the “ordinary-extraordinary” dynamics, single molecule translocation through a protein channel under coupled forces, and the newly discovered topologically frustrated non-diffusive dynamics of charged macromolecules inside charged hydrogels will be discussed.

*Acknowledgment is made to NSF-DMR-1504265, NIH-5R01HG002776-15, and AFOSR Grant No. FA9550-17-1-0160.
1:03PM S51.00004: How structural modifications of pectin affect its gelling and complexation behavior [Invited]
RUTH CARDINAELS (Presenter), Eindhoven University of Technology — Pectin is a plant cell wall polysaccharide that is intrinsically present in many plant-based food products, both in the plant cell particles as well as in the serum phase. In addition, extra pectin is frequently added to food products as a gelling agent and source of dietary fibre. Pectin is a polyelectrolyte with a backbone of galacturonic acid units, organized in linear and branched domains. The detailed pectin structure can be very heterogeneous even within a single cell wall. The galacturonic acid units that originally contain methylester groups can undergo deesterification thereby leaving negatively charged acid groups. Depending on the processing steps that in general include thermal treatment as well as mechanical homogenisation, various degrees and patterns of methylesterification [1,2] as well as degrees of branching can result [3]. These structural features determine the rheological properties of pectin solutions [1] as well as their gelling propensity by viscoelastic network formation [2,3,4]. Moreover, in typical food products pectin is in contact with other polysaccharides and proteins, which can result in complex formation, aggregation or phase separation. The type of interaction, phase boundaries and resulting microstructure are strongly contingent on the structural features of pectin [5]. Here, effects of processing techniques that allow to tailor pectin’s structural features will be discussed along with the relationships between these structural features and pectin’s functional properties.
[1] Moelants et al. (2013), Food and Bioprocess Technology, 6(10), 2870-2883.

1:39PM S51.00005: Network connectivity, viscoelasticity and failure in gel networks: microscopic insights into soft complexity. [Invited] EMANUELA DEL GADO (Presenter), Georgetown University — Gel networks assembled from polymers, biopolymers, small particles or aggregates can be stretched, flow, squeezed or fractured, but controlling and being able to design such processes (think of soft inks for 3D printing technologies) requires a fundamental understanding that is still lacking. We have developed a theoretical/computational approach that addresses in particular the role of the network topology in such materials, its stress-controlled evolution over time and its implications for the mechanics. I will give an overview of the novel insight gained into the origin of the uniquely wide-ranged viscoelastic spectra and the presence of a topologically controlled softness in gel networks. I will discuss how our findings can help understand the nontrivial mechanical response of soft gels in different contexts, further develop constitutive models, and design smart materials.

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Session S52 DPOLY: Block Copolymer Thin Films I: Theory and Simulation
BCEC 253B - Christopher Arges, Louisiana State University - Tag(s): Focus

11:15AM S52.00001: Self-assembly of Bottlebrush Block Polymers at Surfaces using Coarse-grained Molecular Dynamics Simulations  MICHIEL WESSELS (Presenter), ARTHI JAYARAMAN, University of Delaware — Self-assembly of block polymers on surfaces is used to engineer nanostructured materials for electronics, optics, sensing, and chemical separation applications. Past experimental, theoretical, and computational work has extensively focused on the self-assembly of block copolymers with linear architecture, and relatively fewer studies have established the polymer physics underlying self-assembly of non-linear architectures such as bottlebrushes. In this talk, I will present our coarse-grained molecular dynamics simulation study aimed at understanding structure (i.e., chain conformations, assembled morphologies) and thermodynamics (i.e., interactions between monomers vs. interactions with surface) of solutions of amphiphilic bottlebrush block polymers near surfaces. We establish the role of bottlebrush side chain length and side chain grafting density on the backbone on the behavior of amphiphilic bottlebrush block polymers near surfaces.
11:27AM S52.00002: Program the self-assembly of block copolymers for desired mesocrystals

WEI-HUA LI (Presenter), Fudan University — The packing of particles in soft matter as a fundamental problem has been paid a lot of attention. As the enthalpic and entropic contributions to the free energy is comparable and could be readily tuned, the packing of soft particles leads to rich crystalline structures (i.e. mesocrystals). To understand the packing mechanism of various soft particles into different crystalline structures and thus to modulate the packing of soft particles for desired mesocrystals is an important problem to be solved. Block copolymer provides a perfect model for solving this problem due to two main reasons. The first reason is that the self-assembly of block copolymers can be programmed by tuning the molecular architectures and modern synthesis techniques enable the precise control of the architectures. The second one is that the self-assembly of block copolymers can be accurately predicted by the well-established self-consistent field theory (SCFT). In this talk, I will talk about programming the self-assembly of block copolymers for desired mesocrystals or even mesoscale quasicrystals based on SCFT calculations.

*W. Li acknowledges the funding support by the National Natural Science Foundation of China (Grants Nos 21574026 and 21774025).

11:39AM S52.00003: Dynamics at the Interface of Structured Block Co-Polymer Thin Films with Polar Solvents: Molecular Dynamics Simulations Insights

MANJULA SENANAYAKE (Presenter), Department of Chemistry, Clemson University, Clemson, SC, United States, 29634, DIPAK ARYAL, Department of Chemical Engineering, University of Texas at Austin, Austin, TX, United States, 78712, GARY GREST, Sandia National Laboratories, Albuquerque, NM, United States, 87123, DVORA PERAHIA, Department of Chemistry/Department of Physics, Clemson University, Clemson, SC, United States, 29634 — Structured ionic copolymers consist of multiple blocks whose dynamics facilitate their uses. Here, the dynamics at the interface of an ABCBA pentablock co-polymer with polar solvents is studied by molecular dynamics simulations. The ionic block C is a sulfonated polystyrene (sPS) with sulfonation fraction $f=0.55$, B is polyethylene-propylene (PEP), and A is poly(t-butyl styrene) (tBS). Simulations are performed using LAMMPS with the polymer and propanol modeled with OPLS-AA force field. The interface evolution with exposure time to propanol is followed and the results are compared with those for the polymer-water interface. The air interface of the neat polymer is dominated by the PEP block. With exposure to propanol, more ionic groups migrate to the interface, similar to the polymer-water interface. However, in contrast to water exposed films, the interface remains dominated by the PEP blocks. Remarkably, the interfacial width of the membrane-propanol system grows with time while the width of the membrane-water interface decreases. Further, water molecules associate predominantly with the ionic blocks and break the ionic clusters while propanol associates with both the ionic and non-ionic polymer segments.

*Supported in part by NSF DMR 1611136

11:51AM S52.00004: Microphase Separation in Dipolar Diblock Copolymer Melts

RAJEEV KUMAR (Presenter), WEI LI, BOBBY G SUMPTER, Oak Ridge National Laboratory, MURUGAPPAN MUTHUKUMAR, University of Massachusetts, Amherst, MA — Understanding microphase separation in polar-non-polar diblock copolymer melts is a topic of great interest due to its fundamental and technological importance. In this talk, we will present our work related to modeling the effects of dipolar interactions in affecting microphase separation in linear diblock copolymer melts. Results obtained for freely rotating dipoles, applicable to high temperature disordered melts, will be presented. These results will be compared with field theory-based and coarse-grained molecular dynamics simulations for lamellar morphology. Advantages and disadvantages of the field theory-based simulations will be discussed and importance of correlations in orientations of dipoles will be highlighted.

12:03PM S52.00005: DPD simulation of multilayer self-assembly of block-copolymer

HEJIN HUANG (Presenter), ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Self-assembly of block copolymers provides a powerful tool for patterning at small length scale. The chemical incompatibility of the two blocks, which are covalently linked together, leads to microphase separation upon annealing. Depending on the volume ratio of the two block, different morphologies, such as spheres, cylinders and lamellae structure can be obtained. Most researchers use self-consistent field theory (SCFT) as the simulation tool to predict self-assembled structure. Recently, a particle-based simulation method - dissipative particle dynamics (DPD) has been implemented to provide different insights into the self-assembly process of BCP. Here we use DPD to investigate the structural information propagation from layer to layer in a multilayer film. The self-assembly process of the first layer is directed by either graphoepitaxy or chemoepitaxy. After that, by depositing a second BCP layer on top, the structural information of the first layer will propagate and affect the structure of the second layer. By carefully designing the structure, we could achieve different bilayer structure such as dots-on-cylinders, parallel cylinders and nanomeshes.
12:15PM S52.00006: Is Simple Cubic Spherical Phase Possible in Block Copolymers?* YUEMING XIA (Presenter), WEI-HUA LI, Fudan University — The self-assembly of amphiphilic macromolecules into various mesocrystals has attracted abiding interest. Although many interesting mesocrystals have been achieved, the simple cubic mesocrystal is rarely reported. Here we purposely design an AB-type multiblock copolymer composed of an AB diblock copolymer with A-/B-block tethered by an extra B-/A-block at the middle point to target the simple cubic spherical phase based on the self-consistent field theory. Specifically, two sophisticated mechanisms are realized synergistically in the copolymer, i.e. packing frustration release and stretched bridge block, leading to the formation of the simple cubic mesocrystal in a significant parameter space. Moreover, more other unusual phase behaviors are predicted.

*Acknowledges the funding support by the National Natural Science Foundation of China (Grants Nos 21574026 and 21774025).

12:27PM S52.00007: Simulation studies reflecting the importance of kinetics on block copolymer self-assembly [Invited] SU-MI HUR (Presenter), Chonnam National University — The self-assembly in polymeric system is one of core principles to many of advanced nanotechnologies. Success of most of these applications utilizing the self-assembly relies on how well one can adjust, and switch the shape, size and arrangement direction of self-assembled structures. Hence, there have been active research efforts on understanding the underlying physical principles controlling the self-assembly, augmented by theoretical and numerical modeling. Complicated interactions and the wide range of length and time scales related with self-assembled structures make theoretical modeling very challenging. Moreover, many systems are in metastable states, thus kinetics, not just thermodynamics, plays a key role for the ability of a polymeric material to self-assemble into a desired state. In this work, we present our efforts on developing powerful simulation approaches capable to describe experimentally-observed microstructures, to predict new mesophases, as well as to provide the kinetic routes between various microphases in block copolymer films. Special efforts are placed on understanding the motion of defects in block copolymer thin films and their interactions, pursuing fully ordered lamellae for its successful application in nanolithography.

1:03PM S52.00008: Single chain in mean field (SCMF) simulation of flexible and semiflexible block copolymers. SOJUNG PARK (Presenter), DAESEONG YONG, JAEUP KIM, Department of Physics, UNIST — Self-consistent field theory (SCFT) has been a popular tool for the study of equilibrium properties of block copolymer nanostructures. It is a mean field theory, and thus it has limitations in that fluctuation effects are ignored. One suggestion to incorporate fluctuations into the field theoretical calculation is the single chain in mean field (SCMF) simulation which performs explicit Monte Carlo simulation of polymer chains under quasi-instantaneously updated self-consistent field. In this research, we perform SCFT calculation and SCMF simulation of block copolymers in thin film morphology. For the symmetric block copolymers, the phase transition is suppressed when confined by two neutral walls, and the surface-perpendicular lamellar phase becomes slightly preferable to the surface-parallel one. We also perform SCMF simulation of semiflexible polymer chains by adopting angle dependent potential in both bead-spring and freely-jointed chain model, and our results reveal that stiffer chains exhibit higher tendency to self-assemble into ordered structures. For the confined system, it turns out that the surface-perpendicular lamellar phase becomes more stable as the stiffness of the chain increases.

1:15PM S52.00009: Effect of free surface and substrate topography on the self-assembly of block copolymer films VIKRAM THAPAR (Presenter), Chonnam National University, JUAN DE PABLO, University of Chicago, SU-MI HUR, Chonnam National University — Theoretical and numerical studies have provided valuable insights in understanding and controlling the self-assembly of block copolymer systems, providing powerful guidelines to experimentalists. However, complicated geometric surface effects on the self-assembly are often ignored due to the limitation of previous simulation models to capture free surface effects, thus constraining systems to thin films with ad-hoc flat interfaces. In this work, we present our efforts on developing efficient simulation approaches to explore the self-assembly of complex polymeric systems with ability to develop, and interact, with non-flat interfaces. Effects of different substrate topographies and initial polymer volume shapes on the self-assembly kinetics are numerically investigated and compared with experimental data.
1:27PM S52.00010: Rational design of linear-dendritic block copolymer for overwhelming region of spherical phases** YICHENG QIANG (Presenter), WEI-HUA LI, Fudan University — Various ordered structures can be formed by the self-assembly of block copolymer, while the formation of some sophisticated phases among them is usually driven by some sophisticated mechanisms. Several mechanisms have been established to expand the spherical region, thus stabilizing some new spherical phases, e.g. Frank-Kasper phases. However, the effect of these mechanisms is still limited. In order to widen the phase regions of these desired new spherical phases drastically, we start from an intuitive hypothesis, design a kind of linear-dendritic block copolymer and investigate its self-assembly behaviors with the self-consistent field theory (SCFT). Under the optimized control parameters, the spherical phase region is expanded to be overwhelmingly large in the phase diagram and at the same time the regions of Frank-Kasper phases are largely expanded. The most important conclusion is that the discrete spherical domains can be formed by the major component with volume fraction around 0.7. These results renew our insight into the intricate mechanisms of the self-assembly of block copolymer.

**Acknowledges the funding support by the National Natural Science Foundation of China (Grants Nos 21574026 and 21774025).

1:39PM S52.00011: Stability of Dodecagonal Quasicrystalline Tiling in ABC Star Terpolymers** CHAO DUAN (Presenter), YICHENG QIANG, WEI-HUA LI, Department of Macromolecular Science, Fudan University — In this work, the thermodynamic stability of cylindrical dodecagonal quasicrystalline (DDQC) phase in ABC star-shaped triblock terpolymers for both neat and blending systems is investigated. A systematic comparison of our theoretical results to those of experiments by Matsushita’s group is performed using the self-consistent field theory (SCFT). Based on our previous work, SCFT coupled with the Stampfli self-similarity construction is adopted to accurately calculate the free energy of the periodic DDQC approximants and then a cluster model is used to predict the stability of aperiodic DDQC phase. We find that ideal tiling DDQC in these ABC star terpolymers is also metastable. Furthermore we show that the DDQC morphology observed experimentally is a kind of random tiling pattern as the mesoscopic coexistence of the (3,3,4,3,4) Archimedean tiling pattern and the 8/3 approximant. Accordingly, we conclude that the formation of random tiling DDQC structure may be possible in self-assembling block copolymer melts.

**National Natural Science Foundation of China (Grants Nos 21574026 and 21774025)

1:51PM S52.00012: Tiling Patterns Self-Assembled from Rod-Coil Copolymers with Hydrogen Bonds** PING TANG (Presenter), Macromolecular Science, Fudan University, ZHIHUI LI, College of Architecture and Environment, Sichuan University, FAQIANG LIU, HONGDONG ZHANG, YULIANG YANG, Macromolecular Science, Fudan University — Based on self-consistent field theory (SCFT), we demonstrate that X-shaped rod-coil molecules with hydrogen-bonding groups, can self-assemble into Archimedean tiling patterns. The rod blocks form the polygon edges with coil blocks filling in the inner spaces of polygons. The existence of hydrogen bonds further decreases the domain size. A new mechanism is proposed to guide the formation of Archimedean tiling patterns: the fabrication of tiling patterns is controlled by the relationship between the length to diameter ratio and volume fraction of rods in X-shaped supra-macromolecules. This study provides a concept of macromolecular tiling and suggests X-shaped rod–coil supra-macromolecules with hydrogen-bonding groups as an ideal platform for the fabrication of two-dimensional nanoscale patterns.

**National Natural Science Foundation of China (Grant Nos: 21534002, 21574027, 21774027).

2:03PM S52.00013: Self-Assembly Behaviors of B1AB2CB3 MultiBlock Copolymer** QIONG XIE (Presenter), WEI-HUA LI, Fudan University — The self-assembly behavior of linear B1AB2CB3 multiblock copolymers is investigated using the self-consistent field theory (SCFT). It has been revealed that the relative lengths between the three B-blocks are able to tune the packing crystalline lattice of binary spherical or cylindrical phases. Here we focus on the impact of the molecular architecture on more phase behaviors in a wider parameter space. Our SCFT results indicate that the relative lengths of the three B-blocks have significant influences on not only spherical/cylindrical phases but also other phases such as the alternative gyroid and lamellar phases. In particular, the stability region of the gyroid phase varies drastically and non-monotonically, which is accompanied by the drastic change of other phase regions. Furthermore, our results reveal that the change of these phase regions is resulted in by different sophisticated mechanisms associated with the relative lengths of the three B-blocks, i.e. the effect of stretched bridging B2-block, the regulation of packing frustration of the B-blocks and the solubilization of short B-blocks.

*Qiongxie acknowledges the funding support by the National Natural Science Foundation of China (Grants Nos 21574026 and 21774025)
11:15AM S53.00001: Twenty Years of Network Science: From Structure to Control [Invited]  ALBERT BARABASI (Presenter), Northeastern University — Systems as diverse as the cell, the brain, the World Wide Web, or the social systems are described by highly interconnected networks with complex topology, whose structure determines their function and utility. Twenty years of research has shown that these networks are the result of self-organizing processes governed by simple but generic laws, that can be best understood using tools rooted in statistical physics. These studies have also offered evidence of a deep universality, finding that many real networks share multiple common architectural features, from the scale-free property, discovered 20 years ago today, to communities and correlations. I will discuss the order characterizing real networks and its implication, with focus on network control. Indeed, most complex systems have purpose, striving to accomplish some function, from the cell’s ability to reproduce to the brain’s ability to control our motions. For this, the underlying networks must be wired to be able to constantly control the system’s internal processes, in response to external inputs and perturbations. I will show how to adapt the tools of control theory to unveil the control principles of complex self-organized systems. Finally, I will discuss a recently developed analytical framework to study the controllability of an arbitrary complex network, and offer experimental evidence for its direct applicability to neural networks in the brain.

11:51AM S53.00002: Multilayer Networks: Structure and Dynamics [Invited]  GINESTRA BIANCONI (Presenter), School of Mathematical Sciences, Queen Mary University of London — Multilayer networks are emerging as a novel and powerful way to describe complex systems. Multilayer networks are ubiquitous and include social networks, financial markets, infrastructures, molecular networks and the brain.

Uncovering the interplay between multilayer network structure and function is a big theoretical challenge with a vast realm of applications. On the other side the urgency of understanding real-world multilayer network problems requires novel theoretical approaches. In this talk we will show how the statistical mechanics theory beyond multilayer networks reveals the information encoded in these structures and its effect on multilayer network dynamics.

12:27PM S53.00003: Temporal networks [Invited]  PETTER HOLME (Presenter), Tokyo Institute of Technology — The power of any kind of network approach lies in the ability to simplify a complex system so that one can better understand its function as a whole. Sometimes it is beneficial, however, to include more information than in a simple graph of only nodes and links. Adding information about times of interactions—modeling your system as temporal networks—can make predictions and mechanistic understanding more accurate. Just as there can be network structures affecting disease spreading, temporal structures can also govern the spreading dynamics. We will discuss recent developments in the analysis of temporal networks, including community detection, the definition of time scales, random walks and various forms of spreading processes. We argue that adding time to network representations fundamentally changes our usual network concepts—so much that it is perhaps meaningless to think of temporal networks as an extension of the network paradigm.

1:03PM S53.00004: Epidemic threshold on temporal networks [Invited]  VITTORIA COLIZZA (Presenter), INSERM — Our understanding of communicable diseases prevention and control is rooted in the theory of host population transmission dynamics. The network of host-to-host contacts along which transmission can occur drives the epidemiology of communicable diseases, determining how quickly they spread and who gets infected. A large body of epidemiological, mathematical and computational studies has provided a number of insights into the understanding of the process and the identification of efficient control strategies. The explosion of time resolved contact data has however opened the stage to new challenges. What are the structural and temporal aspects, and possibly their non-trivial interplay, that are critical for disease spread? To answer this question, I will introduce the infection propagator approach, a theoretical framework for the assessment of the degree of vulnerability of a host population to disease epidemics, once we account for the time variation of its contact pattern. By reinterpreting the tensor formalism of multilayer networks, this approach allows the analytical computation of the epidemic threshold for an arbitrary time-varying network of host contacts, i.e. the critical pathogen transmissibility above which large-scale propagation occurs. I will apply this framework to a set of empirical time-varying contact networks and show how it can be used to test different intervention strategies for infection prevention and control in realistic settings.
The dynamics of adsorbed polymer chains in polymer nanocomposite melts can be significantly perturbed from the bulk state and can dictate properties in polymer nanocomposites (PNCs). In this work, we directly observe and quantify polymer chain-scale interactions at the surface, which are significant in studying changes in miscibility of the PGNP and might be driving the morphology of the entire brush.

Let's consider the following scenarios:

1. **Effects of Matrix Chain Length on Miscibility of Nanoparticles**
   - **Presenter:** CLEMENT KOH
   - **Institution:** Columbia University, AMISH PATEL, University of Pennsylvania, SANAT KUMAR, Columbia University
   - **Description:** In this simulation, we observe brush collapse due to decreasing the graft/matrix chain ratio (N/M) for PGNPs in a homopolymer matrix of free chains. This effect is observed experimentally by decreasing the graft/matrix chain ratio. While composition profiles of the graft/matrix chains do not reveal any signs of brush collapse, brush heights calculated using a second moment of the segment density highlights a subtle indication of brush collapse. Further, by measuring free chain fluctuations and free energies via indirect umbrella sampling, we are able to suggest that the free chain length varied systematically in a series of simulations, while NP radius, grafting density, and grafted chain length were held constant.

2. **Dynamics of Adsorbed Polymer Chains in Polymer Nanocomposite Melts**
   - **Presenter:** ERIC BAILEY
   - **Institution:** RUSSELL JOHN COMPOSTO, KAREN WINEY, University of Pennsylvania
   - **Description:** The dynamics of polymer chains and chain segments near an enthalpically attractive interface can be significantly perturbed from the bulk state and can dictate properties in polymer nanocomposites. In this work, we directly observe and quantify polymer chain-scale desorption from nanoparticles in the melt using elastic recoil detection and Rutherford backscattering spectrometry on model PNCs comprised of poly(2-vinyl pyridine) and 25-nm diameter silica nanoparticles. We observe polymer desorption ~10^2 times slower than bulk chain diffusion and desorption that is slowest for longer chains and at lower temperatures. In this highly attractive system, we observe bound polymer that persists after more than 10^6 reptation times, even at T_g+100°C. By correlating the measured bound polymer to the nanoparticle concentration, we measure the adsorbed chain areal density as ~0.05 chains per nm^2 and extract a bound layer thickness that extends ~R_g from the nanoparticle surface. Two parameters that have been difficult to experimentally probe in the melt state.

3. **Rational Design of Polymer Nanocomposites to Advance Their Thermomechanical Performance via Predictive Multiscale Modeling**
   - **Presenter:** WENJIE XIA
   - **Institution:** North Dakota State University
   - **Description:** Understanding and predicting the thermomechanical responses of polymer nanocomposites are challenging as they are influenced by many factors, such as interfacial energy and filler volume fraction, giving rise to the presence of nanoscale interfaces. To better design polymer nanocomposites, we have recently established an atomistically informed coarse grained (CG) modeling approach to investigate how the nanoscale interfaces and molecular characteristics influence the mechanical and glass transition properties of polymer nanocomposites. Taking cellulose reinforced polymer nanocomposite as a relevant model system, we present a multiscale materials by design framework using CG modeling combining with advanced computational algorithms for prediction of thermomechanical properties of nanocomposites. Our established framework is validated by recent experiments and breaks new ground in predicting key structure and property relationships for optimum and tailored design of polymer nanocomposite materials.

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Thursday, March 7, 2019 11:15 AM - 2:15 PM

**Session S54 DPOLY: Polymer Nanocomposites V: Thermodynamics and Dynamics**

**11:15AM S54.00001:** Effects of Matrix Chain Length on Miscibility of Nanoparticles

**11:27AM S54.00002:** Dynamics of Adsorbed Polymer Chains in Polymer Nanocomposite Melts

**11:39AM S54.00003:** Rational Design of Polymer Nanocomposites to Advance Their Thermomechanical Performance via Predictive Multiscale Modeling
rheological measurements exhibit 30 decades variation in aT. Further analyses suggest the local rearrangements of PNCs at different time and length scales follow identical temperature dependence with the neat polymer, although the range [1], indicating an unrealistic fast polymer dynamics at high temperatures. In this work, we decoupled the dynamic translated to evaluate the dynamics features of PNCs at different temperatures. These results clearly show the shift factors by the time-temperature superposition principles cannot be directly nanomaterials, especially at high temperatures, lead to the breakdown of the time-temperature superposition principle in transmission electron microscopy (TEM), and correlated to the long-term viscoelastic creep behavior observed by DMA. The effect of these parameters on PNC morphology is quantified by small-angle X-ray scattering (SAXS) and by hydroxyl surface groups capable of hydrogen bonding versus nanoparticle surfaces treated with a phenyl-capping agent. The interaction between nanoparticle surface and the polymer matrix is adjusted by using bare silica featuring silica nanoparticles dispersed in an amorphous polymer matrix of approximately 200,000 g/mol weight-average molecular weight. The interaction between nanoparticle surface and polymer matrix is adjusted by using bare silica featuring hydroxyl surface groups capable of hydrogen bonding versus nanoparticle surfaces treated with a phenyl-capping agent. The effect of these parameters on PNC morphology is quantified by small-angle X-ray scattering (SAXS) and by transmission electron microscopy (TEM), and correlated to the long-term viscoelastic creep behavior observed by DMA.

12:03PM S54.00005: Exchange of the Bound Polymer Layer on Silica Nanoparticles* 
SANAT KUMAR (Presenter), ANDREW JIMÉNEZ, Columbia University, JACQUES JESTIN, CEACNRS, Laboratoire Léon Brillouin — It is now commonly accepted that a bound polymer layer (BL) naturally forms when a polymer melt is mixed with nanoparticles in the limit of favorable interactions. What is unclear is the temporal persistence of this BL – its very name implies that this layer is expected to be irreversibly adsorbed. We use contrast variation methods in conjunction with small angle neutron scattering to probe this issue in the canonical case of poly(2-vinylpyridine) mixed with 14 nm diameter silica nanoparticles. We find that there is essentially no long-term reorganization of the bound layer at 150 °C, but apparently a rapid reduction of the BL thickness at 175 °C. We believe that the dramatic temperature dependence arises from the polyvalency of the binding of a P2VP chain to a NP – that is the fact that each P2VP chain is adsorbed to the NP through multiple monomers. Thus, while the adsorption-desorption process of a single segment is an activated process that occurs over a broad temperature range, the cooperative nature of requiring multiple segments to desorb converts this into a sharp process that occurs over a relatively narrow temperature range.

12:15PM S54.00006: The complexity of linear viscoelastic properties of polymer nanocomposites: polymer dynamics and nanoparticle rearrangement* 
SHIWANG CHENG (Presenter), JIE YANG, Department of Chemical Engineering and Materials Science, Michigan State University, WEI YANG, College of Polymer Science and Engineering, State Key Laboratory of Polymer Materials Engineering, Sichuan University — Polymer nanocomposites (PNCs) are widely used as structural and functional materials, whose lifetime are typically evaluated from the time-temperature superposition. Rheological measurements of PNCs usually show >30 decades variation in the horizontal shift factor, aT, over a finite temperature range [1], indicating an unrealistic fast polymer dynamics at high temperatures. In this work, we decoupled the dynamic spectra of PNCs through a combination of rheology and dielectric measurements. We found that polymer dynamics in PNCs at different time and length scales follow identical temperature dependence with the neat polymer, although the rheological measurements exhibit 30 decades variation in aT. Further analyses suggest the local rearrangements of nanoparticles, especially at high temperatures, lead to the breakdown of the time-temperature superposition principle in PNCs. These results clearly show the shift factors by the time-temperature superposition principles cannot be directly translated to evaluate the dynamics features of PNCs at different temperatures.


*The authors acknowledge the support from Michigan State University. JY acknowledges the support from China Scholarship Council.

12:27PM S54.00007: The Effect of Nanofillers on the Viscoelastic Creep Behavior of Thermoplastics 
FRANCISCO BUITRAGO (Presenter), ANITA S YANG, University of Pennsylvania, PETER A GORDON, ExxonMobil Research and Engineering, ROBERT RIGGLEMAN, KAREN WINEY, University of Pennsylvania — The use of polymer nanocomposites (PNCs) in infrastructure applications requires a comprehensive understanding of the mechanism of nanoparticle reinforcement during viscoelastic creep. Some of the most relevant parameters that impact the mechanical reinforcement of nanoparticles to a thermoplastic matrix are the nanoparticle size and concentration, and the interaction between the nanoparticle surface and the polymer matrix. In this study, the long-term creep behavior of a model nanocomposite system is examined by applying time-temperature superposition to dynamic mechanical analysis (DMA) of PNC films at temperatures between Tg-60 °C and Tg+60 °C. The PNC system is composed of monodisperse 10-nm, 15-nm, and 28-nm silica nanoparticles dispersed in an amorphous polymer matrix of approximately 200,000 g/mol weight-average molecular weight. The interaction between nanoparticle surface and polymer matrix is adjusted by using bare silica featuring hydroxyl surface groups capable of hydrogen bonding versus nanoparticle surfaces treated with a phenyl-capping agent. The effect of these parameters on PNC morphology is quantified by small-angle X-ray scattering (SAXS) and by transmission electron microscopy (TEM), and correlated to the long-term viscoelastic creep behavior observed by DMA.
Thickness Effects on Morphology and Gas Permeability of Polystyrene-Grafted-Silica in a Polystyrene Matrix*  
SOPHIA CHAN (Presenter), CONNOR BILCHAK, MAYANK JHALARIA, ANDREW JIMENEZ, SEBASTIAN RUSSELL, Chemical Engineering, Columbia University, JULIA PRIBYL, BRIAN C BENICEWICZ, Chemistry and Biochemistry, University of South Carolina, SANAT KUMAR, Chemical Engineering, Columbia University — Polymer-grafted-nanoparticles in a polymer matrix can self-assemble into anisotropic morphologies that can be controlled by varying system parameters, such as grafting density and film thickness. The relationships between film thickness, morphology, and gas permeability of these systems, however, are not well-understood. We present the film thickness effects on gas transport properties and the surface and bulk morphologies of polystyrene-grafted-silica (PS-g-SiO₂) in a polystyrene (PS) matrix. Our thinnest films (2.5 μm) of the polymer nanocomposite exhibited a 90% reduction in CO₂ permeability relative to that of PS, while those of bulk films (100 μm) increased by 200%. Morphology characterization suggests lightly grafted PS-g-SiO₂ components are conducive to diffusing to the surface; this effect is more pronounced in thinner films, where distance to the surface is much shorter than bulk films. Nanoparticles at the surface of thinner films would then rearrange into structures that disallow gas transport. Conversely, the enhanced relative permeability in bulk films is likely due to the decreased interfacial density between the nanoparticle and the polymer chains, allowing gas molecules to more easily flow through the film.

*Columbia Soft Matter Grant, NSF GRFP DGE 16-44869

Highly-Mobile Nanoparticles that Strongly Interact with Well-Entangled Polymer Melts Diffuse via the Vehicular Mechanism*  
KAREN WINEY (Presenter), ERIC BAILEY, University of Pennsylvania, PHILIP J GRIFFIN, University of Chicago, RUSSELL JOHN COMPOSTO, University of Pennsylvania — When particles are large relative to the entanglement mesh in well-entangled polymer melts, the Stokes-Einstein (SE) relation predicts that particle diffusion scales as M⁻³.⁴. Using Rutherford backscattering spectrometry, we measure the diffusion coefficient of very small (radius ≈ 0.9 nm) octaaminophenyl silsesquioxane nanoparticles (NPs) in well-entangled poly(2-vinylpyridine) (P2VP) melts of varying molecular weight (1 – 26 entanglements/chain). We demonstrate that these small NPs diffuse between 10–10,000X faster in P2VP melts than predicted by SE, with the diffusion coefficients scaling weakly with molecular weight M⁻⁰.⁷±⁰.¹. Furthermore, we characterize the local segmental relaxation process and chain-scale center-of-mass diffusion and find reductions relative to bulk of ~80% and ~60%, respectively, at a NP concentration of up to 25 vol%. Through the combined study of NP and polymer dynamics in this attractive nanocomposite system, we demonstrate experimentally that small and highly-mobile nanoparticles in well-entangled polymer melts diffuse via the vehicular mechanism, i.e. successive NP adsorption/desorption events that occur on Rouse length and time scales.

*NSF-CBET #1706014; DOE-BES DE-SC0016421; National Science Foundation Graduate Re-search Fellowship Program (Bailey)

Using advanced field-based approaches to predict macroscale polymer nanocomposite phase behavior [invited]  
JASON KOSKI (Presenter), AMALIE FRISCHKNECHT, Sandia National Laboratories, ROBERT RIGGLEMAN, University of Pennsylvania — Predictive phase diagrams significantly improve the refinement and optimization of materials for advanced applications. Unfortunately, theoretical phase diagrams of polymer nanocomposites (PNCs) are lacking, which is a result of limitations with conventional modeling approaches such as computational expense or critical approximations. Here we describe the development of field-based approaches in modeling PNCs and demonstrate their efficacy in modeling macroscale phase behavior. The exciting advances of these field-based approaches have led to the development of phase diagrams for an array of polymer nanocomposite systems. Examples of these systems include grafted nanoparticles in a polymer melt and the assembly of mixed brush nanoparticles in solution. We find the introduction of thermal fluctuations have a significant impact on the overall phase behavior of these systems. Specifically, thermal fluctuations are necessary to properly capture depletion interactions in grafted nanoparticle systems and to describe solution-based assembly where it is understood that thermal fluctuations are significant. Excitingly, we further show the versatility of these methods to other PNC systems and provide comparisons with analogous experiments.

1:39PM S54.00011: Local structure and phase behavior of dense polymer-particle mixtures: improved theory and comparison with simulation  
YUXING ZHOU (Presenter), KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — 
The polymer reference interaction site model (PRISM) has been extensively applied to study the equilibrium behavior of polymer nanocomposites (PNC). The theory predicts three typical phases or states of aggregation: depletion clustering, steric stabilization via discrete adsorbed layers, and polymer-mediated bridging or networking, depending on polymer-particle attractive interaction, size ratio, composition, chain length and total packing fraction. While the existence of such microstructures appears to qualitatively agree with simulations and experiments, the accuracy of the predicted pair correlation functions and phase behavior has not been thoroughly examined. By performing systematic simulations, we find the PRISM pair correlation functions, selected thermodynamic properties and phase behaviors based on the commonly used Percus-Yevick and Hypernetted Chain closures sometimes incur significant errors, especially near bridging and depletion spinodal boundaries. A variety of new closure approximations are explored and we find that over a wide range of parameter space the modified Verlet approximation provides a major improvement in accuracy of structural and thermodynamic behavior for both PNCs and the corresponding atomic or colloidal mixtures.

1:51PM S54.00012: Deforming Interfacial Layers of Bare and Grafted Particle Nanocomposites in Large Amplitude Oscillatory Shear*  
SIYANG YANG (Presenter), PINAR AKCORA, Stevens Institute of Technology — 
Chemical heterogeneity around nanoparticles yields enhancement in mechanical properties in polymer nanocomposites. We have shown interfacial layers composed of two miscible polymers on well-dispersed nanoparticles control the dynamics of chains and their temperature-induced stiffening response. In this work, we examined these interfacial layers and the evolution of entanglements under large amplitude oscillatory shear to reveal the stability of mechanical and structural behavior of attractive composites. Deformation-recovery experiments have shown that particles adsorbed with low rigidity polymer (PMMA) disentangle/re-entangle and reinforcement factor increased significantly, whereas with the high rigidity polymer (P2VP) the modulus recovered to its initial value. Fourier transform rheology results indicated that strain-softening resulted from the arrangement of interfacial PMMA chains, which yielded to a higher entanglement state and stiffening. The non-linear rheology results of the PMMA-grafted particles will be discussed with the results of PMMA-, PC- and P2VP-adsorbed chains with varying rigidity. Large shear-induced entanglements can therefore be explained through the deformability of chains in interfacial layers.

*This work is funded by NSF-CMMI-MEP, Grant #1538725, 1825250.

2:03PM S54.00013: Dissipative Particle Dynamics (DPD) Simulations of Polymer-Filler Blends: Understanding Dispersion and Hierarchical Structure in Polymer Nanocomposites.*  
ASHISH GOGIA (Presenter), University of Dayton Research Institute, University of Dayton, OH, KABIR RISHI, ALEX MCGLASSON, MICHAEL CHAUBY, GREG BEAUCAGE, Dept. Chem. and Mat. Eng, University of Cincinnati, OH, VIKRAM K KUPPA, University of Dayton Research Institute, University of Dayton, OH — 
Nanoscale fillers are widely employed as cheap and effective additions for enhanced properties and functionality in polymeric systems. Such nanocomposites may contain fillers of varying miscibility, such as carbon black, silica, metal oxides, pigments, and/or various combinations thereof. In such systems, a complex partitioning of the components often results from the rich thermodynamics and kinetic history. Hence, the state of dispersion of the polymers and fillers is crucial to the behavior of polymer nanocomposites. In this research, we perform Dissipative Particle Dynamics (DPD) simulation of these blends, varying polymer-polymer, filler-filler and polymer-filler interaction energy, to understand the hierarchical structure and dispersion over multiple length and time-scales. The simulation results are validated against small angle x-ray scattering data to bridge a significant gap in our understanding of how complex hierarchical structure (across several decades in length) develops in these multicomponent systems. Additionally, the influence of parameters such as polymer chain stiffness and chain size on the formation of aggregates and agglomerates are explored.

*NSF CMMI-1635865, 1636036.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S55 DPOLY DBIO GSNP: Polymers and Biopolymers in Very Strongly Confined Environments I: Structure and dynamics of packaged polymers  
BCEC 254B - Zachary Dell, University of Massachusetts Amherst - Tag(s): Focus
11:15AM S55.00001: Distribution of label spacings for genome mapping in nanochannels* DANIEL ODMAN, University of Gothenburg, ERIK WERNER, Zenuity, KEVIN DORFMAN, University of Minnesota, CHARLES R DOERING, University of Michigan, BERNHARD MEHLIG (Presenter), University of Gothenburg — In genome mapping experiments, long DNA molecules are stretched by confining them to very narrow channels, so that the locations of sequence-specific fluorescent labels along the channel axis provide large-scale genomic information. It is difficult, however, to make the channels narrow enough so that the DNA molecule is fully stretched. In practice its conformations may form hairpins that change the spacings between internal segments of the DNA molecule, and thus the label locations along the channel axis. Here we describe a theory for the distribution of label spacings that explains the heavy tails observed in distributions of label spacings in genome mapping experiments. This talk is based on the paper Ödman, E. Werner, K. D. Dorfman, C. R. Doering & B. Mehlig, arxiv:1803.11396.

*Vetenskapsrådet

11:27AM S55.00002: Pathway-dependent nonequilibrium conformations of a polymer globule as a model for chromatin organization* SEULKI KWON (Presenter), BONG JUNE SUNG, Sogang University — The spatial organization of chromatin in nucleus resembles a fractal globule, of which structure differs from an equilibrium polymer globule. Even though there have been efforts to develop a polymer model to describe nonequilibrium structure of tightly-packed chromatin, the dependence of a transition pathway toward a globule has been often ignored. Because biological systems are often in nonequilibrium states, the transition pathway the chromatin would take before it reaches the densely-packed globule would be important. In this study, by using a simple polymer model and Langevin dynamics simulations, we investigate the conformational transition of a single polymer from swollen coil to compact globule in order to elucidate the effect of transition pathway on the final globular structure. We show that a fast collapse induces a nonequilibrium fractal-like structure, whose relaxation toward an equilibriumglobule is extremely slow. Moreover, in strong confinement, polymer conformation never relaxes into equilibrium state, thus the structure of the globule becoming dependent on the transition pathway.

*This work was supported by Samsung Science and Technology Foundation under Project No. SSTF-BA1502-07.

11:39AM S55.00003: Organization and Dynamics of Multiple DNA Chains Confined in a Nanofluidic Compartment* ZEZHOU LIU (Presenter), XAVIER CAPALDI, LILI ZENG, YUNING ZHANG, Physics department, McGill University, THU HA DAO, Physics department, University of Camerino, WALTER REISNER, Physics department, McGill University — The dynamics of multiple chains interacting in a confined environment is a fundamental problem in polymer physics and a model system for understanding confinement in biological systems. Here we present a nanofluidic device with compartments that can be opened and closed via pneumatic actuation of a thin membrane lid. The compartments are elliptical in shape with widths and lengths varying from hundreds of nm to microns. Differentially stained chains are trapped inside the cavities and the chain interactions assessed by monitoring the chain conformation and positioning in real-time via fluorescence videomicroscopy. We observe a transition between different dynamical states as the confinement is varied from quasi-0D (cavity confinement) to quasi 1-D (nanochannel confinement).

*This work was funded through the Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery Grants Program and the Fonds de recherche du Quebec Nature et technologies (FQRNT) Projet d'équipe.
11:51AM S55.00004: Chromatin Rheology Tells a Story: From DNA Damage Loci to Cellular Monolayers* [invited] KRIS DAHL (Presenter), Carnegie Mellon University — Over the past two decades here have been numerous intellectual intersections between polymer physics and modeling of intracellular environments including (i) soft glassy rheology as a description of the numerous relaxation states within the cell and (ii) athermal rheology from the contribution of cellular molecular motors. Within the nucleus we have also observed a powerlaw response of chromatin both by extracellular applied force and by particle tracking microrheology. Global condensation state of the chromatin greatly impacts its rheology, and both can be manipulated with epigenetic modifying drugs (trichostatin A) or growth factors. Locally, chromatin condensation can be manipulated with other methods such as tetracycline responsive elements (TRE) or is altered during transcription. We have developed methods to image changes in these regions using fluorescence lifetime imaging and particle tracking combined with multichannel registration and processing to determine the effects of DNA damage on heterochromatin and euchromatin. Measuring the impact of molecular motors within the cell show that actin-myosin forces produced in the cytoskeleton are transmitted into the nucleus where the athermal motions can be registered by nuclear particle tracking, thus allowing the dense chromatin to be used as a sensor for cellular force generation. This technique, which we refer to as SINK (Sensors from IntraNuclear Kinetics) has allowed us to determine strain variations within heterogeneous monolayers of cells. Mechanical defects in cell monolayers shows exponential propagation, which suggests that monolayers of cells may be better modeled as colloidal crystals than continuum sheets. The study of condensed chromatin inside of cells has provided interesting physical and biological insights into cells at length scales of tens of nanometers to hundreds of micrometers.

*NSF-CMMI-1634888

12:27PM S55.00005: Conformation and Dynamics of Nonconcatenated Ring Polymers under Planar Confinement TIANREN ZHANG (Presenter), KAREN WINEY, ROBERT RIGGLEMAN, University of Pennsylvania — Understanding the segregation of nonconcatenated ring polymers in a restricted volume is important to the biological field, because ring polymers have been proven to be a good model to study DNA organization in the cell nucleus. From our previous study, linear polymers segregate under extreme cylindrically-confined systems due to the strong correlation hole effect that is enhanced by the confining surfaces. Unlike linear polymers, the correlation hole effect of ring polymers is much stronger under confined systems since there are no chain ends. In this study, we use MD simulation to investigate the chain conformations and dynamics of ring polymers under planar confinements with different thicknesses ($H = 5, 7, 10, 14$ and $20\sigma$) that span from extreme confined case to bulk like case. Our results show that conformations of ring polymers are similar to the linear polymers under planar confines, except that ring polymers are less compressed along the direction normal to the walls. On correlation hole effect analysis, we distinguish the segregation regime from the mixing regime based on self-density calculation for ring polymers. From the diffusion and local chain relaxation dynamics, we observe that chain dynamics are primarily affected by the friction from walls.

12:39PM S55.00006: The Kinetoplast as a Model 2D Catenated Polymer ALEXANDER KLOTZ (Presenter), BEATRICE SOH, PATRICK DOYLE, MIT — Genomic length DNA molecules have served as a model system for studying the physics of single polymers, in part due to their large length scales, compatibility with fluorescence optical microscopy, excellent monodispersity, and the commercial availability of complete genomes of the lambda and T4 viruses. There has been theoretical interest in the physics of two dimensional polymers, but robust experimental systems have been lacking. Here, we extend the use of DNA as a model polymer into the second dimension by studying the physics of the kinetoplast in free solution. A kinetoplast is a complex genomic structure found in certain parasites that consists of thousands of topologically linked rings of DNA forming a two-dimensional network. Removed from the cell and viewed in fluorescence microscopy in good solvent conditions, it adopts a form akin to a jellyfish bell approximately 5 microns in diameter. We characterize the equilibrium conformation and dynamics of kinetoplasts and examine their response to flow, confinement, and varying solvent conditions. Due to the commercial availability of kinetoplasts and the possibility of controlling their size using topoisomerase reactions, this study will open the door to a new class of experiments on two-dimensional and catenated polymers.
12:51PM S55.00007: Random Walks in Disordered Environments: Membrane-Induced Confinement of DNA*

XAVIER CAPALDI (Presenter), ZEZHOU LIU, YUNING ZHANG, WALTER REISNER, McGill University — Understanding the conformation and dynamics of DNA in nanoslit structures is a topic of long-standing interest in the physics of nanoconfined polymers, yet introducing molecules into the most confined (sub 20 nm thick) structures is very challenging. Here we use a pneumatically-actuated membrane device to sandwich single DNA molecules between a flexible nitride flap and glass nanochannel floor, forcing the molecules into a degree of confinement limited only by the intrinsic roughness of the channel surfaces. In these environments the molecule undergoes a self-avoiding random walk in the disordered environment created by the surface roughness. We study single-molecule dynamics and conformation as a function of root-mean-square surface roughness and imposed confinement.

*Natural Sci. and Eng. Research Council of Canada (NSERC) Discovery Grants Program (Grant No. RGPIN 386212) and the Fonds de recherche du Quebec Nature et technologies (FQRNT) Projet d’équipe (PR-180418)

1:03PM S55.00008: Molecular Confinement on Nanostructured Polymer Surfaces

SARA HEEDY (Presenter), ALBERT YEE, Chemical Engineering, University of California, Irvine — Polymers have characteristic dimensions of assembly which depend on processing, especially in nanofabrication. These dimensions may be important in properties such as electrical or thermal conductivity. These properties will be strongly affected when fabricated polymer nanostructures have dimensions comparable to the critical length scale of physical phenomena (mean free path of electrons, mass transport, etc.). Enhanced mechanical, optical, and electrical properties of nanostructures, including nanopillar arrays less than 1 μm tall, have been well documented. We fabricated nanostructures on poly(methyl methacrylate) surfaces with nanoimprint lithography. A consequence of such a process is confinement induced reordering of polymer chains which is affected by the mold geometry, surface properties, and imprinting variables. Using thermal imprinting, and the combined topographical and nanoscale chemical mapping of photoinduced force microscopy, we found that nanopillars (100-700 nm range) confine functional groups differently depending on the feature shape, height, and periodicity. These findings suggest that surface chemistry, as well as nanoscale phenomena, can be controlled for use in adhesion and bio-electronic interfaces.

1:15PM S55.00009: Voltage-Driven Translocation through a Nanopore: How can we define a/the Capture Radius?*

GARY W. SLATER (Presenter), LE QIAO, Physics, University of Ottawa — A typical translocation event includes the following three steps: (i) the diffusion, (ii) the capture, and finally (iii) the translocation of the analyte. The capture process remains rather ill-understood because it cannot easily be visualized or inferred from the blockage current measured across the nanopore. To estimate the size of the so-called capture zone, a capture radius $R_c$ is generally defined as the radial distance from the pore where diffusion-dominated dynamics (at large distance) cross over to drift-dominated dynamics (near the pore). However, this definition is ambiguous and the models used are often over-simplified. We investigate several approaches to defining and estimating $R_c$ for the simple case of a charged particle diffusing in a liquid and attracted to the nanopore by an applied electric field. We present a theoretical analysis of the flux and Péclet number methods as well as 2D Lattice Monte Carlo (LMC) simulations with different simulation protocols and boundary conditions, including particle evaporation from the pore under a reversed field conditions. We compare our results to experimental estimates and we stress the fact that the boundary conditions and finite experimental times both matter in the interpretation of $R_c$.

*Funded by NSERC (Canada).

1:27PM S55.00010: Exploring How the Capture Process Affects the Translocation of Polymers through Nanopores*

HENDRICK W DE HAAN (Presenter), KONSTANTINOS KASTRITIS, MARTIN MAGILL, University of Ontario Institute of Technology — The translocation of polymers across membranes through nanopores has received a great deal of attention in recent years. This work is motivated by applications such as sequencing DNA and also characterizing and sorting biopolymers by size. While the great majority of this work has focused on the translocation process itself (i.e., when the polymer is in and passing through the pore), details such as the conformation of the polymer when it arrives at the pore are critical for real-world applications. In this talk I will present results from a simulation study of the capture of semiflexible polymers by nanopores and demonstrate how dynamics that yield non-equilibrium conformations affect the translocation process. The impact of these results will be demonstrated by presenting simulation and experimental results for nanofluidic devices that are designed to sort and count biopolymers. These will include having many nanopores in series connected by nano- or micro-channels and DNA passing through a nano-filtered nanopore device.

*NSERC Discovery Grant
The effects of packaging on the ejection rate of a polymer from a nanopore*  CHUNG BIN PARK (Presenter), BONG JUNE SUNG, Sogang University — DNA ejection and packaging are related in terms of DNA conformation. As the DNA becomes jammed, it cannot undergo dramatic conformational change in the capsid. That is, final conformation after packaging may be correlated with the conformation right before ejected. Then, a scientific question arises; whether a packaging process affects the ejection rate or not. In this work, we find three regimes of ejection processes: (1) knot dominant, (2) non-equilibrium dominant and (3) effective-ejection regime. We perform Langevin dynamics simulations of a semi-flexible single chain with 660 monomers. We package the chain with different packaging rates into a nanopore and eject the chain subsequently. If the chain is packaged slowly enough to be knotted, its ejection process becomes slow (~35%). Also, if the chain is packaged too fast to relax its conformation, its ejection rate decreases (~20%). Then, if a packaging rate is moderate (3), where DNA can relax but cannot be knotted, DNA ejects faster than other regimes. Our results show that ejection dynamics is determined by the history of packaging and suggest that there could be most effective packaging rate for ejection process in nature.

*This work was supported by Samsung Science and Technology Foundation under Project No. SSTF-BA1502-07.

Capture and translocation of a stiff oligomer by a nanopore*  LE QIAO (Presenter), GARY W. SLATER, Department of Physics, University of Ottawa — Both the translational diffusion coefficient \( D \) and the electrophoretic mobility \( \mu \) of an oligomer that is pulled towards a nanopore by an electric field depend on its orientation. Since a charged rod-like molecule tends to orient in the presence of an electric field gradient, \( D \) and \( \mu \) will change as the molecule approaches the nanopore, and this will impact the capture radius (a somewhat ill-defined measure of the efficiency of the nanopore to attract analytes in its vicinity). We present a study of this problem using theoretical arguments and Langevin Dynamics simulations. In particular, we define an alignment radius which we compare to the capture radius, and we examine different physical limits. The hydrodynamic interactions with the wall are also investigated by coupling the Langevin MD oligomer to a Lattice-Boltzmann fluid.

*The authors acknowledge the financial support by CSC and the University of Ottawa.

Towards Single Molecule Protein Sequencing by Nanopore Mass Spectrometry*  NICHOLAS DRACHMAN (Presenter), MATHILDE LEOPOITIEVIN, BENJAMIN WIENER, HANNAH SZAPARY, OLIVER G ISIK, DEREK STEIN, Brown University — Here we describe an approach to sequencing single protein molecules that will combine the advantages of mass spectrometry with those of nanopores. The basic idea is to cleave the individual amino acids from a protein molecule as they transit a small hole in sequence, and then identify each one by determining its mass-to-charge ratio in a mass spectrometer. We present the results of studies of the transfer of single amino acid ions from liquid into vacuum from the nanoscale orifice of a charged needle. We also summarize the development of an instrument featuring a magnetic mass filter and an array of channeltron detectors, which will be able to photo-dissociate single proteins and then measure both the mass and the time of detection of the resulting fragments.

*We acknowledge support from Oxford Nanopore Technologies.

Thursday, March 7, 2019 11:15 AM - 1:51 PM

Session S56 GSNP DPOLY: Interactions of Elastic Structures with Fluids and Granular Matter I  BCEC 255 - Douglas Holmes, Virginia Tech - Tag(s): Focus

Interactions of slender elastic structures with complex media like granular materials [Invited] EVELYNE KOLB (Presenter), NICOLAS ALGARRA, ESPCI, PMMH, ARNAUD LAZARUS, Sorbonne Université, Institut Jean Le Rond d'Alembert, DAMIEN VANDEMBROUCQ, ESPCI, PMMH — Slender elastic structures are extremely flexible and get easily unstable. As a consequence of their high geometrical aspect ratio, slender structures can be sensitive to low forces of various origins and exhibit complex mechanical behaviors due to the associated couplings with the surrounding medium, whatever it is (fluid, elastic medium, gels, frictional substrate, granular material...). The effect of flexibility has recently motivated a growing number of studies. This is in particular the case of the elasto-capillary problems (interaction between slender structures and capillary forces), and of the fluid-structure interaction, where water or air flows induce shape reconfiguration and streamlining of elastic structure, leading to drag reduction. Here we will review various cases of interaction of elastic structures with complex external medium, focusing on granular medium. Direct applications of this problem will be chosen in the bio-physics domain, like the growth of plant roots in structured soils.
11:51AM S56.00002: Elastogranular Packing of a Loop*  DAVID JAY SCHUNTER, JR. (Presenter), REGINA K. CZECH, DOUGLAS PETER HOLMES, Mechanical Engineering, Boston University — Confined thin structures are ubiquitous in nature. Spatial constraints have led to novel packing strategies at both the micro-scale, as when DNA packages inside a capsid, and the macro-scale, observable in plant root development. Previous work has focused on growing thin structures confined by rigid boundaries. Comparatively, much less is known about the behavior of slender growing structures constrained by deformable boundaries, such as granular materials. By varying the arc length of an elastic loop injected into a granular array of mono-disperse, soft, spherical grains of varying initial number density $\phi_0$, we investigate the resulting behavior of this model elastogranular system. At low $\phi_0$, the elastic loop deforms as though it were hitting a flat surface by periodically folding into the array. Above a critical packing fraction $\phi_c$, local re-orientations of grains cause the elastic loop to deform as though striking a curved surface, leading to the emergence of a distinct circular packing morphology. These results will bring new insight into the packing behavior of wires and thin sheets (where the same morphologies have been observed) and will be relevant to modeling animal burrowing & locomotive strategies, and developing smart, steerable needles.

*NSF CMMI -- CAREER #1454153

12:03PM S56.00003: Elastic tweezers for a vibrated granular bead  PAUL RAMBACH (Presenter), University of Mons, THOMAS SALEZ, YACINE AMAROUCHENE, University of Bordeaux, PASCAL DAMMAN, University of Mons — Optical tweezers are usually used to capture colloidal particles. In this talk, we will show that this method can be transferred in the realm of vibrated granular matter. It has been shown that the velocity distribution of mechanically vibrated beads is gaussian provided that a randomization of the collisions is achieved. This can be done via a rough surface, a layer of glued beads for instance. First we checked that a bead on top of a such rough surface undergoes a Brownian motion. Then we attached the bead to a flexible string and analyzed the fluctuations of motion. It revealed the drastic influence of the string elasticity, acting as a confining potential. This being equivalent to the harmonic potential achieved with optical tweezers. This new experimental setup paves the way to study stochastic behavior of small particles that should mimic colloidal suspension in 2D.

12:15PM S56.00004: Using an Olami-Feder-Christensen model with velocity weakened friction and variable stress transfer range to model slip-stick behavior in a sheared granular fault gouge system*  RACHELE DOMINGUEZ (Presenter), Physics, Randolph - Macon College — We present a variant of the Olami-Feder-Christensen (OFC) model with variable stress transfer range and a residual stress modified according to a velocity weakened friction force. The model displays dynamical modes similar to those observed in a sheared granular fault gouge laboratory system. For long stress transfer ranges, we find dynamical phases including a steady sliding state, a stick-slip state with periodic system-wide slipping events, and an intermittent state with both steady sliding and occasional slipping. For medium stress transfer ranges, we find additionally intermediate phases with large slipping events occurring in localized patches of the system. We compare simulation results of the model to laboratory results for the sheared granular fault gauge system.

*Walter Williams Craigie Teaching Endowment; Rashkind Family Endowment; Chenery Research Endowment; Center for Nonlinear Studies, Los Alamos National Laboratory

12:27PM S56.00005: Mechanical properties of jammed elastogranular columns  XIN JIANG (Presenter), MO EYDANI, KATE FLANAGAN, CASEY RICKS, DOUGLAS PETER HOLMES, Department of Mechanical Engineering, Boston University — Composite materials have unique properties due to the creative assemblies of their constituents. A mixture of grains and rods can enable the formation of stable structures via granular jamming. Understanding how these constituents govern the mechanical properties of the jammed structures is crucial for devising relevant engineering designs. Here, we examine freestanding columns composed of rocks and strings, and propose a simple physical model to explain the resulting structure's mechanical behavior. The results indicate that exterior fiber mainly contributes to stiffness, while interior fiber increases the resilience and toughness of the structures. By assembling the grains and rods in a programmable way, structures with robust mechanical properties can be formed. The results provide guidelines that allow the design of jammed elastogranular structures with desired mechanical properties.
12:39PM S56.00006: Scaling Effects in Composite Elastogranular Materials*  MO EYDANI (Presenter), XIN JIANG, CASEY RICKS, KATE FLANAGAN, DOUGLAS PETER HOLMES, Mechanical Engineering, Boston University — Composite elastogranular materials combine the characteristics of their constituents, resulting in interesting and distinct mechanical properties. In this study, the effect of scale on the mechanical properties of composite string-rock materials comprised of elastic fibers embedded in a granular rock matrix is investigated. An experimental study is carried out to explore whether the relative global size of a composite elastogranular medium affects its bulk mechanical properties. In particular, the stiffness, strength and ratcheting-like behavior of string-rock composite is investigated for a cylindrical form. The stiffness of composite string-rock columns is shown to be scale-independent while the strength and compaction are observed to be driven by the scale.

*This work was funded by The Defense Advanced Research Projects Agency (DARPA).

12:51PM S56.00007: Modeling the physical constraints of latch mediated, spring actuated systems*  MARK ILTON (Presenter), ANDRES COOK, NICHOLAS HELLER, Harvey Mudd College, S. N. PATEK, Duke University, ALFRED CROSBY, University of Massachusetts Amherst, SARAH BERGEBREITER, Carnegie Mellon University, EMANUEL AZIZI, University of California Irvine, GREGORY P. SUTTON, University of Bristol, SARAH LONGO, Duke University, SATHVIK DIVI, Carnegie Mellon University, CRYSTAL REYNAGA, Duke University, JEFFREY OLBERDING, University of California Irvine, RYAN ST PIERRE, Carnegie Mellon University, SUZANNE COX, Penn State University — Certain plants and animals utilize elastic structures made of biomaterials to actuate rapid movements. In some of the most extreme cases, which includes mantis shrimp and trap-jaw ants, a latching mechanism is used to control the spatio-temporal flow of energy from the organism to their environment. In this work, we model the physical constraints of latch mediated, spring actuated systems. An integrated approach rooted in physical principles that includes the loading and release of energy from these systems is presented. This approach reveals the inherent tunability of these systems, and is applicable to both biological and synthetic systems. We identify critical transitions that depend on the materials properties and geometry of the spring and latch components. The resulting kinetic energy output of these systems is ultimately limited by physical constraints placed on the organism by interaction with their environment and their control dynamics.

*This material is based upon work supported by the U.S. Army Research Laboratory and the U.S. Army Research Office under contract/grant number W911NF-15-1-0358

1:03PM S56.00008: Elastic feathers spread impact force  SUNGHWAN JUNG (Presenter), KINJAL BHAR, Biological and Environmental Engineering, Cornell University, BRIAN CHANG, Virginia Tech, LORIAN STAKER, Smithsonian Museum, EMMANUEL VIROT, Harvard University, ROMAIN PARIS, CHRISTOPHE CLANET, Mechanics, Ecole Polytechnique — Northern Gannets are seabirds that frequently employ a hunting tactic called ‘plunge-diving’ in which they dive through the water surface at high speeds to catch underwater prey; often reaching speeds of up to 24 m/s at the moment of impact. It can result in forces as high as 500 N acting on the bird’s neck during impact, yet the bird escapes uninjured, despite making 20-100 dives per foraging trip. However, little is known about how such high impact forces affect the rest of the body. The goal of this study is to investigate the role played by the feathers in spreading the hydrodynamic impact force on the skin around the impact zone. We model the feathers as elastic beams taking into account their pre-curvature and non-uniform cross-section. Results from our experiments with polycarbonate beams suggest that the interaction of feathers on the skin patch redistributes the force, thereby reducing the impact on any particular area of the skin.

1:15PM S56.00009: Entanglement of Elastic Fibers in low Reynolds Fluid Flow*  HOSSEIN SHARIFAZADEH (Presenter), YAYUN DU, Department of Mechanical and Aerospace Engineering, University of California, Los Angeles, ALI BEYZAVI, Massachusetts Institute of Technology, MOHAMAD KHALID JAWED, Department of Mechanical and Aerospace Engineering, University of California, Los Angeles — We report a discrete differential geometry based simulation for entanglement of elastic rods that couples the structural elasticity, hydrodynamic loading, and rod-rod contact. In nature, such entanglement can play a beneficial role, e.g. bundling in bacterial flagella; however, can also be a nuisance, e.g. trichobezoar (hairball) in human stomach. We consider a model system where elastic rods are injected, at a controlled velocity, one after another into a spherical tank full of viscous fluid. The simulation tool for this process is a combination of the following four components: the Discrete Elastic Rods algorithm for the elasticity of the rods, the modified mass method to impose the boundary condition, a penalty force-based collision detection and handling algorithm, and the Resistive Force Theory for hydrodynamic loading. We conduct experiments with a collaborative robot that injects the rods at a prescribed velocity and video records the process. In both experiments and simulations, we find that entanglement process is governed by the ratio of the elastic bending forces to the viscous forces. By exploring parameter space, we construct phase boundaries delineating the regions of entanglement.

*We acknowledge support from HSSEAS, University of California, Los Angeles.
Formation mechanism and morphological behavior of high aspect-ratio folds in compressed films

DEREK BREID (Presenter), Engineering Science, Saint Vincent College, SACHIN VELANKAR, Chemical Engineering, University of Pittsburgh — A thin, rigid film that is subjected to compression can exhibit a variety of buckling modes depending on the nature of the applied compression and the boundary conditions at the film surface and edges. Among the lesser-known buckling modes is the development of sharp, tall folds which are typically observed as a response to a swelling stress in a confined region of a larger film. Here, we conduct experiments to identify the essential physics underlying fold growth and the effect of constraints on the mode of buckling. We show that the folding mechanism is not limited to cases of rapid swelling, but emerges more generally in any compressed thin film which is imperfectly bound to a solid substrate. The only essential condition to achieve this mode of buckling is that the film must be able to slide along the substrate without allowing air or fluid to intrude between the film and the substrate. We demonstrate that this can occur through purely mechanical application of stress. We also show the effects of the size of the compressed region, the film thickness, and the stress application rate using swelling-based methods, and characterize our results using a model combining Flory-Rehner swelling theory with buckle initiation mechanics.

AFOSR, Award No. FA9550-10-1-0329

Rate-controlled wrinkling and folding of thin elastic films bonded to viscous substrates

SACHIN VELANKAR (Presenter), SOURAV CHATTERJEE, JUNYU YANG, University of Pittsburgh, RUI HUANG, University of Texas, XIANHENG GUAN, University of Pittsburgh, LUKA POCIVAVSEK, University of Chicago, ENRIQUE CERDA, University of Santiago — We examine the buckling of a thin elastic film floating on a viscous liquid layer which is itself supported on a prestretched rubber sheet. Releasing the prestretch in the rubber at a controlled rate induces viscous stress in the liquid, which compresses the elastic film, causing buckling. This approach allows compressive strains of several ten percent to be applied. Experiments and simulations show that two different buckle modes can appear. The first is that the elastic film develops roughly sinusoidal wrinkles. Wrinkling can be captured qualitatively by a linear stability analysis starting from a stress state that is calculated from a shear lag approach (Chatterjee, Soft Matter, 2015). The second is the appearance of tall, well-spaced folds which tend to appear at small liquid layer thickness. Folds are separated by regions where the film remains more-or-less flat. To our knowledge, the appearance of such folds in elastic films bonded to viscous supports is a new discovery. While their exact origin remains unclear, we argue that folds are energetically favorable (i.e. reduce bending energy more) as compared to wrinkles. But because folds can take a long time to develop, wrinkles may appear as a temporary intermediate state.

AFOSR FA9550-10-1-0329, NSF 1561789

Thursday, March 7, 2019 11:15 AM - 1:39 PM

Session S57 GSNP DBIO: Noise-driven Dynamics in Far-from-equilibrium Systems III BCEC

Probing noisy dynamics at the nanometer scale

DAVID HAVILAND (Presenter), SHAN JOLIN, RICCARDO BORGANI, Applied Physics, KTH Royal Institute of Technology — When driven by a strong pump, a nonlinear oscillator creates correlations in the frequency domain between signal and idler pairs symmetrically placed about the pump frequency. These correlations result in two-mode squeezing and phase-insensitive amplification of the signal. Not only signals but also noise can be squeezed, leading to measurement sensitivity below the standard limits imposed by thermal or quantum fluctuations. There is currently great interest in demonstrating these effects at the quantum limit, but less attention is paid to the squeezing of thermal noise where there is great potential for practical application. We demonstrate two-mode squeezing in dynamic Atomic Force Microscopy (AFM), where the limiting noise at room temperature is the thermal Brownian motion of the cantilever. Unlike previous work on the mechanical amplification of force, we do not use an 'external' nonlinearity to realize gain. Rather the sample itself is the 'gain medium' which causes a widening of the measurement bandwidth over which dynamic AFM is limited by thermal noise.

Affirms the general principle and the possibility of a Brownian ratchet working near room temperature scale. Our work thermally the steady-state dynamics of a simple stochastic electronic system featuring two resistor-capacitor circuits coupled by a third capacitor. The resistors are subject to thermal noises at real temperatures. The voltage fluctuation across each resistor can be compared to a one-dimensional Brownian motion. However, the collective dynamical behavior, when the resistors are subject to distinct thermal baths, is identical to that of a Brownian gyrator, as first proposed by Filliger and Reimann [1]. The average gyrating dynamics is originated from the absence of detailed balance due to unequal thermal baths. We look into the details of this stochastic gyrating dynamics, its dependences on the temperature difference and coupling strength, and the mechanism of heat transfer through this simple electronic circuit. Our work affirms the general principle and the possibility of a Brownian ratchet working near room temperature scale.


*This work has been supported by Ministry of Science and Technology in Taiwan under Grants No. MOST 104-2112-M-008-003-MY3, No.105-2112-M-008-019-MY2, and No. 105-2112-M-008-023. C.-L.L. acknowledges the support from the NCTS thematic group Complex Systems.

Detecting and quantifying non-equilibrium activity is essential for studying complex living systems such as cells. We present a non-invasive approach of measuring activity in a system based on the breaking of time-reversal symmetry. We focus on "cycling frequencies" - the frequencies with which the trajectories of pairs of degrees of freedom circle around in phase space, which is related to the entropy production rate. We test our approach on simple toy-models comprised of elastic networks immersed in a viscous fluid with spatially-varying internal driving. We prove both numerically and analytically that the cycling frequencies obey a power law as a function of distance between the selected degrees of freedom. Moreover, the behavior of the cycling frequencies contains information about the dimensionality of the system and the amplitude of active noise. Finally, we aim to find a mapping between the microscopic properties of a non-equilibrium system and macroscopic observables such as the cycling frequencies by including features such as the active force moments or spatial and temporal correlations of the active noise.

11:39AM S57.00003: Electrical autonomous Brownian gyrator+ KUAN-HSUN CHIANG (Presenter), CHI-LUN LEE, PIK-YIN LAI, YUNG-FU CHEN, Department of physics, National Central University, Zhongli 32001, Taiwan — We study experimentally and theoretically the steady-state dynamics of a simple stochastic electronic system featuring two resistor-capacitor circuits coupled by a third capacitor. The resistors are subject to thermal noises at real temperatures. The voltage fluctuation across each resistor can be compared to a one-dimensional Brownian motion. However, the collective dynamical behavior, when the resistors are subject to distinct thermal baths, is identical to that of a Brownian gyrator, as first proposed by Filliger and Reimann [1]. The average gyrating dynamics is originated from the absence of detailed balance due to unequal thermal baths. We look into the details of this stochastic gyrating dynamics, its dependences on the temperature difference and coupling strength, and the mechanism of heat transfer through this simple electronic circuit. Our work affirms the general principle and the possibility of a Brownian ratchet working near room temperature scale.

11:51AM S57.00004: Experimental observation of fluctuation loops JOHN NEU (Presenter), Mathematics, University of California, Berkeley, JUAN PABLO GONZALEZ, STEPHEN TEITSWORTH, Physics, Duke University — Fluctuation loops arise in the large deviation theory of stochastic dynamical systems. Displacements from a stable critical point to a small destination box about a point many standard deviations away are rare. When they do occur, they closely follow a most probable outward path. The most probable outcome after reaching the destination box is deterministic relaxation back to the stable critical point. The union of the outward and relaxation paths constitutes a fluctuation loop. For linear stochastic dynamics, fluctuation loops can be constructed by simple averaging. Ensemble averaging over forward histories after reaching the destination box obviously recovers the relaxation segment. Less obviously, averaging over back histories prior to reaching the destination box recovers the outbound segment. The characterization of fluctuation loops by averaging means that they can be recovered from experimentally recorded time series of state variables. We demonstrate this for a simple electrical network of two capacitively coupled, noise driven RC circuits. Even when the destinations boxes are not many standard deviations away from the stable critical point, it is striking that clearly resolved fluctuation loops emerge from very noisy data.

12:03PM S57.00005: Hydrodynamic Brownian motion and nanoscale transport efficiency in liquids SEAN SEYLER (Presenter), STEVE PRESSÉ, Center for Biological Physics, Arizona State University — Recent experiments have motivated a reexamination of Brownian motion, as hydrodynamic memory and colored thermal noise arising on short spatiotemporal scales lead to substantially different dynamical behavior. We revisit the problem of particle transport in liquids at low Reynolds number, where we account for the Basset-Boussinesq force and added mass effect induced by unsteady particle motion while reincorporating thermal fluctuations so as to satisfy fluctuation-dissipation. The resulting fluctuating Basset-Boussinesq-Oseen equation is solved numerically using an efficient method based on Markovian embedding, which can simultaneously capture the algebraic decay of the memory kernel and the colored noise spectrum to an arbitrary level of precision. We apply various driving forces to ensembles of submicron spherical particles in different liquids while holding constant the amount of input work; the resulting particle displacements and velocities are analyzed in terms of the magnitude, duration, and shape of different forcing protocols. For each protocol, we compute efficiencies for particle transport—with and without hydrodynamic effects—using the mean displacement and current density as proxies for output work. Implications for subcellular biology and nanofluidics are discussed.
12:15PM S57.00006: Operator dynamics in Brownian quantum circuit*  TIANCI ZHOU (Presenter), XIAO CHEN, Kavli institute of theoretical physics — We view the operator spreading in chaotic evolution as a stochastic process of height growth. The height of an operator represents its spatial extent and a master equation governs the transition to higher operators. We derive and solve a master equation in a random N -spin model with all 2-body interactions. The mean height, being proportional to the squared commutator, will grow exponentially within log N scrambling time and saturates in a manner of logistic function. We propose that the chaos bound at finite temperature could be due to initial height biased towards the high operators, which has smaller Lyapunov exponent.

*XS and TZ are supported by a postdoctoral fellowship from the Gordon and Betty Moore Foundation, under the EPIQS initiative, Grant GBMF4304, at the Kavli Institute for Theoretical Physics. We acknowledge support from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1720256).

12:27PM S57.00007: Operator dynamics in chaotic long-range interaction systems*  XIAO CHEN (Presenter), TIANCI ZHOU, University of California, Santa Barbara — We use out-of-time-order correlator (OTOC) to diagnose the propagation of chaos in one dimensional long-range power law interaction system. We consider a model called Brownian quantum circuit, which allows us to derive the master equation governing the operator dynamics and therefore transforms the evolution of OTOC to a classical stochastic dynamics problem. We find that the chaos propagation relies on the number of qubits N on each site and the power law exponent α. We use OTOC to define light cone and find that in the small N limit (N=1), there are three light cone regimes as we vary α: (1) a log light cone regime when 1<α<2, (2) a sublinear power law light cone regime when 2<α<4 and (3) a linear light cone regime when α>4. We further study the scaling behaviors of OTOC in the vicinity of light cone. Moreover, we also study the operator growth in the large N limit and find it to be remarkably different. Our result provides a unified physical picture for chaos dynamics in power law interaction system and can be generalized to higher spatial dimensions.

*We are supported by postdoctoral fellowships from the Gordon and Betty Moore Foundation, under the EPIQS initiative, Grant GBMF4304, at the Kavli Institute for Theoretical Physics.

12:39PM S57.00008: Anomalous diffusion, infinite measures, and limit distributions in a class of exactly solvable stochastic processes  GUENTER RADONS (Presenter), Institute of Physics, Chemnitz University of Technology, Germany, TAKUMA AKIMOTO, Department of Physics, Tokyo University of Science, Japan, ELI BARKAI, Department of Physics, Bar-Ilan University, Ramat Gan, Israel — We consider stochastic processes, piecewise constant in time, which can be viewed as a gapless sequences of statistically independent box functions of duration τi and height vi. Lengths and heights of the boxes are deterministically coupled, whereas the areas τivi are i.i.d. random variables. These processes are closely related to the velocity process of space-time coupled Levy walks [1,2], but can more generally be viewed as a renewal processes, where the life times τi are not simply drawn from one given distribution, but are determined via a deterministic law by the values vi of a relevant stochastic variable. Despite its simplicity, these processes can show anomalous diffusion, or, more general, anomalous behavior of its moments. The latter can be related either to invariant densities, which are non-normalizable, or, for other parameters, to certain scaling densities. We obtained exact results for these quantities because we were able to derive the exact form of the propagator analytically. In addition, we were able to derive non-trivial exact limit distributions for time-averaged quantities of interest.


12:51PM S57.00009: Optimal Finite Time Erasure: A mass transport perspective*  JAMES MELBOURNE (Presenter), SAURAV TALUKDAR, HARISH DODDI, MURTI SALAPAKA, University of Minnesota — Landauer’s principle states that the average heat dissipation in a bit erasure is atleast kBT ln 2. Recent experiments approach this bound in an asymptotic manner with respect to time. Meanwhile, in the experimentally relevant case that a single bit memory is modeled as a Brownian particle in a bistable well, developments in non-equilibrium thermodynamics and stochastic control predict larger heat dissipation for finite time erasure, dependent on the Wasserstein transportation distance between the initial and final configurations. Inspired by these considerations, we propose an experimentally feasible finite time erasure protocol which approximates a Wasserstein geodesic. Monte Carlo simulations are used to demonstrate the efficacy of the proposed erasure protocol, comparing energetics against existing erasure protocols and the theoretically optimal bounds.

*The research was supported by the National Science Foundation under the grant NSF ECCS 1809194.
1:03PM S57.00010: Exact solutions of dissipative quantum spin chains using Majorana fermions  
NAOYUKI SHIBATA (Presenter), HOSHO KATSURA, Physics, University of Tokyo — The Lindblad equation is the well-known quantum master equation which describes the evolution of open quantum systems. While Lindblad equations have been used in the past mostly to describe few-particle systems in e.g., quantum optics, recent years have witnessed a growing interest in many-body systems in the Lindblad setting. However, very few exact results are available for many-body systems. The main difficulty is that we often need to deal with effective interactions arising from dissipation [1] even when the Hamiltonian itself is reducible to that of a free-particle system. This prevents us from understanding the full dynamics of the system.

In this talk, we construct a new exactly solvable dissipative spin model which maps to an effective non-Hermitian many-body system. By Kitaev's technique [2], this model can be seen as free Majorana fermions in a static Z2 gauge field, allowing us to obtain the full dynamics of this open system sector by sector. With this method, we obtain the Liouvillian gap (the inverse of relaxation time) numerically and exactly. We also obtain a closed formula for the auto-correlation of the edge spin by relating it to the enumeration of lattice paths.


1:15PM S57.00011: Degree heterogeneity increases the probability of rare events in population networks  
MICHAEL ASSAF (Presenter), Hebrew University of Jerusalem, JASON HINDES, Plasma Physics Division, Naval Research Laboratory — There is great interest in predicting rare and extreme events in complex systems, and in particular, understanding the role of network topology in facilitating such events. In this work, we show that degree heterogeneity - the fact that the number of local connections in complex networks is broadly distributed - increases the probability of large, rare fluctuations in population networks generically.

We perform explicit calculations for two canonical examples of rare events: network extinction and switching. When the distance to bifurcation is held constant, and hence stochastic effects are fairly compared among networks, we show that the probability exponent for rare events decreases linearly with the ratio of the degree distribution's standard deviation to its mean.

1:27PM S57.00012: Using a System's Equilibrium Behavior to Reduce Its Energy Dissipation in Non-Equilibrium Processes  
SARA TAFOYA, Biophysics, University of California, Berkeley, STEVEN J. LARGE, Physics, Simon Fraser University, SHIXIN LIU, Rockefeller University, CARLOS JOSE BUSTAMANTE, Molecular & Cellular Biology, Physics, and Chemistry, University of California, Berkeley, DAVID SIVAK (Presenter), Physics, Simon Fraser University — Cells must operate far from equilibrium, utilizing and dissipating energy continuously to maintain their organization and to avoid stasis and death. However, they must also avoid unnecessary waste of energy. Recent studies have revealed that molecular machines are extremely efficient thermodynamically when compared to their macroscopic counterparts. However, the principles governing the efficient out-of-equilibrium operation of molecular machines remain a mystery. A theoretical framework has been recently formulated in which a generalized friction coefficient quantifies the energetic efficiency in non-equilibrium processes.

Moreover, it posits that to minimize energy dissipation, external control should drive the system along the reaction coordinate with a speed inversely proportional to the square root of that friction coefficient. Here, we demonstrate the utility of this theory for designing and understanding energetically efficient non-equilibrium processes through the unfolding and folding of single DNA hairpins.
11:15AM S58.00001: Phospholipid bilayer interleaflet friction from coarse-grained numerical simulations

OTHMÈNE BENAZIEB (Presenter), FABRICE THALMANN, CNRS and University of Strasbourg, France, Institut Charles Sadron — Amphiphilic lipid bilayers modify the friction properties of the surfaces on top of which they are deposited [1]. In particular, the measured sliding friction coefficient is significantly reduced compared with the one of a native surface [2]. We investigate in this work the friction properties of a numerical coarse-grained model [3] of lipid bilayer subject to longitudinal shear. Interleaflet friction coefficients are extracted from out-of-equilibrium pulling and relaxation experiments. In particular we gain access to the transient viscoelastic response of the bilayer subject to normal shear. We then show how our method can be generalized to supported lipid bilayers.


11:27AM S58.00002: Modifying lubrication in micro-patterned and polymer-grafted soft interfaces

LILIAN HSIAO (Presenter), YUNHU PENG, CHRISTOPHER SERFASS, North Carolina State University — Soft contacts are encountered in a variety of natural and technological applications. Two common strategies to modify interfacial friction include the deliberate micropatterning of surfaces and the grafting of charged polymer brushes onto the surfaces. Nevertheless, the connection between macroscopic friction and surface energies on textured substrates is not well understood. We synthesize model poly(dimethylsiloxane) (PDMS) substrates with microtextures and polyzwitterionic brushes, and use them as tribopairs to investigate the effect on elastohydrodynamic (EHL) and boundary lubrication (BL). Our results indicate that patterned surfaces exhibit micro-EHL to EHL transitions in which the critical friction coefficient and Sommerfeld numbers vary as a function of the surface geometry. The experimental data show excellent agreement with a simple scaling theory we developed from Reynold's equations for 1D lubrication flows. Furthermore, we investigate the BL changes in PDMS tribopairs in which betainized poly(2-dimethylamino ethyl methacrylate) (PDMAEMA) brushes are covalently grafted onto the surface. Our preliminary results suggest that the polymer relaxation physics may play an important role in the lubricating efficiency of the PDMAEMA brushes.

11:39AM S58.00003: Ink Transfer in Ultrathin Flexographic Printing Using Nanoporous Stamps

DHANUSHKODI MARIAPPAN (Presenter), KIM SANHA, MICHAEL S. H. BOUTILIER, Mechanical Engineering, Massachusetts Institute of Technology, JUNJIE ZHAO, Chemical Engineering, Massachusetts Institute of Technology, HANGBO ZHAO, JUSTIN BEROZ, Mechanical Engineering, Massachusetts Institute of Technology, HOSSEIN SOJOUDI, KAREN GLEASON, Chemical Engineering, Massachusetts Institute of Technology, PT BRUN, Chemical and Biological Engineering, Princeton University, JOHN HART, Mechanical Engineering, Massachusetts Institute of Technology — Printing of ultrathin layers of liquid and colloidal inks is critical to manufacturing of low-cost electronics on non-conventional substrates such as polymer films and flexible glass. A recent invention from our research group, engineered nanoporous stamps made from polymer-coated carbon nanotube (CNT) forests, are highly porous (>90%) and can retain colloidal nanoparticle inks within their volume. Using these stamps, we have achieved printing of micron-scale features with highly uniform sub-100 nm thickness. In this work, we use high-speed imaging of the contact line motion during printing on transparent substrates to observe the dynamics of liquid spreading during contact, and the evolution of a capillary liquid bridge in the stamp-substrate gap. At high approach speeds, spreading speed increases with approach speed whereas at low approach speeds, flow from the porous medium defined by the fluid and stamp properties determine the spreading speed. After bridge rupture at a critical stamp-substrate gap, liquid respreads to fill the area defined by a precursor film matching the stamp geometry with high precision, and the respreading dynamics follow Tanner's law. The transferred liquid volume decreases with retraction speed enabling speed based process control of layer thickness.
11:51AM S58.00004: Effects of Bidisperse Wettability on Interfacial Viscoelasticity of Particle Laden Interfaces
SYED EHSANUR RAHMAN, GORDON CHRISTOPHER (Presenter), Texas Tech University — Increasing use of Pickering Emulsions has led to increasing study of interfacial particles. It is known that particle contact angle determines emulsion type and modifies interfacial viscoelasticity, effecting emulsion stability and viscosity. Most studies of particle interfaces examine a mono-population of colloids. However, in applications, there can be significant distribution in contact angle. What role such distribution plays on interfacial mechanical properties is unclear.

In this work, the effects of controlled dispersity of wettability on particle laden interfaces is examined. Using hydrophobic and hydrophilic negative polystyrene and hydrophobic non-ionic polystyrene, mixed wettability systems with varying ratios of hydrophobic to hydrophilic particles are studied. An increase in interfacial elasticity is observed when the ratio of hydrophobic to hydrophilic particles reaches 1. This corresponds with an increase in local hexagonal order and decrease in area around particles. Similar but smaller magnitude changes are observed for combinations of hydrophobic particles. We believe these changes occur due partitioning of particles to either side of the interface, creating larger local density and increased resistance to deformation.

*NSF #1437710

12:03PM S58.00005: Particle assembly on an evolving interface
BENJAMIN DRUECKE (Presenter), XIANG CHENG, SUNGYON LEE, University of Minnesota — The behavior of particles on fluid-fluid interfaces has a history extending back to Pickering. Much of the work on these particle rafts treats the fluid as a quasi-static interface and investigates the behavior of the particles on this passive interface. In this work, we investigate the behavior of particle rafts on dynamically evolving interfaces such that there is a strong coupling between the behavior of particles on the interface and the underlying hydrodynamics of the evolving interface. As a prototypical system, we consider a water-oil interface inside a funnel, such that the interface deforms as the water level is varied. We examine the behavior of a variety of particles on such an interface to elucidate the coupling between bulk and interfacial phenomena.

*Funded by the National Science Foundation through the University of Minnesota MRSEC under Award Number DMR-1420013

12:15PM S58.00006: A Computational Method to Study Packing on Deformable Shells
SANJAY DHARMAVARAM (Presenter), Mathematics, Bucknell University, LUIGI E PEROTTI, Mechanical and Aerospace Engineering, University of Central Florida — Many problems in softmatter and membrane biophysics, such as studying equilibrium configurations of protein clusters on cell-membranes, highly defect ridden structures of Gag polyproteins in immature HIV capsids, and the unusual fluid-like state of Archaeal viruses [1] can all be analyzed as systems of interacting particles (typically representing proteins or protein capsomers) on deformable fluid surfaces. The coupled interactions between the particles and the underlying elastic medium to which they are constrained pose significant computational challenges. Existing methods often employ expensive constraints to anchor particles to the surface or artificially restrict their movement yielding spurious equilibrium states. In this talk, we present a new approach that circumvents existing challenges to obtain reliable equilibria. We apply the method to study the generalized Thomson problem of packing interacting particles on a deformable shell. In this context, we investigate particle symmetries, surface tessellation, and surface shape as the fluid membrane is progressively covered by interacting particles.


12:27PM S58.00007: Rigid Bubbles: Novel Instabilities in Colloidal Film Rupture
PHALGUNI SHAH (Presenter), SRISHTI ARORA, MICHELLE R DRISCOLL, Northwestern University — When a soap bubble pops, a rupture opens up and grows on the timescale of milliseconds. Culick (1960) showed that this rupture grows at a constant rate. Recently, Petit et al. (2015) studied films that were rigidified due to their high surfactant concentration. They observed that these films developed crack-like instabilities during rupture, and their rupture velocity was slower than that predicted by Culick. We investigate whether soap films rigidified by adding colloidal spheres show similar instabilities. We rupture a flat film containing surfactant and colloidal spheres using a needle and record it with a high-speed camera at 75,000 frames per second. We control film rigidity by varying particle concentration and find that this dramatically alters rupture dynamics. The rupture opens at a rate that is non-constant and an order of magnitude slower than the Culick velocity. Additionally, we observe a wide variety of instabilities in these rupturing colloidal films. We systematically study film rupture dynamics as a function of colloid concentration and film thickness.
12:39PM S58.00008: Thermally assisted buckling of colloidal assemblies* SIMON STUIJ (Presenter), Institute of Physics, University of Amsterdam, JAN-MAARTEN VAN DOORN, TOM KODGER, JORIS SPRAKEL, Physical Chemistry and Soft Matter, Wageningen University, CORENTIN COULAIS, PETER SCHALL, Institute of Physics, University of Amsterdam — We investigate the effect of thermal fluctuations on the buckling instability of colloidal assemblies. Using laser tweezers to grab the ends of, and push on colloidal chains assembled with critical Casimir forces, we probe the buckling instability analogous to the Euler buckling of macroscopic beams, in the presence of thermal activation. We find that buckling fluctuations diverge upon approaching the buckling point, while their time scale diverges similar to critical slowing down. Molecular dynamic simulations allow quantitative extraction of the corresponding critical exponents, which we identify as the mean-field critical exponents. Using an analytically solvable minimal model, we elucidate the origin of these exponents. The surprisingly rich physics of this simple thermal mechanical system highlights the interplay of thermal fluctuations and elasticity in the buckling stability of micron-scale architectures such as biomaterials.

*P.S. acknowledges support by a Vici grant from the Netherlands Organization for scientific research (NWO).

12:51PM S58.00009: Memory effects in the attachment of thin films to liquid surfaces* DEEPAK KUMAR (Presenter), THOMAS RUSSELL, BENJAMIN DAVIDOVITCH, NARAYANAN MENON, University of Massachusetts Amherst — We study the dynamics of depositing or peeling off a thin polymer film at an air-water surface. In our experiment, we control the velocity of the film withdrawal or attachment while measuring the force required to do so. The observed dynamics is hysteretic, wherein the force depends on the direction of motion even at the lowest attainable velocities, but the magnitude of the hysteresis loop appears to be independent of the velocity. When the motion of the film is halted, the relaxation to equilibrium configuration is extremely slow, and appears to be logarithmic in time. Quite remarkably, the relaxation dynamics retains the memory of velocity history. This behavior, involving hysteresis, slow relaxation and memory effects are hallmarks of glassy systems which have access to a large number of relaxation modes with a broad distribution of dynamics. The surprisingly rich physics of this simple system exhibits some of these features.

*We gratefully acknowledge support from NSF DMR 1507650.

1:03PM S58.00010: Motion of water droplets on oil infused surfaces* SOLOMON ADERA (Presenter), LILIAN MAGERMANS, School of Engineering and Applied Sciences, Harvard University, MUGHEES KHAN, Wyss Institute for Biologically Inspired Engineering, Harvard University, JOANNA AIZENBERG, School of Engineering and Applied Sciences, Harvard University — Controlling the motion of water droplets on solid surfaces has broad technological implications ranging from microfluidics to thermal management. Past approaches utilized topography and chemical composition gradients to manipulate the motion of droplets. Here we show that the motion of droplets on oil infused surfaces can be triggered via asymmetry of the wetting ridge. Our experimental results show that neighboring droplets exert force on each other through their wetting ridge. This interaction causes droplets to coalesce and self propel by releasing free surface energy. Importantly, our experiments show that the motion of water droplets on slippery oil infused surfaces is not random as has been hypothesized in past studies. Instead, the oleoplaning droplets select their path such that the force required to overcome viscous dissipation is minimum. Consequently, droplets move away from oil depleted regions where the lubrication oil thickness is small and the resistance to motion is large. This “sensing” ability of droplets to the thickness of lubrication oil enables them to maneuver by avoiding prior oil depleted paths. This study provides new mechanistic insight into the motion of water droplets on oil infused surfaces.

*The authors acknowledgments funding from the Wyss Institute.

1:15PM S58.00011: Two-wavelength Wrinkling Patterns in Chiral Liquid Crystal Surfaces PARDIS ROFOUIE, ZIHENG WANG, ALEJANDRO REY (Presenter), McGill University — We present a model to investigate the formation of two-length scale surface patterns in biological and synthetic anisotropic soft matter through the high order interaction of anisotropic interfacial tension and capillarity at their free surfaces. Focusing on the chiral liquid crystal (CLC) material model, the generalized shape equation for anisotropic interfaces using the quartic anchoring energy is applied to understand the formation of two-length scale patterns, such as those found in floral petals. Analytical and numerical solutions are used to shed light on why and how simple anisotropic anchoring generates two-lengthscale wrinkles whose amplitudes are given in terms of anchoring coefficients. The proposed new nano-wrinkling mechanisms augment previous models dedicated to understand and mimic biological surface pattern formation. Symmetry relations and scaling laws are used to provide the explicit relations between the anchoring constants and surface profile of the two length scale wrinkles. These new findings establish a new paradigm for characterizing surface wrinkling in biological liquid crystals, and inspire the design of novel functional surface structures.
1:27PM S58.00012: Sculpting high aspect ratio particles from oil-in-water emulsions*  MATHEW GISÓ (Presenter), Physics & Astronomy, Tufts University, HAO DA ZHAO, PATRICK T SPICER, Chemical Engineering, University Of New South Wales, TIM ATHERTON, Physics & Astronomy, Tufts University — Shape is a powerful route to control the transport and rheological properties of particulate media. Here, we present a process to sculpt elongated colloidal particles from an oil-in-water emulsion. Oil droplets are crystallized by reducing the temperature. The rate of cooling determines the rate of crystallization. With the addition of surfactants, it is possible to induce dewetting of the crystals by their own liquid phase. By tuning the relative rates of dewetting and crystallization, a rich variety of crystal shapes can be grown in an easily scalable process using controlled interfacial hydrodynamics. We explain these experimental findings using a non-equilibrium Monte Carlo model that captures both the crystallization and dewetting processes. Our results reproduce the wide range of shapes seen in experiment and provide insights to control their final morphology. Prospects for expanding the space of final shapes will also be discussed.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1654283.

1:39PM S58.00013: Defect screening in faceted emulsion droplets.  IRETH GARCÍA-AGUILAR (Presenter), PIEMARCO FONDA, LUCA GIOMI, Leiden University, ELI SLOUTSKIN, Bar-Ilan University — Oil emulsion droplets in water have been observed to spontaneously deform into polyhedral shapes at temperatures where the surfactant interface freezes while the bulk oil and water remain liquid. The interface monolayer crystalizes into a hexagonal lattice, which is topologically constrained to accomodate a certain number of defects, namely disclinations. Additional defects, called dislocations, are also expected to be found in crystals with large number of particles. Dislocations are not only thermally induced but, more importantly, they are known to screen the large stresses around disclinations by forming chain-like structures at their vicinity. We address the problem of faceting droplets by studying the interplay between the interface geometry and the arrangement of dislocations. We have found that the coupling between the distribution of crystal defects, surface curvature and entropy is key to understand the temperature and size-dependent behaviour of the shape transformations.

1:51PM S58.00014: Statistical Mechanics of Puckered Membranes  ABIGAIL PLUMMER (Presenter), DAVID R NELSON, Harvard University — A triangular lattice of points connected by springs that resists bending and stretching provides a discrete model of a thin elastic plate. We consider such a surface with a superlattice of ‘impurities’— sites that have longer springs connecting them to the rest of the lattice. In the continuum limit, this corresponds to a preferred metric with periodic dilations. These impurities tend to pucker either above or below the lattice. We regard this as an Ising-like degree of freedom, and characterize interactions between neighboring puckers. We find we can tune these puckered membranes from a ‘ferromagnetic’ state to an ‘antiferromagnetic’ state using elastic constants and superlattice structure, and investigate these states theoretically and numerically.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S59 GSOFT: Actuation in Soft Matter II BCEC 257B - Benjamin Gorissen

11:15AM S59.00001: Liquid Crystal Elastomer Micron-Rings with Pre-Designed Molecular Orientations*  HAO YU (Presenter), YUBING GUO, ZIYUAN ZHOU, MIAO JIANG, TARAS TURIV, O D LAVENTOVICH, QI-HUO WEI, Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, Ohio, 44242, USA — Mechanical responses of liquid crystal elastomers (LCEs) to external stimuli are pre-programmable by predesigning molecular orientations, promising applications such as sensors and actuators and micro robotics. Recently we have developed capabilities to photopatterning arbitrary molecular orientations with high spatial resolutions and to fabricating LCEs with well-defined geometric shapes and predesigned 3D molecular orientations. In this talk, we will present studies on LCE micro-rings, especially on how their mechanical deformations and dynamics are affected by their molecular orientations and geometric shapes.

*NSF CMMI-1436565 and DOE, Office of Sciences, DE-SC0019105
**11:27AM S59.00002: Topography from topology in liquid crystal elastomer coatings***
YOUSSEF MOSADDEGHIAN GOLESTANI (Presenter), GREGA BABAKHANOVA, MICHAEL P VARGA, HAO YU, JONATHAN SELINGER, QI-HUO WEI, O D LAVRENTOVICH, ROBIN SELINGER, Kent State University — Liquid crystal elastomer (LCE) free-standing films containing topological defects deform on heating into three-dimensional shapes [1-3]. Attaching such LCE films to a rigid substrate as a coating provides the opportunity to create temperature-responsive surface topography, a phenomenon demonstrated by Babakhanova et al [4]. Using finite element method (FEM) simulation, we model surface deformations produced by LCE coatings with defects as a function of both topological charge and orientational phase angle. We find that, on heating, a radial +1 defect produces an inward depression while a circular +1 produces an outward elevation. The -1 defect and higher order +/- integer defects produce wrinkle patterns with out-of-plane surface deformations. By contrast, +/- half-integer defects give rise to both out-of-plane and in-plane displacements. Theoretical calculations in the limit of small strain elasticity explain these results and are compared with both FEM simulation and experimental data. [1] McConney et al, Adv Mater 25, 5880 (2013); [2] Konya et al, Front Mater 3, 24 (2016); [3] Modes et al Phys Rev E 81, 060701R (2010); [4] Babakhanova et al Nat Commun 9, 456 (2018).

*Supported by NSF DMR-1409658, NSF CMMI-1663041, and Office of Sciences DOE grant DE-SC0019105.

**11:39AM S59.00003: Multi-responsive polymeric microstructures with encoded pre-determined and self-regulated deformability***
YUXING YAO (Presenter), Department of Chemistry and Chemical Biology, Harvard University, JAMES WATERS, Chemical Engineering Department, University of Pittsburgh, ANNA SHNEIDMAN, JIAXI CUI, XIAOGUANG WANG, NIKOLAJ MANDSBERG, John A. Paulson School of Engineering and Applied Sciences, Harvard University, SHUCONG LI, Department of Chemistry and Chemical Biology, Harvard University, ANNA CHRISTINA BALAZS, Chemical Engineering Department, University of Pittsburgh, JOANNA AIZENBERG, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Dynamic functions of biological systems often rely on arrays of actively deformable microstructures undergoing a huge range of pre-determined and self-regulated reconfigurations and motions. Here, we introduce stimuli-responsive microstructures based on liquid crystalline elastomers (LCEs) that display a broad range of hierarchical, even mechanically-unfavored deformation behaviors. Using patterned magnetic fields during polymerization, we encode any desired uniform mesogen orientation into the resulting LCE microstructures, which is read-out upon heating above the nematic-isotropic transition as a prescribed deformation. By further introducing light-responsive moieties, we demonstrate multi-functionality of the LCEs with three actuation modes controlled by different external stimuli. We finally create patterned arrays of microstructures with encoded area-specific deformation modes and show their functions in responsive release of cargo, image concealment, and light-controlled reflectivity. We foresee that this platform can be widely applied in soft robotics and smart buildings.

*This material is based upon work supported by the Department of Energy under Award Number DE-SC0005247 and by the Department of Defense, Army Research Office under Award Number W911NF-17-1-0351.

**11:51AM S59.00004: Electromechanical actuation of dielectric liquid crystal elastomers for soft robotics***
ZOEY S. DAVIDSON (Presenter), HAMED SHAHSAVAN, YUBING GUO, LINDSEY HINES, Physical Intelligence, Max Planck Institute for Intelligent Systems, YU XIA, SHU YANG, Department of Materials Science and Engineering, University of Pennsylvania, METIN SITTI, Physical Intelligence, Max Planck Institute for Intelligent Systems — Liquid crystal elastomers, networks of anisotropic molecules, are two-way reversible shape memory polymers. They have long been considered as intelligent materials reminiscent of biological muscles with orientational order. Despite significant developments in chemistry, processing, and handling methods of liquid crystal elastomers, most demonstrated actuation mechanisms still rely on thermal or optical stimulation, which often suffers low efficiency of energy conversion into useful work. Here, we report fast and efficient electrical stimulation of liquid crystal elastomer actuators with high output work density for potential soft robotics applications. Different from conventional dielectric elastomers, which often require prestrain, the intrinsic elastic anisotropy in liquid crystal elastomers allows us to design complex patterns of locally aligned liquid crystal molecules. In turn, we demonstrate pre-programmed twisting, bending, and other actuations.

*ZSD and YG are supported by the Alexander von Humboldt Foundation, HS is supported by Natural Sciences and Engineering Research Council of Canada. SY also wishes to acknowledge partial support from National Science Foundation (NSF)/EFRI-ODISSEI grant, #EFRI-1331583.
12:03PM S59.00005: Programmed anisotropic transformations of cellular structures  SHUCONG LI (Presenter), GABRIELE LIBRANDI, Harvard University — The physical properties of metamaterials are controlled by the underlying material properties (molecular scale) as well as the design of the periodic structures, including shape, geometry, size, orientation, and arrangement (unit cell scale). Harnessing instabilities in soft materials based periodic structures offers an effective strategy to achieve multifunctionalities. Here, we report the programmable anisotropic transformations of cellular structures made of liquid crystalline elastomers (LCEs) on rigid substrates. By programming the mesogen alignment of liquid crystals (LC) using magnetic fields at the molecular scale, the desired anisotropies are introduced to periodic structures with different geometric designs at the unit cell scale. We demonstrate that the coupling of the two scales of controls leads to various novel deformation modes benefiting from both the mechanical guiding and the chemical guiding, which greatly broadens the design space of metamaterials. The design principle for programmed reconfigurations with prescribed anisotropies in periodic lattices is validated by both mechanics model and finite element simulation.

12:15PM S59.00006: Bioinspired design of vascular artificial muscle+ QIGUANG HE (Presenter), SHENGQIANG CAI, Mechanical and Aerospace Engineering Department, University of California, San Diego — Recently, liquid crystal elastomers (LCEs) have drawn much attention for its wide applications as artificial muscle in soft robotics, wearable devices and biomedical engineering. One commonly-adopted way to trigger deformation of LCEs is using embedded heating elements such as resistance heating wires and photo-thermal particles. To enable the material to recover to its unactuated state, passive and external cooling is often employed to lower down the temperature, which is typically slow and environmentally sensitive. Here, inspired by biology, we design and fabricate a vascular LCE-based artificial muscle (VLAM) with internal fluidic channel in which we inject hot or cool water to heat up or cool down the material to achieve fast actuation as well as recovery. We demonstrate that the actuation stress, strain and cyclic response rate of the VLAM are comparable to mammalian skeletal muscle. Because of the internal heating and cooling mechanism, VLAM shows very robust actuating performance within wide range of environmental temperature.

*The authors acknowledge support from the National Science Foundation through Grant No. CMMI-1554212 and ONR through Grant No. N00014-17-1-2056.

12:27PM S59.00007: Colloidal Micromachines Regulated by Liquid Crystals+ WYATT SHIELDS (Presenter), Harvard University, YOUNG KI KIM, Cornell University, KOOHEE HAN, NC State University, NICHOLAS ABBOTT, Cornell University, ORLIN D VELEV, NC State University — Reconfigurable microdevices have become a subject of intense interest due to their ability to harvest energy and change shape on demand. These attributes allow them to be used as robotic structures, constituents for self-healing materials, and switchable metamaterials. Yet, many of these structures are limited in utility by lack of control over their dynamics. Accordingly, much work has been done to engineer their shape, composition, and actuation as a means to control dynamics; however, little is known about regulation of their dynamics in complex fluid milieu. Here, we show how actuation of microdevices made from the assembly of patchy magnetic microcubes, which we refer to as “microbots”, can be regulated by the anisotropic viscoelastic environment of a liquid crystal (LC). We show that the elastic energy arising from the strain of LC around microbots directly influences their folding dynamics, which can be tuned by tailoring: (i) the far-field orientation of the LC and (ii) the local ordering of the LC at the microbot surfaces. These findings represent a first step towards establishing a general set of design rules to control the dynamics of actuating devices via use of anisotropic fluids.

*This work was supported by the NSF: DMR-1121107, DMR-1121288, and CBET-1604116.

12:39PM S59.00008: Programming Complex and Arbitrary Shape Changes in Liquid Crystal Elastomers+ MORGAN BARNES (Presenter), RAFAEL VERDUZCO, Rice University — Liquid crystal elastomers (LCEs) are reversible shape responsive materials that are promising for many applications including biomedical devices, microfluidic pumps and soft robotics. To date, programming complex shape changes in LCEs requires locally aligning the liquid crystals throughout the material to form a predetermined director profile. Here we demonstrate a straightforward method that does not rely on foresight of the liquid crystal director to program complex reversible shape changes. Using an optimized two-step synthesis method we mechanically deform the LCEs into arbitrary shapes between the first and second cure steps. The resulting competitive double-network LCE is capable of transitioning between its initial shape and its programmed shape when heated and cooled, respectively. We demonstrate the versatility of this method in a variety of shape changes including films capable of transforming into a flower and a face.

*The authors acknowledge support from the Welch Foundation for Chemical Research (C-1888), the Army Research Office Chemical Sciences Division (W911NF1810289), and the Shared Equipment Authority at Rice University.
complex hybrid microstructures. Exceptional agreement with experimental observations, providing insights for further development of soft solids with elastodynamics simulations at the continuum level, we demonstrate this actuation variety based on several key design factors: director orientation, pattern orientation, as well as domain and sample size. Our simulations studies show an elastodynamics simulations at the continuum level, we demonstrate this actuation variety based on several key design factors: director orientation, pattern orientation, as well as domain and sample size. Our simulations studies show an actuation behavior, going from helical twisting to chiral bending and accordion folding. By implementing finite element regions with nematic order and isotropic regions. Depending on patterning design, these materials exhibit a variety of nematic director, no theoretical studies have been made on dual-phase elastomers: samples that combine well-defined complex microstructures in the nematic director field. While most imprinted designs are based on spatial variations of the A wide variety of out-of-plane actuation behavior can be encoded in liquid crystalline polymer networks thru implementing multiple microfluidic regions with nematic order and isotropic regions. Depending on patterning design, these materials exhibit a variety of actuation behavior, going from helical twisting to chiral bending and accordion folding. By implementing finite element elastodynamics simulations at the continuum level, we demonstrate this actuation variety based on several key design factors: director orientation, pattern orientation, as well as domain and sample size. Our simulations studies show an exceptional agreement with experimental observations, providing insights for further development of soft solids with complex hybrid microstructures.

Support by NSF DMR-1409658, CMMI-1663041, CMMI-1436565, Office of Sciences DOE grant DE-SC0019105.

Electrorheological model based on liquid crystals membranes with applications to outer hair cells EDMON HERRERA VALENCE (Presenter), Chemical Engineering, FESZ-UNAM, ALEJANDRO REY, Chemical Engineering, McGill University — Liquid crystal flexoelectric actuation uses an imposed electric field to create membrane bending, this phenomenon is found in Outer Hair Cells (OHC) located in the inner ear, whose role is to amplify sound through generation of mechanical power. Oscillations in the OHC membranes create periodic viscoelastic flows in the contacting fluid media. A key objective of this work on flexoelectric actuation relevant to OHC is to find the relations and impact of the electro-mechanical properties of the membrane, the rheological properties of the viscoelastic Jeffrey's media, and the frequency response of the generated mechanical power output. When the inertia is neglected, the system follows a non-monotonically behavior in the power spectrum. This behavior is associated to the solvent contributions related to the retardation-Jeffreys mechanisms.

Acknowledgments: A.D. Rey is thankful to McGill University for financial support through the James McGill Professorship Program. EEHV is grateful for the financial support of PAPIIT and PAPIPE projects (IN115615 and PE112716) from the Government of Mexico, and to FQNRT (Merit Scholarship for Foreign Students from Ministry of Education and Higher Education, Government of Quebec).

Patterning order and disorder with an angle: Modeling dual-phase nematic elastomer ribbons VIANNEY GIMENEZ-PINTO (Presenter), Physics, Temple University, FANGFU YE, Institute of Physics, Chinese Academy of Sciences — A wide variety of out-of-plane actuation behavior can be encoded in liquid crystalline polymer networks thru implementing complex microstructures in the nematic director field. While most imprinted designs are based on spatial variations of the nematic director, no theoretical studies have been made on dual-phase elastomers: samples that combine well-defined regions with nematic order and isotropic regions. Depending on patterning design, these materials exhibit a variety of actuation behavior, going from helical twisting to chiral bending and accordion folding. By implementing finite element elastodynamics simulations at the continuum level, we demonstrate this actuation variety based on several key design factors: director orientation, pattern orientation, as well as domain and sample size. Our simulations studies show an exceptional agreement with experimental observations, providing insights for further development of soft solids with complex hybrid microstructures.

This work was supported by the Chinese Academy of Sciences (CAS) [the Key Research Program of Frontier Sciences of CAS, Grant No. QYZDB-SSW-SYS003], the National Natural Science Foundation of China (Grant No.11774394).

Design of a Novel Architecture to Improve the Performance of the Dielectric Elastomer Actuators MEHDI TORBATI (Presenter), KATIA BERTOLDI, Harvard University — This work aims to develop a geometry-based strategy to exploit the capabilities of the dielectric elastomer actuators (DEAs) for applications in soft robots. Owing to their fast response, light weight and high strain energy density, DEAs offer a remarkable actuation performance. However, the high voltage required to induce the electromechanical response not only increases the manufacturing cost it may also lead to breakdown of the material. Moreover, DEAs can only generate small amount of force that limits their applications to small scale functions. Here using the nonlinear electromechanical analysis, we optimize the arrangement of the electrodes and the applied boundary conditions to reduce the voltage required to actuate the elastomer. This naturally decreases the possibility of the electromechanical instability. Also, we propose a novel architecture which creates a snap through buckling that can be utilized for variety of functions in robotic applications.
1:39PM S59.00013: Polymer nanocomposites with reversible heat stiffening properties  SHAGHAYEGH KHANI, ELVIS CUDJOE, Case Western Reserve University, STUART J ROWAN, University of Chicago, JOAO MAIA (Presenter), Case Western Reserve University — Inspired by the defense mechanism of sea cucumber, a stimuli-responsive nanocomposite was fabricated that can reversibly increase its stiffness upon exposure to warm water. Experimentally, polymers with lower critical solution temperature (LCST) were grafted on cellulose nanocrystals embedded into a viscoelastic matrix. This material shows reversible heat-stiffening behavior analogous to sea-cucumber dermis. The stiffening behavior was hypothesized to occur due to formation of a percolating network by the nanofillers above the transition temperature. Energy Conserving Dissipative Particle Dynamics (EDPD) simulations were performed to examine the hypothesis. According to experimental data and simulation results, grafted LCST polymers disrupt the interactions between the nanocrystals below the transition temperature and upon exposure to warm water collapse of the LCST chains enhances the interactions between the cellulose nanocrystals and results in the subsequent stiffening.

1:51PM S59.00014: Dynamic Microcapsules from Complex Emulsion Drops*  JOERG WERNER (Presenter), SARAF NAWAR, BRENDAN DEVENEY, DAVID A WEITZ, Harvard University — Microcapsules are widely employed to protect and release sensitive cargo at predetermined trigger-events and rates. Since common release mechanisms involve degradation or destruction of the protective shell, their functionality is one-directional with single-use applicability. We demonstrate the fabrication of microcapsules that reversibly respond to external stimuli by changing the shell membrane's property without structural degradation, enabling the repeated and dynamic change of its permeability upon changing trigger events. The encapsulating shell in our system acts as an active gate-keeper, regulating diffusion in and out of the aqueous core compartment. I will describe microfluidic fabrication methods for complex emulsion drops and the development of a number of polymer chemistries that allow for the synthesis of trigger-responsive hydrogel shells directly around water drops without the need of sacrificial templates. The trigger responsive microcapsules are distinctly different from microgels, as the properties in microcapsules are dictated only by the state of the shell membrane that can make up less than 10% of the microparticle. The shape, size, and permeability of the microcapsules are dynamically and actively tunable with external triggers.

*NSF (DMR-1708729)

2:03PM S59.00015: Modelling discrete differential swelling in a bi-strip rolled gel  OZ OSHRI (Presenter), SANTIDAN BISWAS, ANNA CHRISTINA BALAZS, University of Pittsburgh — We derive an analytical model that allows us to quantitatively predict the features of 2D-to-3D shape changes in polymer gels that encompass different degrees of swelling within the material and thus, can model different regions of growth within the sample. Such gels can be realized, for example, by introducing variations in the cross-link density within the network or polymerizing the chains to be relatively longer in one area of the sample than another. Focusing on a bi-strip gel that swells into a "bi-roll", we determine the radii and amplitudes within a given roll, and the length of the transition layer between the two rolls. The predictions from our model agree quantitatively with available experimental data. In addition, we carry out numerical simulations that account for the complete non-linear behavior of the gel, and show good agreement between the analytical predictions and the numerical results. Models that provide quantitative predictions on the final morphology in such heterogeneously swelling hydrogels are useful not only for understanding growth patterns in biology, but also for establishing how to accurately tailor the structure of gels to meet the requirements of various technological applications.
11:15AM S60.00001: Opportunities for Doing Science at the NIST Center for Neutron Research [Invited] JOSEPH DURA (Presenter), National Institute of Standards and Technology — The NIST Center for Neutron Research, NCNR, operates a national user facility with widespread international usage providing 29 instruments, each optimized for specific measurement capabilities in a variety of disciplines including condensed matter physics, materials science, chemistry, chemical engineering, biology, geology, and others.

Several unique features give neutrons many advantages for probing condensed matter. Unlike optical and electron probes, the scattering length is not proportional to the atomic number, thus there is often good contrast for low Z, and between neighboring elements. Many elements have large isotopic differences in scattering length (notably hydrogen/deuterium and $^7$Li/$^6$Li), enabling control of contrast. Wavelengths from 0.01nm to 10nm can be used to probe length scales from the atomic to tens of microns. Neutrons directly probe magnetic features, from anti ferromagnetic order to large scaled structures such as skyrmions. Inelastic neutron scattering in which energy is exchanged with various excitation in a material enables spectroscopy of vibrational modes without selection rules and can be combined with crystallographic direction information. Neutrons are weakly interacting, enabling penetration into numerous in-operando sample environments, studies of buried structures and in some cases simpler or unique analysis, without beam damage to samples.

The NCNR has sample environments for control of temperature, pressure, magnetic field, and humidity, etc. and many relevant sample processing and pre-characterization capabilities. Users can be trained and supported by instrument scientists. An annual summer school is run to educate graduate students and others on neutron scattering techniques.

I will present an overview of the measurement capabilities available, the types of science they enable, and the modes of accessing these capabilities.

11:51AM S60.00002: Sirius, the new Brazilian Synchrotron Light Source* [Invited] HARRY WESTFAHL (Presenter), Laboratorio Nacional de Luz Sincrotron — The use of synchrotron radiation by a great variety of fields has increased steadily worldwide. This, to a large extent, is a result of the availability of the much brighter third-generation light sources, which allowed the development of new experimental techniques. Recently, new advances in accelerator technology are opening up the possibility of even brighter sources, which are being named fourth-generation light sources. Brazil gave an important contribution to science through the development of the necessary technology and the construction of the first synchrotron in the Southern Hemisphere, the Brazilian Synchrotron Light Laboratory (LNLS), still the only one in Latin America, that operates this installation as an open facility since 1997. Its pioneering activities in synchrotron science gave rise, with time, to the Brazilian Center for Research in Energy and Materials (CNPEM), a complex of four National Laboratories – LNLS itself, the Brazilian Biosciences National Laboratory (LNBio), the Brazilian Bioethanol Science and Technology Laboratory (CTBE) and the Brazilian Nanotechnology National Laboratory (LNNano). CNPEM is a research center that benefits more than two thousand researchers yearly. Sirius, the new Brazilian synchrotron light source being constructed at CNPEM, will be one of the first fourth-generation machines in the world. It will be a 3 GeV storage ring based on a five-bend-achromat (5BA) magnetic lattice that will be able to reach 250 pm.rad emittance (bare machine). It is being planned to be a state-of-the-art light source, providing cutting edge research tools that are nonexistent today in Brazil. In this talk an overview of themain characteristics, potentialities and status of the project will be provided.

Talk presented on behalf of the Sirius team.

*Sirius is funded by the Brazilian Federal Government via a contract with the Ministry of Science, Technology, Innovation and Communications.

12:27PM S60.00003: European Spallation Source: neutron scattering and technology of the XXI century [Invited] CHRISTIANE ALBA-SIMIONESCO (Presenter), European Neutron Scattering Association — TBD
The beamtime allocation is based on proposal system. There were 54 proposals in the first round. Turkey, Pakistan, Egypt, Iran and Jordan submitted the most proposals. The list also included Italy, Cyprus, Kenya, Palestine, France, Sweden, and Colombia. Most of the proposals were submitted in life sciences, chemistry, physics and materials sciences. There were also five proposals in the archeology/cultural heritage studies, indicating strong interest in this field. Half of the proposals are allocated beamtime, already putting SESAME in oversubscription form by a factor of two.

1:39PM S60.00005: New user facilities for condensed matter and material science in China [Invited] LI LU (Presenter), Synergetic Extreme condition User Facility — TBD

Thursday, March 7, 2019 11:15 AM - 2:03 PM

Session S61 GSOFT DFD: Steerable Colloids II BCEC 258B - Stefan Egelhaaf - Tag(s): Focus

11:15AM S61.00001: Role of shape and symmetry in externally driven micromotors [Invited] ALEXANDER LESHANSKY (Presenter), Technion - Israel Institute of Technology — Motion in fluids at the micrometric scale is dominated by viscosity. One efficient propulsion method relies on a weak uniform rotating magnetic field that drives a chiral object. From bacterial flagella to artificial magnetic nanohelices, rotation of a corkscrew is considered as a universally efficient propulsion gait. Although approximate theories concerning dynamics of slender magnetic helices are available, actuation of geometrically achiral particles or random aggregates was not well understood. I will present a general theory of magnetized object of arbitrary shape in a rotating magnetic field. It appears that its propulsion velocity can be written in a compact form as Rayleigh quotient in terms of geometry-dependent chirality matrix Ch, where both the diagonal elements (owing to inherent handedness) and off-diagonal entries (that do not necessitate handedness) contribute in a similar way. The theory anticipates multiplicity of stable rotational states predicting that, e.g., two identical magnetic objects may propel with different speeds or even in opposite directions. However, for a class of simple planar objects, there is particular magnetization whereas the pair of symmetric rotational states degenerates into a unique propulsion gait closely resembling that of an ideal helix. In other words, geometrically achiral object can acquire effective chirality due to its interaction with the external magnetic field. The developed theory was further applied to optimize the geometry/magnetization and to obtain purely geometric constraint on propulsion speed of arbitrary shaped magnetic object. Finally, I will discuss general symmetries (such as parity and charge conjugation) and establish correspondence between propulsive states of geometrically achiral planar objects depending on orientation of the dipolar moment.

11:51AM S61.00002: Programmable self-assembly of magnetic handshake materials* RAN NIU (Presenter), Physics Department, Cornell University, EDWARD PAUL ESPOSITO, James Franck Institute, The University of Chicago, CHRISY DU, School of Engineering and Applied Sciences, Harvard University, WEI WANG, Mechanical Engineering, Cornell University, JAKIN NG, Physics Department, Cornell University, MICHAEL PHILLIP BRENNER, School of Engineering and Applied Sciences, Harvard University, PAUL L MCEUEN, ITAI COHEN, Physics Department, Cornell University — An outstanding intellectual problem in nanoscience is the programmable self-assembly of smart, digital, and mechanically functional structures [1]. We propose to combine magnetic patterning with the design principles of molecular biology for programmable self-assembly. To be specific, we harness magnetic forces from (i) panels with a 2 x 2 pattern of magnetic domains so they bond together using specific, intelligent, interactions, analogous to Watson-Crick base pairs in DNA, and (ii) create programmed global structures, from assembly of magnetically patterned panels as well as strands that link these encoded panels in specific sequences. As a first step towards microscopic machines, we build macroscopic prototypes for proof-of-principle demonstration of information storage capability and programmable self-assembly of magnetic handshake materials.

References

*DMR-1435829

12:03PM S61.00003: Collapse dynamics of chains of paramagnetic particles: the role of the susceptibility.* HAMED ABDI, RASAM SOHEILIAN, RANDALL ERB, CRAIG MALONEY (Presenter), Northeastern University — We use computer simulations to study the dynamics of the collapse of chains of paramagnetic particles subject to rotating magnetic fields at various magnetic susceptibility. The system is initialized at constant magnetic field with particles forming chains along the field axis. The dynamics of the chains depends on the field rotation rate and, surprisingly, the particle susceptibility. At low susceptibility, and at sufficiently high field rotation rate, the particles undergo a period of chaotic motion and finally decay into a periodic orbit, consistent with previous simulations and experiments. Surprisingly, at high enough susceptibility we find a qualitatively different behavior. The initial chain state remains essentially intact for all time with the local moments strongly influenced by the orientation of the chain and less dependent on the applied field than in the low-susceptibility case. Our results should be important for applications of paramagnetic particles where rotating extended structures are desired such as micro mixing and should motivate new experiments on suspensions of paramagnetic particles in regimes of higher susceptibility.

*This material is based upon work supported by the National Science Foundation under Grant No. NSF/CMMI- 1250199.

12:15PM S61.00004: ABSTRACT WITHDRAWN

12:27PM S61.00005: Hurricane dynamics in a membrane NAOMI OPPENHEIMER (Presenter), MICHAEL JOHN SHELLEY, Center for Computational Biology, Flatiron Institute — We study driven microscopic rotors immersed in a membrane. We show that for small distances, interactions between rotors are identical to interactions between vortices in an ideal 2D Euler fluid, while the longer-ranged ones relate to classical models of atmospheric dynamics. Going beyond idealized interactions between rotors, we examine the more realistic setting where rotors also interact through local repulsion. We show that initially random distributions of rotors will rapidly self-organize into rotating uniform lattices or random hyperuniform structures, and exhibit activity-induced phase separation.

12:39PM S61.00006: Optically driven birefringent rotators ALVIN MODIN (Presenter), MATAN YAH BEN ZION, MELISSA FERRARI, MARK D HANNEL II, PAUL M CHAIKIN, New York University — We use circularly polarized light to induce stable rotation in hundreds of colloidal micro-particles simultaneously. The optical angular momentum transferred to the particles creates a torque causing particle rotation. In the past, optical tweezers were used to rotate individual colloids while trapping them to the narrow waist of the focused beam. We use a defocused, circularly-polarized, beam to rotate multiple particles with minimal trapping. We developed a process for synthesizing stable birefringent vaterite particles that can rotate for long periods of times and characterized their optical and physical properties. Altering the handedness and intensity of the laser source allows us to control the frequency and switch between clockwise or counterclockwise rotation. We observe and discuss the interaction between the rotating particles.
12:51PM S61.00007: Light-driven capillary assembly and motion of hydrogel nanocomposite disks at the air/water interface

HYUNKI KIM (Presenter), JI-HWAN KANG, YING ZHOU, ALEXA KUENSTLER, TODD EMRICK, RYAN HAYWARD, University of Massachusetts Amherst — Modulation of capillary forces by active changes in shape is an approach used by a number of insects to achieve propulsion at air-water interfaces. Learning from nature, we have designed light-responsive sub-millimeter hydrogel disks that exhibit: (1) attraction, leading to formation of well-defined assemblies; (2) repulsion; or (3) sustained rotation, depending on the pattern of illumination. Fabrication of light-responsive hydrogel disks containing patterned gold nanoparticles (Au NPs) was achieved by photo-chemical reduction of Au$^{3+}$ ions to metallic Au NPs within micro-patterned temperature-responsive hydrogels. Photothermal deswelling of illuminated Au NP-containing hydrogel regions induced out-of-plane buckling and deformation of the air/water interface, with a characteristic response time of seconds. This provided a versatile means to control capillary interactions in both time and space, thereby leading to a diverse range of behaviors at the air/water interface.

*ARO W911NF-16-1-0119
NSF-CHE 1506839

1:03PM S61.00008: Controlling Colloidal Assembly through Optical Binding

DUSTIN KLECKNER (Presenter), DOMINIQUE DAVENPORT, University of California, Merced — Directed assembly of colloidal particles has attracted considerable interest from both a fundamental and applied perspective. Most approaches to colloidal self-assembly use short range forces, e.g. via patchy or shaped particles. As an alternative, I will discuss the possibility of using 'optical binding' - a long range inter-particle force generated by multiple light scattering - to control the assembly of particles via a tunable external field. Although this approach has many advantages in principle; significant experimental and modelling work is required to make this a practical approach. I will discuss our efforts in both directions.

*This work was supported by a grant from the Hellman Fellows Fund.

1:15PM S61.00009: Observations of Optically Bound Colloidal Assemblies

DOMINIQUE DAVENPORT (Presenter), DUSTIN KLECKNER, University of California, Merced — In recent years there has been growing interest in assembling complex structures from colloidal suspensions for use in both fundamental and applied studies. We are exploring a relatively new and highly tunable inter-particle colloidal force known as the optical binding force. The optical binding force is mediated by light scattering between two or more particles in an intense optical field which can be externally modified. We use experimental methods to impose this optical binding force onto clusters of dielectric colloidal particles. We will discuss unique behaviors that arise from this force, including the formation of multiple extended particle chains and formation of planar arrays.

*This work was supported by the Hellman Fellows Fund.

1:27PM S61.00010: Harnessing Complex Fluid Interfaces to Control Colloidal Assembly and Deposition

XIN YONG (Presenter), MINGFEI ZHAO, WILSON LUO, Mechanical Engineering, Binghamton University — Using lattice Boltzmann-Brownian dynamics (LB-BD) simulations, we model large-scale assembly of nanoparticles on liquid-vapor interfaces with complex geometries and investigate subsequent deposition upon complete evaporation. Particles aggregate into hexagonally close-packed monolayers on flat and spherical interfaces given appropriate value of the interaction parameter that couples fluid hydrodynamics and discrete particle dynamics. Detailed force analysis reveals a long-range attraction between particles, mimicking capillary interactions due to interface disturbance. On curved fluid interfaces with complex curvature fields, the particle dynamics is governed by pair capillary interactions and curvature-induced capillary migration. We develop a minimal theoretical model to predict equilibrium particle distribution on non-evaporating curved interfaces, which agrees well with simulation observation. Finally, we demonstrate that the interplay between evaporation-induced convective flow, particle pair interaction, and curvature-particle interaction results in distinct deposition patterns, which were obtained by using curved fluid interfaces as templates.

*U.S. National Science Foundation Grant No. CMMI-1538090
1:39PM S61.00011: Interstitial Particle Design for Active Colloidal Microstructures*  BRYAN VANSADERS (Presenter), Materials Science and Engineering, University of Michigan, SHARON GLOTZER, Chemical Engineering, University of Michigan — Defect microstructures in colloidal crystals can be viewed as complex localized motifs, distinct from the environments present throughout the bulk of the crystalline phase. These motifs are persistent sites which interstitial particles can adsorb onto and be trapped by. The degree to which interstitial particles are bound to the vicinity of defects can be explored as a function of particle geometry. We present here a method to maximize the strength of the preferential interaction that a rod-like interstitial experiences with defect microstructures that include edge dislocations. We show that for sufficiently strongly bound interstitials, microstructural migration can be induced by applying forces to the designed particle, making it active. This approach opens up many possibilities for dynamically manipulating the microstructure of colloidal crystals, with applications in shape changing colloidal assemblies. Furthermore, the line-like nature of dislocations permits widely separated interstitials to be connected, correlating their transport properties in a manner not typically possible with local particle interactions.

*National Science Foundation, Division of Materials Research Award # DMR 1409620

1:51PM S61.00012: Maze-solving via diffusiophoresis*  TANVI GANDHI (Presenter), University of California, San Diego, SOPHIE RAMANANARIVO, LadHyX, ANTOINE AUBRET, MASSIMO VERGASSOLA, JEREMIE PALACCI, University of California, San Diego — Mazes provide a simple model for many frequently-occurring structures and phenomena (e.g. human circulatory system, traffic in a city). It is often of interest to find the most efficient path in a maze (e.g. in order to transport materials). The problem of maze-solving poses a mathematical challenge: most analytic solutions can become computationally demanding as mazes become more complex, often relying on brute-force methods that involve exploring multiple paths before arriving at the solution. In this work, we present a novel method of solving the problem by exploiting the diffusiophoretic motion of colloids in a maze. We demonstrate our method experimentally via a microfluidic maze.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1554724. J.P. thanks the Sloan Foundation for support through grant FG-2017-9392.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S62 DCMP: Nematic Order and Correlated Electrons in Iron Pnictides and Chalcogenides  BCEC 258C - Ming Yi - Tag(s): Invited

11:15AM S62.00001: Local orthorhombic lattice distortions in the paramagnetic tetragonal phase of superconducting NaFe$_{1-x}$Ni$_x$As*  [Invited]  PENGCHENG DAI (Presenter), Department of Physics and Astronomy, Rice University — Understanding the interplay between nematicity, magnetism and superconductivity is pivotal for elucidating the physics of iron-based superconductors. Here we use neutron scattering to probe magnetic and nematic orders throughout the phase diagram of NaFe$_{1-x}$Ni$_x$As, finding that while both static antiferromagnetic and nematic orders compete with superconductivity, the onset temperatures for these two orders remain well separated approaching the putative quantum critical points. We uncover local orthorhombic distortions that persist well above the tetragonal-to-orthorhombic structural transition temperature $T_s$ in underdoped samples and extend well into the overdoped regime that exhibits neither magnetic nor structural phase transitions. These unexpected local orthorhombic distortions display Curie-Weiss temperature dependence and become suppressed below the superconducting transition temperature $T_c$, suggesting that they result from the large nematic susceptibility near optimal superconductivity. Our results account for observations of rotational symmetry breaking above $T_{s}$, and attest to the presence of significant nematic fluctuations near optimal superconductivity.

*The single crystal growth and neutron scattering work at Rice is supported by the U.S. DOE, BES under contract no. DE-SC0012311 (P.D.). A part of the material’s synthesis and characterization work at Rice is supported by the Robert A. Welch Foundation Grant Nos. C-1839 (P.D.) and C-1818 (A.H.N.). A.H.N. also acknowledges the support of the US National Science Foundation Grant No. DMR-1350237.
**11:51AM S62.00002: Orbital-selective correlations and superconductivity in the nematic FeSe** [Invited] JIAN-XIN ZHU (Presenter), Los Alamos National Laboratory, HAOYU HU, Rice University, RONG YU, Renmin University of China, EMILIAN NICA, University of British Columbia, QIMIAO SI, Rice University — The interplay between electronic orders, orbital-selective electronic correlations and associated superconductivity, has played a central role in the physics of emergent phases and unconventional superconductivity. This interplay has been found to be particularly pronounced in recently discovered iron-based superconductors. Motivated by the recent low-temperature experiments on iron selenide (FeSe), we theoretically study the electronic correlation effects and emerging superconductivity in a multiorbital model for this compound. We propose that the combination of various bond nematic orders with the ferro-orbital order can give rise to a surprisingly large orbital selectivity among the Fe-3d t2g orbitals in the normal state. This enhanced orbital selectivity is also reflected in the superconducting pairing amplitudes, which gives rise to a large gap anisotropy on the Fermi surface. Our results naturally explain the seemingly unusual observation of strong orbital selectivity and related unconventional superconductivity in the nematic phase of FeSe, thereby providing new insight into the nature of both the nematic order and the iron-based superconductivity in general.

*This work has in part been supported by the National Science Foundation of China Grant numbers 11674392 and Ministry of Science and Technology of China, National Program on Key Research Project Grant number 2016YFA0300504 (R.Y.), and by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0018197, the Robert A. Welch Foundation Grant No. C-1411 and a QuantEmX grant from ICAM and the Gordon and Betty Moore Foundation through Grant No. GBMF5305 (Q.S.), and by the U.S. DOE Office of Basic Energy Sciences E3B5 (J.-X.Z.).

**12:27PM S62.00003: Orbital selective magnetism, nematicity, and fluctuations in FeSe** [Invited] RUDOLF HACKL (Presenter), ANDREAS BAUM, Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, HARRISON N RUIZ, Stanford University, NENAD LAZAREVIC, Institute of Physics Belgrade, YAO WANG, Harvard University, THOMAS U BOEHM, Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, THOMAS WOLF, Karlsruhe Institute of Technology, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford University — Iron pnictides and chalcogenides have rich phase diagrams displaying superconductivity, nematic and spin density wave order, fluctuations and short-range magnetism. Yet, the magnetism observed in FeSe, for instance, is not necessarily of the same type as that in the pnictides since the typical nesting conditions of the Fermi surfaces are much less robust in the chalcogenides and the question as to strong versus weak coupling magnetism arises. Raman scattering experiments afford a window into the type of ordering and allow one to distinguish between itinerant and localized magnetism. We show how the response from a weakly coupled itinerant system can be distinguished from that of a Heisenberg-type localized magnet. We present results of light scattering experiments as a function of polarization and temperature. In the pnictides the Raman spectra display all features of a spin density wave while the spectra of FeSe are similar to those of systems with localized spins such as the cuprates. Our numerical simulations using exact diagonalization of a 4x4 cluster reproduce the experiments semi-quantitatively in the limit of a nearly frustrated spin-1 Heisenberg model (localized spins), in particular the low energy peak in B1g symmetry. The results indicate that the electrons in some of the orbitals are more localized in FeSe than in the pnictides and reopen the discussion on the type of nematic fluctuations observed recently.

*Work in Europe was supported by the DFG via SPP 1458 and TRR80, by the Serbian Ministry of Education, Science and Technological Development (Project III45018), by the DAAD, and by BaCaTeC. Work in the SIMES at Stanford University and SLAC was supported by the U.S. DOE, Office of Basic Energy Sciences (DE-AC02-76SF00515) and Office of Science (DE-AC02-05CH11231).

**1:03PM S62.00004: ARPES probe of the electronic structure in the detwinned FeSe** [Invited] DONGHUI LU (Presenter), SLAC National Accelerator Laboratory, Stanford University — TBD
Intertwined and vestigial electronic phases in hole-doped Sr$_{1-x}$Na$_x$Fe$_2$As$_2$ [Invited]  
CHRISTOPH MEINGAST (Presenter), Karlsruhe Institute of Technology — Hole-doped ReFe$_2$As$_2$ (Re = Ba, Sr, Ca) exhibit much richer phase diagrams than the corresponding electron-doped systems. In particular, the phase diagram of Na-doped BaFe$_2$As$_2$ exhibits a small pocket of a double-Q reentrant C4 magnetic phase [1], as well as another yet unidentified magnetic phase [2]. In strong analogy with the charge order observed in underdoped cuprates [3], these additional phases compete strongly with the emerging superconducting order [2,4].

Here we present a detailed phase diagram of the Na-doped SrFe$_2$As$_2$ system using thermodynamic probes (heat capacity, thermal expansion and magnetization). The double-Q C4 reentrant phase is much more stable in this system, and our data demonstrates that the phase diagram of Na-doped SrFe$_2$As$_2$ exhibits even more complexity than the K- and Na-doped BaFe$_2$As$_2$ counterparts.


Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S63 DBIO GSNP: Statistical Physics of Large Populations of Cells: from Microbes to Tissues II

11:15AM S63.00001: Modeling the Solid-Fluid Transition in Ordered Biological Tissues* [Invited]  
PREETI SAHU (Presenter), Syracuse University, JANICE KANG, Hamilton College, GONCA ERDEMCI-TANDOGAN, M. LISA MANNING, Syracuse University — Biological functionality of tissues relies on its rheology. Fluidity of a 2D non-proliferating confluent tissue is contingent on cellular rearrangements which are called T1 transitions. In a 2D vertex model for disordered tissues, the tissue fluidizes when the T1 energy barriers disappear as the target shape index approaches a critical value (~3.81) [Bi 2015]. The linear response also becomes fluidlike (i.e. the shear modulus vanishes) at this same value. However, shear modulus of ordered ground states of 2D vertex models vanishes at a lower value (3.72) [Farhadifar 2007, Staple 2010]. Therefore, an interesting open question is whether the ground states of the 2D vertex model are fluid-like or solid-like between 3.72 and 3.81. In other words, does the “equation of state” for these systems have two branches (like glassy particulate matter) or only one? Using four-cell and many-cell numerical simulations, we demonstrate that for a hexagonal ground state, T1 energy barriers vanish only at ~3.81, indicating that ordered systems have the same critical point as disordered systems. We also develop a simple geometric argument that predicts the correct scaling of energy barriers with T1 edge length in these systems.

*This work was partially supported by NSF-PHY-1607416 and NSF DMR-1757749.

11:51AM S63.00002: Cell size regulation induces sustained oscillations in the population growth rate  
FARSHID JAFARPOUR (Presenter), Physics and Astronomy, University of Pennsylvania — There are negative correlations between the generation time of a biological cell and those of its descendants. If a cell grows for a longer time than expected, its daughter cells will be larger at birth and have to compensate for their sizes by dividing slightly earlier than expected. Otherwise, the noise in the generation times would accumulate over generations in the size of the cells, leading to extremely large cells. This process is known as cell size control. In this talk, I discuss the effect of these correlations on the dynamics of population growth of microorganisms. I show that any non-zero correlation that is due to cell-size control can induce long-term oscillations in the population growth rate. The population only reaches its steady state due to the often-neglected variability in the growth rates of individual cells. The relaxation time scale of the population to its steady state is determined from the distribution of single-cell growth rates independent of the details of the division process or the cell-size regulation. I propose an experimental method to measure single-cell growth variability by observing how long it takes for the population to reach its steady state, a measurement that is significantly easier and less biased than single-cell measurements.
12:03PM S63.00003: Cell-level mechanical heterogeneity promotes rigidity in confluent tissues  XINZHI LI (Presenter), DAPENG(MAX) BI, Northeastern University — Intra-tumor heterogeneity is one of the hallmarks of cancer, which describes the phenotypic differences among cells in a tumor or cellular collective. While genetic heterogeneity has been an intense focus of study, how mechanical variations among cells influence tissue mechanics is not well understood. Here, we investigate the effect of cell-to-cell mechanical heterogeneity on the overall bulk mechanics of a confluent 2d tissue using a vertex model-based approach. We find that the rigidity of a confluent tissue depends on overall statistical properties of single-cell properties such as mean and variance, rather than the specific functional form of its distribution. A single universal parameter - the fraction of mechanically rigid cells, $f_r$, can be used to characterize the tissue mechanical state. As $f_r$ is tuned, the tissue undergoes a rigidity percolation at a critical threshold of $f_r$. Remarkably, this rigidity percolation occurs at a much lower value than what is required for rigid-cell to form a spanning cluster. A mean field model is proposed to explain the discrepancy between rigidity and contact percolations.

12:15PM S63.00004: How diverse forms of phenotypic variability affect microbial growth in changing environments*  ETHAN LEVIEN (Presenter), ARIEL AMIR, School of Engineering and Applied Sciences, Harvard University, JANE KONDEV, Department of Physics, Brandeis University — Numerous organisms utilize phenotypic variability to hedge their bets against unpredictable environmental changes. In microbiology, the most well-studied example of this is bacterial persistence — the phenomenon by which some fraction of the population grows relatively slowly in exchange for decreased susceptibility to antibiotics. Experimental evidence suggests a distribution of many phenotypes, not just two growth states, plays a role in bacterial growth, yet the quantitative consequences of more general forms of phenotypic variability are not well understood. Here we model various forms of phenotypic variability in changing environments, including deterministic variability arising from asymmetric segregation at cell division, to stochastic variability resulting from noisy gene expression. In our model, single-cell growth rates are functions of the phenotype and the environmental state. We derive conditions on these functions that guarantee phenotypic variability will be beneficial to a population.

*Funding was provided by Simons Foundation (Award ID: 400108)

12:27PM S63.00005: Grow or Go? Studying fitness of cell populations using a mathematical model  NOAH REUTER (Presenter), MOUMITA DAS, School of Physics and Astronomy, Rochester Institute of Technology — In nature, no organism lives in an isolated environment. Competition between different organisms is a fact of life, and we are familiar with the famous phrase “Survival of the fittest” as the principle behind natural selection. But what factors decide whether one organism is more fit than another? Similar questions can be asked about cell populations. For a long time “evolutionary fitness” was thought to be simply determined by the rate at which an organism (or cell) reproduced. Recent studies have, however, questioned this view, and have suggested fast migration and invasion as a competing mechanism to fast reproduction. It has been observed that many types of cells and organisms favor either growth and proliferation, or rapid and distant migration. This is referred to as the grow or go hypothesis. We test this hypothesis using a computer simulation of populations of two types of cells, modeled as active, interacting particles. The two cell types have different self-propulsion speeds, and different rates of proliferation and death. The simulation assumes that the faster cells divide at slower rates and have shorter life spans. We investigate the migration and phase separation in this system and look to see which population is more successful in reaching the periphery.

12:39PM S63.00006: Statistics of single cell trajectories in a bacterial swarm  N. S. KARTHIK SOMAYAJI (Presenter), HARSHITHA SHANKAR KOTIAN, AMITH Z. ABDULLA, Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India, SHALINI HARKAR, Robert Bosch Centre for Cyber Physical systems, Indian Institute of Science, Bangalore, India, VARSHA SINGH, Molecular Reproduction, Development and Genetics, Indian Institute of Science, Bangalore, India, MANOJ M. VARMA, Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India — In our work, we analyse the microscopic characteristics of the motion of individual bacterial cells in an advancing bacterial swarm consisting of over 10 million individuals. Statistical analysis of single cell trajectories in the swarm reveals a correlated random walk with a mean growth direction. The trajectory length of the random walk was found to obey a log-normal distribution. The distribution of turning angles revealed an interesting situation with a Gaussian hump centred around zero over a uniform background. The peak in the distribution of turning angles could be reasonably fitted to a truncated normal distribution. The background (angles from [-180, -100] and its mirror [100, 180]) displayed a uniform distribution. Such a distribution can be thought of as arising from a weakly biased random walk where the bias provides the global mean direction of the swarm while the overall uniform background arises from the Brownian (unbiased) portion. The bias results in finite correlation of the current direction with the previous direction resulting in the Gaussian hump centred around zero. The observed statistics of motion at the microscopic level can thus predict the mean directed swarm motion.
12:51PM S63.00007: Big data of big tissues: deep neural networks to accelerate analysis of collective cell behaviors in large populations  JULIENNE LACHANCE (Presenter), DANIEL COHEN, Princeton University — Coordinated cellular motion is crucial for proper tissue organization and function. Biophysical statistics of group behaviors can provide key insights into these behaviors, such as detecting pathological changes. Applying statistical analyses to very large tissues (>50,000 cells) offers exciting potential but requires more versatile feature extraction approaches. Convolutional neural networks are increasingly promising for tasks such as object classification and segmentation (e.g., cells, phenotypes). In this study, we apply a U-Net style architecture for label-free nuclei detection using low-magnification, transmitted light imaging. We utilize UV-excited nuclear labels to achieve automatic annotation of the data. The benefits of label-free image segmentation with transmitted light microscopy are numerous: improved accessibility by allowing for feature extraction without fluorescence imaging; eliminating the phototoxicity that results from typical UV-excited nuclear labels; and unambiguous, rapid post-processing of massive datasets. Here, we assess the accuracy of the reconstructed nuclei, and present preliminary data using this tool to explore cellular distribution and migration statistics (e.g., order, neighbor arrangements, correlations) in large, complex tissue geometries.

1:03PM S63.00008: Effects of curvature and topology on collective cell migration in dense biological tissues  MARGHERITA DE MARZIO (Presenter), Harvard Medical School, JEFFREY FREDBERG, Harvard T.H. Chan School of Public Health, DAPENG BI, Northeastern University — Confluent epithelia line every organ surface and body cavity. The epithelial tissue typically remains quiescent and non-migratory while performing its routine barrier and immune functions but becomes dynamic and migratory during morphogenesis, repair, invasion and metastasis [1]. To model these processes, recent progress has been made using agent-based simulations [2] of multicellular behavior grown in cultures on flat space [3,4]. However, native epithelia typically comprise curved surfaces, such as embryos, and respiratory bronchioles, airways, intestines and embryos. On such curved geometry out-of-plane mechanical forces can influence cytoskeletal organization, cell-cell interaction and thus could influence migration and development. Here, we develop an agent-based cellular model to simulate the collective behavior on curved surfaces, such as spheres, ellipses and tubular structures. We explore how the curvature alters the nature of unjamming and glass transitions in tissues and how topological defects introduce new motion patterns.

[1] Sadati, M et al., Differentiation 2013

1:15PM S63.00009: Failure Propagation in Cooperating Multicellular Systems*  DERVIS CAN VURAL (Presenter), PINAR ZORLUTUNA, University of Notre Dame — From microbial communities to eukaryotic tissues, biological function often hinges on the exchange of diffusing cooperative factors and public goods. When stressors or statistical fluctuations compromise the population locally, this leads to an interruption of these exchanges near by and creates a cascade of failures. Here we present analytical results on how failure propagates through a multicellular system right before its catastrophic end. We find that the failure of the system progresses on two fronts; through the propagation of a wave from the surface inwards, and simultaneously, a decay of the bulk that may or may not finalize with a sudden collapse. We obtain formulas governing the population dynamics and failure propagation velocity, and fit some of these findings to experimental measurements.

*This material is based upon work supported by the National Science Foundation under grant no. CBET-1805157

1:27PM S63.00010: Power-law distributions of T-cell clone abundances in a non-neutral birth-death-immigration model  RENAUD DESSALLES (Presenter), Biomathematics, UCLA, MARIA R D’ORSOGNA, Mathematics, CalState Northridge, THOMAS CHOU, Mathematics, UCLA — T-cells can then die or proliferate to produce new T-cells carrying the same receptor. This process can be described by a stochastic multitype birth-death-immigration (BDI) process. However, predictions of a simple neutral BDI process, where cells of all receptor types have the same immigration, birth, and death rates, do not reproduce the experimentally measured power-law clone size distributions. However, it is known that T-cell proliferation depends on its specific affinity to self-ligands and T-cells of certain receptors are more likely to be produced in the thymus. Here, we study a non-neutral BDI model, in which each clone has a specific immigration rate and a specific peripheral proliferation rate arising from different ligand affinities. Realistic distributions of immigration rates are generated from measured DNA, while hypothetical distributions of proliferations rates are tested. We also include a carrying capacity through the death rate to model the competition of lymphocytes for cytokines and to ensure homeostasis of the system. The effects of sampling of T-cells from an organism are also calculated. We show that a non-neutral model with sampling can describe the experimentally observed clone size distributions provided the appropriate T-cell heterogeneity is employed.
**1:39PM S63.00011: Extreme value analysis of gut microbial alterations in colorectal cancer**  
STEPHANIE SONG (Presenter), Wellesley College, PATRICIO JERALDO, JUN CHEN, NICHOLAS CHIA, Mayo Clinic — Gut microbes play a key role in colorectal carcinogenesis, yet reaching a consensus on which microbes remains challenging in part due to reliance on mean value estimates. We present an extreme value analysis for overcoming these limitations. By characterizing a power law fit to the relative abundances of microbes, we capture the same microbial signatures as more complex meta-analyses. Importantly, we show that our method is robust to the variations inherent in microbial community profiling and point to future directions for developing sensitive, robust analytical methods.

*This work was supported an NIH grant (R01 CA 179243) as well as the Arnold and Mabel Beckman Foundation and Patterson Funds from the Neuroscience Program at Wellesley College.

**1:51PM S63.00012: Characterization of Swarmer Cell Differentiation in *Proteus mirabilis***  
EMRAH SIMSEK (Presenter), MINSU KIM, Emory University — Some bacteria translocate across quasi-solid surfaces via a multicellular type of motility called swarming. Swarming is performed by highly elongated and hyperflagellated differentiated swarmer cells. It is known that swarmer cell differentiation occurs upon surface contact. However, cellular and environmental factors affecting swarmer cell differentiation remain poorly understood. Here, we studied swarmer cell differentiation in *Proteus mirabilis*. We found that swarmer differentiation occurs abruptly at a critical cell density. In order to understand this tight regulation, we have analyzed the gene regulatory network controlling the expression of the master regulator *flhDC*. Interestingly, our single-cell-level experiments show that both initiation of and commitment to differentiation are stochastic. Our efforts to mechanistically bridge this single-cell-level stochasticity in differentiation and its population-level tight regulation will also be discussed.

**2:03PM S63.00013: Optimal segregation of proteins: phase transitions and symmetry breaking**  
JIE LIN, JISEON MIN (Presenter), ARIEL AMIR, Harvard University — In stressed environments, microbial cells such as bacteria or yeast utilize various mechanisms to survive. One important mechanism is the asymmetric segregation of key proteins at cell division, placing one of the two daughter cells in a more favorable condition. We provide a general framework to describe the evolutionary origin of this asymmetric segregation. We compute the population fitness as a function of the protein segregation asymmetry $a$ and show that the value of $a$ which optimizes the population growth manifests a phase transition between symmetric and asymmetric partitioning phases. Surprisingly, the nature of phase transition is different for the case of beneficial proteins as opposed to deleterious proteins: a smooth (second order) transition from purely symmetric to asymmetric segregation is found in the former, while a sharp transition occurs in the latter. Our study elucidates the optimization problem faced by evolution in the context of protein segregation and motivates further investigation of asymmetric protein segregation in biological systems.

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**Thursday, March 7, 2019 11:15 AM - 2:15 PM**

**Session S64 DBIO: Robophysics: Robotics Meets Physics I**  
BCEC 259B - Chen Li, Johns Hopkins University - Tag(s): Undergraduate

**11:15AM S64.00001: Importance of body and leg adjustment for traversing cluttered terrain**  
YAQING WANG (Presenter), RATAN SADANAND OTHAYOTH MULLANKANDY, CHEN LI, Johns Hopkins University — Although robots are good at avoiding obstacles, in critical applications like search and rescue in cluttered terrain like earthquake rubble, they must traverse obstacles using effective physical interaction, an ability still missing from most robots. Here, we study how the ability to adjust body parts and legs contributes to cluttered terrain traversal using animal and robophysical experiments. To traverse grass-like beams, cockroaches adjusted their head, body, abdomen, and legs in coordination. As the animal pushed against the beams, its body pitched up due to terrain interaction. In response, the animal flexed its head repeatedly to reduce body pitching and physically feel out the terrain. In addition, the animal used two hind legs differentially, extending and depressing one more than the other ($P < 0.05$, ANOVA), to roll its body to align with the gap between beams to reduce terrain resistance. Finally, the animal pushed the lower hind leg backward on the ground to propel itself forward while flexing its abdomen to break body rubbing against beams. We developed a robot with the ability to flex its head and abdomen and differentially move its legs and used it as a physical model to study the principles of using reactive motions to modulate physical interaction to traverse.
11:27AM S64.00002: JUMP: Experiment-enabled Modeling of Click Beetle Jumps for Robotic Applications  
OPHELIA BOLMIN (Presenter), LIHUA WEI, University of Illinois at Urbana-Champaign, JAKE J SOCHA, Virginia Tech, MARIANNE ALLEYNE, ALISON DUNN, AIMY A WISSA, University of Illinois at Urbana-Champaign — Click beetles use a unique jumping maneuver to self-right without using their legs. The jump is power-amplified thanks to a hinge situated in the thoracic region. The hinge is composed of a peg and a mesosternal lip, two conformal parts that allow the body to be locked in an arched position before the energy-release phase, which results in a jump. The jump of the beetles is divided into three stages: the pre-jump (latching), take-off (snapping), and airborne (jump) stages. In this paper, we present data extracted from synchrotron x-rays experiments at Argonne National Laboratory. High-speed video recordings (1,000 – 30,000 fps) show the latching phase, the contraction of soft cuticle prior to energy release, and the quick snapping maneuver. To describe the latching and snapping phases of the jump, we integrated experimental and morphological data into new analytical models. A combined mechanical/friction model predicts the initiation of slip between the peg and lip, and a dynamic force analysis model calculates the center of mass accelerations and required torques at the hinge. Understanding the enabling physics of the three jump stages creates numerous opportunities for engineering applications including self-righting robots and power-amplifying actuation systems.

11:39AM S64.00003: A Robophysical Analysis and Gait Development for the NASA Resource Prospector Rover  
SIDDHARTH SHRIVASTAVA (Presenter), ANDRAS KARSAI, YASEMIN OZKAN AYDIN, VERONICA PAEZ, Georgia Institute of Technology, WILLIAM BLUETHMANN, ROBERT O. AMBROSE, NASA Johnson Space Center, DANIEL GOLDMAN, Georgia Institute of Technology — Planetary rovers can become entrapped in soft substrates. The LCROSS lunar mission in 2009 indicated that regolith was less consolidated at the lunar poles than the equator. This led NASA JSC to develop RP-15, a 300 kg rover capable of lifting and sweeping each wheel to develop a crawling behavior. To discover techniques to improve performance, we created a scaled (2.1 kg) robophysical rover, conducting systematic experiments in our autonomous tilting, aerating, and motion capture gantry apparatus. A combination of stepping and wheel rolling produced higher drawbar-pull than wheel rotation alone in any situation (~4x increase on a 0° poppy incline). We validated our findings through experiments on RP-15 at JSC (~2x on a 0° sand incline). On steeper slopes (up to 27°, near max angle of stability), a novel gait generated forward progress via terrain remodeling via controlled avalanches. Rolling front wheels led to substrate mound formation posterior to the rover with stepping/paddling hind wheels generating forward progress; the wheel-only and walking-only gaits led to backward progress. Single paddling/rolling wheel force measurements showed a 2x increase in normal force per gait cycle over pure rolling. Our discoveries generalize to weakened (via aeration) and wet granular media.

11:51AM S64.00004: Micro and nanorobots propelled by science  
JOHANNES SACHS, PEER FISCHER (Presenter), Micro Nano Molecular Systems, Max Planck Institute for Intelligent Systems — Nature has evolved many microorganisms that operate without neurons, yet exhibit remarkably complex behaviors. These are examples of autonomous machines whose function and interaction with the environment is entirely governed by the chemistry and physics at small scales. Since consciousness plays no role, there is thus no fundamental reason why we should not also be able to build and operate analogous synthetic microrobots. One key ingredient is the ability to synthesize and engineer complex 3D parts and ways to organize or assemble these components. Another challenge is to provide energy for activation, which calls for strategies that are entirely different to the many engineering solutions that have been devised at large scales. This talk will describe our efforts in realizing such systems — some with outside control, others that are entirely autonomous — at the smallest of scales.

12:03PM S64.00005: Kirigami pop-up spikes improve soft robot anchoring and locomotion under soil  
BANGYUAN LIU (Presenter), Mechanical Engineering, Georgia Institute of Technology, YASEMIN OZKAN AYDIN, DANIEL GOLDMAN, Physics, Georgia Institute of Technology, FRANK L HAMMOND III, Mechanical Engineering, Georgia Institute of Technology — Earthworms can move beneath soil by expanding parts of their bodies radially; bristles called chetae can work as anchors during surface locomotion but their efficacy during subsurface movement is unknown. We designed a soft, worm-like robot which models the putative earthworm anchoring mechanisms by combining Kirigami skin with radially-expanding pneumatic actuators. The robot consists of three pneumatic actuator segments: head and tail segments that expand radially as anchors, and a middle segment that elongates body. The Kirigami structure pops up when an actuator is radially expanded, forming bristle-like spikes, which penetrate the soil and improve the anchoring ability of segment. Improvements in anchoring are studied by measuring the differences in segment drag forces beneath soil. The performance of robot locomotion in soil terrain with or without Kirigami skin was measured in several terrain conditions (within a wet garden soil channel, buried in wet garden soil, and buried in sand) as the robot dragged payloads behind it. The Kirigami skin-covered robot exhibits a greater maximum drag force (improved from 0.43N to 1.35N), greater forward displacement per gait cycle, and higher traction (e.g., with an 80g payload, the 1.11cm/gait cycle improved to a 2.18cm/gait cycle).
12:15PM S64.00006: The use of robophysical mantis shrimp models to study ultra-fast "impulsive" biological an
synthetic systems*  EMMA STEINHARDT (Presenter), ROB J WOOD, Harvard University — Peacock mantis shrimp are
considered the fastest strikers in the animal kingdom, achieving punches in the range of 14-23 m/s in water – fast enough
to create cavitation bubbles and break clam shells. They accomplish this with a dactyl heel striking appendage only a few
centimeters long. In order to study these remarkable capabilities, we leverage recent breakthroughs in multi-scale, multi-
material rapid fabrication to create a physical model of the mantis shrimp at scale. The rapid release of energy storage is
accomplished through a torque reversal mechanism with a spring in parallel. Our preliminary design is capable of
achieving a 15.5 m/s peak velocity, 67.4% the peak velocity of biological mantis shrimp. We're able to demonstrate the
formation of cavitation bubbles in striking, and can produce peak forces of 100 N. Our analytical dynamic model is capable
of accurately predicting the trajectory and peak velocities of our current design. We will present designs using our model
that maximize velocity. Our simulation results will be accompanied by our experimental results for various fluid loads and
design parameters. These results will then be used to inform us on how the biological system operates and how the
underlying physics contribute to its performance.

*Army Researh Office

12:27PM S64.00007: Coordination of legs and body undulation during turning in quadruped locomotion  BAXI
CHONG (Presenter), YASEMIN OZKAN AYDIN, School of physics, Georgia Tech, GUILLAUME SARTORETTI, Carnegie Mellon
University, JENNIFER RIESER, School of physics, Georgia Tech, HAOSEN XING, CHAOHUI GONG, HOWIE CHOSET, Carnegie Mellon
University, DANIEL GOLDMAN, School of physics, Georgia Tech — Sprawled-postured quadrupeds like lizards and salamanders
must coordinate limb with body movements to adjust their direction of motion while walking in environments with
obstacles. However, their robotics counterpart, the quadrupedal robots, often rely on adjusting their direction of motion
by introducing a lateral asymmetry in leg motion amplitude, making the stable transition between forward and turning
gaits difficult. We hypothesize that using properly-coordinated body undulation and limb movements will enable effective
locomotion and stable transitions between gaits. Using geometric mechanics, we design gaits by prescribing a footfall
pattern and optimizing the body undulation which produces a desired motion. We predict that rotations resulting from
coordination of body undulation and limb movements can simplify gait transitions in legged robots, and we verify our
predictions by measuring displacements and rotations of a robophysical quadruped locomoting through granular media.
We find that the amplitude of body undulation controls the steering angle, and thus controls the turning radius. In
particular, we find that by increasing the body undulation amplitude from $\pi/12$ to $\pi/8$, the turning radius decreased from
10.5±0.3 body lengths (BL) to 2.9±0.1 BL.

12:39PM S64.00008: Robophysical Investigation of Root Circumnutation through Heterogeneous Environment
MASON MURRAY-COOPER (Presenter), YASEMIN OZKAN AYDIN, ENES AYDIN, Georgia Institute of Technology, NICHOLAS
NACLERIO, Mechanical Engineering, UC Santa Barbara, ERIN N MCCASKEY, JENNIFER RIESER, ELLIOT HAWKES, DANIEL
GOLDMAN, Georgia Institute of Technology — Circumnutation, a cyclic endogenous circular pattern exhibited by the tip of a
growing root, occurs in a diversity of plants, but its function is not fully understood. To investigate the hypotheses that
such motion facilitates substrate penetration and exploration, we built a planar soft robot [Hawkes et al. 2017], which
grows from the tip like a plant root and can bend in 2D space by oscillating inflation of the series pneumatic artificial
muscles (sPAMs) arranged on the two sides. Existing work observed force reduction effects from circumnutation in
homogeneous granular material [Dottore et al. 2016]. Here we demonstrated that tip oscillation aids the robot to
penetrate heterogeneous environment, e.g. hard obstacles, by growing the robotic root into a lattice of rough cylinders
(d=8cm) distributed uniformly on a board (120X120cm^2). Systematic variation of initial robot positions revealed that the
non-oscillating tip strategy led to an increased probability to become pinned to obstacles and unable to grow more than
23.8±19.7cm; the oscillating tip penetrated the lattice significantly further, 55.2±24.9cm. The results show that without
complicated control and sensing mechanism, oscillatory movement of a growing structure enables robust navigation in a
heterogeneous environment.
cycles and self-right. Allowed the system to explore more phase offsets, increasing probability and reducing time to escape from failure limit cycles. Added randomness in appendage oscillations was critical to self-righting. Periodic oscillations limited the coupled-oscillator system to visiting only a few phase offsets, causing it to often be trapped near failure limit cycles. Added randomness in appendage oscillations also increases the time to reach the peak force. This is largely due to earlier contact time which causes the sand to fluidize with impacts at the angle of repose producing 55% less force compared to impacts on a flat bed. Greater substrate incline also increases the time to reach the peak force. This is largely due to earlier contact time which causes the sand to fluidize sooner. Results from impacts with different plate angles will also be discussed.

Running up a sand dune is a challenging task due to several factors. First, sand fluidizes when an external force exceeding the material yield stress is applied. Second, at the angle of repose, the sand pile is in a metastable state, such that small perturbations will cause fluidization. Ongoing studies show that sand specialist lizards exhibit lower performance decrements than desert generalist when running up inclined sand. Preliminary evidence suggests that these differences are largely correlated with different impact angles of the feet relative to the sand, indicating that differences in foot movement can have dramatic effects on running ability. In this study, we experimentally examine the vertical impact force of a flat plate (1 in x 1 in) against a glass beads with varying plate and substrate angles. The plate impacted the substrate at 0.6 m/s with a force sensor attachment. Here, we find that impact at higher angles reduces the peak force, with impacts at the angle of repose producing 55% less force compared to impacts on a flat bed. Greater substrate incline also increases the time to reach the peak force. This is largely due to earlier contact time which causes the sand to fluidize sooner. Results from impacts with different plate angles will also be discussed.

Randomness in appendage oscillations helps a robot self-right. We tested this idea using an experimentally validated multi-body dynamics simulation of the robot. As appendage oscillation randomness (coefficient of variation) increased from 1% typical of the well-controlled robot to 20% typical of the animal, the robot self-righted more often (43% vs. 69%) and more quickly (6.8 ± 3.9 s vs. 5.2 ± 3.8 s) (P < 0.001, ANOVA). We discovered that an appropriate phase offset between the two oscillations was critical to self-righting. Periodic oscillations limited the coupled-oscillator system to visiting only a few phase offsets, causing it to often be trapped near failure limit cycles. Added randomness in appendage oscillations allowed the system to explore more phase offsets, increasing probability and reducing time to escape from failure limit cycles and self-right.
1:39PM S64.00013: The stigmatic-start: a rapid non-planar gait in snakes  NICHOLAS CHARLES (Presenter), Harvard University, RAGHUNATH CHELAKKOT, Indian Institute of Technology Bombay, BRUCE YOUNG, Kirksville College of Osteopathic Medicine, MATTIA GAZZOLA, Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, L MAHADEVAN, Harvard University — Newborn and juvenile yellow anacondas exhibit a previously unreported rapid transient gait, which we term the stigmatic-start. This is characterized by the snake first bending its body and then lifting itself partly out of the plane while moving forward about the mid-section. While superficially similar to sidewinding, the stigmatic-start is qualitatively different as it is a very rapid transient gait that allows the snake to move parallel to itself. To understand our observations, we construct a mathematical model for the non-planar locomotion of snakes that shows an interesting gait transition as a function of body size; small (juvenile) snakes can move via stigmatic locomotion but large (adult) snakes cannot, just as seen. In the context of biomimetic applications, the simulations of our model also suggest an avenue for optimal control of soft active filaments.

1:51PM S64.00014: Towards Obstacle-aided Legged Locomotion in Cluttered Environments*  FEIFEI QIAN (Presenter), DIVYA RAMESH, DANIEL E KODITSCHEK, University of Pennsylvania — Modern robots are often required to perform tasks in environments filled with obstacles and disturbances. However, most legged platforms are not yet capable of coping gracefully with unanticipated repeated disturbances, and often rely on active sensing to avoid all engagements with their physical surroundings. In this study, we propose a novel framework wherein we abstract the obstacle-cluttered environment into a horizontal-plane disturbance force field, and we consider robot legs as disturbance selectors. With different gait patterns, the robot can generate different disturbance forces on its center-of-mass from the same physical environment. Our simplified model significantly reduces the complexity of representing interactions between robot and obstacle-cluttered environments, and begins to suggest an approach to using gait space affordances for purposes of generating desirable obstacle responses in multi-legged robot locomotion amidst complex environments.

*This work is supported by NSF INSPIRE Award #1514882 and NSF NRI Award #1734355

2:03PM S64.00015: Mechanics of snake slithering on deformable substrates.*  PERRIN SCHIEBEL (Presenter), JENNIFER RIESER, GEORGIA INSTITUTE OF TECHNOLOGY, HENRY ASTLEY, UNIVERSITY OF AKRON, ALEX M HUBBARD, KELIMAR DIAZ CRUZ, DANIEL GOLDMAN, GEORGIA INSTITUTE OF TECHNOLOGY — Elongate, limbless animals like snakes move in both fluid and terrestrial habitats using flexural waves of the body. Little is known about their movement in materials like mud and granular matter (GM) which provide propulsion while yielding but, unlike fluids, may be permanently deformed by the interaction. We studied the ~40 cm long desert-dwelling snake *C. occipitalis* slithering on the surface of homogeneous GM. The snakes traveled 30-80 cm/s using a stereotyped shape. Surface drag measurements revealed that the ratio of thrust to drag forces, a critical component in undulatory motion, did not depend on speed or depth. We developed a surface resistive force theory (RFT) which revealed their waveform maximized center-of-mass speed given a constraint on peak muscle power. The snakes' motion was non-inertial, so we explored the performance of a robophysical model, a 10-link 70 cm long robot snake. The waveforms RFT predicted would maximize the speed of the robot instead failed to make progress, largely because the robot would re-encounter previously disturbed material. The snakes' waveform was in the regime where motion is like that in a frictional fluid; by limiting material yield the animal avoided contending with the memory-dependent effects that stymied the robot.

*NSF,NDSEG,ARO

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S65 DBIO DPOLY GSNP: Physics of Genome Organization II  BCEC 260 - Alexandre Morozov, Rutgers Univ - Tag(s): Focus
11:15AM S65.00001: Measuring the energetics of transcriptional regulation in living cells using allelic manifolds*

[Invited] JUSTIN KINNEY (Presenter), Cold Spring Harbor Laboratory — Gene expression in all organisms is controlled by cooperative interactions between DNA-bound transcription factors (TFs), but quantitatively measuring TF-DNA and TF-TF interactions remains difficult. Here we introduce a strategy for precisely measuring the Gibbs free energy of such interactions in living cells. This strategy centers on the measurement and modeling of “allelic manifolds”, a multidimensional generalization of the classical genetics concept of allelic series. Allelic manifolds are measured using reporter assays performed on strategically designed DNA regulatory sequences. Quantitative biophysical models are then fit to the resulting data. We used this strategy to study regulation by two *Escherichia coli* TFs, CRP and σ70 RNA polymerase. Doing so, we consistently obtained energetic measurements precise to ~ 0.1 kcal/mol (equivalently, ~0.2 k_BT). We also obtained multiple results that deviate from the prior literature. Our strategy is compatible with massively parallel reporter assays in both prokaryotes and eukaryotes, and should therefore be highly scalable and broadly applicable.

*This work was supported by a CSHL/Northwell Health Alliance grant to JBK and by NIH Cancer Center Support Grant 5P30CA045508.

11:51AM S65.00002: The Influence of Nucleosome Energetics on Chromatin Structure Across Multiple Length-Scales*

JOSHUA MOLLER (Presenter), University of Chicago, JOSHUA LEQUIEU, Chemical Engineering, University of California Santa Barbara, JUAN DE PABLO, University of Chicago — The physics governing nucleosome interactions influence structural features of chromatin across a range of length-scales. Here, we assess the extent of these interactions through Brownian dynamics simulations using a recently-developed coarse-grained model of chromatin. Simulations are used to interpret the hierarchy of interactions in chromatin fibers by quantifying the energetics of small-fibers including di- and trinucleosomes and isolating the factors which facilitate condensed configurations. Among these factors, we consider the influences of DNA sequence, nucleosome repeat length, and inclusion of the H1 linker histone. These small-fiber results are then used to assess the structure of larger chromatin fibers, revealing that nucleosomes in larger fibers favor configurations related to those exhibited in the small-scale systems. Lastly, we show that the linker histone significantly shifts the energetic minima of smaller systems, which corresponds to similar configuration changes of the larger chromatin fiber structure.

*NSF: MCB 1818328
NSF: EFRI CEE 1830969

12:03PM S65.00003: Modeling the spreading of epigenetic marks at the Oct4 promoter*

MELINDA VARGA (Presenter), WILLIAM C. AIRD, Center for Vascular Biology Research and Department of Medicine, Division of Hematology and Oncology, Beth Israel Deaconess Medical Center, Boston, MA, ERZSÉBET RAVASZ REGAN, Biochemistry and Molecular Biology Program, The College of Wooster, Wooster, OH — Epigenetic phenomena govern a wide range of processes in biological systems from cell differentiation to cancer. Genes are activated and inactivated by the presence and absence of various epigenetic marks ranging from histone methylation and acetylation to DNA methylation. Several computational models were developed to shed light on the bistability of the expressed protein, but they are mostly conceptual inventories of mechanisms required for a switch-like behavior of promoters, without an attempt to match experimental data. Here we introduce a computational model of the promoter region of the Oct4 gene, in which we incorporate the processes of histone acetylation, histone methylation and the spreading of silencing marks via the HP1 protein complex, and DNA methylation. We show that our model's dynamics align well with experimental results measured at the Oct4 promoter of mouse embryonic stem cells and can be adapted to describe the behavior of various promoters. We expect our approach to offer an important predictive tool to probe the strength of the epigenetic barrier to turn on a silenced gene and to predict the dependence of this barrier on the spatial organization of CpG sites.

*This work was supported by National Institutes of Health: Lung and Blood Institute grant HL076540.
The role of activity from within and outside of the cell nucleus in nuclear blebbing

KUANG LIU (Presenter), Physics Department, Syracuse University, EDWARD BANIGAN, Institute for Medical Engineering & Science, MIT, ALISON E. PATTESON, Institute for Medicine and Engineering, University of Pennsylvania, J. M. SCHWARZ, Physics Department, Syracuse University — The cell nucleus is an active environment in which molecular motors such as RNA polymerase and condensin continuously remodel chromatin. Outside the nucleus, the cytoskeleton is an active semiflexible polymer network comprised of actin, microtubules, and intermediate filaments, with motors, such as myosin and kinesin, remodeling the network. These two active environments are mechanically coupled via LINC complexes embedded in the nuclear membranes, as well as direct steric interactions at their interface. We numerically study shape fluctuations at the interface of these two active environments. We focus on the formation of nuclear blebs, which are large bulges in the nuclear envelope that frequently occur in the cells of individuals with diseases, such as muscular dystrophy or progeria. In particular, we study how bleb formation depends on the type of activity in the nucleus, be it contractile or extensile, to explain such phenomena as nuclear blebs occurring more frequently for diseased cells in stiffer or more confined microenvironments than in softer ones.

Modeling intrinsic biases in high-throughput sequencing data for chromatin accessibility

SHENGEN HU, CHONGZHI ZANG (Presenter), University of Virginia — Genome-wide profiling of chromatin accessibility with the assay for transposase-accessible chromatin using sequencing (ATAC-seq) or DNaseI hypersensitivity sequencing (DNase-seq) has been widely used for studying regulatory DNA elements and transcriptional regulation in many cellular systems. Efficient and thorough computational analysis is essential for extracting biological information from such high-throughput sequencing data. It has been reported that DNase cleavage of DNA has sequence preferences that can significantly affect the footprint patterns at transcription factor binding sites in genomic profiles. We found that enzymatic sequence biases commonly exist in both bulk and single-cell chromatin accessibility profiling data. Using a regular simplex encoding model, we developed a quantitative approach for accurate characterization and systematic correction of intrinsic sequence biases contained in ATAC-seq and DNase-seq data. This approach can be applied in bioinformatics for improved analysis of high-throughput chromatin accessibility sequencing.

Polymer models of chromosome compaction during cell division

ANTON GOLOBORODKO (Presenter), Massachusetts Institute of Technology, JOHAN H. GIBCUS, Medical School, University of Massachusetts, Worcester, KUMIKO SAMEJIMA, ITARU SAMEJIMA, University of Edinburgh, NATALIA NAUMOVA, Medical School, University of Massachusetts, Worcester, JOHANNES NUEBLER, Massachusetts Institute of Technology, MASATO KANEMAKI, National Institute of Genetics, Shizuoka, Japan, LINFENG XIE, JAMES R. PAULSON, University of Wisconsin-Oshkosh, WILLIAM C. EARNSHAW, University of Edinburgh, JOB DEKKER, Medical School, University of Massachusetts, Worcester, LEONID MIRNY, Massachusetts Institute of Technology —

During mitosis, cells compact their chromosomes into dense rod-shaped structures to ensure their reliable transmission to daughter cells. Our work explores how cells achieve this compaction. In our study, we probe the chromosome organization by microscopy and Hi-C at multiple time points during cell division. We use these data to develop polymer models of chromosomes. We show that our Hi-C data can be explained with a simple analytical model, which accounts for compaction of chromosomes into consecutive loops. We further support our conclusions with large-scale detailed polymer simulations. Finally, we show that the model of loop extrusion can also explain the observed dynamics of chromatin compaction.

As a result, we delineate a detailed pathway of mitotic chromosome folding that unifies many previous observations. In prophase, loop extrusion compacts chromosomes into arrays of consecutive loops. In prometaphase, these loops become compacted into clusters of smaller nested loops and collapsed by chromatin-to-chromatin attraction. These loops adopt a “spiral staircase” structure with a helical scaffold. The combined action of these mechanisms achieves the 10,000-fold compaction of chromatin into linearly organized dense mitotic chromosomes.
The accurate separation of chromosomes during cell division is key to survival and proper development. As the nuclear envelope breaks down, the microtubules within the spindle begin to interact with chromosomes. The disordered chromosomes, then, congress and are aligned in the mid-plane of the bipolar spindle. The underlying active forces that move the chromosomes during this process are poorly understood. We utilize the data from the first full 3D tomographic reconstructions of *C. elegans* mitotic spindle to understand how individual microtubules interact with chromosomes and propose a microscopic theory for chromosome congression. In addition to predicting the observed length distribution of microtubules in tomography, our theory correctly predicts a mechanically stable half spindle structure, as is observed in cells with monopolar spindles. Most remarkably, we find that the shapes (curvature) of microtubules based on our micromechanical theory are in good agreement with the tomography results.
1:39PM S65.00011: Optimizing chromosome disentanglement via chromatin loop organization*  
SUMITABHA BRAHMACHARI (Presenter), Center for Theoretical Biological Physics, Rice University, JOHN FREDERICK MARKO, Physics and Astronomy, and Molecular Biosciences, Northwestern University — Chromosome structure is actively regulated by a concerted action of various proteins to avail vital cellular functions, like the mitotic segregation of chromosomes. We seek to understand the microscopic scheme underlying the structure manipulation that leads to a compact disentangled mitotic state from a less compact and more entangled state in interphase, and vice-versa. We model cellular chromosomes as polymer brushes in a confined volume, and calculate the level of inter-chromosome entanglement in a fluctuating-topology ensemble for various steady-state configurations defined by structural parameters like the grafting density and side chain or loop length. We find that entanglements are minimized for certain brush configurations that depend on net chromosome length. Comparing with existing experimental observations we suggest that chromosomal loops are important for maintaining a low level of entanglement during the cell cycle. Our model provides a steady-state description of chromosomes that is consistent with experimental observations for both the interphase and mitotic stages, where the cell-cycle-specific reorganizations in the structure are accounted for by evolution of the steady state, likely driven by loop extrusion.

*Supported by NIH grants CA193419 and DK107980.

1:51PM S65.00012: Modulation of the DNA accessibility in the nucleosome -- insights from basic physics.*  
ALEXEY ONUFRIEV (Presenter), Virginia Tech — The nucleosome, a complex of 147 base-pairs of DNA with eight histone proteins, must protect its DNA, but, at the same time, allow on-demand access to it when needed by the cell. The exact mechanism of the control remain unclear.

A simplified electrostatic model of the nucleosome reveals that at physiological conditions the complex is extremely stable, but at the same time is close to the phase boundary separating it from the "unwrapped" states where the DNA is accessible. A small drop in the charge (e.g. through acetylation of a lysine) of the globular histone core can significantly lower nucleosome stability, and thus increase DNA accessibility. The finding suggests that charge-altering post-translational modifications in the histone core might be utilized by the cell to modulate accessibility to its DNA at the nucleosome level.

A follow-up, detailed multi-state atomistic model explores virtually all possible charge-altering post-translational modifications (PTMs) in the globular histone core. The model reveals a rich and nuanced picture: the effect of PTMs varies greatly depending on location, including counter-intuitive trends such as decrease of DNA accessibility for some lysine acetylations in the core. A connection to transcription regulation in-vivo is made.

*NSF MCB-1715207

2:03PM S65.00013: How nucleoid associated proteins stabilize supercoiled DNA  
KATELYN DAHLKE (Presenter), CHARLES E. SING, University of Illinois at Urbana-Champaign — Nucleoid associated proteins (NAPs) play an important physical role in prokaryotic cells by manipulating the shape and structure of the DNA within the nucleoid. These NAPs bend or twist DNA, and there are indications that NAPs bind preferentially to DNA that is already locally deformed. We hypothesize that these binding behaviors and local deformations strongly impact the stability and structure of DNA.

We use coarse-grained simulation of NAPs and DNA that allow us to achieve the time and length scales where DNA supercoiling occurs. Supercoils are twist-induced structures that are the result of relaxing highly-twisted DNA by inducing higher degrees of bending and writhe. This model can capture experimentally observed supercoiling behavior, and also shows that NAPs that locally bend DNA enhance DNA supercoiling. We are able to show that NAPs tend to localize along the contour of the supercoil, and this binding preference is capable of stabilizing supercoils that form within the nucleoid. By tracking different energies within the system, such as the energy due to bending, extension, or excluded volume, we gain insights into what is driving this protein-mediated supercoiling.

Thursday, March 7, 2019 11:15 AM - 2:15 PM

Session S66 DBIO: Pathogens and Parasites: Evolution and Immune Response BCEC 261 - Armita

Nourmohammad, Princeton University
11:15AM S66.00001: A statistical ensemble approach to immune discrimination* ANDREAS MAYER (Presenter), Princeton University — The immune system needs to distinguish molecular signatures of pathogens from those found in the organisms’ own proteins. A naive, but universal way to discriminate is to whitelist everything that should not elicit a reaction. Can the immune system do better? To begin to answer this question we characterize the self and pathogen proteomes as statistical ensembles. Probabilistic models reveal how both universal and phyla-specific constraints on protein evolution shape the statistics of the proteomes. The models furthermore allow us to quantify to what extent the ensembles differ systematically. We analyze whether and how these differences might be used for efficient immune defense. Finally, we compare predictions to what is known about epitopes recognized by the immune system.

*A. Mayer was supported by a Lewis-Sigler Fellowship.

11:27AM S66.00002: Force-Induced Ultrasensitivity at Cell-Cell Interfaces* BING LI, STEVEN ABEL (Presenter), Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — Recent experiments have revealed that B cells use mechanical forces transmitted by the actin cytoskeleton to discriminate between antigens of similar binding affinity and to internalize portions of the antigen-presenting membrane. However, there is no unifying theoretical framework to probe the role of forces in antigen discrimination at cell-cell interfaces. In this work, we develop a hybrid computational approach to account for key biophysical properties of immune cell interfaces, including stochastic receptor-ligand binding kinetics, membrane mechanics, and actin-mediated forces on the membrane. We show that the number of B cell receptors (BCRs) bound to antigens increases in an ultrasensitive manner as a function of the binding affinity, and that the stiffness of the antigen-presenting membrane influences the threshold of the response. Above the threshold, antigens are internalized through a mechanism involving BCR clustering. Taken together, our results highlight the importance of forces at B cell interfaces and suggest that affinity discrimination is enhanced by membrane deformations, intracellular forces, and the dynamic spatial organization of surface receptors.

*This work was supported by NSF CAREER Award PHY-1753017.

11:39AM S66.00003: Active tuning of synaptic patterns enhances affinity discrimination MILOS KNEZEVIC, SHENSHEN WANG (Presenter), Department of Physics and Astronomy, University of California Los Angeles, Los Angeles, CA, USA — Immune cells learn about their antigenic targets using tactile sense: during recognition, a highly organized yet dynamic motif, named immunological synapse, forms between immune cells and antigen-presenting cells (APCs). Via synapses, immune cells selectively extract recognized antigen from APCs by applying mechanical pulling forces generated by the contractile cytoskeleton. Curiously, depending on its stage of development, an immune cell exhibits distinct synaptic patterns which appear to strongly impact its capacity of distinguishing antigen affinities. While complete phase separation between receptor-ligand complexes and bound adhesion molecules observed in naïve (antigen-inexperienced) cells can be captured by existing models, how and why maturing cells maintain a multifocal pattern characteristic of arrested phase separation remains an unsolved puzzle. In this talk, I introduce a statistical-mechanical model to show that normal cytoskeletal forces can tune the degree of phase separation and thereby actively control the transition between distinct patterns. What is more, we find that normal forces coupled to lateral organization of receptors provide a robust grading scheme that allows efficient and broad affinity discrimination essential for proper immune function.

11:51AM S66.00004: Electronic Monitoring of Ligands-Induced Conformational Dynamics of Single Lysozymes* JAMES FROBERG (Presenter), MYUNGKEUN OH, YONGKI CHOI, North Dakota State University — We have investigated the dynamic interactions between lysozyme and several potential inhibitors such as peptide-based inhibitors, small-molecule inhibitors, and urea. In particular, the peptide-based inhibitor showed a weak affinity to lysozyme due to the non-covalent interactions between the C-terminus and the active site of lysozyme. Compared to the peptidoglycan substrates, the peptide inhibitor induced large conformational changes of lysozyme as well as stayed longer in the active site pockets while binding. The overall effectiveness of the peptide inhibitor was 20% when tested in the presence of both peptidoglycan substrates and inhibitors. The information gained by this research fundamentally improves our knowledge of lysozyme-inhibitor interactions, potentially paving the way to more effective, mechanism-focused drugs.

*This research was supported by the NIGIM/NIH under Award NO. R15GM122063 and ND EPSCoR Seed Award.
**12:03PM S66.00005: Macrophage phenotype bioengineered by magnetic field interference**  
JAREK WOSIK (Presenter), Electrical and Computer Engineering Department, University of Houston, MARTHA VILLAGRAN, Dept. of Physics and Texas Center for Superconductivity, University of Houston, WEI CHEN, The Houston Methodist Research Institute, Institute for Academic Medicine, PAVITHI WEERASINGHE, JOHN H MILLER, Dept. of Physics and Texas Center for Superconductivity, University of Houston, WANDA ZAGOZDZON-WOSIK, Electrical and Computer Engineering Department, University of Houston, MALGORZATA KLOC, The Houston Methodist Research Institute, Institute for Academic Medicine — Functionally different macrophages have different shape and molecular phenotype that depend on actin cytoskeleton. In all eukaryotic cells the cell shapes and the cell functions are reciprocally related. Thus, the mechanically/magnetically, genetically or biochemically enforced change in cell shape will profoundly reverberate at cell functions. Here we report that an exposure of macrophages to a nonuniform magnetic field causes extreme elongation of macrophages and has a profound effect on their molecular components and organelles. We observed that magnetic force rearranges the macrophage actin cytoskeleton, Golgi complex and cation channel receptor TRPM2 and modifies expression of macrophage molecular markers. We also analyzed magnetic-induced forces acting on macrophages and found that location and alignment of magnetic-field-elongated macrophages correlate very well with the simulated distribution and orientation of such magnetic-force lines. Such bioengineering of the macrophages properties has a potential to be used in development of novel anti-rejection therapies in clinical organ transplantation and anti-cancer and anti-metastatic therapies.

*Texas Center for Superconductivity at University of Houston

**12:15PM S66.00006: Collapse and contingency in phage infections of migrating bacterial populations**  
Derek J Ping (Presenter), Tong Wang, David Fraebel, Sergei Maslov, University of Illinois at Urbana-Champaign, Kim Sneppen, Niels Bohr Institute, Copenhagen University, Seppe Kuehn, University of Illinois at Urbana-Champaign — Natural bacterial populations are subject to constant predation pressure by phages. Since phage are non-motile perhaps the simplest defense against phage is for bacteria to outrun their predators. In particular, chemotaxis may help the bacteria escape slowly diffusing phages. Here we study phage infection dynamics in migrating bacterial populations driven by chemotaxis. We find that expanding phage-bacteria populations support two migrating fronts, an outermost “bacterial” front driven by nutrient uptake and chemotaxis and an inner “phage” front at which bacterial population collapses due to phage infection. We show that with increasing adsorption rate and initial phage population, the rate of migration of the phage front increases, eventually overtaking the bacterial front and driving the system from a regime where bacteria outrun a phage infection to one where they must evolve phage resistance to survive. We suggest that this process requires phages to hitchhike with the migrating bacterial front by repeatedly re-infecting the fastest moving bacteria. A deterministic model recapitulates the transition. Our work opens a new, spatiotemporal, line of investigation into the eco-evolutionary struggle between bacteria and their phage predators.

*NSF PFC (PHY 0822613 and PHY 1430124)

**12:27PM S66.00007: Bacterial Phage Resistance Emergence in Complex Landscapes of Stress**  
Krisztina Nagy (Presenter), Institute of Biophysics, Szged, Hungary, Trung Phan, Matthew Black, Princeton University, Julia Bos, Institute Pasteur, Robert Austin, Princeton University — We have begun studies of the emergence of loss of sensitivity of E. coli to the phages T4 and T4r using a microfabricated stress landscape where phage titers are distributed across an array of localized metapopulations. Sensitivity emerges from local biofilm-like pockets of bacteria and spreads as a form of colony hopping across the landscape. Sequencing on the insensitive bacterial colonies tests for both genetic mutations and additions of viral genome fragments in the CRISPR intervening spacer regions.

*This work was supported by NSF PHY-1659940.

**12:39PM S66.00008: A physical model for the selective assembly of HIV-1.**  
Chen Lin (Presenter), Chemistry and Biochemistry, University of California, Los Angeles, Ioulia Rouzina, Molecular Biology, The Ohio State University, Paola Espinosa, Orlando Guzman, Jose-Antonio Moreno, Department of Physics, UAM (Iztapalapa), Robijn Bruinsma, Physics and Astronomy, University of California, Los Angeles — We report on finding an intramolecular bound state of the structural Gag capsid protein of HIV-1 using a combination of all-atom Molecular Dynamics (MD) simulations and statistical mechanical modeling. The presence of this bound state prevents premature capsid assembly on non-viral host RNA. It would unify numerous observations that have been made on HIV-1. We show that the presence of a GFP sequence inserted into the Gag gene interferes with the formation of the bound-state, suggesting that such constructs can not be considered as representative of the wild-type Gag. The central role of the bound-state for the kinetics suggests a variety of possible routes for interfering with HIV-1 assembly.

*We thank the NSF-DMR for support under Grant 1610384 (SD, BS, RB);
1:27PM S66.00012: Stabilization of fine-scale host-pathogen diversity by spatiotemporal chaos  
ATISH AGARWALA (Presenter), MICHAEL PEARCE, DANIEL S FISHER, Stanford University — DNA sequencing studies have increasingly found that within microbial species, fine-scale genetic diversity coexists. A major open question is how such diversity can develop and be maintained under pervasive selection when the subtypes all compete locally. Host-pathogen interactions are often cited as a cause of diversity. But the behavior with large numbers of closely related (but distinct) types is not understood. We analyze a generalized Lotka-Volterra model of host-pathogen interactions. The set of pathogens are all similar, as are the hosts: we thus assume no explicit specificity and approximate the variations in the host-pathogen interactions as being random. The negative effect of a pathogen on a host is correlated with the positive-effect of that host on the pathogen: thus the full matrix of interactions has antisymmetric correlations. With purely antisymmetric interactions, there is a stable chaotic phase with many types surviving but the population of each type fluctuating wildly. Deviations from this special case cause runaway extinctions. We show that the addition of spatial structure can stabilize the chaos: there are local extinctions, but repopulations from other islands prevent a substantial fraction of the types from going globally extinct.

*We thank the NSF-DMR for support under Grant 1610384 (SD, BS, RB); the Brandeis Center for Bioinspired Soft Materials, an NSF MRSEC, DMR-1420382 (GRL); and the NIH, Award Number R01GM108021 from the National Institute Of General Medical Sciences (GRL and MFH). Computational resources were provided by the NSF through XSEDE computing resources (MCB090163) and the Brandeis HPCC which is partially supported by the Brandeis MRSEC.

1:03PM S66.00010: Investigation of Lymphatic Filariasis via Computational Modeling*  
KI WOLF (Presenter), J. BRANDON DIXON, ALEXANDER ALEXEEV, Mechanical Engineering, Georgia Institute of Technology — Lymphatic filariasis is a disease caused by parasitic worm such as W. bancrofti, which lives and spreads between human and mosquitoes. The condition is prevalent in tropical countries, and its complication such as lymphedema affects millions worldwide. Although the filariasis-causing parasite can be treated, limited understanding of the interaction between lymphatic valve, vessel, and the parasite slows the effort to create an effective treatment for filariasis complications. To further investigate the parasite interaction with the lymphatic system, we present a fully-coupled, three-dimensional fluid-solid computational model that incorporates the parasite movement inside the lymphatic vessel. First, the parasite movement against various flow condition inside lymphatic system is simulated to investigate the mechanism behind worm's ability to stay and navigate complex and constricting flow environment like the lymphatic system. Then, the parasite's interaction with lymphatic valves is investigated under different worm and valve parameters, which helps to understand how the worm's motion inside the lymphatic system may lead to valve damage and complications like lymphedema.

*Financial support from the National Science Foundation (CMMI-1635133) is gratefully acknowledged.

1:15PM S66.00011: A mean-field computational approach to intra-host HIV mutational dynamics  
HANRONG CHEN (Presenter), University of Pennsylvania, MEHRAN KARDAR, Physics, MIT — During HIV infection, the intra-host population is attacked by host cytotoxic T lymphocyte (CTL) responses. CTLs kill HIV-infected cells by recognizing certain HIV peptides presented on their surface. HIV strains with mutations in these regions escape CTL recognition and hence gain a relative fitness advantage. Can the dynamics of HIV mutations during intra-host infection be predicted? The intrinsic fitness landscapes of various HIV proteins, describing replicative capacity as a function of amino acid sequence, have been inferred from the global prevalence of strains infecting diverse hosts. Here, we present a new method to compute intra-host HIV mutational dynamics given an intrinsic fitness landscape and CTL responses, which we designate the evolutionary mean-field (EMF) method. EMF is a high-recombination-rate model of HIV dynamics that outputs effective fields and frequencies of mutations at each residue over time. We show via an example how intrinsic fitness costs and epistatic interactions of longer-term dynamics using the effective fitnesses yielded by EMF. Finally, we extend EMF to stochastic population dynamics and quantify stochasticity in infection outcomes.

12:51PM S66.00009: Gaussian curvature and the budding kinetics of enveloped viruses  
SANJAY DHARMAVARAM, Mathematics, Bucknell University, BAOCHEN SHE (Presenter), Physics and Astronomy, University of California, Los Angeles, GUILLERMO R LAZARO, MICHAEL F HAGAN, Chemistry, Brandeis University, ROBIJN BRUINSSMA, Physics and Astronomy, University of California, Los Angeles — Recent Brownian dynamics simulations of enveloped virus budding (Lazaro et al. 2018) have reproduced the puzzling pausing and stalling phenomena observed on in-vivo viral budding. We show that the pausing/stalling can be understood as a purely kinetic phenomenon associated with a "geometrical" energy barrier. This barrier does not show in the equilibrium thermodynamics of the system but it must be overcome by capsid proteins diffusing along the membrane prior to incorporation into the viral capsid. The barrier is generated by the conflict between the positive Gauss curvature of the capsid and the large negative Gauss curvature of the neck region. The theory is compared with the Brownian simulations of the budding of enveloped viruses.

We thank the NSF-DMR for support under Grant 1610384 (SD, BS, RB); the Brandeis Center for Bioinspired Soft Materials, an NSF MRSEC, DMR-1420382 (GRL); and the NIH, Award Number R01GM108021 from the National Institute Of General Medical Sciences (GRL and MFH). Computational resources were provided by the NSF through XSEDE computing resources (MBC090163) and the Brandeis HPCC which is partially supported by the Brandeis MRSEC.

1:51PM S66.00008: Gaussian curvature and the budding kinetics of enveloped viruses  
K. WOLF (Presenter), University of Pennsylvania, MEHRAN KARDAR, Physics, MIT — During HIV infection, the intra-host population is attacked by host cytotoxic T lymphocyte (CTL) responses. CTLs kill HIV-infected cells by recognizing certain HIV peptides presented on their surface. HIV strains with mutations in these regions escape CTL recognition and hence gain a relative fitness advantage. Can the dynamics of HIV mutations during intra-host infection be predicted? The intrinsic fitness landscapes of various HIV proteins, describing replicative capacity as a function of amino acid sequence, have been inferred from the global prevalence of strains infecting diverse hosts. Here, we present a new method to compute intra-host HIV mutational dynamics given an intrinsic fitness landscape and CTL responses, which we designate the evolutionary mean-field (EMF) method. EMF is a high-recombination-rate model of HIV dynamics that outputs effective fields and frequencies of mutations at each residue over time. We show via an example how intrinsic fitness costs and epistatic effects, skewed CTL responses, etc. impact the identities and time course of HIV escape mutations. We also explain features of longer-term dynamics using the effective fitnesses yielded by EMF. Finally, we extend EMF to stochastic population dynamics and quantify stochasticity in infection outcomes.

1:27PM S66.00012: Stabilization of fine-scale host-pathogen diversity by spatiotemporal chaos  
ATISH AGARWALA (Presenter), MICHAEL PEARCE, DANIEL S FISHER, Stanford University — DNA sequencing studies have increasingly found that within microbial species, fine-scale genetic diversity coexists. A major open question is how such diversity can develop and be maintained under pervasive selection when the subtypes all compete locally. Host-pathogen interactions are often cited as a cause of diversity. But the behavior with large numbers of closely related (but distinct) types is not understood. We analyze a generalized Lotka-Volterra model of host-pathogen interactions. The set of pathogens are all similar, as are the hosts: we thus assume no explicit specificity and approximate the variations in the host-pathogen interactions as being random. The negative effect of a pathogen on a host is correlated with the positive-effect of that host on the pathogen: thus the full matrix of interactions has antisymmetric correlations. With purely antisymmetric interactions, there is a stable chaotic phase with many types surviving but the population of each type fluctuating wildly. Deviations from this special case cause runaway extinctions. We show that the addition of spatial structure can stabilize the chaos: there are local extinctions, but repopulations from other islands prevent a substantial fraction of the types from going globally extinct.

*We thank the NSF-DMR for support under Grant 1610384 (SD, BS, RB); the Brandeis Center for Bioinspired Soft Materials, an NSF MRSEC, DMR-1420382 (GRL); and the NIH, Award Number R01GM108021 from the National Institute Of General Medical Sciences (GRL and MFH). Computational resources were provided by the NSF through XSEDE computing resources (MBC090163) and the Brandeis HPCC which is partially supported by the Brandeis MRSEC.
1:39PM S66.00013: Revealing Determinants for Antibody-Antigen Coevolutionary Outcome Using a Shape-Space Model  JIMING SHENG (Presenter), SHENSHEN WANG, Physics & Astronomy, University of California, Los Angeles — B cells in the adaptive immune system produce antibody molecules that bind foreign antigens for removal. The binding affinity of antibodies for an antigen is improved \textit{in vivo} through affinity maturation (AM) – a speedy Darwinian process occurring in numerous modest-size B cell populations housed by individual germinal centers (GC). A significant challenge arises when highly mutable pathogens (notably HIV) evolve on similar timescales as do B cell populations, evading an effective immune response.

Existing theoretical studies have ignored demographic fluctuations and precluded alternative evolutionary outcomes. In this talk, I extend the classic shape-space model to describe antibody-antigen coevolution via mutation and mutual selection. Using agent-based stochastic simulations, we show that consideration of population dynamics reveals diverse evolutionary outcomes and uncovers key determinants that can potentially be manipulated, including initial antigen diversity and epitope conservation. Moreover, we find population subdivision may slow down mutational escape of antigen. Finally, we suggest a possible route to evolving cross-reactive antibodies amenable to experimental search.

1:51PM S66.00014: Ultra small carbon nanodots as fluorescence markers in primary human cells: uptake and cellular distribution*  THOMAS HEINZEL (Presenter), STEFAN FASBENDER, Department of Physics, University of Dusseldorf, Germany, RAINER HAAS, University Hospital, University of Düsseldorf, Germany — Carbon nanodots (CNDs) are promising candidates for fluorescence labeling of cellular components as well as for drug and gene delivery. Therefore, the uptake dynamics of CNDs and their cellular distribution are of vital interest. Here, we report the preparation of CNDs by a simple pyrolysis process, their structural and spectroscopic characterization, and the observation of cell-specific uptake rates by the leukocyte family as well as for hematopoietic stem cells. Large uptake rates are observed, resulting in up to approximately $10^9$ CNDs per cell after 24 hours of incubation. [1] The CNDs distribute non-uniformly across the cells. In particular, they do not enter the nucleus and have a tendency to accumulate in the Golgi apparatus in living cells. Fixation of the cells leads to a homogenization of the CND distribution across the cytoplasm. We show that this behavior suggests uptake via endocytosis, followed by intra-cellular storage inside nanoscale vesicles. Furthermore, the CNDs have only a small effect on the cell viabilities over a period of 72 hours even at very large CND concentrations.


*The authors acknowledge financial support by the Düsseldorf School of Oncology (DSO) and by the Betz foundation.

2:03PM S66.00015: Antimicrobial activity of sulphur-doped graphene quantum dots coupled with methylene blue for photodynamic therapy applications*  ALI ER (Presenter), KHOMIDKHODZHA Kholikov, ILHOM SAIDJAFARZODA, LAUREN COOPER, ERMEK BELEKOV, Western Kentucky University, OMER SAN, Oklahoma State University — Graphene quantum dots (GQDs) have attracted much attention and are a promising material with potential applications in many fields. One application of GQDs is as a photodynamic therapy agent that generates singlet oxygen. In this work, GQDs were grown by focusing nanosecond laser pulses into benzene and then were later combined with methylene blue (MB) and used to eradicate the Gram-negative bacteria, \textit{Escherichia coli}, and Gram-positive bacteria, \textit{Micrococcus luteus}. Theoretical calculation of pressure evolution was calculated using the standard finite difference method. Detailed characterization was performed with TEM, SEM, FTIR, UV-Vis, and photoluminescence spectra. Combining MB with GQDs caused enhanced singlet oxygen generation. Our results show that the MB-GQD combination efficiently destroys bacteria. The MTT assay was used to determine if GQDs in dark conditions caused human cellular side-effects and affected cancer and noncancer cellular viability. We found that even high concentrations of GQDs do not alter viability under dark conditions. These results suggest that the MB-GQD combination is a promising form of photodynamic therapy.

*This project is fully supported by Kentucky Biomedical Research Infrastructure Network and INBRE (KBRIN) ULRF13-1493C-01.
T70.00001: GENERAL

T70.00002: A Neoclassical Framework That Reunifies Modern Physics
ALAN M. KADIN (Presenter), Consultant, Princeton Junction, NJ 08550 — The unity of classical physics was broken by quantum uncertainty on the micro level and curved spacetime on the cosmic level. In contrast, a novel neoclassical picture is presented*, which incorporates key aspects of quantum and relativistic physics, while maintaining deterministic local reality at all levels. This is based on the following principles:
1) Real rotating vector fields self-organize into soliton-like wave packets with quantized spin; these represent elementary particles.
2) Characteristic frequency and wavelength of these wave packets define time and space, and are modulated by gravity.
3) Wave packets maintain constant frequency for both massive and massless particles, reproducing relativistic trajectories.
4) Transitions are due to continuous interactions between wave packets that conserve total frequency, wavevector, and spin.
This approach maintains quantum discreteness without Hilbert space, and reproduces curved light without spacetime. But this also predicts sharp deviations from some simple predictions of orthodox quantum theory, such as the two-stage Stern-Gerlach experiment.


T70.00003: Mesoscopic RLC Circuit and its Associated Occupation Number and Berry Phase
ERIC GREENWOOD (Presenter), Geology and Physics, University of Southern Indiana — We consider the quantization of the time-dependent harmonic oscillator and its associated Berry phase using the invariant operator method, as well as the occupation number of the induced quasi-particle production. Furthermore, we point out that in the literature there exist different methods for determining the solution to the Milne-Pinney equation, which leads to different results. By measuring the time-dependent occupation number and associated Berry phase, one can, in principle, determine which of these methods leads to physically realized results. As a concrete example, we consider the mesoscopic RLC circuit and derive the occupation number and associated Berry phase for each of these different methods. We find that, the solution to the Ermakov equations leads to a time-dependent occupation number and associated Berry phase, while the particular solution to the Milne-Pinney equation does not.

T70.00004: Tracking UV photolysis and molecular transport induced chemical changes within tissue models treated with a cold atmospheric pressure plasma jet*
BHAGIRATH GHIMIRE (Presenter), PRADEEP LAMICHHANE, EUN HA CHOI, Electrical and Biological Physics, Kwangwoon University — Cold atmospheric plasma jets operated into ambient air provide a rich source of reactive oxygen and nitrogen species (RONS), which are known to influence biological processes important in disease. Despite plasma shown to have effects deep within tissue (e.g. destruction of subcutaneous cancer tumors), it is not understood how the plasma RONS can reach deep-seated diseased cells. In this study, we model the plasma jet delivery of RONS into a tissue target and we delineate two processes: through target delivery of RONS generated (primarily) in the plasma jet and in situ RONS generation by UV photolysis within the target. RONS are rapidly generated in the tissue target's surface by UV photolysis. Once in the target, RONS are transported to millimeter depths via a slower molecular process.

*This work was supported by a grant from National Research Foundation of Korea (NRF- 2016K1A4A3914113, and NRF-2010-0027963), and in part by Kwangwoon University, Korea.

T70.00005: Convolutional Autoencoder for Denoising Images of Active Nematics
ZHENGANG ZHOU (Presenter), PENG-YU HONG, MICHAEL NORTON, SETH FRADEN, Brandeis University — The images produced in active nematics experiments are usually quite noisy. These noises (caused by the activities of materials, lighting, etc.) can significantly influence the downstream analyses and constraint our capability of understanding active nematics. Conventional denoising methods have limited power in improving the quality of those images. In this study, we developed a Deep Learning technique to tackle this problem. We designed a deep denoising model as a deep convolutional auto-encoder with skip-layers. The deep denoising model was trained using randomly chosen clean images of active nematics. We also designed a convolutional reconstruction method that uses our deep denoising model to remove noises in new active nematics images. Experimental results demonstrate the effectiveness of our approach.
T70.00006: Spectral Stability of Gravitationally Interacting Rods  CARLOS OWUSU-ANSAH (Presenter), JOHN LINDNER, College of Wooster — We investigate the spectral stability of equilibrium configurations of two line-masses (slashes or rods) interacting via gravity. The Euler-Lagrange formalism provides the equations of motion. We determine the positions, orientations and angular velocities of the slashes at their equilibrium configurations. All equilibrium solutions are checked using the equations of motion. The spectral stability of each equilibrium configuration is determined by linearizing the equations of motion about the equilibrium configurations and analyzing the path of the slashes when they are perturbed. We illustrate the parameter values that cause equilibrium configurations to be spectrally stable.

T70.00007: Sliding on a Spinning Cuboid*  KIMBERLY PATTERSON (Presenter), JOHN LINDNER, College of Wooster — Which way is downhill on a spinning asteroid? Comet nuclei and asteroids like 67P, Ryuga, and Bennu are too small to gravitationally pull themselves into spheres. As spacecraft like Rosetta, Hayabusa2, and OSIRIS-REx visit them, a better understanding of the surface motion of regolith and boulders, as well as hoppers, landers, and rovers, is needed. For a theoretical overview, previous work studied the frictionless sliding of point masses on spinning asteroids idealized as rotating spheroids. In this work, we concentrate the curvature into 12 edges and study the periodic and chaotic motion of point masses sliding frictionlessly on rotating cuboids.

*NSF DMR 1560093

T70.00008: Three Roads to Quaternion Gravity  DOUGLAS SWEETSER (Presenter), Quaternions.com of Acton, MA — Three roads merge to create a different approach to gravity. Our deepest insights into nature use symmetries because symmetries remain unchanged. Using quaternion algebra instead of tensor calculus, the conservation of space-times-time is the symmetry underlying the quaternion gravity proposal for non-inertial observers in a gravitational field. Where there is a symmetry, there need also be a transformation law to detail how change is permitted to happen. The notion of relaxed relativity holds that in a gravitational field, one observer looking at another observer measuring the speed of light will find the product of wavelength and frequency differs from the speed of light \( c \) in a precise way \( c' = c \gamma^2 \text{esc} \). Lorentz invariance remains for inertial observers, but non-inertial observers are governed by different symmetries. Gravity is different everywhere, so a field theory is also necessary using gravitational escape velocities. With some reasonable guesses constrained by observations, one can form a quaternion gravity proposal that is consistent with weak field gravity tests to first order Parameterize Post Newtonian accuracy. No gravitons are required for this technical variant of special relativity. Pre-print available on line: http://bit.ly/vp-three-roads

T70.00009: Detection of biomarkers in lipidic cubic phases  MUNIR PIRBHAI (Presenter), St. Lawrence University — Lipidic cubic phases have been shown to be versatile platforms for the detection of biomarkers, viruses, bacteria and parasites. This technique produces birefringent crystals during a positive test, which can be detected by placing the sample between crossed-polarizers and shining light through. The intensity of light emerging from the setup constitutes the output signal, and can be related to the concentration of analyte present. In this work, we investigate how the thickness of the sample affects the output signal.

T70.00010: Gravity and Waves and Dimension Reduction  THOMAS MATERDEY, University of Massachusetts Boston, ALBERT MATERDEY (Presenter), Roxbury Community College, ALEXANDER MATERDEY, Quantum FC, Inc. — Gravity can interact with a mechanical wave to convert a 3D object into a 1D string, thus reducing space-time dimensions from 4 to 2. The physics of this gravity-wave interaction could form the basis of a semi-classical approach to quantum gravity.

T70.00011: MEDICAL PHYSICS —
Hyperspectral imaging of human hands and curvature correction

LUKA ROGELJ, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia, URBAN PAVLOVČIČ, Faculty of Mechanical Engineering University of Ljubljana, Ljubljana, Slovenia, JOŠT STERGAR, ROK DOLENEC, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia, MATIJA JEZERŠEK, Faculty of Mechanical Engineering University of Ljubljana, Ljubljana, Slovenia, MATIJA MILANIC (Presenter), URBAN SIMONČIČ, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia.

Hyperspectral imaging (HSI) is a non-contact and non-invasive method that provides spectral and spatial information in a single measurement. It has been recently introduced into the medical imaging as a research tool for determination of physiological parameters distribution (e.g., hemoglobin and oxygenation maps). An imaged surface curvature significantly affects illumination distribution over the surface and thus introduces artifacts in the recorded HSI. Such artifacts markedly affect accuracy of the image analysis, therefore a curvature correction of the images should be performed. In this study, hands of human volunteers were imaged by a HSI system (400–1000 nm spectral range) and a laser triangulation profilomer (LTP) providing 3D surface of the hands. Lambert cosine law and height corrections were applied to the recorded images. The corrected images show improved illumination homogeneity, effectively eliminating the curvature artifacts.

By combining HSI and LTP, hyperspectral images can be successfully corrected for the curvature artifacts, greatly improving accuracy of the further image analysis (original image discrepancy 12 %, corrected image discrepancy 4 %).

Curvature statistics: An underused measure for epithelial to mesenchymal transition classification in pancreatic cancer

JEFFREY LA (Presenter), JONATHAN P CELLI, CHANDRA S YELLESWARAPU, University of Massachusetts Boston — Epithelial to mesenchymal transition (EMT) and mesenchymal to epithelial transition (MET) plays an essential role in the local progression and metastasis of pancreatic cancer, whereby malignant cells undergo a physical transformation associated with increased mobility and resettle in a new site. Discovering EMT and MET's underlying molecular processes have opened new therapeutic agents, however knowledge of this complex network is not complete and design consistencies in literature limit inferences and prevent meta-analysis of data. Instead of focusing on chemical pathways, we revisit ways to characterize cellular shape through cellular curvature distribution. We demonstrate this measure can improve classification models of epithelial, mesenchymal, and transitioning cells, with pancreatic cancer cells by computational analysis of optical microscopy images, which can improve risk stratification and treatment decisions.

Sub-Nano Pulsed Laser Transport through Different Skin Types for Tattoo Removal Application

SHAH FAISAL MAZHAR (Presenter), REGINALD EZE, Math, Engineering & Computer Science, LaGuardia Community College — In this study, a thin scattering tissue layer model developed using modified Monte Carlo method [1] was used as skin model to simulate African American, Asian, and Caucasian skins and different laser transport trends were found for different skin types while running picosecond pulsed laser through the skin model. The optical properties of this skin types were simulated using their optical coefficients (i.e. absorption coefficient) found from the existing literature. The study of laser transport through different skin types and finding associated trends are significant for tattoo removal application in order to optimize the wavelength and pulse width of the laser from different skin types.


Material Design for Near-Infrared Photothermal Therapy

FAITH CHEUNG (Presenter), XUAN LUO, Physics, National Graphene Research and Development Center — Photothermal therapy, as a promising and emerging method of cancer treatment, uses the emission of near-infrared light for tumor ablation. However, current photothermal agents have led to inefficient tumor ablation due to its inability to penetrate deeply into affected tissue. In our research, we perform first-principles calculations to find the optimal materials for near-infrared light emission by doping graphene. Our results show the band gaps corresponding to near-infrared light emission and we claim that oxygen doped graphene is a suitable source for near-infrared light. It is possible to improve the efficiency of photothermal therapy by using these materials, hence our results pave the way for photothermal therapy.
Recently, 3D printing has become more popular due to the availability of new materials. For example, electrically conductive graphene-PLA composites can be used as a shield for electromagnetic interference (EMI); specifically, circuit packages 3D printed using conductive composites could provide shielding. The purpose of this research is to determine how the parameters of 3D printed samples impact the shielding effectiveness. Our previous research has shown that the percentage and orientation of infill has the greatest impact on conductivity. Here, we test shielding effectiveness from 10 MHz to 3 GHz by measuring RF transmission through a sample by sandwiching it between a custom coaxial tester connected to a spectrum analyzer. The data showed that the greater the infill percentage, the less the orientation effects attenuation. For example, 100% infill samples with perpendicular and parallel orientation both attenuated by -15 dB at 1 GHz. However, at lower infill percentages, more varied infill orientations differed in RF attenuation. For example, at 25% infill, samples with perpendicular and parallel infill attenuated by -20 dB and -12 dB at 1 GHz, respectively. The most efficient sample by mass had 25% infill orientated at 4 varying angles.

References:

Limiters, with their optical properties highly dependent on the wavelength and intensity of the incoming light, are often used to protect sensitive optical components. Currently most limiters are sacrificial, destroyed after a single high intensity exposure. As an alternative, this work focuses on photonic limiters because they significantly increase the cost-efficiency by their high damage threshold and reusability. We study a photonic limiter design with phase-change material (PCM) as a key component. To incorporate PCM in the limiter design, we use ellipsometry to characterize PCM optical property at a wide range of wavelength and temperature. An example of such materials is GeSbTe (GST), an alloy consisting of germanium, antimony and tellurium. Around a critical temperature, GST transforms from amorphous to crystalline, thereby switching its optical properties. Besides GST, we also examine the optical properties of other semiconductors such as ZnO and GaAs as possible material for other limiter designs.
T70.00022: Lithium niobate optomechanical crystal*  WENTAO JIANG (Presenter), RISHI N PATEL, FELIX MAYOR, TIMOTHY MCKENNA, PATRICIO ARRANGOIZ-ARRIOLA, CHRISTOPHER SARABALIS, RAPHAËL VAN LAER, AMIR SAFAVI-NAEINI, Department of Applied Physics and Ginzton Laboratory, Stanford University — Lithium niobate (LN) has excellent piezoelectric and electro-optic properties, enabling it as the workhorse material of the essential components for classical communication. Recently LN is also considered for quantum signal transduction and modulation. High-quality LN microring resonator and LN photonic crystal have been demonstrated with quality factor as high as $10^7$ and $10^5$ respectively. Here we demonstrate 1D LN optomechanical crystals with optical quality factor as high as 300,000, 2 GHz mechanical mode with quality factor as high as 37,000 at 4 Kelvin and zero-point optomechanical coupling rate $g/2\pi \sim 120$ kHz. The optomechanical coupling is shown to be tunable down to zero by designing the orientation of the crystal. We further utilize the piezoelectric coupling to drive the mechanical mode directly and optically readout the motion. We identify both the mechanical bandgap and the mechanical modes. The optomechanical coupling and the compatibility of the LN-on-silicon material system with microwave qubits demonstrate the enormous potential of this piezo-optomechanical platform for quantum electro-optic conversion and coupling between microwave nanomechanics and superconducting qubits.

*Work supported by a Packard Fellowship, ONR MURI QOMAND, and Stanford University.

T70.00023: Influence of ZnTe nanocrystals in the laser performance parameters of Yb$^{3+}$ doped phosphate glasses*  ALYSSON MIRANDA FREITAS, RODRIGO FERREIRA FALCI, MARIA JOSE V BELL, Universidade Federal de Juiz de Fora, NOELIO OLIVEIRA DANTAS, Universidade Federal de Alagoas, VIRGILIO ANJOS (Presenter), Universidade Federal de Juiz de Fora — This work reports an optical investigation of a phosphate glass (PZABP) doped with ZnTe semiconductors nanocrystals and co-doped with Yb$_2$O$_3$. ZnTe nanocrystals growing were evidenced by optical absorption spectra and their average radius were estimated via effective mass approach. The emission cross section, absorption cross section and lifetime measurements were performed via Optical Absorption, Photoluminescence and Time-Resolved Photoluminescence techniques. Important performance parameters for solid-state lasers, like the minimum fraction of ions that must be excited ($\beta_{\text{min}}$), the pump saturation intensity ($I_{\text{sat}}$) and the minimum intensity of the pumping laser ($I_{\text{min}}$) were obtained and the product $\sigma_{\text{emi}} \times t_{\text{exp}}$ was defined as a figure of merit to analyses the efficiency of the system. The influence of the ZnTe nanocrystals in the laser performance parameters was studied. The results point the alterations caused by the presence of the nanostructures may be compensated by the intensity gain on the media active and indicates the PZABP glasses as a promising material to applications in high power lasers.

*The authors would like to thank CNPq, CAPES and FAPEMIG for their financial support.

T70.00024: Role of Ni$^{2+}$ in transparent glass-ceramics with semiconductor nanocrystals for optoelectronic applications*  RADHA MADA, SESHADRI MERUVA, MARIA JOSE V BELL, Universidade Federal de Juiz de Fora, NOELIO OLIVEIRA DANTAS, Universidade Federal de Alagoas, VIRGILIO ANJOS (Presenter), Universidade Federal de Juiz de Fora — Phosphate glass doped with 5 wt% Ni$^{2+}$ ions and glass-ceramics containing ZnTe nanocrystals with x wt% of Ni$^{2+}$ ions (x = 0.5, 1.0, 5.0 and 10.0) were prepared by fusion method. The structural analyses were performed through XRD, FTIR-ATR and Raman techniques. The XRD revealed amorphous and ZnTe crystalline phases. Several phosphate groups were observed from FTIR-ATR and Raman spectra showing that Ni$^{2+}$ ions possess octahedral symmetry. The intensity of the 1352 nm band increased with the increase of Ni$^{2+}$ ions in GC which is an indicative of the $^{6}\text{Ni}^{2+}$ coordination. The emission cross-sections ($s_{\text{emi}}$), full width at half maxima for the $^1T_2g(D) \rightarrow ^3T_2g(F)$ and $^3T_2(F) \rightarrow ^3A_2(F)$ emissions were reported. The product of $s_{\text{emi}}$ and $t_{\text{mer}}$ (figure of merit) and $s_{\text{emi}}$ ($^3T_2(F) \rightarrow ^3A_2(F)$) was higher to GC sample with 10.0 wt% of Ni$^{2+}$. Thermal diffusivity (D) and thermal conductivity (K) were obtained through thermal lens and thermal relaxation methods. D and K did not change significantly with the increase of Ni$^{2+}$ ions (0.5 – 5 %) in GCs. The 10.0 wt% Ni$^{2+}$ sample presented the lower variation of the optical path with temperature with good lasing properties suggesting it as good candidate for optoelectronic applications.

*The authors would like to thank CNPq, CAPES and FAPEMIG for their financial support.
**T70.00025: Computational electro-magnetic field modeling of TMS coils with validation in gel-based phantom brain**

JOHN R GERMICK, XIAOJING ZHONG (Presenter), YIFEI WANG, Department of Electrical and Computer Engineering, Iowa State University, AARON BOES, HIROYUKI OYA, Carver College of Medicine, University of Iowa, DAVID C JILES, Department of Electrical and Computer Engineering, Iowa State University — Transcranial magnetic stimulation (TMS) is a noninvasive brain stimulation technique for modulation of cortical neurons in the brain. One challenge with the use of TMS is that it is often difficult to determine the spatial distribution of brain regions receiving stimulation. A popular method of exploring the stimulation profile of TMS coils is through generation of virtual head models and Finite Element Simulations (FEM). However, a limitation of this approach is the models are rarely validated against actual measurements of the magnetic and electric fields. Here, we performed FEM modeling on gel-based phantom brain models with conductive properties that mimic those of the human brain. The phantom brains had implanted electrocorticography electrodes at varying depths to record the stimulation profiles recorded by the electrodes, which were then compared with FEM models of the phantom brain. Ongoing work is focused on validating FEM results relative to a novel paradigm of recording the effects of TMS in neurosurgical patients with intracranial EEG. Taken together, this work highlights the strengths and limitations of using FEM to simulate the magnetic and electric field profiles generated by TMS coils, and propose a new method of testing the performance of novel TMS coils.

**T70.00026: Investigating how coil designs and anatomical variations affect the efficacy of cerebellar TMS**

XIAOJING ZHONG (Presenter), PRIYAM RASTOGI, YIFEI WANG, Iowa State University, ERIK G LEE, Department of Psychiatry, Massachusetts General Hospital, DAVID C JILES, Iowa State University — Transcranial magnetic stimulation (TMS) is a neuromodulation technique a non-invasive treatment for various neurological disorders such as major depressive disorder. Cerebellum is a complex structure connected with almost the entire central nervous system, and TMS has promise for non-invasively probing cerebellar function. Therefore, TMS has been gaining popularity in the field of neurostimulation of cerebellum. Recent studies have reported that cerebellum plays an important role not only in motor planning and behavior but also in the cognitive domain. Nevertheless, few studies have explored how different coil designs and anatomical variations affect the effectiveness of cerebellar TMS. In this work, we investigated the effects of cerebellar TMS with different coil designs positioning on several locations. Finite element modeling was conducted with Figure-of-8 coil and DB-80 coil. Each coil was positioned in the center, 1 cm and 3 cm to the left with respect to the center of the cerebellum and all the locations were tangential to the scalp at a distance of 5 mm. Furthermore, the commercial head model MIDA and 50 MRI derived head models were used in the computer modelling to examine how anatomical variations affect the efficacy of cerebellar TMS.

**T70.00027: Magnetic properties of synthesized Fe_x(Fe_3O_4)_1-x nanoparticles with core-shell structures coated by carbon matrix**

ARAM MANUKYAN, HARUTYUN GYULASARYAN, EDUARD SHAROYAN, Laboratory of Solid State Physics, Ashtarak-2, Laboratory for Physical Research, NAS of Armenia, JENNIFER LYNN GRAY, Materials Characterization Lab, Pennsylvania State University, Materials Research Institute, OSCAR BERNAL, ARMEN KOCHARIAN (Presenter), Department of Physics, California State University Los Angeles — Here we are focused on investigation of magnetic and structural properties of synthesized nanocomposites with iron nanoparticles as effective heat mediators with high thermal energy transfer efficiency suitable for use for magnetic hyperthermia. These nanoparticles have “core-shell” structure, in which the core has a high magnetic moment (such as Fe), and the shell consists of a biocompatible material (e.g. iron oxide or carbide). Complex investigations of structural and magnetic properties of these materials are obtained using X-ray diffraction (XRD), Raman spectroscopy, magnetometry, electron paramagnetic and ferromagnetic resonances (EPR, FMR). The measured magnetization of magnetic saturation and coercivity as well as the specific absorption rate (SAR) show that these materials attractive for magnetic hyperthermia applications. Hysteresis loop of the (Fe-Fe_3C)@C nanocomposites is of special interest as it shows almost square behaviour, where M_r/M(200 Oe) = 0.75.

*This work was supported by a grant from the Russian-Armenian (Slavonic) University at the expense of the Ministry of Education and Science of the Russian Federation. The work at CSULA was supported by the National Science Foundation-Partnerships for Research and Education in Materials under Grant DMR-1523588.
T70.00028: Nucleic Acid Functionalization of Graphene and the Impact on Stem Cell Maturation  VINCENT BATTISINI OLIVIERI, Tufts University School of Medicine, LAN WEI, Molecular Cardiology Research Institute, Tufts University School of Medicine, MICHELLE CHEN (Presenter), Physics and Engineering, Point Loma Nazarene University, HOWARD H CHEN, Molecular Cardiology Research Institute, Tufts University School of Medicine — Stem cells are capable of differentiating into defined cell types, thus hold great promise for medical applications including disease modeling, drug screening, and therapeutics. When integrated with graphene, an extremely conductive and strong atomic sheet of carbon atoms, novel ways to understand and control the differentiation of stem cells may be realized. We hypothesize that nucleic-acid functionalized graphene minimally impact stem cell viability, and can further enhance stem cell differentiation. In our experiments, various nucleic acid constructs were successfully purified and characterized before functionalization onto graphene, which was synthesized on copper via chemical vapor deposition and then transferred onto glass coverslip. Stem cells, primary bone marrow mononuclear cells (BMMCs), were isolated from mice and cultured on nucleic acid functionalized graphene. Preliminary atomic force microscopy revealed prominent 3-dimensional features of greater than 30 nm in height 24 hours after stem cell attachment, suggesting the presence of viable BMMCs. Furthermore, cell topography and significant adhesion to nucleic acid-graphene substrate suggests robust cell viability. Our findings indicate potential enhancement of graphene for stem cell viability and differentiation.

T70.00029: INSTRUMENTATION AND MEASUREMENTS —

T70.00030: Determination of cantilever's spring constant by using single-optic-fiber radiation-pressure technique  HEONHWA CHOI, JAE-HYUK CHOI (Presenter), Korea Research Institute of Standards and Science — We generated sub-femtonewton radiation-pressure forces to drive a very soft silicon-nitride cantilever without highly reflective coating and determine its spring constant in the range of \(10^{-5} \text{ N/m.}\) To be applicable to cantilevers of general dimensions and reflectivity, we built an experimental setup with a single optic fiber accessing a cantilever surface and an in-situ reflectivity measurement feature. A 1320-nm laser from a superluminescent diode was used to generate oscillating forces of 0.2–1 femtonewton, and a tunable laser to measure the cantilever’s displacement and its absolute distance from the fiber. The origin of the discrepancy between the obtained and bulk values of silicon-nitride reflectivity is to be discussed.

T70.00031: Development of the Millimeter-wave Camera with High Time Resolution for Observation of the Vortex Beam  ASAKI TANABE (Presenter), Nagoya University, TOKIHKO TOKUZAWA, National Institute for Fusion Science, SOKENDAI, YUKI GOTO, Nagoya University, TORU II TSUJIMURA, SHIN KUBO, National Institute for Fusion Science — Recently, it has been shown that a charged particle with spiral motion creates a radiation field with vortex property [1]. Since an electron in the magnetic field confinement fusion plasma has a spiral motion (electron cyclotron motion), the electron cyclotron emission (ECE) should have a vortex property. In order to demonstrate the vortex property, we will investigate the ECE from the gyro phase control electron. In this research, radiation pattern measurement of less than millisecond is required, so we are developing millimeter wave camera with high temporal resolution.

The designed camera consists of an array of horn antennas followed by waveguides and microstrip lines for directing the millimeter wave power to an array of high time resolution detectors. Optimization of the coupling from the waveguide to the microstrip line and the detector is performed using the 3D finite difference time domain method (FDTD method). The details of the optimization of the camera design and resultant experimental characteristic of this camera will be discussed.


T70.00032: Extracting Ion Transport Properties from Scanning Probe Measurements on Smectite Clay Nanoparticles  AYDIN WELLS (Presenter), KELSEY YEE, N. E. ISRAELOFF, Northeastern University — Using finite element modelling, electronic simulations under an electrical load can be designed to better understand ion transport properties of smectite clay nanoparticles (NP). Smectite clay is a layered, porous material capable of changing its physical properties when hydrated upon exposure to water vapor. With a conducting atomic force microscope (AFM) tip, scans on the surface of these particles were done; data relating to particle topography and frequency-dependent electric forces was extracted from these experiments. A finite element method (FEM) model and Matlab programs were constructed to facilitate simulation of AFM system parameters, measurements, and computation. The equivalent charge method offered an advanced approach to computing NP electric properties with the irregular shaped AFM tip by modeling the force resulting from a series of test charge-image interactions. FEM simulations revealed that dielectric phase shift followed a power law with increasing voltage frequency on the AFM tip. With different conductivity anisotropy, force derivative and phase shift values were observed to have different frequency dependencies. Computational results were paired with experimental findings to extract frequency dependent NP conductivity to compare to bulk measurements.
The Casimir Effect is a physical manifestation of quantum fluctuations of the electromagnetic vacuum. When two metal plates are placed closely together, typically much less than a micron, the long wavelength modes between them are frozen out, giving rise to a net attractive force between the plates, scaling as $d^{-4}$ (or $d^{-3}$ for a spherical-planar geometry) even when they are not electrically charged. In this work we show that by modifying a post-release MEMS accelerometer, similar to the one in your phone, we can actually measure this effect in ambient conditions. This device is a step towards leveraging the Casimir Effect for cheap, sensitive, room temperature quantum metrology.

*This work is funded by the National Science Foundation grant no. 1708283, the Engineering Research Centers Program of the National Science Foundation through NSF (11) (12) 16 Cooperative Agreement under Grant EEC-0812056, Grant EEC-1647837, and Grant ECCS-1708283, and the DARPA Atoms to Product (A2P) Program/Air Force Research Laboratory (AFRL) contract no. FA8650-15-C-7545.

T70.00034: Superconducting Nanowire Single Photon Detectors for Nuclear Physics+ TOMAS POLAKOVIC (Presenter), Physics Division, Argonne National Laboratory, JOHN E. PEARSON, AXEL F HOFFMANN, Materials Science Division, Argonne National Laboratory, VOLODYMYR YEFREMENKO, CLARENCE CHANG, High Energy Physics Division, Argonne National Laboratory, WHITNEY ARMSTRONG, ZEIN-EDDINE MEZIANI, KAWTAR HAFIDI, Physics Division, Argonne National Laboratory, GORAN KARAPETROV, Department of Physics, Drexel University, VALENTYN NOVOSAD, Materials Science Division & Physics Division, Argonne National Laboratory — Superconducting nanowire single photon detectors (SNSPD) are becoming the most prominent technology in the fields of nanophotonics and quantum information sciences because of their excellent detection efficiency and timing capabilities. The possibility of high detection rates and superior timing jitter, they are also an attractive technology in the field of nuclear and particle physics as a replacement for conventional light detectors or as detectors of charged particles. These applications have unique challenges, as the detectors need to operate in strong magnetic fields and withstand radiation damage.

We present results of characterization of Niobium Nitride SNSPDs fabricated by ion beam assisted sputtering with focus on their detection capabilities in magnetic fields and effects of radiation damage on the material and detection characteristics.

*This work was supported by the U. S. Department of Energy (DOE), Office of Science, Offices of Nuclear Physics, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-06CH11357.

T70.00035: HAXPES Lab: A novel laboratory-based Hard X-ray Photoelectron Spectroscopy System ANNA REGOUTZ (Presenter), Imperial College London, MANFRED MASCHECK, TOMAS WIEL, SUSANNA ERIKSSON, CRISTOPHER LILJENBERG, Scienta Omicron, KORNELIUS TETZNER, Imperial College London, BENJAMIN WILLIAMSON, DAVID SCANLON, University College London, PAUL PALMGREN, Scienta Omicron — Hard X-ray photoelectron spectroscopy (HAXPES) uses X-rays in the 2-10 keV range to excite photoelectrons, which are used to non-destructively probe the local chemistry and electronic structure of materials. It is particularly useful as it can be applied to bulk as well as structured samples. HAXPES is a powerful technique for the study of buried layers and interfaces in multilayer thin film stacks and composite materials. Up to now HAXPES was only available at synchrotron sources, which provide the necessary intense, high energy X-rays. This work presents a new laboratory-based instrument capable of delivering monochromated hard X-rays with an energy of 9.25 keV, giving an excellent energy resolution of <0.5 eV. The instrument behaviour and capability is showcased by experimental results from reference as well as technologically relevant systems, including TiO$_2$ bulk samples and multilayer metal oxide structures used in transistors. Measurements including shallow and deep core levels, Auger lines, and valence bands will be presented, including comparison of valence data with theoretical density of states calculations.

T70.00036: Diffraction of the Millimeter Wave with Vortex Property by a Triangular Aperture YUKI GOTO (Presenter), Nagoya University, TORU II TSUJIMURA, SHIN KUBO, National Institute for Fusion Science — Recently, it has been shown that a radiation from a charged particle with spiral motion has vortex property. Various researches regarding a vortex beam has been carried out not only in the visible region but also in the various frequencies. Since an electron cyclotron motion is also spiral motion, an Electron Cyclotron Emission (ECE) should have vortex property. In order to experimentally demonstrate the vortex property of ECE, we have tried to generate the gyro-phase controlled multi-electron system, which can actively emit the ECE with vortex property. For this experiment, we developed the method to estimate the vortex property and to identify the Topological Charge (TC). This method is successfully checked by using the passively generated vortex beam from Gaussian beam in the millimeter wave region. The diffraction pattern by a triangular aperture of the passively generated vortex beam is observed. Since the diffraction pattern depends on the TC, we can identify the TC of the vortex beam. As a result, we were able to measure the characteristic diffraction patterns of millimeter wave vortex beam by a triangular aperture for the first time in the world. We will show the details of the experimental and calculation results.
T70.00037: Increasing Solution Viscosity in Dynamic Light Scattering to Lower the Detection Limit for the Determination of Nanoparticle Size* HRISTO IVANOV (Presenter), BRYAN AUGSTEIN, ANTON WIGGINS, CLAYTON PALMER, JEFFREY SIMPSON, Towson University — We report on the development of homebuilt Dynamic Light Scattering (DLS) instrumentation to measure the size of monodisperse (MD), spherical nanoparticles (NPs) of gold. HeNe and Ar-ion lasers constitute the excitation sources for the scattering experiment, while an avalanche photodiode detects the scattered light, and an autocorrelation card analyzes the resulting signal to provide a measurement of the translational diffusion coefficient, which allows for the determination of NP diameter. We characterized our instrumentation using commercially-produced gold NPs with diameters ranging from 50nm to 200nm in aqueous solution. Given the strong temperature-dependence of the solution viscosity, periodic ambient temperature measurements were used to produce dynamic values for viscosity and minimize uncertainty in the determination of NP size. Increasing the liquid viscosity slows down the Brownian motion of the NPs and affords measurement of smaller-sized particles that otherwise diffuse too fast for detection. Currently we are suspending NPs in higher viscosity solutions in an effort to lower our size detection floor from approximately 50nm to 10nm.

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T70.00038: Complex Materials Scattering (CMS) Beamline at NSLS II: Recent Developments and Progress toward Autonomous Exploration of Material Structure* MASAFUMI FUKUTO (Presenter), RUIPENG LI, National Synchrotron Light Source II, Brookhaven National Laboratory, KEVIN G. YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory — The CMS beamline at the National Synchrotron Light Source II provides small- and wide-angle x-ray scattering (SAXS/WAXS) capabilities for materials science community. Since 2017, CMS has been supporting user experiments involving a wide range of materials, from polymers, nanocomposites, liquid crystals, biomolecular materials, to self-assembled nanoparticle superlattices and lithographic nanostructures. To promote efficient exploration of material parameter spaces, CMS has implemented a variety of high-throughput and in-situ capabilities. Besides basic transmission and grazing-incidence (GI)SAXS/WAXS capabilities, CMS has demonstrated, and offers, technically demanding capabilities such as specular reflectivity, variable-angle methods (CD-SAXS/CD-GI-SAXS), and grazing-incidence scattering tomography. We will discuss these developments as well as our recent progress with implementing autonomous x-ray scattering experiments in which decision-making algorithms are integrated into a closed-loop beamline workflow pipeline.

*The CMS beamline is operated by NSLS II and CFN, which are U.S. Department of Energy (DOE) Office of Science User Facilities operated for the DOE Office of Science by Brookhaven National Laboratory under Contract No. DE-SC0012704.

T70.00039: Atomically Resolved Probe-type Scanning Tunneling Microscope for Use in Harsh Vibrational Cryogen-free Superconducting Magnet* WENJIE MENG (Presenter), JIHAO WANG, YUBIN HOU, Anhui Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory and Hefei Science Center, Chinese Academy of Sciences, MENGQIAO SUI, Oxford Instruments Technology (Shanghai) Co., Ltd, JUNTING WANG, Anhui Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory and Hefei Science Center, Chinese Academy of Sciences, GANG WU, Oxford Instruments Technology (Shanghai) Co., Ltd, JING ZHANG, Anhui Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory and Hefei Science Center, Chinese Academy of Sciences, JUNYUN LI, Oxford Instruments Technology (Shanghai) Co., Ltd, QINGYOU LU, Anhui Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory and Hefei Science Center, Chinese Academy of Sciences — We present a probe-type scanning tunneling microscope (STM) with atomic resolution that is designed to be directly inserted and work in a harsh vibrational cryogen-free superconducting magnet system. When a commercial variable temperature insert (VTI) is installed in the magnet and the STM is in turn housed in the VTI, a lowest temperature of 1.6 K can be achieved, where the STM still operates well. We have tested it in an 8 T superconducting magnet cooled with the pulse-tube cryocooler (PTC) and obtained atomically resolved graphite and NiSe2 images as well as the scanning tunneling spectrum (STS, i.e. dI/dV spectrum) data of the latter near its critical temperature, which show the formation process of the superconducting gap as a function of temperature. The drifting rates of the STM at 1.6 K in X-Y plane and Z direction are 1.15 and 1.71 pm/min respectively. This is important as a cryogen-free magnet system has long been considered too harsh for any atomic resolution measurement.

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**T70.00040: New Design for Inertial Piezoelectric Motors**

JING ZHANG (Presenter), Anhui Province Key Laboratory of Condensed Matter Physics at Extreme Conditions, High magnetic filed laboratory of the Chinese Academy of Sciences, LIGE LIU, University of Science and Technology of China, WENJIE MENG, JIHAO WANG, YUBIN HOU, QINGYOU LU, Anhui Province Key Laboratory of Condensed Matter Physics at Extreme Conditions, High magnetic filed laboratory of the Chinese Academy of Sciences — We have designed, implemented, and tested the performance details of a new type of piezoelectric motor called the CicadaDrive. It is a new motor design that the total friction force can be dramatically reduced or even canceled by pushing the clamping points at the ends of a piezoelectric tube in the opposite directions during piezoelectric deformation. While our new motor requires the addition of another piezoelectric tube, which leads to an increase in volume of 120% when compared with traditional inertial piezoelectric motors, we can realize far greater performance than two times, including step size, threshold voltage, stability, etc. Its highly integrated structure means that this motor is suitable for use as either a motor or a scanning unit.

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**T70.00041: Terahertz Interferometric Microscopy**

YESENIA A. GARCÍA, NASER QURESHI (Presenter), DAHI LUDIM HERNANDEZ-ROA, JESÚS GARDUÑO-MEJÍA, ICAT, Universidad Nacional Autónoma de México, CARLOS GERARDO TREVIÑO-PALACIOS, INAOE, Puebla, Mexico — We report on the development of a continuous wave near-field scanning microscope operating in the 500-600GHz frequency range. The use of interferometric detection allows for enhanced sensitivity and the use of low cost thermal detectors even when using a low power radiation source. We present representative images of both soft and hard matter samples.

*Work funded by CONACyT CB253754, Fronteras 344 and PAPIIT UNAM IN106316.

**T70.00042: Computing the 3D Radial Distribution Function: An Advanced Analytic Approach**

BERND KOPERA, MARKUS RETSCH (Presenter), Department of Chemistry, University of Bayreuth, 95447 Bayreuth, Germany — The radial distribution function, g(r), is ubiquitously used to analyze the internal structure of particulate systems. Applications range from molecular dynamic simulations to confocal microscopy of colloids. Measured particle coordinates are always confined in a finite sample volume. Computing g(r) is challenging once the radial distance, r, extends beyond the sample boundaries in at least one dimension. State of the art algorithms for g(r) use artificial periodic boundary conditions to circumvent this challenge. Ignoring the finite nature of the sample volume distorts g(r) significantly. Here, we present a simple, analytic algorithm for the computation of g(r) in finite samples. No additional assumptions about the sample are required. The key idea is to use an analytic solution for the intersection volume between a spherical shell and the sample volume. In addition, we discovered a natural upper bound for the radial distance that only depends on sample size and shape.

**T70.00043: In Operando micro-Raman 3D thermometry with diffraction-limit spatial resolution for GaN-based light-emitting diodes**

TAEYOUNG PARK (Presenter), YONG ZHANG, University of North Carolina at Charlotte, YONG-JING GUAN, ZHIQIANG LIU, Chinese Academy of Science, Institute of Semiconductors — Confocal micro-Raman microscopy performed in the transparent spectral region of a semiconductor can in principle be used for *operando* 3D thermometry with optical diffraction-limit spatial resolution. However, when applied to high power GaN-based light-emitting diodes (LEDs), the applicability is hindered by the often strong secondary electroluminescence (EL) in the visible spectral region that overwhelms the Raman signal. We develop a “split-time-window” scheme that can mimic the continuous wave (CW) operation but without the interference of the secondary emission, which allows us to carry out noninvasive 3D temperature profiling, thus, a comprehensive thermal analyses of the whole device, at any operation current. The technique is applied to an InGaN/GaN LED to extract its 3D temperature distribution when operated at 350 mA with µm scale resolution when using 532 nm laser. We show that although a conventional technique can yield reliable average temperature difference between the heat sink and the LED junction (a few degrees), the spatial fluctuations are much larger than the average difference. Furthermore, we show that using anti-Stokes to Stokes Raman intensity ratio as metric can yield more reliable and accurate results than using Raman frequency shift.

*ARO/Electronics & IOS
Chromatographic $^3$He purification system, with an acoustic purity monitor*  

WENGUANG JIANG (Presenter), YOONSEOK LEE, Physics, University of Florida, BRODIE POPOVIC, Physics, Duke University, COLIN BARQUIST, Physics, University of Florida — A system for Helium extraction and purification (SHeEP) is constructed around a chromatographic cylinder filled with activated charcoal to remove $^4$He contamination from $^3$He gas [1]. In order to monitor the composition of the mixture during the process, an acoustic cavity is designed. The acoustic cavity measures the average atomic mass of the mixture by measuring the speed of sound [2][3]. The sensitivity of the acoustic cavity is estimated to be 0.04%. It provides a cheap alternative to a mass spectrometer.


*NSF DMR-1708818

Axisymmetric Neutron Analyzers to Enable Efficient Powder Neutron Diffractometers*  

BORIS KHAYKOVICH (Presenter), IBRAHIM ALNAMI, Massachusetts Institute of Technology, ALEXANDRU STOICA, Oak Ridge National Laboratory, JAY THEODORE CREMER, Adelphi Technology, Inc. — State-of-the-art thermal neutron sources are large expensive national facilities, which serve a diverse community of scientific and industrial users. The need to improve the performance of neutron instruments stems from the fact that most neutron methods are limited by the available flux, even at high-flux facilities. Many neutron methods cannot be used effectively at small sources available at universities and industrial laboratories. Thus, the efficient use of neutron flux is important for the progress and broader use of these neutron techniques. We present a novel design of an axisymmetric analyzer for powder diffraction to enable polychromatic cold and thermal neutron diffractometers, which will have much higher throughput than existing instruments and enable diffractometers at small reactors or even laboratory neutron generators. At the large neutron sources, such analyzers would enable fast screening of multiple samples or measuring kinetic processes.

*Research was supported by the US Department of Energy, Office of Basic Energy Sciences, under Awards no. DE-SC0018454

Mask aligner for ultrahigh vacuum with capacitive distance control  

PRIYAMVADA BHASKAR (Presenter), SIMON MATHIOUDAKIS, TIM OLSCHIEWSKI, FLORIAN MUCKEL, JAN RAFAEL BINDEL, MARCO PRATZER, MARCUS LIEBMANN, MARKUS MORGENSTERN, RWTH Aachen University — We present an ultrahigh vacuum mask aligner driven by three piezoelectric motors which guide and align a SiN shadow mask under capacitive control towards a conductive sample surface. The three capacitors for read out are located at the backside of the thin mask. The mask can be placed in micrometer distance from the sample surface without touching it, while deliberately keeping it parallel to the sample surface. The sample can additionally be displaced laterally with respect to the mask with a precision of few nanometers. Samples and masks can be exchanged in-situ with a wobble stick. We demonstrate an edge sharpness of the deposited structures below 100 nm, which is likely limited by the diffusion of the deposited Au on Si(111).

Characterization of LED Temperature Dependence and Power-Efficient LED Modulation Methods for Use in Fluorescence Absorption Spectroscopy  

PHILLIP KUPLIC (Presenter), LUCAS J KOERNER, Engineering, University of St. Thomas — Temperature characteristics of LEDs impact the performance of optical instruments. We have characterized these effects by powering various colors of high-powered LEDs in constant current mode and analyzing the light output with a spectrometer. Light intensity, center wavelength, and spectral full width at half maximum (FWHM) was recorded as temperature changed, allowing for a better understanding of the relationship between temperature and the characteristics of light. Results show that an increase in temperature (range of 40 °C) decreases the efficiency (average of 15%; peak of 46%), increases the FWHM (average of 6.7%), and causes the center wavelength to shift to the red. Furthermore, we present the impact of sinusoidal current modulation upon the wavelength spread of LEDs. Circuit approaches for power efficient modulation are proposed that minimize changes in LED characteristics and produce pure sine-waves. Temperature characterization measurements and modulation methods are critical for low-cost and portable medical instruments.
T70.00049: Reducing thermal conductivity through lattice softening*  RILEY HANUS (Presenter), MATTHIAS AGNE, JEFF SNYDER, Northwestern University — Two fundamentally different avenues for controlling a materials thermal conductivity are phonon scattering and lattice softening. Lattice softening recognizes that lattice defects alter the phonon dispersion relation and thus reduce the lattice thermal conductivity ($\kappa_L$) by reducing phonon frequencies and group velocities. I will discuss experimental data on several systems (Si, PbTe, and SnTe) which demonstrate that microstructural defects such as grain boundaries, dislocations, and vacancies can significantly softening a materials lattice, reducing the materials speed of sound. By analyzing the data on elasticity and thermal conductivity through transport modeling, it is shown that lattice softening is a dominate mechanism for the reduction of $\kappa_L$ in these systems. Additionally, it will be shown that lattice softening is theoretically expected to be more effective than phonon scattering effects in anharmonic materials and at high temperatures. This work demonstrates how lattice softening is emerging as an important mechanism for controlling a materials thermal conductivity, and provides new avenues to engineer a materials $\kappa_L$, beyond phonon scattering.

*GJS and RH acknowledge EFRC (S3TEC) Grant DE-SC0001299. RH acknowledges support from the Weertman Graduate Fellowship.

T70.00050: Near-field radiative heat transfer in the presence of edge states  GAO MIN TANG (Presenter), JIAN-SHENG WANG, physics, National University of Singapore — We demonstrate that dispersionless electronic edge states substantially enhance near-field radiative heat transfer. An unusual heat flux dependence on vacuum gap separation is found, where the heat transfer can reach local maxima at experimentally feasible gap separation. The underlying mechanisms for the peculiar effects are uncovered from a simple Su-Schrieffer-Heeger model, and we propose zigzag single-walled carbon nanotubes as experimental realizations. Our results offer a novel route to active radiative thermal switch, where the heat flux can be modulated through tuning the presence or absence of edge states.

T70.00051: Thermoelectric Transport at Organic-silicon interface*  NAIMING LIU, MONA ZEBARJADI (Presenter), University of Virginia — Hybrid organic-inorganic materials are among the latest class of materials proposed for thermoelectric applications. The organic-inorganic interface is critical in determining the effective transport properties of the hybrid material. We present results on the thermoelectric properties of the F4TCNQ—silicon interface. Transfer of electrons from silicon to F4TCNQ results in holes trapped within the screening length of the interface that can move parallel to the interface. We report the response of these trapped charges to applied temperature differential and compare the thermoelectric transport properties of the silicon with and without F4TCNQ. The results confirm the presence of interface charges and demonstrate enhanced interface thermoelectric power factor.

*National Science Fundation grant #1653268

T70.00052: First principle study of lithium diffusion pathways in layered oxide Li2La(TaTi)O7  MING YU (Presenter), Physics and Astronomy, University of Louisville, SELORM JOY FANAH, Chemistry, University of Louisville, ASHFIA HUQ, Oak Ridge National Laboratory, FARSHID RAMEZANIPOUR, Chemistry, University of Louisville — Layered oxides, as the Ruddlesden-Popper family, have the potential to be a good lithium-ion conductor as solid electrolytes for lithium ion batteries. Recently, new family member, the layered Li2La(TaTi)O7 has been successfully synthesized [1] and its ionic conductivity has been examined. Our first principle calculations reveal the orientation of lithium diffusion pathways and the energy barriers in these pathways, which are directly correlated with the atomic arrangement of this material. We also found that the energy barriers will be lowered with Li deficiency, indicating that introducing lithium defects can also improve the lithium diffusion, and therefore the ionic conductivity, agreement with our experimental observations. These results have broad implications with regard to the design of a new class of Li-conducting oxides based on Ruddlesden-Popper oxides.

T70.00053: Understanding H-ion transport dynamics in superionic conductor BaH$_2$ * QIANGQIANG GU (Presenter), Peking University, FEIPENG ZHENG, Jinan University, JI FENG, Peking University — Superionic conductors have received increasingly attentions due to the potential applications to energy storage, fuel cells, solid electrolytes, etc. BaH$_2$ was experimentally reported as a superionic conductor which exhibits ionic conductivity of nearly 0.2 S/cm at 630 °C, an order of magnitude larger than that of state-of-the-art proton-conducting perovskites at this temperature [1]. However, the mechanism of H-ion conduction therein still remains investigations. In this work, we use first-principles nudged elastic band (NEB) simulations to compute the energy barriers. The quantum dynamic effects were considered by path-integral Monte Carlo (PIMC) sampling. Free energy surface was calculated using PIMC combined with umbrella sampling method. Furthermore, kinetic Monte Carlo (kMC) simulations were carried out to compute the ionic mobilities and conductivities which match well with the experimental data.


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T70.00054: Crystallization Dynamics of Amorphous Solid Electrolytes using Large Scale Atomistic Simulations * CHRIS ABLITT (Presenter), Department of Materials, Imperial College London, MORDECHAI C KORNBLUTH, JONATHAN P MAILOA, Research and Technology Center North America, Robert Bosch LLC, BORIS KOZINSKY, Harvard University — LiPON ceramic glass electrolytes offer the possibility to increase the energy density of batteries thanks to their resistance to dendrite formation, a problem in batteries using Li-metal anodes, yet the conductivity of oxide glasses is relatively poor. This work studies the fundamental process of amorphization, crystallization, and ion conduction within a wide composition range of lithium phosphate systems. We employ atomistic force fields developed from ab-initio dynamics trajectories and validated on lithium phosphates with comparison to ab-initio trajectories and experimental characterization. Using large-scale dynamics simulations we predict the structural relaxation and conductivity of glass electrolyte materials, reaching timescales and system sizes inaccessible to ab-initio methods. We show how the Li content determines both the ionic conductivity and the degree of corner-sharing, which in turn determines the ease of amorphization and provides insight into optimal glass processing conditions.

*This work is partially supported by the Advanced Projects Research Agency - Energy (ARPA-E), US Department of Energy, and by the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the US Department of Energy.

T70.00055: Photovoltaic and thermoelectric indirect coupling for maximum solar energy exploitation MOHAMMED HAJJI (Presenter), physics, LaMCSi, Faculty of Sciences, Mohammed V University in Rabat, Morocco — Advanced photovoltaic devices with a high performance/cost ratio is a major concern nowadays. In the resent study, we investigate the energetic efficiency of a new concept based on an indirect (instead of direct) photovoltaic and thermoelectric coupling. Using state-of-the-art thermal transfer calculations, we have shown that such an indirect coupling is an interesting alternative to maximize solar energy exploitation. In our model, a concentrator is placed between photovoltaic and thermoelectric systems without any physical contact of the three components. Our major finding showed that the indirect coupling significantly improve the overall efficiency which is very promising for future photovoltaic developments.

T70.00056: High-performance organic solar cells by adding the third component YAO WU (Presenter), THOMAS RUSSELL, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Organic solar cells have attracted much attention over the past decades, which have numerous advantages, including solution-processability, low cost, light weight, and flexibility. Due to the development of non-fullerene acceptors, the efficiencies of organic solar cells were increased to 17% for a tandem junction and 14% for a single junction. To further improve the efficiency of organic solar cells, a third component can be added to the active layer making a ternary blend film. Ternary blend film contains a donor material, an acceptor material, and a third component having complimentary absorption with the donor and acceptor, increasing the light harvesting ability of the devices. Some of the third components have suitable energy levels to reduce the charge transfer barriers between the donor and acceptor. The added component can also induce the crystallization of the donors and change the morphology of the blend film. In our work, a few third components were selected to add in the active layer, which leads to an improvement of the device performance. Also, the absorption, charge transportation and the morphology of the ternary system were carefully investigated to understand how the third component influences the efficiency of organic solar cells.
levels seems to have a larger influence on the efficiency of the cell. Conduction bands would increase the open circuit voltage and possibly the efficiency of these "band-matched" solar cells. It was hypothesized that avoiding energy loss due to large differences between the CdSe and metal oxide nanoparticulate substrates. Metal oxides were chosen to closely match their conduction bands with the conduction bands of the CdSe. We found that the opposite was true and that the improved electron kinetics due to larger differences in conduction band levels seems to have a larger influence on the efficiency of the cell.

*We wish to acknowledge and thank the Neuhoff Summer Science Communities Grant for providing seed funding for this project.

**T70.00058: Light absorption induced band bending in p-type Cu$_2$(Zn,Sn)(S,Se)$_4$ thin-film photovoltaic cells: local Raman imaging and scanning probe microscopy** JURAN KIM (Presenter), Department of Physics, Ewha Womans University, KEE-JEONG YANG, DAE-HWAN KIM, JIN-KYU KANG, Convergence Research Center for Solar Energy, Daegu Gyeongbuk Institute of Science & Technology (DGIST), WILLIAM JO, Department of Physics, Ewha Womans University — Kesterite-structured Cu$_2$ZnSn(S,Se)$_4$ (CZTSSe) is one of the most promising materials for highly efficient and low-cost thin-film solar cells because of its appropriate optical and electrical properties. The best efficiency of CZTSSe solar cells is 12.6%, which was obtained using a hydrazine process, while the materials used in this study showed efficiency of 12.3%. Note that the CZTSSe thin-films were grown by sputtering and subsequent sulfur-selenium treatment. Raman spectroscopy imaging was utilized to measure local built-in voltage and its local composition. According to the surface potential results, we were able to observe upward band bending near grain boundaries, meaning intra-grains take a role as current path by collected electrons. Unlike Cu(In,Ga)Se$_2$, defects in CZTSSe thin-films have deep energy levels, which can be charge carrier recombination center and cannot be suitable for a current path. By measuring surface photo-voltage, we observed the significant changes in energy band bending under illumination, implying the existence of these interfacial states. The main contribution of the research is related to the realization of new way for carrier separation enhancing power conversion efficiency of the kesterite-based thin-film solar cells.

**T70.00059: Scalable Transparent Metal-polymer Hybrid Metamaterial for Enhanced Greenhouse Effect** TAO LI, YIN GAO, Institute of Engineering Thermophysics, Chinese Academy of Sciences, KUN ZHENG, YONGMEI MA, Institute of Chemistry, Chinese Academy of Sciences, XIULAN HUAI, Institute of Engineering Thermophysics, Chinese Academy of Sciences, DING DING (Presenter), Agency for Science, Technology and Research, HANG ZHANG, Institute of Engineering Thermophysics, Chinese Academy of Sciences — Tailoring the emissivity of optically engineered materials in both the solar and the ambient blackbody radiation wavelength has led to significant day-time radiative cooling. It is conceivable that manipulating the optical spectrums in the opposite way will lead to enhanced greenhouse effect, as demonstrated in current commercial low-emissivity (low-E) window coatings. In this work, based on Mie scattering and the principle of surface plasmon polaritons for enhanced transparency, metallic nanowire/polymer hybrid structures were designed to achieve the goal of enhancing day-time heating. This metal-polymer hybrid metamaterial can enhance solar heating in enclosed environment or reject thermal radiation for energy saving in air-conditioned environment. The resulted metamaterial can reflect the mid-infrared spectrum effectively(~80%) and be transparent(transmittance of about 85%) to sunlight spectrum at the same time. Comparing our metamaterial with commercial low-E glasses, our metamaterial is more transparent in the visible and less emissive in the infrared. In addition, this type of metamaterials is flexible and can be scalable-manufactured with lower cost than that of low-E glasses.

**T70.00060: Effects of Prolonged Heat Exposure on the Performance Characteristics of Monocrystalline Silicon Photovoltaic Cells** AMANDA PORTOFF (Presenter), ANDREW D VENZIE, JUSTIN L SMOYER, PAUL QUINN, Kutztown University of Pennsylvania — Solar energy is a rapidly growing field of study since alternative energy sources, especially those that are renewable and economically feasible, are highly sought after. Silicon photovoltaic cells are the most commonly used type of cell, yet limitations in their efficiency place a restraint on overall effectiveness. The objective of this research was to observe the effects on the performance characteristics of monocrystalline silicon photovoltaic cells after being exposed to high temperatures for fixed periods of time. In particular, we examined the open-circuit voltage, $V_{oc}$, and short-circuit current, $I_{sc}$. To observe these changes, the cells were heated at temperatures ranging from 200°C to 280°C for a duration of 20 minutes. An analysis of various IV curves was used to determine changes in performance characteristics of the cells exposed at different temperatures. Our study revealed that this heat exposure yielded a permanent alteration in the performance of the cell. Ultimately, this exposure led to an increase in the overall performance of the monocrystalline silicon photovoltaic cell. Such an increase in performance occurred with existing cells, requiring no significant changes to the manufacturing process.
Morphology Controlled Electrospun Fibers as the Catalyst Layer for Polymer Electrolyte Membrane Fuel Cells

LIKUN WANG (Presenter), Stony Brook University, GUAN HAO CHEN, St. George's School, Vancouver, Canada, DANIELLE KELLY, Friends Academy, Locust Valley, NY, ZIPEI LIU, Shenzhen Middle School, Shenzhen, China, AUDREY SHINE, Plainview Old-Bethpage JFK High School, Plainview, NY, KAO LI, MIRIAM RAFAILOVICH, Stony Brook University — The efficient operation of Polymer Electrolyte Membrane Fuel Cells (PEMFCs) largely relies on a costly and easily-degradable platinum catalyst layer. Although air spraying techniques has previously served as the main method of catalyst deposition, electrospinning deposition may provide a more promising method by granting users precise control over 3-D structures by manipulating fiber diameter, porosity, and alignment. 12wt% of poly(acrylic acid) (PAA) and Nafion (1:4 weight ratio) solution was used to obtain a semi-viscous base solution for electrospinning. Through Laser Optical Microscopy and Scanning Electron Microscopy, optimal fiber diameter of 1 μm was found when incorporated with Pt/C, allowing uniform catalyst nanoparticles attachment. The fuel cell performance tests indicate that the morphology optimized electrospun electrodes exhibited a 108% increase in max power output over air-sprayed electrodes of comparable loading. This enhancement is attributed to its unique interwoven surface morphology, which increases the specific surface area of electrode and promotes the efficiency of the reactant and proton transport to catalytic sites. Thus, electrospinning can be used as a potential strategy to improve power output of PEMFCs by altering the catalyst electrode morphology.
Battery Performance and Reaction Mechanism in Tin Sulfide as Negative Electrode: First-Principles Calculations

HIROKI KOTAKA (Presenter), Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, HIROYOSHI MOMIDA, Institute of Scientific and Industrial Research, Osaka University, AYUKO KITAJOU, Organization for Research Initiatives, Yamaguchi University, SHIGETO OKADA, Institute for Materials Chemistry and Engineering, Kyushu University, TAMIO OGUCHI, Institute of Scientific and Industrial Research, Osaka University — Sodium (Na) ion batteries have been recently expected as a next-generation battery in which Li-ion batteries is replaced with Na. Tin sulfide (SnS) has been expected to have a high energy density and be a candidate for anode materials of Na-ion batteries. In this study, we investigate the battery characteristics of SnS as a negative electrode for Na-ion batteries by first-principles calculations. We calculate a phase diagram of Na-Sn-S ternary systems from energy analyses, and clarify a possible reaction route considering intermediate products in charge and discharge reactions. We theoretically estimate the voltage-capacity curves of Na/SnS half-cell systems based on the Na-SnS reaction path obtained from the ternary phase diagram, and compare with the experimental result. From the comparison between calculated and experimental results, the Na₂S reaction product can precipitate in the SnS electrodes after discharging, and it is expected that the electrode can recover to be SnS again after charging. Therefore, the conversion reactions in which Na₂S precipitates in the SnS electrodes are considered to occur reversibly.

Structural mechanisms in complex oxides enabling high-rate lithium-ion energy storage*

KENT GRIFFITH (Presenter), Northwestern University, KAMILA WIADEREK, Advanced Photon Source, Argonne National Laboratory, GIANNANTONIO CIBIN, Diamond Light Source, LAUREN MARBELLA, Department of Chemical Engineering, Columbia University, CLARE GREY, Department of Chemistry, Cambridge University — The maximum power output and minimum charging time of a lithium-ion battery depend on mixed ionic-electronic conduction. We show that complex niobium tungsten oxides with frustrated polyhedral arrangements and dense μm-scale particle morphologies can rapidly and reversibly intercalate large quantities of lithium. Analysis of high-rate and multi-electron energy storage will be discussed with insights from operando X-ray diffraction, solid-state nuclear magnetic resonance spectroscopy, and multi-edge X-ray absorption spectroscopy for the recently reported crystallographic shear structure and bronze-like oxide phases[1]. Materials and mechanisms that enable lithiation of μm particles in minutes have implications for high power applications, fast charging devices, all-solid-state batteries, and general approaches to electrode design and materials discovery.

Electrochemical kinetics of SEI growth in porous electrodes*

SUPRATIM DAS (Presenter), MICHAEL FORSUELO, MARTIN BAZANT, Chemical Engineering, Massachusetts Institute of Technology — Growth of the solid electrolyte interphase (SEI) is a major driver of capacity fade in LIBs. Despite its importance, the fundamental mechanisms remain unclear, primarily because of the complicated reaction pathways involved. SEI growth can be both electrochemical and chemical in nature, and thus, it is a strong function of the potential and degree of lithiation of the electrode. In this work, we model the early-stage and long-term growth of SEI by accurately capturing the potential dependence of its formation kinetics as well as long term rate limiting steps, and validating it against extensive experimental data. This is done using the Multiphase Porous Electrode Theory (MPET) framework on graphite (phase separating) and carbon black (non phase separating) particles. Results indicate that the peak SEI-forming currents are higher for higher driving currents. Counterintuitively, despite higher peak SEI-forming currents, the highest differential capacities or ‘extent of SEI growth’ are seen for lower driving currents, which implies that SEI formation is a stronger function of potential and cycling time, than the driving current. This work holds promise for the predictive design of procedures for manufacture and formation of LIBs.

*This project is being funded by the TRI
**T70.00068: Structure of lithium dendrite in polymer electrolytes**  
FUDONG HAN (Presenter), TIANCHENG YI, University of Maryland College Park, ROBERT GREGORY DOWNING, National Institute of Standards and Technology, ROBERT BRIBER, CHUNSHENG WANG, HOWARD WANG, University of Maryland College Park — The structure of Li dendrites grown in solid polymer electrolytes (SPE) has been studied using a symmetric sandwich cell of Li / poly(ethyleneoxide) (PEO) : lithium bis(trifluoromethane) sulfonamide (LiTFSI) / Li as a model system. In situ neutron depth profiling (NDP) during directional Li pumping and plating shows that dendrites start to grow, and eventually short-circuit the battery. Li dendrite 3D mapping reveals rather heterogeneous lateral distribution of Li over wide length scales from below a millimeter to centimeters. While the lateral mobility of Li appears to be large, most dendrites grow from the plating electrode, with the overall composition decreases linearly from the electrode interface to the bulk of the electrolyte. It is observed that dendrites also grow from the bottom electrode, where presumably only Li oxidation reaction occurs. The revelation poses new design and engineering challenges in using Li metal electrode in future batteries.

**T70.00069: Flexible Graphene-Carbon Nanotube Supercapacitors**  
KAREN PEARSON, FIT, VLADIMIR SAMUILOV (Presenter), SHI FU, Stony Brook University — A carbon fiber textile has been utilized as flexible supercapacitor electrodes with cost-effective graphene nanoplatelet composite material (GNP) as model material for coating the electrodes. GNP represent a new class of carbon nanoparticles with very high intrinsic electrical conductivity in plane and accessible surface area. Multi wall carbon nanotube (MWCNT) at the concentration 50:50 of CNT to GNP were added to take advantage of the high surface area of the composite of these two carbon nano-materials. The first experimental results without optimization showed promising supercapacitor behavior of the carbon fiber textile with bare pads, better than in [1]. GNP – MWCNT (50:50) electrode material has improved the capacitance density approximately 10 times. Our newly designed high energy supercapacitors [2] allows increasing the operational voltage window from 3V (natural restriction by the Debye length voltage drop for standard supercapacitors) to the value higher than 20V.

References:

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**T70.00070: Applying a 1D Plasma Profile Simulator to COMPASS to Model Sawtooth Instabilities**  
MARTIN LIZA (Presenter), Mechanical and Aerospace Engineering, Old Dominion University — Being able to control the plasma state and its evolution in real time is crucially important for the confinement stability. However, the complex physics that needs to be solved requires a high amount of computational power.

If experimental data is combined with a model that predicts the transport behavior of a tokamak (COMPASS), then accurate predictions can be used to develop an integrated control system that ensures the control of the plasma state and confinement stability.

An active control for the plasma instabilities will be developed using a 1D RApid Plasma Transport simulatOR (RAPTOR) code. This code solves two coupled 1D partial differential diffusion equations for the electron temperature and the poloidal magnetic flux. The RAPTOR code will be implemented in COMPASS to model and simulate sawtooth instabilities; this simulation will take into consideration Neutral Beam Injectors (NBI).

The RAPTOR code will be used as a state observer system that will predict the behavior of the plasma before it actually happens. This prediction will later be used for implementing a real time sawtooth instability control system for COMPASS and/or COMPASS-U.
T70.00071: Computational fluid dynamics modeling of a microchannel-type reactor for the coupling of OCM and reforming reactions* MYUNG-JUNE PARK (Presenter), MINJI SON, HAE LIN YANG, Ajou University, SEON-JU PARK, YUN-JO LEE, Korea Research Institute of Chemical Technology — Oxidative coupling of methane (OCM) is a reaction that converts methane to high-value added ethylene and ethane. However, strong exothermic heat of reaction leads to thermally unstable operation and lowers the selectivity of the desired species. To control the heat of OCM, we developed a microchannel-based reactor that couples OCM with the steam reforming of methane (SRM), one of strong endothermic reactions.

The computational fluid dynamics model clearly showed that temperature increase in the OCM bed was maintained below 80 °C and the reaction temperature was close to the optimal one (820 °C). However, the temperature profile in the SRM bed showed abrupt decrease due to strong endothermic characteristic. To expand the kinetically controlled region of the SRM bed, the effects of the operating conditions and structure parameters were evaluated.

In conclusion, the modeling approach in the present study could determine the optimal operation strategy, and provide important information on the design of industrial microchannel based reactors.

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T70.00072: Raman Spectroscopy of Diesel and Gasoline Engine-Out Soot* ZHIPENG YE (Presenter), HAIWEN GE, RUI HE, Texas Tech University — We studied engine-out soot samples collected from a heavy-duty direct-injection diesel engine and a port-fuel injection gasoline spark-ignition engine. The two types of soot samples were characterized using Raman spectroscopy with different laser power. A Matlab program using least-square-method with trust-region-reflective algorithm was developed for curve fitting. We used a DOE (design of experiments) method to avoid local convergence. This method was used for two-band fitting and three-band fitting. The fitting results were used to determine the intensity ratio of D and G Raman bands. We find that high laser power may cause oxidation of soot samples, which gives higher D/G intensity ratio. Diesel soot has consistently higher amorphous/graphitic carbon ratio and thus higher oxidation reactivity, in comparison to gasoline soot, which is reflected by the higher D/G intensity ratio in Raman spectra measured under the same laser power.

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T70.00073: Fundamentals of the photocatalytic activity of conjugated polymers for hydrogen evolution reaction: optical and thermodynamic aspects GIANE DAMAS (Presenter), CLEBER F. MARCHIORI, C. MOYES ARAUJO, Department of Physics and Astronomy, Uppsala University — Harvesting sunlight is a convenient approach to meet the global demand of energy, a process that makes use of a suitable photo-electro-catalyst to convert solar energy into chemical fuels[1]. In this context, conjugated polymers have emerged as a subclass of materials with potential applicability as photocatalysts for hydrogen evolution reaction (HER). [2] In this work, we use density functional theory-based methods to evaluate the thermodynamic and optical properties of a set of conjugated polymers containing fluorene, cyclopenthathiophene or thiophene-based donor units and benzothiadiazole-based acceptor units. Optimizations and frequencies were held in Gaussian 09 [3] at the M06-6-31G* level of theory, whereas the excitation, solvation and electronic energies were obtained with the 6-311G** basis set. Our preliminary results show that the polymers containing benzo(triazole-thiadiazole) or benzo(triazole-selenodiazole) acceptor units present a broad absorption spectrum and a suitable reduction potential for photocatalytic HER. In particular, PFO-DSeBTrT has maximum peak at 950 nm, while showing a hydrogen binding free energy (0.02 eV) that is lower in absolute values than Pt (-0.10 eV).

T70.00074: ELDOR-detected NMR Spectroscopy at 115/230 GHz* ZAILI PENG (Presenter), SUSUMU TAKAHASHI, University of Southern California — Electron-electron double resonance (ELDOR)-detected NMR (EDNMR) spectroscopy is one type of the EPR based hyperfine spectroscopy techniques, which is used to detect hyperfine couplings between magnetic nuclei and unpaired electrons, which are too small to be resolved in the conventional EPR spectrum. Compared with other commonly used hyperfine spectroscopy, for instance, ESEEM (electron spin echo envelop modulation) and ENDOR (electron nuclear double resonance), HF EDNMR has advantages of higher sensitivity and finer spectral resolution enabling high-resolution hyperfine spectroscopy at room temperature. In this presentation, we present the principle and implementation of EDNMR in our 115/230 GHz EPR spectrometer at USC, and demonstrate the strategies to obtain high quality EDNMR spectrum by the employment of EDNMR on a standard sample. In addition, we discuss applications of HF EDNMR on the study of solid-state spin systems.

*This work was supported by the Searle Scholars Program and the National Science Foundation (DMR-1508661 and CHE-1611134).

T70.00075: TOPOLOGICAL MATERIALS —
T70.00076: Floquet generation of higher order topological phases and its quenching dynamics  TANAY NAG
(Presenter), Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, VLADIMIR JURICIC, NORDITA, Nordic Institute for Theoretical Physics, Stockholm University and KTH, Stockholm, Sweden, BITAN ROY, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — We discuss a non-equilibrium Floquet scheme to generate the higher-order topological (HOT) phases. In particular, we find that if a $d$-dimensional regular topological phase involves $m$ Hermitian matrices then a kick in the discrete symmetry breaking Wilsonian mass term, which is composed of additional $p-1$ anti-commuting matrices, can give rise to $n^{th}$ order Floquet HOT phases (with $n=1,...,p$). We demonstrate explicitly this mechanism in the cases of three-dimensional spin-1/2 Dirac semimetal, 2nd order topological insulator and nodal loop semimetal. We give analytical support for the numerical findings by using the Floquet effective Hamiltonian. Additionally, we study the relaxation dynamics of the above phases by calculating the survival probability for a topological phase followed by a sudden quench. Our results suggest that survival probability for quenching from a higher-order to a lower-order phase depends on the system size while the reverse quenching does not show any system size dependence.

T70.00077: Edge states across the topological phase transition due to approximate chiral symmetry in quantum anomalous and spin Hall systems*  DENIS CANDIDO (Presenter), Sao Carlos Institute of Physics at the University of Sao Paulo, MAXIM KHARITONOV, Institute for Theoretical Physics and Astrophysics, University of Wurzburg, CARLOS EGUES, Sao Carlos Institute of Physics at the University of Sao Paulo, EWELINA HANKIEWICZ, Institute for Theoretical Physics and Astrophysics, University of Wurzburg — In this work we demonstrate that a quantum anomalous Hall system (Chern insulator) always exhibits edge states right at the phase transition (except when the system becomes charge-conjugation symmetric), where the Hamiltonian is gapless, and in the vicinity of the topologically trivial and non-trivial gapped phases. We show that the origin of these edge states can be attributed to the approximate chiral symmetry of the Hamiltonian. Additionally, we demonstrate that while the non-trivial quantum Hall topology is responsible only for the existence of these edge states within the energy gap region, the approximate chiral symmetry is the ingredient responsible for the edge state existence in the remaining energy range in both topological and trivial phases. This behavior is described by the realistic one block of the BHZ model of a quantum spin Hall system, which was already noticed but remained unexplained.

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T70.00078: Observation of multiple Dirac states in EuMg$_2$Bi$_2$*  FIROZA KABIR (Presenter), MD MOFAZZEL HOSEN, University of Central Florida, FAIROJA CHEENICODE-KABEER, ALEX APERIS, Department of Physics and Astronomy, Uppsala University, GYANENDRA DHAKAL, KLAUSS DIMITRI, CHRISTOPHER SIMS, SABIN REGMI, University of Central Florida, TOMASZ DURAKIEWICZ, Los Alamos National Laboratory, PETER OPPENEER, Department of Physics and Astronomy, Uppsala University, DARIUSZ KACZOROWSKI, Polish Academy of Science, MADHAB NEUPANE, University of Central Florida — Initiated by the discovery of topological insulators, topologically non-trivial materials especially topological semimetals and metals have emerged as a new frontier in the field of quantum materials. In this work, we perform a systematic measurement of EuMg$_2$Bi$_2$, a compound with antiferromagnetic transition temperature at 7K. By utilizing angle-resolved photoemission spectroscopy in concurrence with first principle calculation, we observe Dirac cones at the corner and the zone center of the Brillouin zone. From our experimental data odd number of Dirac states are observed per Brillouin zone. Our experimental investigation of detailed electronic structure of EuMg$_2$Bi$_2$ could potentially provide the platform to study the interplay between topology and magnetism.

*This work is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415 and the startup fund from UCF (M.N.).

T70.00079: Tunable Topological Phase Transition in 2D Heterostructures*  ANH PHAM (Presenter), PANCHAPAKESAN GANESH, Oak Ridge National Laboratory — Two dimensional (2D) materials can host a wide range of properties, such as magnetism [1], high mobility and a wide range of topological properties [2]. Recently, it has been experimentally shown that heterostructures of 2D materials can be synthesized. This leads to the exciting possibility of interfacing 2D materials in heterostructure geometries to design new and exotic quantum-materials for dissipationless quantum-transport. In this study, we theoretically demonstrate that vertical heterostructures of magnetic and topological 2D materials can give rise to quantum anomalous Hall (QAH) effect. In addition, we show that electric-fields can be used to tune the interfacial coupling to drive the system to the QAH regime. We demonstrate this concept in 2D heterostructures such as CrI$_3$/Sb/CrI$_3$, CrI$_3$/Si/CrI$_3$, and CrI$_3$/Ge/CrI$_3$.


*This research was funded by ORNL-LDRD (Project ID: 8988)
**T70.00080: Two-Step Growth Method for High Quality (Bi0.5Sb0.5)2Te3 and Cr doped (Bi0.5Sb0.5)2Te3 on Nb surfaces for Topological Josephson Junctions**  
HE REN (Presenter), University of Waterloo, HUI ZHANG, XIAODONG MA, University of Science and Technology of China, DELER LANGENBERG, University of Waterloo — It has been theoretically predicted that Majorana bound state can appear at the interface between topological insulators and superconductors. To obtain high quality (Bi0.5Sb0.5)2Te3 films on superconducting Nb surface, a two-step growth method was developed to promote proper nucleation on Nb surfaces in the early growth stage, where Bi, Sb and Te clusters were firstly evaporated at a relatively low temperature and then annealed to form a crystallized passivation layer, and a standard (Bi0.5Sb0.5)2Te3 film was grown under the normal deposition temperature secondly. Based on the two-step method, we also grew high quality Cr doped Bi-Sb-Te films on Nb surface with a similar procedure. Reflection high-energy electron diffraction (RHEED), high resolution transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) were used to characterize the quality of the films. Finally, a top Nb film was deposited by magnetron sputtering at the room temperature. The Hetero-Nb/epitaxial (Bi0.5Sb0.5)2Te3 (with and without Cr doped)/ Nb stacks were further fabricated into micro Josephson junctions and the results of transport measurement also demonstrate a good quality of the multi-layer stacks.

**T70.00081: Magnetic Weyl Points and Symmetry Protected Nodal Loops in 5d Cubic Double Perovskites**  
YOUNG-JOON SONG (Presenter), KWAN-WOO LEE, Department of Applied Physics, Graduated School, Korea University — 5d systems show abundant physical phenomena due to an interplay between strong spin-orbit coupling (SOC) and moderate correlation, viz. the Dirac-Mott metal-insulator transitions in Os-based oxides. In topological characters, various symmetries, SOC, and (sometimes) strength of correlation are key ingredients to generate topologically nontrivial phases. Using the *ab initio* approach, we have investigated topological characters in the Os-based cubic double perovskites of 5d1 and 5d2 which have a strong SOC, moderate correlation, and plentiful crystal symmetries. In our GGA results of both nonmagnetic(NM) and ferromagnetic(FM) cases, there are nodal lines around W and K points. Even for considering SOC, in the TRS-broken cases the nodal lines are robust on kz=0 plane, which is perpendicular to the direction of [001] SOC, whereas these disappear in the NM cases. Besides, in the TRS-broken cases, 14 pairs of Weyl points with opposite chirality on the mirror planes appear. Applying correlation as well as SOC, the nodal lines remain protected, while the WPs vanish. In this presentation, we will analyze the mechanisms of topological characters in the Os-based cubic double perovskites.

*This research was supported by NRF-2016R1A2B4009579.

**T70.00082: Thermoelectric Imaging of Domain Boundary States in Epitaxial Graphene**  
SANGHEE CHO, Korea Research Institute of Standards and Science, YONG-HYUN KIM, Physics, KAIST, HO-KI LYEO (Presenter), Korea Research Institute of Standards and Science — We investigated electronic states associated with the boundary structure between domains of two carbon layers in epitaxial graphene. The topological structure formed between AB and BA stacking domains could be observed in microscopic thermoelectric measurements down to the atomic length scale. Measurements show that the boundary structure observed from epitaxial bilayer graphene is associated with point defects of carbon pentagon-heptagon and the structure forms a closed loop. Such structural patterns define soliton-like domain walls driven by strain in epitaxial graphene, which gives rise to prominent contrast in the thermoelectric measurement. The contrast observed over the domain walls in the measurement of thermoelectric response is the direct consequence of chiral boundary modes expected for tensile-strained boundaries, which is similar to the structures observed in exfoliated and CVD-grown bilayer graphene. These results will help to elucidate how the topological band plays in epitaxial graphene.

**T70.00083: Bulk and surface states carried supercurrent in ballistic Nb-Dirac semimetal Cd3As2 nanowire-Nb junctions**  
CAIZHEN LI (Presenter), School of Physics, Peking University, CHUAN LI, MESA+ Institute for Nanotechnology, University of Twente, LIXIAN WANG, School of Physics, Peking University — A three dimensional Dirac semimetal has bulk Dirac cones in all three momentum directions and Fermi arcs like surface states, and can be converted into a Weyl semimetal by breaking time-reversal symmetry. However, the highly conductive bulk state usually hides the electronic transport from surface state in Dirac semimetal. Here, we demonstrate the supercurrent carried by bulk and surface states in Nb-Cd3As2 nanowire-Nb short and long junctions, respectively. For the ~1μm-long junction, the Fabry-Pérot interferences-induced oscillations of the critical supercurrent are observed, suggesting the ballistic transport of the surface states carried supercurrent, where the bulk states are decoherent and the topologically protected surface states still stay coherent. Moreover, a superconducting dome is observed in the long junction, which is attributed to the enhanced dephasing from the interaction between surface and bulk states as tuning gate voltage to increase the carrier density. The superconductivity of topological semimetal nanowires is promising for brading of Majorana fermions toward topological quantum computing.

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T70.00084: Gate-tuned Aharonov-Bohm interference of surface states in a quasiballistic Dirac semimetal nanowire*  
BENCHUAN LIN (Presenter), SHUO WANG, ZHI-MIN LIAO, Peking University, DAPENG YU, South University of Science and Technology of China — We report an observation of a topologically protected transport of surface carriers in a quasiballistic Cd$_3$As$_2$ nanowire. The nanowire is thin enough for the spin-textured surface carriers to form 1D subbands, demonstrating conductance oscillations with gate voltage even without magnetic field. The $\pi$-phase shift of Aharonov-Bohm oscillations can periodically appear/disappear by tuning gate voltage continuously. Such a $\pi$-phase shift stems from the magnetic field induced helical modes in the surface subbands.

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T70.00085: Fano Interference between Bulk and Surface States of a Dirac semimetal Cd$_3$As$_2$ nanowire*  
SHUO WANG (Presenter), BENCHUAN LIN, ZHI-MIN LIAO, Peking University, DAPENG YU, South University of Science and Technology of China — Dirac semimetals possess Fermi-arc surface states, which will be a set of discrete surface subbands in a nanowire due to the quantum confinement effect. Here, we report a tunable Fano effect induced by the interference between the discrete surface states and continuous bulk states of a Dirac semimetal Cd$_3$As$_2$ nanowire. The discrete surface bands lead to a zero bias peak in conductance as the Fermi level is tuned across the surface subbands. The Fano resonance results in an asymmetric line shape in the differential conductance $dI/dV$ spectrum. Furthermore, the Fano interference would introduce an additional phase into the Weyl orbits and lead to a modification of the oscillation frequency. The results are valuable for further understanding the exotic quantum transport properties of topological semimetals.

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T70.00086: Observation of Dirac States in Superconducting Materials*  
KLAUSS DIMITRI (Presenter), MD MOFAZZEL HOSEN, GYANENDRA DHAKAL, University of Central Florida, HONGCHUL CHOI, Theoretical Division, Los Alamos National Laboratory, FIROZA KABIR, CHRISTOPHER SIMS, University of Central Florida, DARIUSZ KACZOROWSKI, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, TOMASZ DURAKIEWICZ, National Science Foundation, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, MADHAB NEUPANE, University of Central Florida — The massive shift in interest towards Topological Superconductors (TSC) and their potential to host Majorana fermions has been a major point that connects the rhetoric of both quantum computation and topological materials. Following this narrative, superconducting Pd-Bi binaries have large spin orbit coupling strength and can develop a TSC phase peaking the interests of both fields. Here, we report a high-resolution angle-resolved photoemission spectroscopy (ARPES) study on the normal state electronic structure of superconducting $\alpha$-PdBi2 ($T_c=1.7$ K). Our results show the presence of Dirac states at higher-binding energy with the Dirac point 1.26 eV below the chemical potential at the zone center. Furthermore, the ARPES data indicate multiple band crossings at the chemical potential, consistent with the metallic behavior of $\alpha$-PdBi2. Our experimental studies are complemented by first-principles calculations, revealing the presence of surface Rashba states in the vicinity of the chemical potential. Our study extends to other superconducting materials providing an opportunity to investigate the relationship between superconductivity and topology.

*This work is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415 and the startup fund from UCF (M.N.).
T70.00087: Dynamical correlation functions and the related novel physical effects in 3D topological semimetals*  
JIANHUI ZHOU (Presenter), Hefei Institutes of Physical Science, HAO-RAN CHANG, Sichuan Normal University, DI XIAO, Carnegie Mellon University, HONG GUO, McGill University — We present a unified derivation of the dynamical correlation functions including density-density, density-current and current-current, of 3D Weyl/Dirac semimetals by use of the Passarino-Veltman reduction scheme at T=0K. The generalized Kramers-Kronig relations with arbitrary order of subtraction are established to verify these correlation functions. Our results lead to the exact chiral magnetic conductivity and directly recover the previous ones in several limits. We also investigate the magnetic susceptibilities, the orbital magnetization, and briefly discuss the impact of electron interactions on these physical quantities within the random phase approximation. Recently, we develop a gauge invariant theory of chiral magnetic plasmons and discuss the impact of the chiral anomaly. Our work provides a starting point for the investigation of the nonlocal transport and optical properties due to the higher-order spatial dispersion in 3D Weyl/Dirac semimetals.  
*the National Natural Science Foundation of China, the 100 Talents Program of Chinese Academy of Sciences, the China Scholarship Council, the NSERC of Canada, and FQRNT of Quebec.

T70.00088: Hydrothermal Synthesis of Tellurium Nanoflakes with Post Growth Thinning*  
ANNE HERBERT (Presenter), ASU ROLLAND, GIRIRAJ JNAWALI, IRAJ ABBASIAN SHOJAEI, SAMUEL M LINSER, Department of Physics, University of Cincinnati, ANJALY NANATTUCHIRAYIL, PENG ZHANG, Department of Chemistry, University of Cincinnati, HOWARD E JACKSON, LEIGH SMITH, Department of Physics, University of Cincinnati, RUOXING WANG, School of Industrial Engineering, Purdue University, GANG QIU, School of Electrical and Computer Engineering, Purdue University, WENZHUO WU, School of Industrial Engineering, Purdue University, PEIDE (PETER) YE, School of Electrical and Computer Engineering, Purdue University — Tellurium is a hexagonal chiral crystal with covalently bonded left- or right-spiral chains of atoms along the c-axis, with much weaker van der Waals interactions between the chains. The lowest conduction bands exhibit Weyl node crossings with different chiralities at the H and H' points in the Brillouin zone. We synthesize 40 nm-thick Tellurium nanoflakes via the hydrothermal method, and confirm the quality of our samples with Raman spectroscopy. The flakes were thinned through a basic NaOH solution with acetone. Thicknesses was measured with Raman spectroscopy, via peak shift, and confirmed using atomic force microscopy.  
*UC acknowledges NSF grants ECCS-1509706, DMR-1531373, and DMR-1507844. PY acknowledges NSF/AFOSR 2DARE, ARO and SRC. WZW acknowledges Purdue University and ORAU.

T70.00089: Electronic structure and optical responses of chalcopyrite semiconductors ZnSnX_2 (X = P, As, Sb)  
BANASREE SADHUHKAN (Presenter), IFW Institute for Theoretical Solid State Physics, Leibniz Institute for Solid State and Materials Research — Ternary compounds having the chalcopyrite structure are of considerable interest because of their semiconducting, electrical, structural, mechanical and nonlinear optical properties. Chalcopyrite semiconductors ZnSnX_2 (X = P, As, Sb) lack an inversion symmetry. Under strong light irradiation, the noncentrosymmetric material exhibits photocurrents as nonlinear functions of the electric field of the light. The spontaneous photocurrent is due to the topological character of the constituting electronic bands; the Berry connection. The photogalvanic effect rectifies light to dc currents and often plays a crucial role in optical devices and solar cells. Under linearly polarized light, the induced photocurrent is usually called shift current originated due to the charge center shift between the valence and conduction bands in the optical excitation. We study the electronic structure, linear and nonlinear optical response, specially the shift current of chalcopyrite semiconductors ZnSnX_2 (X = P, As, Sb) using Kubo formulism via a multiband approach using first principles. We analyze the relationship between the response and the materiars properties which serves as a deep understanding of the shift current effects in noncentrosymmetric materials over linear response.
Angle-resolved photoemission spectroscopy study of the topological Kondo insulator candidates CeRhX (X=As, Sb)

SEUNGOH SEONG, Physics, The Catholic University of Korea, KYOO KIM, 2MPPHC CPM, EUNSOOK LEE, Physics, The Catholic University of Korea, CHANG-JONG KANG, TAESIK NAM, BYUNG IL MIN, physics, Pohang University of Science and Technology, TAKENOBU YOSHINO, TOSHIRO TAKABATAKE, Department of Quantum Matter, Hiroshima University, JONATHAN DENLINGER, ALS, Lawrence Berkeley National Laboratory, JEONGSOO KANG (Presenter), Physics, The Catholic University of Korea — Topological Kondo insulators (TKIs) belong to a class of symmetry-protected topological phases arising from the strong correlation. CeNiSn, CeRhSb, and CeRhAs are known as Kondo insulators with the large anisotropy [1]. Recently CeNiSn and CeRhSb are predicted to be the novel TKIs having the Möbius-twisted surface states [2]. A unique feature in these systems is the non-symmorphic glide and screw axis symmetries, which bring about the new topological surface band structures. We have investigated the electronic structure of CeRhX (X=Sb, As) employing ARPES and DFT/DMFT band calculations. The Fermi surfaces (FSs) and band structures are successfully measured for the three orthogonal crystallographic directions. For X=Sb, the metallic FSs are obtained for all three different planes. Both the FSs obtained at the Ce 4f resonance and the ARPES data are described well by the unfolded DFT FSs and the DMFT band structures, respectively. The temperature-evolution of the Ce 4f peak agrees with that of the Ce 4f Kondo resonance. The photon energy map provides evidence for the 3D character of the Fermi-edge states unlike the theoretically predicted surface states.

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Discovery of topological nodal-line fermionic phase in a magnetic material GdSbTe

SABIN REGMI (Presenter), MD MOFAZZEL HOSEN, GYANENDRA DHAKAL, KLAUSS DIMITRI, University of Central Florida, PABLO MALDONADO, ALEX APERIS, Uppsala University, FIROZA KABIR, CHRISTOPHER SIMS, University of Central Florida, PETER RISEBOROUGH, Temple University, PETER OPPENEER, Uppsala University, DARIUSZ KACZOROWSKI, Polish Academy of Sciences, TOMASZ DURAKIEWICZ, National Science Foundation, MADHAB NEUPANE, University of Central Florida — Topological semimetals with accidental band touching between conduction and valence bands protected by time-reversal (TR) and inversion symmetry are at the frontier of modern condensed matter research. Mostly, the discovered topological semimetals are non-magnetic and preserve TR symmetry. Here, we report the systematic electronic structure study of the antiferromagnetic GdSbTe using angle-resolved photoemission spectroscopy (ARPES) as well as first-principles calculations. Our study reveals the presence of nodal-line semimetallic state along the Γ-M direction of the Brillouin zone (BZ). Our data also reveal a robust Dirac like state at X point of the BZ both below and above the magnetic transition temperature (T_N = 13K). With a relatively high transition temperature, GdSbTe can prove to be an archetypical platform to study the interaction between magnetism and topological states of matter.

* This work is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415 and the startup fund from UCF (M.N.)

Observation of Nodal Loops in HfP2

CHRISTOPHER SIMS (Presenter), MD MOFAZZEL HOSEN, GYANENDRA DHAKAL, Physics, University of Central Florida, Orlando, Florida 32816, USA, HUGO ARAMBERRI, Physics and Astronomy, California State University, Northridge, California 91330, USA, KLAUSS DIMITRI, FIROZA KABIR, Physics, University of Central Florida, Orlando, Florida 32816, USA, DARIUSZ KACZOROWSKI, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, 50-950 Wroclaw, Poland, XIAOTING ZHOU, TAY-RONG CHANG, Physics, National Cheng Kung University, Tainan, 701, Taiwan, HSIN LIN, Physics, Academia Sinica, Taipei 11529, Taiwan, NICHOLAS KIOUSSIS, Physics and Astronomy, California State University, Northridge, California 91330, USA, MADHAB NEUPANE, Physics, University of Central Florida, Orlando, Florida 32816, USA — Topological nodal-line semimetals that arise due to band touching which are protected by crystalline symmetries are materials that are currently being pushed to further understand topology in crystals protected by different symmetries. Here we report the experimental observation of three topological nodal loops in the transition metal pnictide HfP2 using angle resolved photoemission spectroscopy. Our systematic study reveals the detailed electronic structure of HfP2 which is protected by glide symmetry. Our calculations reveal three unique nodal loops, one of which is protected by glide symmetry in the center and two non-trivial topological nodal loops in finite k-space. Our experimental data and calculations both reveal the existence of these non-trivial loops which warrants further symmetry analysis in the non-symmorphic space group.

*This work is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415 and the startup fund from UCF (M.N.).
T70.00093: Temperature-dependent coherent phonon dynamics in Bi$_2$Te$_3$*  
HSUAN-YIN CHEN, Department of Photonics, National Sun Yat-sen University, JUNG-CHUN HUANG, Department of Physics, National Cheng Kung University, MENG-QING LEE, CHAO-KUEI LEE, Department of Photonics, National Sun Yat-sen University — In this work, temperature-dependent(78K~290K) coherent phonon dynamics in topological insulator Bi$_2$Te$_3$ are investigated. Four coherent phonon types(A$_{1g}^1$, A$_{1g}^2$, E$_g$, coherent acoustic phonon) with strong temperature dependency are observed in transmission pump-probe spectroscopy at low temperature(78K, 90K). These could be attributed to temperature dependent gradient force which resulting in the coherent phonons generation. Especially, lifetime of around 2.87ps for E$_g$ phonon mode is observed for the first time. The depressing signal of reflective pump probe due to the enhancing absorption of surface state for thin film topological insulator will be accordingly increasing as temperature cooling is proposed.

*The authors would like to thank financial support by the grant of Ministry of Science and Technology under the project number of MOST 106-2112-M-110-006-MY3 and MOST 107-2218-E-110-016.

T70.00094: Optical nonlinearity investigation of Bi$_2$Te$_3$*  
MENG YU WU (Presenter), MENG-YUAN CHUANG, WEI-HENG SUNG, PENG LEE, JUN-PENG QIAO, CHAO-KUEI LEE, National Sun Yat-sen University — To realize 2-D material nonlinear optical applications, including wavelength generation, ultrafast optical processing, and saturable absorber for ultrafast laser, the information of optical nonlinearity property for given material is very important. In this work, ultra-low peak intensity (10$^3$ to 10$^5$ W/cm$^2$) z-scan measurement was proposed and buildup for studying the discontinuity of conventional nonlinear transmission with low and high pulse energy. The two photon absorption behavior was observed and is with tremendous large coefficient of 2.03x10$^{-2}$ cm/W for excitation power of 100uW. This can be used to interpret and resolve the discontinuity.

*The authors would like to thank financial support by the grants of Ministry of Science and Technology under project number of MOST 106-2112-M-110-006-MY3 and MOST 107-2218-E-110-016-.

T70.00095: Modulation of the universal conductance fluctuations by broken time-reversal symmetry in topological insulator  
SHUAI ZHANG, FENGQI SONG (Presenter), Nanjing University — In topological insulator BiSbTeSe$_2$ nanowire device, we extract the conductance fluctuations and study their magnetic field dependence in the gate-dependent transport of topological electrons. With the magnetic field increasing, the conductance fluctuation magnitudes are found to reduce by a ratio of $\sqrt{2}$ and form a quantized step, and this is observed both in n-type and p-type transport. This is related to the breaking of the time reversal symmetry of three-dimensional topological insulators, which reveal a crossover of the symmetry classes.

T70.00096: Magnetoresistance from Quantum Interference Effects in Topological Materials  
BO FU (Presenter), HUANWEN WANG, SHUNQING SHEN, Department of Physics, The University of HongKong — A large amount of experimental results about the longitudinal magnetoresistance (LMR) in Weyl semimetal and topological insulator systems display a nonmonotonic behavior over a wide range of magnetic field conditions. At small fields close to zero, a sharp increase of the LMR is observed. When the magnetic field exceeds some threshold value, the LMR is found to decrease as the magnetic field increases. In experiment, this crossover from positive to negative magnetoresistivity is commonly attributed to the competition between Chiral anomaly and weak antilocalization. This negative magnetoresistivity is viewed as the signature of chiral anomaly and the evidence for the existence of Weyl fermion. Using the Feynman diagram techniques, we derive the magnetoconductivity formulae from the quantum interference effects for disordered three-dimensional Dirac materials. By including all the possible contributing Cooperon modes, we can reproduce such nonmonotonict magnetoresistance behavior. We also find that by changing the chemical potential, topological trivial and non-trivial insulators exhibit distinctly different magnetoconductivity behavior. It can help us to directly distinguish the different topological phases through the bulk states transport measurement.
**T70.00097: Compressibility of the quantum spin Hall insulator HgTe**  MATTHIEU DARTIAILH (Presenter), Physics, New York University, SIMON HARTINGER, Physikalisches Institut (EP3), Universität Würzburg, ALEXANDRE GOURMELON, HUGO BARTOLOMEI, JEAN-MARC BERROIR, Laboratoire Pierre Aigrain, Ecole Normale Supérieure, CNRS, PSL Research University, Université Pierre et Marie Curie, Sorbonne Universités, Université Denis Diderot, HARTMUT BUHMANN, LAURENS W MOLENKAMP, Physikalisches Institut (EP3), Universität Würzburg, BERNARD PLAÇAIS, ERWANN BOCQUILLON, Laboratoire Pierre Aigrain, Ecole Normale Supérieure, CNRS, PSL Research University, Université Pierre et Marie Curie, Sorbonne Universités, Université Denis Diderot — Quantum spin Hall (QSH) insulators are two-dimensional electron systems which host spin-polarized edge states while the bulk remains insulating. These helical edge states provide a potential support system to encode information in 'topological quantum bits' robust to the decoherence. Despite immense theoretical and experimental efforts, the rise of these new materials has however been hampered by strong difficulties to clearly observe their predicted topological properties. These challenges motivate the investigation of the dynamics of their topological edge states using microwave techniques. Here we report on the compressibility of the QSH insulator HgTe, measured in metal-oxyde-HgTe capacitors. The quantum capacitance reflects the expected band structure of the HgTe quantum wells. A capacitance minimum associated to a resistance maximum signal the QSH regime. We analyse the dependence of this minimum as a function of the capacitor size and identify both 2D and 1D contributions, which can be used to estimate the 1D channel size. Similar measurements performed on non-topological quantum wells do not show any sizable 1D contributions in agreement with the absence of edge states.

*We acknowledge support from the ERC StG Castles (Grant 758077)

**T70.00098: Vertical Topological Josephson Junciton**  YUTONG DAI (Presenter), GUOXING MIAO, IQC, University of Waterloo — Topological Josephson junciton holds a promising platform for pursuing Majorana zero mode. Due to the proximity effect, the topological insulator layer sandwiched by two superconducting layers can be considered as topological superconductor. We explored the Andreev bound states of this heretrostructure, and observed teh 2pi periodic Andreev states, arising from the paring potential in topological superconductor. We also calculated the transport properties and compared simulation results with experimental measurements.

**T70.00099: ABSTRACT WITHDRAWN**

**T70.00100: ABSTRACT WITHDRAWN**

**T70.00101: WITHDRAWN ABSTRACT**

**T70.00102: Generalized Lieb-Schultz-Mattis theorem on bosonic symmetry protected topological phases**  SHENGHAN JIANG (Presenter), Physics, Caltech, YANG QI, Physics, Fudan University, YUAN-MING LU, Physics, OSU — We propose and proof a generalized Lieb-Schultz-Mattis (LSM) theorem for symmetry protected topological (SPT) phases on boson/spin models in any dimensions. The "conventional" LSM theorem, e.g. spin-1/2 per unit cell on square lattice, disallows symmetric short-range-entangled (SRE) phase. Here, we focus on systems with fractional spins, but have no LSM anomaly. Thus, it is possible to have symmetric SRE phases in the long wavelength. We show that, symmetric SRE phases obtained in these systems must be nontrivial SPT phases of both on-site and spatial symmetries. Depending on models, they can be either strong or higher-order SPT phases, characterized by nontrivial edge/corner states. Furthermore, given global symmetry group and fractional spins, we are able to determine all possible SPT phases by using a spectral sequence expansion of group cohomology. We also provide examples in various dimensions, and discuss possible physical realization of these SPT phases based on topological defects/quasiparticles condensation picture.

*This work is supported by the IQIM, NSF under award number DMR-1653769, MOST of China under grant numbers 2015CB921700, and NSF of China under grant number 11874115.
T70.00103: Charge-spin response and collective excitations in Weyl semimetals*

SAYANDIP GHOSH (Presenter), CARSTEN TIMM, Institute of Theoretical Physics, TU Dresden — We present analytical expressions for all components of the frequency- and wave-vector-dependent charge-spin linear-response tensor of Weyl fermions. The spin-momentum locking of the Weyl Hamiltonian leads to a coupling between charge and longitudinal spin fluctuations, while transverse spin fluctuations remain decoupled from the charge. Based on the response tensor, we investigate the low-energy collective excitations of interacting Weyl fermions. For a local Hubbard interaction, the charge-spin coupling leads to a dramatic change of the zero-sound dispersion: its velocity becomes independent of the interaction strength and the chemical potential and is given solely by the Fermi velocity. In the presence of long-range Coulomb interactions, the coupling transforms the plasmon modes into spin plasmons. Using a lattice model with two Weyl nodes, we show that the collective modes are strongly affected by the presence of parallel static electric and magnetic fields due to the chiral anomaly. We discuss possible experiments that could provide smoking-gun evidence of Weyl physics.

*Deutsche Forschungsgemeinschaft through Collaborative Research Center SFB 1143

T70.00104: Non-linear optical response and HHG in 3D Dirac semimetals

JEREMY LIM (Presenter), YEE SIN ANG, LAY KEE ANG, Singapore University of Technology and Design — Attosecond-duration pulses of extreme ultraviolet to X-ray light, generated via high harmonic generation (HHG), have proven to be highly useful tools in the study of the smallest and quickest fundamental phenomena. The study of HHG in condensed matter systems has attracted much interest due to its potential to realize novel solid-state optical technologies, as well as greater brightnesses compared to gas-phase HHG. We will present results on high harmonic generation in topological materials like 3D Dirac and Weyl semimetals, which exhibit strong, non-linear response to incident fields, which result in efficient generation of odd harmonics. We consider the massless Dirac quasiparticle limit, previously used to predict the harmonic spectra of 2D graphene due to its simplicity and physical transparency, and extend it to 3D Dirac semimetals. We study its non-linear response due to incident fields, and predict its harmonic spectra. A comparison of our results with graphene as well as potential novel photonic applications will be discussed.

T70.00105: Probing Weyl nodes by inelastic neutron scattering*

MICHAEL BJERNGAARD (Presenter), Johns Hopkins University, BOGDAN GALILO, Lancaster University, ARI MARK TURNER, Technion — We present how to detect Weyl nodes in a material by inelastic neutron scattering, taking into account realistic anisotropic properties. A generic material will not have relativistic symmetry. However, under circumstances not too limiting, the dynamics of the excitations can be mapped to a relativistic symmetry. It is then possible to separate out universal properties reflecting this in the cross-section. In a fully unpolarized experiment it is possible to detect the spin-momentum locking of Weyl states, their linear dispersion, principal axis and a sum-rule independent of the material parameters. Furthermore, with polarized neutrons, it is possible to experimentally control the momentum and spin of the excited Weyl particle-hole pairs, with the consequence that the scattered neutron beam is fully polarized in a direction determined by the coupling parameters of the material. This allows one to determine cleanly the coupling parameters as well as to measure the chirality of the Weyl nodes involved in the scattering.

*The research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544.

T70.00106: Solutions to the Chiral Fermion Problem from Topological Orders and Floquet Non-Hermition Field Integrals*

MICHAEL DEMARCO (Presenter), XIAO-GANG WEN, Physics, MIT — Defining a chiral gauge theory non-perturbatively on a lattice has posed a longstanding issue for a non-perturbative definition of the standard model. However, recent insights connecting quantum anomalies with topologically ordered states have led to a breakthrough in lattice formulations of chiral gauge theories: any anomaly-free chiral gauge theory may be formulated as the edge theory of a 2+1 slab with topogical order that is reduced to trivial order by interactions. We keep the `width' of the sla finite so that the system is truly 1+1d. We can then develop a recipe for defining chiral gauge theories that can be extended to higher dimensions. In a parallel development, our recent formulations of discrete-time field integrals allow us to formulate several chiral Floquet phases as local field integrals in discretized spacetime. Intriguingly, these field integrals have unitary correlation functions, even though their Lagrangians are non-Hermitian operators. This provides a second non-perturbative definition of a chiral field theory in 1+1d, with possible generalizations to higher dimensions.

*This material is based upon work supported by NSF Graduate Research Fellowship Program Grant No. 1122374, Grant No. DMR-1506475, and NSFC 11274192.
T70.00108: Quantum criticality preempted by nematicity

SHIXIN ZHANG (Presenter), SHAO-KAI JIAN, HONG YAO, Tsinghua University — Exotic physics often emerges around quantum criticality in metallic systems. Here we explore the nature of topological phase transitions between 3D double-Weyl semimetals and insulators (through annihilating double-Weyl nodes with opposite chiralities) in the presence of Coulomb interactions. From renormalization-group (RG) analysis, we find a non-Fermi-liquid quantum critical point (QCP) between the double-Weyl semimetals and insulators when artificially neglecting short-range interactions. However, it is shown that this non-Fermi-liquid QCP is actually unstable against nematic ordering when short-range interactions are correctly included in the RG analysis. In other words, the putative QCP between the semimetals and insulators is preempted by emergence of nematic phases when Coulomb interactions are present. We further discuss possible experimental relevance of the nematicity-preempted QCP to double-Weyl candidate materials HgCr$_2$Se$_4$ and SrSi$_2$.

[1] Shi-Xin Zhang, Shao-Kai Jian and Hong Yao, arXiv: 1809.10686

T70.00109: How to braid mobile with immobile non-Abelian anyons in a topological superconductor

ANTON AKHMEROV (Presenter), Kavli Institute of Nanoscience, Delft University of Technology, CARLO W J BEENAKKER, PAUL S BAIREUTHER, Lorentz institute for theoretical physics, Leiden University, INANC ADAGIDELI, Faculty of Engineering and Natural Sciences, Sabanci University, YAROSLAV HERASYMENKO, Lorentz institute for theoretical physics, Leiden University — Majorana zero-modes in a superconductor are midgap states localized in the core of a vortex or bound to the end of a nanowire. They are anyons with non-Abelian braiding statistics, but when they are immobile one cannot demonstrate this by exchanging them in real space and indirect methods are needed. As a real-space alternative, we propose to use the chiral motion along the boundary of the superconductor to braid a mobile vortex in the edge channel with an immobile vortex in the bulk. The measurement scheme is fully electrical and deterministic: edge vortices (p-phase domain walls) are created on demand by a voltage pulse at a Josephson junction and the braiding with a Majorana zero-mode in the bulk is detected by the charge produced upon their fusion at a second Josephson junction.

*the Netherlands Organization for Scientific Research (NWO/OCW), the European Research Council (ERC)

T70.00110: Higher-order topological superconductivity: possible realization in Fermi gases and Sr$_2$RuO$_4$

ZHIGANG WU, Shenzhen Institute for Quantum Science and Engineering and Department of Physics, Southern University of Science and Technology, ZHONGBO YAN (Presenter), School of Physics, Sun Yat-sen University, WEN HUANG, Institute for Advanced Study, Tsinghua University — We propose to realize second-order topological superconductivity in bilayer spin-polarized Fermi gas superfluids. We focus on systems with intralayer chiral $p$-wave pairing and with tunable interlayer hopping and interlayer interactions. Under appropriate circumstance, an interlayer even-parity $s$- or $d$-wave pairing may coexist with the intralayer $p$-wave. Such mixed-parity phases do not carry one-dimensional gapless Majorana modes on the boundary, but could support Majorana zero modes at the corners of the system geometry, the end points of superconducting domain walls, as well as certain bulk defects. We show how the number and location of the Majorana zero modes can be tuned by the interlayer pairing and hopping. Generalized to spinful systems, we further propose that the putative $p$-wave superconductor Sr$_2$RuO$_4$ when placed under uniaxial strains, may also realize the desired topological phase.

T70.00111: Principal component analysis of quantum Hall wave functions

HENGXI JI (Presenter), NA JIANG, XIN WAN, Zhejiang University — The fractional quantum Hall effect demonstrates the robustness of topological properties in many-body systems. The effect of mass and interaction anisotropy can be understood in terms of a geometrical description. We present a study of the evolution of quantum Hall wave functions with interaction anisotropy by a statistical learning technique known as the principal component analysis (PCA). We show that the topological and geometrical aspects of a family of wave functions can be readily separated by the PCA. We discuss how to use the PCA to extract wave function metric and to determine the stability of a fractional quantum Hall phase.
T70.00112: Anyonic statistics of quantum impurities in two dimensions  
ENDERALP YAKABOYLU (Presenter), MIKHAIL LEMESHKO, Institute of Science and Technology, Austria — We demonstrate that identical impurities immersed in a two-dimensional many-particle bath can be viewed as flux-tube-charged-particle composites described by fractional statistics. In particular, we find that the bath manifests itself as an external magnetic flux tube with respect to the impurities, and hence the time-reversal symmetry is broken for the effective Hamiltonian describing the impurities. The emerging flux tube acts as a statistical gauge field after a certain critical coupling. This critical coupling corresponds to the intersection point between the quasiparticle state and the phonon wing, where the angular momentum is transferred from the impurity to the bath. This amounts to a novel configuration with emerging anyons. The proposed setup paves the way to realizing anyons using electrons interacting with superfluid helium or lattice phonons, as well as using atomic impurities in ultracold gases [1].  

T70.00113: Composite Fermion Insulator in Opposite-Fields Quantum Hall Bilayers*  
YAHUI ZHANG (Presenter), Massachusetts Institute of Technology — We consider a quantum Hall bilayers from opposite magnetic fields close to the filling $1/2 + 1/2$. We add inter-layer repulsive interaction starting from two decoupled Composite Fermion Liquids (CFL) with opposite chiralities. In this case physical exciton is frustrated from condensation, unlike the conventional quantum Hall bilayers. We argue that more natural phases are the exciton condensates between composite fermions or between slave bosons. The resulting states are insulators with neutral Fermi surfaces coupled to an emergent $U(1)$ gauge field without Chern-Simons term. This insulating state is a generalization of the well-known CFL state. We also comment on the possibility of a topological superconductor in this system. Finally we give experimental proposals to simulate this novel system in a graphene moire system consisting of two nearly flat bands with opposite Chern numbers 1 and -1.

*The work is supported by NSF grant DMR-1608505 to Senthil Todadri.

T70.00114: Quantum Hall stripes with a reduced transport anisotropy at half-filled Landau levels in GaAs quantum wells*  
MICHAEL ZUDOV (Presenter), XIAOJUN FU, QIANHUI SHI, University of Minnesota, GEOFFREY GARDNER, JOHN WATSON, MICHAEL MANFRA, Purdue University, K. W. BALDWIN, LOREN PFEIFFER, KENNETH WEST, Princeton University — It is well known that the hard (easy) resistance due to formation of quantum Hall stripes in high Landau levels of a two-dimensional electron gas exhibits a maximum (minimum) at half-integer filling factors. Here, we report the opposite behavior, namely a local minimum (maximum) in the hard (easy) resistance at half-filling. This talk will discuss our experimental observations in several samples including the temperature dependence of the resistance anisotropy and the response to the in-plane magnetic field applied parallel or perpendicular to the native stripes.

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T70.00115: SEMICONDUCTORS, INSULATORS, AND DIELECTRICS —

T70.00116: Diamond magnetic sensing and imaging*  
ABDELGHANI LARAOUI (Presenter), ILJA FESCENKO, Dept. of Physics and Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106, JANIS SMITS, University of Latvia, Riga, LV-1586, Latvia, Laser Center, NAZANIN MOSAVIAN, JOSHUAT DAMRON, NATE RISTOFF, Dept. of Physics and Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106, PAULI KEHAYIAS, Sandia National Laboratories, Albuquerque, NM 87185, USA, ANDREY JARMOLA, Department of Physics, University of California-Berkeley — Diamond magnetic sensing has emerged as a powerful tool to detect nanomagnetism in biological and solid-state samples, as well to measure weak signals from nuclear spins and spin textures of molecules. We report ongoing experiments that explore several applications of diamond magnetic sensing. These include: (i) microfluidic nuclear magnetic resonance spectrometer capable of sensing small quantities (< 1 pL) of analyte [1], achieving spectral resolutions capable of distinguishing proton with heteronuclear ] splitting; (ii) a wide-field magnetic microscope able to measure the stray magnetic fields produced by individual malarial hemoglobin biocrystals (size < 300 nm) [3] and magnetization relaxation of single magnetic nanoparticles (size < 25 nm) at room temperature and as a function of applied field up to 350 mT. [1] P. Kehayias*, A. Jarmola*, N. Mosavian, I. Fescenko, F. M. Benito, A. Laraoui, J. Smits, L. Bougas, D. Budker, A. Neumann, S. R. J. Brueck, V. M. Acosta, Nature Commu. 8, 188 (2017). [2] I. Fescenko, A. Laraoui, J. Smits, N. Mosavian, P. Kehayias, J. Seto, L. Bougas, A. Jarmola, V. M. Acosta, arxiv:1808.03636 (2018).

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T70.00117: Magnetic noise due to interactions between bulk impurities and electrons in nitrogen vacancy center diamonds

BRUCE BARRIOS (Presenter), SHOU LI, D H SANTAMORE, Department of Physics and Engineering Physics, Delaware State University, Dover, Delaware 19901 — Nitrogen Vacancy (NV) Centers diamond present great interest as robust atomic-scale magnetic field sensors. One of the serious problems of NV center diamond devices is electric and magnetic field noise. The noise causes ODMR line-broadening, which reduce sensitivity of the devices. In this work we theoretically study the magnetic field noise caused by the magnetic dipole-dipole interactions between the impurities of carbon-13 and nitrogen-14 and the electron in the NV center. We use the cluster correlation expansion method to calculate the magnetic field fluctuations, and then, obtain the noise spectrum. The noise is greater at lower frequencies but rapidly decrease at higher frequencies.

*NSF DMR-150641

T70.00118: Interfacial treatment of 4H SiC/SiO2 interface by shallow boron ion implantation

MD. HAIDER SHAIM, HANI ELSAYED-ALI (Presenter), Old Dominion Univ — Shallow boron ion implantation at the 4H SiC/SiO2 interface was performed using boron multicharged ions from laser plasma. A Q-switched Nd:YAG laser (wavelength 1064 nm, pulse width 7 ns, and fluence 135 J/cm2) was used to ablate a boron target generating a dense plasma source of multicharged ions. Ions up to B5+ are generated. The ions are deflected by an electrostatic field to separate them from the neutrals. SRIM simulation was used to estimate the ion penetration depth in the SiC substrate. The optical bandgap of the 4H SiC was reduced by boron ion implantation. Several MOSCAP devices were fabricated. High-low C-V measurements were used to characterize the MOSCAPs. Shallow boron implantation in the SiC/SiO2 interface reduces the flatband voltage from 4.5 V to 0.04 V.

*This material was based on the work supported by the National Science Foundation under Grant No. MRI-1228228 and a seed grant from the Virginia Microelectronics Consortium.

T70.00119: Noble gas defects in ZnO: interaction with the localized defect states

OLEKSANDR MALYI (Presenter), Centre for Materials Science and Nanotechnology, Department of Physics, University of Oslo, KOSTIANTYN SOPIHA, Department of Engineering Sciences, Uppsala University, CLAS PERSSON, Centre for Materials Science and Nanotechnology, Department of Physics, University of Oslo — Owing to fully occupied orbitals, noble gases are often considered to be chemically inert and to have limited effect on materials properties under typical synthesis conditions. However, using first-principles calculations, we show that the insertion of noble gases (i.e., He, Ne, and Ar) in ZnO results in destabilization of electron density of the material driven by minimization of the unfavorable overlap of atomic orbitals of noble gases and its surrounding atoms. Specifically, the noble gas defect (interstitial or substitutional) in ZnO pushes electron density of its surrounding atoms away from its vicinity. Simultaneously, the host material confines electron density of the inserted noble gas. Because of this, the interaction of He, Ne, or Ar with O vacancies of ZnO in different charge states (ZnO:VOq) affects the vacancy stability and electronic properties. In particular, we reveal that to minimize the unfavorable overlap of atomic orbitals of the noble gases and surrounding atoms, the noble gases can occupy the vacancy site delocalizing the otherwise localized ZnO:VOq states.

*The work is supported by RCN #251131.

T70.00120: Theoretical study on atomic and electronic structures of vacancy-defect complexes in Ga2O3

KENTA CHOKAWA (Presenter), Graduate school of engineering, Nagoya University, KENJI SHIRAISHI, Institute of materials and systems for sustainability, Nagoya University — Ga2O3 has been studied as a next generation power semiconductor material which can realize lower energy consumption power devices than those using GaN and SiC.[1] Although some theoretical studies have already clarified the atomic and electronic structures of the point defects such as vacancies,[2] there are few knowledge of the defect complexes in Ga2O3. Therefore, we perform the first principles calculations by using VASP code,[3] and examine the atomic and electronic structures of the vacancy-defect complexes in Ga2O3. We made some vacancy-defect complexes in the α-Ga2O3 and β-Ga2O3 models and determined stable defect structures. We also study the stability of defects in the Mg-doped Ga2O3 models.

Reference:
T70.00121: First-principles prediction of p-type doping of β-Ga2O3 ultrawide bandgap semiconductors

BENJAMIN TATTERSFIELD (Presenter), STEVEN HARTMAN, GUANGFU LUO, JOHN CAVIN, ROHAN MISHRA, Mechanical Engineering and Materials Science, Washington University in St. Louis — β-Ga2O3 is an ultra-wide-band-gap semiconductor with a large intrinsic band gap of 4.8 eV and a high breakdown field of 8 MV/cm. These properties when combined with the availability of high-quality large-area single crystals of β-Ga2O3, make it attractive for power electronic applications than conventional wide-band-gap semiconductors such as GaN and SiC. However, the efficiency of β-Ga2O3 devices is currently limited by the lack of good p-type dopants. We present evidence based on first-principles density-functional theory calculations that β-Ga2O3 can be efficiently doped p-type by bismuth. Based on formation energies, we predict that bismuth acts as a substitutional dopant at the gallium site. At low concentrations, bismuth leads to delocalized states just above the valence band edge of β-Ga2O3. These states arise due to the antibonding interaction between the occupied 6s2 lone pair electrons of bismuth and the 2p states of oxygen. The occupancy of these delocalized defect states can be controlled by moving the Fermi level, which can lead to efficient p-type doping.

T70.00122: Development of Room Temperature Multiferroic SmFeO3 Thin Films

YUAN-CHIH WU (Presenter), YI-DE LIOU, Physics, National Cheng Chung University, CHANG-YANG KUO, ZHIWEI HU, CHUN-FU CHANG, Max-Planck-Institute for Chemical Physics of Solids, TAY-RONG CHANG, Physics, National Cheng Chung University, HENG-JUI LIU, National Chung Hsing University, YI-CHUN YANG, Physics, National Cheng Chung University — Multiferroic materials are very popular in recent decades due to its versatile functionalities for applications. A result development of new materials that possesses multiferroicity is of great importance. SmFeO3 (SFO) has been considered as new room temperature single-phase multiferroic material for few years. SFO exhibits anti-ferromagnetism and significant magnetization below $T_N \sim 670$ K. However, the existence of ferroelectricity of single crystal SFO is still under debate.

In this work, we focus on the growth of epitaxial SFO thin films on different single crystalline substrates (LaAlO3 and NdGaO3) in order to trigger the presence of room temperature ferroelectricity. Atomic force microscopy has been used to check the surface morphology to prove the layer-by-layer epitaxy growth. To certify the interfacial strain between two different oxide materials, high resolution XRD is adopted. The ferroelectricity of SFO grown on NdGaO3 substrate has been identified by the piezoresponse force microscopy (PFM). Multiple techniques have been exploited to verify the ferroelectricity in the strained SFO thin films. The existence of the ferroelectricity is further supported via density functional theory. Out results identify a new room temperature single-phase multiferroic system.

T70.00123: Epitaxial growth and multiglass order in room-temperature relaxor multiferroics*

WEICHUAN HUANG (Presenter), Department of Materials Science and Engineering, University of California at Berkeley, YEN-LIN HUANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, SUJIT DAS, Department of Materials Science and Engineering, University of California at Berkeley, YUN-LONG TANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, R RAMESH, Department of Materials Science and Engineering, University of California at Berkeley — Multiferroic materials with simultaneous ferroelectricity and magnetism provide a pathway to achieving strong magnetoelectric (ME) coupling with voltage control of magnetism, leading to compact and power efficient electric-field tunable magnetic devices. In recent years, substantial progress in finding room-temperature (RT) relaxor multiferroics, a new perspective for low-power spintronics, displaying strong ME coupling coefficients has been made [1-3]. Here, we present electric and magnetic properties of single-phase $x$Pb(Fe,W)O3-(1-x)Pb(Zr,Ti)O3 (PFW-PZT) films epitaxially grown on (001) SrTiO3 and (220) GdScO3 substrates using pulsed laser deposition. It is demonstrated that the PFW-PZT films show good ferroelectric and piezoelectric properties by measuring macroscopic polarization and local piezoelectric as a function of electric-field. In addition, weak ferromagnetism via magnetic hysteresis loops was also observed at RT.

References


*This work was supported by the Center for Probabilistic Spin Logic for Low-Energy Boolean and Non-Boolean Computing (CAPSL), a SRC program sponsored by the NSF.
T70.00124: Characterization of $\text{Ta}_x\text{Ti}_{(1-x)}\text{O}_y$ thin film and its applications in RRAM devices. YU SHI (Presenter), RABIUL ISLAM, GUOXING MIAO, Electrical and Computer Engineering, University of Waterloo — The movement of oxygen ions plays an important role in the resistive switching behavior of $\text{TiO}_x$ based devices, therefore the designed distribution of oxygen ions may help enhance the oxygen ion's movement and improve the resistive switching performance. In this work, we dope the $\text{TiO}_x$ thin film with a graded concentration of $\text{Ta}$ in depth, to generate a spatial gradient of oxygen activation energy. Detailed characterization of the structural changes and resistive switching performance has been carried out, our result may suggest a new way to use dopants to help improve the resistive switching performance.

T70.00125: Temperature and field dependent Raman Studies on Cupric Oxide Single Crystals RAJEEV GUPTA (Presenter), BARNITA PAUL, Indian Institute of Technology Kanpur — Cupric oxide is a well known oxide material which shows two successive magnetic transitions at 230 K ($T_{N2}$) and 213 K ($T_{N1}$). Interestingly, it has been reported in recent times that a small electric polarization of $160 \mu\text{C/m}^2$ develops along the b axis between 213-230 K. The origin of the observed macroscopic polarization is attributed to the noncollinear arrangement of spins and breaking of inversion symmetry via the Dzyaloshinskii-Moriya interaction. This mechanism is rather unusual and was suggested that spin-lattice coupling plays a crucial role. In the current work, we present temperature dependent Raman measurements on single crystalline CuO in presence of a magnetic field. Room temperature Raman measurements reveal three prominent Raman modes at 302 cm$^{-1}$, 350 cm$^{-1}$ and 635 cm$^{-1}$ consistent with earlier reports. Interestingly, we find a new mode appearing at 240 cm$^{-1}$ below 175 K. This mode splits into two modes on an application of a small magnetic field. Our experiments suggests that the mode observed at 240 cm$^{-1}$ is a combination of a magnon mode and a zone folded phonon contrary to the earlier reports.

T70.00126: Point defects at ferroelectric domain walls in hexagonal YMnO$_3$* DIDRIK SMÅBRÅTEN, SANDRA SKJAERVOE, DENNIS MEIER, Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, THOMAS TYBELL, Department of Electronic Systems, NTNU Norwegian University of Science and Technology, SVÆRRE SELBACH (Presenter), Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology — Understanding how point defects influence the domain wall (DW) mobility and properties in ferroelectrics is desirable both to control the macroscopic ferroelectric properties and to develop DW-based nanoscale electronic circuitry. Here we use DFT calculations to study the interplay between neutral ferroelectric DWs in improper ferroelectric YMnO$_3$ and lattice imperfections like aliovalent dopant cations and oxygen defects like vacancies and interstitials. We find that the DW mobility and conductivity strongly couples to the defect chemistry of the material, and our simulations are supported by experimental reports. The overall aim of this study is to obtain chemical guidelines from first principles calculations for how to control the DW mobility and conductivity through defect chemistry. YMnO$_3$ displays great chemical flexibility, where donor and acceptor doping of both cation sublattices as well as both oxygen deficiency and excess is possible, making hexagonal manganites an ideal model system for this purpose.

T70.00127: Crystal structure and dielectrical behavior of $\text{YFe}_{1-x}\text{Ti}_x\text{O}_3$* MAURY SOLORZANO (Presenter), BASIC SCIENCE, UNIVERSIDAD JUÁREZ AUTÓNOMA DE TABASCO, ALEJANDRO DURAN, Materiales Avanzados, Centro de Nanociencia y Nanotecnologia, RICHARD FALCONI, BASIC SCIENCE, UNIVERSIDAD JUÁREZ AUTÓNOMA DE TABASCO — Yttrium orthoferrite, $\text{YFeO}_3$, is a multiferroic system despite having a $\text{Pnma}/\text{Pbnm}$ centrosymmetric structure. The mechanism that gives rise to ferroelectricity is under discussion, but it is believed to be associated with the breakdown of inversion symmetry. In this work, the synthesis, structural characterization, as well as the dielectric properties of the Ti - doped $\text{YFeO}_3$ are reported. Structurally it was found that doping with Ti generates an increase in the volume of the unit cell. The relative permittivity, $\varepsilon_r$, increases with the Ti content and has a diffuse phase transition at a temperature that decreases with x. In the same way, both the dielectric loss and the activation energy decrease with Ti doping. These results are discussed considering geometrical aspects and the occupation of the d orbitals.

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**T70.00128: Enhanced charge carrier lifetime in layered 2D hybrid perovskites**  
POLLY J PIERONE (Presenter),  
Department of Physics, Wesleyan University, NOOR TITAN PUTRI HARTONO, JUAN-PABLO CORREA-BAENA, TONIO BUONASSISI,  
Massachusetts Institute of Technology, MENG-JU SHER, Department of Physics, Wesleyan University — Lower dimensional layered perovskite exhibited better environmental stability than 3D organic-inorganic hybrid perovskite materials such as methylammonium lead iodide (MAPbI₃). Due to the reduced dimensionality, one drawback of these layered 2D perovskite is the reduced charge carrier mobility. Currently, using layered 2D perovskite materials, no improvement in solar cell performance has been reported. In this study, we synthesized layered 2D lead-halide perovskite samples using different ratios of t-butylammonium and methylammonium as the organic cation, creating a set of samples spanning the 3D to 2D transition. We used time resolved terahertz conductivity measurements, a non-contact conductivity probe, to study both charge carrier mobility and lifetime in these materials. We confirmed the reduced charge carrier mobility but found enhanced carrier lifetime, indicating a possibility of finding optimal composition to maximize carrier diffusion length. The increased carrier lifetime supports efficient exciton dissociation and long-lived free carriers recently reported on other 2D Ruddlesden-Popper perovskites. Lastly, we compared the device performance of the 2D perovskite solar cells with the charge carrier dynamics measured.

**T70.00129: Ultrafast Charge Transfer at CH₃NH₃PbI₃ and MoS₂ Interface**  
WISSAM SAIDI (Presenter), University of Pittsburgh, YONGLIANG SHI, JIN ZHAO, University of science and technology of China — To achieve higher power conversion efficiency of promising hybrid organic-inorganic perovskites (HOIP), interface engineering must be applied to optimize the charge carrier pathway from absorber to electron and hole transport layers. Fast charge transfer can largely avoid charge accumulation at the interface, and suppress recombination. Further, optimized band alignment between charge transfer material and adsorber would reduce the “potential loss” in the conversion efficiency of the solar cell. Herein, we employ nonadiabatic molecular dynamics (NAMD) within time dependent density functional theory to study hole transfer from CH₃NH₃PbI₃ to monolayer MoS₂. Our results show that there is an ultrafast hole transfer channel in agreement with a recent experimental study. Because of the existence of a fast charge transfer and minimal band mismatch between CH₃NH₃PbI₃ and MoS₂ at the same time, MoS₂ is a promising hole transfer material in HOIP.

**T70.00130: Epitaxial growth of MoSe₂ and MoTe₂ monolayer on GaAs by molecular beam epitaxy**  
YIPU XIA,  
Department of physics, The University of Hong Kong, HAILONG WANG, State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, ZE MEN (Presenter), JUNQIU ZHANG, Department of physics, The University of Hong Kong, HU XU, Department of Physics, Southern University of Science and Technology, WINGKING HO, Department of physics, The University of Hong Kong, HAO TIAN, Department of Physics, Southern University of Science and Technology, JIANHUA ZHAO, State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, MAOHAI XIE, Department of physics, The University of Hong Kong — Molybdenum diselenide (MoSe₂) and molybdenum ditelluride (MoTe₂) are promising transition metal dichalcogenides (TMDs) that have attracted great interests in recent years because of their unique electrical and optical properties. In this work, we fabricate crystallographically aligned MoSe₂ and MoTe₂ monolayers on gallium arsenide (GaAs) (111) surface by MBE as revealed by low energy electron diffraction (LEED) measurements. Unlike TMDs growth on van der Waals (vdW) substrates such as the highly oriented pyrolytic graphite (HOPG) and graphene, the interface interactions between GaAs and the epitaxial TMD films are electronically stabilized surface as suggested by X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations. Ultraviolet photoelectron spectroscopy (UPS) measurements are also performed to provide additional evidence and results.

*This work is financially supported by a Collaborative Research Fund (C7036-17W) sponsored by the Research Grant Council (RGC), Hong Kong Special Administrative Region, China.
**T70.00131: Transport and photoresponse study of Bulk MoS\textsubscript{2}**

MEHDI PAKMEHR (Presenter), MOJTABA EBRABIMI, HAJAR KAZEMI, ZOHREH MOHAMMADI, Physics, Shiraz University — Molybdenum disulfide (MoS\textsubscript{2}) or Molybdenite were known as an indirect gap semiconductor with energy gap of 1.8 eV. More recently, it turns out that in 2D morphology (atomic thin film case) MoS\textsubscript{2} hosts novel physical properties including high optical absorption coefficient. To be used as a common semiconductor material within electronic and optoelectronics industry, one needs to know the types of impurity atoms within by-product powder of MoS\textsubscript{2} from copper extraction factory. We investigated structural properties of powder MoS\textsubscript{2} through PXRD, which confirm MoS\textsubscript{2} with reasonable purity. The powder used for bulk polycrystalline sample growth through common melting techniques. Transport measurements at cryogenic temperatures done to check conductivity of our bulk sample. Due to unintended dopant species, we observed conductivity dependence on temperature in range of 80-300 K. We plan to present our finding through a poster at APS march meeting 2019 being held at Boston.

*M. Pakmehr would like to Acknowledge National Elite Foundation of Iran and Shiraz University Dean Office for supporting our research work.*

**T70.00132: Thermal and Electrical Transport Properties in bulk Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}**

MING YIN (Presenter), JERESHIA BUSH, Physics/Engineering, Benedict College, LEI WANG, TIMIR DATTA, Physics & Astronomy, University of South Carolina — The remarkable ability of certain solids, the Phase Change materials (PCM), to reversibly and rapidly switch between amorphous and crystalline states with large differences in electrical, thermal and optical properties was discovered exactly half a century ago [S.R. Ovshinsky PRL, 21,1450 (1968)]. Currently ambient temperature operable PCM’s are used in electronic flash memory as well as optical data storage. Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} is such a PCM alloy; in which, we have previously reported Noritheim-Gorter like scaling between Seebeck coefficient (S) and electrical conductivity (σ). Here we report that in the room temperature regime, thermal conductivity (κ) of this material is a linear function of temperature with a slope ~ 1e-3 W/mT\textsuperscript{2}; whereas, electrical conductivity falls off with rising temperature; Remarkably, despite this deviation from Wiedemann-Franz Law, the value of Lorenz number estimated from the experimental (κ and σ) data ranges between 2-2.47 e-8 WWK\textsuperscript{-2}, not much off from the ideal kinetic theory value of 2.44e\textsuperscript{-8}. Further experimental details and results will be discussed.

*DOE DE-NA0002630*

**T70.00133: Photoexcited dynamics in tellurium probed by coherent phonons**

YU-HSIANG CHENG (Presenter), Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, SAMUEL W TEITELBAUM, FRANK GAO, KEITH ADAM NELSON, Department of Chemistry, Massachusetts Institute of Technology — We studied the photoexcited dynamics in tellurium films using ultrafast pump-probe spectroscopy. Photoexcitation with femtosecond laser pulses produces carriers that modify the interatomic potential and thus excite coherent phonons. The phonon frequency strongly depends on the carrier density and the lattice temperature. We estimated the carrier density and the corresponding electronic bond softening using the diffusion equation. We also measured the phonon dynamics at different temperatures from 80 to 500 K. Based on these measurements, the lattice temperature within 1 ns after the pump pulse can be estimated using the frequency of the coherent phonons, excited by a second pump pulse. In addition, we modified the two-temperature model to simulate the dynamics of the carrier density, carrier temperature, lattice temperature, and phonon motion at different depths.

**T70.00134: On the pitfalls of applying isotropic mobility spectrum analysis to conductors with weak anisotropy**

KENNETH S. STEPHENSON (Presenter), YAROSLAW BAZALIY, University of South Carolina — It is shown that applying isotropic quantitative mobility analysis (QMSA) to anisotropic materials can lead to drastic qualitative errors, even in the case of modest anisotropy. The procedure may provide not only wrong values for carrier mobilities and concentrations, but even a wrong number of carrier species.
T70.00135: Multiscale study on Phase Transformation of Ceramic Materials* YUHUAN FEI (Presenter), College of Engineering, Qufu Normal University — Compared with their microstructures, phase analysis of ceramic materials is rarely reported. Generally, phase analysis includes experimental phase structure determination and theoretical simulation, which are quite challengeable and require a heavy workload. Here, we proposed a series of simulation methods to analyze the phase transformation during the sintering process of Al₂O₃-ceramic materials. The structures of generated Al-Mg phases were simulated using XPFC method. The obtained potential function of Ti-C-N was applied to simulate the formation of generated Ti-C-N phases with MD methods employed. Combined with corresponding experimental results, the relationship between specific phases and mechanical properties were established.

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T70.00136: In situ investigation of electric field and stress control of ferroelectric phases in PIN-PMN-PT single crystal* PETER FINKEL (Presenter), MARGO STARUCH, United States Naval Research Laboratory, MARKYS CAIN, Electrosciense, Ltd — We explored stability of relaxor ferroelectric single crystals with composition near a morphotropic phase boundary (MPB) using the three-pronged approach offered by this project of in situ, stress, temperature and E field whereby a bias of any one of these parameters can move the operating point in almost any direction. This MPB can be moved through the application of stress or electric field. In this work we demonstrate an induced rhombohedral (R) to orthorhombic (O) phase transition in [011] cut Pb(In₁/₂Nb₁/₂)O₃-Pb(Mg₁/₃Nb₂/₃)O₃-PbTiO₃(PIN-PMN-PT) single crystal relaxor ferroelectric, that can be simultaneously tuned through combination of stress and applied electric field. Direct observations of this phase transition with X-ray and Raman scattering reveal the local symmetry while sweeping through the transition with a low applied electric field when the crystal is near a critical value of stress. A coexistence of R and O phases was observed and these microscopic measurements mirror the bulk strain in the sample. Remarkably, cycling through this transition can generate reversible strain >0.35% for tens of millions of cycles with little fatigue. Details of these results and their implications will be presented.

*Office od Naval Reserach

T70.00137: Ab initio studies of electronic and vibrational properties of transition metal dichalcogenides systems under hydrostatic pressure TOMASZ WOZNIAK (Presenter), Department of Theoretical Physics, Wroclaw University of Science and Technology, JAN KOPACZEK, ROBERT OLIVA, Department of Experimental Physics, Wroclaw University of Science and Technology, PAWEL SCHAROCH, Department of Theoretical Physics, Wroclaw University of Science and Technology, JORDI IBANEZ, Instituto de Ciencias de la Tierra Jaume Almera, ROBERT KUDRAWIEC, Department of Experimental Physics, Wroclaw University of Science and Technology — We study from first principles (DFT) the electronic structure of MoTe₂ and WS₂ under hydrostatic pressure in comparison to photoreflectance spectra. The analysis based on pressure coefficients allowed for identification of several optical transitions in bulk and multilayer systems. The calculated pressure coefficients for K and H point transitions are in good agreement with the experimental values. [1]

Lattice dynamics of bulk HfS₂ and MoS₂ in comparison to high pressure Raman scattering measurements is studied. From the calculated phonon dispersions we derive linear pressure coefficients which are then compared to experimental data. DFT calculations were performed using various functionals, vdW corrections and lattice dynamics calculations methods. We find that GGA properly describes the high pressure lattice dynamics of these compounds when vdW interactions are taken into account. In contrast, we show that LDA, which is widely used to predict structural and vibrational properties at ambient conditions in 2D compounds, fails to reproduce the Raman modes evolution under compression. [2]

[1] J. Kopaczek, T. Wozniak, R. Kudrawiec, to be submitted

T70.00138: WITHDRAWN ABSTRACT
T70.00139: Modeling and Simulation of GaTlAs Quantum Well Solar Cells

Ahmed Zayan (Presenter), Thomas Vanderwende, Electrical and Computer Engineering, Tufts University — Multiple Quantum Wells (MQW) have been an ongoing topic of research and discussion for the scientific community with structures like InGaAs/GaAs and InGaP/GaAs quantum wells producing promising results that could potentially improve overall solar energy conversion. Here, we use WEIN2K, a commercial density functional theory package, to study the ternary compound Ga$_{1-x}$TlxAs and determine its electronic properties. Using these results combined with experimental confirmation we extend these properties to simulate a MQW GaAs/ Ga$_{1-x}$TlxAs solar cell. Ga$_{1-x}$TlxAs is a tunable compound, with its bandgap being strongly dependent on the concentration of Tl present. Concentrations of Tl as low as 7% can reduce the bandgap of Ga$_{1-x}$TlxAs to roughly 1.30 eV at room temperature with as little as a 1.7% increase in lattice constant. The change in bandgap, accompanied by the relatively small change in lattice constant makes Ga$_{1-x}$TlxAs a strong candidate for a MQW cell with little to no strain balancing required within the structure to minimize unwanted defects that impede charge collection within the device. Our GaAs photodiode with TlGaAs MQWs shows an expanded absorption band and improved conversion efficiency over the standard GaAs photovoltaic cell.

T70.00140: Charge carrier lifetime dependence on annealing conditions in copper oxide thin films: A transient absorption study

Lenny Shenje (Presenter), Suzanne Ullrich, University of Georgia — Ultrafast transient absorption spectroscopy has been used to study charge carrier dynamics in Copper(I) and Copper(II) oxide thin films as a function of annealing conditions. 16 samples were deposited on glass substrates and then subsequently annealed at temperatures 150 to 380 C for periods ranging from 2 to 24 hrs. Clear evidence of oxidation from the copper(I) to the copper(II) phases was observed by steady state and time-resolved spectroscopies as well as x-ray diffraction. Thin film transient absorption spectra were recorded by exciting the samples across the band gap and probing subsequent carrier dynamics with a white light continuum. The mixed Cu$_2$O/CuO thin film transient spectra were compared to those of pure Cu$_2$O and CuO to investigate the influence of annealing conditions on the films' optical properties. All samples showed multi-exponential decay kinetics with a fast component (ranging from 0.2 – 0.5 ps) and a long-lived component (>1 ns); an additional 0.8 to 3 ps intermediate time constant was observed in mixed Cu$_2$O/CuO and pure CuO films. These kinetics are attributed to carrier relaxation in the conduction band, trapping and recombination.

T70.00141: Spatially-resolved photoluminescence of Si$_2$Te$_3$ nanostructures*

Andrew Mendizabal (Presenter), Alexis Buzzell, Patrick Devlin Fitzgerald, Kateryna Kushnir, Physics Department, Worcester Polytechnic Institute, Mengjing Wang, Chemistry Department, Brown University, Teng Shi, Physics Department, Worcester Polytechnic Institute, Kristie Koski, Chemistry Department, University of California Davis, Lyubov Titova, Physics Department, Worcester Polytechnic Institute — Silicon telluride (Si$_2$Te$_3$) is a unique 2D material: it has strong optical absorption across the visible spectrum, optical emission in the red, p-type conductivity and processing compatibility with silicon and silicon oxide. It's potential application range from energy storage, thermoelectric devices and chemical sensors to light emitting diodes. It is possible to grow Si$_2$Te$_3$ nanostructures of different morphology, from nanometer-sized nanoplates to ribbons up to 10 μm long by either vapor-liquid-solid or layer-by-layer vapor solid growth[1]. Here we present spatially-resolved photoluminescence spectroscopy of 50-1000 nm-thick Si$_2$Te$_3$ nanoplates and Si$_2$Te$_3$ ribbons that are ca. 300 nm wide and 10 μm long. Correlating morphology, thickness and lateral dimension of Si$_2$Te$_3$ nanostructures to their optical emission provides important insights into their electronic and optical properties, and lays the foundation to their potential applications.


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T70.00142: Two-dimensional Fourier Transform Spectroscopy on Bulk GaAs in High Magnetic Fields*

Christopher E Stevens, Varun Mapara (Presenter), Jagannath Paul, Dept. of Physics, University of South Florida, Myron Kapetanakis, Dept. of Physics, University of Alabama at Birmingham, Stephen A McGill, National High Magnetic Field Laboratory, Florida State University, Ilias Perakis, Dept. of Physics, University of Alabama at Birmingham, Denis Karaiskaj, Dept. of Physics, University of South Florida — Two-dimensional Fourier transform spectroscopy was performed on Bulk GaAs in the presence of magnetic fields up to 10T. The polarization dependent exciton dynamics were studied in addition to the effects of an applied external magnetic field. The experimental results were then modeled using the optical Bloch equations.

*We acknowledge National Science Foundation for financial support.
A ferroelectric semiconductor field-effect transistor (FeS-FET) was proposed and experimentally demonstrated for the first time. In this novel FeS-FET, a 2D ferroelectric semiconductor α-In$_2$S$_3$ is used to replace conventional semiconductor as channel. α-In$_2$S$_3$ is identified due to its proper bandgap, room temperature ferroelectricity, the ability to maintain ferroelectricity down to a few atomic layers and the feasibility for large-area growth. An atomic layer deposited (ALD) Al$_2$O$_3$ passivation method was developed to protect and enhance the performance of the α-In$_2$S$_3$ FeS-FETs. The fabricated FeS-FETs exhibit high performance with a large memory window, a high on/off ratio over $10^8$, a maximum on-current of 671 μA/μm, high electron field-effect mobility with $\mu_{FE} = 312$ cm$^2$/Vs in forward sweep and $\mu_{FE} = 488$ cm$^2$/Vs in reverse sweep, and the potential to exceed the existing Fe-FETs for non-volatile memory applications.
T70.00147: Minimal double quantum dot in ZnO*  JUNYI ZHANG, Princeton University, HAO ZHENG (Presenter), School of Physics and Astronomy, Shanghai Jiao Tong University, RICHARD BERNDT, Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — Minimal double quantum dots (DQDs) are prepared in ZnO, a wide band-gap semiconductor matrix. The DQDs are of the atomic scale that is difficult to achieve for for conventional microfabrication techniques. It is comprised of a pair of strongly coupled donor atoms that can each be doubly charged. Using scanning tunneling microscopy and spectroscopy, we mapped out the donor excitation diagram of this system which mimicks the charge stability diagram observed in transport measurements of DQDs. The charge and spin degrees of freedom of the minimal DQDs may also be used as quantum bits. The DQDs can be prepared in the quantum entangled state, e.g., in a Bell state. The results open an intriguing perspective for quantum electronics with atomic-scale structures.

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T70.00148: Resistance drift of metastable amorphous and crystalline fcc GeSbTe memory devices*  HELENA SILVA (Presenter), NAFISA NOOR, SHALINI TRIPATHI, C. BARRY CARTER, University of Connecticut — Phase-change memory is an emerging technology that utilizes the electrical resistivity contrast between the amorphous and crystalline phases of chalcogenide glasses to store data. The most commonly used material for PCM has been GeSbTe (GST), which has metastable amorphous and crystalline fcc phases and a stable crystalline hcp phase [1]. One difficulty with the implementation of PCM is the upward resistance drift of the metastable amorphous and crystalline fcc phases. We are using electrical characterization together with transmission electron microscopy and finite-element electrothermal simulations [2] to study the physical mechanisms that give rise to the electrical resistance drift of GST cells.


*This work was supported by NSF under award DMR-1710468. The devices were fabricated at IBM Watson Research Center. The TEM analysis is performed at the CINT, a DOE User Facility operated by Los Alamos and Sandia National Laboratories (DE-AC52-06NA25396 and DE-NA-0003525).

T70.00149: SUPERCONDUCTIVITY —

T70.00150: Iron based superconductors on flexible coated conductor templates*  ALEENA THOMAS (Presenter), KORNELIUS NIELSCH, DR. RUBEN HÜHNE, Leibniz Institute of Solid State and Materials Research (IFW Dresden), Helmholtzstr. 20, 01069 Dresden, Germany — The discovery of high temperature superconductivity in layered iron-based material has ignited also significant scientific interest for technological applications. Iron based superconductors are particularly promising for high field applications due to its high upper critical field and low anisotropy. To realize such applications, the coated conductor technology based on textured IBAD (Ion beam assisted deposition) layers can be used. Additionally, such templates might be applied to investigate the influence of uniaxial strain on the superconducting properties. Therefore, we deposited pure as well as Te doped FeSe with a thickness of up to 200 nm on buffered IBAD substrates having a final cap layer of either CeO2 or LaMnO3. We found that FeSe1-xTex (FST) and FeSe is grown epitaxially on these buffered metal tapes under optimized conditions with a superconducting transition temperature of up to 16 K for textured FST film on CeO2 buffered metal tape. Finally, we will present first results on the influence of uniaxial strain on the superconducting transition using these templates.

*This work was supported by the German research foundation (DFG) within the research training group GRK 1621.
T70.00151: Measurements of Superconducting Anisotropy in FeSe with Resonance Frequency Technique

RONGXING CAO (Presenter), JUN DONG, College of Physics Science and Technology, Yangzhou University, D. A. CHARIEV, Institute of Experimental Mineralogy, Russian Academy of Sciences, A. N. VASILIEV, Low Temperature Physics and Superconductivity Department, Lomonosov Moscow State University, GUOQING WU, XIANGHUA ZENG, College of Physics Science and Technology, Yangzhou University — Utilizing a novel method with the resonance frequency of a LC circuit, we measured the superconducting anisotropy of single crystals of Fe-based superconductor FeSe. We found that the temperature dependence of the upper critical field $H_{c2}(T)$ of FeSe coincides with the Werthamer-Helfand-Hohenberg (WHH) model when taking the Maki parameter $\alpha$ into consideration, which suggests an important role played by spin-paramagnetic effect in suppressing the superconductivity. When temperature $T \to 0$, the values of $H_{c2,||}(0)$ and $H_{c2,\perp}(0)$ derived from the WHH fitting are close to and within the range of the Pauli limit, for field $H_0$ applied parallel to the c-axis and to the ab-plane, respectively. As compared with other typical iron-based high-Tc superconductors, lower values of $H_{c2}(0)$ and higher superconducting anisotropy were found in FeSe.

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T70.00152: Phases and Phase Transitions of an Anisotropic Ising-O(3) Model

ANZUMAAN CHAKRABORTY (Presenter), THOMAS VOJTA, Physics, Missouri University of Science and Technology — The two-dimensional anisotropic Ising-O(3) model is an effective Hamiltonian for the square-lattice J1-J2 Heisenberg model, with nearest-neighbor coupling J1 along with frustrated and dominant next-nearest-neighbor coupling J2. We employ Monte Carlo simulation of the Ising-O(3) model to determine its phase diagram as a function of the anisotropy of the O(3) spins and the temperature. For sufficiently large anisotropy, there is a direct transition from the paramagnetic high-temperature phase to the low-temperature phase that breaks both spin and nematic (Ising) symmetries. This transition splits into two separate transitions as the anisotropy is lowered, leading to the appearance of an Ising-ordered intermediate phase. We also determine the orders of the phase transitions. These results can be related to the experimental observations of the orders and sequences of magnetic and structural transitions in quasi-2D ferropnictide materials.

*This work was supported in part by the NSF under Grant numbers DMR-1506152 and DMR-1828489.

T70.00153: Magnetic properties of bulk and monolayer FeSe : A DFT+DMFT study

CHANG-YOUN MOON (Presenter), Korea Research Institute of Standards and Science — FeSe is unique among other iron-based superconductors, which shows no magnetic ordered state and becomes superconducting below 8 K in the undoped bulk system while the superconducting transition temperature soars by an order of magnitude for a monolayer FeSe on SrTiO3 substrate. Using a DFT+DMFT method, we perform a comparative study on the magnetic properties of FeSe systems and LaFeAsO, another representative iron-based superconducting material. Calculated magnetic moment in the typical stripe-type magnetic ordering pattern is finite for LaFeAsO while negligible for bulk FeSe, consistently with experiments, and is also finite for monolayer FeSe suggesting the magnetic order is restored in monolayer FeSe. We suggest a mechanism explaining why the systems with the similar magnitudes of fluctuating spin $\langle S_2^2 \rangle$ have very different magnitude of ordered moment $\langle S_z \rangle$ focusing on the different aspects of local charge fluctuation. Our work provides a comprehensive understanding of magnetism in iron-based superconducting materials, and also emphasizes on the potential importance of magnetism in the high superconducting transition temperature of monolayer FeSe on SrTiO3 substrate.
The nematicity induced $d$-symmetry charge density wave in electron-doped iron-pnictide superconductors*  
HONG-YI CHEN (Presenter), National Taiwan Normal University — The interplay among the nematicity, the stripe spin-density-wave (SDW) order and superconductivity in iron-pnictides is studied in a self-consistent Bogoliubov-de Gennes equations. Our calculations have shown that the nematic-order breaks the degeneracy of $d_{x^2-y^2}$ and $d_{yz}$ orbitals and causes the elliptic Fermi surface near the $\Gamma$ point in the normal state. In addition, the appearance of the orthorhombic magnetic fluctuations generates two uneven pairs of peaks at $(\pm\pi,0)$ and $(0,\pm\pi)$ in its Fourier transformation. All these are comparing favorably with experimental measurements. In the nematic phase, our results indicate that the charge density and its spatial image in the local density of states exhibit a $d_{x^2-y^2}$-like symmetry. Finally, the complete phase diagram is obtained and the nematic phase is found to be in a narrow region close to the SDW transition in the electron-doped iron-pnictide superconductors.

*MoST of Taiwan under Grant No. 104-2112-M-003-003-MY3 and 102-2112-M-002-003-MY3, and National Center for Theoretical Science of Taiwan.

Point Contact Spectroscopy of Iron Pnictides: Probing Superconductors to Observe the Gap Structures of (P, Co, K) Doped Iron Pnictides*  
BRETT CONTI, OBERON O WACKWITZ, KEERAN RAMANATHAN (Presenter), GABRIELLE MOSS, University of the Sciences, CHENG LIN ZHANG, YU SONG, GUOTAI TAN, PENGCHENG DAI, Rice University, ROBERTO RAMOS, University of the Sciences — We used a four-wire point contact spectroscopy system to obtain differential conductance ($dI/dV$) measurements in order to observe the energy gap structures of phosphorus, cobalt, and potassium doped iron-pnictides with varying doping levels at 2K. We were motivated to study the iron pnictides because they were only recently discovered to be superconducting (~2007) due to the presence of iron which is traditionally expected to quench all superconducting properties, and also because the iron pnictides can exhibit multi-gap structures like those of magnesium di-boride. Our goal was to obtain the differential conductance measurements for varying $x$ values of phosphorus, cobalt, and potassium, and observe the gap structures of the various families to further characterize and understand the superconducting transition of these iron pnictides. We observed both single and double gap structures for various $x$ values, with delta $1 \approx 2-5$ meV, and delta $2 \approx 7-10$ meV. We will report additional results from this ongoing work.

*National Science Foundation (NSF) DMR #1555775
Charles Kaufman Foundation

Growth of ultra-thin high-Tc FeSe$_{0.5}$Te$_{0.5}$ film with high Tc on piezoelectric Pb(Mg$_{1/3}$Nb$_{2/3}$)$_{0.7}$Ti$_{0.3}$O$_3$ substrates by pulsed laser deposition  
LIN ZHU (Presenter), physics, florida state university, YONGGANG ZHAO, physics, Tsinghua University — The influence of strain on the electrical transport properties of iron chalcogenide superconductors FeSe$_x$Te$_{1-x}$ may offer insight into the mechanism of superconductivity. The inverse piezoelectric effect from a piezoelectric substrate provides a method of continuous tuning of the lattice deformation on one and the same sample. Single-crystalline piezoelectric Pb(Mg$_{1/3}$Nb$_{2/3}$)$_{0.7}$Ti$_{0.3}$O$_3$ (PMN-PT) substrates have been shown to allow reversible and dynamic control of biaxial strain in epitaxially grown thin functional films. Here we present an effective method to significantly improve the epitaxy of superconducting FeSe$_1$-xTex thin films via the introduction of a semiconducting buffer layer of FeSe$_1$-xTex. The buffer layer enables subsequent growth of superconducting FeSe$_1$-xTex at reduced deposition temperatures ($275\degree$C) on PMN-PT by pulsed laser deposition. The films exhibit consistently high critical temperatures ($\geq 16$ K); the FeSe$_1$-xTex thin films show Tc as high as 15 K even when the thicknesses are less than 10 nm. This work demonstrate a versatile platform to investigate the relationship between structure and superconductivity in FeSexTe$_1$-x thin films.

Direct Visualization of the Nematic Superconductivity in Cu$_x$Bi$_2$Se$_3$  
RAN TAO (Presenter), Physics, Fudan University — Cu$_x$Bi$_2$Se$_3$ hosts both topological surface states and bulk superconductivity. It has been identified recently as a topological superconductor (TSC) with an extraordinary nematic, i. e. $C_2$-symmetric, superconducting state and odd-parity pairing. Here, using scanning tunneling microscopy (STM), we directly examine the response of the superconductivity of Cu$_x$Bi$_2$Se$_3$ to magnetic field. Under out-of-plane fields ($B_\perp$), we discover elongated magnetic vortices hosting zero-bias conductance peaks consistent with the Majorana bound states expected in a TSC. Under in-plane fields ($B_//$), the average superconducting gap exhibits two-fold symmetry with field orientation; the long $C_2$ symmetry axes are pinned to the dihedral mirror planes under $B_//=0.5$ T but rotate slightly under $B_//=1.0$ T. Moreover, a nodeless $\Delta_4^x$ gap structure is semi-quantitatively determined for the first time. Our data paint a microscopic picture of the nematic superconductivity in Cu$_x$Bi$_2$Se$_3$ and pose strong constraints on theory.
T70.00158: SUPERCONDUCTING TRANSITION TEMPERATURE OF A BORON NITRIDE LAYER WITH A HIGH TITANIUM COVERAGE.*

FERNANDO MAGANA (Presenter), GERARDO J VAZQUEZ, National Autonomous University of Mexico — We explore the possibility of inducing superconductivity in a Boron Nitride (BN) sheet, by doping its surface with Ti atoms sit on the center of the BN hexagons. Defining the coverage M as the ratio of the number of atoms of titanium to the number of hexagons of BN per cell, we take the cases of M = 1 and 1/3. We used first-principles density functional theory in the general gradient approximation. The Quantum-Espresso package [1] was used with norm conserving pseudopotentials. The structure considered was relaxed to their minimum energy configuration. Phonon frequencies were calculated using the linear-response technique on several phonons wave-vector mesh. The electron-phonon coupling parameter was calculated with several electron momentum k-mesh. The superconducting critical temperature was estimated using the Allen-Dynes formula with μ* = 0.1 - 0.15. We note that Ti is a good candidate material to show a superconductor transition for the BN-metal system.


*We thank Mitzli Super-Computing center the technical assistance.

T70.00159: Superconductivity in Niobium Nitride

TSU-LIEN HUNG (Presenter), MIN-NAN OU, FAN-YUN CHIU, TING-KUO LEE, YANG-YUAN CHEN, Institute of Physics, Academia Sinica — Niobium nitride is a well-known superconductor with many excellent physical properties, such as high hardness, high shear rigidity, high bulk modulus. It has several structure phases, including cubic, hexagonal, and tetragonal. Among these phases, the cubic phase has been extensively studied the superconductivity with a wide range of $T_c$, 9 ~ 17 K. In our work, the cubic phase specimens of NbN were been measured by X-ray diffraction, magnetic susceptibility, resistivity, and specific heat. We observed that the $T_c$ of cubic phase appeared 13.6 K from magnetic and specific heat measurements. Very recently the hexagonal phase of epsilon-NbN (ε-NbN) has been reported to have the superconducting transition temperature about 11 K [1]. A micron sized NbN crystal was obtained from commercial product, and confirmed to be epsilon phase by electron back-scattering diffraction (EBSD) technique. However, no superconductivity was found in the micron sized epsilon-NbN crystal. We inferred that the superconductivity of epsilon-NbN reported in literature may have shorter Nb-N bond length as that of the cubic NbN phase which is about 0.02 Å shorter than our epsilon-NbN crystal.


T70.00160: ABSTRACT WITHDRAWN

T70.00161: Crystalchemistry and Thermodynamics in ZnMgO$_2$, Zn$_2$MgO$_3$ and Zn$_3$MgO$_4$ compositions.

DANIEL IVÁN GUILLEN CARRILLO (Presenter), ELIZABETH CHAVIRA, RICARDO ERNESTO PANIAGUA, JOSE ANTONIO HURTADO, KARLA ERISETH MORALES, ADRIANA TEJEDA, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, JESÚS ÁNGEL ARENAS, JORGE BARRETO, Instituto de Física, Universidad Nacional Autónoma de México, ROBERTO YSACC SATO, Instituto de Ciencias Aplicadas y Tecnología, Universidad Nacional Autónoma de México — In 2016 was reported the ZnMgO$_2$ 115 K, Zn$_2$MgO$_3$ 132 K y Zn$_3$MgO$_4$ 152 K superconductors. Our interest was study the thermodynamic behaviour, which did not reported jet. Of course, also study their crystal structure and magnetic properties. Searching in the phase diagrams thermodynamic equilibrium, we found the binary ZnO-MgO system. Then the SC compositions were in the region of the mixture of zincite-periclase solid solutions.

By simultaneous SDT (DCS-TGA) analysis it is observe the reactions and oxygen changes temperature. The solid solution mechanism was complex, occurs a cationic substitution and instantaneous accepted our lost of anions.

XRD was used to determine the reagents purity, crystal structure and reactions results. Gives the information of the formation of the mixtures of the solid solutions. CIF data helps to determined (hkl) displacement in the wurtzite crystal structure, that shows what planes happened the cation substitution. For example, (110) indicates Zn$^{2+}$ ions substitution by Mg$^{2+}$ cation. RAMAN gives only ZnO vibration, because are in a high proportion in the studied compositions. SQUID corroborate that the compositions worked were not superconductors.
SYNTHESIS OF (Bi$_{1.7}$Pb$_{0.3}$)Sr$_2$Ca$_2$Cu$_2$O$_{10}$ NANOMATERIAL SUPERCONDUCTOR. RICARDO ERNESTO PANIAGUA MARTINEZ (Presenter), ELIZABETH CHAVIRA, DANIEL IVAN GUILLEN CARRILLO, RODOLFO IVAN CRUZ HERNANDEZ, ADRIANA TEJEDA, KARLA ERISETH MORALES, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México., JESÚS ÁNGEL ARENAS, JORGE BARRETO, Instituto de Física, Universidad Nacional Autónoma de México. — The purpose of the study of the synthesis of the compound (Bi$_{1.7}$Pb$_{0.3}$)Sr$_2$Ca$_2$Cu$_2$O$_{10}$ is to characterize the properties of the superconductivity in the (Bi$_{1.7}$Pb$_{0.3}$)Sr$_2$Ca$_2$Cu$_2$O$_{10}$ when it is found as a nanocrystal in the stabilized 110 K superconducting compound, which will be induced in a single superconducting compound with the addition of lead that will substitute in the proportion of 15% of a bismuth, the final product will be characterized by XRD and SQUID.

To obtain the polycrystals of the material, solid state reaction was used with PbO, CuO, CaCO$_3$, SrCO$_3$, Bi$_2$O$_3$ by reagents, which were crushed by hand with an agate mortar.

To obtain nanocrystals from the sample, the wet crushing technique will be used, which consists of placing the sample with methanol and a magnetic stirring bar for a period of 68:22 hours.

The polycrystalline and nanocrystalline products were characterized with SQUID to see their hysteresis curves interpreting whether they present superconductivity or not.

Pairing in quantum-critical systems: $T_c$, $\Delta$ and their ratio* YI-MING WU (Presenter), University of Minnesota, ARTEM G ABANOV, Physics, Texas A&M U, ANDREY CHUBUKOV, University of Minnesota — We calculate the ratio of the pairing gap $\Delta$ at $T=0$ and $T_C$ for a set of quantum-critical models in which the pairing interaction is mediated by a gapless boson (the $\gamma$ model, where different $\gamma$ corresponds to different pairing models). The ratio $2\Delta/T_C$ has been recently computed numerically for $0<\gamma<2$ within Eliashberg theory and was found to increase with increasing $\gamma$ [T-H Lee et al, arXiv:1805.10280]. We argue that the origin of the increase is the divergence of this ratio at $\gamma = 3$. We obtain an approximate analytical formula for the ratio for $\gamma<3$ and show that it fits numerical data well. We also consider in detail the opposite limit of small $\gamma$. Here we obtain the explicit expressions for $T_c$ and $\Delta$, including numerical prefactors. We show that these prefactors depend on fermionic self-energy in a rather non-trivial way. The dependence is, however, the same for $T_c$ and $\Delta$, and the ratio $2\Delta/T_c$ approaches the BCS value 3.53 when $\gamma$ approaches to 0.

*We thank T-H Lee, G. Kotliar for fruitful discussions. The work by YW and AVC was supported by NSF-DMR-1523036.

Thermodynamic Properties of a nano-gram NbN crystal by 3ω Method FAN-YUN CHIU (Presenter), MIN-NAN OU, CHIA-SENG CHANG, YANG-YUAN CHEN, Institute of Physics, Academia Sinica — Niobium nitride is a well-known superconductor, which has several structure phases, including cubic, hexagonal, and tetragonal. Among them, the cubic phase has been extensively studied, and shows a superconductivity transition temperature ($T_C$) in a wide range of $T_C = 9 \sim 17$ K. In order to study the superconductivity of a single crystalline NbN, a NbN crystal with um size was selected from a commercial powder. The phase of selected crystals were confirmed by powder x-ray diffraction and electron backscatter diffraction (EBSD) analysis. In this work, crystals placed on a nanowire-device (ND) for studying its thermodynamic properties by 3ω method. The fabricated ND (30 μm × 600 nm × 100 nm) was carried out by means of thermal and sputtering deposition, and optical and e-beam lithography on a Si$_3$N$_4$/Si wafer. The chemical etching techniques followed up to realize the sagging of the ND from the membrane for thermal isolation. By 3ω technique, the temperature dependent specific heat and thermal conductivity of a NbN crystal at low temperatures were investigated. The details will be discussed in the presentation.

Structural and electronic behaviors of YBa$_2$(Fe$_{1-x}$Mn$_x$)$_3$O$_{8+\delta}$* RICHARD FALCONI (Presenter), MAURY SOLORZANO, Basic Science, Universidad Juárez Autónoma de Tabasco — In this work, the synthesis, structural, electrical and magnetic characterization of the set of polycrystalline samples: YBa$_2$(Fe$_{1-x}$Mn$_x$)$_3$O$_{8+\delta}$, with $x = 0$, 0.025, 0.05, 0.10 and 0.15 are reported. From the structural point of view, it was found that Mn doping generates a decrease in cell volume which is related to an oxidation state different from Mn$^{3+}$ as corroborated by XPS analysis. On the other hand, the magnetic behavior of the YBa$_2$Fe$_2$O$_{8+\delta}$, system presents a weak ferromagnetic transition around 16 K. Doping with Mn, results in a considerably decrease of the magnetic transition temperature. Oxygen content slightly decreases under Ti doping, but it seems not to be related to magnetic changes. Instead magnetic behavior is routed to changes in the oxidation state of Mn ion.

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SOORAN KIM (Presenter), Physics Education, Kyungpook National University, XI CHEN, WILLIAM FITZHUGH, XIN LI, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Since the discovery of high-temperature superconductivity in hole-doped La$_2$CuO$_4$, the mechanism of cuprate superconductors has been one of the most important problems in condensed matter physics. In this talk, we show, using ab initio simulations, a new trend that the bonding strength between the apical cation (e.g. La, Hg, Bi Ti) and apical anion (O, Cl) is positively correlated with experimental $T_{c,max}$ across the hole-doped cuprates. The “apical structure unit” formed by the apical anion and the apical cation, the in-plane Cu and its nearest oxygen neighbors is a fundamental building block that can couple dynamically to control the superconductive properties. We present the underlying fundamental phenomena of coupled apical charge flux and the phonon/lattice dynamics of apical oxygen. Cooperative apical charge fluxes modulate the in-plane transport property by dynamically change both hopping integral and charge transfer energy. We believe our understanding here can shed light on the understanding of the complicated phenomena in cuprates, especially how the transport properties are controlled by the coupled electronic and ionic dynamic oscillations.

Reference

CHUN-CHIH HSU (Presenter), Department of Physics, National Taiwan University, Taipei, Taiwan, BO-CHAO HUANG, Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan, CHIA-SENG CHANG, Institute of Physics, Academia Sinica, Taipei, Taiwan, YA-PING CHIU, Department of Physics, National Taiwan University, Taipei, Taiwan; and Institute of Physics, Academia Sinica, Taipei, Taiwan — Short-range charge density wave (CDW) order is found universally among underdoped high-$T_c$ superconductors. However, a picture on how CDW order propagates through CuO$_2$ planes remains ambiguous. In this work, we presented cross-sectional scanning tunneling microscopy and spectroscopy measurement on YBa$_2$Cu$_3$O$_6$8.81 thin film and probed both atomic and electronic structure simultaneously along the $c$-axis. Our real-space observation reveals the existence of the charge modulation on CuO$_2$ plane and CuO chain layers. The periodicity of charge modulation exhibits a wide distribution with peak value $\lambda \approx 1.3$ nm and is correlated across layers, implying a close connection of CuO$_2$ plane and CuO chain layer.

*This work was supported by Ministry of Science and Technology of Taiwan, ROC under contracts MOST 106-2628-M-002-011-MY3.

KEVIN HAUER (Presenter), MASAFUMI HORIO, Physics, University of Zurich, YASMINE SASSA, Department of Physics and Astronomy, Uppsala University, ZARINA MINGAZHEVA, DENYS SUTTER, KEVIN KRAMER, ASHLEY COOK, Physics, University of Zurich, ELISABETTA NOCERONI, OLA KENJI FORSLUND, MARTIN MÅNSSON, OSCAR TJERNBERG, Materials and Nano Physics, KTH Royal Institut of Technology, MASAKI KOBAYASHI, ALLA CHIKINA, THORSTEN SCHMITT, VLADIMIR STROCOV, Swiss Light Source, Paul Scherrer Institut, SUNSENG PYON, TAKAGI TAKAYAMA, HIRONORI TAKAGI, Department of Advanced Materials, University of Tokyo, O.J. LIPSCOMBE, STEPHEN HAYDEN, H.H. Wills Physics Laboratory, University of Bristol, TITUS NEUPERT, Physics, University of Zurich, CHRISTIAN MATT, Physics Department, Harvard University, JOHAN CHANG, Physics, University of Zurich — On this poster, we present a soft x-ray angle-resolved photoemission spectroscopy study of the high-temperature superconductors La$_2$-Sr$_x$CuO$_4$ (LSCO) and La$_{1.8-x}$Eu$_{0.2}$Sr$_x$CuO$_4$. Mapping in-plane and out-of-plane components of the Fermi surface reveals a distinct $k_z$ dispersion, that was parametrizing a tight binding model [1]. In this fashion, we quantify the contribution of the van Hove singularity to specific heat found in over doped LSCO can't be assigned to the van Hove singularity and is therefore taken as evidence of quantum criticality.

T70.00169: Vortex dynamics and hysteretic flux losses due to pinning*  
DANILIO LIARTE (Presenter), DANIEL HALL, PETER N. KOUFALIS, Cornell University, AKIRA MIYAZAKI, CERN, ALEN SENANIAN, MATTHIAS ULF LIEPE, JAMES PATARASP SETHNA, Cornell University — We use a model of vortex dynamics and collective weak pinning theory to study the residual dissipation due to trapped magnetic flux in a dirty superconductor. Using simple estimates, approximate analytical calculations, and numerical simulations, we make predictions and comparisons with experiments performed in CERN and Cornell on resonant superconducting radio-frequency NbCu, doped-Nb and Nb3Sn cavities. We invoke hysteretic losses originating in a rugged pinning potential landscape to explain the linear behavior of the sensitivity of the residual resistance to trapped magnetic flux as a function of the amplitude of the radio-frequency field. Our calculations also predict and describe the crossover from hysteretic-dominated to viscous-dominated regimes of dissipation. We propose simple formulas describing power losses and crossover behavior, which can be used to guide the tuning of material parameters to optimize cavity performance.

*DBL and JPS were supported by the US National Science Foundation under Award OIA-1549132, the Center for Bright Beams. DH, PNK and ML were supported by DOE Award No. DE-SC0008431, and NSF Award No. NSF PHY-1416318 and NSF PHY-1734189.

T70.00170: Vortex dynamics in temperature gradients: Magnetic flux expulsion in type-II superconductors.*  
ALEN SENANIAN (Presenter), DANILO LIARTE, JAMES PATARASP SETHNA, Cornell University — How do vortices in type-II superconductors get expelled as they are cooled down to the Meissner state? Experiments at Fermilab and Cornell on superconducting radio-frequency cavities suggest thermal gradients are the main mechanism behind flux expulsion. Trapped flux significantly contributes to power losses in particle accelerators, thus understanding expulsion is vital to optimizing cavity performance. Here we re-derive the thermal gradient force acting on vortices and study vortex dynamics when this force is offset with pinning forces and vortex-vortex interactions. We show that a thermal gradient acting on interacting vortices is sufficient for flux expulsion in the absence of impurities. We then introduce collective weak pinning and use recent results to obtain analytic expressions for the balance of these forces for isolated vortices. We further explore flux trapping mechanisms by modeling pinning of vortices on strong, but local, pinning centers. By including vortex-vortex interactions in addition to vortex-impurity interactions, we numerically explore their implications on trapped magnetic flux. Finally, we consider the consequences of dendritic inhomogeneity in the cooling temperature-front on flux trapping.

*National Science Foundation OIA-1549132 Center for Bright Beams.

T70.00171: Josephson Junctions Containing Antiferromagnetic FeMn and IrMn for Cryogenic Memory Application*  
ROBERT MICHAEL KLAES (Presenter), BETHANY M NIEDZIELSKI, THOMAS JOSEPH BERTUS, REZA LOLOEE, NORMAN OWEN BIRGE, Michigan State University — The study of ferromagnetic Josephson junctions for cryogenic memory applications is an area of intense research interest. The prototypical memory device takes the form of an S/F/F'/S spin valve where the two ferromagnetic layers [F, F'] have different switching fields. Switching the relative magnetizations of the two layers between parallel and antiparallel tunes the ground state phase difference across the junction to either 0 or π [1], and corresponds to a bit in a proposed memory cell [2]. It is necessary to design a device where the magnetization of the hard F' layer is robust within the switching field range of the soft F layer. A traditional method of accomplishing this in MRAM applications is to exchange-bias one of the layers by pinning its magnetization with an adjacent antiferromagnetic layer. To determine if that method can be used in cryogenic memory, we have fabricated Josephson junctions containing FeMn/NiFe and IrMn/NiFe bilayers. We present the results in this poster.


*This work was supported by IARPA via ARO Contract W911NF-14-C-0115
T70.00172: Terahertz Emission From Annular Microstrip Antennas

AMANDA VASQUEZ (Presenter), SHEILA BONNOUGH, RICHARD KLEMM, University of Central Florida — One of the most promising proposed sources of terahertz (THz) electromagnetic radiation is superconductor-based devices. These superconductors work by utilizing the intrinsic Josephson junctions (IJJs) present in single crystals of the superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ (BSCCO). To exploit the Josephson effect, a groove is inscribed in a crystal of BSCCO, producing a mesa about 1 μm thick of any shape, the geometry of which determines the emission spectrum. Alternatively, much more efficient stand alone mesa structures can be built in the desired geometry. The mesa or mesa cavity effectively functions as a microstrip antenna, which can be analyzed using standard antenna theory.

In this project, we study the one and two-dimensional wave functions of a thin annular antenna, with inner and outer radii $p_1$ and $p_2$, respectively. This involves constructing the wave functions from products of Bessel functions of the radial coordinate and trigonometric functions of the angular coordinate, finding expressions for the energy eigenvalues, and producing contour plots of the emitting wave functions. We then employ the Love equivalence principles to integrate the emission phase factor around the circumference and produce plots of the emission power patterns.

Reference:

T70.00173: Characterization of cavity mode and radiation pattern in superconducting coherent terahertz emitters

KAVEH DELFANAZARI (Presenter), University of Cambridge, RICHARD KLEMM, University of Central Florida, MANABU TSUJIMOTO, University of Tsukuba, DANIEL CERKONEY, Rutgers University, TAKASHI YAMAMOTO, Delft University of Technology, TAKANARI KASHIWAGI, KAZUO KADOWAKI, University of Tsukuba — We discuss the broadly tunable terahertz (THz) radiation in solid state terahertz (THz) emitters based on high-temperature superconducting Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ (Bi-2212). We experimentally measure the current-voltage characteristics (IVC) of mesas of different geometries, such as triangular-, pentagonal-, hexagonal-, and elliptical- cavities, and compare the IVC of the radiating and no-radiating cavities. The THz emission spectra in radiating THz cavities was measured using the Fourier transform infrared spectrometer in order to elucidate the radiation mechanism of the emitters. Moreover, we experimentally and theoretically study the angular dependence of the emission intensity obtained in mesas’ plane at various frequencies and detection angles, by rotating the sample holder relative to the detector, to identify the excited EM cavity modes within the cavities that participate in the emitter output power enhancement.

T70.00174: Towards Measuring Vacuum Polarization of Quantum Electrodynamics with Superconducting Junctions

ALI RAD (Presenter), Physics, University of Maryland, College Park — In this proposal, we present an experimental setup based on superconducting circuits and Josephson junctions to explore the modification of Josephson coefficient in the presence of external magnetic field due to vacuum polarization of quantum electrodynamics. This robust experiment can be considered as one of the few possible chances to observe the fine quantum field theory corrections in the low energy regimes of condensed matter systems. It can also be a new check for the universality of Josephson constant which is important in metrology. We will expect the signal to noise ratio of the read-out signal to increases quadratically by running time of the experiment. This characteristic of the output signal the will guarantee the feasibility of measurements with desired precision.

T70.00175: Device for extraction of Majorana current by means of Fraunhofer diffraction in proximitized superconducting arrays*

XIANGYU SONG (Presenter), YANG BAI, JAMES ECKSTEIN, ALEXEY BEZRYADIN, Physics, University of Illinois at Urbana-Champaign — We propose a geometry in which the supercurrent carried by Majorana zero modes dominates the ordinary supercurrent. The devices is tunable through the Fraunhofer diffraction. The contribution of the Majorana current is further amplified by organizing an array of conducting channels. This system can act as a tunable source of Majorana current.

We performed transport experiment on superconductor-topological insulator-superconductor Josephson junctions array consisting of square niobium islands on a Bi$_2$Se$_3$ film.

According to a Fraunhofer diffraction model, when perpendicular magnetic field is applied such that there is exactly one flux quantum in each junction we should achieve the desired regime where Majorana current is the only supercurrent in the sample. Our results indicate that the conductance peak corresponding to ordinary supercurrent indeed disappears at such magnetic flux bias. Yet, even at this flux bias (frustration f=2) the sample resistance approaches zero rapidly with cooling. This divergence of the conductance at the flux when the ordinary superconductivity is suppressed is taken as evidence for Majorana mode supercurrent.

Geometrical inhomogeneity has been modelled and, apparently, cannot account the observed zeroing of the resistance.

*NSF DMR 18-36710
T70.00176: Ferromagnetic Resonance Properties of NbCrFeCrNb multilayer stacks* MURAT CUBUKCU, London Centre for Nanotechnology, University College London, SACHIO KOMORI, Department of Materials Science and Metallurgy, University of Cambridge, ALEXANDER VANSTONE, Blackett Laboratory, Imperial College London, JULIET JOHNSON, Department of Materials Science and Metallurgy, University of Cambridge, ALEXANDER CHAN (Presenter), Blackett Laboratory, Imperial College London, KUN-ROK JEON, MARK BLAMIRE, JASON ROBINSON, Department of Materials Science and Metallurgy, University of Cambridge, LESLEY COHEN, Blackett Laboratory, Imperial College London, HIDEKAZU KUREBAYASHI, London Centre for Nanotechnology, University College London — It is by now well established that the presence of a spatially varying magnetization at a SC/FM interface can generate long range spin-polarized triplet supercurrents into the FM via the proximity effect in combination with spin mixing and spin rotation processes. Indeed junctions made up of Nb/Cr/Fe/Cr/Nb layers have been shown to carry supercurrents through significant thicknesses of Fe, showing that this combination of layers supports the generation of long range spin triplet superconductivity [1]. Quite separately, it has been recently demonstrated that spin pumping by ferromagnetic resonance (FMR) of Py when embedded in a Pt/Nb/Py/Nb/Pt stack also supports the formation of long range triplet superconductivity [2]. The characteristic signature of a spin triplet supercurrent in the latter case was an anomalous broadening of the FMR linewidth below the superconducting critical temperature \((T_C)\). In the current work we report on the FMR properties of Nb/Cr/Fe/Cr/Nb stacks, to study the behaviour of the intrinsic linewidth above and below \(T_C\) and to establish characteristics indicative of triplet superconductivity.


*Uk EPSRC SuperSpintronics Programme grant

T70.00177: Time-dependent Ginzburg-Landau model for light-induced superconductivity in the cuprate LESCOt/8 ROSS TAGARAS, JIAN WENG, ROLAND ALLEN (Presenter), Texas A&M University — Cavalleri and coworkers have discovered evidence of light-induced superconductivity and related phenomena in several different materials [1]. Here we suggest that some features may be naturally interpreted using a time-dependent Ginzburg-Landau model. In particular, we focus on the lifetime of the transient state in \(La_{1.675}Eu_{0.2}Sr_{0.125}CuO_4\) (LESCOt/8), which is remarkably long below about 25 K, but exhibits different behavior at higher temperature. A reciprocity inherent in the free energy makes the superconducting phase just as effective in blocking the stripe phase as vice-versa, and in the simulations at low temperature (coherent 3-dimensional) superconductivity persists as a robust metastable phase for an indefinitely long period of time after the femtosecond-scale laser pulse has destroyed the (coherent 3-dimensional) stripe phase. On the other hand, as the temperature, stoichiometry, and other parameters vary, there may be no ordered phase, or either, or both coexisting, as is consistent with a large body of experimental and theoretical work.


T70.00178: High field charge order across the phase diagram of \(YBa_2Cu_3O_y\)* DAVID LEOBEUF (Presenter), FRANCIS LALIBERTÉ, MEHDI FRACHT, SIHAM BENHABIB, LNCMI, TOSHINAO LOEW, JUAN PORRAS, MATHIEU LE TACON, BERNHARD KEIMER, max planck inst., CYRIL PROUST, LNCMI, STEFFEN WIEDMANN, HFML — In hole-doped cuprates there is now compelling evidence that inside the pseudogap phase, charge order breaks translational symmetry. In \(YBa_2Cu_3O_y\) (YBCO) charge order emerges in two steps: a 2D order found at zero field and at high temperature inside the pseudogap phase, and a 3D order that is superimposed below the superconducting transition \(T_c\) when superconductivity is weakened by a magnetic field. Several issues still need to be addressed such as the effect of disorder, the relationship between those charge orders and their respective impact on the Fermi surface. Here, we report high magnetic field sound velocity measurements of the 3D charge order in underdoped YBCO in a large doping range. We found that the 3D charge order exists over the same doping range as its 2D counterpart, indicating an intimate connection between the two distinct orders. Moreover, our data suggest that 3D charge order has only a limited impact on low-lying electronic states of YBCO.

*CNRS, European Magnetic Field Laboratory (EMFL), French ANR (SUPERFIELD, contract ANR-12-BS04-0012-02) the Laboratoire d’Excellence NEXT (ANR-10-LABX-0037-NEXT), French ANR (project UNESCO COS, contract ANR-14-CE05-0007), the Laboratoire d’Excellence LANEF (ANR-10-LABX-0037-NEXT), and the Université Grenoble-Alpes (SMing-AGIR).
Pressure tuning of structure, superconductivity and novel magnetic order in the Ce-underdoped electron-doped cuprate T'-Pr$_{1.3-x}$La$_{0.7}$Ce$_x$CuO$_4$ ($x = 0.1$)

ZURAB GUGUCHIA (Presenter), Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, TADASHI ADACHI, Department of Engineering and Applied Sciences, Sophia University, ZURAB SHERMADINI, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, JOHAN CHANG, Physics Institute, University of Zürich, EMIL BOZIN, Brookhaven National Laboratory, FABIAN O VON ROHR, Department of Chemistry, University of Zürich, ANTONIO M. DOS SANTOS, JAMIE MOLAIISON, Oak Ridge National Laboratory, REINHARD BOEHLER, Carnegie Institution of Washington, YOJI KOIKE, Department of Applied Physics, Tohoku University, JEDRZEJ WIETESKA, Columbia University, BENJAMIN FRANDSEN, Brigham Young University, ELVEZIO MORENZONI, ALEX AMATO, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, SIMON J L BILLINGE, YASUTOMO J UEMURA, Columbia University, RUSTEM KHASANOV, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute — High-pressure neutron powder diffraction, muon-spin rotation and magnetization studies of the structural, magnetic and the superconducting properties of the Ce-underdoped superconducting (SC) electron-doped cuprate system T’-Pr$_{1.3-x}$La$_{0.7}$Ce$_x$CuO$_4$ with $x = 0.1$ are reported. A strong reduction of the lattice constants a and c is observed under pressure. However, no indication of any pressure induced phase transition from T’ to T structure is observed up to the maximum applied pressure of $p = 11$ GPa. Large and non-linear increase of the short-range magnetic order temperature $T_{so}$ in T’-Pr$_{1.3-x}$La$_{0.7}$Ce$_x$CuO$_4$ ($x = 0.1$) was observed under pressure. Simultaneously pressure causes a non-linear decrease of the SC transition temperature $T_c$. All these experiments establish the short-range magnetic order as an intrinsic and a new competing phase in SC T’-Pr$_{1.2}$La$_{0.7}$Ce$_0.1$CuO$_4$. The observed pressure effects may be interpreted in terms of the improved nesting conditions through the reduction of the in-plane and out-of-plane lattice constants upon hydrostatic pressure.

Vortex structures in a mesoscopic unconventional superconductors*

DAE HAN PARK, NAMMEE KIM, HEESANG KIM (Presenter), Department of Physics, Soongsil University — We investigate the vortex structures in unconventional superconductors of mesoscopic size. It is well-known that, in such small systems, the size as well as the shape have a profound influence on the formation of the vortex structure, leading to interesting phenomena such as giant vortex and anti-vortex. We present unusual vortex structures when the order parameters are unconventional and multi-dimensional. Especially, we focus on the vortex structures in mesoscopic unconventional superconductors. The results are compared with those in conventional ones. For concreteness, the order parameter which transforms according to the $E_{1g}$ representation of $D_{6h}$ is chosen. The vortex structures are obtained by minimizing the Ginzburg-Landau free energy, using the simulated annealing method.

*This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education (no. 2018R1D1A1B07046338).

Superconductivity in BiS$_2$-based layered compound REO$_{0.5}$F$_{0.5}$BiS$_2$ with high-entropy-alloy-type (HEA-type) blocking layers*

YOSHIKAZU MIZUGUCHI (Presenter), RYOTA SOGABE, Tokyo Metropolitan University — We have synthesized BiS$_2$-based superconductors with high-entropy-alloy-type (HEA-type) REO (RE: rare earth) blocking layers [R. Sogabe et al., APEX 2018]. In the HEA-type samples, the RE site of REO$_{0.5}$F$_{0.5}$BiS$_2$ was occupied with five RE elements with a compositional range of 5–35%. Notably, the superconducting properties were enhanced by making HEA-type REO blocking layer as compared to the BiS$_2$-based superconductors with a conventional REO blocking layer. We will discuss about the interlayer interaction in the HEA-type REO$_{0.5}$F$_{0.5}$BiS$_2$ superconductors by examining the samples having similar lattice parameters and different mixing entropy for the RE site. [R. Sogabe et al., 1808.04090]

*This study was partially supported by the Grants-in-Aid for Scientific Research (Nos. 15H05886, 16H04493, 16K17944, and 17K19058).
T70.00182: MgB₂ and NbTiN-based hyperbolic metamaterial superconductors*  
WILL KORZI (Presenter), GRACE YONG, BRYAN AUGSTEIN, Physics, Towson University, WENURA K WITHANAGE, FEI QIN, KANISHKA WIJESEKARA, NARENDR  
ACHARYA, XIAOXING XI, Physics, Temple University, ANNE-MARIE VALENTE-FELICIANO, Thomas Jefferson National Accelerator  
Facility, JOSEPH PRESTIGIACOMO, MICHAEL OSOSKY, United States Naval Research Laboratory, IGOR SMOLYANINOV, Saltena  
LLC, VERA SMOLYANINOVA, Physics, Towson University — Recent experiments have demonstrated that the metamaterial  
dielectric function engineering is capable of enhancing superconducting properties, such as tripling the critical  
temperature Tc in Al-Al₂O₃ epsilon near zero (ENZ) core-shell metamaterial superconductors. Similar effects have been  
observed in hyperbolic (superconductor/dielectric) metamaterials. In order to expand this approach to superconductors  
with higher Tc, MgB₂/MgO, MgB₂/AlN, and NbTiN/AlN multilayers were fabricated. Dielectric constants of these  
metamaterials measured via polarization reflectometry will be reported. Correlation of the results of the transport  
measurements and the hyperbolic properties of the multilayers will be discussed.  
*This work was supported by the DARPA grant W911NF1710348.

T70.00183: Non-centrosymmetric superconductivity in Re-based solid solutions*  
FABIO ABUD (Presenter), Physics, University of Sao Paulo, MILTON S TORIKACHVILI, Physics, San Diego State University, JAMES VALLES, Physics, Brown University,  
RENATO F JARDIM, Physics, University of Sao Paulo — Rhenium based superconducting compounds Re₃M (M = W, Mo, Nb, Ta)  
crystallize in the non-centrosymmetric cubic α-Mn structure and have critical temperatures Tc ranging from ~ 4 to 9 K.  
Polycrystalline samples of Re₃M and its solid solutions were synthesized through an arc-melting furnace and subsequently  
heat treated at 1700 °C. Atomic substitutions of W by Ta or Nb in Re₃W lead to single phase materials even in as-cast  
samples, a feature not observed in the parent compound. From the superconducting point of view, the low temperature  
heat capacity cp(T) data suggest conventional s-wave pairing, which is also supported by magnetization M(T), electrical  
resistivity ρ(T), and thermal conductivity κ(T) measurements. The estimated upper critical fields Hc2(0), however, are  
sizeable in comparison with the Pauli limiting field, and may be related to either a possible triplet channel or even  
disorder. Electron tunneling measurements of the superconducting density of states of Re₃M materials are also presented  
and provide further insight into the superconducting pairing mechanism. The results are discussed within the context of the  
emergence of superconductivity in non-centrosymmetric materials.  
*This work is sponsored by the Capes Foundation within the Ministry of Education, Brazil.

T70.00184: Analysis of tunneling spectroscopy measurements of Assymetrical all-MgB₂ Thin Film Josephson  
Junctions*  
JOSEPH LAMBERT, National Radio Astronomy Observatory, KEERAN RAMANATHAN (Presenter), University of the  
Sciences, MASAHITO SAKODA, MICHIO NAITO, Tokyo University of Agriculture and Technology, ROBERTO RAMOS, University of  
the Sciences — We have previously reported high-resolution tunneling spectroscopy measurements of substructure within  
the two superconducting energy gaps of Magnesium diboride (MgB₂) [1,2]. The samples used consisted of 1-gap/2-gap  
heterojunctions, where the counter-electrode is a conventional single-gap superconductor (Pb or Sn). Here, we report  
similar measurements of 2-gap/2-gap all-MgB Josephson junctions. The crystal orientations of the two MgB films are  
mostly c-axis parallel to the tunneling direction, with very small contribution from the larger σ gap. Due to differences in  
growth conditions, we find that the two MgB electrodes have different Tc’s and gap values. We represent this physical  
system using a modified tunneling model where each electrode is represented as a weighted sum of two BCS densities of  
states. We report results of this ongoing analysis that focuses on (1) a transition from SIS to NIS behavior as temperature  
increases past the lower Tc electrode, and (2) the presence of multiple quasiparticle peaks due to the sums and  
differences in pairwise combinations of disparate π and σ gap values within each electrode.  
*R.C.Ramos acknowledges support from the National Science Foundation DMR 1555775 and the Charles Kaufman  
Foundation.
T70.00185: Possible three-dimensional nematic odd-parity superconductivity in Sr₂RuO₄

WEN HUANG (Presenter), HONG YAO, Institute for Advanced Study, Tsinghua University — The superconducting pairing in Sr₂RuO₄ is widely considered to be chiral $p$-wave with $\tilde{\Delta}_k \sim (k_x + ik_y)\tilde{\hat{z}}$, which belongs to the $E_u$ representation of the crystalline $D_{4h}$ group. However, this superconducting order appears hard to reconcile with a number of key experiments. In this paper, based on symmetry analysis we discuss the possibility of odd-parity pairing with inherent three-dimensional character enforced by the inter-orbital interlayer coupling and the sizable spin-orbit coupling in the material. We focus on a yet unexplored $E_u$ pairing, which contains finite $(k_x\tilde{\hat{x}}, k_y\tilde{\hat{y}})$-component in the gap function. Under appropriate circumstances a novel time-reversal invariant nematic pairing can be realized. This nematic superconducting state could make contact with some puzzling observations on Sr₂RuO₄, such as the absence of spontaneous edge current and no evidences of split transitions under uniaxial strains.


T70.00186: Rashba and Ising superconductors

DAVID MÖCKLI (Presenter), MAXIM KHODAS, Hebrew University of Jerusalem, YOUICHI YANASE, Kyoto University, MANFRED W SIGRIST, ETH Zürich — This poster addresses the parity-mixed superconductivity in a locally noncentrosymmetric multilayer system (Rashba), and in monolayer transition metal dichalcogenides (Ising). For the Rashba system, we investigate the magnetic field dependence of an ideal superconducting vortex lattice in the parity-mixed pair-density wave phase of multilayer superconductors within a circular cell Ginzburg-Landau approach. In multilayer systems, due to local inversion symmetry breaking, a Rashba spin-orbit coupling is induced at the outer layers. On the other hand, Ising materials like monolayer NbSe₂ are nodal topological superconductors at magnetic in-plane fields exceeding the Pauli limit, with nodal points strictly on high symmetry lines in the Brillouin zone. We use a combined numerical and group-theoretical approach in real-space to characterize the unconventional superconducting state in monolayer transition metal dichalcogenides. Even with a conventional pairing interaction, the superconducting state is intrinsically parity-mixed and robust against on-site disorder. The interplay between the Zeeman magnetic field, strong spin-orbit interaction, and electronic orbital content confer the unique superconducting and topological properties.

T70.00187: Superconductivity in NbX₂

JUNYE HUANG (Presenter), DEYI FU, BARBAROS OEZYILMAZ, Centre for Advanced 2D Materials, National University of Singapore — NbX₂, X=S, Se, Te is a family of superconducting transition metal dichalcogenides. Recently, the advent of 2D materials brought new insights into the study of superconducting TMDCs, such as gate tunability and layer dependence study, revealing rich interplay of charge density waves, spin orbit coupling and superconductivity. Ising superconductivity arises in few-layer NbSe₂ due to coexistence of SOC and superconductivity, showing strongly enhanced in-plane critical field and 2nd order superconductor-insulator transition under in-plane magnetic field. In this work, we explored the cousins of NbSe₂ in the NbX₂ family: NbS₂ and NbTe₂, using transport measurements down to milliKelvin. We will show magnetoresistance measurement in normal and superconducting states, as well as angle dependence of critical field.


*NRF Investigatorship Award (NRFI001-20)
T70.00189: Magnetoelastic coupling in multiferroic CaBaCo$_4$O$_7$  BARNITA PAUL (Presenter), RAJEEV GUPTA, Indian Institute of Technology Kanpur — A large change in magnetic field induced polarization of $\Delta P \sim 8 \text{ mC/m}^2$ around $T_C$ was discovered in multiferroic CaBaCo$_4$O$_7$ suggesting a giant linear magnetoelastic effect. The crystal structure of CaBaCo$_4$O$_7$ contains alternating triangular and kagome layers along c axis with distorted corner shared CoO$_4$ tetrahedra that makes these oxides a unique class of geometrically frustrated systems. It is assumed that the large magnetoelastic coupling arises from their atypical crystal structure and the mixed valence state of Co cations. It is well known that specific spin-lattice interaction can control the direction of the electrical polarization with a magnetic field. Although strong magnetoelastic coupling is expected in these improper ferroelectrics, there are hardly any studies to investigate the same. In this work we carry out a detailed investigation on magnetoelastic coupling using temperature dependent Raman measurements. We observe anomalous deviation of phonon frequencies and line-width from anharmonicity in the magnetic ordered phase. The maximum deviation is observed across $T_C$. This study suggests a strong magnetoelastic coupling in this compound in the ferrimagnetic phase and indicates the role of lattice in the gigantic spin induced polarization along c axis.

T70.00190: Spin-orbital-lattice entangled states in cubic $d^1$ double perovskites  NAOYA IWAHARA (Presenter), VEACHESLAV VIERU, LIVIU F CHIBOTARU, KU Leuven — The magnetism of cubic 4/5$d^1$ double perovskites has been intensively investigated due to their geometrical frustration and multipolar exchange interaction, whereas many puzzling phenomena related to the lattice degrees of freedom, e.g. “violation of the JT theorem” in structural data [1] and “breaking of local point symmetry” accompanying the ferromagnetic order [2], have not been understood. In this work, the interplay of spin-orbit coupling and vibronic coupling on the heavy $d^1$ site is investigated by $ab$ initio calculations [3]. The stabilization energy of spin-orbital-lattice entangled states is found to be comparable to or larger than the exchange interactions, suggesting the presence of nonadiabatic Jahn-Teller dynamics in the systems. The entanglement of the spin and lattice degrees of freedom induces a strong magnetoelastic response. This multiferroic effect is at the origin of the recently reported breaking of local point symmetry accompanying the development of magnetic ordering in Ba$_2$NaOsO$_6$.


T70.00191: Spin Seebeck Effect in insulating SrFeO$_3$-$\delta$ films*  DESHUN HONG (Presenter), CHANGJIANG LIU, JOHN E. PEARSON, AXEL F HOFFMANN, DILLON D FONG, ANAND BHATTACHARYA, Argonne National Laboratory — SrFeO$_3$ is a metal with cubic structure and is a helicoidal antiferromagnet (AF) at low temperatures (< 134 K) [1]. Recently, an anisotropic double $q$ spin spiral and isotropic quadruple $q$ spiral hosting a three-dimensional lattice of hedgehog singularities in SrFeO$_3$ [2] was found suggesting a topologically non-trivial magnetic structure. Upon reduction, SrFeO$_3$-$\delta$ becomes insulating while retaining long wavelength incommensurate AF order. In this work we measured the spin Seebeck effect (SSE) in SrFeO$_3$-$\delta$ films synthesized by molecular beam epitaxy, and detected an SSE signal below ~120 K, near the ordering temperature of incommensurate antiferromagnetism found in SrFeO$_3$-$\delta$ bulk [3]. Control experiment were used to verify that the signal arises from a spin current originating in SrFeO$_3$-$\delta$ and to rule out magnetic proximity effect. By comparing the second derivative of the SSE signal with respect to magnetic field and comparing to a Brillouin function, we find large deviations that suggest strong spin correlations in oxygen reduced SrFeO$_3$-$\delta$ for temperatures below 120 K. Our work suggests SSE an effective way of probing magnetic correlations in non-ferromagnetic insulating films.

*This work was supported by the U.S. DOE, BES.
**T70.00192: Quantum percolation of monopoles and the response of quantum spin ice**

VADIM OGANESYAN, Physics and Astronomy, CSI and GC, CUNY, MATTHEW STERN, Physics and Astronomy, SUNY, Stony Brook, CLAUDIO CASTELNOVO (Presenter), TCM, University of Cambridge, SARANG GOPALAKRISHNAN, Physics and Astronomy, CSI and GC, CUNY — The low-temperature (magnetic) response of quantum spin ice is dominated by the coherent motion of a dilute gas of monopoles. Contrary to conventional modelling that assumes a uniform distribution of hopping amplitudes for such dynamics, recent work by Tommasello et al. has demonstrated that the distribution is in fact bimodal, and strongly correlated with the surrounding spin configuration. The larger of the two amplitudes occurs on average 2/3 of the times, and is responsible for the coherent motion of monopoles. The smaller one, on the other hand, induces dynamics that is far slower than the expected decoherence time scales in a solid state system. We exploit this structure to construct a theory of quantum monopole motion in spin ice in the limit where the slow hopping terms are set to zero. The monopole wavefunctions are fractal. The non-ergodic nature of monopole motion manifests itself in the low-frequency behaviour of spin response, and is consistent with experimental observations. We further extend our results to the case of disordered spin ice.

*This work was supported in part by Engineering and Physical Sciences Research Council (EPSRC) Grant No. EP/P034616/1, and by NSF grant DMR 1653271 and NSF DMR Grant No. 1508538

**T70.00193: Many-body-localization transition in the one-dimensional SYK model at finite N**

SHAOKAI JIAN, HONG YAO, Tsinghua University — We study the generalized Sachdev-Ye-Kitaev (SYK) chain consisting of N (complex or Majorana) fermions per site with random interactions and hoppings between neighboring sites. In the limit of vanishing SYK interactions, from both supersymmetric field theory analysis and numerical calculations we find that the random-hopping model exhibits Anderson localization at finite N, irrespective of the parity of N. Moreover, the localization length scales linearly with N, implying the absence of Anderson localization only at $N=\infty$. For finite SYK interactions, by performing the exact diagonalization we show that there is a dynamic phase transition from many-body localization to thermal diffusion as interaction strength exceeds a critical value $J_c$. In addition, we find that the critical interaction strength $J_c$ decreases with the increase of $N$, consistent with the analytical result of $J_c/t \sim 1/(N^{4/5}/\log N)$, derived from the weakly interacting limit.

[1] Xin Dai, Shao-Kai Jian, Hong Yao, arXiv:1802.10029

**T70.00194: Electrically conducting rock-salt LuO epitaxial thin film**

KENICHI KAMINAGA (Presenter), WPI-AIMR, Tohoku Univ., DAICHI OKA, Graduate School of Science, Tohoku Univ., TETSUYA HASEGAWA, Graduate School of Science, University of Tokyo, TOMOTERU FUKUMURA, WPI-AIMR, Tohoku Univ. — Lutetium sesquioxide Lu$_2$O$_3$ is known as a widegap insulator with the highly stable closed shell trivalent ions. On the other hand, lutetium monoxide LuO has been recognized as gaseous phase. In this study, solid-phase rock-salt LuO was synthesized in a form of epitaxial thin film by pulsed laser deposition method for the first time [1]. LuO possesses unusual valence of Lu$^{2+}$ ($4f^{14}5d^1$). In contrast with transparent and highly insulating Lu$_2$O$_3$, LuO exhibited dark-brown color and metallic conduction with high electrical conductivity at room temperature (~60 S.cm$^{-1}$). A cusp-shaped positive magnetoresistance originating from the weak antilocalization effect suggested a significant spin-orbit coupling in LuO manifested by Lu 5$d$ electron carriers. [1] K. Kaminaga et al., ACS Omega 3, 12501-12504 (2018).

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**T70.00195: Structure-property relationships in lacunar spinels from band theory**

YIQUN WANG (Presenter), JAMES M RONDINELLI, Northwestern University — The A-site deficient lacunar spinel GaM$_4$X$_8$ (M=Mo,V,Nb,Ta; X=S,Se) are ideal candidates to achieve novel electrical materials exhibiting metal-insulator transitions and may find use in resistive random-access memories (RRAM). They are experimentally narrow-bandwidth semiconductors, and undergo structural, electrical and magnetic phase transitions with external stimuli, e.g. temperature, pressure, electric pulse.

We systematically study the structure-property relationships within the lacunar spinels using ab initio density functional theory (DFT). We find that semi-local GGA functionals are able to predict insulating states with the low-symmetry rhombohedral phase without static correlation, but the high-temperature cubic phase is metallic due to orbital degeneracy. Spin-orbit coupling together with on-site Coulomb interactions are shown to reduce the local symmetry and open a small band gap within the cubic lattice. Our findings will assist understanding of the nature of these transitions and design new materials with tunable electronic states.

*This work is supported by the National Science Foundation (NSF) under award number DMR-1729303.
T70.00196: High-pressure synthesis, crystal structure, and magnetic properties of Ba$_3$CuOs$_2$O$_9$

JIE CHEN (Presenter),
National Institute for Materials Science, HAI LUKE FENG, Max Planck Institute for Chemical Physics of Solids, YOSHITAKA MATSUISHITA, ALEXEI A BELIK, YOSHIHIRO TSUJIMOTO, YOSHIO KATSUYA, MASAHIKO TANAKA, National Institute for Materials Science, MAN-RONG LI, HONGBIN LIANG, School of Chemistry, Sun Yat-sen University, LIRONG ZHENG, Institute of High Energy Physics, Chinese Academy of Sciences, KAZUNARI YAMAURA, National Institute for Materials Science — The triple perovskite Ba$_3$CuOs$_2$O$_9$ crystalizes into an orthorhombic structure (Cmcm) and shows a manifest antiferromagnetic transition at 47 K [1], while it crystalizes into a hexagonal structure (P6$_3$/mmc) when treated under a high-pressure and high-temperature condition (typically 6 GPa and 1100 °C). The change of structure gains a 1.3% increase in structural density. The hexagonal phase was quenched at ambient condition and the magnetic and electrical properties were investigated via measurements of the ac and dc magnetic susceptibilities, electrical resistivity, and specific heat capacity. The data indicated that the magnetic transition temperature increased to 290 K by the structure change. We discuss details of the magnetic and electrical properties of the newly synthesized hexagonal Ba$_3$CuOs$_2$O$_9$.


T70.00197: Strong Pseudospin-Lattice Coupling in Sr$_3$Ir$_2$O$_7$: Coherent Phonon Anomaly and Negative Thermal Expansion*

LILI HU, MENG YANG, YANLING WU, QIONG WU, HUI ZHAO, FEI SUN, WEI WANG, Chinese Academy of Sciences, RUI HE, Texas Tech University, SHAOLONG HE, Chinese Academy of Sciences, HONG ZHANG, Sichuan University, RONGJIN HUANG, LAIFENG LI, YOU GUO SHI, JIMIN ZHAO (Presenter), Chinese Academy of Sciences — The similarities with cuprates make iridates interesting materials to investigate superconductivity. Equivalently attractive is their puzzling intrinsic complex interactions. Here, we report an ultrafast optical spectroscopy investigation of the coherent phonon in Sr$_3$Ir$_2$O$_7$, a bilayer Ruddlesden-Popper perovskite iridate. An anomaly in the $A_{1g}$ optical phonon ($\nu = 4.4$ THz) is unambiguously observed below the Néel temperature ($T_N$), which we attribute to pseudospin-lattice coupling (PLC). Significantly, we find that PLC is the dominating interaction at low temperature, and we directly measure its coefficient to be $\lambda = 150 \pm 10$ cm$^{-1}$, which is two orders of magnitude higher than that in manganites (< 2.4 cm$^{-1}$) and comparable to that in CuO (50 cm$^{-1}$, the strongest PLC or spin-lattice coupling known so far). Moreover, we find the strong PLC induces an anisotropic negative thermal expansion. Our finding identifies essential role of PLC in iridates at low temperature and uncovers a possible novel similarity with cuprates.

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T70.00198: Electronic Transport in Thin Crystals of Ruthenium Chloride*

NAOMY MARRUFO (Presenter), AMIRARI DIEGO, JOSUE RODRIGUEZ, Physics & Astronomy, California State University, Long Beach, GILBERT LOPEZ, Physics, University of California, Berkeley, NICHOLAS BREZNAY, Physics, Harvey Mudd College, ROBERT KEALHOFER, Physics, University of California, Berkeley, FRANCISCO RAMIREZ, SAMANTHA CROUCH, Physics & Astronomy, California State University, Long Beach, JAMES G. ANALYTIS, Physics, University of California, Berkeley, CLAUDIA OJEDA-ARISTIZABAL, Physics & Astronomy, California State University, Long Beach — Ruthenium chloride (RuCl$_3$) has gathered significant interest in the recent years, as it is a layered material that presents key features such as a honeycomb geometry and bond-directional interactions, making it a promising candidate for the experimental realizations of the Kitaev-Heisenberg model. Exciting ground states have been predicted for this system, such as quantum spin liquids, consistent with recent inelastic neutron scattering experiments as well as long ranged magnetic ordered states. Here we present preliminary electronic transport experiments on exfoliated thin crystals of RuCl$_3$ and the effects of ionic liquid gating.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences. Award number: DE-SC0018154. Additional funding was supported by the National Institute of General Medical Sciences of the National Institutes of Health Under Award Number T34GM008074. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health.
T70.00199: Doping driven spin-flop transition in mixed 3d-5d compounds*  WEIGUO YIN (Presenter), WENHU XU, ROBERT KONIK, Brookhaven National Laboratory — The in-plane magnetization of the layered iridate Sr$_2$IrO$_4$ turns to out-of-plane upon partial substitution of ruthenium or manganese atoms for iridium. Based on first-principles electronic structure analysis, we present an effective low-energy Hamiltonian to model this doping effect. We found that the spin-flop transition originates from the M-Ir bond direction changes from the local easy axis to the hard axis as M changes from Ir to Ru or Mn.

*U.S. DOE-BES, Division of Materials Science and Engineering, under Contract No. DE-SC0012704.

T70.00200: Semi-classical Theory of Large N Tensor Model Chaos  JAEWON KIM (Presenter), EHUD ALTMAN, THOMAS SCAFFIDI, University of California, Berkeley — Lately, the Sachdev-Ye-Kitaev (SYK) model has become increasingly important due to its chaotic dynamics and its approximate conformal symmetry. The model's conformal symmetry suggests the existence of a holographic dual, rendering the model important in the study of quantum gravity. Tensor models have been found to be similar to the SYK model, in that they exhibit the dominance of melonic diagrams. In this paper, we study the chaotic dynamics of the Tensor Models semi-classically, by finding the spectrum of the Lyapunov exponent. We introduce a classical version of the Tensor model for which chaos can be understood as arising from nonlinear dynamics of the equation of motion.

T70.00201: 2D fermi gases under the microscope  AIRLIA SHAFER-MOAG (Presenter), CEDRIC WILSON, BISWAROOP MUKHERJEE, PARTH PATEL, ZHENJIE YAN, RICHARD J FLETCHER, MARTIN ZWIERLEIN, MIT — Confining a quantum fluid in two dimensions (2D) profoundly changes its behavior and leads to a host of new phenomena, for example the possibility of topological superfluid transitions and quantum Hall states. Here we report our progress towards creating a uniform 2D fermionic gas of 6Li confined in a highly flexible optical potential. The homogenous density enables the study of physics typically difficult to access in harmonically trapped samples, such as critical phenomena, correlation functions, superfluid properties and the spectroscopic response. Incorporating a dual-objective high-resolution imaging system allows us to both manipulate and image the gas with sub-micron resolution, permitting the projection of tailored potentials and in situ imaging of topological defects.

T70.00202: Machine learning of quantum phase transitions  XIAOYU DONG (Presenter), California State University, Northridge, USA, XUEFENG ZHANG, Chongqing University, Chongqing, People's Republic of China, FRANK POLLMANN, Technische Universität München, Garching, Germany — Machine learning algorithms provide a new perspective on the study of physical phenomena. In this paper, we explore the nature of quantum phase transitions using multi-color convolutional neural-network (CNN) in combination with quantum Monte Carlo simulations. We propose a method that compresses (d + 1)-dimensional space-time configurations to a manageable size and then use them as the input for a CNN. We test our approach on two models and show that both continuous and discontinuous quantum phase transitions can be well detected and characterized. Moreover we show that intermediate phases, which were not trained, can also be identified using our approach.

T70.00203: Unbinding slave spins in the Anderson impurity model*  DANIELE GUERCi (Presenter), International School for Advanced Studies, ADRIANO AMARICCI, Democritos National Simulation Center, Istituto Officina dei Materiali del CNR and International School for Advanced Studies, MICHELE FABRIZIO, International School for Advanced Studies — We show that a generic single-orbital Anderson impurity model, lacking, for instance, any kind of particle-hole symmetry, can be exactly mapped without any constraint onto a resonant level model coupled to two Ising variables, which reduce to one if the hybridization is particle-hole symmetric [1]. The mapping can be straightforwardly extended to a multiorbital impurity model where the isolated impurity Hamiltonian does not include Coulomb exchange terms. We also demonstrate how single-particle Green's functions of the physical fermions can be calculated without constraints, which would, for instance, allow exploiting DMFT to study in the slave-spin representation Hubbard-like models in lattices with infinite coordination. The generality of the mapping allows to study a wide range of problems varying from the Mott-transition in infinite-dimensionality to transport in quantum dots.


*This work has been supported by the European Union under H2020 Framework Programs, ERC Advanced Grant No. 692670 “FIRSTORM”.

T70.00204: ABSTRACT WITHDRAWN —
T70.00205: Local electrodynamics of disordered conductor model systems measured with scanning microwave impedance microscopy

HOLGER THIERSCHMANN (Presenter), Quantum Nanoscience, Delft University of Technology, HALE CETINAY, Faculty of Electrical Engineering, Mathematics and Computer Science, Delft University of Technology, MATVEY FINKEL, MARC P. WESTIG, ALLARD J. KATAN, Quantum Nanoscience, Delft University of Technology, PIET VAN MIEGHEM, Faculty of Electrical Engineering, Mathematics and Computer Science, Delft University of Technology, TEUN M Klapwijk, Quantum Nanoscience, Delft University of Technology — We have measured the local impedance of disordered conductor model systems at GHz frequencies in order to study the electrodynamic response of systems around the metal-insulator phase transition for non-trivial patterns of conductive and insulating regions at small scales. We realize the disordered conductors through nano patterning of metallic thin films into networks which exhibit a phase transition from the conducting to the insulating state through bond percolation. The electrodynamic response is measured with a scanning microwave impedance microscope at room temperature. When the networks are patterned out of aluminum with highly conductive bonds, we observe a correlation of the local signal and the size of the respective cluster, at different degrees of percolation. When the bonds are made more resistive through using NbTiN, the signal varies within a cluster, depending sensitively on the local network topology. Our results are well reproduced within a network model of resistors and capacitors that takes into account the specific network topologies as well as the electric and dielectric environment.

*We acknowledge funding from the ERC (METIQUM, grant 339306). T.M.K. further acknowledges support from the Russian Science Foundation (RSF) Project No.17-72-30036.

T70.00206: Mesoscopically confined 2D holes with strong correlation

CHIEH-WEN LIU (Presenter), Case Western Reserve University, LOREN PFIEFFER, KENNETH WEST, Princeton University, XUAN GAO, Case Western Reserve University — We present a transport study on the mesoscopic confinement effects on a strongly interacting two-dimensional holes (2DH) in a GaAs quantum well with low density (~2×10¹⁰/cm²) and high mobility. By applying a voltage to a split-gate, the 2DH underneath the gate is depleted, leaving a narrow (~2 μm wide) channel conducting. The channel formation is reflected in the evolution of the temperature (T)-dependent resistance at various gate voltages \( V_g \) as well as the \( V_g \) dependent resistance. Interestingly, when the mesoscopic channel starts to form, a strong magneto-resistance peak with an insulating-like \( T \) dependence was observed before the \( ν = 1 \) quantum Hall (QH) state. When the channel is further depleted, the magnetic field induces a rapidly increasing magneto-resistance and a ‘metal-to-insulator’ transition appears at a moderate magnetic field (~ 0.2 T) where the sample resistivity \( ρ_{xx} < h/e^2 \) along with the destruction of the \( ν = 1 \) QH state. Our results suggest that mesoscopically constricted dilute 2D systems can be a rich playground for exploring interaction effects and phase transitions in 2D.

*The work at CWRU was funded by the NSF (DMR-1607631). The work at Princeton University was funded by the Gordon and Betty Moore Foundation, and by the NSF MRSEC (Grant# 1420541).

T70.00207: Optical control of magnetism in NiFe/VO₂ heterostructures

GUODONG WEI, XIAOYANG LIN (Presenter), Beihang University, STEPHANE MANGIN, University of Lorraine, WEISHENG ZHAO, Beihang University — Optical methods for magnetism manipulation have been considered as a promising strategy for ultralow-power spintronics. Strategies based on all optical switching (AOS), hot electrons and photosensitive-material-based devices have already generated exciting new prospects both for fundamental physics and technological applications. However, a widely applicable method to combine optical operation with magnetic modulation is still highly desired. Here, the strongly correlated electron material VO₂ is introduced to realize phase-transition based optical control of the magnetism in NiFe. [1] The heterostructure features appreciable modulations both in electrical and magnetic properties. Utilizing this optically controlled magnetism modulation feature, programmable Boolean logic gates (AND, OR, NAND, NOR, XOR, NXOR and NOT) for high-speed and low-power data processing are demonstrated based on this engineered heterostructure. As a demonstration of phase-transition spintronics, this work may pave the way for next-generation electronics in the post-Moore era.

1) arXiv: 1805.02453.

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demonstrate the ability to tune the insulating behavior of TiSe$_2$ with different synthesis parameters. We confirm the metallicity in single crystalline TiSe$_2$ grown by the transition forms, but there has been little reported on the low temperature resistivity, where there is large discrepancy been paid to the anomalous feature in temperature dependent resistivity near 150 K where a charge-density-wave interaction is not the sole driving force of these transitions and that lattice degrees of freedom play an important role. Our analysis indicates that the electron–electron interaction is not the sole driving force of these transitions and that lattice degrees of freedom play an important role.

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**T70.00212: Exploring “hidden order” (HO) through Re and Rh co-substitution in URu$_2$Si$_2$**

KALYAN SASMAL (Presenter), University of California, San Diego, SHENG RAN, University of Maryland, College Park, TREVOR KEIBER, BOB WANG, ROBERT A ROBINSON, M BRIAN MAPLE, University of California, San Diego — The identity of the mysterious “hidden-order” (HO) phase in the correlated $f$-electron superconductor (SC) URu$_2$Si$_2$ has eluded researchers for more than three decades. Substitution of transition metals into URu$_2$Si$_2$ at the Ru sites reveals how factors such as lattice parameters, charge carrier concentration, disorder and $d$-$f$ electron hybridization influence the HO phase and SC. We discuss the effects of the co-substitution of equal amounts of Re and Rh, which are isoelectronic on average, into URu$_2$Si$_2$ to form URu$_2$$_{2-x}$Re$_x$Rh$_x$Si$_2$, pseudo ternary alloys based on the physical properties including structure and lattice parameters, electrical resistivity, magnetic susceptibility, and specific heat. The features in the physical properties that characterize the energy gap associated with the HO phase (e.g., exponential $T$-dependence of the specific heat) are suppressed rapidly with Re and Rh co-substitution level so that by $x = 0.11$, the HO phase transition is no longer discernible. The HO phase transition temperature ($T_{HO}$) and the gap decrease monotonically with Re-Rh concentration $x$.

*This research was supported by US DOE DE-FG02-04ER46105 and NSF DMR-1810310

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**T70.00213: A Dirac Fermion Hierarchy of Composite Fermi Liquids**

JIE WANG (Presenter), Princeton University — Composite Fermi liquids (CFLs) are compressible states that can occur for 2D interacting fermions confined in the lowest Landau level at certain Landau level fillings. They have been understood as Fermi seas formed by composite fermions which are bound states of electromagnetic fluxes and physical fermions due to the celebrated work by Halperin, Lee and Read [Phys. Rev. B 47, 7312 (1993)]. At half filling, an explicitly particle hole symmetric theory based on Dirac fermions [Phys. Rev. X 5, 031027 (2015)] was proposed by Son as an alternative low energy description. In this work, we propose an effective theory, which generalizes Son’s Dirac fermion theory, by internal gauge flux attachment, from half filling to all fillings that CFLs for fermions can occur. We also numerically investigated the Berry curvature of CFL model wave functions at fillings not being one half, and observed that it is uniformly distributed on the Fermi sea except at the center where an additional $\pi$ phase was found. The numerical results support the idea of internal gauge flux attachment.

*Princeton University graduate student Compton Fund.

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**T70.00214: First-principles study of charge and magnetic ordering in monolayer NbSe$_2$**

ZHIMOU ZHOU (Presenter), Peking University, FEIPENG ZHENG, Jinan University, XIAOQIANG LIU, JI FENG, Peking University — Monolayer NbSe$_2$ has recently been shown to be a two-dimensional superconductor, with a competing charge-density wave (CDW) order. This work investigates the electronic structure of monolayer NbSe$_2$ based on first-principles calculations, focusing on charge and magnetic orders. It is found that decreased screening in the monolayer NbSe$_2$ with a perfect lattice exhibits magnetic instability, which is removed by the formation of CDW. Two energetically competitive but distinct $3 \times 3$ CDW structures are revealed computationally, which have a significant impact on the Fermi surface. The relations of the potential CDW phases with experimental structure and the coexisting superconductivity are discussed.

*This work was supported by National Natural Science Foundation of China (Grant No. 11725415), Ministry of Science and Technology of the People's Republic of China (Grant No. 2016YFA0301004), and the Key Research Program of the Chinese Academy of Sciences (Grant No. XPDPB08-4).

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**T70.00215: Fermionic retro reflection, hole jets, and magnetic steering in 2D electron systems**

LEV KENDRICK (Presenter), Physics, Massachusetts Institute of Technology, PATRICK J. LEDWITH, Massachusetts Institute of Technology, ANDREY SHYTOV, Physics, Massachusetts Institute of Technology, LEONID LEVITOV, Massachusetts Institute of Technology — The combination of fermion exclusion and momentum conservation leads to unusual dynamics in two-dimensional Fermi liquids. We show that the response of a 2D Fermi liquid to an injected beam of current includes hole jets centered at the backscattering direction. We propose a magnetotransport measurement to probe the angular structure of the hole jets.
T70.00216: SmB\textsubscript{6} in-gap states encoded inside the hybridization*  EDWIN RAMOS, JERESON SILVA VALENCIA, ROBERTO FRANCO, Physics Department, National Colombian University, MARCOS FIGUEIRA (Presenter), Physics Department, Federal Fluminense University — In this article we investigate the effects of short-range anti-ferromagnetic correlations on the gap opening of topological Kondo insulators. We add a Heisenberg term to the periodic Anderson model at the limit of strong correlations. This new model [1] is adequate for studying the topological Kondo insulator SmB\textsubscript{6}.

We solve the problem on a two dimensional square lattice considering the $\Gamma_8$ symmetry group representation that already encoded the spin-orbit coupling of the $J=5/2$ multiplet structure of the Samarium ions orbitals. We investigate the role of the hybridization on the generation of in-gap states inside the topological gap. We also discuss the effects of those in-gap states over the band structure, the density of states, the differential conductance and the optical conductivity, comparing them with recent Arpes experimental results [2,3,4].

references:

*We are thankful for the financial support of the Brazilian agencies CNPq and Capes and Colombian agencies Dieb and Colciencias.

T70.00217: Quantum effects in the system of Boltzmann hard spheres*  SERGEI STISHOV (Presenter), Institute for High Pressure Physics, Moscow, Troitsk, Russia — The quantum contribution to the energy of the Boltzmann gas of solid spheres turns out to be practically constant to the highest temperatures, when the De Broglie thermal wavelength is only a small fraction of the diameter of the solid sphere. Accordingly, the heat capacity of the system is not much different from the classical value of $3/2 \ k$ everywhere except for the region of the lowest temperatures, where the dependence of the heat capacity of the system on temperature has a Debye appearance, but with a very low "Debye" temperature of the order of several degrees.

The quantum crystal-liquid equilibrium line of the "Boltzmann" system of hard spheres coincides with the classical one except for the region of very low temperatures. In the system under consideration, high-temperature quantum effects appear in a kind of "naked" form, while in the case of more realistic systems or models they can be masked by the complex behavior of the other components of the total energy.

*The work was supported by the Russian Science foundation (Grants No. 17-12-01050).

T70.00218: Spontaneous symmetry breaking from anyon condensation*  MARCEL BISCHOFF, Mathematics, Ohio University, COREY JONES, Mathematics, Ohio State University, YUAN-MING LU (Presenter), Physics, Ohio State University, DAVE PENNEYS, Mathematics, Ohio State University — As a cornerstone for condensed matter physics, Landau theory of symmetry breaking dictates that the symmetry group G of a physical system can spontaneously breaks down to any subgroup H, characterized by a local order parameter valued in the quotient group G/H. However this paradigm breaks down when topological orders and anyons come into play. What is the relation between symmetry groups G and H of two symmetry enriched topological orders (SETOs), if they are connected to each other through a continuous quantum phase transition (QPT)? To address this issue, we develop a mathematical framework within the category theory of topological orders, which determines the compatibility of symmetry groups G and H for two SETOs connected by a QPT driven by anyon condensation. We identify two symmetry obstructions for such anyon-condensation transitions. which are demonstrated by many examples.

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Identification of low-lying energy states in quantum critical Ce(Fe$_{0.76}$Ru$_{0.24}$)$_2$Ge$_2$

THOMAS HEITMANN (Presenter), WOUTER MONTFROOIJ, University of Missouri, YIMING QIU, SHANNON M WATSON, ROSS WEBB ERWIN, WANGCHUN CHEN, National Institute of Standards and Technology, YANG ZHAO, University of Maryland - College Park — The compound Ce(Fe$_{0.76}$Ru$_{0.24}$)$_2$Ge$_2$ has long been known to be a quantum critical point system. One of the features discovered in this material is hyperscaling of the dynamic response of the system. Chemical doping is used to prepare the system at the quantum critical point, which results in a distribution of local Kondo temperatures and consequently the formation of magnetic clusters. We present direct evidence for the spin-flipping of these magnetic clusters, which provides the low energy states required to explain the hyperscaling at the quantum critical point. The superspin flipping was first identified using spin-polarized neutron spectroscopy on the BT7 triple-axis spectrometer at the NIST Center for Neutron Research, then—once the magnetic signal was separated from that of the lattice—tracked using unpolarized neutron spectroscopy on the TRIAX thermal neutron triple-axis spectrometer at the University of Missouri Research Reactor.

Braiding of worldlines in Monte Carlo configurations as nonlocal probe for quantum phase transitions

LIANA SHPANI (Presenter), Clark University, WEI WANG, Max Planck Institute for the Physics of Complex Systems, FABIO LINGUA, BARBARA CAPOGROSSO-SANSONE, Clark University — We propose to use the braiding of particles’ trajectories in path-integral Monte Carlo configurations, to characterize entanglement “patterns” in strongly-correlated hardcore lattice bosons. By extracting certain statistical properties of worldline configurations, we are able to detect the SF-insulator transition and SF-Z2 topological insulator transition.

Ultrafast transient interference in pump-probe spectroscopy of band and Mott insulators

KAZUYA SHINJO (Presenter), TAKAMI TOHYAMA, Tokyo University of Science Katsushika Campus — Ultrafast pump-probe spectroscopy with high temporal and spectral resolutions provides new insight into ultrafast nonequilibrium phenomena. We propose that transient interference between pump and probe pulses is realized in pump-probe spectroscopy of band and Mott insulators, which can be observed only after recent developments of ultrafast spectroscopic techniques [1]. A continuum structure in the excitation spectrum of band insulators is found to act as a medium for storing the spectral information of the pump pulse, and the spectrum detected by the probe pulse is interfered with by the medium, generating the transient interference in the energy domain. We also demonstrate the transient interference in the presence of electron correlations in a one-dimensional half-filled Hubbard model. Furthermore, bosons coupled to electrons additively contribute to the interference. Our finding will provide an interpretation of probe-energy-dependent oscillations recently observed in the pump-probe spectrum for a two-dimensional Mott insulator [2].


Dynamical t/U Expansion Theory of a Doped Hubbard Model

WENXIN DING (Presenter), School of Physics and Materials Science, Anhui University, RONG YU, Physics Department, Renmin University — In this work, we construct a new U(1) slave representation for the single band Hubbard model in the large-U limit. By employing a dynamic Green’s function method for the slave spins, we formulate a dynamic t/U expansion for the Hubbard model which reduces the model to a t-J-type low energy effective theory for the spinons and an XXZ-type effective theory for the slave spins. This new approach recovers our previous slave rotor results for the Mott insulating state at half-filling, and is more amenable to describe the strong correlation effects in the finite doping regime. By solving the slave spin theory at the mean field level for finite doping, we find that the superexchange interaction strength J, as well as the effective spinon hopping amplitude, develops doping dependence. More interestingly, pairing-type interaction in the dynamic Green’s function shows up, which solely stems from quantum fluctuations of the doping driven Mott-insulator-to-metal transition.

Energy-Momentum Photoluminescence Spectroscopy of Quantum Emitters in Hexagonal-Boron Nitride

YANG WANG (Presenter), JUAN LIZARAZO FERRO, RASHID ZIA, Brown University — Defects in hexagonal-boron nitride(h-BN) have recently been characterized and identified as light emitters that are ideal for quantum information applications. These photostable emitters have narrow and tunable emission spectra, operate at room temperature, and exhibit high quantum efficiency. However, the electronic structure of these quantum emitters are still under intense debate. In this presentation, we use angle- and polarization-resolved photoluminescence spectra to study the origin of light emission from a range of point emitters in h-BN.
T70.00225: Visualization of domain and interfacial structures of Monolayer semiconductors by Nonlinear Optical Microscopy*  
CHUN AN CHEN (Presenter), YING-YU LAI, National Tsing-Hua University, National Tsing Hua University, PO-YEN LIN, Academia Sinica, Taiwan, XIN-QUAN ZHANG, MENG-HSI CHUANG, YI-HSIEN LEE, National Tsing-Hua University, National Tsing Hua University — Domain and interfacial structures of the monolayer transition metal dichalcogenides (TMD) are significant to diverse physics and performances. Unique carrier transportation and bandgap tunability could be engineered with inter-grain twisting, which provide an extra degree of freedom for device designing. Here, the correlation between GBs and inter-grain twisting in monolayer WS2 is studied using nonlinear microscopy. With the change of inter-grain twisting, domain and interfacial structures of the monolayer is monitored and studied.

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T70.00226: Energy transfer in van der Waal stacked MoS2 – Graphene Quantum Dots with Ab-initio validation  
RAJARSHI ROY (Presenter), Plasma Technologies, CEITEC MU — Graphene based van der Waals (vdW) heterostructures can facilitate enticing charge transfer dynamics in between the layers with emission of excitonic quasi-particles. In this work, an attempt has been made to probe such van der Waal (vdW) heterostructures between few layer MoS2 sheet embedded quantum dot (QD) and amine-functionalized graphene quantum dot (GQD) to explore the energy transfer mechanism. Our findings reveal interesting non-radiative Forster type energy transfer with quenching of functional GQD PL after GQD/MoS2 hetero interface formation and validates the existing charge transfer shown that is analogous between a 0D and 2D system. This non-radiative type energy transfer characteristics from GQD into MoS2 layer through vdW interaction has been confirmed by with a combination of photoluminescence and time decay analyses with ab-initio calculation affirms the same observation with shifting of Fermi level in density of states towards conduction band in van der Waals distance separation limit. This result encourage exploration of optical properties in other QD/2D based heterostructures for understanding the charge transfer mechanism and luminescence quenching for future optoelectronic device and optical sensing applications.


T70.00227: When graphene meets electrolyte: how does graphene sense proton (H+)?  
XIAOYU JIA (Presenter), ZHAOYANG LIU, ZONGPING CHEN, AKIMITSU NARITA, MÜLLEN KLAUS, Max Planck Institute for Polymer Research, KLAAS-JAN TIELROOIJ, ICFO - The Institute of Photonic Sciences, MISCHA BONN, I. HAI WANG, Max Planck Institute for Polymer Research — Graphene has been extensively used as electrodes in electrochemical applications [1,2,3]. Despite its relevance for these various applications of graphene, the effect of electrolyte solutions on the electronic properties, specifically conductivity, of graphene remains poorly understood. In the few available studies using graphene field effect transistors (FETs) for ionic sensing, conflicting results have been reported [4,5]. One major challenge is to separate contributions to the overall FET conductance from bulk electrolyte conductivity and from graphene itself, as the FET contacts are typically also exposed to the electrolyte. Here we introduce THz spectroscopy as a contact-free, all optical means to track the intrinsic carrier conductivity of silica-graphene in contact with protons (H+) in water. Our report provides new insight on the graphene's proton sensing mechanism, and highlights the importance and impact of proton transfer though graphene and interfacial charge screening on the graphene conductivity enhancement.

References  
5 W. Fu et al Nano Lett. 11, 3597 (2011).
T70.00228: Thermal conductivity of TMPS₃ (TM=Fe, Ni, and Mn): role of a boundary scattering  
HWIIN JU (Presenter), YOUNGGWAN CHOI, DOGYEOM JEONG, Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Gwangju, South Korea, SUNGMIN LEE, JE-GUEN PARK, 2 Center for Correlated Electron Systems, institute for Basic Science; and 3 Department of Physics and Astronomy, Seoul National University, Seoul, South Korea, JONGSEOK LEE, Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Gwangju, South Korea — Among various van der Waals (vdW) materials, a TMPS₃ (TM=Fe, Ni, Mn) group undergoes an antiferromagnetic transition at about 100 K, and hence can be an important magnetic layer in realizing multi-functional heterostructure. Although a thermal conduction through vdW materials is a fundamental issue in optimizing device performances, thermal properties of TMPS₃ has rarely been studied. In this work, we measured the thermal conductivity of TMPS₃ materials with a time-domain thermoreflectance method. We found that the cross-plane thermal conductivity of TMPS₃ is relatively low compared to other vdW materials, such as graphite and transition-metal dichalcogenides. By comparing the temperature–dependent thermal conductivities of these materials, we demonstrated that effective boundaries caused by a stacking fault of vdW layers act as a main scattering channel in the heat conduction in these materials.

T70.00229: Transition metal dichalcogenide phase-change materials for infrared photonics  
AKSHAY SINGH (Presenter), YIFEI LI, JIAN ZHOU, Massachusetts Institute of Technology, HESHAN YU, ICHIRO TAKEUCHI, University of Maryland, JU LI, RAFAEL JARAMILLO, Massachusetts Institute of Technology — Transition metal dichalcogenides (TMD) exist in 2H (usually semiconducting) and 1T’ (semi-metallic) polymorphs. Switching between these polymorphs offers a new paradigm for controlling light. However, energy required for phase-change (PC) in pure phases is large. Alloying 2H and 1T’ materials, for example MoS₂ and TiS₂, could offer low-energy PC. This low energy transformation would especially be useful for infrared (IR) integrated photonics.

We present a combined experimental and theoretical study of IR properties of MoS₂, TiS₂ and alloys thereof. Our density functional theory (DFT) calculations predict a large refractive index contrast in the 1-1.5 μm spectral range, between 2H and 1T’ phases, for optimized alloys. We experimentally test our DFT predictions using spectroscopic ellipsometry and Fourier-transform IR spectroscopy (FTIR). We measure the complex dielectric constants of bulk crystals, and of synthesized (many-layer) thin films. We characterize the quality of our samples – including wafer-scale combinatorial composition spreads - using Raman and X-ray diffraction mapping. Our work lays the foundation for thin-film TMD PC active IR materials that can be switched optically, electrically, or mechanically.

T70.00230: Large area synthesis of GaSe and GaS monolayers by Chemical Vapor Deposition*  
ALGENE FYER, TARIQ AFANEH, HUMBERTO RODRIGUEZ GUTIERREZ (Presenter), Department of Physics, University of South Florida — Two-dimensional crystals of group-III metal monochalcogenides [i.e. MX where M=In, Ga] and X=S, Se,Te] have gained attention in the last years as alternative 2D semiconductors. They present high carrier mobility, thickness dependent electronic properties, as well as good photoresponse and on/off ratio. To date, most of the fundamental studies in these materials have been performed on mechanically exfoliated samples and few groups have reported chemical vapor deposition (CVD) synthesis of these materials. The implementation of practical electronic applications will rely on developing approaches to deposit high quality films over large areas. The CVD approaches reported to date usually involve low pressure environment and MX powders with the right stoichiometry (pre-synthesized in vacuum sealed ampules) used as evaporation sources, as well as. Here we report large area deposition of GaSe and GaS monolayers, using atmospheric pressure CVD and commercially available precursors. We systematically studied the influence of the growth parameters on the quality of the as grown materials. The samples were characterized using micro-Raman spectroscopy, scanning electron microscopy and atomic force microscopy.

*This work was supported by startup funds from the University of South Florida.

T70.00231: A Novel Method for Thermal Conductivity Measurements in Atomically Thin Materials*  
TALIP KASIRGA (Presenter), ONUR ÇAKIROĞLU, HAMID REZA RASOULI, Bilkent University — Study of thermal properties of materials are crucial for applications and fundamental science. There are many techniques available in the literature to measure thermal conductivity. Measuring the thermal conductivity of atomically thin materials however, is a major challenge. The most common method is to measure the temperature calibrated shift of a well-defined Raman peak with increasing laser power over a suspended sample. Thea fit to the measured data with a temperature profile yields the thermal conductivity. Applicability of this method is limited to materials with relatively low thermal conductivity and well established Raman peaks. In this presentation, I will talk about the method we developed for measuring the thermal resistivity of atomically thin materials relies on a laser beam and two terminal resistivity measurement. The technique can be applied to any conductive material.

*This work is supported by TUBITAK Grant NO: 118F061
T70.00232: Origin of anisotropic negative Poisson's ratio in graphene  ZHENZHEN QIN (Presenter), Zhengzhou University, GUANGZHAO QIN, RWTH Aachen University, MING HU, University of South Carolina — Negative Poisson's ratio (NPR) in auxetic materials is of great interest due to the typically enhanced toughness, shear resistance, and sound and vibration absorption, which enables plenty of novel applications such as aerospace and defense. Insight into the mechanism underlying NPR is significant to the design of auxetic nanomaterials and nanostructures, and a thorough and fundamental understanding is lacking. In this paper, we report anisotropic differential NPR in graphene for uniaxial strains applied along both zigzag and armchair directions based on first-principles calculations. The mechanism underlying the emergence of NPR in graphene (evolution of bond length and bond angle) is found to be different from the conclusions from previous classical molecular dynamics simulations with empirical potential. We propose that the decentralized electron localization function (ELF) driven by strain leads to ELF coupling between different types of bonds, which results in the counter-intuitive anomalous increase of the bond angle and thus the emergence of NPR in graphene. Moreover, the NPR phenomenon can be anticipated to emerge in other nanomaterials or nanostructures with a similar honeycomb structure as that of graphene, where the ELF coupling would also be possible.

T70.00233: Magnetic doping of 2D semiconductor crystals* NALAKA KAPURUGE (Presenter), VIJAYSANKAR KALAPPATTIL, FLORENCE A NUGERA, MANH-HUONG PHAN, HUMBERTO RODRIGUEZ GUTIERREZ, Department of Physics, University of South Florida — Recently reported ferromagnetism in two dimensional crystals have gain increasing interest due to its potential for developing a new generation of 2D spintronic devices. Doping transition metal dichalcogenides with magnetic atoms such as Cr, Mn and Fe, is another approach worth exploring. High doping levels can lead to 2D diluted magnetic semiconductors with crystalline structure compatible with the TMDs that can be connected laterally to create in-plane lateral heterostructures with potential for spin valves or spin-FETs applications. In this work, we report on the Mn magnetic doping of Transition metal dichalcogenides (e.g MoSe2) using a chemical vapor deposition approach. The optical properties of the as grown films were studied by micro-Raman and PL spectroscopy. Morphology and thickness of the samples were characterized via SEM and AFM, respectively. The samples display room-temperature magnetism and a clear temperature dependent ferromagnetic characteristic.

*This work was partially supported by startup funds from the University of South Florida and by the National Science Foundation Grant DMR-1557434

T70.00234: Electronic and Structural Properties of Defects in Few Layer Molybdenum Disulfide Films* MARCUS FORST (Presenter), DAN TRAINER, Department of Physics, Temple University, MARIAN PRECNER, TOMAS POLAKOVIC, Department of Physics, Drexel University, QIAO QIAO, YIMEI ZHU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, XIAOXING XI, Department of Physics, Temple University, GORAN TRIPUN KARAPETROV, Department of Physics, Drexel University, MARIA IAVARONE, Department of Physics, Temple University — Molybdenum disulfide (MoS2) has emerged as an attractive candidate for next-generation 2D electronic devices yet the exact role of defects on its electronic properties is still not well understood. In this study we employ scanning tunneling microscopy and spectroscopy, transmission electron microscopy and kelvin probe force microscopy to obtain quantitative measurements of the local density of states, work function and nature and mobility of these defects. The defects investigated include individual point defects such as sulfur and molybdenum vacancies and extended defects like grain boundaries and film edges.

*This work was supported as part of the Center for Complex Materials from First Principles, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Grant No. DE-SC0012575. The electron microscopy facilities at BNL were supported by the Materials Science and Engineering Divisions, Office of Basic Energy Sciences of the U.S. Department of Energy under Contract # DE-SC0012704.
T70.00235: Inversion-domain-free growth of epitaxial MoS$_2$ on hBN assisted by substrate defects: towards full orientation control*  
YUANXI WANG (Presenter), FU ZHANG, NASIM ALEM, VINCENT HENRY CRESPI, Pennsylvania State University — Progress in growing exceptionally high-quality single crystals has long been impeded in polar 2D materials by the ubiquitous presence of inversion domain boundaries caused by what are often near-degenerate 0° and 180° orientations with respect to their substrate. For transition metal dichalcogenides (TMD), it has not yet proven possible to lift this degeneracy, even when grown on lattice-matched polar substrates. We perform a systematic structural search for a TMD/hBN heterostack system using density functional theory and hybrid functional calculations to identify a new mechanism to lift this near-degeneracy: the energetic distinction between eclipsed and staggered configurations during nucleation at a point defect in the substrate. Orientation control is then verified in experiments that achieve ~90% consistency in the orientation of as-grown MoS$_2$ flakes on hBN, as confirmed by aberration-corrected scanning/transmission electron microscopy. [arXiv:1801.00487]

*We acknowledge support from NSF under EFRI 2-DARE Grant 1433378 and DMR-1420620. The computational work is supported by the 2-Dimensional Crystal Consortium Materials Innovation Platform under NSF DMR-1539916, and by XSEDE under TG-DMR170050 for allocation on the LSU superMIC cluster.

T70.00236: Gunther Martin, Maxwell Rabe, Dr. Alem Teklu: Investigation of the mechanical properties of MOS2 and ReSe2 using an AFM.  
GUNTHER MARTIN (Presenter), College of Charleston — We measured the mechanical properties of MOS2 and ReSe2 using an AFM. MOS2 and ReSe2 are promising materials for their flexibility combined with their optical and electronic properties. Values relevant to their commercial use were obtained for Young's Modulus, stiffness, and hardness.

T70.00237: Electronic properties, dynamical stability and mechanical properties of zeolite-templated carbon Schwarzites*  
ROSS SIEGEL, KORY BEACH, ZACHARY WARD, MICHAEL C LUCKING, HUMBERTO TERRONES (Presenter), Rensselaer Polytechnic Institute — Periodic crystalline carbon structures, with negative Gaussian curvature, have been recently obtained theoretically by the simulated impregnation of microporous zeolite templates in an attempt to address the nature of porous carbon materials obtained by this method in the lab. While encouraging, more work needs to be done to make the connection between the structures obtained by theory and those which have been synthesized. Here, we report the results of first principles and classical molecular dynamics simulations on the electronic and mechanical properties of the theoretically proposed structures that are identified as Schwarzites and potentially synthesizable. Through a comparison of electron and phonon density of states, we confirm that these structures are dynamically stable, graphitic in nature and can be regarded as semimetals. Their mechanical properties including the bulk moduli and the universal anisotropy indices are calculated. Our results serve to guide and supplement experimental work on zeolite-templated carbon Schwarzites.

*We are grateful to the National Science Foundation (EFRI-1433311).

T70.00238: Characterization of 2D Hybrid Systems: Graphene and Beyond*  
SAJEDEH POURIANEJAD (Presenter), JSNN, UNC Greensboro, FREDERICK ARYEETEY, JSNN, North Carolina A&T State University, ADEYINKA ADESINA, JSNN, UNC Greensboro, SHYAM ARAVAMUDHAN, JSNN, North Carolina A&T State University, TETYANA IGNATOVA, JSNN, UNC Greensboro — High-quality junction between semiconductor and metallic contact with no energy barrier is crucial for high-performance device, which is hard to achieve for 2D MoS$_2$ because of its large bandgap. The heterostructure of single-layers MoS$_2$/graphene has been demonstrated. However, a critical challenge has emerged: to develop reliable methods to transfer this graphene from its growth substrate to the application substrate without damaging the fragile patchwork or leaving undesired residues on the graphene surface. To ascertain the MoS$_2$ and graphene layer number and their defects, Confocal Raman spectroscopy and photoluminescence measurements were conducted before and after transfer. To identify the thin film thickness atomic force microscopy (AFM) was performed. Scanning electron microscopy was used to investigate the surface morphologies of MoS$_2$ and Graphene. To confirm the low surface defect results, X-ray Photoelectron Spectroscopy (XPS) was also carried out. We speculate that the tunable Fermi level in graphene allows excellent work-function to be well-matched with MoS$_2$, resulting in low contact resistance.

*Funding Acknowledgement: Samples for this paper were provided by The Pennsylvania State University 2DCC-MIP supported by NSF cooperative agreement DMR-1539916
T70.00239: Healing a Topological Scar*  
BENJAMIN KATZ (Presenter), VINCENT HENRY CRESPI, Pennsylvania State University  
— A novel defect type in two-dimensional systems is presented, which changes the local coordination number of an atom in an otherwise regular structure. While point-like by itself, such a ‘coordination defect’ has an unusually large number of involved atoms and a potentially dramatic influence on the growth of the system following its formation, due to its introduction of a mismatch between bond network topology and physical ring size. The potential growth pathways after the occurrence of such a defect in graphene are followed using molecular dynamics and first-principles calculations; the inherent conflict between the topological requirements and the actual chemical/physical structure that occurs as the system heals the defect can result in varied morphologies, including a runaway feedback that spawns one or more semi-infinite grain boundaries. Energy comparisons from first principles are used to evaluate the likelihood of this result under various conditions. The appearance of this defect type is predicted to have similar ramifications across a broad array of two-dimensional systems, potentially providing a new method of controlling grain boundary behavior and location.

*Research performed under a training fellowship for CoMET, an NRT at Penn State funded by NSF.

T70.00240: Gate-defined Quantum Confinement in few-layer Black Phosphorus Transistor  
JIAWEI YANG, RUOYU CHEN (Presenter), SHI CHE, Ohio State University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, SEONGPHILL MOON, DMITRY SMIRNOV, Natl High Magnetic Field Lab, CHUN NING LAU, Ohio State University — Black phosphorus is a novel two-dimensional(2D) semiconductor which has attracted considerable research interest due to its tunable band gap and high electron mobility. Here we demonstrate quantum confinement defined by split gate in devices based on few-layer black phosphorus. The tunability of split gate can be illustrated by the fact that a device can be tuned off by split gate alone. In quantum Hall regime, gate-controlled pinching off of quantum Hall states(with filling factor ν = -1, -2, -3, -4) indicates the realization of strong confinement and the potential of manipulation of edge states. The work opens the door for using black phosphorus as platform for electronic and optoelectronic applications.

T70.00241: Polarized Raman spectroscopy in monolayer ReSe2*  
GEOVANI CARVALHO DE RESENDE, Universidade Federal de Minas Gerais, BRUNO R CARVALHO (Presenter), Departamento de Física Teórica e Experimental, Universidade Federal do Rio Grande do Norte, MARCOS PIMENTA, Universidade Federal de Minas Gerais — Raman spectroscopy is a powerful tool to study two-dimensional compounds and has been widely used to obtain important information of their electronic and vibrational structures. In the case of graphene and MoS2-type compounds, the Raman spectrum is isotropic when the light polarization lies in the layer plane. However, for low-symmetry materials such as black phosphorus and triclinic transition metal dichalcogenides, the spectra are polarized dependent and polarized Raman spectroscopy should be used. By changing the angle between the light polarization and the crystallographic axes, the elements of the Raman tensors for the different phonon modes can be determined. Previous studies in black phosphorus showed that Raman tensor elements are complex numbers, but the physical origin of the phase differences are not yet well understood. In this work, polarized Raman spectroscopy is used to investigate the anisotropic behavior in monolayer ReSe2. The angular dependence of the polarized Raman spectra using different polarization configurations is obtained for the 18 Raman active modes as well as the Raman tensor elements for each mode. It was also observed that the principal axes of those Raman tensors are not along the crystallographic axes.

*CNpq, CAPES, FAPEMIG and INCT-Nanocarbono

T70.00242: Magnetoplasmons and magnetoexcitons in doped double-layered α-T₃ lattice in a strong magnetic field  
GODFREY GUMBS (Presenter), DIPENDRA DAHAL, Physics and Astronomy, Hunter College/CUNY, ANDRII IUROV, Center for High Technology, University of New Mexico, DANHONG HUANG, Advanced E/O Space Sensors Group, Air Force Research Laboratory — We investigate the conditions for the occurrence of Bose-Einstein condensation and superfluidity of indirect magnetoexcitons for a pair of quasi-two-dimensional spatially separated α-T₃ layers. The energy dispersion of collective excitations, the spectrum of sound velocity, and the effective magnetic mass of magnetoexcitons are obtained in the integer quantum-Hall regime for strong magnetic fields. The superfluid density and the temperature of the Kosterlitz-Thouless phase transition are probed as functions of the excitonic density, magnetic field and the interlayer separation.
T70.00243: Exciton luminescence efficiency and dynamics in flux-growth MoSe2 monolayers  HONGHUA FANG, BO HAN, CEDRIC ROBERT, DELPHINE LAGARDE, XAVIER MARIE, BERNHARD URBASZEK (Presenter), CNRS/INSA, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS Tsukuba, SEFAATTIN TONGAY, ASU — Monolayers of transition metal dichalcogenide like MoS2 are promising materials for optoelectronics applications due to their exceptionally strong light-matter interaction governed by very robust excitons (Coulomb bounded electron hole pairs). Nevertheless, practical usage has been hindered by their relatively low quantum efficiency (0.1-1%) due to the presence of non-radiative recombination channels (defects, exciton-exciton annihilation, relaxation to dark states ...). In this work, we compare the optical properties of monolayers of MoSe2 exfoliated from different bulk crystals: commercially available crystals from 2D Semiconductors and bulk crystals synthetized with the low temperature flux-growth technique. We perform temperature dependent photoluminescence (PL) and time resolved PL measurements and observe strong differences between the materials in terms of doping level, the PL intensity evolution with temperature and the exciton dynamics at both cryogenic and room temperature. These results are interpreted evoking the lower defect density measured in our flux-growth samples.

T70.00244: Diverse Strain Dependent Thermal Transport in 2D Materials  GUANGZHAO QIN, MING HU (Presenter), Department of Mechanical Engineering, University of South Carolina — Manipulation of thermal transport is in increasing demand as heat transfer plays a critical role in a wide range of practical applications. While 3D bulk materials usually exhibit decreased lattice thermal conductivity upon mechanical stretching and enhanced thermal transport by compression, the thermal response of 2D materials to mechanical strain is not that simple. Perfectly planar atomically-thin materials such as graphene have reduced thermal transport ability when stretched. In contrast, some 2D materials with intrinsic buckled structure will possess enhanced thermal conductivity upon tension. However, many exceptions exist in other 2D materials. The thermal conductivity of 2D planar group III-nitrides (h-BN, h-AlN, h-GaN) is tremendously enhanced by stretching. By deeply analyzing the orbital projected electronic structure, we establish a microscopic picture of the lone-pair electrons driving strong phonon anharmonicity in group III-nitrides. However, the lone-pair electrons do not necessarily lead to enhanced thermal conductivity in strained penta-like 2D materials. Our findings offer perspectives of modulating thermal transport properties of broad 2D materials for applications such as thermoelectrics, thermal circuits, and nanoelectronics.

T70.00245: Band Gaps and Optical Spectra of Fluorinated and Hydrogenated Graphenes*  FRANTISEK KARLICKY (Presenter), Department of Physics, University of Ostrava — Two-dimensional (2D) materials derived from graphene by attachment of hydrogen and halogens have attracted considerable interest over the past few years because of their potential applications (e.g., in electronic devices or sensing)[1]. Here, we consider the effect of electron-electron and electron-hole correlation on the electronic/optical properties of materials under study. Large difference between the experimental optical gap and the electronic band gap from many-body GW theory for fluorographene CF, fluorographite, and graphane CH is explained by unusual large binding energies of excitons obtained by solution of Bethe-Salpeter equation (BSE)[2,3]. Fluorographane C2FH is found as material with the widest electronic gap (~10 eV) and a largest binding energy of exciton (~3 eV) in the class of currently known 2D materials [4]. Finally, we show the importance of careful computational setup for reliable usage of many-body methods.


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**T70.00246: Impact of structure on exciton physics in organic-inorganic 2D perovskites**  
JEAN-CHRISTOPHE BLANCON (Presenter), Rice University, JACKY EVEN, INSA Rennes, ANDREAS STIER, Technical University of Munich, CLAUDINE KATAN, Universite de Rennes, JARED CROCHET, Los Alamos National Laboratory, ADITYA D. MOHITE, Rice University  
Organic-inorganic (hybrid) 2D perovskites is a new class of 2D layer materials that feature unique structural characteristics related to their hybrid nature, which includes soft and dynamic lattice structure and organic-inorganic interfaces. There is still little knowledge of the interplay between, on the one hand, their photo-excited states and electronic properties and, on the other hand, their structural characteristics. Here, using optical spectroscopy and 60-Tesla magneto-absorption, we report the dependence of the formation, dynamics, and recombination of exciton states on the structural and compositional details of hybrid 2D perovskites [Nature Communications 9, 2254, 2018 & Science 355, 1288, 2017]. Our work reveals the changes in the exciton properties due to the tuning of the thickness of the 2D perovskites and the size of the organic molecules in the lattice. The exciton characteristics are explained by an advanced model which includes quantum and dielectric confinement. Moreover, we demonstrate the existence of unique electronic states located at the edges of the 2D perovskite layers, which result from local distortions of the lattice at the edges. Finally, we will provide insight into the hetero-coupling between 2D perovskites and transition metal dichalcogenides.

**T70.00247: Refractory metals as alternate contact metals for 2D/3D Heterostructures**  
MAHESH NEUPANE (Presenter), DMITRY A RUZMETOV, ROBERT A BURKE, MATTHEW L CHIN, MIKE D VALENTIN, A. GLEN BIRDWELL, TERRANCE O'REGAN, TONY IVANOV, US Army Rsch Lab - Adelphi  
Vertical three-terminal complex devices based on 2D/3D heterostructures require metal contacts that can withstand high temperature and harsh chemical environment brought about by the 2D/3D material synthesis that follows the metal contact fabrication [1, 2, 3]. Refractory metals, such as Mo, W and Cr, are candidates for this purpose and have been used by our team for the fabrication of contacts to the Base (MoS₂) in a vertical GaN/MoS₂/GaN heterojunction bipolar transistor. Since refractory metals exhibit endurance toward high temperature, abrasion and degradation, they are expected to form sharp, high-quality interface with 2D materials. Motivated by this, we have performed first principle simulation study of refractory metals/2D/3D systems and analyzed structural and electronic properties, such as binding energies, Schottky barrier heights (SBH), and mid-gap charge densities, and investigated the feasibility of using refractory metals as contact metals in 2D/3D systems. Furthermore, we have made an attempt to establish a correlation between the metal type and degree of Fermi level pinning using theoretical as well as in-house experimental data. 1. ACS Nano 10, 3580, 2016, 2. App. Phys. Lett 111, 051602, 2017, 3, 2D Materials 5, 045016, 2018

**T70.00248: Electric-field tunable fine-structure splitting in monolayer semiconductors**  
CHITRALEEMA CHAKRABORTY (Presenter), Electrical Engineering and Computer Science, MIT, NICHOLAS R JUNGWIRTH, GREGORY FUCHS, School of Applied and Engineering Physics, Cornell University, NICK VAMIVAKAS, The Institute of Optics, University of Rochester  
Semiconducting quantum dots (QDs) are among the most promising source of on-demand, indistinguishable single and entangled photon source which are the basic ingredients for quantum communications and computing applications. The most common approach to generate entangled photon pairs in QDs is to utilize the bieexciton to exciton radiative cascade. Recently, single confined exciton and bieexciton emission have been demonstrated at locally strained sites in semiconducting two-dimensional (2D) materials. The 2D host makes them ideal for integrated quantum photonics studies. However, a sizable fine-structure splitting (FSS) (~800 μeV) due to anisotropic electron-hole exchange interaction in these quantum-confined excitons and bieexcitons poses a limit to the indistinguishability of the generated photon pairs. We demonstrate a suppression of the FSS by leveraging on van der Waals heterostructure and fabricate a voltage tunable device to minimize the effect of exchange interaction.

T70.00249: Spin transistors built on 2D van der Waals heterostructures  SHENGWEI JIANG, LIZHONG LI, ZEFANG WANG (Presenter), JIE SHAN, KIN FAI MAK, Cornell University — A transistor based on spin rather than charge (spin transistor) was first proposed by Datta and Das in 1990. Such a spin-based device promises non-volatile data storage and a faster and more energy-efficient performance than present transistors. Many approaches have been pursued to realize spin transistors, but they remain a formidable challenge. Recent discovery of two-dimensional magnetic insulators such as CrI$_3$ with electrically switchable magnetic order and effective spin filtering effect inspires a new operational principle for spin transistors. Here we demonstrate spin field-effect transistors based on dual-gated graphene/CrI$_3$/graphene tunnel junctions. These devices show an ambipolar behavior and tunnel conductance that is dependent on the magnetic order in the CrI$_3$ tunnel barrier. The gate voltage switches the tunnel barrier between an interlayer antiferromagnetic and ferromagnetic state under a constant magnetic bias near the spin-flip transition, thus effectively altering the device between a low and a high conductance state with a large hysteresis. Based on the electrically controlled spin-flip transition in the magnetic tunnel barrier, these new spin transistors achieve spin injection, control and detection in a single device with a conductance ratio approaching 400%.

T70.00250: High Photo-response in Conformally Grown Monolayer MoS$_2$ on Rugged Substrate* YONG SOO KIM (Presenter), TRI NGUYEN, TAM CHINH LE, FARMAN ULLAH, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, KYO-IN KOO, Department of Biomedical Engineering, University of Ulsan, ZEESHAN TAHIR, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, EUNAH KIM, DONGWOOK KIM, Department of Physics, Ewha Womans University, JOON JANG, Department of Physics, Sogang University — Conformal growth of atomic-thick semiconductor layers on patterned substrates can boost up the performance of electronic and optoelectronic devices remarkably. However, conformal growth is a very challenging technological task, since the control of the growth processes requires utmost precision. Herein, we report on conformal growth and characterization of monolayer MoS$_2$ on planar, micro-rugged, and nano-rugged SiO$_2$/Si substrates via metal-organic chemical vapor deposition. The continuous and conformal nature of monolayer MoS$_2$ on the rugged surface was verified by high-resolution transmission electron microscopy. Strain effects were examined by photoluminescence (PL) and Raman spectroscopy. Interestingly, the photo-responsivity (~254.5 mA/W) of as-grown MoS$_2$ on the nano-rugged substrate was 59 times larger than that of the planar sample (4.3 mA/W) under a small applied bias of 0.1 V. Such enhancement in the photo-responsivity arises from a large active area for light-matter interaction and local strain for PL quenching, where the latter effect is the key factor and unique in the conformally grown monolayer on the nano-rugged surface.

*This research was supported by the NRF of Korea (2009-0093818; 2014R1A4A1071686; 2017R1E1A1A01075350).

T70.00251: Monolithic image sensor and optoelectronics of monolayer.* CHEN PO-HAN (Presenter), CHANG-NING LIAO, MENG-HSI CHUANG, KUAN-CHANG CHIU, MENG-CHYI WU, CHIH-CHAO YANG, YI-HSIEN LEE, National Tsing Hua University — Development of advanced optoelectronic devices for ultrahigh speed, low power consumption, and low cost image sensors are emergent applications of Internet of Things (IoT). To achieve ultrasensitive image sensors, high responsivity, fast response speed, and low power consumption are required. Monolayer transition metal dichalcogenides (TMD) crystals are potential candidates for high performance optoelectronic devices with high responsivity and low power consumption. Here, persistent photoconductivity (PPC) of the monolayer TMD are studied and improved. Monolithic image sensor and optoelectronic transport properties of the MoS$_2$ are demonstrated.

*The authors acknowledge support from AOARD grant (co-funded with ONRG) FA2386-16-1-4009, Ministry of Science and Technology (MoST-106-2119-M-007-023-MY3, MoST-105-2811-M-007-093, MoST-105-2112-M-007-032-MY3, MoST-105-2119-M-007-027, and MoST-105-2633-M-007-003)

T70.00252: Study of graphene/hBN heterostructures using Raman Spectroscopy* JESSICA SANTOS LEMOS (Presenter), LEANDRO MALARD MOREIRA, DANIEL CUNHA ELIAS, Universidade Federal de Minas Gerais — In this work, heterostructures of graphene and hexagonal boron nitride (hBN) were built using the pick-up method and dry-transferred to an insulator substrate (glass). Then, electric contacts were made in order to control the charge carrier concentration applying a voltage between graphene and the golden contact deposited on hBN. In this way, it was possible to access charge concentrations higher than $10^{13}$ cm$^{-2}$. Aligned sample was desired in order to obtain a Moiré patterning such that the cloning of the Dirac cones would occur for small energy values, being accessible by voltage application. In order to check the formation of the cloning of the Dirac cones due to the Moiré patterning, Raman spectroscopy was used. It was observed a frequency reduction and width increase in the G band for three distinct values of the voltage applied in the sample. The electron-phonon coupling effect was investigated to explain such experimental observations between the different Dirac points and the G band phonons.

*The authors thank to CNPq, CAPES, FAPEMIG and INCT-Nanotubo.
Electrical properties of graphene field-effect transistors functionalized with aryldiazonium salts

Among functionalization strategies, aryldiazonium salts are often chosen to form stable covalent adducts. Here we analyze the effect of this chemistry on the electrical properties of graphene field-effect transistors (G-FETs). First, we conducted an extensive review of published experiments and developed a theoretical framework to compare data obtained under different conditions (channel size, reagent concentration, incubation time). From the aggregated dataset, we found that the electronegativity of the para group seems to have little impact on the electrical response, which contrasts with conclusions found in the literature. We also found that the type of graphene (exfoliated, CVD, RGO) seems to have a much more dominant impact, which could explain strong differences between previous studies. Finally, we argue that device-to-device variations are significant, and we propose an experimental design based on multiple GFET arrays and statistical analysis to unambiguously characterize the effect of aryldiazonium functionalization on graphene transport properties.

*IRIC (Institute for Research in Immunology and Cancerology) Next Generation Award
T70.00257: Graphene-based catalytic mats for Belousov Zhabotinsky reaction* D JAYA PRASANNA KUMAR (Presenter), SACHIN VERMA, KABEER JASUJA, PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Use of hybrid materials that have morphological features at various length scales has opened up new avenues to design multi-functional materials. Here, we synthesize graphene-based catalytic mats and harness their unique properties to tune the kinetics of self-oscillating BZ reactions. In particular, we create catalytic mats containing 0D-2D heterostructures by decorating Ce, Ru, Ag, and Au nanoparticles (NPs) onto the graphene sheet and subsequently, use these nanocomposites to catalyze the BZ reaction. The NPs attached on the graphene function as spacers by increasing the interlayer distance to several nanometers and thus, prevent the stacking of individual graphene sheets. Moreover, the presence of NPs on highly conductive graphene sheets provides enhanced access to active catalytic sites and reveals a multi-fold increase in the number of chemical oscillations frequency in BZ reactions. We also validate the kinetic model of the BZ reaction with our experimental results and identify key parameters to model the reaction kinetics for our BZ system. We expect that our findings will offer a novel approach to design synthetic smart materials with tunable dynamic behavior.

*DST-SERB: EMR/2016/007778

T70.00258: Nanoelectromechanical resonators from thin superconducting crystals of BSCCO SUDHIR SAHU (Presenter), Department of Physics, Indian Institute of Science Bangalore, JAY KUMAR VAIDYA, DIGAMBAR JANGADE, ARUMUGAM THAMIZHAVEL, MANDAR DESHMUKH, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, VIBHOR SINGH, Department of Physics, Indian Institute of Science Bangalore — High transition-temperature superconductors host a rich variety of quantum phases. Cavity optomechanics techniques could be helpful in a sensitive detection of long-wavelength phonon modes carrying imprints of the electronic phases. Here we present mechanical resonators fabricated with thin exfoliated crystals of BSCCO at low temperatures. For mechanical readout, we couple their motion to a coplanar waveguide microwave cavity fabricated with a superconducting alloy of molybdenum-rhenium. We perform spectroscopic and time-domain measurements to understand dissipation in these systems. Our results suggest that the performance of these devices is limited by the contact resistance arising from the insulating outer layer, and interlayer friction.

T70.00259: Superconductivity from Valley Fluctuations and Approximate SO(4) Symmetry in a Weak Coupling Theory of Twisted Bilayer Graphene YIZHUANG YOU (Presenter), ASHVIN VISHWANATH, Department of Physics, Harvard University — We develop a weak coupling approach to superconductivity in twisted bilayer graphene, starting from the Fermi liquid regime. A key observation is that near half filling, the fermiology consists of well nested Fermi pockets derived from opposite valleys, leading to enhanced valley fluctuation, which in turn can mediate superconductivity. This scenario is studied within the random phase approximation. We find that inter-valley electron pairing with either chiral (d+id mixed with p-ip) or helical form factor is the dominant instability. An approximate SO(4) spin-valley symmetry implies a near degeneracy of spin-singlet and triplet pairing. On increasing interactions, commensurate inter-valley coherence wave (IVCW) order can arise, with simultaneous condensation at the three "M" points in the Brillouin Zone, and a 2 × 2 pattern in real space. In simple treatments though, this leads to a full gap at fillings ±(1/2 + 1/8), slightly away from half-filling. The selection of spin-singlet or spin triplet orders, both for the IVCW and the superconductor, arise from SO(4) symmetry breaking terms. Mott insulators derived from phase fluctuating superconductors are also discussed, which exhibit both symmetry protected and intrinsic topological orders.

T70.00260: Realizing Td phase at room temperature in ultrathin MoTe2* GAIHUA YE (Presenter), ZHIPENG YE, RUI HE, Texas Tech University, LOGAN WINFORD, University of Northern Iowa, SHAZHOU ZHONG, HYUN HO KIM, ADAM TSEN, University of Waterloo, Canada — MoTe2 emerges as a new type of transition metal dichalcogenide (TMD) whose different polymorphs show very different properties. In bulk MoTe, both hexagonal 2H phase (semiconducting) and monoclinic 1T' phase (semimetallic) can be formed at room temperature depending on the growth conditions. When temperature is lowered to 250K, the 1T' phase transforms into an orthorhombic Td phase in which the MoTe2 crystal is a type-II Weyl semimetal with novel quantum phenomena. We exfoliated 1T'-MoTe2 flakes on SiO2 substrates and protected them with boron nitride from oxidation. Electrical transport measurements show that the ultrathin flakes do not show a phase transition below 250K. Raman studies reveal that the MoTe2 ultrathin flakes exhibit a Td phase even at room temperature, making it a potential host material for realizing type-II Weyl semimetal at room temperature.

*NSF (CAREER Grant No. 1760668, RUI Grant No. DMR-1410496, and MRI Grant No. DMR-1337207) and NSERC Discovery grant (RGPIN-2017-03815)
Electronic properties of bare and functionalized 1- and 2-Dimensional Tellurene structures

Daniel Wines (Presenter), Fatih Ersan, Jaron Kropp, Gracie M Chaney, Can Ataca, University of Maryland, Baltimore County — Recently, 1D and 2D Tellurene structures have been experimentally synthesized. These structures possess high mobility and air stability which make them ideal candidates for applications in electronics, optoelectronics and energy devices. We performed density functional theory and molecular dynamics simulations to investigate the stability and electronic structure of 1D α, β and Γ Tellurene chains, 2D α and β Tellurene sheets, and hydrogen, oxygen, and fluorine functionalized counterparts, including spin-orbit coupling effects. Our calculations show that bare α and β Tellurene sheets are stable and have direct band gaps of 0.56 eV and 1.02 eV respectively. When hydrogenated, α-Tellurene displays metallic properties while the direct band gap of β-Tellurene increases to 1.72 eV. Our calculations also show that α and β Tellurene chains are unstable while Γ Tellurene chains are stable. Our molecular dynamics calculations indicate that Γ Tellurene chains gain kinetic energy and rotate around the chain growth direction. This rotation provides stability to the Γ Tellurene chains. Our results indicate that functionalized-Tellurene chains and monolayers are not only suitable for future optoelectronic devices, but they can be used as metallic contacts in nanoscale junctions.
T70.00265: Interaction of the system titanium-borophene with lead substrate with water molecule. **GREGORIO RUÍZ-CHAVARRIA** (Presenter), Universidad Autonoma Chapingo — In this work I made an computational study of the interaction of the system titanium-borophene with lead substrate with water. I first established the stability of the borophene system with lead substrate, then added titanium, studying the stability of this system, which was stable. Finally, an water molecule is added, studying the evolution of the interaction between this molecule and the system titanium-borophene with lead substrate. To do this work, I use Density Functional Theory, Born-Oppenheimer Approximation, atomic pseudopotentials and molecular dynamics. The results obtained are compared with experimental results, as well as with similar calculations.

T70.00266: Critical electronic and many-body properties of $\alpha$-T$_3$ nanoribbons **PAULA FEKETE** (Presenter), United States Military Academy, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, Albuquerque, NM, GODFREY GUMBS, Hunter College, City University of New York, New York, NY, DANHONG HUANG, Kirtland Airforce Base, Air Force Research Laboratory, Albuquerque, NM — Quasi-one-dimensional nanoribbons of finite width could be produced from the recently proposed $\alpha$-T$_3$ materials with variable hub-rim coupling parameter similarly to nanoribbons fabricated from graphene. We investigate their critical electronic and collective properties, such as plasmons, based on the tight-binding model for the low-lying energy bands and spin-1 Dirac-Weyl equation with the proper boundary conditions. Our results strongly depend on the type of boundary which our nanoribbon has. We believe that the novel electronic properties we obtained will significantly benefit the field of currently existing carbon-based nanoelectronics and nanodevices.

T70.00267: A First-Principles Investigation of Spintronic Capabilities of Nitrophosphorene Doped With 3d Transition Metals **LAWRENCE SHI** (Presenter), XUAN LUO, National Graphene Research and Development Center — There has been search for materials with spintronics properties as they have potential advantages in data transfer and storage over their conventional electronics counterparts. Notably, phosphorene is at the center of such material search with its widely tunable band gap and high carrier mobility. Nitrophosphorene (PN), a newly discovered material in 2017, is considered to be a superior semiconductor to Black Phosphorene (BP) because of its larger band gap. However, unlike BP, whose spintronic properties have been well studied, little is known about the spintronic properties of PN. We present strong evidence that PN is potentially an even better material for spintronics than BP. Specifically, we used first-principles calculations to investigate the spintronic properties of 3d transition metal-doped PN. Sc, Cr, and Co doping result in a DMS. V, Mn, and Fe doping result in a half metal, and Ti and Ni doping result in a semiconductor with no magnetization. We also compared the spintronic properties of interstitial Mn-doped PN and interstitial Mn-doped BP. Although both of them are half-metals, Mn-doped PN has a higher magnetization and band gap. Our discovery in PN spintronics contributes to the recent advances in the fundamental studies and search for spintronics materials.

T70.00268: Predicting Synthesizable Functional Edge Reconstructions in 2D Monolayers* **GUOXIANG HU** (Presenter), XIAHAN SANG, RAYMOND UNOCIC, PANCHAPAKESAN GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Two-dimensional (2D) transition metal dichalcogenides (TMDCs) have attracted tremendous interest due to their exceptional electronic and optical properties. More interestingly, it has been found that edges of 2D TMDCs are responsible for their promising catalytic activity, while the basal plane is chemically inert. In addition to the conventional armchair and zigzag edges, more complex edge reconstructions have recently been realized by various experiments. Therefore, it is highly desirable to computationally predict the family of stable edges so as to screen their functional properties. Here we report development of such a computational approach and demonstrate it on the 2D TMDC family of systems such as MoS2 & MoSe2. Starting from configuration ensemble generations, we screen for stable edges using cheaper force-fields or surrogate (Neural-Network-based) models, which are then further refined using DFT-level of theory. We predict many stable edges that are superior for hydrogen evolution reaction (HER). Our study thus provides a comprehensive yet tractable computational approach for predicting synthesizable functional edges in 2D monolayers.

*This work was supported by the ORNL-LDRD program.
JARVIS (Joint Automated Repository for Various Integrated Simulations) is a unique integrated framework to accelerate material design using classical force-fields (FF), density functional theory (DFT) and machine learning (ML). The JARVIS-DFT hosts data for more than 30000 materials. We discovered more than 1500 2D materials using lattice parameter criteria and exfoliation energy calculations. We charted improved lattice parameters, formation energies and elastic tensors using van der Waals functional for more than 12000 materials and established relation between exfoliation energies and elastic constants. To alleviate bandgap underestimation in conventional DFT and improve frequency dependent dielectric function predictions, we evaluated meta-GGA based approaches for more than 10000 materials. We use spectroscopic limited maximum efficiency approach to identify potential photovoltaic materials. Using spin-orbit spillage criteria, we discovered more than 1500 potential topological materials including topological insulators, Weyl and Dirac semimetals, and topological crystalline insulators. The database is publicly available at https://jarvis.nist.gov/.

While theoretical modeling of the atomic scale structure of non-crystalline solids has become well developed, deriving functional properties from these models still faces challenges. In order to address this deficit, we analytically demonstrate a decomposition of the non-equilibrium glassy macrostate into a statistical ensemble of crystalline microstates with an effective temperature. Crystalline microstates are calculated as local potential energy minima using density functional theory. With the radial distribution function and powder diffraction intensity as signatures of short- and long-range order respectively, we show that the glassy states of both silicon and silica can be reproduced with remarkable fidelity using crystalline microstates with unit cells on the order of just a few dozen atoms. Our approach offers a complementary view to the conventional supercell-based continuous random network model, which typically singles out a single representative microstate for the purposes of modeling. By contrast, our model presents the glassy state as an effective liquid, which visits crystalline potential energy minima ergodically, opening the door to new predictive methods for property calculations based on ensemble averaging and to the rational design of glassy solids.

MSCD Framework A Novel Computational Design Software for High-Temperature Superconductors

We present recent results on stable and reliable synthesis of boron nitride nanotubes (BNNTs) in volume by an anodic arc discharge at near atmospheric pressure of nitrogen. This arc was operated with the boron-rich anode and the cathode made from a refractory metal which has a melting temperature above the melting point of boron. Ex-situ characterization of synthesized BNNTs with electron microscopy and Raman spectroscopy revealed that independent of the cathode material, the tubes are primarily single and double walled. Ex-situ analysis results also show evidence of root-growth of BNNTs produced in the arc discharge. In order to understand nanostructure formation we needed to determine the plasma and gas composition conditions in the nucleation and growth region. We determined plasma parameters in the growth region using plasma diagnostics and thermodynamic modelling. Previous atomistic simulations helped to analyse crucial processes in nanomaterial synthesis. References are available at nano.pppl.gov

*The arc modeling was supported by the US DOE Office of Science, Fusion Energy Sciences. Experiments and simulations of synthesis processes were supported by the US Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
T70.00273: Towards Understanding of Arc-Based Synthesis of Carbon Nanotubes*  
YEVENY RAITSES, SHURIK YATOM, ALEXANDER KRABRYI, VLAD VEKSELMAN, IGOR KAGANOVICH (Presenter), Princeton Plasma Phys Lab — This work reports on studies of arc-based synthesis of carbon nanomaterials. Applying a set of the in-situ diagnostics of plasma and nanoparticles, our synthesis experiments revealed that the carbon arc forms a highly inhomogeneous plasma consisting of distinguishable regions with different dominant species, including ions, atoms, molecules and clusters, and nanoparticles. Measurements revealed clouds of nanoparticles in the arc periphery bordering the region with a high density of diatomic carbon molecules. Two-dimensional CFD simulations of the arc combined with thermodynamic modeling show that this is due to the interplay of the condensation of carbon molecular species and the convection flow pattern. The formation of nanoparticles is strongly affected by unstable arc behavior.
References are available at nano.pppl.gov

*The arc modeling was supported by the US DOE Office of Science, Fusion Energy Sciences. Experiments and simulations of synthesis processes were supported by the US Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

T70.00274: Multilayer graphene shows intrinsic resistance peaks in the carrier density dependence: experiments in tetra- and hexlayer graphene  
RYUTA YAGI (Presenter), TAIKI HIRAHARA, RYOYA EBISUOKA, TAKUSHI OKA, SHINGO TAJIMA, AdSM, Hiroshima Univ., KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science (NIMS) — Since the advent of graphene, a variety of studies have been done to elucidate its fundamental physics, or to explore its practical applications. Gate-tunable resistance is one of the most important properties of graphene and has been studied in 1-3 layer graphene in a number of efforts to control the band gap to obtain a large on-off ratio. On the other hand, the transport property of multilayer graphene with more than three layers is less well understood. Here we show a new aspect of multilayer graphene. We found that four-layer shows intrinsic peak structures in the gate voltage dependence of its resistance at zero magnetic field. Measurement of quantum oscillations in magnetic field confirmed that the peaks originate from the specific band structure of graphene and appear at the carrier density for the bottoms of conduction bands and valence bands. Similar but different peak structures were observed in six-layer graphene. The intrinsic peak structures should generally be observed in AB-stacked multilayer graphene. The present results would be significant for understanding the physics of graphene and making graphene FET devices. (Sci. Rep. 8, 13992 (2018). DOI: 10.1038/s41598-018-32214-7)

T70.00275: Controlling graphene structures and electronic properties by Ion beam irradiation*  
KOSUKE NAKAMURA (Presenter), KAZUYUKI TAKAI, TOMOAKI NISHIMURA, HIROKI YOSHIMOTO, Hosei University — Irradiation of ion into graphene is interesting in view of defect-introduction and chemical modification. In this study, we attempted 200 keV Au or I ion injection to graphene. Irradiation to bare graphene will cause damage, so a sacrificial layer protecting graphene was designed and fabricated on the surface. NaCl thin-film was applied for sacrificial layer, where it has been confirmed NaCl hardly affects structural and electronic properties of graphene after removal process. Raman spectroscopy of Au or I ion irradiated graphene by using NaCl thin-film as a sacrificial layer, shows peculiar G band intensity of graphene near 1580 cm-1, indicating honeycomb structure of graphene was preserved after irradiation. Also defects that cause significant intervalley scattering (D band : 1340 cm-1) and intravalley scattering (D’ band : 1620 cm-1) appeared after irradiation. Field effect transistor (FET) of graphene was fabricated after irradiation, and the mobility of irradiated graphene was measured by applying gate voltage sweep range. The mobility of Au and I irradiated graphene decreased down to 0.114 cm2 / Vs and 0.034 cm2 / Vs respectively, being responsible for extremely less conductivity.

*This work was supported by JSPS KAKENHI Grant No. 16K05758 and 26107532
Defects introduction is one of the important strategy to tune graphene properties. Especially, it is known that an ion beam irradiation can introduce atomic vacancies in graphene. Although, the number of defects is usually focused, the chemical structure of defects has been not well considered. Actually, for hydrogenated atomic vacancies, the theoretical calculation shows a low energy barrier and little adsorption heat for the additional adsorption of hydrogen molecules, suggesting an efficient hydrogen storage and release in this system. In this study, hydrogenated / oxygen-terminated atomic vacancies are introduced into epitaxial graphene and the amount of hydrogen and carrier scattering related to vacancies are evaluated. Hydrogenated and oxygen-terminated atomic vacancies were introduced into epitaxial graphene by ion beam sputtering, followed by exposing to H2 gas and air, respectively. After introducing hydrogenated vacancies, the increment of hydrogen is comparable to the upper limit for the number of vacancies. The smaller Raman D-band for hydrogenated vacancies than that for oxygen terminated vacancies suggests the inter valley scattering depends on the chemical structure of defects in graphene.

*This work was supported by JSPS KAKENHI Grant No. 16K05758 and 26107532.

Free radical ions generated at the surface can cleave a cross-linked polymer mesh that holds together colloidal assemblies or can polymerize acrylic acid monomer at the particle surface (viz. bond breaking or bond formation). Proximity of polymeric amine groups allows photo-induced electron transfer from excited dye molecules, to form free radical ions. Formation of free radical ions is not a function of the size of the colloid, neither is it restricted to a specific fluorophore. Fluorophores with redox potentials that allow photo-induced electron transfer with amine groups show formation of free radical ions.

*SERB, DST-India.

How atoms acquire three-dimensional bulk character is one of the fundamental questions in materials science. Before addressing this question, how atomic layers become a bulk crystal might give a hint to the answer. While atomically thin films have been studied in a limited range of materials, a recent discovery showing how to mechanically exfoliate bulk crystals has opened up the field to study the atomic layers of various materials. Here, we show systematic variation in the band structure of high mobility graphene with one to seven layers by measuring the quantum oscillation of magnetoresistance. The Landau fan diagram showed distinct structures that reflected differences in the band structure, as if they were finger prints of multilayer graphene. In particular, an even-odd layer number effect was clearly observed, with the number of bands increasing by one for every two layers and a Dirac cone observed only for an odd number of layers. The electronic structure is significantly influenced by the potential energy arising from carrier screening associated with a gate electric field. (Sci. Rep. 8, 13018 (2018). DOI:10.1038/s41598-018-31291-y)
**T70.00279: Magnetic Proximity Effect in Graphene/BiFeO$_3$ Hybrid System**

HUA-DING SONG (Presenter), ZHI-MIN LIAO, Department of Physics, Peking University, DAPENG YU, Department of Physics, Southern University of Science and Technology — Graphene, a very intriguing 2D massless fermionic system with high carrier mobility, is promising for spintronics. However, the spin splitting is always weak in pristine graphene. Here, we report the transport properties of graphene coupled to an antiferromagnetic insulator BiFeO$_3$. It is found that the magnetic proximity effect results in a strong Zeeman splitting in graphene with the obvious spin splitting in Landau levels. $\nu=0$ quantum Hall state of the coupled system undergoes quantum phase transitions as a result of the combined effect of exchange field and external field. The direction of the external magnetic field also shows its capability to adjust the proximity effect at the interface, by tuning the interfacial magnetization. We also achieve the electrical control of the magnetic proximity effect via strong magneto-electric coupling in BiFeO$_3$ nanoplates. Our findings in graphene/BiFeO$_3$ heterostructure are therefore promising for future spintronics.

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**T70.00280: Thermal Conductivity of Pure and Doped Graphene**

GIRIJA DUBEY (Presenter), Department of Earth & Physical Sciences and Department of Physics & Engineering Physics, York College of CUNY and Fordham University, New York, NY, USA, SARITA MANN, Department of Physics, Punjab University, Chandigarh, India, VASSILIOS FESSATIDIS, Department of Physics and Engineering Physics, Fordham University, Bronx, New York, USA, HITESH SHARMA, Department of Physics, Punjab Technical University, Kapurthala, India, GODFREY GUMBS, Department of Physics & Astronomy, Hunter College of CUNY, New York, NY, USA, VIJAY JINDAL, Department of Physics, Punjab University, Chandigarh, India — In this work we have studied the thermal conductivity of both pure graphene and boron-doped graphene structure. The calculations have been performed using ab-initio density functional perturbation theory, implemented in VASP software, to study structural properties and calculated the interatomic forces/force constants of pristine/doped graphene. Thermal conductivities are calculated by solving linearized Boltzmann transport equations (LBTE) using single mode relaxation time approximation (RTA). The phonon density of states and thermal conductivity were calculated using phonopy and phono3py. A graphene sheet of 32 atoms was considered for calculating second order force constants while an 8 atom sheet was used to calculate third order force constants. A smaller sheet was used for third order force constant calculation as it requires high computation. Doping concentrations of 12.5% and 25% B dopants were used in this work since higher concentration of dopants lead to unstable structures.

Using this approach, we have obtained thermal expansion results for pure graphene which match well earlier calculations using similar approach. The results have suggested that the thermal properties could be highly tuneable and have interesting application prospects.

**T70.00281: Infrared Spectroscopy of Dual-Gated Bilayer Graphene**

JORDAN RUSSELL, JORDAN PACK (Presenter), YASHIKA KAPOOR, Washington University in St. Louis, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ERIK HENRIKSEN, Washington University in St. Louis — We have performed infrared transmission spectroscopy measurements on dual-gated encapsulated bilayer graphene. In these measurements, we have observed intra- and inter-band resonances of bilayer graphene which we study as a function of magnetic field, filling factor, and displacement field. We will share comparisons between measurements of devices with metal and graphite gates. Methods of distinguishing sample resonances from resonances observed in the silicon and graphite gates will also be discussed.
**T70.00282: Energy Relaxation of Hot Dirac Carriers in CVD Graphene-based Heterostructures**

JINGGAO SUI (Presenter), Department of Physics, University of Cambridge, JACK ALEXANDER-WEBBER, YE FAN, Department of Engineering, University of Cambridge, HIROMU GAMOU, Department of Materials Science, University of Tokyo, S HOFMANN, Department of Engineering, University of Cambridge, MALCOLM CONNOLLY, CHARLES G SMITH, Department of Physics, University of Cambridge — The two dimensional character of graphene makes it a promising material to be used in the post-silicon electronics era. Despite the exceptional electronic properties, the lack of a bandgap in monolayer graphene limits its potential applications. The creation of heterostructures based on graphene and other two-dimensional crystals can help overcome some limitations. We present a fabrication process and magnetotransport measurements to study the hot carrier dynamics in scalable bilayer CVD graphene and graphene-on-WSe2 heterostructures. Energy relaxation of hot Dirac fermions in these systems is experimentally investigated by Shubnikov–de Haas oscillations and weak localization\(^1\). Energy loss rates in graphene-based heterostructures have been found to follow the predicted Bloch–Grüneisen power-law behaviour. The electron-phonon relaxation time has also been observed to be carrier density dependent. Hot carrier dynamics in graphene has considerable importance in determining the performance of high frequency and high power electronics, high-speed sensors and quantum Hall metrology for accurate measurements\(^2\).

\(^1\) J. Huang et al., J. Phys.: Condens. Matter 27, 164202 (2016)

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**T70.00283: Electronic transport in graphene decorated with Bi2Te3 nanoparticles**

JOSHUA COHEN (Presenter), JAMIE ELIAS, Department of Physics, Washington University in St. Louis, 1 Brookings Dr, St. Louis, MO 63130, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0044, Japan, FUDONG WANG, WILLIAM BUHRO, Department of Chemistry, Washington University in St. Louis, 1 Brookings Dr, St. Louis, MO 63130, ARASHDEEP S THIND, ROHAN MISHRA, Department of Mechanical Engineering and Materials Science, Washington University in St. Louis, 1 Brookings Dr, St. Louis, MO 63130, ERIK HENRIKSEN, Department of Physics, Washington University in St. Louis, 1 Brookings Dr, St. Louis, MO 63130 — We investigate the electronic transport in monolayer graphene Hall bars in which the graphene surface is carefully cleaned and then decorated with a dilute coating of Bi2Te3 nanoparticles. The devices include both monolayer-on-silicon oxide and monolayer-on-boron nitride variants. The Bi2Te3 nanoparticles are high quality with few defects, and mono-disperse with a diameter of approximately 15 nm. Initial measurements were made on graphene with a low coverage of \(~1\) nanoparticle per \(10^4\) nm\(^2\), and indicate transport not dissimilar from standard for graphene. Upon annealing the sample in Ar to promote removal of the nanoparticle polymer coating, a small leftward shift indicating electron doping was observed. Results in devices with higher nanoparticle densities will be presented.

**T70.00284: STATISTICAL THERMODYNAMICS OF DICE LATTICE CARRIERS**

NORMAN J.M. HORING (Presenter), Physics, Stevens Inst. of Tech., Hoboken, NJ, USA, M LAWRENCE GLASSER, Physics, Clarkson University, Potsdam, NY, USA, JAY D MANCINI, Physical Sciences, Kingsborough Community College, Brooklyn, NY, USA — We have developed the retarded and thermodynamic Greene’s functions for Dice Lattice carriers and employed them in the determination of the Dice Lattice statistical thermodynamic functions, including the Helmholtz Free Energy, grand partition function, ordinary partition function, and entropy. These evaluations are carried out for arbitrary temperature and chemical potential, including the degenerate and nondegenerate statistical regimes.
T70.00285: Are freestanding Xene monolayers excitonic insulators in their ground state?* MATTIAV BRUNETTI (Presenter), CUNY Graduate Center, OLEG BERMAN, ROMAN KEZERASHVILI, Physics, CUNY - City Tech — We present evidence that monolayers of Xenes (silicene, germanene and stanene) suspended in vacuum behave as excitonic insulators in their ground state, by drawing upon well-established ab initio and theoretical models of the electronic structure of these materials. By solving the Schrödinger equation for electrons and holes interacting via the Rytova-Keldysh potential, it is shown that the direct exciton binding energy exceeds the band gap when the external electric field is small or zero [1]. We propose a phase transition in freestanding monolayer Xenes from the semiconducting phase to the excitonic insulating (EI) phase can be induced by reducing an external electric field below some critical value which is unique to each material. Our calculations show the coexistence of the semiconducting phase of A excitons with the EI phase of B excitons for a particular range of electric field. Enhanced dielectric screening in supported or encapsulated monolayer Xenes precludes the existence of the EI phase in those scenarios.


*This work is supported by U.S. Department of Defense under Grant No. W911NF1810433.

T70.00286: Mechanical and electronic properties of 2D green phosphorene, a first-principles study GUANG YANG, Arizona State University, TIANXING MA, Beijing Normal University, XIHONG PENG (Presenter), Arizona State University — Recently, a phosphorus isomer named green phosphorus was theoretically predicted with a similar interlayer interaction compared to that of black phosphorus, thus indicating that individual layers can be mechanically exfoliated to form two-dimensional (2D) layers known as green phosphorene. The 2D structure shows high stability and was predicted to have a direct band gap up to 2.4 eV. First-principles density functional theory calculations were used to investigate the mechanical properties and strain effect on electronic band structure of the 2D green phosphorene along two perpendicular in-plane directions. Remarkably, it was found that the material can sustain a tensile strain in the armchair direction up to a threshold of 35% which is larger than that of black phosphorene, suggesting that green phosphorene has more puckered structure. The results also showed that the Young's modulus and Poisson's ratio in the zigzag direction are four times larger than those in the armchair direction, which confirms the anisotropy of the material. Furthermore, uniaxial strain can trigger the direct-indirect bandgap transition in the material, and the critical strains for the bandgap transition are revealed.


T70.00287: Van-der-Waals-gap tunneling spectroscopy for low dimensional materials* DONG HWAN CHOI (Presenter), JU-JIN KIM, Physics, Chonbuk National University, MYUNG-HO BAE, Korea Research Institute of Standards and Science, KYUNG-AH MIN, SUK-LYUN HONG, Physics, Sejong University — Field-effect transistors based on low-dimensional materials such as carbon nanotubes (CNTs), graphene, and transition metal dichalcogenides have been developed in order to provide enhanced electronic performance, with significant efforts to overcome the van der Waals (vdW) gap between the metal and inert material components. We report a new method that offers a high resolution tunneling spectroscopy by adopting tunnel barrier as the vdW interface indium (In) metal and low-dimensional nano-structures without an artificial insulating tunnel barrier. We show that multiple differential conductance peaks for varying bias voltages correspond to the van Hove singularities existing in the electronic density of states of CNTs. For the multi-layer MoS2 FET, conductance shoulders were observed at the source-drain voltage ($V_{sd}$) of $-0.9$ V and were attributed to a semiconducting gap. For the 1T-TaS2 case, Mott-gap induced conductance peaks at $V_{sd} \sim 0.2$ V were observed at $T = 4$ K, which coexist with the commensurate charge-density-wave phase.

*This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) (Grant NRF-2016R1A2B4008525)

T70.00288: Temperature-dependent optical and transport conductivities in doped silicene* ANDRII IUROV (Presenter), University of New Mexico, GODFREY GUMBS, Hunter college, DANHONG HUANG, Air Force Research Labs. — We examined the thermal transport properties of silicene, germanene and other buckled honeycomb lattices with finite electron doping. Both Boltzmann and optical conductivities are computed based on the finite-temperature polarization function, Such thermally convoluted polarizability is calculated using temperature-dependent chemical potentials. We have analyzed the frequency dependence of both real and imaginary parts of the optical conductivity. Specific features of the obtained spectral dependence can be used for analyzing plasmon damping in silicene and ultrafast light modulations. We also calculated transport conductivities for various doping concentrations and band gaps using the second-order Born approximation and derived several important analytical expressions for the inverse relaxation times.

*D.H. would like to acknowledge the support from the Air Force Office of Scientific Research (AFOSR). D.H is also supported by the DoD Lab-University Collaborative Initiative (LUCI) program. G.G. would like to acknowledge the support from the Air Force Research Laboratory (AFRL) through Grant #12530960.
T70.00290: Low-energy bandstructure, electronic states and Berry phases in α-T₃ materials under external irradiation

* LIUBOV ZHEMCHUZHNA (Presenter), Hunter college, ANDRII IUROV, University of New Mexico, GODFREY GUMBS, Hunter college, DANHONG HUANG, Air Force Research Labs. — Electron dressed states, or interacting Floquet states, have been derived analytically for α-T₃ materials. These arise from the off-resonant coupling of Dirac pseudospin-1 electrons to the external irradiation. Results will be presented over the allowable range of values of the interaction parameter $\alpha_0 < \alpha < 1$ and for all possible types of incoming light polarizations. For elliptical and circular polarizations, an energy band gap could be opened, there is no longer symmetry between the valence and conduction bands, and the obtained low-energy bandstructure directly depends on the valley index $\tau$. In contrast, applying linearly polarized light could induce $\alpha$-dependent anisotropy of the dispersions, but there is no change to the flat band. We have obtained and examined the corresponding wave functions, their structure and Berry phases.

*D.H. would like to acknowledge the support from the Air Force Office of Scientific Research (AFOSR). D.H is also supported by the DoD Lab-University Collaborative Initiative (LUCI) program. G.G. would like to acknowledge the support from the Air Force Research Laboratory (AFRL) through Grant #12530960.

T70.00290: Exploration of exciton behavior in atomically thin WS₂ layers by ionic gating

XIN HE (Presenter), ZEHUI ZHANG, CHENHUI ZHANG, Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), YANG YANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, MING HU, Institute of Mineral Engineering, Division of Materials Science and Engineering, Faculty of Georesources and Materials Engineering, RWTH Aachen University, WEIKUN GE, School of Physics, Peking University, XIXIANG ZHANG, Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST) — The photoluminescence spectra of mono- and bilayer WS₂, gated by the ionic liquid, were systematically studied at 77 K. Interesting phenomena, such as a redshift of the exciton peaks and a change in the spectral weight of the exciton, trion, and biexciton peaks, were observed at intermediate doping levels. By increasing the doping level, all the exciton, trion, and biexciton peaks vanished, which is attributed to the phase-space filling effect and the Coulomb screening effect. The variation in the band structure, which was induced by the quantum-confined Stark effect in both the mono- and bilayer WS₂, was also studied using first-principle calculations.

T70.00291: The control of the double-slit silicene interferometer by the spin-Hall effect

BARTLOMIEJ RZESZOTARSKI (Presenter), BARTLOMIEJ SZAFRAN, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology — Silicene [1] is a novel 2D-material similar to the graphene with buckled structure that provides spin-orbit coupling (SOC) which is a source of topological physics. In silicene zigzag nanoribbons for low Fermi energy the quantum spin Hall effect [2] occurs and the charge currents for both spin orientation flow along opposite edges of the ribbon. Here, we present an idea for the double-slit-interference device with one input lead that splits to double channels (Y-shape) based on the atomistic tight-binding approach [3]. The double channel is connected to an unconfined silicene half-plane with a third lead used as a detector. The double-slit interference can be detected with the external magnetic field that triggers the Aharonov-Bohm conductance oscillations only when the electron wave functions passes through both the arms of the split input channel. The Aharonov-Bohm oscillations are attenuated when the system is driven in the quantum spin Hall regime, when the wave functions passing through both the channels have opposite spins.


T70.00292: Polarization charge coupling effect in 2D van der Waals-ferroelectric heterostructure

HYE-JIN JIN (Presenter), JAYEONG KIM, YEJIN KIM, SEOKHYUN YOON, Department of Physics, Ewha Womans University, YANGJIN LEE, KWANPYO KIM, Yonsei University, WILLIAM JO, Department of Physics, Ewha Womans University. — In two-dimensional (2D) layered semiconducting materials, charge distribution is controlled by ferroelectric polarization and inequivalent charge distribution is obtained vertically. Ferroelectric polarization induced accumulation or depletion in 2D semiconductors resulting in polarization charge coupling effect. In this study, 2D semiconductors ($n$-type MoS₂ and $p$-type WSe₂) and ferroelectric PbTiO₃ (PTO) thin films were integrated vertically. We used conductive atomic force microscopy to study vertical transport and light illumination effect is also studied. Enhanced resistive switching effect was obtained and polarization was exploited to control resistive switching characteristics. In addition, charge separation is effectively obtained due to built-in interfacial electrical field at interface between 2D semiconductor and PTO thin films. In particular, photovoltaic response is obtained in the heterostructure and polarization can behave as a physically-doped electrode. Polarization gives stable and additional separation of electron-hole pairs in 2D semiconductors and increase of photoresponse is obtained. Therefore, we can expect application for a photo-memristor and suggest new memory and photovoltaic devices by integrating 2D semiconductors and ferroelectrics.
T70.00293: Tunnelling spectroscopy of localized states in WS₂ based van der Waals heterostructures*  
NIKS  
PAPADOPOULOS (Presenter), PASCAL GEHRING, Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, Delft 2628 CJ, The Netherlands, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan, HERRE S.J. VAN DER ZANT, GARY STEELE, Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, Delft 2628 CJ, The Netherlands — Defects in semiconductors and dielectrics can provide rich physics with technological potential such as quantum photon emission, spin control and they might be potential platforms for realizing quantum entanglement. In transition metal dichalcogenides, defects have been found to play important role as they affect the doping and the spin-valley relaxation dynamics. Herein we study localized states in WS₂ by means of tunnelling spectroscopy using van der Waals heterostructures of h-BN/graphene/WS₂/metal. The monolayer graphene electrodes provide for weak screening of electric-fields, which allows us to tune the chemical potential of WS₂ with the back-gate. The obtained conductance maps as a function of bias and gate voltage reveal single-electron transistor behaviour (Coulomb blockade) with a rich set of transport features like excited states and negative differential resistance regimes. Moreover, by applying a perpendicular magnetic field, we study the spin ground- and excited states of single defects.  
*This work is part of the Organisation for Scientific Research (NWO) and the Ministry of Education, Culture, and Science (OCW). Growth of hexagonal boron nitride crystals was supported by the Elemental Strategy Initiative conducted by the MEXT, Japan and the CREST (JPMJCR15F3), JST.

T70.00294: Spin Polarized Excitonic Superfluids in Topological Insulators*  
HENRY TRAVAGLINI (Presenter), University of California, Davis —  
Topological insulators (TIs) are a remarkable class of materials due to their linear dispersion relation and exotic spin textures at the surface, and have recently been proposed as a candidate system for achieving a condensate state of excitonic particles. We use scanning photocurrent microscopy to study Sb doped Bi₂Se₃ at varying temperature, wavelength, polarization, and incident angle. This suite of measurements confirm that electrons and holes form bound states at low temperature, and demonstrate ballistic transport at temperatures up to 40 K, as evidenced by millimeter exciton transport lengths. Furthermore, photocurrent magnitude is drastically different depending on which side of the channel the photoexcitation occurs, which we attribute to spontaneous magnetization of the exciton condensates and spin momentum locking. We also explore spin polarization at the TI surface from the dependence of photocurrent distributions on the polarization of the photoexcitation at oblique-incidence-angle.  
*This work was supported by National Science Foundation Grant DMR-1838532.

T70.00295: Finite-Size Effect in the Photonic Topological System  
YUHAO KANG (Presenter), Physics, The Graduate Center of the City University of New York, AZRIEL Z GENACK, Physics, Queens College of the City University of New York — Measurements of the transmission matrix of a topological system supporting edge state between metacrystal emulating quantum valley-Hall and spin-Hall effects show the disruption of ballistic propagation. We observe a decrease of transmission and an increasing of the dwell time for the edge mode in a finite topological system. The non-linear spatial decrease of the logarithm of the intensity along the edge highlights the differences between transport statistics of an edge state and normal 1D channel.

T70.00296: Effect of band-offsets on the valley polarization properties of WSe₂ lateral homojunctions  
ANIL RAJAPITAMAHUNI (Presenter), NEREA ONTOSO, LUIS HUESO, FELIX CASANOVA FERNANDEZ, JOSE IGNACIO PASCUAL, REYES CALVO, CiC nanoGUNE — We have studied the effect of band-offsets on the valley polarization of lateral homojunctions composed of 1L/n-layer WSe₂ flakes. WSe₂ flakes are transferred onto SiO₂/Si substrates using elastic film assisted micromechanical exfoliation. Optical microscopy combined with Raman spectroscopy is used to identify and determine the layer number of 1L/n-layer WSe₂ structures. We worked with naturally occurring 1L/n-layer lateral homojunctions to eliminate the band-offsets resulting from twist angles and stacking order. Spatially-resolved photoluminescence (PL) spectroscopy measurements are performed using a scanning confocal microscope at low temperatures down to 4.2 K and in magnetic fields up to 5T. The intensity and energy position of the different excitation peaks in the PL spectra are mapped to determine the effects of inhomogeneities and band-offsets on the valley polarization properties of the lateral homojunctions. We intend to study the valley Zeeman effect in the lateral homojunctions via polarization-resolved PL spectroscopy. Our work will facilitate in understanding the effects of band alignment on the valley polarization phenomena in TMD homo/heterostructures for valleytronic applications.
T70.00297: Valleytronics in two-dimensional merging Dirac cone system: Universal reversible Boolean gate* YEE SIN ANG (Presenter), LAY KEE ANG, SHENGYUAN YANG, Science and Math, Singapore University of Technology and Design — Due to the logical irreversibility, the energy efficiency of Boolean logic gates is fundamentally capped by the Landauer’s waste heat energy generation limit of $k_B T \log_2 p$ per bit of irreversible operation. Here we show that valley degree of freedom in two-dimensional (2D) material can be harnessed to reassert the logical reversibility of classical two-input Boolean logics. The valley index manifests macroscopically in the electrical current as three distinct polarization states: two opposite valley polarizations plus a null state. These triplet of valley polarization states can be used to encode additional information, thus removing all ambiguity and recovering logical reversibility in Boolean logic gates. We use 2D merging Dirac cone system, which occurs in few-layer black phosphorus, strained graphene, and 2D topological Dirac semimetal, as a toy model to demonstrate three fundamental valleytronic building blocks: valley filter, valve, and logic gates. We show that the all-important universal reversible gate, such as the NAND gate, can be realized using this valleytronic approach. Our findings provide a new valleytronic route towards ultimately energy-efficient classical reversible computing.

*This work is supported by A*STAR IRG (A1783c0011) and AFOSR AOARD (FA2386-17-1-4020).

T70.00298: SUPERLATTICES, NANOSTRUCTURES, AND OTHER ARTIFICIALLY STRUCTURED MATERIALS —

T70.00299: Solvent and Concentration Effects Governing the Hierarchical Organization of Asphaltenes: A Small-Angle X-Ray Scattering Study HASAN RAHMAN (Presenter), Physics, New Mexico State University, JOSE L BANUELOS, Physics, The University of Texas at El Paso — Asphaltenes are a group of planar molecules found in crude oil and are prone to aggregation which causes blockage of pipes along the oil production stream. The solution-state nanostructure of various asphaltene solutions was studied using small-angle x-ray scattering (SAXS) (over a Q-range of 0.008 - 0.4 Å⁻¹) in order to understand solvent and concentration effects on asphaltene hierarchical organization. The fractal aggregate structure of asphaltene was characterized as a function of concentration in toluene (1-50 mg/ml), tetrahydrofuran (1-500 mg/ml), and benzene (1-100 mg/ml). In toluene, the varying cutoff length, primary radius parameters, and the growing mass fractal dimension, all suggest that at a certain chain length, asphaltene nano-aggregates (NA) begin to collapse onto themselves to form a larger and denser aggregate. The experimental data has also been fit with several models including the Unified Power Law and the Ellipsoidal/Spherical Hayter Mean Spherical Approximation models to compare their characteristic parameters such as the ‘Guinier Radius’ and ‘Porod Slope’ to develop a consistent view of the hierarchical structure of asphaltene which will aid as a valuable input to develop strategies to mitigate the effects of asphaltene aggregation.

T70.00300: A generalised shapelet-based method for analysis of nanostructured surface imaging NASSER ABUKHDEIR (Presenter), THOMAS AKDENIZ, Chemical Engineering, University of Waterloo — The determination of quantitative structure-property relations is a vital but challenging task for nanostructured materials research due to the presence of large-scale spatially varying patterns resulting from nanoscale processes such as self-assembly and nano-lithography. Focusing on nanostructured surfaces, recent advances have been made in automated quantification methods for translational order using shapelet functions, originally developed for analysis of images of galaxies, as a reduced-basis for surface pattern structure.

In this work, a method combining shapelet functions and a machine learning clustering method is developed and applied to a representative set of images of self-assembled surfaces from experimental characterization techniques including SEM, AFM, and TEM. The method is shown to be computationally efficient and able to quantify salient pattern features including deformation, defects, and grain boundaries from a broad range of patterns typical of self-assembly processes.

T70.00301: Second Harmonic Generation On Hydrothermal Grown Zno Nanowires And Colloidal Nanostructures Films DOMINIC TRAN (Presenter), CHRISTOPHER VALDES, MOSTAFA SADOQI, St. John's University, IWAN KITYK, Electrical Engineering Department, Czestochowa University Technology, GEN LONG, St. John's University — We report a non-linear optical study on ZnO nanowires grown on FTO substrate and spin-cast colloidal nanostructures (PbS and PbS-Au) based films for the first time. Zinc oxide (ZnO) nanowire was grown by hydrothermal method on pre-cleaned, seeded FTO substrates, placed facedown in the aqueous solution of zinc nitrate hydrate and HMTA (Hexamethylenetetramine) for a few hours. The diameters diameters, lengths and density of ZnO nanowires could be controlled by varying seedling concentration, growth temperature and growth time. Non-linear optical measurement was done using a systems of mirrors M1, M2, M3 stable for the power densities up to 1.5 GW/cm², the laser fundamental beam of Nd:YAG laser was frequency doubled by a-BiB₃O₆ second harmonic crystals. Second harmonic generation was observed on the ZnO-nanowire-grown substrates. It was also noted the SHG pattern showed same pattern as the ZnO nanowire growth pattern. The general origin of the observed effect is caused by local acentricity of the titled compounds. Further studies will be done on nanostructures based devices. Similar studies were also done on spin-cast films made of colloidal nanostructures such as PbS and PbS-Au nanoparticles. SHG was also observed in such films.
T70.00302: Ion-implanted silver nanoparticles for metal-enhanced fluorescence SHAHID IQBAL (Presenter), MOHAMMAD HATSHAN, PRASHANTA NIRAULA, ABUBKAR ARZAQ, HASNA ABDULLAH, RAMAKRISHNA GUDA, ASGHAR KAYANI, Western Michigan University — Metal Enhanced Fluorescence (MEF) has promising applications in the field of optical displays, bio-sensing and photodynamic therapy. In this work, we exploit the plasmons of embedded silver nanoparticles (Ag-NPs) fabricated by ion implantation to enhance the fluorescence of Coumarin 515 dye (C515) via MEF. Ion implantation of 70 keV Ag ions in quartz matrix at different fluences was carried out to synthesize Ag-NPs inside quartz matrix. The formation of Ag-NPs is characterized by the optical absorption measurements. Rutherford Backscattering Spectrometry (RBS) measurement was used to obtain the depth profile and concentration of silver within the substrate. From the RBS results, it was determined that front edge of the layer containing Ag was formed at an average depth of 16 nm below the surface, which closely agreed with Stopping and Range of Ions in Matter (SRIM) calculations. The MEF of drop casted C515 dye was studied using steady-state emission and excitation spectra measurements. Photoluminescence (PL) enhancement factor ranging from 1.2 to 2.1 with a maximum enhancement for the largest fluence was obtained. The observed MEF was ascribed to a combination of plasmon enhancement with larger nanoparticles due to increase in fluence and to increase plasmonic hot spots.

T70.00303: Reflection from bare and gold coated InP nanowire arrays* CHIAWEI TU (Presenter), Department of Physics, University of Cincinnati, Cincinnati, OH 45221, U.S.A., QIAN GAO, HOE TAN, CHENNUPATI JAGADISH, Department of Electronic Materials Engineering, Research School of Physics and Engineering, Australian National University, Canberra ACT 0200, Australia, MASOUD KAVEH-BAGHBADORANI, Department of Physics and Astronomy, James Madison University, Harrisonburg, Virginia 22807, U.S.A., HEIDRUN SCHMITZER, Department of Physics, Xavier University, Cincinnati, OH 45207, U.S.A., MARTIN FRAENZL, Department of Physics, University of Leipzig, 04103 Leipzig, Germany, HANS-PETER WAGNER, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, U.S.A. — We investigated the spectral and angle resolved reflectance from bare and gold coated (plasmonic) InP nanowire (NW) arrays which were grown by selective area epitaxy. The NWs in the arrays have diameters of 180 nm, heights of ~2 and ~1 micrometers and a pitch of 666 and 500 nm (named areas NWA-1 and NWA-2), respectively. In NWA-2 the NWs additionally possess a 10 nm thick surrounding Al2O3 layer to reduce surface state and metal induced band-bending. A nominally 10 nm thick gold layer was deposited around the NWs in both arrays to study the influence of plasmonic effects. The NW arrays were illuminated with a cw laser at 880 nm for the angle resolved reflectance measurements and with an incandescent light sourced ranged from 500 nm to 1000 nm spectrally resolved experiments. The incident light beams were polarized in p- and s-orientation. The measured spectral and angle resolved reflectance of both uncoated arrays is in very good agreement with finite-difference-time-domain (FDTD) simulations. The MEF of drop casted C515 dye was studied using steady-state emission and excitation spectra measurements. Photoluminescence (PL) enhancement factor ranging from 1.2 to 2.1 with a maximum enhancement for the largest fluence was obtained. The observed MEF was ascribed to a combination of plasmon enhancement with larger nanoparticles due to increase in fluence and to increase plasmonic hot spots.

*T70.00304: Compact localized states in open scattering media FABRIZIO SGRIGNUOLI (Presenter), Boston University, MALTE RÖNTGEN, CHRISTIAN MORFONIOS, PETER SCHMELCHER, Zentrum für optische Quantentechnologien, Universität Hamburg, LUCA DAL NEGRO, Boston University — In this work, we study the compact localized scattering resonances of periodic and aperiodic chains of dipolar nanoparticles by combining the powerful Equitable Partition Theorem (EPT) of graph theory with the spectral dyadic Green's matrix formalism for the engineering of embedded quasi-modes in non-Hermitian open scattering systems in three spatial dimensions. We provide analytical and numerical design of the spectral properties of compact localized states in electromagnetically coupled chains and establish a connection with the distinctive behavior of Bound States in the Continuum. Our results extend the concept of compact localization to the scattering resonances of complex open systems with aperiodic order beyond tight-binding models, and are relevant for the efficient design of novel photonic and metamaterials architectures with enhanced light-matter interactions.

T70.00305: Simulations of Nanostructure Plasmonic Resonators PARVEEN KUMAR (Presenter), University of California, Merced, 95353, USA — Semiconductor nanostructures with and without plasmon enhancement are studied and explored extensively for nanodevice applications ranging from bio/chemical sensors to medical monitors and photovoltaics. Plasmonic resonances strongly depends on the size, shape, spacing and interaction of metal nanoparticles with semiconductor nanostructure. A lot of resources as well as efforts are required to realize plasmonic resonator devices and optimization with different shapes and sizes. In contrast, device modeling and simulations offer a much economical substitute to tackle such challenges. To solve this problem in most economical and reliable mode, is to use Maxwell equation solver which helps in simulating the nanoparticles as surface plasmon resonator on the top of semiconductor nanostructures. The sharp features as well as the nanoparticle asymmetry is usually used for reported the enhancement of the electric field. To enhance the absorption rate as well as the photocurrent signal, I report the simulation the electrical field profile for spherical, cylindrical, and bipyramidal nanoparticles (of different materials) and model the interaction of these nanoparticles with semiconductor nanostructures.
T70.00306: Novel Two-Dimensional Tellurium Allotropes from the First-principles Predication*  CHUNYAO NIU, CHUNXIANG ZHAO, XIAOLIN CAI, CHAOSHENG LIAN, ZHILI ZHU, YU JIA (Presenter), School of Physics and Engineering, Zhengzhou University — Very recently, the successful predication and synthesis of α-, β-, and γ- tellurene have extended the two-dimensional (2D) materials family to group-VI elements and provided new candidates for next-generation electronic and optoelectronic applications. Based on our previous work, we have further predicted 33 newly 2D tellurium allotropes with mono- and multi-layers of tellurium atoms using the particle-swarm crystal structure searches methods and the first-principles calculations. The stability of these 2D structures is well verified by the total energy calculations, as well as phononspectrum calculations. Four kinds of new allotropes are found energetically more stable than the β-Te phase which already has been synthesized experimentally. Among these structures, we found three of them exhibit topological properties and two with superconductor properties. The present findings enlarge the family of tellurene and will stimulate future experimental studies to synthesize novel group-VI 2D materials.

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T70.00307: Light stops at exceptional points†  TAMAR GOLDZAK (Presenter), Massachusetts Institute of Technology, ALEXEI A MAILYBAEV, Instituto Nacional de Matemática Pura e Aplicada-IMPA, NIMROD MOISEYEV, Technion - Israel Institute of Technology — Light travels in vacuum with a constant speed of 300,000,000m/sec, almost twenty years ago the light was slowed down to less than 10⁻⁷ of its vacuum speed in a cloud of ultracold atoms of sodium. Upon a sudden turn-off of the coupling laser, a slow light pulse can be imprinted on cold atoms such that it can be read out and converted into photon again. Alternatively, the light can be stopped at the band edge in photonic-crystal waveguides. Here we extend the phenomenon of stopped light to the new field of parity-time (PT) symmetric systems.

We show that zero group speed in PT symmetric optical waveguides can be achieved if the system is prepared at an exceptional point, where two optical modes coalesce. This effect can be tuned for optical pulses in a wide range of frequencies and bandwidths, as we demonstrate in a system of two coupled waveguides with gain and loss. We also investigate how the structure of multiple coupled wave guides affect the dispersion relation of the two coalesced modes.


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T70.00308: Quantum to Classical Transitions in Multilayer Plasmonic Metamaterials*  EVAN SIMMONS (Presenter), University of Massachusetts Lowell, KUN LI, ANDREW BRIGGS, SETH BANK, DANIEL WASSERMAN, Electrical and Computer Engineering, University of Texas at Austin, VIKTOR PODOLSKIY, University of Massachusetts Lowell, EVGENII NARIMANOV, Electrical and Computer Engineering, Purdue University — Electromagnetic response of noble metals, transparent conducting oxides, and highly doped semiconductors are all dominated by the dynamics of their free electron plasma. AlInAs/InGaAs heterostructures have emerged as a reliable platform that provides epsilon-near-zero, plasmonic, and hyperbolic responses in the important mid-infrared frequency range. The electromagnetic properties of semiconductor multilayers can be related to the properties of individual layers via effective medium theory (EMT). It is typically assumed that the validity of EMT improves as the layers in metamaterials become thinner. However, quantum-confinement is expected to affect the dynamics of the free charges in ultra-thin layers. In this work, we analyze, experimentally, analytically, and numerically, the optical response of semiconductor designer metal multilayers that undergo transition from bulk to quantum-confined regime. We demonstrate that this transition can be used as a doping-independent control mechanism to engineer the optical response of designer metals and the optical topology of the resulting multilayer metamaterials.

*This research is sponsored by NSF-DMREF program
T70.00309: Interlayer excitons at the tunable Moire line defect*  JIANJU TANG (Presenter), HONGYI YU, WANG YAO, The University of Hong Kong — Van der Waals stacking of two monolayers semiconducting transition metal dichalcogenides is a powerful approach to create semiconductor heterojunctions for engineering functional devices. The inevitable mismatch in lattice constants and crystallographic axes leads to the formation of Moire pattern, giving new possibilities to tailor the material properties. Interlayer excitons in such Moire pattern experience an effective superlattice potential and have a nanoscale patterned light-coupling properties. The low energy physics of those excitons can be described by a tight binding model with giant spin-orbit coupling. Here, we investigate interlayer excitons in such Moire pattern with a line defect due to the twin domain boundary in one of the layers, which can localize one-dimensional excitonic modes of topological origin. We show that the defect configuration in the Moire superlattice can be tuned by the interlayer translation, twisting angle and reflects the atomic configuration of the domain boundary. The effects of the Moire line defect configuration on the exciton modes are systematically investigated. We also find the defect exciton mode has distinct light-coupling properties on the two sides of the twin domain boundary.

*Research Grant Council of HKSAR (HKU17302617, C7036-17)

T70.00310: Photoluminescence studies of lysozyme mediated zinc oxide (ZnO) nanoparticles  NIKESH MAHARJAN (Presenter), MIM L NAKARMII, Department of Physics, Brooklyn College and The Graduate Center of the CUNY, Brooklyn, NY 11210, USA, DEEPENDRA DAS MULMI, Department of Physics, Nanomaterials Research Laboratory, Faculty of Science, Nepal Academy of Science and Technology, Khumaltar, Lalitpur, GPO Box 3323, Nepal, NARESH M SHAKYA, Department of Applied Physics, New York University, NYU - Tandon School of Engineering, Brooklyn, NY 11201 — Ultraviolet Photoluminescence spectroscopy was employed to study optical properties of lysozyme mediated zinc oxide (ZnO) nanoparticles. The Zinc oxide nanoparticles using lysozyme (L: ZnO) were prepared through a facile synthesis. The samples were annealed at 550 °C for 2 hours. Third harmonic laser (260 nm) generated from the Ti: sapphire laser was used for optical excitation in the experiments. Photoluminescence spectrum measured at low temperature has emission peaks around 3.3 eV and a broad emission around 2.45 eV. We performed temperature and excitation power dependent photoluminescence measurements to identify the origin of the emission peaks in the spectra. We will present our findings on the optical properties of lysozyme mediated zinc oxide nanoparticles and discuss the effect of lysozyme in the optical properties of ZnO nanoparticles.

T70.00311: Phonon induced resistance oscillations (PIRO) caused by THz laser  BEATE HORN-COSFELD (Presenter), MIHAII CERCHEZ, THOMAS HEINZEL, Condensed Matter Physics, Heinrich-Heine University Düsseldorf — PIRO terms the magneto-resistance (MR) oscillation originating from the resonant interaction of 2D electrons with thermal acoustic phonons [1], observed only in very high mobility samples (>10⁷ cm²V⁻¹s⁻¹) [2]. This manifests itself as a 1/B periodic oscillation of the MR of GaAs/AlGaAs heterostructure, in a temperature range of 4-10 K and high filling factors (magnetic fields below 500 mT).

In this work we use THz excitation of the acoustic phonon branch of GaAs by means of a 1.8 THz pulsed quantum cascade laser, so the acoustic phonons are excited by the THz radiation rather than thermally. Electrons resonantly absorb the acoustic phonons accompanied by a 2 kF momentum transfer, causing indirect transitions between Landau levels.

The thermally induced PIRO's are not observable in our samples, probably due to the electron mobility being about a factor of two lower than those given in [2].


T70.00312: Tunability of thermal conductivity in low-dimensionality chalcogenide and perovskite heterostructures*  MACK ADRIAN DELA CRUZ (Presenter), NICK BOECKER, GARY PENNINGTON, Towson University — Recent work in lead chalcogenide alloys of PbSe, PbS, and PbTe has shown interesting electronic properties. Perovskites, such as SrTiO₃, have been the focus of much research in the past few years. The thermal properties of such materials are of interest for thermoelectric applications. We further consider low-dimensionality heterostructures, which generally have lower thermal conductivities compared to bulk. We use a computationally efficient shell model to find the phonon dispersion of bulk, and approximate the heterostructure phonon dispersions. Phonon Transport is modeled with a Monte Carlo formulation of the Boltzmann transport equation using an interfering particle method with phonon-phonon scattering, boundary scattering, defect scattering, interface scattering, and quantum confinement. We will report on the tunability of thermal conductivity by manipulating low-dimensionality heterostructures of these lead chalcogenide alloys and perovskites.

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*This work was supported by AME Young Individual Research Grants by the Agency for Science, Technology and Research under Proposal No. 17284017.

T70.00314: Phonon backaction in diatomic molecular junctions: Negative differential conductance, quantum interference and super-Poissonian noise  TAE-HO PARK (Presenter), HAN-YONG CHOI, Sungkyunkwan University — We present a study of the non-equilibrium electron transport through diatomic molecular junctions employing the full counting statistics (FCS) in combination with the self-consistent Born approximation (SCBA). Here, we consider two different types of electron-phonon coupling in a molecule. One is the coupling of the molecular vibration to the electrons in each orbital (intra-orbital coupling) and the other is to the transferring electrons (inter-orbital coupling). We show that the super-Poissonian noise is enhanced by increasing the electron-phonon coupling in the presence of the phonon backaction. In the weak coupling regime for the inter-orbital coupling, the negative differential conductance (NDC) can take place in the resonant tunneling regime. It turns out that the current fluctuation suppresses NDC, but induces the quantum interference in molecular conductance.

T70.00315: Molecular Architecture’s Impact on Directional Charge and Energy Transfer within Organic Assemblies*  SARAH MARQUES (Presenter), MICHAEL D BARNES, Chemistry, University of Massachusetts Amherst — The goal of my work is to understand the connection between molecular architecture and directional charge and energy transfer within organic assemblies. Organic optoelectronic devices are based on a materials ability to directionally transfer charge and energy after excitation. Our group has found that extended crystals of 7,8,15,16-tetrazaterrylene (TAT) can produce charge separated states when directionally excited, but the mechanism be it intrinsic or extrinsic in which charge separation occurs is still unknown. To disentangle these mechanisms, we have isolated different stages of TAT crystal growth and probed their molecular orientation (order) using defocused imaging and polarization anisotropy, as well as, their interchromophore interactions and exciton recombination kinetics using photoluminescence spectroscopy and time resolved measurements. We found that even though the spectral signatures of extended crystals (microns) and small clusters (<250 nm) are incredibly different, TAT intrinsically forms ordered assemblies that have a 1D coupling mechanism. These results support an optoelectronic device design based on a monomolecular design platform that intrinsically generates directional charge transport.

T70.00316: Phonon-Plasmon Scattering and Localization in Graphene Structures  BRAHMANANDAM JAVVAJI, DEBIPROSAD ROY MAHAPATRA (Presenter), Indian Institute of Science — In this paper we discuss about a self-consistent model of phonon-plasmon coupled dynamics and investigate the nature of the coupling in the graphene nanostructures. Effect of length-scale in three types of structures namely graphene nano-ribbon, graphene on silicon and graphene defects are investigated. Nonlinear conversion arising from aperiodic localization of phonon modes in the nanoribbon are observed. We show how the chirality plays a role on this relationship. Effect of silicon substrate atoms on the dynamics are analyzed. We then review the present understanding and new ways to design thermal energy transport in graphene based optoelectronic devices. Another aspect of phonon generation is plasmonic extinction due to RF, field emission or lasing with application in filters or sensors. In context of these ideas, we show how the structure of defects in graphene alters the plasmonic extinction. The charge localization around the defects are studied in details and the stability limits of the defects in terms of size and shape are analyzed. To this end, new results showing signature of these instabilities in the optical spectra and phonon spectra will be discussed.
T70.00317: Nanoscopic Hyperlensing from Natural and Monoisotopic Hexagonal Boron Nitride Crystals*

SWATHI IYER (Presenter), ALEXANDER GILES, United States Naval Research Laboratory, SAI SUNKU, Department of Physics, Columbia University, New York 10027, THOMAS FOLLAND, Mechanical Engineering Department, Vanderbilt University, Nashville, TN, USA, NICHOLAS SHARAC, United States Naval Research Laboratory, SONG LIU, JAMES H. EDGAR, Tim Taylor Department of Chemical Engineering, Kansas State University, Manhattan, Kansas 66506, USA, DIMITRI BASOV, Department of Physics, Columbia University, New York 10027, JOSHUA D CALDWELL, Mechanical Engineering Department, Vanderbilt University, Nashville, TN, USA — Hyperbolic media, where the permittivity is opposite in sign along orthogonal axes, support highly directional propagation of volume-confined, hyperbolic polaritons (HPs) for use in super-resolution imaging via the hyperlens concept. Hexagonal boron nitride (hBN), a natural hyperbolic material, supports deeply subdiffractional, low-loss HPs in both planar slabs and nanoscale resonators within the mid- to long wavelength IR. These losses could be reduced even further by using monoisotopic (i.e. material with just a single boron isotope) hBN. Here we exploit these ultralow losses and natural hyperbolic response to realize unprecedented spatial resolution in hyperlensing with long-wavelength IR light. We provide a direct comparison of the imaging power of hyperlens designs using flat slabs of naturally abundant and monoisotopic hBN via scattering-type near field optical microscopy (s-SNOM). Our experimental (s-SNOM) and simulated results show the ability to resolve features as small as 50 nm with 6-7.1 µm free-space wavelength light, providing at least l/125 spatial resolution. We complement this with electromagnetic field simulations of the hyperlens response to demonstrate and quantify the improvements from the monoisotopic over the naturally abundant materials.

*ASEE

T70.00318: Thermal transport in holey silicon membranes investigated with optically-induced transient thermal gratings*

RYAN DUNCAN (Presenter), GIUSEPPE ROMANO, Massachusetts Institute of Technology, MARIANNA SLEDZINSKA, Catalan Institute of Nanoscience and Nanotechnology, ALEXEI MAZNEV, Massachusetts Institute of Technology, JEAN-PHILIPPE PERAUD, Lawrence Berkeley National Laboratory, OLLE HELLMAN, Linköping University, CLIVIA SOTOMAYOR TORRES, Catalan Institute of Nanoscience and Nanotechnology, KEITH ADAM NELSON, Massachusetts Institute of Technology — In semiconductor nanostructures with feature sizes on the order of 100 nm, thermal transport is expected to be well-described by the phonon Boltzmann transport equation (BTE) with diffuse boundary scattering. However, over the past several years there have been reports of anomalously low effective thermal conductivity values in one- and two-dimensional semiconductor nanostructures. In this study, we investigate thermal transport in nanostructured holey silicon membranes using the non-contact optical transient thermal grating (TTG) technique. We compare the experimental results with two ab-initio BTE numerical techniques. We obtain excellent agreement between theory and experiment, indicating that semiclassical Boltzmann transport theory for phonons is adequate for describing thermal transport in semiconductor nanostructures with feature sizes on the order of 100 nm.


T70.00319: OpenBTE: A Multiscale Solver for the Phonon Boltzmann Transport Equation

GIUSEPPE ROMANO (Presenter), Department of Mechanical Engineering, Massachusetts Institute of Technology — We present OpenBTE, an open-source tool to compute heat transport in nanostructured materials with arbitrary shape and dimensionality. The code solves the space-dependent Boltzmann transport equation taking into account the material's Brillouin's zone and diffuse boundaries. For phonon mean-free-paths (MFP) that are much smaller than the characteristic length of the material, we employ a heat diffusion solver so that we lift most of the computational load with negligible loss in the accuracy [1,2]. After an introduction to OpenBTE's main features, we will show the software architecture, including parallelization and interfaces to popular first-principles phonon solver. Then, we illustrate key examples and comparison with experiments. A brief tutorial will conclude the talk.

T70.00320: Symmetry selective oxygen orbital polarization in spinel Al$_2$O$_3$ films* RUYI ZHANG (Presenter), YANG SONG, YANWEI CAO, Key Laboratory of Magnetic Materials and Devices, Ningbo Institute of Industrial Technology, Chinese Academy of Sciences. — Orbital polarization is common for the 3$d$ orbitals of cations as a result of strain, symmetry breaking, or charge transfer, but very rare for 2$p$ orbitals of simple anions. Here, we report a symmetry-selective measurement of orbital polarization for O 2$p$ orbitals in γ-Al$_2$O$_3$/SrTiO$_3$ thin films via linearly polarized X-ray absorption spectroscopy (XAS) at the O K-edge. The O 2$p$ orbitals with octahedral coordination exhibit a large subband splitting exceeding ~ 0.35 eV, while those with tetrahedral coordination show a very weak orbital polarization. These results pave a new way to engineer band structure and quantum states of functional oxide materials via local symmetry effects on anion orbitals.

*National Natural Science Foundation of China (No:11874058)

T70.00321: d-orbital symmetry of BaTiO$_3$ thin film* YANG SONG (Presenter), RUYI ZHANG, YANWEI CAO, Key Laboratory of Magnetic Materials and Devices, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences — A high-quality BaTiO$_3$ thin film was grown on a DyScO$_3$ single crystal substrate using pulsed laser deposition. Soft X-ray absorption spectroscopy was performed at the Ti $L_{2,3}$ edges of the film to characterize the d-orbital symmetry. Novel split Ti d-orbital $e_g$ and degenerate $t_{2g}$ subbands of the BTO film have been observed. The energy of $d_{x^2-y^2}$ orbital is lower than the $d_{3z^2-r^2}$ orbital by about 100 meV, the opposite of what would normally be expected for Jahn-Teller octahedral distortion. This is likely a result of the displaced Ti cation. This novel d-orbital symmetry is very likely to be found in other perovskite-based ferroelectric materials.

*National Natural Science Foundation of China (No:11874058)

T70.00322: Synapse-like modulation of photoconductance at the LaAlO$_3$/SrTiO$_3$ interface. YU CHEN, BLAI CASALS, FLORENCIO SANCHEZ, GERVASI HERRANZ (Presenter), Institute for Materials Science of Barcelona ICMAB-CSIC — We analyze the properties of LaAlO$_3$/SrTiO$_3$ interfaces in relation to its persistent photoconductance (PPC). In this phenomenon the conductance is increased after excitation with visible or ultraviolet light, so that the initial value prior to the photoexcitation is recovered only after prolonged periods of time. Among applications, an interesting prospect for PPC is to exploit its modulation capability to emulate the plasticity of biological synapses using optical stimuli. This requires knowing the dynamical PPC response and its magnitude with respect to illumination conditions so that the potential for neuromorphic vision can be evaluated. Our experiments show that the LaAlO$_3$/SrTiO$_3$ interface is sensitive to 100-millisecond-scale timing of pairs of light stimuli, causing long-term changes of photoconductance. We show that the PPC changes plastically in response to optical stimuli of varying strength and duration, demonstrating that fine-tuning of the photoconductive signal is feasible over a diversity of cumulated timespans. Based on these remarkable observations, we propose that complex information can be extracted from patterns imprinted as spatiotemporal modulations of PPC.

T70.00323: Modulation doping in SrSnO$_3$/BaSnO$_3$ heterostructures* ABHINAV PRAKASH (Presenter), Chemical Engineering and Materials Science, University of Minnesota - Twin Cities, NICHOLAS F QUACKENBUSH, Materials Measurement Science Division, National Institute of Standards and Technology, HWANHUI YUN, JACOB T HELD, TIANQI WANG, K. ANDRE MKHOYAN, BHARAT JALAN, Chemical Engineering and Materials Science, University of Minnesota - Twin Cities — Through a combination of MBE growth, hard X-ray photoelectron spectroscopy (HAXPES), magnetoresistance measurements and transport modeling, we report on the realization of two-dimensional electron gas (2DEG) at SrSnO$_3$/BaSnO$_3$ (SSO/BSO) heterointerfaces. The HAXPES revealed the valence band offset between SSO and BSO to be 0.7 eV resulting in a favorable conduction band offset for modulation doping of BSO using SSO as a spacer layer. Two-channel conduction suggested by the non-linear transverse hall resistance as a function of magnetic field revealed the transfer of electrons from La-doped SSO to BSO. The sheet carrier density on the BSO side was measured to be 5×10$^{12}$ cm$^{-2}$ consistent with the value obtained using a self-consistent solution to one-dimensional Poisson and Schrödinger equations. The role of band offset, interface roughness and threading dislocations in BSO will be discussed with the goal to obtain high mobility oxide heterostructures.

*Work supported by NSF DMR and AFOSR YIP
**T70.00324: Magnetic Structure in Entropy Stabilized Single Crystal Spinel Ferrite Films**

YOGESH SHARMA (Presenter), ALESSANDRO MAZZA, ELIZABETH SKOROPATA, LIAM COLLINS, ZHENG GAI, THOMAS WARD, Oak Ridge National Laboratory —

“Entropy-stabilized oxides” possess large configurational entropy driven by the multi-cation disorder which dominates over the enthalpy of formation. The random distribution of constituent elements into the cation sublattice(s) enhances the configurational entropy. These oxide systems possess new possibilities for generating complex electronic and magnetic states due to the near degeneracies of cation spin-charge-orbital order parameters. Here, we grow single-crystal epitaxial thin films of extremely configurationally disordered spinel ferrites. We find that high entropy spinel oxide (HESO) films of (Mg₀.₂Ni₀.₂Fe₀.₂Co₀.₂Cu₀.₂)Fe₂O₄ grown on various substrates—MgAl₂O₄ (MAO), MgO, and SrTiO₃ (STO)—demonstrate an interesting array of magnetic properties in terms of long-range stripe domains, strain-controlled magnetic anisotropy, unusual element-specific magnetization, and magnetic phase transition well above room temperature. The extreme number of cations and configurational degeneracy is expected to open many new avenues for fundamental physics and applied works.

*This work was supported by the DOE Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division and the Office of Science Early Career Research Program.

**T70.00325: Theoretical study of piezotronic metal–insulator–semiconductor tunnel devices**

XIAOLONG FENG (Presenter), Singapore University of Technology and Design — Piezotronics has been an emerging concept coupling piezoelectric and semiconducting properties with potential applications in sensors, flexible electronics and nanoelectromechanical systems. Piezoelectric field is created under an applied strain, which controls the carrier generation, transport, separation or recombination processes at the interface or junction of the semiconductor devices. Based on the piezotronic theory, we present a 1D model for the metal–insulator–semiconductor (MIS) tunnel diode based on the piezoelectric semiconductor. Analytical solutions of piezoelectric modulated tunneling are described to reveal the piezotronic effect on the MIS tunnel junction. A numerical simulation of the carrier transport properties is provided for demonstrating the piezotronic effect on MIS tunnel devices.

**T70.00326: Rare-earth metal organic frameworks for quantum information applications**

DONNY PEARSON (Presenter), Physics, University of Maryland, College Park, ELIZABETH GOLDSCHMIDT, Army Research Lab, HAQUAN FAN, Physics, University of Maryland, College Park — Rare-earth atoms in solids are excellent candidates for atomic ensemble-based quantum memory due to their long-lived optical and spin lifetimes, high density of emitters, and suitability for photonic integration. In rare-earth doped systems, a major problem implementing long-lived, efficient quantum memory is the inhomogeneous broadening of the energy levels due to the site-to-site variations, which in doped materials is primarily caused by the dopant itself. Crystals that are stoichiometric in the rare-earth atom, i.e. the rare-earth species is part of the chemical formula of the crystal rather than a substitutional dopant for some element, have demonstrated the potential for smaller inhomogeneous line widths due to the lack of doping induced disorder. We investigate the potential of metal organic frameworks to host rare-earth atoms with narrow optical inhomogeneous linewidth as a platform for quantum memory and other related applications. We will present progress towards growing macroscopic single crystals and initial optical measurements of these high-density, rare-earth ensembles.

**T70.00327: Spectroscopy of Erbium-167 doped yttrium orthosilicate for quantum photonic technologies**

MI LEI (Presenter), IOANA CRAICIU, JAKE ROCHMAN, JONATHAN KINDEM, JOHN BARTHOLOMEW, ANDREI FARAON, Caltech — Rare-earth ions in crystals are one of the most promising candidates for quantum memories due to their long optical and spin coherence times. They have been used to realize solid-state quantum memories in bulk crystals and in nanophotonics devices. Erbium is of particular interest because it has an optical transition in the telecom band, which allows integration with silicon photonics and telecommunication compatibility. Recently, erbium-167 doped yttrium orthosilicate has been shown to have good properties for quantum memories. With a nuclear spin of 7/2, erbium-167 has 16 hyperfine levels in the optical ground state manifold, which can be used as shelving levels for spectral holeburning, and to store coherence in the nuclear spin.

We study erbium-167 doped yttrium orthosilicate at dilution refrigerator temperatures and in a magnetic field. We obtain long hyperfine lifetimes approaching 30 minutes, observe good spectral hole burning and characterize the optical coherence properties. These properties point to a very promising material for optical quantum memories.

*We would like to acknowledge funding support from the Air Force Office of Scientific Research.*
Materials that couple electric and magnetic ordering create interesting possibilities for the next generation of data storage technologies. However, there are few of these multiferroic materials that exist at room temperature, and even fewer with strong, coupled polarization and magnetization. One promising avenue to develop these materials is through oxide molecular beam epitaxy, which can generate new combinations of properties through heterostructures and interface phases. Here, we combine the ferroelectric LuFeO$_3$ with the ferrimagnetic CoFe$_2$O$_4$ into a superlattice to develop a material with spontaneous polarization and magnetization above room temperature. To study how these materials are layered at the atomic scale, we use scanning transmission electron microscopy (STEM) combined with x-ray energy dispersive spectroscopy (EDS) and electron energy-loss spectroscopy (EELS). We map the elemental profiles through the film and across the bottom electrode to determine the relation between interdiffusion and growth conditions, which provides critical feedback for further growths.

*Thanks to the NSF for funding under DMR-1539918 as part of the Materials Innovation Platform program.

**T70.00329: Epitaxial Growth of Phosphorus Nanostripe Arrays on Cu(110)**

SHUO SUN (Presenter), JIALIN ZHANG, National University of Singapore, SONGTAO ZHAO, University of Science and Technology of China — Black phosphorus has attracted significant attention as a new emerging two-dimensional (2D) material in recent years. New 2D phosphorus allotropes with various structures have also been predicted by theoretical calculations. It has been theoretically predicted that substrate plays a critical role in stabilizing phosphorus nanoflakes on surface. Here, we report a molecular-beam-epitaxial growth of phosphorus nanostripe arrays on Cu(110) by using black phosphorous as precursor, through the combination of in-situ low temperature scanning tunneling microscopy (STM), low energy electron diffraction, X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations. Atomically resolved STM image and the corresponding DFT simulations reveal that phosphorus atoms are adsorbed on top of the valley copper atoms and arranged periodically to form nanostripe arrays. XPS and Bader charge analysis confirm a significant charge transfer from the Cu(110) substrate to P atoms on top.

**T70.00330: Nitrogen-Vacancy (NV) centers in Nano diamonds: Toward optimization and photo stability**

RAVI KUMAR (Presenter), Advanced Carbon Products and Metrology, CSIR-National physical Laboratory, New Delhi, DILIP KUMAR SINGH, Physics, BIT Mesra, SANJAY R. DHAKATE, Advanced Carbon Products and Metrology, CSIR-National physical Laboratory, New Delhi — Nitrogen-Vacancy (NV) centers in Nano diamonds (NDs) are one of the most promising room temperature atom like system for an array of present and future technological applications. These include bio imaging, nano metrology and quantum information processing (QIP). All of these applications depend upon the optimized concentration of NV centers (NV- ) in NDs and their photo stability over continuous excitation. Both of these factors i.e. optimization of concentration of NV centers and their stable photo-physical behavior are major hurdles for different applications. In the present work, we have optimized the fabrication condition for the efficient creation of NV centers. Interestingly, we have successfully created the uniform concentration of NV centers in NDs by dispersed low energy ion irradiation . While investigating the effect of surface functionalization, it was revealed that different degree of surface oxidation of NDs leads to different photo-stability of NV centers. With the optimized concentration of NV centers, we have observed the single photon emission at room temperature and optical bio imaging. Our findings provide new insight to achieve the optimized as well as photo-stable concentration of NV centers and prepare the platform for wide range of applications of NDs.

**T70.00331: Tin catalyzed-silicon nanowires prepared by solid-liquid-solid mechanism**

KAIGUI ZHU (Presenter), KHAMIS MASOUD, Beihang University — The fabrication of silicon nanowires (SiNWs) catalyzed by low melting metal through solid-liquid-solid (SLS) mechanism makes it very useful in electronic device applications. However, little research has been done in combining SLS mechanism with Sn catalyst deposited as continuous film by magnetron sputtering system to grow SiNWs. The growth of Sn catalyzed-SiNWs through SLS mechanism by thermal annealing technique on a Si <100> substrate was investigated, and initially Sn catalyst was deposited as a continuous film by magnetron sputtering system. Randomly and voluminous SiNWs are observed on the Si substrate after 1000 0C annealing process with a feature that looks like a tree having many numbers of long branches of SiNWs. These confirm the growth of Sn catalyzed-SiNWs through SLS mechanism, with Sn catalyst initially being deposited as a continuous film.
T70.00332: Modeling the Growth of Salt Nano-Wires* CHARLES AY (Presenter), GARY PENNINGTON, Towson University — The purpose of our research has been to successfully model the growth of NaCl nano-wires from a supra-molecular gel. The interest in these wires is the ease of growth and the potential application of integrating them into electrical circuitry. Our model is based off of diffusion driven crystal formation through evaporation. We used two different crystallization constants to represent the overall mass-transfer rate of the process. The first crystallization constant is a reaction constant; this is present during the initial formation of the seed crystals directly below the gels surface. The second constant is the diffusion crystallization constant. The first constant is taken to be at its maximum before it deforms the gel. This is calculated from the salt mass ratio the gel in which the gel is deformed in the initial growth phase. While the second constant is derived from the supporting material. The main two parameters that we are observing are the height of the wires and width of the wires, where we see experimentally a maximum width of 5.64 Angstroms, which is the reported width of a single NaCl crystal lattice.

*The authors acknowledge support from the NSF Grant DMR 1709781 and PAGS Department of Towson University specifically Dr. Pennington and Dr. Kolegani.

T70.00333: Synthesis and characterization of Co-based magnetic nanowires POK LAM TSE (Presenter), University of Southern California — Pure Co, pure Cu and Co/Cu two-segment nanowires with high pore filling rate and uniform sizes were successfully synthesized through the direct electrochemical deposition in Anodic Aluminum Oxide (AAO) membrane. By applying different deposition currents in a single mix bath, nanowires with different materials and different crystal structure were fabricated. The length of the nanowires is several micron and diameter is between 80-100 nm. The pure Co nanowires and the Co segment in the Co/Cu nanowires show hexagonal close packed (hcp) crystal structure. The pure Cu nanowires and the Cu segments in Co/Cu nanowires show face centered cubic (fcc) structure. Magnetic force microscopy (MFM) analysis illustrates the quasi-periodic magnetization modulation along the pure Co wires and the Co segment in Co/Cu two-segment nanowires. A pair of Co/Cu two-segment nanowires partially in contact showed magnetization interactions at the Co segments. The magnetization modulation is explained by the competition between shape anisotropy and magnetocrystalline anisotropy.

T70.00334: Interaction Effects in Open Nanoelectromechanical Systems* BILAL TANATAR (Presenter), Department of Physics, Bilkent University, VALERIU MOLDOVEANU, RADU DRAGOMIR, STEFAN STANCIU, National Institute of Materials Physics — We discuss the transient and steady-state transport properties of nanoelectromechanical systems (NEMS) in the quantum regime. The system consists of quantum wire electrostatically coupled to a nearby nanoresonator (NR). The intertwined dynamics of the open NEMS is described within a generalized master equation which is exact with respect to the electron-vibron coupling. The eigenfunctions of the nanoelectromechanical system are found using configuration-interaction methods. We introduce an improved description of the electron-vibron coupling by taking into account the sample specific single-particle functions. We analyze how the electron-vibron coupling and the Coulomb interaction affect the energy spectrum of the NEMS. This fact causes the removal or the onset of the Coulomb blockade as the distance between the NR and the mesoscopic system is changed. The time-dependent filling of the vibronic states is analyzed as a function of bias.

*This work is supported by TUBITAK, TUBA and CNCS-UEFISCDI.
T70.00335: Topological Insulator Sb$_2$Te$_3$ and Phase Change Material GeTe Nanowires Synthesis and their Electrical Properties Measurements  
POK LAM TSE (Presenter), Materials Science, University of Southern California — Sub-100nm topological insulating(TI) Sb$_2$Te$_3$ nanowires(NWs) and phase change material GeTe nanowires were fabricated by Catalytic Chemical Vaporized Deposition(CVD). The Vapor-Liquid-Solid(VLS) growth mechanism in the fabrication process effectively decreased the growth temperature to around 400°C from around 600-800°C. The stoichiometry ratios of Sb$_2$Te$_3$ NWs(2:3) and GeTe NWs(1:1) had been measured by energy-dispersive X-ray Spectroscopy(EDX) analysis along the NW samples. For the electron spin transports in TI, Magnetic Tunnel Junction contacts at 4K showed a sharp conductance change of non-local magnetoresistance at ±0.5kG, indicates the spin momentum locking effect of topological insulator. P-type conduction property of Sb$_2$Te$_3$ nanowire$^1$ was measured by the field effect transistor(FET) measurement at 68K with back gate voltage up to 100V across 300nm SiO$_2$ dielectric layer. Phase change property of GeTe nanowire was tested for crystalline and amorphous transition by applying 3V to 5V voltage few hundred ns width voltage pulses, the crystalline form had a resistance at about few kilo-ohm and the amorphous form was at about 30k ohm to 1M ohm range. Preliminary results showed 10 to 20 cycles of switching with no degradation.


T70.00336: The observability of Quantum Pinch Effect in the magnetized semiconducting Quantum Wires  
MANVIR KUSHWAHA (Presenter), Rice University — We investigate a two-component, cylindrical, quasi-one-dimensional quantum plasma subjected to a \( \Omega \)-radial confining harmonic potential and an applied magnetic field in the symmetric gauge. It is demonstrated that such a system as can be realized in semiconducting quantum wires offers an excellent medium for observing the quantum pinch effect at low temperatures. An exact analytical solution of the problem allows us to make significant observations: surprisingly, in contrast to the classical pinch effect, the particle density as well as the current density display a \( \Omega \)-determinable maximum before attaining a minimum at the surface of the quantum wire. The effect will persist as long as the equilibrium pair density is sustained. Therefore, the technological promise that emerges is the route to the precise electronic devices that will control the particle beams at the nanoscale.

T70.00337: Collective excitations in quantum wires made up of vertically stacked quantum dots  
MANVIR KUSHWAHA (Presenter), Rice University — We report on the theoretical investigation of the elementary electronic excitations in a quantum wires made up of vertically stacked self-assembled InAs/GaAs quantum dots. The length scales (of a few nanometers) involved in the experimental setups prompt us to consider an infinitely periodic system of two-dimensionally confined (InAs) quantum dot layers separated by GaAs spacers. Since the wells and barriers are formed from two different materials, we employ the Bastard's boundary conditions in order to determine the eigenfunctions along the z direction. We compute and discuss the behavior of the single-particle and collective excitations and finally size up the importance of studying the inverse dielectric function in relation with the quantum transport phenomena. It is remarkable to notice how the variation in the barrier- and well-widths can allow us to tailor the excitation spectrum in the desired energy range. Given the advantage of the vertically stacked quantum dots over the planar ones and the foreseen applications in the single-electron devices and in the quantum computation, it is quite interesting and important to explore the electronic, optical, and transport phenomena in such systems.

T70.00338: Single-Molecule Super-Resolution Fluorescence Lifetime Microscopy  
ZACHARY HALLENBECK (Presenter), NATHAN KIMMITT, ESTHER A WERTZ, Rensselaer Polytechnic Institute — The environment of an emitter has a remarkable impact on its emission properties, and on its lifetime in particular. Emitters coupled with plasmonic nanoparticles show enhanced emission rates, dependent on their proximity and orientation with respect to the nanoparticles, and on the overlap in wavelength between emission and plasmon resonance. We propose a method that combines fluorescence lifetime imaging microscopy with single-molecule super-resolution microscopy to study these properties with spatial resolution below the diffraction limit and picosecond time domain resolution. In order to study single molecule emission in these environments, a nanoscale emitter must be immobilized long enough to confocally scan over its diffraction limited emission. This challenge will be overcome using fast scanning speeds and careful dye deposition. Combining single-molecule super-resolution microscopy with fluorescence lifetime imaging techniques allows for a new level of precision and isolation that avoids the loss of information associated with ensemble averaging. Our study will provide new insight into the physics of plasmonic environments which will be essential to the development of plasmonic technology in growing fields like biomedicine, nanoscale imaging, and quantum information.
All-inorganic halide perovskites at an ambient atmosphere. We reported the conversion from three-dimensional CsPbBr3 nanocrystals has until now, been too complex. Our newly developed saponification approach was employed to synthesize applications in optoelectronic devices because of their excellent photophysical properties, however, the synthesis of those nanocrystals has until now, been too complex. Our newly developed saponification approach was employed to synthesize all-inorganic halide perovskites at an ambient atmosphere. We reported the conversion from three-dimensional CsPbBr3 to lead depleted zero-dimensional Cs4PbBr6 nanocrystals by altering the amount of Cs-oleate precursor at a low-temperature synthesis so that the transformation remarkably changes the properties of the nanocrystals. The XRD spectra, TEM images, absorption and photoluminescence spectra have been taken for the systematic study of properties of CsPbBr3 and Cs4PbBr6 nanocrystals. The CsPbBr3 emitting a strong blue emission (460 nm) and is shifted to the green region (528 nm) for Cs4PbBr6, which demonstrates the intrinsic luminescence nature of the Cs4PbBr6 nanocrystals. In addition, the lead depleted Cs4PbBr6 structure is of great interest that minimizes the chemical instability, and particularly, toxicity issues. These exciting properties offer them an advantage to be used in optoelectronic devices.

*The University of Tulsa faculty start-up fund

**T70.00340: Hydrostatic pressure effect on the intraband absorption coefficient in a core-shell spherical GaAs/AlxGa1-xAs quantum dot**

K. A. RODRÍGUEZ-MAGDALENO (Presenter), JUAN CARLOS MARTINEZ OROZCO, Unidad Académica de Física, Universidad Autónoma de Zacatecas — In this work we present the intraband absorption coefficient calculation in a core-shell spherical GaAs/AlxGa1-xAs quantum dot. The quantum dot is composed of GaAs and surrounded by three shells of AlGaAs and GaAs, respectively. The electronic structure is calculated within the effective mass approximation and considered the hydrostatic pressure effect using a numerically stable transfer matrix method. The intraband absorption coefficient is computed by means of the Fermi’s Golden rules under the dipolar matrix approximation. We reported the absorption coefficient between the 1s and 1p states as a function of the internal and external radius size, Aluminium concentration and the hydrostatic pressure. The results show that the absorption coefficient undergoes a change in the magnitude as well as in the resonance peak location. These results can be used to improve the absorption tuning and could be useful for enhance the solar devices.

*K. A. Rodriguez-Magdaleno acknowledge to CONACyT México for is postdoctoral position at the Universidad Autónoma de Zacatecas.

**T70.00341: Color Tunable All-Inorganic Mixed Halide Perovskites for Optoelectronic Applications**

SAROJ THAPA (Presenter), GOPI ADHIKARI, HONGYANG ZHU, PEIFEN ZHU, University of Tulsa — All-inorganic lead halide perovskites have attracted tremendous attention in recent years due to their superior optical properties such as tunable bandgap, narrow line-width emission, and high photoluminescence quantum yield (PLQY). Herein, CsPb(Br1-xIx)3 [0 x<1] perovskite nanocrystals with tunable emission (464-667 nm) and narrow line-width emission (23-47 nm) were synthesized at an ambient atmosphere employing a newly developed saponification technique in our laboratory. The inert gas-glovebox free protocol adopted in this technique offers a simplicity in the preparation of high-quality perovskite nanocrystals. The application of these nanocrystals in white light-emitting diodes (LEDs) leads to tunable correlated color temperature (CCT) with a high color rendering index (CRI).

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**T70.00342: Auto-Desiccating Synthesis of Lead Halide Perovskite Nanocrystals via a Saponification Process**

PRESTON VARGAS (Presenter), GOPI ADHIKARI, HONGYANG ZHU, PEIFEN ZHU, University of Tulsa — In this work, a new process is developed to synthesize lead halide perovskite nanocrystals with the goal of reducing the manufacture cost. By using a saponification reaction to create the cesium precursor solution, synthesis can be achieved at room temperature and without the use of a vacuum oven. Blue-green tunable emission is obtained by varying the synthesis temperature. The crystal phase of the nanocrystals exhibit an increasingly directionally aligned orthorhombic phase with increasing temperature. Also, the saponification process uses low-cost compounds to produce the cesium precursor. Furthermore, the moisture instability of halide perovskite nanocrystals is well managed by this process because the highly hygroscopic by-products in this process auto-desiccate the reactants. Therefore, the nanocrystals can be efficaciously synthesized in an air atmosphere without interference from local humidity. This provides an accessible and low-cost pathway for synthesizing this material outside of controlled laboratory conditions.

*Acknowledgement: The University of Tulsa faculty start-up fund, University of Tulsa Faculty Development Summer Fellowship, and University of Tulsa Student Research Grant.
Nonlinear optical properties of double asymmetric Al_xGa_{1-x}N/GaN quantum wells considering strain effects

FLAVIO MANUEL NAVA MALDONADO (Presenter), JOSE GUADALUPE ROJAS BRISEÑO, Universidad Autónoma de Física, Universidad Autónoma de Zacatecas, MIGUEL EDUARDO MORA RAMOS, Centro de investigación en Ciencias, Universidad Autónoma de Morelos, JUAN CARLOS MARTINEZ OROZCO, Universidad Autónoma de Física, Universidad Autónoma de Zacatecas — A theoretical study has been carried out to investigate the optical absorption coefficient and the relative change in the refraction index in asymmetric double zinc-blende Al_xGa_{1-x}N/GaN quantum wells. Highlighting the effect of lattice strain on these properties.

The electronic energy structure is determined in the scheme of the effective mass and parabolic band approximations while the strain effects are incorporated with the use of the model solid theory. Optical coefficients are calculated through the expressions obtained within the compact matrix density formulation. In general we conclude that the strain effects are of paramount importance for the cubic phase of the considered heterostructure, because this contribution considerably affect the band offset of the system and, despite the ground, and the first excited, state are not modified significantly, the studied optical properties becomes slightly affected, particularly for narrow well widths.

Principal transport properties of α-T3 model in the presence of external irradiation.

DIPENDRA DAHAL (Presenter), CUNY Graduate Center, GODFREY GUMBS, Physics and Astronomy, Hunter college, CUNY, ANDRII IUROV, DANHONG HUANG, Physics, University of New Mexico — Using a simplified s-wave approximation approach for the conventional Boltzmann conductivity equation, we have obtained the transport properties of pseudospin-1 electrons in the α-T3 lattice irradiated by external light with linear or circular polarization. Basic transport properties of such dressed states significantly depend on their low-energy band structure and the corresponding wave functions. These electronic states are mainly determined by the polarization of the incident dressing field. For instance, circularly-polarized radiation leads to opening an energy gap, which could substantially suppress the conductivity. Electron transport also shows dependence on the coupling strength parameter α of an α-T3 lattice, which has also been thoroughly investigated.

Effective Plasma Frequency in Graphene-Based Photonic Crystals

IVAN FUENTECILLA-CARCAMO (Presenter), FELIPE RAMOS-MENDIETA, Universidad de Sonora, MARTHA PALOMINO-OVANDO, ALEJANDRO HERNÁNDEZ-López, Facultad de Ciencias Físico-Matemáticas, Benemérita Universidad Autónoma de Puebla — Photonic crystals, based on graphene-dielectric multilayers, have been shown to exhibit tunable Bragg gap opening due to Fermi level tunability at each graphene layer. At low Frequencies (THz regime), a metallic-like gap is also observed with a doping dependent cutoff frequency which marks the beginning of the first transmission region. In this work, we numerically analyze this cutoff frequency as a function of Fermi level, interlayer distance and immersing dielectric constant for an equally doped graphene stack immersed in homogeneous dielectric. We give an analytical approach to deduce a Drude-like effective index for a graphene-dielectric unit cell which in turn, allows to obtain an analytical formula for this cutoff frequency. We determine parameter ranges where our analytical model fits better with the data obtained by numerical computation.

IFC aknowledge Financial support from CONACYT M'èxico.

Transverse Electric Mode Excitation in Graphene-Based Multilayers Through Attenuated Total Reflection Technique

FELIPE RAMOS-MENDIETA, IVAN FUENTECILLA-CARCAMO (Presenter), Universidad de Sonora, MARTHA PALOMINO-OVANDO, ALEJANDRO HERNÁNDEZ-López, Facultad de Ciencias Físico-Matemáticas, Benemérita Universidad Autónoma de Puebla — Graphene monolayer can support transverse electric plasmonic modes where in-plane current oscillations are present and parallel to electric field vector. These modes, as recently shown, can be excited by Attenuated Total Reflection (ATR) Technique where mode coupling is obtained above a cutoff distance between prism and graphene. In this work, we extend this analysis by considering a graphene (equally doped)/dielectric stack immersed in homogeneous dielectric. We show that Surface Plasmonic (SP) modes are excited through this technique showing smaller cutoff distances than those reported for monolayer graphene. We found that cutoff distance, \( d_c \), decreases as the number of stacked layers grows following the rule \( d_c = \alpha / (2n) \), where \( \alpha \) is the decaying length and \( n \) is the number of graphene layers. We prove surface plasmon excitation, corresponding to minima in the ATR, by numerical calculation of dispersion relations of SPs for two, three and four graphene layers in the stacking.

IFC aknowledge financial support from CONACyT M'èxico.
In this study, we examine the interaction of Dirac fermions and bosons, we investigated the electronic and magnetic properties of rare-earth-metal intercalated in bilayer graphene. Using density functional theory, we determined the electronic structure, density of states, magnetic moment, and total energy for lanthanum (La), gadolinium (Gd), holmium (Ho), and erbium (Er) in a honeycomb configuration. An analysis of the total energy and magnetic structure, shows that the Gd and Ho substitutions obtain a FM ground state, while the La and Er substitutions have an AFM ground state, which means that Gd and Ho layered sandwiches may have possible Dirac boson interactions. The electronic structure provides information on Dirac fermionic interactions. We find that the presence of rare-earth materials shifts the Dirac cone in the electronic structure into the valence band, and while Lanthanum does not provide any f-orbital interactions, Gd, Ho, and Er have strong f-orbital characteristics. However, this seems to be at the expense of the Dirac fermionic cone.

*Institute for Materials Science at Los Alamos National Laboratory

**T70.00348: Ordered Particle Arrays via a Langmuir Transfer Process: Large Area Access to Any Two-Dimensional Bravais Lattice**

MIRIAM MAUER, CHRISTIAN STELLING, BERND KOPERA, FABIAN NUTZ, Department of Chemistry, University of Bayreuth, 95447 Bayreuth, Germany, MATTHIAS KARG, Physical Chemistry I, Heinrich-Heine-University, 40204 Düsseldorf, Germany, MARKUS RETSCH (Presenter), Department of Chemistry, University of Bayreuth, 95447 Bayreuth, Germany, STEPHAN FÖRSTER, JCSN-1/ICS-1, Forschungszentrum Jülich, 52425 Jülich, Germany — The preparation of particle arrays on solid substrates is an essential step for the fabrication of functional surfaces and thin-film devices with applications in lithography, optics, photonics, high-density data storage and as adhesive/non-adhesive surfaces. Colloidal self-assembly represents an attractive and scalable route towards hexagonally close-packed particle arrays. To significantly broaden the structural variability, the fabrication of non-close-packed and also non-hexagonal particle arrays are required. Here, we demonstrate how to fabricate non-close-packed particle arrays with symmetries of all possible Bravais lattices in a simple solution-based process. Our process starts with readily self-assembled, hexagonally close-packed monolayers, which are immobilized on an air/water interface. Upon transfer onto the target substrate, stretching along a specific crystallographic direction occurs. This yields non-close-packed structures with non-hexagonal symmetry. We demonstrate how to control the stretching factor by interfacial modification of the target substrate to access all possible Bravais lattices.

*This work was funded by the German Research Foundation (DFG) by the SFB840.

**T70.00349: High energy particles detection through high mobility GaAs/Al0.3Ga0.7As QW Hall bar sensor**

MEHDI PAKMEHR (Presenter), MUHAMMAD ASTERAKI, Physics, Shiraz University — GaAs as a well-known semiconductor has been used widely for detection and different types of sensor fabrication for diverse purposes within last decades. We used high carrier density GaAs/Al0.3Ga0.7As QW with relatively high mobility with an ultimate goal of being used to fabricate high energy particles detector. The carrier density of our samples are relatively high \( n_c = 6.24 \times 10^{11} \text{ cm}^{-2} \) with hall mobility of \( 1.5 \times 10^5 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \). The large Hall bars samples were fabricated form modulation doped MBE grown wafer used for our experimentations. The sample sits at the bottom of probe stick within VTI at Liquid nitrogen temperature (T=77 K) while chopped high energy particle beams (positrons) from Na22 source hit it. Through common lock-in technique we detected signal due to interaction of beam particles with 2DEGs confined within QW of our samples. We plan to present our findings through a poster at March 2019 APS meeting being held at Boston

*M. Pakmehr would like to acknowledge Shiraz University office of Dean for supporting our research work.

**T70.00350: SURFACES, INTERFACES, AND THIN FILMS**

**T70.00351: The coordination of Metal-Salen to diatomic molecules**

DAN LIU (Presenter), Peking University — Salen is a Schiff base complex which is condensed from salicylaldehyde and ethylenediamine. The chemical, electronic and magnetic properties of metal-salen could be altered by adjusting the central metals. These metal-salen register wide applications in materials science, heterogeneous catalysis, geology, biology and so on due to the diversity of their properties. Thanks to the invention of scanning tunneling microscopy (STM) in 1980s, people are able to observe the single atoms and molecules. Up to date, the morphological and electronic properties of metal-salen have been systematically studied in surface science. However, their catalytic performances have not been fully explored. Therefore, this proposal focuses on the coordination of several metal-salen complexes to diatomic molecules (such as CO) as well as analyses of its morphological and electronic properties with STM and surface science techniques. Specifically, Metal-Salen as a surface model catalyst will be extensively explored to uncover its catalytic properties towards small molecules.
In this work, we investigate the icing and deicing characteristics of a sessile droplet on an Al-based superhydrophobic surface and aim to understand the surface and interface phenomena occurred during icing and deicing. During icing, ice front always propagates from the bottom of the droplet, finally forming a singular tip at the droplet top, while the nucleation position is various under different conditions. When the surround air is very humid, the nucleation tends to appear at the solid-liquid interface of the droplet; otherwise, the nucleation appears at the liquid-air interface of the droplet. During deicing, melting also first occurs at the bottom of the freezing droplet, but the ice-water interface is more flexible compared with that during icing with obvious swaying and rotating behavior of the unmelted ice cover. The possible Marangoni effect occurred during deicing may be the reason for these behavior.

T70.00353: Ionic effectiveness in the self-assembly and crystallization of polymer grafted Au nanoparticles at the gas-liquid interface* WENJIE WANG, Ames Laboratory, Iowa State University, WEI BU, NSF's ChemMatCARS, University of Chicago, DAVID VAKNIN (Presenter), Ames Laboratory, Iowa State University — Salts in solutions promote aqueous surface self-assembly of gold nanoparticles (AuNPs) that are grafted with non-ionic and water soluble polymers such as poly(ethylene glycol) (PEG) or poly(N-isopropylacrylamide) (PNIPAM). Using AuNPs functionalized with PEG (PEG-AuNPs) as a model system, previous studies have demonstrated that ions can be ranked in their effectiveness to promote the two-dimensional superlattice formation of PEG-AuNPs. Similar ranking for the aqueous biphasic system (ABS) of PEG in salt solutions. However, we show that ionic species that do not readily induce ABS at ambient temperatures can lead to surface crystallization of PEG-AuNPs. Synchrotron x-ray reflectivity and grazing incidence small angle x-ray scattering methods are used to determine the structures of the surface assembly for various ionic species. Here, we report on grazing incidence x-ray fluorescence spectroscopic measurements that in conjunction with Compton and Thomson scattering reveal ion-specific distributions at the surface and in the bulk in the presence of PEG-AuNPs suspensions and compare them to salt solutions without NPs. We find that the ion distributions of CsCl and NaI correlate with the quality of surface PEG-AUNPs crystallization.

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T70.00354: First-Principles Prediction of Temperature Dependence of Surface Wettability and Interfacial Tension in Multiphase Systems QIAOYU GE, JIN-YOU LU, AIKIFA RAZA, TIEJUN ZHANG (Presenter), Mechanical Engineering Department, Masdar Institute, Khalifa University — Temperature dependences of solid surface wettability and liquid-liquid interfacial tension play important roles in many applications involving interfaces or thin films working at elevated temperature, such as subsurface energy production and organic solar cell fabrication. In this work, a first-principles approach based on ab initio molecular dynamics is proposed to reveal the insightful effect of temperature on solid surface wettability and liquid-liquid interfacial tension. Temperature-dependent adhesion and cohesion energies are calculated from ab initio molecular dynamics and used to evaluate the temperature dependency of interfacial properties. A system of calcite-water-decane is simulated to predict the contact angle of water on calcite surface in presence of decane, as well as water-decane interfacial tension at different temperatures. The predicted reduction rates of contact angle and interfacial tension with temperature agree well with our experimental validation. The first-principles nature of this method makes the prediction accurate and intrinsic, meanwhile it provides physical insight into experimental multiphase behaviors and prediction of new wetting phenomena.
**T70.00355: Resistive switching in La$_{0.3}$Ca$_{0.7}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-\delta}$ devices**

JOHN BETANCOURT (Presenter), Physics, Center of excellence on novel materials, JOHN E ORDONEZ, MARIA GOMEZ, CARLOS WILLIAM SANCHEZ, WILSON LOPERA, KATHERINE GROSS, Physics, Thin Films group, JUAN RAMIREZ, Physics, Universidad de los Andes — We have deposited La$_{0.3}$Ca$_{0.7}$MnO$_3$ (LCMO) /YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) on SrTiO$_3$ (STO) (100) oriented substrate by sputtering technique at pure oxygen atmosphere at high pressure (4 mbar) to study the resistive switching response. We grew systematically the insulator LCMO film with different thicknesses ($t_{LCMO} = 60, 30$ and $15$ nm) on YBCO layer ($t_{YBCO} = 60$ nm), which acts as bottom electrode. For the electric characterization, we deposited Ag circles on top of the heterostructures as top electrode. From XRD we found that the LCMO and YBCO layers grew textured aligned with substrate. The electrical properties with temperature measurements indicated the LCMO insulator behavior and the YBCO conduction at room temperature. I versus V curves at room temperature showed hysteric behavior and the presence of two resistive states, whose electrical transport mechanism could be associated with space charge limited conduction (SCLC). The performed resistance switching with applied voltage tests indicate a dependence of the high resistance state (HRS)/ low resistance state (LRS) ratio with LCMO thicknesses.

*This work has been supported by intern research projects CI 71109, CI 71136 and Center of Excellence on Novel Materials-CENM at Universidad Del Valle.

**T70.00356: Realizing Narrow Band Thermal Emitters in the Mid-Infrared by Utilizing Polaritonic Metasurfaces.**

DIEGO GARCIA (Presenter), Department of Physics and Astronomy, University of Texas at Rio Grande Valley — The purpose of this study is to show evidence that surface phonon polaritonic(SPhP) metasurfaces can produce a well-defined thermal emission signal in the optical phonon band of Silicon Carbide to realize narrow band emitters in the mid-IR wavelengths. Preliminary data and results have demonstrated strong localized SPhP resonances of these devices, so there is a high possibility that a well-defined emission signal will be obtained if we apply Kirchhoff’s Law of Heat Radiation. To observe the thermal radiation from the polaritonic metasurface patterns, an optical setup was built in which the beam path of the visible light and thermal radiation would be equivalent. This was done primarily for the precise alignment of the metasurface and to maximize the collection of thermal radiation. The device was heated conventionally and data analysis was attained using a FTIR Spectrometer. Initial results showed an emission spectrum with broad resonances from 820 cm$^{-1}$ to 960 cm$^{-1}$ and it was determined the resonances were from multiple patterns on the metasurface. Currently, we have improved the setup to collect emissions from single patterns.

*Research was supported by the NSF-REU program at the University of Texas Rio Grande Valley, and the University of Texas system STARs award.

**T70.00357: Set of Techniques for High-Q Noble Metals Deposition: from Continuous Ultrathin to Single-crystalline Films**

ALEKSANDR BABURIN (Presenter), AIDAR R. GABIDULLIN, DMITRIY O. MOSKALEV, EVGENIY LOTKOV, MICHAEL ANDRONIC, ANTON I. IVANOV, REC FMN, Bauman Moscow State Technical University, ILYA A. RYZHIKOV, ITAE RAS, ILYA A. RODIONOV, REC FMN, Bauman Moscow State Technical University — Losses are the most serious challenges, which impede high-Q plasmonic devices rapid development. There are numerous types of plasmonic devices with conflicting requirements for the films. One can conclude that most devices require continuous silver and gold films with ultra-low losses, extremely low roughness, single-crystalline structure and maximum possible surface plasmon polarization wave (SPP) propagation length on various substrates including amorphous.

We present a full row of techniques as contribution to material platform. Among them single-crystalline ultra low loss (SCULL) sub-50 nm single-crystalline silver films, which provide SPP propagation length 200 μm (at wavelength 780 nm) [1] and allow ultra-bright single photon sources fabrication [2]. For amorphous substrates, we proposed polycrystalline big grain film deposition with high aspect ratios between grain size and film thickness that ensured high-Q light source fabrication [3]. Finally, for ultrathin films, less than 15 nm thick, we developed technologies to reduce percolation threshold of gold and silver without using wetting layers.

References
Resistive switch on Iron oxides thin films* RAFAEL SILVA GONÇALVES, ROMUALDO SANTOS SILVA JUNIOR, PETRUCIO BARROZO DA SILVA (Presenter), Physics Department, Federal University of Sergipe — The resistive switch properties on binary oxides has largely studied due to the non-volatile properties and its potential to be used to develop data storage devices. The resistive switch has been attributed to the percolation of a conductor pathway across the insulator matrix. However, the properties of the growth of the conductor pathways and the speed of the switch between the different resistive states on iron oxide has not yet been reported. In this work, we describe the mechanism of the resistive switch on the thin films of iron oxide growth by sputtering. The dynamics of growth of the conductor pathways in iron oxide and the speed of switch also will be reported.

*Thanks to Brazilian fund agencies CNPq and CAPES.

Nanoscale Imaging Studies of Cobaltite Thin Films Using X-Ray Nanodiffraction* GEOFFERY IAN RIPPY (Presenter), LACEY L TRINH, ALEXANDER MICHAEL KANE, ALEKSEY IONIN, MICHAEL STEVEN LEE, RAJESH V CHOPDEKAR, University of California, Davis, DUSTIN GILBERT, ALEXANDER GRUTTER, National Institute of Standards and Technology, PEYTON MURRAY, University of California, Davis, MARTIN HOLT, ZHONGHOU CAI, Argonne National Laboratory, KAI LIU, YAYOI TAKAMURA, ROOPALI KUKREJA, University of California, Davis — The perovskite (ABO3) and closely related brownmillerite (ABO2.5) phase of cobaltites possess a wide range of functional properties, which makes them promising candidates for solid oxide fuel cells, ionically-gated devices, and magneto-ionic devices. However, the role played by nanoscale morphology, i.e. phase separation and defects in these oxide thin films and heterostructures, remains unknown. This poster presents nanoscale imaging studies of emergent structural phases and their morphology in cobaltite heterostructures using x-ray nano-diffraction. Gd/La0.67Sr0.33CoO3 heterostructures were ionically and stoichiometrically controlled via the thickness of the Gd oxygen-gettering layers. Our measurements, using the hard x-ray nanoprobe at the Advanced Photon Source, show lateral and transverse nanoscale separation of the perovskite and brownmillerite phases. These nanoscale heterogeneities were characterized and strain mapped in real space with a spatial resolution of 25 nm. Our studies provide insights into the nanoscale morphology which can be utilized to tune the macroscopic functional properties of cobaltite heterostructures.

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Steering on the high-temperature oxidation of Ru(0001) HAORAN CHEN (Presenter), Peking University — Ruthenium oxide is the active phase and plays a significant role in many catalytic reactions. By virtue of ultrahigh vacuum low temperature scanning tunneling microscopy, it has been observed that Ru(0001) could be oxidized to several novel kinds of ruthenium oxide films at different temperatures. High-resolution STM images showed that these films resulted from the novel structures formed at surface. Interestingly, these oxidation structures were inter-changeable upon reduction in hydrogen at different temperatures. After series of studies, the structural evolutions of Ru(0001) surface caused by high-temperature oxidation and reduction were revealed.

Chemical Reactivity at the Co/CuO interface* ANIL CHOURASIA (Presenter), Texas A&M University - Commerce — The chemical reactivity at the Co/CuO interface has been investigated using the technique of x-ray photoelectron spectroscopy. Thin films of hafnium have been deposited on CuO substrates at room temperature by the e-beam method. The Oxford Applied Research EGN4 was used for this purpose. The spectral data in the hafnium 4f core level and copper 2p core level were investigated by XPS. The copper oxide was observed to get reduced to elemental copper while cobalt was observed to get oxidized to CoO. The thickness of the cobalt overlayer resulting in no chemical reactivity has been determined. The investigation was also performed at substrate temperatures of 100, 200, 300, 400, 500, and 600°C. The diffusion of copper through the overlayer was observed. The interface consists of a mixture of elemental cobalt, CoO and elemental copper. The amount of these materials is governed by the processing conditions. The results of the investigation will be presented.

*Texas A&M University-Commerce
**T70.00362: Modeling of molecular stripe formation on insulating surfaces**  
CHRISTOPH SCHIEL (Presenter), University of Osnabrück, MAXIMILIAN VOGLTAND, ANGELIKA KÜHNLE, University of Bielefeld, PHILIPP MAASS, University of Osnabrück — We discuss theoretical approaches to model molecular stripe formation on dielectric surfaces as observed for 3-hydroxybenzoic acid (3-HBA) and 3-aminobenzoic acid (3-ABA) on calcite (104). For the self-assembly of the 3-HBA and 3-ABA molecules it is argued that adsorption-induced dipolar interactions cause an ordering towards a regular spacing between the molecular stripes. Measured stripe distance distributions show a good agreement with analytical results for a simplified one-dimensional model [1]. In this model scaling relations for the distance distribution are predicted that can be tested experimentally. In a refined approach, we further study the stripe formation on a two-dimensional lattice by an anisotropic Ising model with dipole-dipole interactions. For this model, stripe length and distance distributions as well as spatial correlation properties are determined by Monte Carlo simulations and compared with experimental data.


**T70.00363: The Effect of Au Nanoparticles on the Photovoltaic Conversion Efficiency in CdTe/CdS Thin Films**

YUNIS YILMAZ (Presenter), OLIVIA RODGERS, ANTHONY J VISCOVICH, RALPH NUNEZ, MEHMET ALPER SAHINER, Seton Hall University — In our previous studies, we've worked on the effects silver nanoparticles have on the efficiency of CdS/CdTe thin film solar cells. In short, the addition of the nanoparticles in the np affects junction light scattering in a way that have a positive effect on efficiency of photovoltaic conversion. Currently, we’re testing gold nanoparticles on the same solar cells and plan on comparing the effects of different deposition times, particle sizes, and how they compare to the efficiencies of that of silver. The deposition method used to create these thin film solar cells is Pulsed Laser Deposition (PLD). The laser shoots at the target material we want to deposit (CdS/Au/CdTe) turning it into a plume of plasma that deposits onto a slide of ITO (indium tin oxide) coated glass. Varying how long the laser shoots at the gold changes the amount of gold deposited. The more gold in the np junction, the more light scattering happens, increasing the efficiency of the solar cell. However, the efficiency cuts off with enough gold added. The Au embedded CdS/CdTe thin film solar cells were characterized by XRD, AFM, SEM/EDX and the photovoltaic conversion efficiency were determined by Ketihley Sourcemeter setup.

*TThis work is supported by NSF Award #:DMI-0420952 and TUBITAK-2221Award and NJSGC (NASA)

**T70.00364: Electrical and Physical Properties of Pulsed Laser Deposited Thin Films of YSZ**

MATTHEW MELFI (Presenter), WILLIAM E COCKERELL, ERICA WILEY, KELLEN MURPHY, MEHMET ALPER SAHINER, Seton Hall University — Solid Oxide Fuel Cells, SOFC’s, are devices that convert chemical energy from fuel into electricity from a series of electrochemical reactions. These fuels can be H₂, CO, O₂, etc. with a high efficiency of conversion. Comparing SOFC’s to coal power plants, the SOFC’s produce a higher electrical conversion efficiency. However, SOFC’s high temperatures create a lower ionic conductivity of the electrolytes. When decreasing the temperature, the ohmic resistance is increased hurting the performance. The method we are trying to take is decrease the ohmic resistance as a thin-film. An Yttria Stabilized Zirconia, YSZ, layer is produced from the fine dimple grain structure allowing high flow of oxygen ion mobility. The goal of our research is to optimize Pulsed Laser Deposition and determine the synthesis conditions which lead to minimum ohmic resistance in these films. We will also use different substrates and monitor the effect of the choice of the substrate on the YSZ thin-film properties. These thin-films will be characterized through electrical measurements such as 4 pt. probe resistivity measurements, Hall Effect, and structural and compositional characterization such as AFM, SEM, and EDX.

*New Jersey Space Grant Consortium- NASA fellowship
NSF-DMR 0420952, TUBITAK-2221
T70.00365: Structural stability and electronic levels of carbon-associated defects in SiO₂: First-principles study*  
YU-ICHIRO MATSUSHITA (Presenter), Tokyo Institute of Technology, ATSUSHI OSHIYAMA, Nagoya University — Silicon Carbide (SiC) attracts much attention as the power semiconductor materials due to its superior material properties such as wide-band gap and high breakdown electric field [1]. In spite of the great materials properties, SiC has a big issue to be solved. That is the low electron mobility of SiC-MOS(Metal-oxide semiconductor) devices caused by the high density of interface traps (Dit). In particular, carbon-associated defects staying around the SiC/SiO₂ interface are the strong candidate for the Dit. In this study, we have clarified the structural stability and electronic levels of C-associated defects near the SiC/SiO₂ interface on the basis of the density-functional theory (DFT). Consequently, we have found that near the SiC/SiO₂ interfaces the carbon clustering is likely and some particular carbon defects cause defect levels near the conduction-band edge of SiC rendering them a strong candidate of the mobility killer.


*We acknowledge the support from JSPS Grant-in-Aid for Scientific Research (A) (Grant No. 18H03873) and Grant-in-Aid for Young Scientists(B) (Grant No. 16K18075).

T70.00366: Surface Morphology Studies of Strained and Oxygen Deficient Epitaxial Thin films of Strontium Titanate and Calcium Manganese Oxide*  
ANTON WIGGINS (Presenter), AZRIEL WEINREB, FRANCIS WALZ, JOSEPH CARTELLI, DAVID HOUSTON, BRIDGET M LAWSON, JESSICA L SIZEMORE, RAJESWARI M KOLAGANI, GARY PENNINGTON, DAVID SCHAEFER, Towson University — Calcium Manganese Oxide (CMO) and Strontium Titanate (STO) are technologically important materials for applications. Our recent work on epitaxial thin films of CMO have shown that films with a tensile lattice mismatch strain exhibit structural and electrical properties that indicate oxygen deficiency. Our Atomic Force Microscopy studies of CMO thin films reveal time dependent surface morphological changes accompanying oxygenation and de-oxygenation of the CMO films. AFM images indicate possible ordering of oxygen vacancies on the surface. Currently we are extending these studies to epitaxial thin films of STO to investigate strain-oxygen stoichiometry coupling. We will report the results of our systematic studies of the evolution of surface morphology with changes in the strain state and oxygen stoichiometry

*We acknowledge support from the NSF grant DMR 1709781 and support from the Fisher General Endowment Grant from the Jess and Mildred Fischer College of Science and Mathematics at Towson University.

T70.00367: Structural characterization of BaSnO₃ thin films via x-ray scattering  
CLAUDIA LAU (Presenter), Yale Univ, YOUJUNG KIM, KOOKRIN CHAR, Seoul National University, CHARLES H AHN, FREDERICK J WALKER, Yale Univ — The alkaline earth stannate BaSnO₃ is a semiconductor with high carrier mobility at room-temperature when doped with La³⁺. BaSnO₃ can be easily integrated with other perovskites for use in oxide electronic devices such as field effect transistors and sensors. We study the crystalline structure of BaSnO₃ thin films grown on SrTiO₃ substrates by pulsed laser deposition and molecular beam epitaxy via a variety of x-ray scattering techniques. With high intensity synchrotron scattering, we measure crystal truncation rods. Analysis of these rods yields information on structural distortions at the thin film surface and interface. We also measure rocking curves of BaSnO₃ fundamental Bragg peaks for H+K+L=even and odd, where the intensity of the odd peaks are particularly sensitive to minute structural changes in the BaSnO₃ film. These measurements have high accuracy, with a coefficient of variation within 5 percent for symmetrically identical peaks in the four quadrants of reciprocal space. We fit the integrated intensity of these fundamental even and odd peaks to a kinematic model of x-ray diffraction and determine parameters, including the Debye-Waller factor and the stoichiometry.

T70.00368: Computational study of the adsorption of bi-metallic clusters*  
NUSAIBA ZAMAN (Presenter), KARIMA LASRI, ABDELKADER KARA, University of Central Florida — It was shown that small silver clusters can control the rate of LiO₂ formation in Li-O₂ batteries. The gap near the fermi energy was shown to control the oxygen reduction, an important reaction for LiO₂ formation. Controlling the gap would ultimately control the rate of LiO₂ formation. One can vary the size of the cluster to control the gap, however, this “knob” provides limited variance. Alloynig, in combination with size variation offer a much wider control of the LiO₂ formation. Here, we investigate the effect of Pd₃M₂ (where M varies from Ag, Au, Co, Cu, Mn, Ni, Pt, and Ru) clusters on the rate of O₂ reduction at the hydroxylated alumina surface. Using DFT, we calculated the binding energies of these clusters on the alumina substrate which ranges from depending upon the composition of the alloy-cluster, its orientation and the adsorption site. We also find that Pd atom binds strongly with the substrate oxygen atom with a short bond-length of about 2.2 Å. We explore how the gap between the HOMO of the cluster and the Fermi energy of the system varies as a function of elemental composition. These preliminary results will open the door for more systematic studies of alloy clusters of different size and stoichiometry.

*Argonne National Laboratory.
T70.00369: Development of Disordered and Ordered Nanoscale Terraced Topographies on Si Under Oblique Incidence Xe⁺ Ion Bombardment*  
EMMETT RANDEL (Presenter), CARMEN SUSANA MENONI, RICHARD M BRADLEY, Colorado State Univ — We explored disordered and ordered nanoscale terraced topographies that develop when a solid surface is bombarded by an ion beam at oblique incidence. It is shown that a flat Si surface when bombarded with 1500 eV Xe⁺ ions at 75° off normal incidence develops a disordered terraced topography. Using a Si surface pre-patterned with 500 nm pitch lines, it is demonstrated that ordered terraced topographies with sub-nanometer roughness on the facets develop under the above conditions. Ordered terraced substrates can be used in the fabrication of EUV multilayer blazed gratings. This work was performed in tandem with theory in an effort to refine models.

*NSF DMR Grant No. 1508745

T70.00370: Graphene-oxide monolayers at the air-water interface  
BRENT LA MURO (Presenter), MICAH VANDERSTEEN, Augsburg University, Minneapolis MN, ISSAM ISMAIL, Khalifa University of Science and Technology, BENJAMIN STOTTRUP, Physics, Augsburg University, Minneapolis MN — Graphene-oxide is a novel material with tremendous applications to coatings and electronics. We utilize investigations of self-assembled GO monolayers at the air-water interface as the basis for experimental investigations in an undergraduate laboratory experience partnered with Augsburg University’s sophomore level Modern Physics course. A Langmuir trough with dual tensiometers oriented parallel and perpendicular to the barrier compression is used to measure the anisotropic forces during the compression and expansion of the monolayer. Investigations of size distribution and pH modulation of the aqueous subphase are presented here. Scanning electron microscopy of Langmuir-Blodgett deposited GO films provides a complementary look at GO morphology. Finally, we present the feasibility of GO studies at liquid-liquid interfaces.

T70.00371: Equating Cu(111) Stepped Surface and Nanoparticle Oxidation Energetics: A Multiscale Computational Study*  
MATTHEW CURNAN, JUDITH YANG, WISSAM SAIDI (Presenter), University of Pittsburgh — Understanding how to inhibit oxide formation on Cu interfaces is critical to corrosion prevention and catalyst deactivation. Oxide growth on metal surfaces is supplied by diffusing O atoms, such that anisotropy in O diffusion rates along different surface structures proportionally affects their observed growth. Structural defects, such as Cu(111) surface steps and similarly faceted nanoparticles (NPs), selectively oxidize with respect to adjacent flat surfaces and differently oriented defects. Previous research suggests that differences in defect atomic coordination, attributed to dangling surface Cu bonds, yield this selective oxidation. In this study, we confirm that these oxidation preferences are conserved over morphologically distinct, equivalently oriented, Cu(111) stepped surfaces and NPs with shared edge orientations. O diffusion energetics are calculated via density functional theory, cross-validated via reactive force field molecular mechanics, and reconciled with molecular dynamics simulations. Equating surface step and NP oxidation energetics furthers the understanding of how defect structure impacts selective oxidation.

*This work is supported by NSF DMR-1410055.

T70.00372: Unconventional properties of superconductivity in SrTiO₃/LaAlO₃/SrTiO₃  
YONGSU KWAK, JONGHYUN SONG (Presenter), Chungnam National University, JINHEE KIM, Korean Research Institute for Stand Science — The 2-Dimensional Electron Gases (2-DEGs) observed at the LaAlO₃/SrTiO₃ (LAO/STO) hetero-interface exhibits superconductivity, which has phase diagram as function of carrier density like high-temperature superconductor. However, the superconducting energy gap in LAO/STO has conventional superconductivity because the temperature dependence of superconducting energy gap follows Bardeen-Cooper-Schrieffer (BCS) theory. Here we report unconventional properties of superconductivity in STO/LAO/STO. We have fabricated vertical Josephson junction to measure the superconducting energy gap. We found that the superconducting energy gap estimated from the Andreev reflection of the Josephson junction did not follow BCS theory from the gap ratio, Δ/k_BTc = 1.31. Additionally, we found evidence of unconventional superconductivity from the magnetic field dependence of superconducting critical current. It has opposite hysteresis, when it was compared with the hysteresis of magnetoresistance in STO/LAO/STO.
T70.00373: Ethylene Epoxidation on Ag(100), Ag(110), and Ag(111) - A First-principles and Kinetic Monte Carlo Study
MATEJ HUS, Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, ANDERS HELLMAN (Presenter), Chalmers University of Technology — Ethylene epoxidation is commercially one of the most important selective oxidation reactions. Silver-based catalysts are the most common catalyst formulation in industry, albeit with significant doping. In this work, we present results from first-principles and kinetic Monte Carlo (kMC) modeling of the reaction on three pristine silver surfaces Ag(100), Ag(110), Ag(111), and on the missing-row reconstructed Ag(110). To better understand the kinetics on different surfaces and veraciously describe the surface coverages, we explicitly take into account the lateral interactions between the adsorbates and their effect on the activation barriers. Comparing with experimental data shows a good agreement with the modeling data especially for Ag(111) and somewhat worse for Ag(100). We show that Ag(100) offers better activity and activity than Ag(111). Differences in the active intermediates surface coverage were also studied. Furthermore, we studied the influence of alkali metals on selectivity. Our calculations show that the combination of electronegative Cl and electropositive Cs offers an optimal compromise between activity and selectivity.

T70.00374: Upgrading scanning tunneling microscopy with a radio-frequency modulation system for the detection of ferromagnetic resonance
HUNG-HSIANG YANG (Presenter), KANTA ASAKAWA, FUMIKAZU OGURO, YUDAI SATO, Institute for Solid State Physics, University of Tokyo, SUSUMU TAKAHASHI, Department of Chemistry, University of Southern California, YUKIO HASEGAWA, Institute for Solid State Physics, University of Tokyo — Scanning tunneling microscope (STM) usually provides us with only static information of material surfaces. Recently, however, dynamics of a single electron spin can be successfully detected by using STM through the resonance under the irradiation of radio-frequency wave [1]. We are developing radio-frequency STM (RF-STM), intending to detect ferromagnetic resonance of nanosize ferromagnetic island structures and to generate spin waves around them. One of the key issues for the development is to generate constant-amplitude radio frequency sweeps at the tunneling junction [2]. Because of magnetostriction-induced drift, sweeping magnetic fields is not preferable. In the presentation, we will discuss the progress of the development and its performance.


T70.00375: Carrier Dynamics and Ultrafast Zero-Bias Photocurrents in SnS2 Single Crystals*
ERIN MORISSETTE (Presenter), KATERYNA KUSHNIR, ALEXIS BUZZEL, CURTIS DOIRON, RONALD GRIMM, LYUBOV TITOVA, Worcester Polytechnic Institute — Moderate band gaps, high carrier mobility, and environmental stability make layered transition metal dichalcogenides attractive for optoelectronic and solar energy conversion applications. Of these materials, SnS2 demonstrates promise as a photocatalyst for visible light water splitting and in field-effect devices, with reported on-off current ratios >10^6 and carrier mobilities up to 230 cm^2 V–1 s–1 [1,2]. Further progress in application of this emergent material requires the understanding of the dynamics of photoinjected carriers and optical excitations.

We present the synthesis of single-crystal SnS2 and its subsequent characterization by terahertz (THz) spectroscopy of carrier dynamics with sub-picosecond time resolution. Emission spectroscopy of photoinduced ultrafast currents probe the presence of shift currents, or zero-bias photocurrents, that appear to be a function of crystal orientation. The observation herein of zero-bias photocurrents indicates the viability of SnS2 nanosheets for third generation shift current photovoltaics.

[1] Huang et. al., ACS Nano 8, 10743 (2014)

*We acknowledge funding from the Clare Boothe Luce Foundation.
T70.00376: Molybdenum Nitride Thin-Film Development and Screening* MUHAMMAD SAJID (Presenter), ASIM KHANIYA, WILLIAM KADEN, ABDELKADER KARA, University of Central Florida — Hydrodenitrogenation (HDN), the process of through which nitrogen groups are removed from organic molecules present in petroleum and coal feedstocks, is a preliminary step in petroleum refinement. With shifts towards renewable biomass feedstocks, which may be harvested free of sulfur impurities, HDN optimization could become an increasingly relevant industrial challenge. HDN proceeds with greater activity and long chain selectivity on molybdenum nitride powders than conventional Co-Mo hydrotreatment catalysts. δ-MoN is suggested to be the most active phase, but more thorough experimental as well as computational studies are needed to better understand the correlation of activity and atomic structure of catalysts.

Using Density Functional Theory (DFT) and Ultra-High Vacuum surface science techniques, we are actively screening/developing different phase-pure MoN thin-films as model catalysts to isolate and explore reaction pathways associated with hydrodenitrogenation of simple nitrogen-containing aromatic molecules. This will aid us towards reaching to the subtle connection between properties at the atomic level with desired catalytic properties.

*American Chemical Society Petroleum Research Fund (ACS-PRL)

T70.00377: Fluctuation Dynamics of Ferroelectric Nano-domains in BaTiO3 Thin Films JIANHENG LI (Presenter), RAHUL JANGID, GEOFFERY IAN RIPPY, CHRISTOPHER KOHNE, Materials Science and Engineering, University of California, Davis, ARNOUD EVERHARDT, Materials Science and Engineering, University of California, Berkeley, BEATRIZ NOHEDA, Zernike Institute for Advanced Materials, University of Groningen, ANDREI FLEURASU, National Synchrotron Light Source II, SYLVIA MATZEN, CNRS, University of Paris - Sud 11, ROOPALI KUKREJA, Materials Science and Engineering, University of California, Davis — Ferroelectric materials possess a thermodynamically stable polarization which can be controlled using temperature, voltage, and recently with optical pulses, enabling numerous device applications including non-volatile memories, actuators, and sensors. Ferroelectric domain structure plays an important role in manipulating polarization switching behavior and depends upon factors including strain, temperature and interfacial properties. In this study, we focused on understanding domain dynamics and fluctuations in BaTiO3 (BTO) thin films, which show ordered 90° alternating in-plane and out-of-plane domain from 50 °C to 130 °C (Curie Temperature). We utilized X-ray photon correlation spectroscopy (XPCS) to probe domain fluctuations by accessing satellite peaks formed by ordered stripe domain in Bragg geometry. Our measurements show a two-step behavior, where from 50 °C to 90 °C, a slowing down of fluctuation timescales was observed due to stabilization of a/c domains. Above 90 °C, an increase in fluctuation timescales was observed as the material undergoes ferroelectric to paraelectric transition. This research demonstrates the characteristic behavior and timescales of nano-domain fluctuations in BTO thin films which have not been previously studied.

T70.00378: Intermetallic formation at deeply supercooled Ni/Al multilayer interfaces: a molecular dynamics study* PENG YI (Presenter), MICHAEL FALK, TIMOTHY P. WEIHS, Johns Hopkins University — Reactions at interfaces between solids are critical processing steps for applications including microelectronics, coatings on turbine blades, and reactive materials. It is established experimentally that the first phase to form through an interfacial reaction need not be the most stable phase. Understanding the thermodynamics and kinetics of the solid-state reaction at interface is crucial for device engineering.

We study the formation of the intermetallic NiAl in the Ni/Al multilayer system, focusing on how composition gradients at the interfaces impact intermetallic formation. High composition gradients (10^9-10^10 m^-1) were generated to mimics Ni/Al interface. Simulation temperatures below 800K were chosen so that both Ni and Al remain crystalline. We observed melting/amorphization at the interface region due to intermixing and stress. The intermetallic phase then forms at the interface from the melted/amorphous region through heterogeneous nucleation. Kinetics of the transformation follows the Johnson-Mehl-Avrami model. The NiAl formation is growth-controlled and the growth rate is found to increase with decreasing composition gradient. Our finding supports a growth-competition mechanism of phase selection for interfacial reactions.

*National Science Foundation (DMR-1308966)
T70.00379: Evident effects of Hofstadter-type energy spectra of modulated bilayer graphene  
DANHONG HUANG (Presenter), Air Force Research Lab - Kirtland, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, GODFREY GUMBS, LIUBOV ZHEMCHUZHNA, Hunter College of the City University of New York, Department of Physics and Astronomy — When a uniform perpendicular magnetic field is applied to a graphene layer, a two-dimensional periodic scatter array only mixes the Landau levels from the same valley to form split electron-hole Hofstadter-type energy spectra. However, in the case of bilayer graphene, this periodic array is able to mix different sets of Landau levels originating from the two separate valleys. Such a valley mixing effect has been carefully investigated in this work using a projected model Hamiltonian which includes an interlayer effective mass, interlayer coupling and different on-site energies. The computed Hofstadter-type energy spectra and associated density-of-states are employed for further calculations of the ballistic conductance of electrons in bilayer graphene.

T70.00380: Valley splitting in a van der Waals heterostructure WSe2/CrI3: A first-principles study*  
ZHIIYA ZHANG (Presenter), National & Local Joint Engineering Laboratory for Optical Conversion Materials and Technology, Lanzhou University, XIAOJUAN NI, HUAQING HUANG, LIN HU, FENG LIU, Department of Materials Science and Engineering, University of Utah — Atomically thin transition metal dichalcogenides (TMDs) have been considered as a wonderland for the research of valleytronics. Lifting the ±K valley degeneracy in TMDs has become an important research topic in the field of valleytronics. It is crucial to achieve large valley polarization for the development of valleytronics devices. In this work, we investigate the effects underpinning the ±K valley splitting in a van der Waals heterostructure WSe2/CrI3 based on first-principles calculations. We demonstrate that the stacking configuration affects the valley splitting dramatically and the influencing factors are discussed in details. The findings would further our basic understanding of the substrate effect on the valley degeneracy lifting in TMDs-based heterostructures beyond the WSe2/CrI3 and provide a useful guide to the valleytronic control in realistic applications.

*We acknowledge financial support from the China NSFC (No. 11874189) and U.S. DOE-BES (No. E-FG02-04ER46148). We also acknowledge DOE-NERSC and CHPC at the University of Utah for providing the computing resources.

T70.00381: Ion gating of the charge density wave order in two-dimensional NbSe2  
DIFEI ZHANG (Presenter), Physics, Nanjing University — Recent experimental advances in atomically thin transition metal dichalcogenide (TMD) metals have unveiled a range of interesting phenomena including the coexistence of charge-density-wave (CDW) order and superconductivity down to the monolayer limit. The atomic thickness of two-dimensional (2D) TMD metals also opens up the possibility for control of these electronic phase transitions by electrostatic gating. Here, with the ionic liquid gate we tune the carrier density in 2D NbSe2 with the expectation to bring up a CDW phase, which is detailedly characterized with the Raman spectroscopy. We also investigate the variation of CDW order with the change in carrier density and complement phase diagram of 2D NbSe2, including CDW order and superconducting phase.

T70.00382: A first principle investigation on the surface properties of β-Ga2O3 with a focus on the stability mechanism and electronic characteristics: GGA and hybrid DFT studies*  
SAJIB BARMAN (Presenter), MUHAMMAD NURUL HUDA, University of Texas at Arlington — β - Ga2O3 a transparent wide band gap semiconductor which has gained wide attention due to its suitability to a wide range of applications. Even though this is not a van der Waals material, it has shown that this material can be mechanically cleaved and exfoliated easily along favorable surfaces to make ultra-thin layers and used in device fabrications. One of the interesting properties of this material is that thin layers preserve the pristine bulk-like electronic properties, which makes it even more promising for applications in power devices. However, detail mechanism for such ultra-thin exfoliation is not known. Hence, a systematic study on the surface properties is essential. In this presentation, we have employed both GGA and HSE employed DFT to investigate surface properties. We are going to present our calculated surface stability, electronic band structures and electrons effective mass as a function of layer thickness for both (100)A and (100)B surfaces of this material. The understanding based on this study will provide a better control to fabricate thin film 2D devices.

*All the computational work was done at TACC in Austin, TX.
**T70.00383: Cross-plane thermal transport in SrRuO₃ thin films investigated by time-domain thermoreflectance technique**  
DOGYEOM JEONG (Presenter), YOUNGWAN CHO, HWIIN JU, Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Korea, SUNGMIN WOO, WOO SEOK CHOI, Department of Physics, Sungkyunkwan University, Korea, JONGSEOK LEE, Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Korea — A SrRuO₃ thin film has been widely used as a metal electrode in electronic devices based on transition metal oxides, and hence it is important to understand thermal transport properties through the SrRuO₃ thin film to minimize a thermal degradation problem during the device operation. Using the time-domain thermoreflectance measurement technique, we investigate the cross-plane thermal conductivity of the SrRuO₃ thin films with a thickness variation from 1 um to 8 nm. We find that the thermal conductivity becomes reduced from 5.0 W/m-K for the 1 um thick film to 0.94 W/m-K for the 8 nm thick film, and attribute such a large reduction of the thermal conductivity to the boundary scattering of thermal carriers, i.e., electron and phonon. In addition, we find a signature of the ballistic phonon transport at low temperature particularly when the film thickness becomes much smaller than the phonon mean free path.

**T70.00384: Nonlinear optical responses of Rashba spin-split GeTe thin films**  
SOON-HEE PARK (Presenter), JEONG GI CHO, CHANG JAE ROH, Gwangju Institute of Science and Technology, SEONG WON CHO, SUYOUN LEE, KIST, JONGSEOK LEE, Gwangju Institute of Science and Technology — Ferroelectric alpha-phase germanium telluride (α-GeTe) has been known to have a giant Rashba spin split band, and hence can be a promising material for the spintronic application. We prepare α-GeTe thin films on a Si substrate with a thickness variation from 2 to 100 nm, and investigate their structural and electrodynamic properties by using second harmonic generation (SHG) and terahertz emission spectroscopy. From the azimuth-dependent anisotropy observed in the SHG responses, we find that all the films have a non-centrosymmetric crystal structure identified as a 3m point group. From the THz emission results, we demonstrate that a fairly strong built-in field exists at the film interface with the Si substrate. In particular, we observe a non-negligible helicity-dependence in the THz emission which can be a possible signature of a spin-polarized photocurrent arising from the spin-split Rashba bands.

**T70.00385: METALS AND METALLIC ALLOYS**

**T70.00386: Imaging magnetic and non-magnetic metal nanostructures using a field emission SEM.**  
STEPHEN BLAMA (Presenter), Dept. of Physics Astronomy and Geosciences, Towson University, MARY SAJINI DEVADAS, Dept. of Chemistry, Towson University — An electron microscope can be used to image materials of nanoscale dimensions allowing for examination of size and shape characteristics, and chemical composition. We use an FEI Apreo scanning electron microscope to image magnetic (using electromagnetic mode) and nonmagnetic nanostructures (using electrostatic mode) of various metals (Au and Ag) and metal alloys (Fe/Co, Fe/Au) using different sample preparation methods, and varying system parameters for optimal image quality and resolution. Samples are prepared with spin coating followed by plasma cleaning, with controlled plasma composition. System parameters of spot size and accelerating voltage for different built-in detectors (ETD, EBSD, in-column BSD detectors, and STEM) are studied. Methods for obtaining optimal EDX maps are also investigated, as EDX is prone to sample charging and image drift due to extended exposure of the sample to the electron beam. Details of the imaging parameters and sample preparation for these nanostructures will be presented.

*We acknowledge funding from NSF MRI 1626326, Fisher Endowment Grant, Fisher Chair Grant and FDRC, GSA Research and travel grants and FCSM travel award from Towson University.

**T70.00387: Dynamic behavior of carbon in steel by using soft X-ray absorption spectroscopy and spectrum simulation**  
KAKERU NINOMIYA (Presenter), KAZUTAKA KAMITANI, Kyushu University, YUSUKE TAMENORI, KAZUKI TSURUTA, Japan Synchrotron Radiation Research Institute, TOSHIHIRO OKAJIMA, DAIKUKE YOSHIMURA, Kyushu Synchrotron Light Research Center, HIDEAKI SAWADA, KEISUKE KINOSHITA, Nippon Steel & Sumitomo Metal Corporation, MAIKO NISHIBORI, Kyushu University — The ferritic steel with supersaturated solid solution carbon remarkable increase in hardness by heat treatment (so-called aging) at low temperature. This has been considered to cause by the formation of the carbon cluster in ferritic steel.¹ In this study, we aimed to understand the low temperature aging behavior of low-carbon steel focusing on carbon atoms, and the chemical state and local structural changes of carbon in low-carbon steel with aging were observed by soft X-ray absorption spectroscopy. Furthermore, we tried to clarify the structure of carbon cluster from the observed absorption spectrum by first principles calculation and spectrum simulation. As a result, we succeeded in clarifying the relationship between microscopic chemical state and macroscopic hardness change. Furthermore, it was found that the chemical state of carbon related to form carbon clusters changes dynamically in the early stage of heat treatment. The results of the spectral analyses suggested that solid solution carbon was interacted with the vacancies in bcc lattice. Therefore, it is suggested that vacancies may play an important role in the formation of carbon clusters.

ASH (Presenter), Biology, Misericordia University, GOPAL VERMA, JEAN-PIERRE DELVILLE, LOMA, University of Bordeaux — Current compaction. Understanding this pathway has implications in biomaterial, epigenetic, and fertility research.

by protamine, we expect a change in the standard deviation of the DNA tether's movement due to further DNA microscopy, we track the motion of the bead and measure the length of the tether over time. When histones are replaced attached to a 1 μm “polystyrene bead on one end and is attached to a glass coverslip on the other. Using video study this phenomenon, we utilize a Tether Particle Motion (TPM) assay. In the TPM assay, a single DNA molecule is specifically, we are interested in reconstructing the direct histone-protamine replacement pathway that occurs in fish. To protected. In this study we aim to understand the mechanics of DNA condensation in the nucleus of sperm cells. More structure that is packed inside the nucleus. However, during human spermatogenesis approximately 85-90% of the histones in the DNA are replaced by an arginine rich protein called protamine. This allows for more efficient packaging of the DNA in the sperm cell. As a result, the sperm cell's movement is more hydrodynamic and the genetic material is protected. In this study we aim to understand the mechanics of DNA condensation in the nucleus of sperm cells. More specifically, we are interested in reconstructing the direct histone-protamine replacement pathway that occurs in fish. To study this phenomenon, we utilize a Tether Particle Motion (TPM) assay. In the TPM assay, a single DNA molecule is attached to a 1 μm “polystyrene bead on one end and is attached to a glass coverslip on the other. Using video microscopy, we track the motion of the bead and measure the length of the tether over time. When histones are replaced by protamine, we expect a change in the standard deviation of the DNA tether's movement due to further DNA compaction. Understanding this pathway has implications in biomaterial, epigenetic, and fertility research.

*Thank you to the NSF Career Grant for funding this experiment.

T70.00391: Creating a viscoelastic spectrum of aqueous polyacrylamide gel at varying concentrations* MICHELLE ASH (Presenter), Biology, Misericordia University, GOPAL VERMA, JEAN-PIERRE DELVILLE, LOMA, University of Bordeaux — Current methods to obtain microrheological measurements inside liquid materials hold the problem of contaminating samples with an internalized foreign particle, especially problematic for intracellular microrheological measurements. Optical interferometry solves this problem by allowing for pico- and nanoscale rheological measurements without coming into contact with the interior system of a sample. Aqueous polyacrylamide (PAAm), a non-Newtonian gel can be used as a model of a cell, mirroring the experimental setup needed to study cellular systems. With a simple setup, a high-power green pump laser is incident on a PAAm droplet, inducing droplet height deformation via radiation pressure, then detected by interferometry using a low-power red probe laser. Firing a pump laser pulse deforms the gel droplet height between maxima and minima, from which the viscosity is calculated. Comparison of our experimental viscoelastic data of PAAm at a single pulse and varying frequencies to literature values confirms an accurate viscoelastic spectrum of PAAm. Based on our measurements and the noninvasiveness of this technique, mechanical perturbation of a gel surface demonstrates possibility of replication for cellular measurements.

*National Science Foundation Grant PHY-1359195
Lehigh University
We propose a disordered ladder spin model which can be designed in a scalable cold atom setup at the hard-core boson limit to dynamically detect out-of-time order correlators (OTOC) and hence information scrambling. Our protocol utilizes the Hamiltonian sign reversal for the evolution backward in time by applying single spin gates successively. We study different limits of disordered Ladder-XY model with focusing on its OTOC behavior and level statistics. We show that in its chaotic limit, disordered ladder-XY model decays exponentially in early-time with power-law tails before its scrambling time and it demonstrates a range of lightcones due to local spin-spin interactions. Based on our results, one can observe how the ladder systems could be useful to understand and experiment information scrambling in the transition from well-studied 1D models to unexplored 2D models.

*This work was supported by the AFOSR MURI program.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V01 DCMP: Frontiers of Topological Materials: Mostly Theory

2:30PM V01.00001: Magnetic quadrupole moment in higher order topological semimetals* JACOPO GLIOZZI (Presenter), College of William & Mary, MAO LIN, TAYLOR HUGHES, University of Illinois Urbana-Champaign — One characteristic feature of conventional two dimensional Dirac semimetals is the bulk orbital magnetic dipole moment (MDM), which is proportional to the energy separation of the bulk nodes, and manifests as boundary circulating currents. In this presentation, we instead consider the magnetic quadrupole moment (MQM) in the three dimensional higher order topological semimetals (HOTS). In contrast to all semimetals considered previously, the bulk energy bands of a HOTS could be gapped, and its surfaces form one (or half of a) two dimensional Dirac semimetal with surface Dirac nodes. By adding perturbations, an energy difference can be created between pairs of surface nodes. We show analytically and numerically that the nodal energy difference generates a bulk MQM and is associated with circulating hinge currents. We discuss possible experiments in solid state systems as well as in metamaterials to verify our predictions.

*ML thanks NSF Emerging Frontiers in Research and Innovation NewLAW program Grant EFMA1641084 for support. TLH thanks NSF CAREER Grant DMR-1351895 for support. JG thanks NSF Grant No.1659598 for support.

2:42PM V01.00002: 't Hooft anomalies in symmetry-enriched U(1) gauge theories* SHANGQIANG NING (Presenter), Institute for Advanced Study, Tsinghua University, LIUJUN ZOU, Department of Physics, Harvard University, MENG CHENG, Department of Physics, Yale University — The 3+1D U(1) gauge theory is the effective field theory of a three-dimensional U(1) quantum spin liquid, which is an exotic gapless phase with emergent gapless photon and also gapped fractionalized electric charges and magnetic monopoles. In the presence of global symmetries, these fractionalized excitations can transform in different fractionalization patterns, which can be captured by projective representations of the symmetry group. Symmetry properties of these gapped excitations determine the universal properties of a symmetric U(1) quantum spin liquid, as well as the nature of its proximate phases. However, certain patterns of symmetry fractionalization cannot be realized in strictly 3+1D . Instead, they can only be realized on the boundary of 4+1D symmetry-protected topological phases. This type of symmetry fractionalization patterns are referred to as possessing 't Hooft anomalies. We obtain the classification of the patterns of symmetry fractionalization in symmetry-enriched U(1) gauge theories, and, in particular, an explicit formula to determine the relevant 't Hooft anomalies in terms of the fractionalization patterns.

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2:54PM V01.00003: Type-II Fracton Models with Gapped Boundaries DANIEL BULMASH (Presenter), University of Maryland, College Park, ARPIT DUA, Yale University, THOMAS IADECOLA, University of Maryland, College Park, DOMINIC WILLIAMSON, Yale University — Type-II fracton systems are exotic models whose pointlike excitations are strictly immobile at zero temperature and have locally indistinguishable degenerate ground states, and unusual error correction properties. We study gapped boundaries of such models, including Haah's code. After enumerating the set of possible gapped boundaries, we study the ground state degeneracy and logical operators in the presence of these boundaries. Although these properties are complicated on the torus, they simplify dramatically for certain open boundary conditions. We discuss the interpretation of the degeneracy in terms of surface line defects, i.e. the domain walls between distinct gapped boundaries.
3:06PM V01.00004: Variational Monte Carlo study on a magnetization process of the Kitaev honeycomb model under a magnetic field  KOTA IDO (Presenter), TAKAHIRO MISAWA, ISSP, University of Tokyo — Recently, the Kitaev model under a magnetic field has been intensively studied, because the magnetization processes offer useful information for characterizing the nature of the quantum spin liquid. It was reported that an intermediate state appears in the antiferromagnetic coupling Kitaev model (AF KM) under a magnetic field by several numerical methods such as Majorana mean field, exact diagonalization, and DMRG. However, these methods are not appropriate for highly accurate analyses of physical properties in the 2D system with large system sizes. To identify whether the intermediate state exists as the ground state of the AF KM under a magnetic field in the bulk limit, it should be necessary to use an accurate numerical method which is applicable to the large 2D system.
In this talk, we will report the magnetization process of the AF KM obtained by using the variational Monte Carlo (VMC) method. The trial wave function we used is the BCS wave function with the Jastrow correlation factor, which can exactly represent the ground state of the pure Kitaev model fermionized by the Jordan-Wigner transformation. We will also explain the details of VMC and its accuracy.

3:18PM V01.00005: Model of spin liquids with and without time-reversal symmetry  JYONG-HAO CHEN (Presenter), CHRISTOPHER M MUDRY, Condensed Matter Theory Group, Paul Scherrer Institute, CLAUDIO CHAMON, Boston University, ALEXEI TSVELIK, Brookhaven National Laboratory — We study a model in (2+1)-dimensional spacetime that is realized by an array of chains, each of which realizes relativistic Majorana fields in (1+1)-dimensional spacetime, coupled via current-current interactions. The model is shown to have a lattice realization in an array of two-leg quantum spin-1/2 ladders. We study the model both in the presence and absence of time-reversal symmetry, within a mean-field approximation. We find regimes in coupling space where Abelian and non-Abelian spin liquid phases are stable. In the case when the Hamiltonian is time-reversal symmetric, we find regimes where gapped Abelian and non-Abelian chiral phases appear as a result of spontaneous breaking of time-reversal symmetry. These gapped phases are separated by a discontinuous phase transition. More interestingly, we find a regime where a non-chiral gapless non-Abelian spin liquid is stable. The excitations in this regime are described by relativistic Majorana fields in (2+1)-dimensional spacetime, much as those appearing in the Kitaev honeycomb model, but here emerging in a model of coupled spin ladders that does not break SU(2) spin-rotation symmetry.

3:30PM V01.00006: Monolayer Mg2C: Negative Poisson's ratio and unconventional two-dimensional emergent fermions  SHAN-SHAN WANG (Presenter), SHENGYUAN YANG, Singapore University of Technology and Design — We analyze the phonon spectrum, reveal the Raman-active modes, and show that it has small in-plane stiffness constants. Particularly, the Mg2C monolayer shows an intrinsic negative Poisson's ratio $\sim -0.023$ along zigzag. The material is metallic at its equilibrium state. A moderate biaxial strain can induce a metal-semimetal-semiconductor phase transition, during which several types of 2D unconventional fermions emerge, including Dirac fermions, the 2D double Weyl fermions in the semimetal phase, and the 2D pseudospin-1 fermions around which three bands cross at a single point on the Fermi level. In addition, uniaxial strains along the high-symmetry directions break the threefold rotational symmetry and reduce the number of Dirac points. Interestingly, it also generates 2D type-II Dirac points. We construct effective models to characterize the properties of these fermions. Our result reveals Mg2C monolayer as an intriguing platform for the study of 2D unconventional fermions, and also suggests its great potential for nanoscale device applications.

3:42PM V01.00007: Unconventional Pairing Induced Anomalous Transverse Shift in Andreev Reflection  ZHI-MING YU (Presenter), YING LIU, Singapore University of Technology and Design, YUGUI YAO, Beijing Institute of Technology, SHENGYUAN YANG, Singapore University of Technology and Design — Superconductors with unconventional pairings have been a fascinating subject of research, for which a central issue is to explore effects that can be used to characterize the pairing. The process of Andreev reflection—the reflection of an electron as a hole at a normal-metal-superconductor interface—offers a basic mechanism to probe the pairing. Here we predict that in Andreev reflection from unconventional superconductors, the reflected hole acquires an anomalous spatial shift normal to the plane of incidence, arising from the unconventional pairing. The transverse shift is sensitive to the superconducting gap structure, exhibiting characteristic features for each pairing type, and can be detected as voltage signals. Our work not only unveils a fundamentally new effect with a novel underlying mechanism, but also suggests a possible new technique capable of probing the structure of unconventional pairings.
3:54PM V01.00008: Goos-Hänchen-like shifts at a metal/superconductor interface  YING LIU (Presenter), ZHI-MING YU, Engineering Product Development, Singapore University of Technology and Design, HUA JIANG, Soochow University, SHENGYUAN YANG, Engineering Product Development, Singapore University of Technology and Design — At a normal-metal/superconductor interface, an incident electron from the normal-metal (N) side can be normally reflected as an electron or Andreev reflected as a hole. We show that pronounced lateral shifts along the interface between the incident and the reflected quasiparticles can happen in both reflection processes, which are analogous to the Goos-Hänchen effect in optics. Two concrete model systems are considered. For the simplest model in which the N side is of the two-dimensional electron gas, we find that while the shift in Andreev reflection stays positive, the shift in normal reflection can be made either positive or negative, depending on the excitation energy. For the second model with the N side taken by graphene, the shift in Andreev reflection can also be made negative, and the shifts have rich behavior due to the additional sublattice pseudospin degree of freedom. We show that the shift strongly modifies the dispersion for the confined waveguide modes in an SNS structure. We also suggest a possible experimental setup for detecting the shift.

4:06PM V01.00009: Dynamical Localization and Delocalization in Floquet Systems*  TILEN CADEZ (Presenter), RUBEM MONDAINI, Beijing Computational Science Research Center, PEDRO D. SACRAMENTO, CeFEMA, Instituto Superior Técnico, Universidade de Lisboa, Portugal — We study the localization aspects of a kicked noninteracting one-dimensional quantum system of spinless fermions and a topological superconductor subject to either time-periodic or aperiodic pulses. The universality class of the transition from delocalized to localized regimes is studied in the case of time-periodic and spatially quasi-periodic kicks. In the case of aperiodic kicks, delocalization ultimately sets in and a diffusive spreading of an initial wave packet is obtained even for small time-aperiodicity of the driving. In the case of Floquet topological superconductors, one finds both Majorana and fermionic localized edge modes in the topological regime. In the intermediate driving period regime, one can identify a region in the phase diagram with a mobility edge between critical and localized states. Finally, we analyze the robustness of the Majorana modes to deviations on the driving period, finding they are stable in a small set of the parameters.

*RM is supported by the NSFC Grant No. 11674021 and No. 11650110441 as well as N.SAF-U1530401. PDS acknowledges partial support from FCT through grant UID/CTM/04540/2013.

4:18PM V01.00010: Prethermalization and topological transport in slowly driven Floquet systems*  NETANEL LINDNER (Presenter), TOBIAS GULDEN, Physics, Technion - Israel Institute of Technology, EREZ BERG, Physics, Weizmann Institute of Science, MARK RUDNER, Physics, University of Copenhagen — Topological phenomena in periodically driven quantum many body systems are difficult to obtain due to the generic tendency of such systems to heat up and tend towards an infinite temperature-like state. We investigate a mechanism to transiently stabilize topological phenomena over a long-time window for systems driven at low frequencies. We derive an analytical bound for the rate of change in the number of particles populating the Floquet bands of the system. The bound is exponentially small in the ratio between the instantaneous bandgap and the maximum between the driving frequency, interaction strength, and the bandwidth. Within the resulting prethermal time window, a quasi-steady state is stabilized, characterized by maximum entropy density subject to the constraint of fixed number of particles in each band. This mechanism provides a route for obtaining long-lived prethermal states with anomalous topological properties, unattainable in equilibrium, such as universal chiral currents in one dimension and magnetoelectric transport in three dimensions.

*This work was supported by European Research Council (ERC) under the European Union Horizon 2020 Research and Innovation Programme (Grant Agreement No. 678862 and 639172), the Israeli Science Foundation and the Villum Foundation

4:30PM V01.00011: Bulk-edge correspondence of periodically driven 2D systems with time-reversal symmetry*  XU LIU (Presenter), FENNER HARPER, RAHUL ROY, Physics & Astronomy, University of California, Los Angeles — We propose an edge invariant for two-dimensional Floquet systems with time-reversal symmetry. This edge index is physically motivated and locally computable. In addition, we generalize an existing construction of a bulk invariant to systems with disorder. Finally, we derive a bulk-edge correspondence which relates the nontrivial bulk behavior with the edge modes present on a boundary at the end of the evolution. Our results provide the first bulk-boundary correspondence for Floquet systems in this symmetry class.

*Bhaumik Institute, NSF
4:42PM V01.00012: FLOQUET ENGINEERING OF EXCHANGE INTERACTIONS IN 2D MAGNETIC MATERIALS*  SWATI CHAUDHARY (Presenter), GIL REFAEL, DAVID HSIEH, California Institute of Technology — Periodic drive can be used to modify the spin exchange interactions in some magnetic materials. These effects arise mainly due to photon-assisted hopping and can be understood within the framework of periodically driven Fermi-Hubbard model. In real materials, these interactions are usually mediated by the non-magnetic ions, and many different channels are available for the exchange process. We take into account the presence of these ligand ions, and investigate the effects of the periodic drive on magnetic coupling strengths between different neighboring spins in transition metal trichalcogenides for a variety of exchange pathways available in these materials. Additionally, the strength of these interactions depends on the orbitals involved in the superexchange process. We also provide a novel method to control the exchange interactions by manipulating the properties of these orbitals with a periodic drive. In this case, the magnetic coupling strength is altered due to the AC stark shift of the states available for virtual excitations. We discuss two different orbital floquet engineering schemes involving the orbitals of ligand ions and the magnetic ions.

*This work was supported by ARO Grant No. W911NF-16-1-0361

4:54PM V01.00013: Light driven magnetic and topological phase transitions in magnetic topological insulator thin films  XIAOYU LIU (Presenter), Institute for advanced study, Tsinghua University, PEIZHE TANG, HANNES HUEBENER, Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, DUAN WENHUI, Institute for advanced study, Tsinghua University, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science — The external manipulation of the magnetism in topological materials would be important both for fundamental interests and practical applications. Herein, we predict that topological and magnetic properties in magnetically doped topological insulator thin films can be well tuned by the laser field. With increasing the strength of the circularly polarized laser (CPL), we can observe a topological phase transition in such system. Remarkably, the CPL could even induce the magnetic phase transition driving thin films from ferromagnetism to paramagnetism. Its critical behavior strongly depends on the quantum quenching, indicating that different Curie temperatures can be observed in different time scales and experimental setups. Furthermore, we propose an all-optical transistor device in which the on-off signal from polar Kerr-rotation angle can be controlled by the applying laser field. Our discoveries not only deepen our understanding of the relationship between topology and magnetism in the magnetic topological insulator in the non-equilibrium regime, but also extend optoelectronic device applications in topological materials.

5:06PM V01.00014: Stability of Periodically Driven Topological Phases against Disorder*  RAMIS MOVASSAGH (Presenter), IBM Thomas J. Watson Research Center, OLES SHTANKO, Physics, Massachusetts Institute of Technology — Time-dependent periodic fields are used to create exotic topological phases of matter with potential applications ranging from quantum transport to quantum computing. These nonequilibrium states, at high driving frequencies, exhibit the quintessential robustness against local disorder similar to equilibrium topological phases. However, proving the existence of such topological phases in a general setting is an open problem. We propose a universal effective theory that leverages on modern free probability theory and ideas in random matrices to analytically predict the existence of the topological phase for finite driving frequencies and across a range of disorder. We find that, depending on the strength of disorder, such systems may be topological or trivial and that there is a transition between the two. In particular, the theory predicts the critical point for the transition between the two phases and provides the critical exponents. We compare with exact diagonalizations for driven-disordered 1D Kitaev chain and 2D Bernevig-Hughes-Zhang models and find excellent agreement. This Letter may guide the experimental efforts for exploring topological phases.


*ExxonMobil-MIT Energy Initiative. IBM Research.

5:18PM V01.00015: Surface Acoustic Wave Study in Microwave-Induced Non-Equilibrium Electron System  JIANLI WANG, International Center for Quantum Materials, Peking University, CHI ZHANG (Presenter), SKLSM, Institute of semiconductors, Chinese Academy of Science, LOREN PFIEFFER, KENNETH WEST, K. W. BALDWIN, Electrical Engineering, Princeton University — Microwave-induced resistance oscillations (MIRO) and zero-resistance states (ZRS) occur under microwave irradiation in the ultrahigh mobility two-dimensional electron gas (2DEG) in GaAs/AlGaAs quantum wells (QW). We employed the surface acoustic wave (SAW) to study the structure of MIRO and ZRS. We observe that the velocity shift ($\Delta v/v$) shows minima at the peak resistance regime ($j = \omega/\omega_C \sim 1, 2, 3, \text{etc}$). And in the ZRS regime, an increase of the velocity shift appears at $j = 5/4$. The results conform to the theoretical and experimental studies of current domains at ZRS under high power microwave.

Thursday, March 7, 2019 2:30 PM - 5:18 PM
2:30PM V02.00001: Pressure Induced Fermi Surface in Sb$_2$Se$_3$ *

UMA GARG (Presenter), NATHANIEL SMITH, WILLIAM CHRISTOPHER REXHAUSEN, Department of Physics, University of Wisconsin Milwaukee, Wisconsin 53211, AUDREY GROCKOWIAK, ALEXEY SUSLOV, STANLEY W TOZER, National High Magnetic Field Laboratory, Tallahassee, Florida 32310, PRASENJIT GUPTASARMA, Department of Physics, University of Wisconsin Milwaukee, Wisconsin 53211 — Studies of a new class of Topological Insulators, believed to be a new quantum phase of matter with a 2-dimensional Fermi surface, have led to a search for other insulators or semi-metals in which topologically non-trivial properties can be tuned using a chemical, structural, or external thermodynamic parameter. Here, we report studies of Shubnikov-de Haas oscillations as a function of pressure and magnetic field orientation on single crystals of antimony selenide (Sb$_2$Se$_3$). Sb$_2$Se$_3$ is a band insulator with a 1 eV bandgap under ambient conditions; it is metallic above 3 GPa, and superconducting above 10 GPa. Our Sb$_2$Se$_3$ single crystals are orthorhombic, unlike rhombohedral Bi$_2$Se$_3$ and Sb$_2$Te$_3$. Following up on our previous collaborative studies of Raman spectroscopy and first-principles DFT, which revealed an electronic topological transition (ETT) with pressure, we performed non-contact conductivity measurements using a tunnel diode oscillator (TDO) circuit under high pressure in a diamond anvil cell. A Fermi Surface (FS) is found to appear at 6.4 GPa. We also find evidence for a Berry phase ($\beta$) of value $\pi$ independent of magnetic field orientation, indicating possible non-trivial topologies.

*AFOSR-MURI; NSF DMR-1157490; State of Florida; UWM

2:42PM V02.00002: Electronic Transport Properties of few-layer PdTe$_2$

GUIXIN CAO (Presenter), RUOYU CHEN, DONGYING WANG, MARC BOCKRATH, CHUN NING LAU, Ohio State University — The interplay of superconductivity and topological states in layered transition-metal dichalcogenide materials have attracted much attention due to their possible promise to realize topological superconductors. PdTe$_2$ is one of such compounds that exhibit coexistence between two-dimensional superconductivity and topological states. We report experimental investigations on the electrical transport and magnetic properties of mechanically exfoliated single crystal PdTe$_2$ bulk and few layers. Latest data as function of layer thickness, temperature and magnetic field will be reported.

2:54PM V02.00003: Observation of Quantum Oscillations in PdTe$_2$ Single Crystals

RAMAKANTA CHAPAI (Presenter), Louisiana State University, DAVID E GRAF, National High Magnetic Field Lab, Tallahassee, FL, JOHN DITUSA, RONGYING JIN, Louisiana State University — Transition-metal dichalcogenide PdTe$_2$ exhibits superconductivity and topologically non-trivial surface states. Here, we present a detailed study of the de-Haas van Alphen (dHvA) oscillations in single crystalline PdTe$_2$. In analyzing the magnetic field dependence of the magnetization and magnetic torque, we identify two frequencies from the oscillations: $F_\alpha = 8$ T and $F_\beta = 117$ T. Using the Lifshitz-Kosevich equation to fit experimental data, the effective masses are obtained with $m^*_\alpha = 0.059m_0$ and $m^*_\beta = 0.067m_0$ ($m_0$ is the free electron mass). Further analysis of the dHvA oscillations reveals that the $\alpha$ band possesses a non-trivial Berry phase (~ 0.94$\pi$) while the $\beta$ band consists of a smaller Berry phase (~ 0.32$\pi$). This indicates that the $\alpha$ band is likely responsible for the topological properties.

3:06PM V02.00004: Surface Repair and Passivation of InAs Quantum Wells with ALD*

SEBASTIAN PAUKA (Presenter), JAMES WITT, School of Physics, Univ of Sydney, CIOFFI NICOLE MURPHY, Microsoft Station Q Sydney, GEOFFREY C. GARDNER, SERGEI GRONIN, TIAN WANG, CANDICE THOMAS, MICHAEL MANFRA, Microsoft Station Q Purdue, DAVID REILLY, MAJA C CASSIDY, Microsoft Station Q Sydney — The two-dimensional electron gas formed in InAs quantum wells and proximitized with epitaxially grown Aluminium has attracted interest as a possible host for Majorana zero modes. This is due to the strong spin-orbit coupling and large Landé g-factor in this material. However, the need to induce superconductivity in the quantum well requires it to be grown close to the surface (~12nm), making the 2DEG highly sensitive to any processing. In particular, the aluminium etch, typically a Transene-based wet etch, has limited measured mobility in InAs quantum wells.

In this work, we report on the use of Al$_2$O$_3$ grown by ALD, with in-situ surface pre-treatment via TMA pulses or an Ar/H plasma, to repair and passivate the surface after processing, and demonstrate the reduction of charged surface states. We show that by this method, we are able to enhance the measured carrier mobility of these devices up to ~45000 cm$^2$/V s. Finally, the spin orbit length is extracted as a function of density, controlled using a global top-gate, to determine spin-scattering mechanisms. Our results provide a path towards high quality, shallow 2DEG-based Majorana devices.

*This work was supported by funding from Microsoft Station Q.
3:18PM V02.00005: Core-Shell Nanowires of 3D Topological Insulators  KEVIN GEISHENDORF (Presenter), Leibniz IFW and TU Dresden, TOMMI PAAVO TYNELL, Leibniz IFW, KORNELIUS NIERSCH, Leibniz IFW and TU Dresden, ANDY THOMAS, Leibniz IFW — Topological insulators (TI) are promising candidates for next generation electronic/spintronic devices. The gapless surface states (SS) in TI exhibit a very high mobility and strongly suppressed backscattering due to spin-momentum locking. However, to exploit those advantageous one has to decrease the finite bulk conductance present in most TI systems.

One approach to achieve this reduction is to utilize band bending which occurs at the interface between two materials with different Fermi levels. The band bending leads to a charge depletion/ or accumulation near the interface. It therefore provides a tool to shift the fermi energy closer to the Dirac point.

In this work, we have grown core-shell NW using Vapor-Liquid-Solid (VLS) growth and Atomic Layer Deposition (ALD). As core material Bi2Se3 and as shell materials Al2O2 and Sb2Te3 were employed. The uniformity, crystallinity and composition of those core-shell NW was investigated using transmission electron microscopy, nanodiffraction and EDX. Furthermore, devices for transport experiments were built using optical lithography and lift-off techniques. With those devices magneto transport measurements have been performed revealing quantum interference effects such as weak-antilocalization and universal conductance fluctuations.

3:30PM V02.00006: Measurement of g-factor in InAs and InAs0.5Sb0.5 Surface Quantum Wells* MEHDI HATEFIPOUR (Presenter), JOSEPH YUAN, WILLIAM ANDREW MAYER, KAUSHINI WICKRAMASINGHE, Physics, New York University, WENDY L. SARNEY, STEFAN P. SVENSSON, US Army Research Laboratory, JAVAD SHABANI, Physics, New York University — The rising interest into topological superconductors has led to the exploration of hybrid superconductor-semiconductor structures. In these structures two dimensional electron gases are confined near surface and can make epitaxial contact to superconducting thin films. Large Zeeman splitting and spin orbit coupling are necessary ingredients to look for when choosing the semiconductor. Here we present findings of our experiments on two prime candidates with strong spin orbit interaction and high g-factor: InAs and InAs0.5Sb0.5. We measure weak anti-localization signal and integer quantum hall energy gaps as a function of carrier density in near surface quantum wells of both materials. We use fitting of weak anti-localization to determine strength of spin orbit interaction and the energy gaps of odd Integer quantum Hall states (v=3 and v=5) to extract g-factors.

*We acknowledge support for this research from NSF and Darpa TEE.

3:42PM V02.00007: Current-induced nuclear spin polarization effects in Bi(111) film flakes with strong spin-orbit interaction* ZIJIAN JIANG (Presenter), VICTORIA SOGHOMONIAN, JEAN HEREMANS, Physics Department, VIRGINIA POLYTECHNIC INSTITUTE — The influence on quantum transport of nuclear spin polarization, induced by hyperfine interactions and the Edelstein effect, was investigated in individual micrometer-size 40 nm thick Bi(111) film flakes. The flakes were obtained by exfoliation and PDMS stamping from epitaxial Bi(111)-on-mica films. The growth method will be discussed. AFM and SEM micrographs of the Bi(111) film clearly show micrometer-size triangular structured islands with 0.4 nm step height (Bi(111) bilayer height). At low temperatures a high current density is applied to generate nonequilibrium carrier spin polarization by the Edelstein effect, which then induces nuclear polarization by hyperfine interactions and dynamic nuclear polarization. The low-temperature quantum transport measurements are carried out both before and after the current application. The quantum phase coherence time and the spin-orbit scattering time are obtained by fitting of weak-antilocalization magnetotransport data. In our Bi(111), the phase coherence time and the spin-orbit scattering time show a dependence on the nuclear spin polarization obtained by hyperfine interactions with the spin-polarized carriers, in turn obtained by the Edelstein effect.

*DOE DE-FG02-08ER46532
Topological Hall Effect in Dual-gated Magnetic Topological Insulator Heterostructures

XIAO (Presenter), DI XIAO, JUE JIANG, MORTEZA KAYYALHA, JAE HO SHIN, FEI WANG, LING ZHANG, JIANXIAO ZHANG, CHAOXING LIU, MOSES H W CHAN, CUI-ZU CHANG, NITIN SAMARTH

Physics, Penn State University

Magnetic chiral spin textures in real space serve as excellent model systems for fundamental studies of Berry curvature physics. The interaction of itinerant charge carriers with chiral spin textures induces an excess Hall voltage known as a ‘topological Hall (TH) effect,’ providing an indirect signature of non-trivial spin textures in transport measurements. Here, we report the observation of a possible TH effect in a heterostructure that sandwiches a topological insulator (TI) layer in between two magnetic TI layers. By varying the chemical potential using top and bottom gates, we map out the behavior of the TH effect and show that it is greatly enhanced when the chemical potential difference between the two surfaces is increased. This observation suggests that the excess Hall voltage is a result of a finite Dzyaloshinskii-Moriya interaction induced by the magnetization asymmetry in two magnetic layers. Apart from providing new insights into the TH effect, our study paves a new route for demonstrating proof-of-concept topological spintronic devices that rely on the interplay between momentum- and real-space spin textures.

Surface State Transport in 3D Topological Insulators

NADYA MASON (Presenter), University of Illinois at Urbana-Champaign

In this talk, I will discuss transport measurements of the topological surface state of the 3D TI Bi2Se3. By carefully configuring devices and controlling doping levels, we are able to demonstrate the unique properties of surface transport. In particular, we show that the supercurrent flows primarily through surface states in TI-superconductor junctions, that there is ballistic surface transport in nanowires exhibiting Aharonov-Bohm effects, and that finite momentum shifts of Cooper pairs is evident in superconducting junctions studied via Fraunhofer spectroscopy.

Accessing the intrinsic spin transport in a topological insulator with a four-probe scanning tunneling microscope

WONHEE KO (Presenter), GIANG NGUYEN, HOIL KIM, JUN SUNG KIM, AN-PING LI, XIAOGUANG ZHANG

Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

The electrical transport through topologically protected surface states in topological insulators is expected to exhibit superior mobility from prohibited backscattering and spin-polarized current from spin-momentum locking. However, access to the intrinsic transport properties of surface states remains an experimental challenge, due to the extrinsic effects such as device geometry and environmental contaminations. Here, we directly access the intrinsic surface conductance of topological insulators by using a four-probe scanning tunneling microscope to tune the crossover of bulk-to-surface conductance. By controlling the probe-spacing and temperature, we realize 100% surface conductance on the bulk single crystal of Bi2Te2Se. It allows us to measure more than an order of magnitude higher surface carrier mobility than the bulk, and a spin polarization approaching theoretically predicted value. A scattering-free spin transport is revealed at micrometer scale through topological surface states. In this manner, we achieve a direct and quantitative measurement of the intrinsic spin-polarized transport associated with topological surface states.

This work is supported by 2DCC-MIP (DMR-1539916), DOE (DE-SC0019064 and DE-SC0019331), ONR (N00014-15-1-2370), and the Alfred P. Sloan Research Fellowship.

This work was supported by the ONR under grant N14-17-1-3012 and the NSF under NSF-DMR 17-10437.

This research was performed at the Center for Nanophase Materials Sciences which is a DOE Office of Science User Facility.
4:54PM V02.00011: Acoustic Polaron on the Surface of Topological Insulators  JIANTAO KONG (Presenter), ALEXANDER SHVONSKI, KRZYSZTOF KEMPA, Boston College — We report a plasmon-polaron mode of a 2D electron gas occupying the surface states of a 3D topological crystal. This new, low-frequency, acoustic plasmon mode splits-off from the conventional spin-plasmon mode [1], as a result of the strong interactions between surface electrons and bulk phonons. We show that, like in the case of the conventional spin-plasmon, the scattering of this mode is strongly suppressed in some regions of the phase space. This signature of the topological protection leads to an Umklapp-free mode dispersion at the Brillouin zone boundary. Such a plasmon-polaron mode has indeed been recently observed in the topological metal Be 2 Se 3 [2].


5:06PM V02.00012: Energy Dependence of the Photogalvanic Effect in a Bi$_2$Se$_3$ Nanoflake Device* SEYYEDESADAF POURNIA (Presenter), GIRIRAJ JNAWALI, HOWARD E JACKSON, LEIGH SMITH, Department of Physics, University of Cincinnati, RYAN NEED, STEPHEN WILSON, Materials Department, University of California, Santa Barbara — Bi$_2$Se$_3$ is a prototypical topological insulator exhibiting gapped bulk states with topologically protected conducting surface states. Here we study the linear photogalvanic effect (LPGE) in a Bi$_2$Se$_3$ nanoflake device as a function of energy from 0.3 to 1.8 eV. At 800 nm (1.5 eV) with the laser polarized parallel to the current, we measure a positive or negative response when the laser excitation is close to one of the contacts. Fixing the laser at the peak response, we measuring the energy dependence of the LPGE as we scan from 0.3 eV to 1.8 eV. Peaks are seen at 0.35 eV, and other higher lying optical transitions. We modulate the 800 nm excitation laser between left and right circularly polarized light observing, when current flows, positive and negative peaks at the edge of the nanosheet in line scans, consistent with a spin-Hall effect.

*UC acknowledges NSF grants ECCS-1509706, DMR-1531373, and DMR-1507844. S.D.W. acknowledges the support of NSF DMR 1505549.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V03 DCMP GMAG: Topological Spin Liquids BCEC 107B - Etienne Lefrancois, Universite de Sherbrooke

2:30PM V03.00001: Solvable 3D classical statistical models and a spin-fermion mapping ZHIYUAN WANG (Presenter), KADEN R A HAZZARD, Rice University — In this talk, I will describe an exactly solvable classical statistical model on a 3D lattice. The model has two classical topological phases (one of which has been introduced previously [1]), and a finite-temperature phase transition between them. In contrast to prior 3D solvable statistical models [2], our system is much simpler, yet does not trivially reduce to a 2D model, and thus displays genuinely 3D correlations. Excitingly, this provides the first exactly solvable model in which to explore genuinely 3D critical phenomena; a caveat, however, is that the model Hamiltonian has imaginary terms. The construction and solution of this model are the first application of a new method that we introduce, developing ideas of [3], to map between a locally interacting fermionic Hamiltonian and a locally interacting spin Hamiltonian, in arbitrary dimension, in a simple way based on the use of algebraic isomorphisms. We expect that the spin-fermion mapping can be used not only for exact solutions, but for other applications such as numerical algorithms or perturbative calculations.

References:
Higher Order Bosonic Topological Phases in Spin Models

OLEG DUBINKIN (Presenter), TAYLOR HUGHES, Department of Physics and Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign — Motivated by the recent discovery of the higher order topological phases in the fermionic systems we propose a natural extension of these phases to bosonic systems. We discuss two bosonic models for a second-order topological phase protected by a global $Z_2 \times Z_2$ symmetry. One model is built from layers of an exactly solvable cluster model for a one-dimensional $Z_2 \times Z_2$ topological phase. The other is built from more conventional spin-couplings (XY or Heisenberg) and repeats the structure of the quadrupole model. These models host gapped, but topologically protected, edges, as well as protected corner modes that fall into a projective representation of the symmetry. Using Jordan-Wigner transformations we show that our models are both related to a bilayer of free Majorana fermions that form a fermionic second-order topological phase. In fact, the XY model was shown to be in exact correspondence with the fermionic Quadrupole model. We also discuss possible extension to 3D bosonic models for 2nd and 3rd order topological phases.

*We acknowledge support from the US National Science Foundation under grant DMR 1351895-CAR.

The Cyclotron resonance as a smoking gun for U(1) spin liquids with gapless fermions

PENG RAO (Presenter), INTI SODEMANN, Max Planck Institute for the Physics of Complex Systems — Certain U(1) spin liquids with gapless neutral fermions are expected to have the mind-boggling property that their optical conductivity vanishes as a power law of frequency. Thus, they are insulators to DC electric fields but without a "hard" optical gap, allowing them to absorb light at low frequencies. Additionally, they can also develop Landau levels in a magnetic field. In this work, we show that they can also have cyclotron resonance peaks in their optical spectrum analogous to metals, even though they are charge insulators. Interestingly, we have found that in contrast to metals, the principal Kohn harmonic of the cyclotron resonance is missing. The cyclotron resonance could therefore serve as a beautiful smoking gun test for the existence of these states which have been proposed in 2D organic materials and SmB$_6$.

A Microscopic Definition of the F-symbol

KYLE KAWAGOE (Presenter), MICHAEL LEVIN, University of Chicago — The theory of anyons is a powerful tool for studying interacting topological phases of matter in two spatial dimensions. In this approach, topological phases are characterized by the properties of their anyonic excitations --- in particular, the statistical phases associated with braiding or fusing anyons. Some of these statistical phases, however, are missing a precise definition that would allow for their computation from a microscopic Hamiltonian. In this talk, we will address this issue by giving a microscopic definition of the “F-symbol” --- one of the most poorly understood pieces of data that characterize anyons. We will show that our definition is consistent with known values of the F-symbol and can easily be applied to new systems as well.

*We thank the NSF for their support of this work under grant NSF DMR-1254741.

Symmetric gauge theories and Lieb-Schultz-Mattis-type constraints

XU YANG (Presenter), YING RAN, Boston College — It is known that certain symmetric gauge theories can only exist on the surface of a higher dimensional symmetry protected topological (SPT) state, in which case the symmetric gauge theory is anomalous. The anomaly class of such a gauge theory is represented by the bulk SPT index. Given an anomaly class, what kind of the symmetric gauge theories are allowed? Based on physical arguments and tensor-network constructions, we point out a sharp mathematical relationship between the symmetry properties of Abelian gauge theories and the anomaly class: the cup product. When the physical system hosts Lieb-Schultz-Mattis-type constraints, which is a specific type of anomaly class, our result sharply determines the physically allowed symmetric gauge theories via the preimage of the cup product. As applications, we algebraically compute the physically allowed skyrmion quantum numbers in various Neel states in 2+1D, and gauge charge/monopole projective representations in U(1) quantum spin liquids in 3+1D. We also compute the allowed Z2 gauge theories in several 2+1D quantum spin systems.

*XY and YR acknowledge support from the National Science Foundation under Grant No. DMR-1712128.
3:30PM V03.00006: A model of symmetry enriched topological phases and its symmetry breaking gapped boundaries* BOWEN SHI (Presenter), YUANMING LU, Ohio State University — We present a model of symmetry enriched topological phases (SET) based on the toric code model, with symmetry group being the tensor product of translation and a $Z_2$ onsite unitary symmetry. The symmetry does not permute anyon types and the model is in a nontrivial symmetry fractionalization class. We also discuss a gapped boundary with spontaneous symmetry breaking (SSB). This boundary condenses an anyon in the usual way, and the excitations at the boundary are domain walls. A domain containing an even number of effective spins could be created locally and a domain with an odd number of effective spins carry m charge. On a cylinder with an odd circumference, the $Z_2$ symmetry permutes the minimal entangled states (MESs). A boundary with odd circumference could absorb an m by flipping all its effective spins. This leads to a correlation of symmetry breaking sectors at the boundary to the bulk MES sectors.

*This work is supported by the National Science Foundation under Grant No. NSF DMR-1653769.

3:42PM V03.00007: Gapped Boundaries of (3+1)-Dimensional Gapped Quantum Liquids FAROOGH MOOSAVIAN, HEIDAR MORADI, Perimeter Institute, APOORV TIWARI (Presenter), Department of Physics, University of Zurich — We study gapped boundaries of $3+1$ gapped quantum liquids with topological order. From a field-theory perspective, we derive a generalization of the concept of Lagrangian subgroups to $3+1d$ and discuss properties of condensed and confined operators. More generally, we show that for a general $3+1d$ topological order defined by a 2-group $G$, the gapped boundaries are labeled by $(\mathbf{H}, \psi)$ such that $\mathbf{H}$ is a 2-subgroup of $G$ and $\psi$ is a cohomological twist. We interpret both these pieces of data physically. We study string and particle like excitations for gapped boundary theories and differentiate between anomalous and non-anomalous boundaries. Finally we study domain walls between two different boundaries.

3:54PM V03.00008: Thermal Transport Study of the Dimerized Quantum Magnet Strontium Copper Borate* COLIN TINSMAN (Presenter), ZIJI XIANG, LU CHEN, DMITRI MIHALIOV, Physics, University of Michigan, SARA HARAVIFARD, Physics, Duke University, LU LI, Physics, University of Michigan — Strontium Copper Borate (SrCu$_2$(BO$_3$)$_2$, or SCBO) has a unique crystal structure in which pairs of copper atoms with spin-1/2 states hybridize to form spin-1 dimers, making it a realization of the Shastry Sutherland model. This compound has a singlet ground state at each dimer separated by an energy gap from a triplet excited state. It is predicted that this system should contain topologically-protected edge states consisting of itinerant triplets known as triplons, making SCBO a bosonic topological insulator. Since these triplons do not carry charge, thermal measurements are required to observe them. We report on the field-dependent thermal conductivity of this material as well as our progress in observing triplon states using the thermal Hall effect.

*This work was mainly supported by the Office of Naval Research through the Young Investigator Prize under Award No. N00014-15-1-2382.

4:06PM V03.00009: Entanglement Spectra of Stabilizer Codes: A Window into Fracton Order and Sub-System Symmetry Protected Topological States* ALBERT SCHMITZ (Presenter), SHENG-JIE HUANG, University of Colorado, Boulder, ABHINAV PREM, Princeton University — We discuss the entanglement spectrum (ES) for stabilizer Hamiltonians with arbitrary weak local perturbations to contrast the entanglement features of gapped topological phases. In particular, we compare fracton order to both conventional topological order and sub-system symmetry-protected topological (SSPT) order. Our results show that non-local surface stabilizers (NLSS)—a set of symmetries of the Hamiltonian formed along the boundary of the entanglement cut—protect the universal non-local features of the ES. In conventional topological and fracton orders, some NLSS retain a form of topological invariance, whereas subsystem symmetric systems—fracton and SSPT phases—show a non-trivial geometric dependence corresponding to the sub-system symmetries. This demonstrates the interplay of geometry and topology in fracton phases as encoded in the ground states of the phase. We further show a version of the edge-entanglement correspondence in three dimensions.

*The authors acknowledge support from the Air Force Office of Scientific Research under award number FA9550-17-1-0183, the U.S. Department of Energy, Office of Science, Basic Energy Sciences (BES) under Award number DE-SC0014415 and the Princeton Center for Theoretical Science at Princeton University.
α-RuCl₃ and other materials with Kitaev spin interactions are thought to be proximate to spin liquid phases although they exhibit magnetic order under normal conditions. An important question is thus what features in the spectral function seen in neutron and THz spectroscopy can be understood as precursors of the nearby spin liquid. We address this question by using a simplified model: a strongly-anisotropic Kitaev honeycomb model supplemented by Ising interactions. In certain limits this model is exactly solvable and shows a topological transition with reduced dimensionality. Using numerical simulations and perturbation theory we extend our conclusions to the more generic situation.

Classification of Symmetry Enriched Topological Phases Under Spatial Groups Interchanging Anyons* TIANFU FU (Presenter), ANDRIY NEVIDOMSKYY, Department of Physics and Astronomy, Rice University, FIONA BURNELL, Department of Physics, University of Minnesota Twin Cities — Symmetry classification of 2d topologically ordered phases, such as topological spin liquids, has received much attention in the past. Previous works have focused on the trivial group action, where symmetries (spatial or internal) do not exchange the anyons. In this work, we extend classification to cases where the group action is nontrivial so that a subset of symmetry elements exchanges the anyon types. We formulate a general framework, based on the theory of group extensions, and apply it to the Z₂ topological phases considering the 17 2d space groups under all possible nontrivial group actions. We demonstrate that the symmetry localization is no longer possible, meaning that two-particle symmetry operations cannot be written as a direct product of the one-particle actions. Moreover, because the anyons are exchanged by the symmetry group, it is no longer possible to discuss symmetry fractionalization that would assign a symmetry class for each anyon independently, and instead projective representations of different anyon types become intertwined. We show that the symmetry classification can nevertheless be formulated in a mathematical rigorous way, and prove its application to the Wen plaquette model on a square lattice as a special case.

Foliated Quantum Field Theory of Fracton Order and String-Membrane-Net Condensation* KEVIN SLAGLE (Presenter), Physics, Caltech, DAVID AASEN, University of California, Santa Barbara, DOMINIC WILLIAMSON, Yale University — Foliated fracton order is a new kind of phase of matter which is similar to topological order, but where a layered structure, referred to as a foliation, plays an essential role (in addition to topology) and determines the mobility restrictions of the topological excitations characteristic of fracton phases. I will introduce a new kind of field theory to describe these phases: a foliated field theory. I will also introduce a new string-membrane-net condensation picture of these phases, which is analogous to the string-net condensation picture of topological order.

Thermal Hall effect in the quantum spin liquid candidate α-RuCl₃ ETIENNE LEFRANCOIS (Presenter), GAEL GRISSONNANCHE, University of Sherbrooke (Canada), PAULA J KELLEY, University of Tennessee (Knoxville, USA), CHRISTIAN BALZ, JIAQIANG YAN, Oak Ridge National Laboratory (USA), DAVID GEORGE MANDRUS, University of Tennessee (Knoxville, USA), STEPHEN NAGLER, Oak Ridge National Laboratory (USA), LOUIS TAILLEFER, University of Sherbrooke (Canada) — Kasahara et al. have reported the observation of a quantized thermal Hall conductivity κₓᵧ in the Kitaev spin-liquid candidate α-RuCl₃ at low temperature, when antiferromagnetic order is suppressed with an in-plane magnetic field [1]. The reported magnitude of κₓᵧ / T is consistent with the quantized value expected from topologically protected chiral edge currents of charge-neutral Majorana fermions [2]. If confirmed, this is major advance in the physics of quantum spin liquids. Given that the magnitude of both κₓᵧ and the longitudinal thermal conductivity κₓₓ varies greatly from sample to sample [3,4], we report further measurements of heat transport in α-RuCl₃, with the aim of shedding light on the factors responsible for this considerable variability.

5:06PM V03.00014: Electrical probes of the non-Abelian spin liquid phase in α-RuCl₃*  DAVID AASEN (Presenter), Kavli Institute for Theoretical Physics, University of California, Santa Barbara, ROGER MONG, Physics, University of Pittsburgh, BENJAMIN MATTHEW HUNT, Physics, Carnegie Mellon University, DAVID GEORGE MANDRUS, Department of Materials Science and Engineering, University of Tennessee, JASON ALICEA, Physics, California Institute of Technology — Recent thermal-transport experiments indicate that the Kitaev material α-RuCl₃ realizes a non-Abelian spin liquid with Ising topological order over a range of magnetic fields. We propose a series of measurements for electrically detecting the hallmark chiral Majorana edge states and bulk anyons in the spin-liquid phase — despite the fact that α-RuCl₃ is a good Mott insulator. In particular, we introduce circuits that exploit interfaces between electronic systems and α-RuCl₃ to convert physical fermions into emergent fermions, thus enabling analogues of transport probes of non-Abelian-anyon physics in topological superconductors. We further propose detection of individual bulk neutral fermions via a spin counterpart of charge sensing. Our results illuminate a partial pathway towards using Kitaev materials for topological quantum computation.

*DA is supported by the Gordon and Betty Moore Foundation, under the EPiQS initiative, Grant GBMF4304. BH acknowledges support from the Department of Energy Early Career program under award number DE-SC0018115. DGM acknowledges support from the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4416. JA acknowledges support from the Army Research Office Grant Award W911NF-17-1-0323; NSF grant DMR-1723367.

5:18PM V03.00015: Thermal Hall effect in square-lattice spin liquids*  RHINE SAMAJDAR (Presenter), Department of Physics, Harvard University, SHUBHAYU CHATTERJEE, Department of Physics, University of California, Berkeley, MATHIAS SCHEURER, SUBIR SACHDEV, Department of Physics, Harvard University — The extension of the notion of a topology-driven Hall effect to charge-neutral excitations has been an exciting theoretical development. Motivated by recent experimental observations in high-Tc cuprate superconductors in a magnetic field, we study the thermal Hall conductivity in materials with topological order, focusing on the contribution from the deconfined neutral gapped spinons in the insulating state. More specifically, we examine different Schwinger-boson mean-field ansätze for the Heisenberg antiferromagnet on the square lattice, allowing for both Dzyaloshinskii-Moriya interactions and additional terms that break time-reversal and reflection symmetries but preserve their product. We show that the bosonic bands acquire nontrivial Chern numbers and evaluate the thermal Hall coefficient. On top of a significantly enhanced conductivity, which should yield a sizable experimental signal, we also observe an anomalous contribution.

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Thursday, March 7, 2019 2:30 PM - 4:30 PM

Session V04 DMP DCOMP: Dielectric & Ferroic Oxides -- Structure, Phase Stability, and Competition II  BCEC 107C - Cyrus Dreyer, Stony Brook University - Tag(s): Focus

2:30PM V04.00001: Nature of the Phase Transitions Leading to Hybrid Improper Ferroelectricity in Ca₃X₂O₇*  SIZHAN LIU, HAN ZHANG, New Jersey Institute of Technology, SANJIT GHOSE, Brookhaven National Laboratory, MALI BALASUBRAMANIAN, Argonne National Laboratory, ZHENXIAN LIU, Brookhaven National Laboratory, SUYIN GRASS WANG, YUSHENG CHEN, Argonne National Laboratory, BIN GAO, JAEWOOK KIM, SANG-WOOK CHEONG, Rutgers University, ELIZABETH NOWADNICK, TREvor TYSOn (Presenter), New Jersey Institute of Technology — Detailed structural and optical measurements reveal that the tilt and rotation distortion relative to the high symmetry phase driving ferroelectricity in the system Ca₃X₂O₇ (X=Mn and Ti) condense at different temperatures. The condensation of the rotation and tilt distortions at distinctly different temperatures is unexpected. Experimental results, combined with DFT simulation of the atomic force constants, suggest that this loss of a polar state is driven by the relative strength of the A-O bonds to the X-O bonds. Raman measurements under isotropic pressure are used to assess the stability of the tilt and rotational distortions.

*This work is supported by NSF Grant No. DMR-1809931.
Lattice dynamics of hybrid improper ferroelectric (Ca,Sr)3Ti2O7*
DIPANSHU BANSAL (Presenter), Mechanical Engineering, Indian Institute of Technology Bombay, JENNIFER L NIEDZIELA, Oak Ridge National Laboratory, XING HE, TYSON LANIGAN-ATKINS, Mechanical Engineering and Materials Science, Duke University, AYMAN SAID, AHMET ALATAS, Argonne National Laboratory, DOUGLAS L ABERNATHY, Oak Ridge National Laboratory, YANG REN, Argonne National Laboratory, BIN GAO, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics & Astronomy, Rutgers University, OLIVIER DELAIRE, Mechanical Engineering and Materials Science, Duke University — In hybrid improper ferroelectric (Ca,Sr)3Ti2O7, the anharmonic coupling between a stable zone-center polar phonon mode and two unstable zone-boundary non-polar modes, and quasi-2D behavior of c-polarized acoustic modes are theoretically proposed but remain to be experimentally validated. We have performed comprehensive T-dependent single-crystal diffraction, calorimetry, and phonon measurements in (Ca,Sr)3Ti2O7 for x = 0, 0.6, and 0.9, including the behavior across the ferroelectric transition Tc. We also performed first-principles phonon simulations. Our results revealed a strong broadening but little shifting of mean phonon energy on heating across Tc. Among two unstable modes, rotational mode remains robust, but the tilt mode shows substantial softening on heating, consistent with previous studies. However, contrary to previous simulations, our momentum and energy resolved inelastic x-ray scattering measurements did not show a quadratic dispersion of acoustic modes, theoretically associated with a quasi-2D character. Our detailed lattice dynamics study enables to benchmark simulations of anharmonic phonons and associated thermodynamic properties such as thermal expansion and thermal conductivity.

*DOE BES DE-SC0016166, DE-AC02-06CH11357, DE-AC02-05CH11231.

Effect of cation ordering and pressure on n=2 Ruddlesden-Popper oxides from first principles
SRIRAM POYYAPAKKAM RAMKUMAR (Presenter), ELIZABETH NOWADNICK, Physics, New Jersey Institute of Technology — Octahedral tilts and rotations are ubiquitous in perovskite oxides and couple strongly to the electronic and magnetic properties. Furthermore, the interplay of octahedral rotations and layering can enable novel functionalities. For example, it has recently been shown that in n=2 Ruddlesden-Popper A3B2O7 layered perovskites, two octahedral rotations of different symmetries can induce a polarization via a trilinear coupling mechanism, known as hybrid improper ferroelectricity. While there has been extensive work on engineering octahedral rotation amplitudes and patterns in ABO3 perovskites, this has been much less studied in the Ruddlesden-Popper phases. By performing first-principles density functional theory calculations for a range of A3B2O7 materials, we explore two different approaches for engineering octahedral rotations in these systems. First, we consider the impact of A-site cation ordering (e.g. A2A′B2O7) on the energetics of a range of structural phases. Second, we elucidate the effect of hydrostatic pressure on octahedral rotation amplitudes and in turn on the energetics of the phases. We hence provide possible mechanisms to control the stability between polar and non-polar phases as well as tune structural distortions necessary for hybrid improper ferroelectricity.

First principles study of structure and electronic properties of a stannate Hybrid Improper Ferroelectric*
SHUTONG LI (Presenter), TURAN BIROL, Department of Chemical Engineering and Material science, University of Minnesota — Hybrid improper ferroelectricity provides a means to design lead-free ferroelectrics. Sr3Sn2O7, which is recently shown to be ferroelectric, can bring together the low electronic effective mass observed in stannates with the robust, switchable polarization of hybrid improper ferroelectricity. In this talk, we are going to present a systematically investigation on structure and electronic properties of Sr3Sn2O7 under biaxial strain. We find that the biaxial strain has significant effect on ground state structure, polarization switching, as well as the electronic structure.

*This work was supported primarily by the National Science Foundation through the University of Minnesota MRSEC under Award Number DMR-1420013.

Ultra-Small SrTiO3 Nanoparticles: Understanding the Polar Phases and Possible Ferroelectricity*
SIZHAN LIU, New Jersey Institute of Technology, NATHANIEL HURLEY, Stony Brook University, VITALI PRAKAPENKA, ERAN GREENBERG, Argonne National Laboratory, ZHENXIAN LIU, MILINDA ABEKYKOON (Presenter), Brookhaven National Laboratory, STANISLAUS S WONG, Stony Brook University, TREVOR TYSON, New Jersey Institute of Technology — Previous work revealed that 10 nm SrTiO3 (STO) nanoparticles host a polar and possibly ferroelectric phase stable under high pressure and over a broad range of temperatures. In this work, a full range of free standing nanoparticle samples between 2 and 60 nm have been studied and compared to bulk STO. Detailed structural and optical measurements are used to explore the evolution of the structure and corresponding phonon modes for varying temperatures and pressures. To understand the nature of the polar state and the existence of ferroelectricity, nonlinear optical measurements were conducted.

*This work is supported by NSF Grant No. DMR-1809931.
3:30PM V04.00006: Pressure Induced Unusual Multiferroicity in Perovskite PbCoO₃  
FENG LOU (Presenter), fudan university — We develop a global structure search approach to predict the ground state of magnetic materials based on the genetic algorithm. With this new approach, we predict that the unusual phase transitions can happen in the recently synthesized perovskite oxide PbCoO₃ [J. Am. Chem. Soc. 139, 4574 (2017)] under the different hydrostatic pressure. At low pressure, the PbCoO₃ phases are polar and weakly ferromagnetic, indicating that these phases are multiferroic. When the pressure is increased to 13 GPa, a polar-to-nonpolar transition takes place, which is associated with the charge order transition. The simultaneous A-site and B-site charge ordering pattern in the nonpolar phase is in agreement with the experimental result.

3:42PM V04.00007: In-situ lego-like construction of Ruddelsden-Popper surfaces using octahedra building blocks.* 
PRAHALD SIWAKOTI (Presenter), MOHAMMAD SAGHAYEZHIAN, ZHEN WANG, Department of Physics and Astronomy, Baton Rouge, Louisiana 70803, US, Louisiana State University, YIMEI ZHU, Department of Energy Science and Technology, Upton, New York 11973, USA, Brookhaven National Laboratory, ROSALBA FITTIPALDI, ANTONIO VECCHIONE, CNR-SPIN Unità di Salerno and Dipartimento di Fisica “E.R. Caianiello”, I-84084 Fisciano, Salerno, Italy, Università di Salerno, JIANDI ZHANG, Department of Physics and Astronomy, Baton Rouge, Louisiana 70803, US, Louisiana State University — The surface of Ruddelsden-Popper (RP) ruthenates provides a rich playground to study the emergent phenomena originating from the coupling of lattice, charge and spin, mediated through RuO₆ octahedron network. Because of the octahedra rotation, Sr₂RuO₄ surface shows a (√2 ×√2)R45° reconstruction. In addition to enhanced bulk-like octahedral rotation, Sr₃Ru₂O₇ surface displays octahedral tilt as well. In this work, using ultra-high-vacuum cleaved surface of Sr₂RuO₄ as a platform, we have sequentially grown different number of SrRuO₃ unit cells (u.c.) thin films, to mimic progression of “surface layer/s” of Sr₂RuO₄ to those of higher RP ruthenates (i.e. one u.c. is equivalent to Sr₃Ru₂O₇, two u.c. for Sr₄Ru₃O₁₀ surface and so on). Combining low energy electron diffraction with transmission electron microscopy, we systematically study the evolution of the lattice structure and discuss their properties.

*Supported by U.S.NSF under Grant No. DMR1608865.

3:54PM V04.00008: Computational discovery of Bi-based perovskite oxide polymorphs* 
OSWALDO DIEGUEZ (Presenter), AKANSHA SINGH, VIVEKA NAND SINGH, Tel Aviv University, ENRIC CANADELL, ICMAB-CSIC, JORGE INIGUEZ, LIST — In this paper we present our recent study[1] of the energy surface of BiScO₃, BiCrO₃, BiMnO₃, BiFeO₃, and BiCoO₃. In normal conditions, the bulk crystals of these materials show three very different variations of the perovskite structure: an antipolar phase, a rhombohedral phase with a large polarization along the space diagonal of the pseudocubic unit cell, and a supertetragonal phase with even larger polarization. With the aim of understanding the causes for this variety, we have used a genetic algorithm to search for minima in the energy surface of these materials. Our results show that the number of these minima is very large when compared to that of typical ferroelectric perovskites like BaTiO₃ and PbTiO₃, and that a fine energy balance between them results in the large structural differences seen. As byproducts of our search we have identified charge-ordering structures with low energy in BiMnO₃, and several phases with energies that are similar to that of the ground state of BiCrO₃. We have also found that a inverse supertetragonal phase exists in bulk, likely to be favored in films epitaxially grown at large values of tensile misfit strain.


*This work is supported by the Army Research Office through Grant No. W911NF-15-1-0017.
Correlation between Rietveld refinement yielded spontaneous polarization and experimentally obtained polarization data for Bi$_2$Mo$_{1-x}$W$_x$O$_6$ nanomaterials

*ANURAG PRITAM (Presenter), VAIBHAV SRIVASTAVA, Shiv Nadar University — Single phase perovskite Bismuth Molybadate, Bi$_2$Mo$_{1-x}$W$_x$O$_6$ [x=0.00, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.08 and 0.10] compositions were prepared using microwave sintering in air for 5 hours. The prepared compacted ceramics were characterized by X-ray diffraction (XRD) at room temperature and obtained XRD data was fitted for Rietveld refinement. The analysis of results confirmed the formation of the orthorhombic crystal structure with the space group of pca21. The atomic displacements for various sites a, b, c yielded close spontaneous polarization and indicated about schematic tilting of octahedrons atmospheric carbon adsorption as contamination on nano open surfaces. Reduced direction cosines indicated about increased strength of MoO$_6$ octahedrons against IR absorptions as shown by FTIR analysis, due to large oxygen bond strength of tungsten W than molybdenum Mo in BMO materials. Contaminated carbon groups were confirmed via additionally appearing FTIR peaks

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V05 DMP: Topological Superconductivity: General I

2:30PM V05.00001: Gauge-Invariant Variables Reveal the Quantum Geometry of Fractional Quantum Hall States

RUDRO BISWAS (Presenter), YINGKANG CHEN, Purdue University — We introduce the framework of gauge invariant variables to describe fractional quantum Hall (FQH) states, and prove that the wavefunction can always be represented by a unique holomorphic multi-variable complex function. We use this representation to combine the quantum geometry of charged particles in a magnetic field with the theory of coherent states and provide an analytical route, hitherto elusive, for deriving the properties of fractional quantum Hall phases from experimentally relevant microscopic Hamiltonians.

2:42PM V05.00002: Connecting the responses of quantum Hall states to gravitational and electric fields

YINGKANG CHEN (Presenter), GUODONG JIANG, RUDRO BISWAS, Physics and Astronomy, Purdue University — We introduce the framework of gauge invariant variables to describe quantum Hall states. This representation exploits novel aspects of the quantum geometry of charged particles in a magnetic field. We use this representation to reveal the geometric response of cyclotron orbits to non-uniform electric fields. We visualize the known connection between the gravitational response of quantum Hall states and their current response to nonuniform electric fields. We also conjecture that gravitational response is connected to the charge response of quantum Hall states to non-uniform electric fields.

2:54PM V05.00003: Dephasing dynamics of noisy Majorana-based qubits: Topological versus Andreev

RYAN MISHMASH, UC Berkeley, BELA BAUER, Microsoft Station Q, FELIX VON OPPEN, Freie University, JASON ALICEA (Presenter), Caltech — Topological quantum computation schemes encode quantum information nonlocally through non-Abelian anyons separated by macroscopic distances $L$, typically spanning the length of the constituent qubit device. This nonlocality renders topological qubits exponentially immune to dephasing from all sources of classical noise with operator support local on the scale of $L$. We explore detailed theoretical and numerical analyses of a time-domain Ramsey-type protocol for noisy Majorana-based qubits which is designed to validate this coveted topological protection in near-term nanowire devices. By assessing dependence on wire length $L$, our proposed protocol can sharply distinguish a bona fide Majorana qubit from one constructed from Andreev bound states, which can otherwise closely mimic the true Majorana scenario in local probes; for a fixed wire length, the protocol can also inform which scenario is likely realized. This proposed experiment requires no pulsing and only (relatively slow) measurement of two nearby Majorana modes for both initialization and readout---achievable, for example, by tunnel coupling to a nearby quantum dot---and thus serves as an enticing pre-braiding experiment aimed at quantifying the utility of Majorana-based qubits.

3:06PM V05.00004: Vortices in a Monopole Superconducting Weyl Semimetal

CANON SUN (Presenter), SHU-PING LEE, YI LI, Johns Hopkins University — A monopole superconductor is a novel topological phase of matter with topologically protected gap nodes as a result of Cooper pairs acquiring a non-zero Berry phase. We study the vortex structure of a Weyl semimetal with broken time-reversal symmetry in the monopole superconducting phase. Within each single isolated vortex, there exists a zero-energy Majorana bound state. The spin up and down components of the Majorana zero mode exhibit a non-trivial winding as a consequence of spin-orbit coupling.

*C.S., S.-P. L., and Y. L. are supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, Grant No. DE-FG02-08ER46544. Y. L. also acknowledges the support from the Alfred P. Sloan Research Fellowships.
3:18PM V05.00005: Phases and phase transitions in Kitaev ladders: symmetries and finite size scaling  KE WANG (Presenter), TIGRAN SEDRAKYAN, Physics, Umass Amherst — We discuss phases and phase transitions in Kitaev ladders with and without interactions. In the noninteracting system, the phase diagram of a two-leg Kitaev ladder with time-reversal (TR) symmetry contains three distinct phases possessing 0, 2, and 4 Majorana edge modes and one tricritical line separating these phases. We discuss the finite-size corrections to energy along the tricritical line and finite-size scaling away from it which exhibits a non-trivial universal shape. Upon breaking the protecting TR symmetry, we find that the phase described by four Majorana edge modes in TR protected state crosses over to a trivial phase with no edge modes via symmetry broken path G in parameter space. The energy gap remains finite along G indicating that Z-classification (class BDI) reduces to Z_2 (class D) classification upon breaking of TR. Remarkably, the finite size scaling function in the vicinity of a critical line separating trivial phase from the nontrivial one in TR broken phase, exhibits a new nontrivial behavior. We also show that there is a phase transition of Ising universality in an interacting Kitaev chain and discuss its implications in ladder models.

3:30PM V05.00006: Spin-Orbit Coupling Effects on the Current-Phase Relation of a DC SQUID*  ALEX MATOS ABIAGUE (Presenter), NARAYAN MOHANTA, Department of Physics and Astronomy, Wayne State University, WILLIAM ANDREW MAYER, SICHAO YU, KAUSHINI WICKRAMASINGHE, JOSEPH YUAN, JAVAD SHABANI, Department of Physics, New York University, IGOR ZUTIC, Department of Physics, State University of New York at Buffalo — We consider a dc superconducting quantum interference device (SQUID) composed of two Josephson junctions (JJs) in a loop threaded by a magnetic flux. The JJs are built on a heterostructure where a semiconducting two-dimensional electron gas (2DEG) is partially covered by a conventional superconductor. Due to proximity effect, superconductivity is induced in the covered 2DEG, while the uncovered region remains in the normal state. Top gates allow for tuning both the carrier density and Rashba spin-orbit coupling (RSOC) strength in the normal region of each JJ, individually. We theoretically investigate the effects of self-inductance, charge density, and RSOC as well as their distinctive signatures on the current-phase relation (CPR) of the device. The sizable effects of RSOC tuning on the CPR make the considered SQUID a promising device not only for the detection of RSOC fields in proximitized materials but also for studying tunable topological transitions and the potential formation of Majorana bound states upon the application of a Zeeman field. The theoretical results are in good agreement with recent experimental measurements of the CPR in SQUIDs composed of InAs/Al JJs.


3:42PM V05.00007: Spontaneous Edge Current in Higher Chirality Superconductors*  XIN WANG (Presenter), ZHIQIANG WANG, CATHERINE KALLIN, McMaster University — The effects of finite temperature, Meissner screening and surface roughness on the spontaneous edge current for higher chirality quasi-two dimensional superconductors are studied in the continuum limit using the quasiclassical Eilenberger equations. We find that the total spontaneous current is non-zero at finite temperature T and maximized near $T=T_c/2$, where $T_c$ is the transition temperature, although it vanishes at $T=0$. In the presence of surface roughness, we observe a surface current inversion in the chiral d-wave case that can be understood in terms of a disorder induced s-wave pairing component in the rough surface regime. This conclusion is supported by a Ginzburg-Landau analysis. However, this current inversion is non-universal beyond the continuum limit as demonstrated by self-consistent lattice Bogoliubov-de Gennes calculations.

*This work is supported by NSERC and CIFAR.

3:54PM V05.00008: Unconventional Josephson Effect in a topological Kondo insulator  XUECHENG YE, Physics, Missouri University of Science and Technology, JACOB COOK, Physics, University of Missouri, ERIK HUEMILLER, Physics, University of Illinois at Urbana-Champaign, AARON D FINCK, IBM Thomas J. Watson Research Center, POUYAN GHAEMI MOHAMMADI, Physics, The City College of New York, CUNY, THOMAS VOJTA, Physics, Missouri University of Science and Technology, SHANTA SAHA, JOHNPIERRE PAGLIONE, Physics, University of Maryland, CIHAN KURTER (Presenter), IBM Thomas J. Watson Research Center — Proximity-induced superconductivity in three dimensional (3D) topological insulators forms a new quantum phase of matter and harbors exotic quasiparticles such as Majorana bound states. One of the biggest drawbacks of the commonly studied 3D topological insulators is having conducting bulk that obscures the role of surface states. Introducing superconductivity in topological Kondo insulators such as SmB$_6$ is particularly promising due to their robust insulating bulk at low temperatures. In this work, we develop an unconventional Josephson junction by coupling superconducting Nb leads to the surface states of a SmB$_6$ crystal. We observe a distinct critical current at low temperatures that exhibits a Fraunhofer diffraction pattern with the application of an out-of-plane magnetic field. The appearance of Shaprio steps under microwave irradiation gives further evidence of a Josephson Effect. The Fraunhofer patterns show an anomalous hysteresis with magnetic field sweep direction suggesting coexistence of ferromagnetism with superconductivity in the topological surface states of SmB$_6$. The experimental work will advance the current understanding of topologically nontrivial superconductors and emergent states associated with such unconventional superconducting phases.
4:06PM V05.00009: Simulating the spectral response of a Majorana-transmon device  ANNA KESELMAN (Presenter), BERNARD VAN HECK, BELA BAUER, Microsoft — We perform a numerical study of a toy-model for the Majorana-transmon device, obtaining its spectral response across the topological phase transition. To this end, we employ the DMRG and TEBD techniques. We model the superconducting wires on either end of the Josephson junction as spinful fermions hopping on a 1D lattice with Rashba spin-orbit coupling in a Zeeman field perpendicular to the spin-orbit direction. As the Zeeman field is increased and the superconducting wires are driven across the topological phase transition, we observe the splitting of the plasma mode due to the zero-energy Majorana modes forming at the ends of the wires. Interestingly, the spectral function is largely unaffected by the gap closing in the bulk of the superconducting wires. When the length of the junction is finite, additional Andreev bound states can form. We show that the appearance of these states gives rise to additional spectral lines, obscuring the signatures of the topological phase.

4:18PM V05.00010: Prediction of Hall effects from geometrical properties of the Fermi surface  ELENA DERUNOVA (Presenter), MAZHAR ALI, Max Planck Institute for Microstructure Physics, YAN SUN, Max Planck Institute for Chemical Physics of Solids, STUART S PARKIN, Max Planck Institute for Microstructure Physics — Recently, the intrinsic Hall effects (e.g. spin, anomalous, and planar Hall effects) have been investigated as topological properties stemming from a material's electronic band structure. In our work we show the connection of these properties to the local geometry of the Fermi surface. Specifically we introduce the concept of geodesic flow of the Fermi surface and using this concept we link the Berry curvature term in the semiclassical equation of motion of Bloch electrons with the evolution of the Riemannian metric in the tangent bundle of the Fermi surface. As an example, we consider the comparison of Kubo formalism for the spin Hall effect with the geometrical analysis of the Fermi surface for Pt and Beta-W. Such geometrisation of topological properties can be applied to an algorithmic material search in crystallographic databases, paving the way for high throughput analysis of materials and topologically driven properties.

4:30PM V05.00011: Parafermions in the Fractional Quantum Hall Spin Transitions*  JINGCHENG LIANG (Presenter), GEORGE E SIMION, LEONID ROKHINSON, YULI LYANDA-GELLER, Purdue University — Parafermion zero modes are promising for universal topological quantum computation because of their richer non-Abelian braiding properties. However, physical systems that are predicted to host these exotic excitations are rare and difficult to realize in experiments. In this work, we show that parafermion zero modes can emerge in the spin transitions in the fractional quantum Hall regime. Exact diagonalization of the Hamiltonian in a disk and torus geometries demonstrates formation of counter-propagating edge states with different spin polarizations at a boundary between polarized and unpolarized ν=2/3 phases. By analytical and numerical methods we find conditions for parafermion zero modes to emerge when these edge states are coupled to an s-wave superconductor. The phase diagram shows that the parafermionic phase, which is represented by the six-fold ground state degeneracy, is separated from gapped phases by a topological phase transition. Parafermion modes in fractional quantum Hall systems coupled to s-wave superconductors are experimentally feasible.

*Authors acknowledge support by the U.S. Department of Energy, Office of Basic Energy Sciences under Award DE-SC0010544 (Y.L-G and J.L.); by the Office of Naval Research Award N000141410339 (Y.L-G, G.S. and LPR).

4:42PM V05.00012: Blurring the boundaries between topological and non-topological phenomena in dots*  DENIS CANDIDO (Presenter), Sao Carlos Institute of Physics at the University of Sao Paulo, MICHAEL FLATTÉ, Department of Physics and Astronomy and Optical Science and Technology Center, University of Iowa, CARLOS EGUES, Sao Carlos Institute of Physics at the University of Sao Paulo — In this work we investigate the electronic and transport properties of topological and non-topological InAs0.85Bi0.15 quantum dots (QDs) described by a Bernevig-Hughes-Zhang (BHZ) model with cylindrical confinement, i.e., "BHZ dots". We analytically show that (it non-topological) dots have discrete helical edge states, i.e., Kramers pairs with spin-angular-momentum locking similar to topological dots. These unusual and unexpectedly non-topological edge states are geometrically protected due to confinement in a wide range of parameters and are not guaranteed to exist by the bulk-edge correspondence. In addition, for a conduction window with four edge states, we find that the two-terminal conductance G vs. the QD radius R and the gate Vg controlling its levels shows a double peak at 2e^2/h for both topological and trivial BHZ QDs. Our results blur the boundaries between topological and non-topological phenomena for conductance measurements in small systems such as QDs thus showing an equivalence between the BHZ QDs in different topological phases.

*This work was supported by CNPq, CAPES, UFRN/MEC, FAPESP, PRP-USP/Q-NANO and the Center for Emergent Materials, an NSF MRSEC under Award No. DMR-1420451.
Topological Superconductivity in a Phase-Controlled Josephson Junction

HECHEN REN (Presenter), FALKO PIENTKA, SEAN J HART, ANDREW T PIERCE, MICHAEL KOSOWSKY, Harvard University, LUKAS LUNCZER, RAIMUND SCHLERETH, BENEDIKT SCHARF, EWELINA HANKIEWICZ, LAURENS W MOLENKAMP, Wuerzburg University, BERTRAND I. HALPERIN, AMIR YACOBY, Harvard University — While signatures of Majorana bound states have been observed in one-dimensional systems, there is an ongoing effort to find alternative platforms that do not require fine-tuning and can be easily scalable. Using a Josephson junction made of HgTe quantum well coupled to thin-film aluminum, we can tune between a trivial and a topological superconducting state by controlling the phase difference $\phi$ and an applied in-plane magnetic field, as we measure the tunneling conductance at the edge of the junction. At low magnetic fields, we observe a minimum in the tunneling spectra near zero bias, consistent with a trivial superconductor. As the field increases, the tunneling conductance develops a zero-bias peak which persists over a range of $\phi$ that expands systematically with increasing magnetic fields. Consistent with theoretical predictions for this system, our observation establishes this system as a promising platform for realizing topological superconductivity and for creating and manipulating Majorana modes in two-dimensional systems.

Army Research Office: W911NF-18-1-0316. DoD NDSEG.
German Research Foundation, EU ERC-AG program, the Bavarian Ministry of Education, and the Elitenetzwerk Bayern program “Topologische Isolatoren”.

Proximity-Induced Superconductivity in a Topological Crystalline Insulator

BRYAN RACHMILOWITZ (Presenter), HE ZHAO, Boston College, JOHN SCHNEELOCH, RUIDAN ZHONG, GENDA GU, Brookhaven National Lab, ILIJA ZELJKOVIC, Boston College — Inducing superconductivity at the surface of topological crystalline insulators (TCIs) can give rise to new topologically protected phases. These phases are theorized to be different than the ones observed at the surface of superconducting $\mathbb{Z}_2$ topological insulators. Here we report molecular beam epitaxy synthesis of a heterostructure involving a prototypical TCI SnTe and a high temperature superconductor Fe(Fe,Se). Using low-temperature scanning tunneling microscopy and spectroscopy, we provide a strong evidence for proximity-induced superconductivity at the surface of a few bi-layer thick SnTe films. Our work provides a platform for investigating the emergent phenomena in superconducting TCIs.

*We gratefully acknowledge the support from the Army Research Office Grant No. W911NF-17-1-0399 and the NSF Grant No. 1654041.

Spectroscopic visualization of aluminum islands in the Coulomb blockade regime deposited on InAs nanowires

HAIM BEIDENKOPF (Presenter), JONATHAN REINER, ABHAY K NAYAK, AMIT TULCHINSKY, YUVAL OREG, HADAS SHTRIKMAN, NURIT AVRAHAM, Weizmann Institute of Science — Hybrid InAs/Al nanowires are studied as a platform for topological superconductivity. Here we visualize spectroscopically the Coulomb blockade regime of aluminum islands deposited in situ on InAs nanowires. We find no changes in the chemical potential before and after aluminum deposition signifying absence of charge doping and of local band bending at the immediate vicinity of the islands. On the aluminum islands we find Coulomb blockade features typical to double barrier tunneling junction. From these we characterize the resistive and capacitive properties of the nanowire-aluminum interface. We identify a finite barrier for tunneling of electrons across that interface. Our observations strongly reflect on the ability to induce robust topological superconductivity by deposition of aluminum on InAs nanowires.

*We acknowledge funding by the ERC (Project TOPONW).

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V06 DCMP: Correlations in Helium and Hydrogen

BCEC 109A - Paul Sokol, Indiana University

Bloomington
2:30PM V06.00001: Neutron Scattering Studies of superfluid helium confined in preplated nanoporous materials.*

PAUL SOKOL (Presenter), GARFIELD WARREN, Indiana University Bloomington, TIMOTHY PRISK, NCNR, NIST, NATHAN NICHOLS, ADRIAN DEL MAESTRO, Physics, University of Vermont — One dimensional systems have been of long standing interest due to a profound difference from their 2 and 3 dimensional counterparts whose properties can be described in terms of quasi-particles. This quasi-particle picture breaks down completely in one dimension where the fundamental excitations are collective and described by the universal Tomonaga-Luttinger liquid (TLL) theory. Superfluid helium confined in one-dimensional templated materials, such as MCM-41, provide an attractive model system for studying the properties of a TLL. Unfortunately, the pore size attainable in these materials is too large to reach the one-dimensional limit. Preplating these porous materials with an adsorbate offers a route to smaller pore sizes where one-dimensional confinement can occur. We will present the results of neutron scattering studies of the excitations of superfluid helium confined in MCM-41 preplated with a monolayer of Argon. The observed scattering departs dramatically from the bulk superfluid and may be consistent with a TLL.

*This work was supported by the NSF through grants DMR-1809027 and DMR-1808440

2:42PM V06.00002: The Damping of a Micro-electromechanical Resonator in the Presence of Quantum Turbulence in He II*

COLIN BARQUIST (Presenter), WENGUANG JIANG, KEEGAN GUNTHER, YOONSEOK LEE, University of Florida, HO BUN CHAN, Physics, Hong Kong University of Science and Technology — A micro-electromechanical plate resonator was immersed in ⁴He down to 13 mK at saturated vapor pressure. The resonator consists of a 125x125x2 μm³ plate suspended 2 μm above a substrate. Due to its small mass and large surface area it is sensitive to vortices in the fluid and vortices pinned to the surface of the device. The device is studied in the presence of fully developed quantum turbulence generated by a quartz tuning fork and in the presence of remnant vortices pinned to the device. Specifically, the velocity dependent damping of the device in these conditions is measured and reported.

*This work is supported by the National Science Foundation through DMR-1708818.

2:54PM V06.00003: The Use of ³He in Obtaining Ultra-Low Temperatures at the NHMFL High B/T Facility*

ANDREW WOODS (Presenter), CHAO HUAN, NAOTO MASUHARA, JIAN-SHENG XIA, NEIL SULLIVAN, Department of Physics and NHMFL, University of Florida — The High B/T Facility at the National High Magnetic Field Laboratory (NHMFL) provides access to unique ultra-low temperature, high magnetic field and ultra-quiet environments. The facility operates nuclear demagnetization refrigerators capable of reaching 0.5 mK at 16 T and 0.1 mK at 8 T. This enables user experiments in diverse fields including ultrasound studies, FQHE studies in tilted fields, high sensitivity NMR, high sensitivity dielectric measurements, sub-mK susceptibility measurements, novel states (Bose glass, Wigner crystals) and studies of superfluid ³He. These experiments require that the ³He, the electrical leads and samples be efficiently cooled to ultra-low temperatures. In this talk I will discuss the use of liquid ³He in cooling at the High B/T Facility, experimental platforms developed to make best use of this method, recent experimental results obtained, and potential future developments.

*Work supported by the NSF DMR-164479 and the State of Florida

3:06PM V06.00004: Mass Flux Measurements in Solid 4He.*

VALENTYN RUBANSKYI, ROBERT HALLOCK (Presenter), University of Massachusetts Amherst — We previously explored the characteristics of mass flux through solid 4He that takes place from one superfluid-filled reservoir to the other through a solid-filled experimental cell off the melting curve (1). We measured flow characteristics that appear to match expectations for one-dimensional Luttinger-Liquid conductivity (2) and we documented the effects that various concentrations of 3He impurity have on the temperature dependence of the flow (3). Our most recent experiments show that reducing the interface between superfluid helium in the Vycor rods and solid helium reduces the flux and that significantly blocking the cross section of the channel filled with solid 4He further suppress the flux. These results further support the possibility that the observed mass flux is due to the superfluid cores of edge dislocations.


*Support: NSF DMR 1205217 and 1602616.
3:18PM V06.00005: Dynamics of 1D $^3$He adsorbed in $^4$He plated MCM-41: NMR Studies*  
JOHNNY ADAMS (Presenter), MARC L. LEWKOWITZ, CHAO HUAN, NAO TO MASUHARA, NEIL S. SULLIVAN, Department of Physics and NHMFL, University of Florida — We report the results of NMR studies of the dynamics of $^3$He confined to 1D in the interior of the hexagonal nanochannels of MCM-41. The walls of the MCM-41 were coated with a monolayer of $^4$He and $^3$He was added afterwards to form a 1D $^3$He line density of 0.1 Å$^{-1}$. The nuclear spin-lattice relaxation times were measured for temperatures 0.050 $<$ $T$ $<$ 3.0 K. A distinct peak is observed at 95 mK which is interpreted as the expected maximum of the “spin-drag” relaxation time predicted by theory for $T$ = 2$T_F$ where $T_F$ is the Fermi degeneracy temperature.

*The measurements were carried out at the High B/T facility of the National High Magnetic Field Laboratory which is supported by the NSF through DMR-1644779 and the State of Florida.

3:30PM V06.00006: Measuring Corrections to the Amplitude Mode Masses in Superfluid $^3$He*  
MAN NGUYEN (Presenter), ANDREW ZIMMERMANN, WILLIAM HALPERIN, Northwestern University — Superfluid $^3$He has a rich spectrum of collective modes with both massive (gapped) and massless (gapless) excitations. The masses of these modes can be precisely measured with acoustic spectroscopy and fit to theoretical models to extract interaction strengths of the underlying superfluid. Prior comparisons between theory and experiment accounted for Fermi-liquid effects, $f$-wave interactions, and the strong-coupling energy gap. However, strong-coupling corrections to the mode mass itself were not included. In this work, we employ a simple procedure to incorporate these corrections$^{[1]}$ to the mode which improve the determination of the $f$-wave pairing strength, $(1/x_3)$. Results from several independent experiments are brought into better agreement with the improved theoretical model.


*This work is supported by the National Science Foundation, DMR 1602542

3:42PM V06.00007: The Polar Phase of Superfluid $^3$He in the Limit of Small Anisotropy*  
ANDREW ZIMMERMANN (Presenter), MAN NGUYEN, WILLIAM HALPERIN, Northwestern University — The polar phase of superfluid $^3$He is characterized by a single orbital component of the p-wave order parameter, and is favored by the breaking of the orbital rotational symmetry. This can be achieved by introducing anisotropic impurities into pure superfluid. Prior comparisons between theory and experiment accounted for Fermi-liquid effects, $f$-wave interactions, and the strong-coupling energy gap. However, strong-coupling corrections to the mode mass itself were not included. In this work, we employ a simple procedure to incorporate these corrections$^{[1]}$ to the mode which improve the determination of the $f$-wave pairing strength, $(1/x_3)$. Results from several independent experiments are brought into better agreement with the improved theoretical model.


*This work is supported by the National Science Foundation, DMR-1602542.

3:54PM V06.00008: Simplified calculations of the frequencies of Higgs modes in superfluid $^3$He-B using N-point Padé approximants  
JOHN PALIOTTA (Presenter), JOSEPH W SERENE, Georgetown University — Previous calculations of the frequencies of the Higgs modes in superfluid $^3$He-B have been done on the real-frequency axis, most recently using the Keldysh formalism. Recently Sauls and Mizushima$^{[1]}$ showed how the unperturbed weak-coupling mode frequencies can be found by solving the imaginary-frequency version of the kinetic equation, followed by standard analytic continuation to real frequencies and evaluation of remaining integrals there. We show that perturbed frequencies due to magnetic fields or strong-coupling effects can be calculated on the imaginary axis and the final results can then be obtained, to high accuracy, by N-point Padé approximants, which greatly simplifies these calculations. $^{[1]}$J.A. Sauls and Takeshi Mizushima, On the Nambu fermion-boson relations for superfluid 3He, Phys. Rev. B 95, 094515 (2017)
4:06PM V06.00009: Quantum Monte Carlo simulation of superfluid helium confined inside pre-plated nanoporous materials*  
NATHAN NICHOLS (Presenter), ADRIAN DEL MAESTRO, University of Vermont, TIMOTHY PRISK, NCNR, NIST, GARFIELD WARREN, PAUL SOKOL, Indiana University Bloomington — In one spatial dimension, enhanced thermal and quantum fluctuations should preclude the existence of any long range ordered superfluid phase of matter. Mesoporous ordered silica-based structures such as the molecular sieve MCM-41 offer an experimental route towards the observation of this effect through the physical confinement of superfluid helium inside quasi-one-dimensional channels. However, the angstrom-scale coherence length of the wavefunction away from the bulk superfluid transition temperature requires novel nano-engineering approaches to reach the one-dimensional limit. In this talk we will describe ab initio quantum Monte Carlo simulations of superfluid helium confined inside MCM-41 that has been pre-plated with adsorbates to reduce the diameter of the confining media. We will describe how the choice of adsorbate (e.g. argon, neon, krypton) can be modified to obtain different types of helium structures inside the pores. Phase and density correlations may be further tuned via the external pressure of helium with the goal of realizing an emergent one-dimensional quantum liquid.

*This work was supported by the NSF through grants DMR-1809027 and DMR-1808440. Simulations performed on the Vermont Advanced Computing Core were partially supported by NSF grant OAC-1827314.

4:18PM V06.00010: Anomalous attenuation of piezoacoustic surface waves by liquid helium thin films*  
KOSTYANTYN NASYEDKIN (Presenter), HEEJUN BYEON, JUSTIN LANE, LIANGJI ZHANG, NIYAZ BEYSENGULOV, REZA LOLOEE, JOHANNES POLLANEN, Michigan State Univ — We report on the experimental observation of an anomalously high attenuation of high frequency surface acoustic waves (SAW) by thin films of liquid 4He [1]. The piezoelectric SAW propagate along the surface of a lithium niobate substrate, which is covered by liquid helium films of varying thicknesses. When the thickness of the helium layer is much larger than the wavelength of the SAW on the substrate the SAW attenuation is dominated by emitting compressional waves into the bulk liquid, in good agreement with theory and previous measurements. However, for sufficiently thin helium films, we find that the SAW attenuation significantly exceeds that measured with the substrate submerged in bulk liquid. Possible mechanisms for this enhanced attenuation are discussed.


*This work was supported by the NSF (Grant no. DMR-1708331).

4:30PM V06.00011: Elastic Anomaly of Helium, Hydrogen and Neon Films on Disordered Substrate  
TAKAHIKO MAKIUCHI (Presenter), KATSUYUKI YAMASHITA, MICHIHIRO TAGAI, YUSUKE NAGO, KEIYA SHIRAHAMA, Keio University — We report systematic elasticity measurements of helium (4He and 3He), hydrogen (H2, HD, D2) and neon films physisorbed on a porous glass substrate. The elastic constant and dissipation as a function of temperature were measured by means of torsional oscillator technique with changing the film coverage. We have found that films of all species (4He, 3He, H2, HD, D2, Ne) showed an increase of the elastic constant accompanied by a dissipation peak at low temperatures, which we call the elastic anomaly. This suggests that any atomic and molecular films adsorbed on disordered substrates exhibit a crossover from a soft state at high temperature to a stiff state at low temperature. Only 4He and 3He films exhibit insulator-(super)fluid quantum phase transitions at critical coverages corresponding to about 2 atomic layers. Helium films below those critical coverages are in a gapped and compressible ground state. Hydrogen films show multiple dissipation peaks depending on the film coverage. The elastic anomaly of neon has single dissipation peak, and the peak temperature did not decrease below 5 K which signifies quantum phase transition does not occur in neon films.

4:42PM V06.00012: Transition in Wave Behavior on a Superfluid Vortex at Large Excitation Amplitude*  
RENA ZIEVE (Presenter), JOSEPHINE SPIEGELBERG, ANDREW DIGGS, University of California, Davis — We study a single quantized vortex stretched between a wire and the wall of a cylindrical container. The wire serves both as a probe and as a means of exciting the system. Vibrating the wire creates oscillations along the vortex. One consequence of these oscillations is that the spot where the vortex joins the wire moves. This in turn changes the normal modes of the wire's vibration, which lets us detect the vortex location. We find a qualitative change in behavior at sufficiently large excitation. Below the crossover, clear vortex waves are induced, with amplitude near the expected threshold for instability. As the excitation increases, the signal becomes much less regular. Higher-frequency oscillations appear, as well as a slow feature that may indicate recurrence. The vortex appears to undergo significant length changes during the process.

*This work was supported in part by NSF through the award PHY-1560482.
The condensed phases of molecular hydrogen are systems of fundamental importance in quantum many-body physics. Zero-point motion makes a large contribution to the kinetic energy and mean-squared displacement $<u^2>$ of hydrogen molecules in the liquid and solid phases. At present, there is a significant disagreement between theory and experiment about the relative importance of thermal and quantum effects near the liquid-solid phase transition of parahydrogen. Path Integral Monte Carlo calculations predict that $<u^2>$ increases as the melting temperature is approached from below, implying a combination of thermal and quantum effects [Phys. Rev. B 95, 104518 (2017)]. However, an inelastic neutron scattering study of the rotational transitions in solid parahydrogen suggests that $<u^2>$ is independent of temperature, and is thus determined by quantum-mechanical zero-point motion alone [Phys. Rev B 86, 144524 (2012)]. In this presentation, we report new inelastic neutron scattering measurements of $<u^2>$ obtained using the ARCS spectrometer at Oak Ridge National Laboratory and the DCS spectrometer at the NIST Center for Neutron Research.

The effect of confinement on the thermodynamic properties and phase transitions of liquids and solids in confinement has been of long-standing interest and recent interest has focused on the effects of dimensionality. Hydrogen has been of interest due to the importance of quantum effects, in particular zero-point motion, and has been studied extensively in a variety of porous media. Templated porous materials, such as MCM-41, provide an attractive model system for studying the effects of confinement due to their highly uniform one-dimensional pores with variable pore size. Unfortunately, the minimum pore diameter is typically limited to a few nanometers which limits our ability to approach the one-dimensional limit. We will present measurements of adsorption isotherms and heat capacity of hydrogen confined in MCM-41. We will present the results for both bare MCM-41 and samples that have been preplated with noble gases to reduce the effective pore diameter.

*This work was supported by the NSF through grants DMR-1809027.

Supersolids are theoretically predicted quantum states that break the continuous rotational and translational symmetries of liquids while preserving superfluid transport properties. Over the last decade, much progress has been made in understanding and characterizing supersolid phases through numerical simulations for specific interaction potentials. The formulation of an analytically tractable framework for generic interactions still poses theoretical challenges. By going beyond the usually considered quadratic truncations, we derive a systematic higher-order generalization of the Gross-Pitaevskii mean-field model in conceptual similarity with the Swift-Hohenberg theory of pattern formation. We demonstrate the tractability of this broadly applicable approach by determining the ground state phase diagram and the dispersion relations for the supersolid lattice vibrations in terms of the potential parameters. Our analytical predictions agree well with numerical results from direct hydrodynamic simulations and earlier quantum Monte-Carlo studies. The underlying framework is universal and can be extended to anisotropic pair potentials with complex Fourier-space structure.
2:30PM V07.00001: Tricritical Points in the Underscreened Anderson Lattice Model*  PETER RISEBOROUGH (Presenter), Temple University, ANA LAUSMANN, Fisica, USFM Santa Maria, ELEONIR CALEGARI, Fisica, USFM Santa Maria, SERGIO G MAGALHAES, Fisica, UFRG, Porto Alegro — We report calculations on the Underscreened Anderson Lattice Model that has been proposed to describe the Hidden Ordered phase of URu2Si2. Since the proposed Hidden Ordered Phase is associated with a spin-orbital density wave, in which the spins condense in a spontaneously chosen plane, the magnetic properties become anisotropic in the low temperature phase. The anisotropy is similar to that found by magnetic torque measurements. We examine the field-temperature phase diagram. At zero field, the transition to the Hidden Ordered phase is second order. The application of a magnetic field has the effect of reducing the transition temperature towards zero. However, at a critical value of the applied field, the transition becomes first-order in agreement with high field measurements. We present an analysis of the tricritical point, which shows that the upper critical dimension of the model is reduced to d=3. Therefore, the transition may be reasonably described by a Gaussian approximation.

*This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Materials Science through award DE FG02 ER45872

2:42PM V07.00002: Schwinger boson approach to the Kondo lattice model  JIANGFAN WANG (Presenter), YUNG-YEH CHANG, Department of Electrophysics, National Chiao Tung University, CHUNG-YU MOU, Department of physics, National Tsing-Hua University, STEFAN B. KIRCHNER, Department of Physics, Zhejiang University, SILKE BUEHLER-PASCHEN, Institute of Solid State Physics, Vienna University of Technology, CHUNG-HOU CHUNG, Department of Electrophysics, National Chiao Tung University — The microscopic mechanism of the heavy-fermion systems close to anti-ferromagnetic quantum critical point constitutes an outstanding open problem in correlated electron systems. To address this issue, we employ a distinct route from the dynamical mean-field theory by solving the 2D Kondo-Heisenberg model via a dynamical large-N multichannel Schwinger boson approach. We identify the quantum critical point separating the anti-ferromagnetic long-ranged ordered and the heavy Kondo-screened Fermi-liquid phases. Various thermodynamical observables near criticality show non-Fermi liquid behaviors and agree qualitatively well with the experiments seen in CeCu_{6-x}Au_x and YbRh_2Si_2.

2:54PM V07.00003: The splitting of electrons on the Kondo lattice  EOIN QUINN (Presenter), LPTMS, Université Paris-Sud, ONUR ERTEN, Arizona State University — We demonstrate that strong correlations in Kondo lattice models can be organised around a splitting of the electronic degree of freedom. This provides a fresh perspective on the behaviour of local moment systems, in which the formation of a heavy fermion band and violation of the Luttinger sum rule are naturally accounted for.

3:06PM V07.00004: The 4f electron character on core-level spectroscopies of AuCu_3-type Ce intermetallics  NORIMASA SASABE (Presenter), Japan Synchrotron Radiation Research Institute — The 3d transition metal compounds and 4f rare earth compounds show attractive phenomena, such as superconductivity and Kondo effect, due to strong electron correlations among localized 3d and 4f electrons. Especially, the 4f electron state of Ce intermetallics causes the various phenomena of Ce intermetallics, Kondo effects and magnetic ordering, for example. X-ray core-level spectroscopy is an efficient technique to investigate the electronic states of strongly correlated systems. Recent years, experimental techniques have been rapidly developing and, especially, the progress in experimental resolution has enabled us to observe fine spectral features, which were not formerly observed. These advantages will enable us to observe spectral fine features related with the 4f electron state related to Kondo and/or magnetic ordering of the Ce intermetallics. In this study, we discuss 4f electron character of AuCu_3-type Ce intermetallics by means of X-ray spectra, especially paying attention on the polarization dependence and the incident photon energy. In order to simulate the electronic state of AuCu_3-type Ce intermetallics, we use an impurity Anderson model including realistic valence structure.

3:18PM V07.00005: Synchrotron-Mossbauer study of the pressure-driven magnetic evolution in EuGa_4  ANJANA KRISHNADAS (Presenter), Okinawa Institute of Science and Technology, STEPHEN ARMSTRONG, Caltech, WENLI BI, JIYONG ZHAO, ESEN ALP, APS, Argonne National Lab, RIKI KOBAYASHI, MASATO HEDO, TAKAO NAKAMA, YOSHICHIKA ONUKI, University of The Ryukyus, THOMAS F ROSENBAUM, Caltech, YEJUN FENG, Okinawa Institute of Science and Technology — Rare-earth Eu compounds represent an intriguing class of magnetic materials that provide a competing playground of Kondo physics, RKKY exchange interactions, and valence evolution. Here, we explore the evolution of antiferromagnetism under pressure via synchrotron-based Mossbauer spectroscopy. Contrary to previous electrical transport results, our observation provides direct evidence of a magnetic ground state at high pressure, continuous through a first order phase transition at 5 GPa and persisting to at least 13.6 GPa. We discuss this result in the framework of a potential interaction between evolution of the valence condition and an increase in the ordering temperature.
3:30PM V07.00006: Order fractionalization and the two channel Kondo lattice  
ARI WUGALTER (Presenter), YASHAR KOMIJANI, PIERS COLEMAN, Physics and Astronomy, Rutgers, The State University of New Jersey — The symmetric two-channel Kondo lattice, involving two separate conduction electron seas, interacting with a lattice of local moments, provides an idealized model for the novel cubic heavy electron superconductors, PrX$_2$Al$_2$O$_{10}$, (X=Ti, Va) and UBe$_{13}$. There are many indications that two-channel Kondo lattice is unstable to the development of broken channel symmetry, in which the Kondo effect develops selectively in one channel giving rise to a \( \text{\textbackslash channel magnetization} \) We study this novel phase using the large N expansion. One of the remarkable features of the resulting mean-field theory, is the emergence of a two-component spinor describing the channel magnetization, suggesting the possibility of order fractionalization. Using the large N expansion, we show that the long-wavelength physics of the two-channel Kondo lattice is described by the principle chiral model, in which the skyrmion density of the channel magnetization couples to the difference of the electromagnetic and internal gauge fields. We will discuss the implications of these results for the order fractionalization conjecture and possible observable consequences.

3:42PM V07.00007: Impact of Rashba spin-orbit coupling on f-electron materials  
YOSHIHIRO MICHISHITA (Presenter), ROBERT PETERS, Kyoto University — We study the interplay between Rashba spin-orbit coupling (RSOC) and the Kondo screening in noncentrosymmetric f-electron materials. We show that the Kondo interaction of the f-electrons becomes anisotropic at high temperatures due to the RSOC in these materials leading to a suppression of the Kondo temperature. However, an isotropic Kondo effect is restored at low temperature which leads to a complete Kondo screening. We furthermore demonstrate that the Kondo effect has influence on the Rashba splitting in the band structure, which becomes temperature dependent. We show that although f electrons are localized at temperatures above the Kondo temperature, already at these temperatures a helical spin polarization emerges. With decreasing temperature, the Kondo screening occurs, which leads to drastic changes in the band structure. Remarkably, these changes in the band structure depend on the helical spin polarization. For strong RSOC, we observe that one of the helical bands becomes gapped at low temperature and a helical half-metal is formed.

3:54PM V07.00008: Charge and heat transport in a charge 2 channel Kondo device  
LARS FRITZ (Presenter), GERWIN VAN DALUM, Physics, Utrecht University, ANDREW K MITCHELL, School of Physics, University College Dublin — Recently, the charge two channel effect was realized in an experimental setup for the first time. Remarkably, the scaling curve of the critical conductance was measured over many decades and was in excellent agreement with theoretical calculations. In this talk we focus on the heat transport in the setup. We theoretically show a violation of the Wiedemann-Franz law and point out an interesting connecting to the central charge of one dimensional Majorana fermions.

4:06PM V07.00009: Coupled charge-Kondo quantum dot devices  
ANDREW K MITCHELL (Presenter), School of Physics, University College Dublin — Exquisite experimental control over exotic states of quantum matter has recently been demonstrated in charge-Kondo quantum dot devices [1,2]. These systems constitute a new paradigm for circuit realizations of fundamental models of quantum criticality, with essentially perfect agreement between experiment and theory for fractionalized two-channel and three-channel Kondo physics [2,3].

Here we study theoretically a device comprising two charge-Kondo quantum dots, coupled together by a quantum point contact. This system is the first step towards constructing more elaborate nanodevices using charge-Kondo building blocks, which could eventually lead to quantum simulations of exotic lattice models.

Depending on dot occupation, different variants on the classic two-impurity Kondo model can be realized, and clear signatures of quantum criticality show up in measurable conductance as a function of tunable parameters.


*AKM acknowledges funding from the Irish Research Council through the Laureate Award "Quantum-boosted functionality in single-molecule transistors" (IRCLA/2017/169).
Using this model, we investigated the effect of interaction and the applied magnetic field near the half-filled region. We consider a Two-Impurity Anderson model. In the non-interacting limit (U=0), the AB orbital is decoupled from the site at the center of the wire and to its nearest neighbors. Taking advantage of the dot symmetry, we work with the bonding and anti-bonding (AB) levels resulting from the symmetric and antisymmetric combinations of the dot levels. We consider a Two-Impurity Anderson model. In the non-interacting limit (U=0), the AB orbital is decoupled from the conduction band and is hence a BIC. For U≠0, our Numerical Renormalization-Group results show that the interaction couples the bonding and anti-bonding orbitals and hence broadens the latter. The RKKY interaction between the magnetic moments of the two dots can either be ferro- or antiferromagnetic, to form a singlet or a triplet, which affects the formation of the Kondo cloud. In the strongly particle-hole asymmetric coupling limit, the AB orbital is reduced to a singly occupied level that is decoupled from the continuum, i.e., a Spin-BIC.

*DFG-SFB 1170, project B04 and ERC-StG-TOPOLECTRICS-336012.

4:42PM V07.00012: Correlation effects in the emergence of Bound Spin State in the Continuum* LUIZ H. GUESSI (Presenter), LUIZ OLIVEIRA, Sao Carlos Institute of Physics, University of Sao Paulo — Bound States in the Continuum (BICs) are states with localized wave-function even though lying in the continuum. Here, we explore theoretically the emergence of a Spin-BIC in a system comprising two identical quantum dots side-coupled to a quantum wire. The dots are symmetrically coupled to the site at the center of the wire and to its nearest neighbors. Taking advantage of the dot symmetry, we work with the bonding and anti-bonding (AB) levels resulting from the symmetric and antisymmetric combinations of the dot levels. We consider a Two-Impurity Anderson model. In the non-interacting limit (U=0), the AB orbital is decoupled from the conduction band and is hence a BIC. For U≠0, our Numerical Renormalization-Group results show that the interaction couples the bonding and anti-bonding orbitals and hence broadens the latter. The RKKY interaction between the magnetic moments of the two dots can either be ferro- or antiferromagnetic, to form a singlet or a triplet, which affects the formation of the Kondo cloud. In the strongly particle-hole asymmetric coupling limit, the AB orbital is reduced to a singly occupied level that is decoupled from the continuum, i.e., a Spin-BIC.

*Supported by FAPESP (2015/26655-9) and CNPq (grant 312658/2013-3).

4:54PM V07.00013: Maximally Localized Wannier Orbitals and the Anderson Impurity Model for Twisted Bilayer Graphene* XI CHEN (Presenter), Center for Computational Quantum Physics, Flatiron Institute, EMANUEL C GULL, Physics, University of Michigan, ANDREW MILLIS, Center for Computational Quantum Physics, Flatiron Institute — We developed an effective Anderson impurity model to describe the low energy electronic properties of the twisted bilayer graphene. By using the method of selectively localizing Wannier orbitals, we construct a model that captures the key energetic and symmetry features of the original low energy bands and is possible for further calculation with non-perturbative methods. Using this model, we investigated the effect of interaction and the applied magnetic field near the half-filled region.

*This project is funded by Simons Foundation.
5:06PM V07.00014: Impact of Quenched Disorders on The Holstein Model*

BO XIAO (Presenter), University of California, Davis, NATANAELE DE CARVALHO COSTA, Instituto de Física, Universidade Federal do Rio de Janeiro, EHSAN KHATAMI, Department of Physics and Astronomy, San Jose State University, GEORGE BATROUNI, Institut de Physique de Nice, Universite de Nice-Sophia Antipolis, RICHARD THEODORE SCALETTAR, University of California, Davis — Over the last few decades, there has been considerable interest in the effects of disorder on the competition between superconductivity and charge order wave (CDW) in underdoped cuprates. Similar questions arise in the study of the interplay of polaron formation and ordering with Anderson localization in disordered electron-phonon systems such as superconducting peroskites, and colossal magnetoresistance manganites. Many interesting phenomena are observed including non-Fermi liquid behavior and metal-insulator transitions (MIT) due to the opening of a CDW gap or due to Anderson localization. The combination of electron-phonon coupling and randomness leads to rich phase regimes as the phonon frequency $\omega$, electron-phonon coupling $\lambda$ and disorder strength $\Delta$ vary. Here we present results from the DQMC method for the two-dimensional disordered Holstein model. We focus on the dependence of sizes of domain walls as well as the correlation length of density fluctuations. We also show the results for the temperature dependence of the conductance and compare to existing dynamical mean field theory results.

*R.T.S. and B.X. were supported by the DOE Grant DE-SC0014671, E. K. was supported by the NSF Grant DMR-1609560 and OAC-1626645, N.C. was supported by the Brazilian funding CNPq and CAPES.

5:18PM V07.00015: Universal entanglement of typical states in constrained systems*

SIDDHARDH MORAMPUDI, ANUSHYA CHANDRAN, CHRISTOPHER LAUMANN (Presenter), Boston University — We develop a formalism to exactly evaluate the bipartite entanglement of random states in large Hilbert spaces with local and global constraints. We solve the simplest class of constraints which includes the much studied Rydberg-blockaded/Fibonacci chain. The resulting entanglement spectra may be classified into `phases' depending on their singularities. Our results predict the entanglement of infinite temperature eigenstates in thermalizing constrained systems and provide a baseline for numerical studies.

*C.R.L. and A.C. acknowledge support from the Sloan Foundation through Sloan Research Fellowships, and from the NSF through grants PHY-1752727 and DMR-1752759, respectively.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V08 DCMP: Superconducting Heterostructures and Quantum Dots

BCEC 150 - James Eckstein, Univ of Illinois - Urbana

2:30PM V08.00001: Towards the Kitaev model with quantum dot chains in semiconductor nanowires

HAO WU (Presenter), PO ZHANG, JUN CHEN, University of Pittsburgh, SASA GAZIBEGOVIC, ROY OP HET VELD, GHADA BADAWY, ERIK P. A. M. BAKKERS, Eindhoven University of Technology, SERGEY M FROLOV, University of Pittsburgh — We experimentally explore whether chains of quantum dots in semiconductor nanowires can be used to emulate important one-dimensional Hamiltonians such as Kitaev model that describes a topological p-wave superconductor. In our devices, quantum dots are electrostatically confined in an InSb nanowire by an array of closely spaced narrow gates. Quantum dots are coupled to NbTiN superconducting leads. We study transport properties and magneto-spectroscopy of Andreev bound states in these quantum dots with magnetic fields parallel to the nanowire axis. Up to three quantum dots and three superconducting contacts are defined in a single nanowire. We compare results from quantum dot chain experiments to those of experiments on closely related Majorana nanowires.

2:42PM V08.00002: Analytical Noise Spectra Calculations for High-Temperature Superconducting Nanowires*

COREY OSTROVE (Presenter), LINDA E REICHL, University of Texas at Austin — In this talk we present analytical results for the noise spectrum of a superconducting heterostructure formed by a high temperature superconductor (HTS) nanowire. The scattering matrix is calculated from first principles using the Bogoliubov-de Gennes equations with appropriate boundary conditions and without the Andreev approximation. The current-current correlation function is calculated directly using the scattering coefficients and from this the noise spectrum (and in particular the shot noise contribution) is generated. The effects of the anisotropy of the order parameter in the scattering properties of the structures are investigated. We also consider some of the consequences of the quasi-1d geometry in terms of the restrictions on allowed propagation modes through the nanowire. Recent advances in materials synthesis have brought the production of high quality HTS nanowires closer widespread use in the design and construction of superconducting devices, which makes theoretical characterization of these structures of particular importance.

*The authors thank the Robert A. Welch Foundation (Grant No. F-1051) for support of this work.
2:54PM V08.00003: Competition between the Yu-Shiba-Rusinov and Kondo screening in double quantum dot based Cooper pair splitters*  
IRENEUSZ WEYMANN (Presenter), KACPER WRZESNIEWSKI, Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — The Andreev transport properties of double quantum dot based Cooper pair splitters with one superconducting and two normal leads are studied theoretically in the Kondo regime. The influence of the Yu-Shiba-Rusinov screening resulting from superconducting pairing correlations on the local density of states, Andreev transmission coefficient, and Cooper pair splitting efficiency is thoroughly analyzed. It is shown that finite superconducting pairing potential quickly suppresses the SU(2) Kondo effect, which can however reemerge for relatively large values of coupling to superconductor. In the SU(4) Kondo regime, a crossover from the SU(4) to the SU(2) Kondo state is found as the coupling to superconductor is enhanced.


3:06PM V08.00004: Andreev Blockade in a Double Quantum Dot with a Superconducting Lead*  
DAVID PEKKER (Presenter), SERGEY M FROLOV, Department of Physics and Astronomy, University of Pittsburgh — A normal metal source reservoir can load two electrons onto a double quantum dot in the spin-triplet configuration. We show that if the drain lead of the dot is a spin-singlet superconductor, these electrons cannot form a Cooper pair and are blockaded on the double dot. We call this phenomenon Andreev blockade because it arises due to suppressed Andreev reflections. We identify transport characteristics unique to Andreev blockade. Most significantly, it occurs for any occupation of the dot adjacent to the superconductor, in contrast with the well-studied Pauli blockade which requires odd occupations. Andreev blockade is lifted if quasiparticles are allowed to enter the superconducting lead, but it should be observable in the hard gap superconductor-semiconductor devices. Andreev blockade should be considered in the design of topological quantum circuits, hybrid quantum bits and quantum emulators.

*DP and SMF acknowledge Charles E. Kaufman foundation, NSF PIRE-1743717. SMF acknowledges NSF DMR-1252962, NSF DMR-1743972, ONR and ARO.

3:18PM V08.00005: Transport in superconductor/ferromagnet multilayers with Néel-type domain walls*  
XAVIER PALERMO, ANKE SANDER (Presenter), SOPHIE D'AMBROSIO, SALVATORE MESORACA, K BOUZEHOUANE, SOPHIE COLLIN, NICOLAS REYREN, VINCENT CROS, JAVIER VILLEGAS, Unité Mixte de Physique, CNRS, Thales, Université Paris-Sud, Université Paris-Saclay, Palaiseau, France — We experimentally investigate the coupling between magnetization reversal and magneto-transport in the metallic superconductor/ferromagnet multilayers. The ferromagnet consists itself of a multilayer in which the materials' stack (Co, Pt, Ir and Ru) is engineered in order to tailor i) the magnetic domains morphology and ii) their size. These variables have a striking effect on the magneto-transport properties below the superconducting critical temperature. In particular, in the presence of magnetic domains the mixed-state resistance is radically diminished to an extent that depends on the domains structure morphology. Contrarily, when the ferromagnet is saturated, an excess resistance is observed. Furthermore, and interestingly, those changes in the longitudinal resistance are accompanied by an anomalous transverse resistance which strongly depends on the applied magnetic field direction and magnetic history. We will discuss the mechanisms contributing to that behavior, which include Pearl vortex pinning and generation, as well as inhomogeneous superconductivity induced by the magnetic template.

*Work supported by the ERC grant No. 647100, French ANR grant ANR-15-CE24-0008-01 and COST “Nanoscale Coherent Hybrid Devices For Superconducting Quantum Technologies” - Action CA16218.

3:30PM V08.00006: Anisotropic purity of entangled photons from Cooper pairs in heterostructures*  
HAE-YOUNG KEE (Presenter), JACOB S. GORDON, University of Toronto — It has been theoretically proposed that a forward-biased p-n junction with a superconducting layer (P-N-S) would produce pure, polarization-entangled photons due to inherent spin-singlet pairing of electrons. However, any heterostructure interface generically induces Rashba spin-orbit coupling, which in turn generates a mixed singlet-triplet superconducting order parameter. Here we study the effect of triplet pairing on the purity of photons produced through Cooper pair recombination. A unique directional dependence of the state purity is found: in a triplet superconductor with fixed d-vector, pure, entangled photons are produced when the photon polarization axis is parallel to d, with diminished purity for other directions. Induced triplet pairing in a singlet superconductor is shown to degrade the state purity, while induced singlet pairing in a triplet superconductor is shown to enhance the production of entangled pairs. These considerations may aid the design of functional devices to produce entangled photons.

*This work was supported by the Natural Sciences and Engineering Research Council of Canada, and the Center for Quantum Materials at the University of Toronto.
3:42PM V08.00007: Subgap states and Dynes parameter in hard-gap tunnel junctions* CHRISTIAN SCHELLER (Presenter), Department of Physics, Univ of Basel, MARIO PALMA, Department of Physics, University of Wisconsin-Madison, LUCAS CASPARIS, Niels Bohr Institute, Univ of Copenhagen, TARAS PATLATIUK, Department of Physics, Univ of Basel, LUCA CHIROLLI, IMDEA-Nanoscience, ANNA V FESHCHENKO, Department of Applied Physics, Aalto University, DARIO MARADAN, Physikalisch-Technische Bundesanstalt (PTB), MATTHIAS MESCHKE, JUKKA P PEKOLA, Department of Applied Physics, Aalto University, DOMINIK ZUMBUHL, Department of Physics, Univ of Basel — Normal metal – insulator - superconductor (NIS) tunnel junctions are the basic building blocks for Josephson junctions, superconducting qubits and many other applications. Ideally, the single particle current is zero within the superconducting gap; while photon assisted tunneling (PAT) can lead to sub-gap currents (Dynes parameter). Here, we examine hard gap NIS tunnel junctions in a well filtered and shielded environment where PAT is negligible. We observe discrete, sharp current steps in the sub-gap regime which can be used as a primary thermometer, in excellent agreement with regular NIS thermometry [1], but cooling as low as 4 mK on a nuclear refrigerator [2]. In an in-plane magnetic field, the steps exhibit Zeeman splitting with g = 2 and display diamagnetic shifts. We model the steps as geometric resonances within the weakly disordered normal metal giving enhanced Andreev reflection due to multiple reflections. The model shows that disorder is a possible microscopic origin for Dynes-type linear leakage current.


*This work acknowledges founding from the Swiss NSF, NCCR QSIT, the Swiss Nanoscience Institute, the European Microkelvin Platform

3:54PM V08.00008: Induced superconducting gap vs. barrier thickness in hybrid Al/Al0.15In0.85As/InAs heterostructures SAEED FALLahi (Presenter), Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907 USA, RAY KALLAHER, SERGEI GRONIN, Microsoft Quantum at Station Q Purdue, Purdue University, West Lafayette, Indiana 47907, USA, CANDICE THOMAS, TIAN WANG, Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907 USA, GEOFFREY C. GARDNER, Microsoft Quantum at Station Q Purdue, Purdue University, West Lafayette, Indiana 47907, USA, GEOR W. WINKLER, Station Q, Microsoft Research, Santa Barbara, California 93106-6105, USA, JAN GUKELBERGER, JOHN GAMBLE, Quantum Architecture and Computation Group, Microsoft Research, Redmond, Washington 98052, USA, ANDREY ANTIPOV, ROMAN LUTCHYN, Station Q, Microsoft Research, Santa Barbara, California 93106-6105, USA, ANTONIO FONIERI, ALEXANDER WHITICAR, ASBJORN C. C. DRACHMANN, Eoin C O'FARRELL, FABRIZIO NICHELE, CHARLES M MARCUS, Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark, MICHAEL MANFRA, Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907 USA — The two dimensional electron gas (2DEG) in InAs proximitized by aluminum (Al) is a promising platform for scaling topological qubits based on Majorana zero modes. The 2DEG lies in an InAs quantum well and is separated from the epitaxial Al layer by a barrier of Al0.15In0.85As with thickness d. Due to hybridization between the wave functions of 2DEG and superconductor, the strength of induced gap in the 2DEG will largely depend on the barrier thickness. We present a systematic study of the strength of the induced gap in hybrid Al/Al0.15In0.85As/InAs superconductor/semiconductor heterostructures as a function of barrier thickness. We estimate the induced gap by analyzing multiple Andreev reflections in SNS junctions and differential conductance measurement in S-QPC-N junctions in the tunneling regime. We compare our results with self-consistent calculations of induced gap for our particular geometry.

4:06PM V08.00009: Interaction of Skyrmions and Pearl Vortices in Superconductor-Chiral Ferromagnet Heterostructures* SAMME DAHIR, ANATOLY F. VOLKOV, ILYA EREMIN (Presenter), Ruhr University Bochum — We investigate a hybrid heterostructure with magnetic skyrmions (Sk) inside a chiral ferromagnet interfaced by a thin superconducting lm via an insulating barrier. The barrier prevents the electronic transport between the superconductor and the chiral magnet, such that the coupling can only occur through the magnetic elds generated by these materials. We nd that Pearl vortices (PV) are generated spontaneously in the superconductor within the skyrmion radius, while anti-Pearl vortices (PV) compensating the magnetic moment of the Pearl vortices are generated outside of the Sk radius, forming an energetically stable topological hybrid structure. Finally, we analyze the interplay of skyrmion and vortex lattices and their mutual feedback on each other. In particular, we argue that the size of the skyrmions will be greatly a ected by the presence of the vortices o ering another prospect of manipulating the skyrmionic size by the proximity to a superconductor.

*The authors acknowledge support from the DFG Priority Program SPP2137, Skyrmionics, under Grant No. ER 463/10.
4:18PM V08.00010: Tunneling Anomalous Hall Effect (TAHE) in Ferromagnet/Superconductor Junctions* ANDREAS COSTA (Presenter), University of Regensburg, ALEX MATOS ABIAGUE, Wayne State University Detroit, JAROSLAV FABIAN, University of Regensburg — The competition of two antagonistic interactions, spin-singlet superconducting pairing and ferromagnetic exchange, in one heterojunction leads to extraordinary phenomena. Owing to the additionally broken inversion symmetry, not only the interplay of superconductivity and ferromagnetism, but also the induced strong interfacial spin-orbit fields (SOFs) offer interesting subjects for experimental and theoretical investigations; several studies unraveled an intriguing impact of interfacial SOFs on transport already in normal-conducting systems, e.g., TAMR1 and TAHE2 effects. Our theoretical work focuses on ferromagnet/superconductor junctions, demonstrating the existence of a superconducting TAHE effect. While the effect's fundamental characteristics are comparable to what has been found in the normal-conducting analog2, our numerical simulations predict a much larger tunability of the TAHE conductance in the superconducting scenario, mostly due to the presence of Andreev reflection. Together with a simultaneously generated transverse supercurrent response in the superconductor, these findings might offer an interesting future perspective for experimentalists.

1 PRL 99, 056601 (2007)
2 PRL 115, 056602 (2015)

*This work was supported by ENB IDK Top. Insulators and DFG SFB 1277 (B07).

4:30PM V08.00011: Optimizing spin-triplet supercurrent through a ferromagnetic Josephson junction* VICTOR AGUILAR (Presenter), JOSEPH A GLICK, REZA LOLOEE, WILLIAM P PRATT, NORMAN OWEN BIRGE, Michigan State University — Ferromagnetic Josephson junctions show promise for application to energy efficient cryogenic memory [1]. Both spin-singlet and spin-triplet supercurrents are being studied by our group for this purpose. Engineering adjacent F layers in a three-layer system to have perpendicular magnetizations allows singlet pairs to convert to spin-aligned triplet pairs. Recent work in our group exploited a synthetic antiferromagnet (SAF) with perpendicular magnetic anisotropy (PMA) for the middle F layer [2]. These junctions exhibit phase control [2], but have a low critical current when compared to singlet junctions. To make the triplet junction a viable option for memory we show that removing the SAF while maintaining the PMA increases the critical current. To estimate the fraction of the supercurrent carried by spin-triplet pairs in our junctions, we also fabricate comparison junctions with the order of the F layers shuffled to suppress generation of spin-triplet pairs.


*This research is supported by the ODNI, IARPA, via US Army Research Office contract W911NF-14-C-0115.

4:42PM V08.00012: Geometry and pairing-symmetry effects in superconductor/half-metallic ferromagnet vertical junctions* SALVATORE MESORACA (Presenter), SOPHIE D'AMBROSIO, XAVIER PALERMO, Unité Mixte de Physique, CNRS/Thales, Université Paris Sud, Université Paris-Saclay, Palaiseau, France, DAVID SÁNCHEZ-MANZANO, FABIAN CUELLAR, GFMC, Dpto. Física de Materiales, Universidad Complutense de Madrid, Spain, SOPHIE COLLIN, ANKE SANDER, Unité Mixte de Physique, CNRS/Thales, Université Paris Sud, Université Paris-Saclay, Palaiseau, France, JACOBO SANTAMARIA, GFMC, Dpto. Física de Materiales, Universidad Complutense de Madrid, Spain, JAVIER VILLEGAS, Unité Mixte de Physique, CNRS/Thales, Université Paris Sud, Université Paris-Saclay, Palaiseau, France — The interactions between superconductors (S) and ferromagnets (F) are widely studied nowadays due to the possibility of obtaining equal-spin triplet pairing, which is immune to the exchange field and therefore can propagate over long distances into the F. This effect has fundamental interest as well as a potential for spintronic applications. In this context, we study vertical S/F/S junctions made of a half-metallic F (La_{0.7}Sr_{0.3}MnO_{3} or La_{0.7}Ca_{0.3}MnO_{3}) with either a d-wave S (YBa_{2}Cu_{3}O_{7}) or a s-wave one (Mo_{80}Si_{20}), aiming to understand to role of the pairing symmetry on the proximity effect and, particularly, on the generation of equal-spin triplet correlations. We will compare low-temperature magneto-transport measurements made in vertical micro-junctions having different geometries, namely three-probe vs. a novel four-probe junction scheme, which is designed to separate conductance features linked to the top electrode's contact resistance from effects due to transport across the entire S/F/S junction.

*Work supported by the ERC grant N. 647100 “SUSPINTRONICS“ and French ANR grant ANR-15-CE24-0008-01 “SUPERTRONICS“.
4:54PM V08.00013: Transport in ferromagnetic/superconducting heterostructures* EVAN MOEN (Presenter), ORIOL TVALLS, University of Minnesota — We consider the transport theory in nano-scale ferromagnetic/superconducting heterostructures with multiple ferromagnetic layers. We do so using fully self consistent, numerical methods in the clean limit. Many properties unique to these systems arise due to the proximity effects between ferromagnets and superconductors. We determine the conductance in each spin channel and analyze its dependence on the magnetic misalignment angle between the ferromagnets, as well as on other physical parameters pertinent to multi-layered systems. We quantitatively describe some of these properties and we discuss our results in connection to proposed experiments.

*This work was supported in part by DOE Grant No. DE-SC0014467

5:06PM V08.00014: Thermoelectric effects in superconductor-ferromagnetic hybrids* KIRSTEN BLAGG (Presenter), ZACHARY PARROTT, Colorado Sch of Mines, MICHAEL P LILLY, Sandia National Labs, MEENAKSHI SINGH, Colorado Sch of Mines — The conflicting spin order in superconductor-ferromagnetic systems has lead to a host of fascinating phenomena. However, most experimental studies have focused on electrical and spin transport measurements. While there have been numerous theoretical predictions of exciting thermal phenomena, thermal properties of these systems remains largely unexplored. In particular, thermoelectric effects which are usually negligible in superconductors have been predicted to increase dramatically in superconductor hybrid structures when in the presence of a spin splitting exchange field. This presentation will focus of the experimental design and measurement of the Seebeck coefficient in superconductor-ferromagnetic hybrids.

*This work is supported by NSF DMR 1807583, user proposal 2018AC0054 at the Center for Integrated Nanotechnologies at Sandia National Laboratories, and startup funds from the Colorado School of Mines.

5:18PM V08.00015: High-critical-field superconducting heterostructures using anodic oxidation ASBJØRN DRACHMANN (Presenter), HENRI J SUOMINEN, Center for Quantum Devices, University of Copenhagen, ALEX R HAMILTON, School of Physics, University of New South Wales, SERGEI GRONIN, TIAN WANG, GEOFFREY GARDNER, CANDICE THOMAS, Department of Physics and Astronomy, Purdue University, ALEXANDER WHITICAR, ANTONIO FORNIERI, Center for Quantum Devices, University of Copenhagen, MICHAEL MANFRA, Department of Physics and Astronomy, Purdue University, CHARLES M MARCUS, FABRIZIO NICHELE, Center for Quantum Devices, University of Copenhagen — In-situ growth of Al on top of shallow InAs 2DEG heterostructures gives close to perfect proximity effect [1-2]. The transparent super/semi interface combined with customizable 2DEG lithography hold promise to many interesting applications, e.g. topological quantum computation [3-4].

When the aluminum is chemically etched the underlying InAs is degraded by surface impurities. [2] Instead of etching the aluminum, here we show that controllably oxidizing the Al through anodic oxidation (AO) gives up to a factor 2 increase in InAs mobility and Quantum Hall effect emerges before 3 Tesla.

We will also show how AO can be used to controllably thin down Al, thus increasing its superconducting properties [2,5-6], obtaining an in-plane critical field > 6 T and a perpendicular critical field > 3T on a mesoscopic structure.

Besides enhancing superconducting properties of established devices, this technique paves the way to new research topics, e.g. Quantum Hall edge states proximitized by the surface Al with close to unity transparency.


Thursday, March 7, 2019 2:30 PM - 5:18 PM

Session V09 DCMP: Nanowires and One-Dimensional Structures: Optical and Electronic Properties BCEC 151A - Patrick Vora, George Mason Univ - Tag(s): Focus
The ultraviolet region indicates: a) that the B1l mode is related to a resonance effect, i.e. Fröhlich interaction plays a role in infra-red spectroscopies. However, the B1l mode appears with a small linewidth in the Raman scattering spectra on high and b) the mechanism allowing the appearance of the B1l does not allow the observation of the B1h. After performing

2:30PM V09.00001: Turning light-guiding nanowires into a fluorescence-based biosensing assay* MOHAMMED ALMOKHTAR, Department of Physics, Assiut University, Egypt, WILFREDO IBARRA-HERNANDEZ, Faculty of Engineering, BUAP, Mexico, MAURICIO MORAIS.DE LIMA JR., Molecular Science Institute, University of Valencia, Spain, CANTARERO (Presenter), SIMON FRASER UNIVERSITY, DAMIANO VERARDO, Division of Solid State Physics, Lund University, MARTIN J. ZUCKERMANN, NANCY FORDE, Simon Fraser University, HEINER LINKE, Division of Solid State Physics, Lund University — In some designs, semiconductor nanowires act as nanoscale optical fibres. Their quasi-1D structure can allow for the coupling of photons, which are then guided along the central axis of the nanowire structure to be emitted through its tip. In this talk, I will discuss our collaborative effort to passivate the surface of nanowires with cleavage-activated fluorogenic peptides, thereby turning a lattice of GaP nanowires into a high-throughput biosensing assay. I will present our results showing that we are able to detect the presence and activity of enzymes free in solution. This detection happens via the increase in light intensity at the nanowire tips as the surface-tethered substrates are cleaved and become fluorescent. The generality of this finding is further improved with use of our newly developed triblock-copolymer surface chemistry, which enables both specific modification of nanowire surfaces and the blocking of undesired nonspecific adhesion (e.g. of quantum dots from solution).

*NSERC Discovery Grant, NanoLund and the People Programme (Marie Curie Actions) of the European Union’s Seventh Framework Programme

2:42PM V09.00002: Size dependent surface band bending in GaN nanowires* SANTANU PARIDA (Presenter), KISHORE K. MADAPU, SANDIP DHARA, Indira Gandhi Centre for Atomic Research — Group III-nitride nanowires (NWs) are recently emerged as a potential candidate for the single nanostructure high-performance optoelectronic devices because of the unidirectional conduction of charge carriers and absence of extended defects. However, surface states play important role in nanostructure-based device performance. The role of surface states and Fermi-level pinning is still unclear for III-nitride semiconductors. Therefore, the present study intends to investigate the effect of surface states on the band bending of the unintentionally doped n-GaN NW using Kelvin probe force microscopy (KPFM) with high spatial resolution. The KPFM measurements were carried out at high vacuum (~10^-7 mbar) to avoid the effect of surface adsorbents. Single-pass imaging was adopted for the simultaneous measurement of topography, and the contact potential difference (CPD). Several measurements were carried out for the NWs with different diameter and the corresponding surface band bending were calculated. The surface band bending value was found to depend on the diameter of the NWs. Diameter dependent surface band banding of the NWs is attributed to the variation in the density of surface states in the NWs.

*Department of Atomic Energy, Government of India and FIP, APS

2:54PM V09.00003: Electronic homogeneity of III-Nitride nanowire Light Emitting Diodes (LEDs) grown on amorphous and nanocrystalline metals CAMELIA SELCU (Presenter), BRELon J MAY, ROBERTO CORREA MYERS, Ohio State University — Conductive atomic force microscopy (c-AFM) is a powerful technique to probe electrical inhomogeneities at nanometer scale in as-grown nanowire ensembles without introducing uncertainty due to additional device processing steps. Using c-AFM, we investigated the nanoscale current uniformity of III-Nitride nanowire LEDs grown on Pt thin films and amorphous metal foil. In this talk, I will discuss the variation of the current distributions in GaN nanowire LEDs grown on p-Si and Pt thin films. By taking IVs on individual nanowires, we found that there is a reduction in the threshold voltage for the GaN nanowire LEDs grown on Pt films compared to those grown on p-Si.

3:06PM V09.00004: Crop up of the B_{11} mode in high quality GaN nanowires due to isotopic disorder* ANDRES CANTARERO (Presenter), CARLOS RODRIGUEZ-FERNANDEz, Molecular Science Institute, University of Valencia, Spain, MOHAMMED ALMOKHTAR, Department of Physics, Assiut University, Egypt, WILFREDO IBARRA-HERNANDEz, Facultad de Ingeniería, BUAP, Mexico, MAURICIO MORAIS.DE LIMA JR., Molecular Science Institute, University of Valencia, Spain, ALDO ROMERO, Applied Physics Department, West Virginia University, USA, HAJIME ASAHI, Institute of Scientific and Industrial Research, Osaka University, Japan — The B_{11} and B_{1h} vibrational modes of GaN are silent, i.e. they cannot appear neither in Raman nor in infra-red spectroscopies. However, the B_{11} mode appears with a small linewidth in the Raman scattering spectra on high quality ultra-narrow GaN nanowires, while the B_{1h} mode does not. The simultaneous appearance of the A_{11}(LO) and B_{11} in the ultraviolet region indicates: a) that the B_{11} mode is related to a resonance effect, i.e. Fröhlich interaction plays a role and b) the mechanism allowing the appearance of the B_{11} does not allow the observation of the B_{1h}. After performing density functional theory calculations and discarding several options we have concluded that the only difference between both modes is the isotopic composition [1]. While Ga, which contributes to the B_{11} mode, has mainly two isotopes, $^{69}$Ga and $^{71}$Ga, N, the main contributor to the high frequency mode, has basically one isotope, i.e. it is isotopically ordered. [1] C. R-F et al., Nano Lett. 18, 5091 (2018).

*The research was carried out under the projects MAT2015-63955-R and MAT2016-82015-REDT of Spain, DMREF-NFS 1439847, OCI-1053575 and OAC-1740111 from NSF, and DE-SC0016176 from Department of Energy. We thanks Texas Advance Computer Center and Pittsburgh Supercomputer Center for providing us computing time.
Harnessing the magneto-optics of quantum wires for designing the optical amplifiers

MANVIR KUSHWAHA (Presenter), Rice University — Quantum wires occupy a unique status among the semiconducting nanostructures with reduced dimensionality. No other system seems to have engaged researchers with as many appealing features to pursue. This letter aims at a core issue related with the magnetoplasmon excitations in the quantum wires characterized by the confining harmonic potential and subjected to a longitudinal electric field and a perpendicular magnetic field in the symmetric gauge. Despite the substantive complexity, we obtain the exact analytical expressions for the eigenfunction and eigenenergy, using the scheme of ladder operators, which fundamentally characterize the quantal system. Crucial to this inquiry is an intersubband collective excitation that evolves into a magnetoroton -- above a threshold value of magnetic field -- which observes a negative group velocity between maxon and roton. The evidence of negative group velocity implies anomalous dispersion in a gain medium with the population inversion that forms the basis for the lasing action of lasers. Thus, the technological pathway that unfolds is the route to devices exploiting the magnetoroton features for designing the novel optical amplifiers and hence paving the way to a new generation of lasers.

ABSTRACT WITHDRAWN

Magneto-Chiral Anisotropy in Carbon Nanotubes

NEDA LOTFIZADEH (Presenter), Department of Physics and Astronomy, University of Utah, MITCHELL J. SENGER, DANIEL MCCULLEY, ETHAN D. MINOT, Department of Physics, Oregon State University, VIKRAM V. DESHPANDE, Department of Physics and Astronomy, University of Utah — Chiral conductors exist in two forms which are mirror images of each other and have different handedness. The nonlinear term in powers of voltage is an odd function of magnetic field and its coefficient in chiral conductors depends on the handedness and electron-electron interactions. Due to the importance of electron-electron interactions in carbon nanotubes and their large magneto-chiral anisotropy, they are one of the best candidates to study nonlinear magneto-transport in chiral conductors. In this work we use ultra clean suspended carbon nanotubes to investigate electrical magneto-chiral anisotropy in these materials, which can be used as a probe to deduce the electron-electron interaction strength and handedness of the tubes. Using photocurrent spectroscopy, we identify our nanotubes’ structure to compare the transport data with the existing theories.

Ultrafast Stimulated Raman Scattering in Carbon Nanotubes

STEVEN DRAPCHO (Presenter), CHAW KEONG YONG, University of California, Berkeley, AVISHEK SAHA, STEPHEN K. DOORN, Los Alamos National Lab, FENG WANG, University of California, Berkeley — We perform ultrafast transient absorption spectroscopy on (6,5) carbon nanotubes in aqueous solution, using a near-IR pump and supercontinuum near-IR probe. We observe stimulated Raman scattering between the pump and probe light involving the nanotube G phonon mode, and examine the dependence of this Raman feature on the pump and probe wavelengths and pump fluence. We find that the stimulated Raman process is enhanced when the probe energy is near the nanotube exciton resonance, allowing us to investigate exciton-phonon coupling in the nanotubes.

Modification of Second Harmonic Generation Signals From Multiferroic Nanofibers Under Changing Magnetic Field

SABA ARASH (Presenter), BRYAN CHAVEZ, Department of Physics and Astronomy, University of South Carolina, MATTHEW BAUER, JENNIFER ANDREW, Department of Materials Science & Engineering, University of Florida, THOMAS M CRAWFORD, YANWEN WU, Department of Physics and Astronomy, University of South Carolina — Multiferroic materials have recently attracted widespread attention as a novel class of materials due to their diverse multifunctional properties and applications. In particular, multi-phase structures are easier to synthesis and more common at room temperature in comparison to the single-phase materials. The hybrid structures investigated in this study are Janus nanofibers consisting of two hemi-cylinders of ferroelectric barium titanate (BTO) and ferrimagnetic cobalt ferrite (CFO). The mechanism involved in the magnetoelastic (ME) coupling between the two phases for this particular system is strain. In this study, we used the optical second harmonic generation (SHG) technique to monitor changes in the ferroelectricity of the BTO half while modifying the magnetization of the CFO half. The optical investigation was performed on an ensemble of pre-aligned nanofibers. In addition, the polarizations of the SHG signal were analyzed at different magnetic field orientations. We observed a clear signature of the SHG polarization rotation as the magnetic field direction was changed. This result suggests the existence of a measurable ME coupling between the two phases of this hybrid structure at room temperature which is essential for realizing devices with multiferroic applications.
4:18PM V09.00010: Intrinsic quality of InSb NWs grown in template pores  
ABHAY SINGH (Presenter), USHA PHILIPOSE, University of North Texas — InSb NWs were grown in two different types of templates: nanoporous anodic aluminum oxide (AAO) and polycarbonate. In this talk, the difference in the structural quality of the as-grown NWs in both cases will be presented. NWs grown in commercially available AAO templates were found to have rough surfaces attributed to non-uniform pores in the membrane. On the other hand, InSb NWs grown in the polycarbonate track-etched membranes showed very uniformly, smooth surfaces. Both types of NWs were characterized by Raman spectroscopy, which showed different Raman spectrum. The strong defect related peak in the polycarbonate-grown InSb NWs attest to the fact that they are possibly amorphous. Temperature-dependent measurements on these NWs also show very different behavior. The NWs grown in the polycarbonate membrane show Mott Variable Range Hopping in the low-temperature regime and Arrhenius (thermally activated) transport in the high-temperature regime. This is contrary to the AAO template grown InSb NWs which shows thermally activated conduction mechanism in both low and high-temperature regime.

4:30PM V09.00011: Investigating surface migration energy barriers of self-assembly ZnO nanorods by multi-optical methods  
FENG-MING CHANG (Presenter), ZONG-ZHE WU, JING-HENG HUANG, WEI-TING CHEN, SANJAYA BRAHMA, KUANG YAO LO, National Cheng Kung University — Post-annealing treatment plays an important role for self-assembly (SA) metal oxide by providing thermal energy for oxygen atoms to overcome the migration energy barrier. With theoretical methods, it's hard to calculate the height of migration energy barrier from the surface to bulk which depends on depth. Due to the high surface-to-volume ratio of SA ZnO nanorods (ZNRs), the optical properties and structural evolution on the surface obtained by ultraviolet/X-ray photoemission spectroscopy (UPS/XPS) and photoluminescence (PL) could be well investigated and reveal mutual agreement in all results in PL, XPS and UPS. In this work, we first demonstrated structural variation on the surface of SA-ZNRs by scanning over a range of annealing temperatures and durations by rapid thermal annealing (RTA) system and then characterized the multi-optical properties by integrating the results of PL, XPS and UPS. Finally, the model of migration energy barriers reveals the well ZNRs formed at 570°C and the further oxidation process with formation of hydroperoxide on the Zn-rich surface of ZNRs at 640°C.

4:42PM V09.00012: Maximizing Photonic Response with Simple Resonating Structures in Various Geometries*  
CONSTANTINOS VALAGIANNOPOULOS (Presenter), ARSEN SHEVERDIN, ADILKHAN SARSEN, AIVAR ABRASHULY, Nazarbayev University — Resonances are all over us in multiple forms concerning the collaboration of two (or more) parts in order to maximize an output. In Photonics, the effect is interpreted as an optimally balanced regime between electric and magnetic response in domains with different optical axes or opposite-sign permittivities. In this talk, we examine simple structures of different geometries serving various purposes from large wave polarization conversion to efficient absorbance and maximal scattering.

Firstly, we consider a planar structure consisting of two slabs positioned back-to-back with different thicknesses but the same binary multilayered texture. By rotating in-plane the two slabs, we aim at tilting the linearly polarized incident field by 90 degrees; it is a particularly challenging task when working with such simple configurations.

Secondly, an isolated core-shell nanowire, where the resonance occurs between the metallic cylinder and the semi-conducting coat, is regarded. The potential of these realistic designs to operate as switches, sensors or as components in filtering and tagging optical systems, is also identified by evaluating the corresponding frequency responses.

*NU Small Grant 090118FD5349. MES RK BR05236454.

4:54PM V09.00013: Dark vertical conduction of cavity-embedded semiconductor heterostructures*  
CASSIA NAUDET-BAULIEU (Presenter), NICOLA BARTOLO, GIULIANO ORSO, CRISTIANO CIUTI, Laboratoire MPQ, Université Paris Diderot - Paris 7 — We present a linear-response theory for the electronic transport along the growth direction of an arbitrary semiconductor heterostructure coupled to a photonic resonator in its vacuum state (no real photons are injected or created). To ensure a coupling between intersubband and photonic excitations, the cavity field is assumed to be polarized along the growth direction. We point out how the light-matter and electron-electron interactions hybridize the (confined) many-body ground state with the continuum, showing how this can affect the conduction properties in the growth direction. Our findings are relevant, for instance, in the development of cavity-embedded quantum-well infrared photodetectors (QWIP).

*We thank the Doctoral School EDPIF for the PhD scholarship of C. N-B.
Arrays of gratings can be multiplexed to create multi-view backlights, where each super-pixel is composed of several angularly directive beams. However, real applications of this technology are hampered by a limited field of view. In particular, diffractive optics are incapable of efficiently radiating light perpendicular to the plane of the array. This causes a hole in the center of the field of view because the refracted beam intensity from a diffraction grating coupler at wavelengths near cut-off. The grating is unable to produce a beam at the broadside, due to a standing wave formed in the plane of the array.

To overcome this limitation, we have developed metasurface-based pixel. The design consists of an array of high-index dielectric pillars, which exhibit simultaneous electric and magnetic resonances. The resulting metasurface supports leaky waves above the light line, which efficiently radiate into the broadside at telecom and visible frequencies. The Dirac-cone metasurface can produce beams over a continuous range of angles around the broadside due to its linear dispersion at the center of the Brillouin zone. By carefully tuning the interference of multiple bound modes, we can independently control the radiative efficiency, beam width, and beam angle.
**3:06PM V10.00002: DFT+eDMFT study of lattice dynamics in FeSe**

GHANASHYAM KHANAL (Presenter), KRISTJAN HAULE, Physics and Astronomy, Rutgers University — Effect of electron-electron interactions in the high-temperature superconductivity has been one of the challenging issues in condensed matter physics. We study the lattice dynamics of one of the iron-based high-temperature superconductors FeSe using ab-initio Density Functional Theory (DFT)+ embedded Dynamical Mean-Field Theory (eDMFT) functional approach. We found that the electron-electron interaction plays an important role in determining the phonon frequencies of different vibrational modes in this material. The phonon frequencies are in a very good agreement with the experimentally reported values in particular when compared to previously reported DFT results. The agreement extends also in the phonon band structure along with the phonon density of states.

*We acknowledge the support of NSF DMR-1709229.

**3:18PM V10.00003: Quantum Phase Transitions in a Multi-Orbital Hubbard Model for Iron Pnictides**

WENJUN HU (Presenter), Rice University, LUCA FAUSTO TOCCHIO, Institute for condensed matter physics and complex systems, HSIN-HUA LAI, Rice University, RONG YU, Renmin University of China, FEDERICO BECCA, International School for Advanced Studies, QIMIAO SI, Rice University — Quantum criticality in iron pnictides was proposed within an effective field theory that contains both antiferromagnetic and nematic order parameters [1,2]. Its proposed realization in P-doped BaFe2As2 has received extensive experimental evidence [3,4]. Here we study this problem within a multi-orbital Hubbard model containing both the Hubbard and Hund's interactions. We analyze the effect of electron correlations in a non-perturbative way, through a variational Monte Carlo method that is based on a Jastrow-Slater wave function. We study the evolution of the electronic orders as the interaction strength is varied, report evidence for concurrent antiferromagnetic and nematic quantum critical points, and discuss the implications for superconducting pairing.


*This work is supported by the DOE Award # DE-SC0018197 and Welch Foundation.

**3:30PM V10.00004: Quantum dynamical screening of the local magnetic moments in the different families of Fe-based superconductors**

CLEMENS WATZENBÖCK, Institute of Solid State Physics, TU Wien, MARTIN EDELMANN, University of Würzburg, DANIEL SPRINGER, Institute of Solid State Physics, TU Wien, ANDREAS HAUSOEL, GIORGIO SANGIOVANNI, University of Würzburg, ALESSANDRO TOSCHI (Presenter), Institute of Solid State Physics, TU Wien — The formation of localized magnetic moments and their dynamical screening represents one of the crucial ingredients of the physics of correlated metals. Their theoretical treatment is, in fact, crucial to correctly predict the spectroscopic observations in several important classes of correlated materials [1,2]. In this talk, we investigate [3] the local spin dynamics in different families of Fe-based superconductors by means of realistic dynamical mean-field theory calculations: We compute the dynamic magnetic correlations on the Fe sites both in real frequency and in real time domain. The former allows for a direct comparison with inelastic neutron spectroscopy, explaining the trends observed in the experiments on the different families of Fe-based superconductors. The latter allows to identify the characteristic time scales of the spin dynamics in these materials, which is useful for the interpretation of the discrepancies between different experimental probes, and, in perspective, for the analysis of future non-equilibrium experiments.

3:42PM V10.00005: Symmetry analysis of magnetoelastic couplings in the Fe-based superconductors* WILLIAM MEIER (Presenter), ANDREAS KREYSSIG, PAUL CANFIELD, Ames Laboratory and Dept. of Physics, Iowa State University — Antiferromagnetism (AFM) is a reoccurring theme in the Fe-based superconductors. The stripe-type AFM on the Fe lattice in these compounds is accompanied by a sympathetic orthorhombic distortion of the tetragonal structure. This is not the only kind of magnetoelastic coupling possible between magnetic and structural degrees of freedom. Based on a symmetry analysis of the crystal structures we obtain the symmetry-allowed coupling terms in the Landau free energy. We propose that many of the compounds in this family (including FeSe, BaFe₂As₂ and CaKFe₄As₄) will develop a periodic structural modification when a magnetic field is applied to the AFM ordered phase. This should produce additional Bragg peaks which could provide a sensitive indicator of the AFM order under extreme conditions, such as in high pressure cells.

*We thank M. H. Christensen, R. M. Fernandes, S. L. Bud'ko, R. Flint, and P. P. Orth for their insightful discussions. This work is supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4411 and the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

3:54PM V10.00006: Simple transport models for the temperature-dependent linear magnetoresistance of pnictide and cuprate superconductors* JOHN SINGLETON (Presenter), National High Magnetic Field Laboratory, Los Alamos National Laboratory — Taken in conjunction with the temperature (T) dependence of the zero-field resistivity, simple transport models invoking e.g., realistic variations in charge-carrier density are shown to be sufficient to explain the linear magnetoresistance and field-temperature resistance scaling recently observed in high-temperature pnictide and cuprate superconductors. Hence, though the T-linear zero-field resistance is a definite signature of the "strange metal" state of high-temperature superconductors, their linear magnetoresistance and its scaling need not be; instead they may merely be signatures of disorder. Straightforward experimental tests of these assertions are proposed.

*Supported by the US DoE BES FWP Science in 100 T, and carried out at NHMFL, which is funded by NSF Cooperative Agreement DMR-1157490, the State of Florida and U.S. DoE.

4:06PM V10.00007: Pairing symmetry and topological surface state in iron-chalcogenide superconductors LUN HU (Presenter), CONGJUN WU, Department of Physics, University of California, San Diego — The gap function symmetries remain an important question in the study of iron-based superconductors. Motivated by the recent ARPES experiments, we investigate the gap function symmetries by examining the behavior of the surface Dirac cone of the iron-chalcogenide superconductors.

Whether the surface Dirac cone can be gapped when entering the superconducting state provides a constraint on the pairing symmetries, based on which possible time-reversal symmetry breaking gap functions are analyzed. This study provides a helpful connection between the gap function symmetries and surface state topology.

4:18PM V10.00008: Theory for quasiparticle interference in the presence of spin-orbit coupling in strongly electron-doped iron-based superconductors JAKOB BÖKER (Presenter), Ruhr University Bochum, PAVEL VOLKOV, Ruhr-University Bochum and Rutgers University, PETER HIRSCHFELD, Department of Physics, University of Florida in Gainesville, ILYA EREMIN, Ruhr University Bochum — Motivated by recent experimental reports on sizable spin-orbit coupling (SOC) and a sign-changing order-parameter in the Li₁₋ₓFeₓ(OHFe)₁₋₂ZnₓSe superconductor with only electron Fermi surface present, we study the possible Cooper-pairing symmetries and their quasiparticle interference (QPI) signatures. We find that each of the resulting states - s-wave, d-wave and helical p-wave - can have a fully gapped density of states (DOS) consistent with ARPES experiments and, due to spin-orbit coupling, are a mixture of spin singlet and triplet components leading to intra- and inter-band features in the QPI signal. Analyzing predicted QPI patterns we find that only the s- and d-wave pairing states with a dominant even parity triplet component can fit the experimental data with the two dominant peak positions in the DOS roughly correspond to the gap sizes at each pocket. Moreover we show that pairing states with dominant triplet component can be further verified using spin-resolved STM.
4:30PM V10.00009: Broken time-reversal symmetry in s+is and s+id states of multi-band superconductors: vortices, skyrmions, domain walls and spontaneous magnetic fields.*  
EGOR BABAEV (Presenter), KTH the Royal Institute of Technology, JULIEN GARAUD, CNRS Tours, MIHAIL SILAEV, Jyvaskyla University, ALBERTO CORTICELLY, KTH the Royal Institute of Technology — The recent experiments on Iron-based superconductors reported two interesting situations: the formation of s-wave superconducting state in Ba1−xKxFe2As2 that breaks time-reversal symmetry (BTRS) (i.e. the so-called s+is state) and disorder-driven crossover from s− to s++ state. Both of these situations should be accompanied by unconventional physics that will be discussed in this talk. I will discuss the origin of the spontaneous magnetic fields in the s+is state [1], unconventional topological excitations arising due to BTRS such as domains walls and Skyrmions [2], the breakdown of type-I/type-II dichotomy due to a divergent coherence lengths at the s− to s+is transition causing the magnetic field penetration length to be intermediate length scale: ξ1<λ< ξ2 [3,4] resulting in vortex clustering, and a rather generic coexistence of the s− and s++ states near the s− to s++ crossover [5].


*Supported by the Swedish Research Council and the Goran Gustafsson Foundation

4:42PM V10.00010: Interplay of structural properties and van der Waals forces in presence of magnet disorder in FeSe and FeTe by density-functional theory calculations  
FELIX LOCHNER (Presenter), Max Planck Institute for Iron Research GmbH, ILYA EREMIN, Theoretische Physik III, Ruhr-University Bochum, TILMANN HICKEL, JÖRG NEUGEBAUER, Max Planck Institute for Iron Research GmbH — We investigate the structural origin of the iron-based superconductors FeSe and FeTe in the presence of several magnetic orders, where we focus on the competition between stripe-type anti ferromagnetism (AFM) and paramagnetic disorder (PM). Here, the PM state is implemented by using the spin-space average approach [1] in combination with constrained magnetic moments for our density-functional calculations (DFT). To predict the correct ground state in respect to the lattice parameters, we use the similarity of the AFM and PM state to transfer the correlations for specific structural properties of the AFM picture to those correlation for the PM approach.

Moreover, we found that the specific energy-volume behavior of FeSe, which looks like an “L”, leads to a weak inter-layer interaction. Therefore, we include several approaches of van der Waals (vdW) interactions to these systems to correct the Se-Se interactions and Te-Te interactions respectively. Our results show, that the additional vdW forces are as necessary to reduce the lattice mismatch between experimental and predicted values as magnetic order is [4].


4:54PM V10.00011: Anomalous Non-Superconducting Time-Reversal-Symmetry Breaking State in Multicomponent Superconductors*  
DANIEL WESTON (Presenter), EGOR BABAEV, KTH Royal Institute of Technology — Multicomponent superconductors can break time-reversal symmetry, either due to phase frustration in Josephson-coupled superconductors with at least three components, or due to higher-order Josephson coupling in superconductors with at least two components. Beyond mean-field theory, such systems may have an anomalous phase in which time-reversal symmetry is broken despite superconducting order being absent. Models of the aforementioned type have been argued to describe the multiband superconductor Ba1−xKxFe2As2. We report properties of the fluctuation-induced precursory normal state that breaks time-reversal symmetry.

*The work was supported by the Swedish Research Council Grant No. 642-2013-7837 and by the Göran Gustafsson Foundation for Research in Natural Sciences and Medicine.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

2:30PM V11.00001: Peculiar spectra of dark and bright excitons in alloyed nanowire quantum dots*  
MICHAL ZIELINSKI (Presenter), Institute of Physics, Nicolaus Copernicus University, Torun, Poland — Excitons in alloyed nanowire quantum dots have unique spectra as shown here using atomistic calculations. The bright exciton splitting is triggered solely by alloying and despite cylindrical quantum dot shape reaches over 15 μeV, contrary to previous theoretical predictions, however, in line with experimental data. This splitting can however be tuned by electric field to go below 1~μeV threshold. The dark exciton optical activity is also strongly affected by alloying reaching notable 1/3500 fraction of the bright exciton and having large out-of-plane polarized component.

*Support from the Polish National Science Centre based on decision No. 2015/18/E/ST3/00583 is kindly acknowledged.

2:42PM V11.00002: Precision Displacement Measurement Using a Shearing Interferometer*  
RAJU KC (Presenter), CAINAN NICHOLS, JAXON LEE, EDWARD B FLAGG, West Virginia University — The emission spectra from semiconductor quantum dots consists of closely spaced spectral peaks, which cannot be resolved by a conventional grating spectrometer. An alternative solution is to use a scanning Fabry-Perot interferometer (FPI), which functions as a narrow bandwidth tunable filter, to enhance the resolution. This technique demands very precise control of the distance between the two FPI mirrors with a resolution of 1 nm. Direct optical feedback would be ideal, but would require an expensive frequency-tunable laser. We demonstrate an economic way to achieve the required precision by mechanically connecting the FPI cavity to a shearing interferometer where fluctuations in the mirror separation can be measured using the interference pattern formed by a relatively inexpensive single-frequency laser. We are able to stabilize the RMS displacement fluctuation between the two mirrors in the shearing interferometer to 0.11 nm. This precision was sufficient to keep the FPI stable for ~40 minutes.

*This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0016848.

2:54PM V11.00003: Spin-selective AC Stark shifts in a charged quantum dot*  
TRISTAN WILKINSON (Presenter), DILLION COTTRILL, JOSHUA CRAMLET, COLE MAURER, COLLIN FLOOD, Department of Physics and Astronomy, West Virginia University, Morgantown, West Virginia 26506, USA, ALLAN S BRACKER, Naval Research Laboratory, Washington, DC 20375, USA, EDWARD B FLAGG, Department of Physics and Astronomy, West Virginia University, Morgantown, West Virginia 26506, USA — The energy levels of an optically active quantum system can be shifted via the AC Stark effect by applying a strong, far-detuned laser. We achieve an AC Stark shift of up to 20 GHz in a single negatively charged InGaAs quantum dot. In addition to the AC Stark shift we observe a small Overhauser shift of <1 GHz which we attribute to dynamic nuclear polarization via electron spin pumping induced by the high power, although far-detuned AC Stark laser. Both shifts are polarization selective, meaning polarization control of the applied laser provides control over the energy level structure of the system. Applying a circularly polarized laser therefore allows for a spin-selective modification to the energies, shifting one spin manifold and not the other. The reconfiguration of the energy levels is reversible and can be applied or removed rapidly on the timescale of a few nanoseconds. In principal this ability to rapidly and coherently reconfigure the energy structure and polarization selection rules may enable single-shot fluorescence readout in a small transverse magnetic field.

*Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0016848.
Superconducting transport in InAs nanowire double quantum dots

DANIEL BOUMAN (Presenter), RUBEN VAN GULIK, DOMINIQUE LAROCHE, QuTech, Delft University of Technology, JESPER NYGÅRD, PETER KROGSTJUP, Niels Bohr Institute, ATTILA GERESDI, QuTech, Delft University of Technology — Quantum dot arrays in narrow-gap semiconductors coupled to superconducting reservoirs can serve as a platform for studying the interaction between solitary spins and the Cooper pair condensate, which can give rise to topologically protected Majorana modes.

We define double quantum dots (DQDs) in InAs nanowires with epitaxial aluminum shell. We demonstrate that we can reach both the strongly and weakly coupled regimes owing to the five wrap-around electrostatic gates on the nanowire. We characterize the Josephson coupling via the DQD as a function of the charge occupation of the islands, and find abrupt changes which are possible experimental signatures of the change in the ground state spin configuration of the device. Finite voltage bias spectroscopy reveals Yu-Shiba-Rusinov states below the superconducting gap exhibiting the weakly and strongly coupled behavior at different gate configurations.

Charging of a Single InAs QD with Electrically-Injected Holes using a Lateral Electric Field*

XIANGYU MA (Presenter), YUEJING WANG, JOSHUA ZIDE, MATTHEW F DOTY, University of Delaware — InAs/GaAs quantum dot (QD) and quantum dot molecules (QDM) are self-assembled semiconductor nanostructures that can trap a single electron or hole in a 3-D potential-well. Grown by molecular beam epitaxy (MBE), they have excellent optical qualities that can be used in applications of quantum information processing and quantum computing. The property of a single QD can be tuned by external electric field, giving it great potential for scalable quantum photonic applications. Deterministically charging a QD with a single electron or hole has been demonstrated by embedding the QD in a diode structure and applying growth direction electric fields. Here, we report a new charging mechanism of a single QD using lateral electric field with a 3-electrode device. We designed a 3-electrode device that embeds a single QD in an unintentionally doped GaAs matrix. We fabricate the device with E-beam lithography and characterize a single QD’s photoluminescence under different bias configurations. We observe charging of a single hole through the lateral electric field, supported by device simulation using COMSOL. We will discuss the potential applications of a 2-D electric field on a single QD using a 3-electrode device.

*We acknowledge financial support from NSF (DMR-1505574)

Quantum mechanics on a torus: Energy levels, Zeeman splitting and transport properties*

DEBANIK DAS (Presenter), SATHWIK BHARADWAJ, SIDDHANT PANDEY, Department of Physics, Worcester Polytechnic Institute, Worcester, MA 01609, L RAMDAS RAM-MOHAN, Department of Electrical and computer engineering, Worcester Polytechnic Institute, Worcester, MA 01609 — Carrier confinement and transport in novel geometries have generated immense theoretical and experimental interest in recent years. Here we investigate the properties of an electron constrained to move on the surface of a torus. We derive the Schrodinger-Riccati equation on a torus using differential geometry. We construct the corresponding action and obtain the eigensolutions through a generalized varational approach. We show that the dual circular symmetries related to the minor and major radii give rise to at most a 4-fold degeneracy. We obtain the level splitting pattern in the presence of a perpendicular magnetic field. We investigate the transport properties for an electron on a torus with two contacts attached. The torus being a multiply connected topology shows the Ahronov-Bohm effect in presence of a magnetic vector potential and manifests the interference occurring due to electron waves travelling through two different paths. Semiconductor quantum dots and carbon nanotori, for certain chirality, have bandgaps at K-points in the Brillouin zone. Hence they obey nonrelativistic equations, making our study relevant for experimentally amenable outcomes.

*We thank the Center of Computational NanoScience (CCNS) at WPI for the computational resources used for these calculations.
3:42PM V11.00007: Spectroscopy of Quantum-Dot Orbitals with In-Plane Magnetic Fields* LEON CAMENZIND (Presenter), LIUQI YU, University of Basel, PETER STANO, Center for Emergent Matter Science, RIKEN, JERAMY D. ZIMMERMAN, ARTHUR C GOSSARD, Materials Department, UC Santa Barbara, DANIEL LOSS, DOMINIK ZUMBUHL, University of Basel — While spins in quantum dots have received a lot of attention for the development as a qubit, the orbitals which are hosting the qubit have largely been ignored. However, important processes such as electric-dipole spin resonance and spin relaxation depend sensitively on the dot shape due to the anisotropic nature of the spin-orbit interaction. Here, we present a method which allows quantifying the in-plane orientation angle and the strength of the hard confinement perpendicular to the 2D gas in which the gate-defined single-electron GaAs dot is formed. Using a piezo electric rotator, we control the direction of the magnetic field in the 2D plane and measure the in-plane orbital energies using pulse gate spectroscopy. Based on a model of the orbitals, we extract the orientation angle of the dot in the 2D plane, quantify the strong confinement and characterize deviations from a harmonic oscillator potential. Our measurements demonstrate a versatile tool for quantum dots with one dominant axis of strong confinement.

*This work was supported by the Swiss Nanoscience Institute (SNI), NCCR QSIT, Swiss NSF, ERC starting grant and the European Microkelvin Platform (EMP).

3:54PM V11.00008: Toward exploring multichannel charge Kondo effects for investigating quantum criticality CONNIE HSUEH (Presenter), Department of Applied Physics, Stanford University, ASBJORN C. C. DRACHMANN, Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, CANDICE THOMAS, Department of Physics and Astronomy and Station Q Purdue, Purdue University, GEOFFREY C. GARDNER, Microsoft Quantum at Station Q Purdue, Purdue University, TIAN WANG, Department of Physics and Astronomy and Station Q Purdue, Purdue University, SERGEI GRONIN, Microsoft Quantum at Station Q Purdue, Purdue University, CHARLES M MARCUS, Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, DAVID GOLDHABER-GORDON, Department of Physics, Stanford University — Recent proposals[1,2] have demonstrated a non-Fermi liquid fixed point in superconducting and topological superconducting islands, analogous to the charge Kondo effect in normal metallic islands. The topological Kondo effect is predicted to be robust against channel detuning and to have a heightened crossover temperature when tuned to charge degeneracy, making this an especially attractive regime for investigating quantum criticality and for demonstrating nonlocal quantum phenomena through Majorana modes. I will talk about our efforts in experimentally realizing new multichannel charge Kondo devices on InAs 2DEG platforms.


4:06PM V11.00009: Transient dynamics of a quantum-dot: From Kondo regime to mixed valence and to empty orbital regimes* YONGXI CHENG (Presenter), ZHEN-HUA LI, Simulation of Physical Systems, Beijing Computational Science Research Center, JIAN-HUA WEI, Department of Physics, renmin university of China, YI-HANG NIE, Institute of Theoretical Physics, Shanxi university, YIJING YAN, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China — Based on the hierarchical equations of motion approach, we study the time-dependent transport properties of a strongly correlated quantum dot system in the Kondo regime (KR), mixed valence regime (MVR), and empty orbital regime (EOR). We find that the transient current in KR shows the strongest nonlinear response and the most distinct oscillation behaviors. Both behaviors become weaker in MVR and diminish in EOR. To understand the physical insight, we examine also the corresponding dot occupancies and the spectral functions, with their dependence on the Coulomb interaction, temperature, and applied step bias voltage. The above nonlinear and oscillation behaviors could be understood as the interplay between dynamical Kondo resonance and single electron resonant tunneling.

*This work was supported by the NSF of China (Grant Nos. 11747098, 11504017, 11774418, 11374363, and 21633006) and the Research Funds of Renmin University of China (Grant No. 11XNJ026).
4:18PM V11.00010: Fano and Fano-Kondo resonance in double quantum dot in parallel  YUJIE ZHANG (Presenter), MIKIO ETO, Faculty of Science and Technology, Keio University — It has been a controversial issue whether the Fano resonance is observed or not in the transport through a mesoscopic ring with an embedded quantum dot, so-called Aharonov-Bohm interferometer. To address this issue, we theoretically examine the nonequilibrium transport through a double quantum dot (DQD) in parallel: resonant tunneling at the Coulomb peak or Kondo effect in the Coulomb valley in quantum dot 1, with a broad linewidth in quantum dot 2. Our model is more tractable than a model for the AB interferometer [1]. We stress the importance of multiple channels in external leads to simulate the experimental systems, which was often neglected in previous studies. In the case of single channel in the leads, we find an asymmetric Fano resonance or Fano-Kondo resonance as a function of energy level in quantum dot 1. With an increase in the number of channels, these approach the symmetric Breit-Wigner resonance or Kondo plateau. This is because the coherence between the quantum dots is weakened, which can be characterized by the off-diagonal element normalized by the diagonal elements in a two-by-two matrix of the linewidth function.


4:30PM V11.00011: Single-Electron Charging Effects in Sketched LaAlO3/SrTiO3 Single-Electron Transistors* PHILIP SHENK (Presenter), Department of Physics, University of Pittsburgh, JOHN MAIER, Department of Physics, University of Notre Dame, JULIANA SEBOLT, Department of Physics, Allegheny College, JUNGWOO LEE, HYUNGWOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, JIANAN LI, PATRICK IRVIN, JEREMY LEVY, Department of Physics, University of Pittsburgh — Mesoscopic devices like the single-electron transistor (SET) exhibit quantum behavior by forcing electrical current through a point-like constriction with quantized energy levels. Such devices typically require extreme nanofabrication techniques. Complex-oxide heterostructures such as the LaAlO3/SrTiO3 system support conductive interfaces that can be controlled using a reversible conductive-AFM lithography technique. These interfaces have richer properties than III-V or silicon-based systems, and support intrinsic magnetic, superconducting and structural phases. Here we describe renewed efforts to explore the properties of “sketched” SETs at the LaAlO3/SrTiO3 interface, focusing on the temperature and magnetic-field dependence of transport. We observe non-equilibrium conductances that cleanly resolve addition energies in nanoscale quantum dots, and track interactions between electronic states vs. experimental parameters such as gate voltage, temperature and magnetic field. These results yield new insights into intrinsic interactions between electrons confined within the quantum dot.

*JL acknowledges a Vannevar Bush Faculty Fellowship, funded by ONR (N00014-15-1-2847). C-BE acknowledges support from NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-4046).

4:42PM V11.00012: Ultra-stable atomically precise single electron transistors in Silicon RANJIT KASHID (Presenter), ANDREW MURPHY, JONATHAN WYRICK, PRADEEP NAMBOODIRI, XIQIAO WANG, SCOTT SCHMUCKER, RICHARD M. SILVER, NEIL ZIMMERMAN, Atom Scale Device Group, Nanoscale Device Characterization Division, National Institute of Standards and Technology — Single electron transistor devices (SETs) in solid-state quantum computing architecture serve as sensitive electrometers for realizing spin selective initialization & single shot readout during spin manipulation, & demand very stable operation. In this context, we demonstrate fully functional, ultra-stable atomically precise SETs fabricated using scanning tunneling microscope (STM) lithography on the Si (100) 2x1: H surface. Low-temperature transport measurement of SETs reveal highly stable Coulomb blockade oscillations. To better understand low-frequency time instabilities we have measured charge offset drift over a period of 4.5 days. SETs fabricated using STM lithography exhibit low charge offset drift magnitude (less than 0.02 e over 4 days, at both base temperature & 6 K) as compared to conventional metal & Silicon based SETs. The low charge offset drift magnitude likely results from the lack of a nearby interface & suggests low defect density in the STM fabrication process & low temperature epitaxial overgrowth. However, at elevated temperatures above 3 K a glassy relaxation is observed in response to gate voltage changes with a settling time that is strongly temperature- dependent.
4:54PM V11.00013: Tunnel Junction Design and Characterization in Si:P Single Electron Transistors  JONATHAN WYRICK (Presenter), XIQIAO WANG, RANJIT KASHID, PRADEEP NAMBOODIRI, SCOTT W SCHMUCKER, RICHARD M. SILVER, National Institute of Standards and Technology — Atomically precise Si:P quantum devices are a promising architecture for scalable solid-state quantum computing. Quantification and control of the tunnel coupling between device components at the atomic scale is essential to successful donor-based quantum information processing (e.g. gate-tunable exchange coupling, electron spin readout, and ultrasensitive charge sensing all require precise control over tunnel coupling). We report on reproducibility of tunnel coupling as measured in atomically precise single electron transistors (SETs). We systematically vary gap separations on the nanometer scale, observing orders of magnitude changes in resistance. Combining low-temperature transport measurements with the orthodox theory of Coulomb blockade, we have extracted tunnel resistances in SETs and analyze to what degree resistances depend on applied voltages. We analyze the relationship between the tunnel conductance and physical barrier parameters and will discuss the limits of lithographically defining an atomically abrupt Si:P tunnel junction. We find the behavior of the tunnel junctions in these devices to be of exceptional quality and will discuss potential reasons for these improvements compared to previous devices fabricated in a similar manner.

5:06PM V11.00014: Fabrication and Measurement of Atomically Precise Single Electron Islands*  DANIEL WARD (Presenter), DEANNA CAMPBELL, MICHAEL MARSHALL, TZU-MING LU, LISA A TRACY, LEON MAURER, ANDREW BACZEWSKI, SHASHANK MISRA, Sandia National Laboratories — Phosphorous donor devices fabricated in silicon with a scanning tunneling microscope (STM) are used as a discovery platform for everything ranging from quantum physics to ultra-efficient tunnel field effect transistors because the underlying hydrogen lithography step can be performed with atomic precision. Many of these devices designs rely on electrostatic gating to tune electrical tunneling through the device. It is expected that out-of-plane gates will be more efficient at gating than in-plane gates. We present on fabrication techniques for adding top gates to devices and the resulting low-temperature measurements on tunnel junctions and single electron islands.

*This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories, and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility.

Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

5:18PM V11.00015: The role of confinement and interaction in the emergence of aromatic features in nanoscale synthetic molecules*  ANTHONY RUTH (Presenter), DAVID B GREEN, KENJIRO KIMURA GOMES, BOLDIZSAR JANKO, University of Notre Dame — It has recently been demonstrated that the electronic structure of polyaromatic hydrocarbons can be qualitatively reproduced by quantum corrals made via atomic manipulation. This presents a quandary since the electronic structure of these molecules has been ascribed to a resonating valence bond like state requiring strong confinement to molecular orbitals and significant electron-electron interactions. However, quantum corrals fundamentally exhibit single-electron physics as evidenced by a short lifetime for an electron in a corral, resulting in the absence of Coulomb effects between electrons. We examine this problem from the experimental data obtained via scanning tunneling spectroscopy and topography, tight-binding modeling of hopping and interaction Hamiltonians, as well as density functional theory calculations to determine what aspects of the fully-interacting picture can be produced by the single-electron approach.

*A. R. thanks support from a NASA Space Technology Research Fellowship

Thursday, March 7, 2019 2:30 PM - 5:18 PM

Session V12 DCMP: Optical and Electronic Properties of Graphene Nanoribbons and Nanowires  BCEC 153A - Vikram V. Deshpande - Tag(s): Focus
Flexible electronics has directed development and research of unique instrumentation and measurement to achieve conformable sensors for a wide range of applications. Conventional high-performance electronic materials such as silicon are not flexible, whereas flexible materials such as conducting polymers, are often characterized by poor electric properties. Thus, high mobility materials in a flexible configuration are desirable, and carbon nanotubes (CNTs) are promising due to their excellent electric properties and flexibility. Here, we present an all-solid state flexible and stretchable pressure sensor composed of vertically aligned CNTs (VACNTs) partially embedded in polydimethylsiloxane (PDMS). VACNTs are grown via chemical vapor deposition (CVD) and transferred onto PDMS as a stretchable electrode. Two electrodes are placed face-to-face and increased pressure is directly proportional to a detectable change in resistance, enabled by increased contact between opposing electrodes. The resistance is maintained at stretching up to 180%, with a rapid response time during loading and unloading. As a proof-of-concept, the sensor is successfully tested for medical and e-skin applications by measuring biological signals of a person.

We report the reflection contrast spectra of atomic-precise armchair graphene nanoribbons (GNRs) on insulating substrates. As-grown GNRs are transferred from gold to an insulating substrate by the “bubbling” method. Polarization control of light is employed to directly probe the one-dimensional (1D) optical resonances of armchair GNRs with different ribbon widths by the reflection contrast spectroscopy. We observed well-defined 1D optical resonances which are identified as optically-bright inter-band transitions in GNR samples. Our experimental interpretations are further supported by theoretical calculations within the GW framework, which reveals a strong exciton effect with exceptionally large exciton binding energies.

Graphene nanoribbons (GNRs) exhibit an electronic bandgap due to the lateral confinement of charge carriers and edge effects. They can be fabricated by bottom-up on-surface synthesis from molecular precursors resulting in atomically precise structures [1]. This approach promises tunable optical and electronic properties [2]. We use Raman spectroscopy to characterize different types of GNRs and investigate their interaction with growth and devices substrates. In particular, we investigate new geometry-dependent signatures beyond the radial breathing like mode (RBLM) and how they are correlated with charge transport properties.


*JO and MC acknowledge funding by the Swiss Nanoscience Institute.

It is known that 7-armchair graphene nanoribbon (AGNR) holds topological end states at its zigzag ends. A superlattice with such end states is predicted to give rise to in-gap bands whose energies differ from the bulk states’ significantly, which will form a well-isolated subspace. Utilizing these characters of the topological states, we develop a novel AGNR superlattice that possesses two zigzag edges per unit cell. We further show using first principle calculations that, by modifying the geometry of such GNRs, it is possible to get metallic GNRs with tunable bandwidth. Explicitly, the occurrence of five-membered rings would change the bandwidth drastically. After including substrate effects, we reach good agreement with experimental results. In addition, we predict that one of the structures would have ferrimagnetic orders based on Lieb’s theorem and confirmed by density functional theory (DFT) calculation.

*This work is supported by the NSF, DOE, and Office of Naval Research under MURI program, and computational resources from NERSC and XSEDE.
3:18PM V12.00005: Quantum Resonant Tunneling in In-Plate Graphene Nanoribbon/h-BN Heterojunctions
MITSUYOSHI TOMIYA (Presenter), SHOICHI SAKAMOTO, Faculty of Science and Technology, Seikei University — The first principle calculations of the electrical properties of in-plate hetero-junctions of armchair graphene nanoribbon/hexagonal boron nitride(AGNR/h-BN)s are presented. They are carried out using SIESTA package, which consists of numerical codes of the density functional theory(DFT) and the non-equilibrium Green’s function(NEGF). The center part is made of two in-plate hetero-junctions of two transverse h-BN arrays embedded into the conductive (3n-1)-family of AGNR((3n-1)-AGNR) and remains two-dimensional. Adopting (3n-1)-AGNR to the both side lead parts, which must be metallic. Two transverse arrays of h-BN, which is wide-gap semi-conductor, act as a double barrier system. The quantum resonant tunneling through the double barrier system is found in the transmission function(TFs) clearly and I-V characteristics of 8, 11, 14-AGNR/h-BN. The TF has sharp peaks in a neighborhood of the Fermi energy due to the tunneling and the I-V characteristics becomes step-wise. The one-dimensional(1D) Dirac equation model is proposed to study double barrier system. Though the 1D Dirac model is very simple, it reproduces most of the peaks of the TF nearby the Fermi energy. The in-plate hetero-junctions of zigzag graphene nanoribbon/h-BN are also discussed.

3:30PM V12.00006: Resonance Raman Spectroscopy of 7-Atom Wide Armchair Graphene Nanoribbons*
VIVIANE VALQUÍRIA DO NASCIMENTO (Presenter), ELIEL GOMES DA SILVA NETO, Departamento de Física -ICEx, Universidade Federal de Minas Gerais, JUAN P LLINAS, Department of Electrical Engineering and Computer Sciences, University of California, CRISTIANO FANTINI, Departamento de Física -ICEx, Universidade Federal de Minas Gerais, GABRIELA BORIN BARIN, Empa, AKIMITSU NARITA, MÜLLEN KLAUS, Max Planck Institute for Polymer Research, ROMAN FASEL, Empa, JEFFREY BOKOR, University of California — Graphene Nanoribbons (GNRs) exhibit interesting electronic and optical properties strongly dependent on their width and edge. The bottom-up approach to fabricate graphene nanoribbons leads to a precise width and extremely high edge quality, and, as a consequence of this uniformity, the quantum confinement plays a significant role in its electronic and optical properties. This work reports the optical response of armchair graphene nanoribbons of width N=7 atom (7AGNR) on Si/SiO2 substrate using Raman spectroscopy. The 7AGNR presents a rich Raman spectrum, with more than 20 peaks, in good agreement with the theoretical predictions. At room temperature, the nanoribbons degrade in a few seconds under laser exposition as shown by time series Raman experiments. Under nitrogen atmosphere and low temperature, the degradation process is shown to be much slower, allowing us to perform resonance Raman spectroscopy of the 7AGNR in a wide range of excitation energies. The results show a strong dependence of the Raman spectrum with the excitation energy, with a resonance peak around 2.3 eV in agreement with reflectance experiments.

*We thank the financial support given by CAPES, Fapemig, CNPq and INCT/Nanomaterials de Carbono.

DEBORAH PREZZI (Presenter), CLAUDIA CARDOSO, ANDREA FERRETTI, Nanoscience Institute of the National Research Council (CNR-NANO) — Graphene nanoribbons (GNRs) have attracted increasing attention in the last decade as a viable route for graphene-based opto-electronic applications, especially in view of the successful production of ultranarrow and atomically precise structures by means of bottom-up techniques. While GNR absorption properties have been addressed in depth [1, 2], emission properties are still largely unexplored. We here report on the optical response of finite-length GNRs as resulting from state-of-the-art ab initio calculations beyond mean field [3, 4]. Our results indicates that bulk-like excitations coexist with below-bandgap states localized at the GNR extremities, which are almost independent on the length. By investigating both the presence of defects and the coupling with a gold tip, our simulations allow us to identify unpredicted optical transitions in GNRs and to elucidate the origin of below-bandgap STM-induced light emission recently observed in suspended GNRs [3], providing a promising route for the realization of bright, robust, and controllable graphene-based light-emitting devices.

3:54PM V12.00008: Evolution of bandgap with size in armchair and zigzag graphene quantum dots* LUDMILA SZULAKOWSKA (Presenter), YASSER SALEEM, LOUIS NAJERA BALDO, ALAIN DELGADO GRAN, PAWEL HAWRYLAK, University of Ottawa — We present here the evolution of the bandgap energy with size in armchair and zigzag graphene quantum dots (GQDs). The results of the tight binding model are analyzed by dividing zigzag graphene quantum dots into concentric rings. For each ring, the solutions are obtained analytically and then the effect of inter-ring tunneling on the energy gap is determined. The growth of zigzag terminated GQD into armchair GQD is shown to be associated with the addition of a one-dimensional Lieb lattice of carbon atoms with a shell of energy levels in the middle of the energy gap of the inner zigzag GQD. This causes a difference in the nature of the wave functions between zigzag and armchair GQD which manifests itself in the oscillation of the energy gap with increasing size. The evolution of the bandgap with the number of carbon atoms is compared with the notion of confined Dirac Fermions and tested against ab-initio calculations of Kohn-Sham and TD-DFT energy gaps.

*PH, YS, AD and LS acknowledge support from NSERC and uOttawa University Research Chair;

4:06PM V12.00009: Photoluminescence Quantum Efficiency of III−V Nanowires on Silicon Substrates YUI CLIFFORD (Presenter), JIARONG CUI, HO VINH, YIFEI WANG, VINH Q NGUYEN, Department of Physics & Center for Soft Matter and Biological Physics, Virginia Tech — The III−V nanowires monolithically grown on silicon substrates provide promising technologies for integrating advanced photonic technologies on a silicon microelectronics. We report the photoluminescence quantum efficiency of nanowires as well as the thermal quenching mechanism in nanowires prepared by vapor−liquid−solid method. High-resolution spectroscopy, quantum yield and temperature dependence measurements of photoluminescence intensity from nanowires were performed. The data provides a picture of the quantum efficiency, thermal quenching processes and activation energy levels of nanowires. The results provide an important step in the realization of III−V quantum information and photonic devices on silicon platform.

4:18PM V12.00010: Gate-tunable Aharonov-Bohm interference in Bi2O2Se nanowires JIANGHUA YING (Presenter), HUAIXIN YANG, FANMING QU, LI LU, Institute of Physics, Chinese Academy of Sciences — Semiconducting Bi2O2Se shows excellent air stability and high carrier mobility. High-quality single-crystalline Bi2O2Se nanowires were synthesized by means of gold-catalyzed vapor-liquid-solid growth. We fabricated nanowire-based devices and performed electron transport measurements down to low temperatures. Oscillations in magnetoresistance under the magnetic field oriented parallel to its axis with a period of the magnetic flux quantum were observed. The quantum oscillations which demonstrate the existence of coherent transport through closed-loop quantum states encircling the wire axis also show a tunable phase shift by the gate voltage. The results indicate clear gate-tuned Aharonov-Bohm interference of surface states in a semiconductor nanowire.

4:30PM V12.00011: Structural and optical properties of Si2Te3nanowires* JIYANG CHEN (Presenter), JINGBIAO CUI, XIAO SHEN, THANG HOANG, University of Memphis, KEYUE WU, College of Electrical and Photoelectronic Engineering, West Anhui University — Si2Te3 has recently attracted attention as a new class of layered 2D materials, which promise useful applications in thermal electrics and chemical sensing. Here, we report a study of the structural and optical properties of Si2Te3nanowires (NW) at various conditions. Single-crystalline Si2Te3NWs were synthesized by using gold nanoparticles as catalysts through the vapor-liquid-solid (VLS) mechanism. It was observed that these NWs prefer to grow along the [0001] direction, which is perpendicular to the 2D layers. Spectral and temporal characteristics of photoexcited carriers in these Si2Te3 NWs were investigated at various temperatures and excitation powers. Photoluminescence spectrum of Si2Te3 NWs was dominated by defect and surface states related emissions at both low and room temperatures. Consequently, the decay time of photoexcited carries strongly depends on the measurements at different temperatures and excitation powers. Our results quantitatively elucidate decay mechanisms that are important towards understanding and controlling of the electronic states in Si2Te3nanostructures for optoelectronic applications.

*National Science Foundation (DMR 1709528),
Natural Science Foundation of Educational Commission of Anhui Province of China (KJ2015A150).
4:42PM V12.00012: Electrically Driven Structural Phase Transition in Single Ag₂Te Nanowire Devices* KASUN PREMASIRI, Case Western Reserve University, WEI ZHENG (Presenter), YUE WU, Iowa State University, XUAN GAO, Case Western Reserve University — Exploring new phase-change materials are instrumental in the progression of electronic memory devices. Ag₂Te with its reversible structural phase transition, and in the form of nanowires becomes an apt candidate to potentially use in nanoscale memory devices. Here we report a study on the temperature- or electrically-driven phase change properties of crystalline Ag₂Te nanowires. We first demonstrate that this structural phase change can be achieved via heating up the nanowires, which results in a sharp drop in conductance. Then we show that a DC voltage (< 1V) induced Joule heating can be used to reach the phase transition, even without any external heating. This work shows the potential of using Ag₂Te nanowires as a phase-change material in low voltage and low power nanoscale devices.

*X. G. thanks the National Science Foundation (DMR-1151534) for its financial support. Y. W. thanks the Office of Naval Research (N00014-16-1-2066).

4:54PM V12.00013: Theoretical Study on VO₂ Nanowire Structures for Energy Applications* PRABAL BHUYAN, Department of Physics, Gujarati University, Ahmedabad, India, SANJEEV K. GUPTA (Presenter), Department of Physics, St Xavier’s College, Ahmedabad, India, YOGESH SONVANE, Department of Applied Physics, SV National Institute of Technology, Surat, India, P. N. GAJJAR, Department of Physics, Gujarati University, Ahmedabad, India — Recent studies on electronic, magnetic and optical properties of VO₂ (vanadium dioxide) material motivates to explore one-dimensional VO₂ nanowire. We have studied the structural and electronic, optical properties of monoclinic and rutile phase of VO₂ nanowire by performing first-principles calculations. The monoclinic phase showed semiconducting behaviour with a band gap of 1.17eV, while its bulk form showed a band gap of 0.7eV. The rutile phase behaves like as spin gapless semiconducting material. The rutile phase of VO₂ NW could find its applications in spintronic devices. We have also investigated the effect of SO₂, CO₂ and N₂ gas dopant on the monoclinic structure of VO₂ nanowire. The optical properties, density of states (DOS) have been investigated to understand the effect of dopant. It is clear from our results that the VO₂ monoclinic NW could likely to open up its application as an optical gas sensor.

*We would like to thank Science and Engineering Research Board (SERB), India for the financial support (Grant no.: YSS/2015/001269).

5:06PM V12.00014: Nano-wire to Film Transitions During Pulsed-Laser Deposition: the Role of Plasma Plume Expansion* DAVIDE DEL GAUDIO (Presenter), Materials Science and Engineering, University of Michigan, CARL T BOONE, SELFIA, KAITLYN SALLANS, Materials Science and Engineering, University of Michigan, ERICA MASON, University of Texas, ANDREW WILLIAMSON, SNEHA YARLAGADDA, JOHN HERON, Materials Science and Engineering, University of Michigan, ILAN SHALISH, Electrical and Computer Engineering, Ben Gurion University, RACHEL GOLDMAN, Materials Science and Engineering, University of Michigan — Due to their high conductivity, optical transparency, and high surface/volume ratio, indium-tin oxide (ITO) nanowires (NWs) are promising for flexible transparent electronics and gas sensors. During pulsed laser deposition (PLD) of ITO, NWs vs. films are typically selected via inert vs. reactive atmospheres. In other studies, both NWs and films are observed during PLD in inert atmospheres. Here, we consider the influence of the plasma plume expansion on NW vs film formation. For low pressure N₂, we hypothesize that oxygen is strongly scattered, leaving a metal-rich plume, resulting in metal droplet formation, followed by vapor-liquid-solid growth of NW. As the N₂ pressure is increased, the plasma plume and its metal rich core are compressed, resulting in a transition to films growth. This approach is likely applicable to a wide variety of metal-oxide NW core-shell structure for nanoscale devices.


*We gratefully acknowledge the support of NSF grant # ECCS-1610362 and BSF grant #2015700.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V13 DMP DCMP: 2D Materials -- Optical Properties BCEC 153B - Xiaohui Qiu, Chinese Academy of Sciences - Tag(s): Focus
Toward Quantum Optoelectronics and Optomechanics in Flatland

HONGKUN PARK (Presenter), Dept. of Chemistry and Chemical Biology and Dept. of Physics, Harvard University — Transition metal dichalcogenide monolayers and multilayers are atomically thin semiconductors that support tightly bound intra- and inter-layer excitons. In this presentation, I will describe our recent efforts to realize solid-state quantum optoelectronic devices using these atomically thin materials. In particular, I will describe how we prepare high-quality van der Waals heterostructures that feature spatially homogeneous, nearly lifetime-broadened excitons. I will then discuss the spectroscopy of intra- and inter-layer excitons in these structures and how we use them to realize atomically thin, electrically tunable mirrors. I will also describe a new approach for dynamically manipulating the exciton dynamics in these structures via electromechanical control over the suspended structures. I will end the presentation by discussing the ongoing efforts in my group to realize new quantum optical/optoelectronic/optomechanical effects in these structures.

THz Electrical Response of Graphene Antennas

DAVID CAREY (Presenter), MOJTABA DASHTI, University of Surrey — Studies of high frequency electrical properties offer an important route in exploring the underexplored unique characteristics of graphene. Here the GHz to THz response of graphene is investigated as a proof of principle concept for use as an ultrawide band patch antenna as part of a graphene based near-field communication system. We show that it is possible to produce a graphene multimode variable surface impedance microstrip antenna with several hundred GHz bandwidth via careful selection of the antenna geometry and substrate, and via engineering the relative contributions of the intra- and interband transitions. For an operating frequency of 2 THz an optimized return loss of -26 dB, bandwidth of 504 GHz and an antenna efficiency of -3.4 dB are calculated. Arising from the circular nature of the antenna structure higher order modes are possible and at 3.5 THz the antenna efficiency improves to -0.36 dB however this is accompanied by a reduction in the bandwidth to 200 GHz. Calculations of the real and imaginary parts of the dielectric constant between 1 and 10 THz have been performed which may be important for metamaterial applications.

Attosecond Dynamics and Electronic Rehybridization in MoS2

OLIVER MONTI (Presenter), CALLEY EADS, SARA ZACHRITZ, BRENT MAUGHAN, University of Arizona, DENNIS NORDLUND, SLAC, Stanford — Two-dimensional transition metal dichalcogenides exhibit highly unusual and layer-dependent electronic structure, caused by quantum confinement effects. The results of these changes have been widely documented in their valley-dependent optical properties. The impact of electron-electron interactions on the carrier dynamics is however at present less clear. Here we report on the attosecond dynamics in MoS2 as a function of carrier density in the conduction band. We show that increased electron density in the conduction band leads to orbital rehybridization, which is the source of the observed layer decoupling. These effects are also clearly observed in the electronic structure in the conduction band region. Our results uncover the many-body effects that govern the electronic properties of MoS2 and likely other 2D materials.

Quantum optics with atomically thin materials

NICK VAMIVAKAS (Presenter), University of Rochester — Two-dimensional, atomically-thin, materials have received enormous interest as a result of their unique mechanical, electrical and optical properties. Although these materials have been investigated for applications in optoelectronics, not much work has focused on these systems as a platform for quantum photonics and quantum optics. In this talk I will describe some approaches that leverage atomically thin semiconductors, and other two-dimensional materials, assembled in layered van der Waals heterostructures for applications in these areas. In the first part of the talk I will describe the unique photophysical properties of quantum emitters hosted by single layer two-dimensional materials. I will describe our recent efforts to controllably charge the quantum emitters and realize a localized spin-valley-photon interface. I will also present results on valley-polaritons that are a manifestation of many body physics arising when coupling an atomically thin semiconductor to a planar optical cavity.

AFOSR FA9550-16-1-0020, NSF CAREER DMR 1553788, NSF EFRI EFMA-1542707, and the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875)
4:06PM V13.00005: Tunable nonlinearity in a Graphene-Silicon Nitride hybrid resonator  RAJAN SINGH (Presenter), ARNAB SARKAR, CHITRES GURIA, Department of Physics, Indian Institute of Technology Kanpur, India, RYAN J NICHOLL, Department of Physics and Astronomy, Vanderbilt University, United States, SAGAR CHAKRABORTY, Department of Physics, Indian Institute of Technology Kanpur, India, KIRILL BOLOTIN, Department of Physics, Freie Universität Berlin, Germany, SAIKAT GHOSH, Department of Physics, Indian Institute of Technology Kanpur, India — Silicon Nitride (SiNx) resonators with high Q have garnered attention due to their strong promise of operation in the quantum regime at room temperature. Simultaneously, graphene resonators with high Young's modulus leading to large and tunable mechanical nonlinearity, have opened up possibilities of mixing and manipulating frequency modes. Here we propose a hybrid system that integrates high Q of SiNx resonator with nonlinearity of graphene resonator. When both resonator modes are tuned on resonance, the motional backaction of graphene induces nonlinear response in SiNx. The hybrid mode, when driven parametrically at twice the resonant frequency, demonstrates parametric amplification and cascaded four wave mixing. Generated peaks and their dispersion reveal the rich interplay between nonlinear damping and cubic nonlinearity. Observations match well with numerical simulations. Furthermore, in direct analogy with optomechanics, the graphene acts as an auxiliary cavity leading to induced nonlinearity on SiNx at resonance. These results indicate that such a hybrid mechanical system can be an efficient, alternate platform for coherent control of modes, in the growing field of opto and electromechanics.

4:18PM V13.00006: Ambient effects on hysteresis and photogating in MoS2 photodetectors* PEIZE HAN (Presenter), ELI ADLER, YIJING LIU, LUKE ST. MARIE, A EL FATIMY, PAOLA BARBARA, Georgetown University — Transition metal dichalcogenides (TMDs) are ideal candidates to create ultra-thin optoelectronics that can be flexible and semitransparent. Photodetectors based on TMDs have demonstrated remarkable performance, with high responsivity and high detectivity [1], however these devices are hindered by a slow response time caused by charge trapping. Gas adsorbents which create charge traps, are a main contribution to hysteresis and photogating [2,3]. Here we study the effect of ambient conditions on the performance of MoS2 photodetectors through vacuum pumping and illumination.

Reference:

*NSF (ECCS-1610953)

4:30PM V13.00007: Temperature Dependence of the Photoconduction in the Few-Layered ReSe2 Field-Effect Transistor* PRASANNA DNYANESHWAR PATIL (Presenter), MILINDA WASALA, RANA ALKHALDI, LINCOLN WEBER, Department of Physics, Southern Illinois University Carbondale, IL-62901, USA., KIRAN KUMAR KOVI, BHASWAR CHAKRABARTI, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL-60439, USA., DANIEL A RHODES, National High Magnetic Field Laboratory, Tallahassee, FL-32310, USA., DANIEL ROSENMANN, RALU DIVAN, ANIRUDHA SUMANT, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL-60439, USA., LUIS BALICAS, National High Magnetic Field Laboratory, Tallahassee, FL-32310, USA., NIHAR R PRADHAN, Department of Chemistry, Physics and Atmospheric Science, Jackson State University, Jackson, MS-39217, USA., SAIKAT TALAPATRA, Department of Physics, Southern Illinois University Carbondale, IL-62901, USA. — We will present the photo response of the few-layered ReSe2 field-effect transistor fabricated using mechanically exfoliated crystals grown using the chemical vapor transport method. The temperature dependence of the photoconductivity was measured as a function of temperature from 20 K to 300 K using a continuous laser source (λ = 640 nm; E = 1.94eV), over a broad range of illuminating laser power, P_{eff} (0.2 nW < P_{eff} < 84 nW). We measured the power dependence of the steady state photocurrent (I_{ph}) on P_{eff} (I_{ph} ~ (P_{eff})^{\gamma}, where 0.3 < \gamma < 0.8). The highest responsivity (R) and external quantum efficiency (EQE) obtained from the few-layered ReSe2 phototransistors at P_{eff} = 0.2 nW were ~ 2150 A/W and 10^5 %, respectively. These findings and the temperature dependence of the photoconductivity as a function of gate voltage will be presented.

*This work was performed, in part, at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, and supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357. This work was also supported by NSF-PREM through NSF-DMR # 1826886 and partially supported by the U.S. Army Research Office MURI grant # W911NF-11-1-0362.
4:42PM V13.00008: Temperature dependent electrical and photoconductive properties of few-layer Indium Selenide (InSe) FETs* MILINDA WASALA (Presenter), PRASANNA DNYANESHWAR PATIL, SUJOY GHOSH, RANA ALKHALDI, LINCOLN WEBER, Department of Physics, Southern Illinois University Carbondale, Carbondale, IL, USA, SIDONG LEI, Department of Materials Science and Nano Engineering, Rice University, Houston, TX, USA, HANSIKA SIRIKUMARA, THUSHARI JAYASEKERA, Department of Physics, Southern Illinois University Carbondale, Carbondale, IL, USA, ROBERT VAJTAI, PULICKEL M AJAYAN, Department of Materials Science and Nano Engineering, Rice University, Houston, TX, USA, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University Carbondale, Carbondale, IL, USA — Here we report on the temperature dependent electrical and photoconductive properties of n-type few-layer InSe Field Effect Transistors (FETs), micromechanically exfoliated from bulk crystal grown using chemical vapor transport method. The temperature dependent electrical conduction in these InSe FETs shows two distinct conduction mechanisms. At high temperatures electrical conduction is governed by thermally activated behavior, while at low temperatures electrical conduction follows Mott’s 2D variable range hopping mechanism. Further, photoconductivity measurements show that these InSe FETs display room temperature photo-responsivities of ~0.05 AW⁻¹ when illuminated with a laser of wavelength λ = 658 nm and a power of ~23 nW. The photo-responsivities of these FETs showed several orders of magnitude improvement (up to ~ 15 AW⁻¹) upon application of a gate voltage (VG = 60 V). These key findings and temperature dependent photoconductivity study will be presented and discussed.

*This work was supported by the U.S. Army Research Office MURI grant # W911NF-11-1-0362.

4:54PM V13.00009: Electric field effect studies of atomically thin crystals of ferroelectric In2Se3 JUSTIN RODRIGUEZ (Presenter), YIXUAN CHEN, SENG HUAT LEE, KAZUNORI FUJISAWA, TIANYI ZHANG, MAURICIO TERRONES, WILLIAM MURRAY, ZHIWEN LIU, YING LIU, Pennsylvania State University — Ultrathin films of ferroelectric materials are important for applications, including non-volatile memories, electromechanical actuators, and sensors. For a ferroelectric film of transition metal oxide to possess electrically switchable polarization, a minimal film thickness is required. In2Se3 is a layered III–VI compound with the unit cell consisting of a quintuple layer (QL) of In and Se ions in a triangular lattice featuring covalent bonding within the unit cell but van der Waals bonding between neighboring unit cells. It was predicted recently that In2Se3 is ferroelectric down to single unit-cell thickness, possessing both in- and out-of-plane polarizations in the a- and b-phases of In2Se3 polymorphism, respectively. We have carried out electric field effect studies of atomically thin crystals of a-In2Se3 down to liquid helium temperatures. These 2D crystals were prepared by mechanical exfoliation and characterized by Raman spectroscopy, photoluminescence, and second harmonic generation measurements. We found that the crystals are easily gated to possess a finite electrical conductivity characterized by thermally activated behavior. Source-drain current vs. gate voltage measurements revealed a hysteresis loop in the transfer characteristic, typical for ferroelectric devices.

5:06PM V13.00010: Crossover between Photochemical and Photothermal Oxidations of Atomically Thin CrPS4 SU HYEON KIM (Presenter), SUNMIN RYU, Pohang University of Science and Technology — Two-dimensional (2D) semiconductors represented by transition metal dichalcogenides have optical bandgaps that can be tuned via thickness, strain, dielectric screening and intercalation, and thus stand promising candidates for optoelectronic devices. Despite the potential, however, many including phosphorene and CrI3 lack photostability even in the ambient air. Here, we studied photoreaction mechanisms of 2D chromium thiophosphate (CrPS4), an antiferromagnetic semiconductor, using Raman spectroscopy and atomic force microscopy (AFM). Few-layer CrPS4 underwent photodegradation which accelerated with increasing partial pressure of O2. Topographic analysis by AFM showed that 2D CrPS4 is photo-oxidized at a laser power density two orders of magnitude lower than that required for MoS2 obeying a photothermal mechanism. Based on various control experiments over photon energy, power density and humidity, we propose that the low-power photoreaction of CrPS4 is a one-photon photochemical oxidation mediated by CrPS4-sensitized generation of singlet O2 and is switched over to a photothermal oxidation in a high-power regime. Additionally, the efficacy of thin Al2O3 films will be discussed as protecting layers of 2D CrPS4.
Spectroscopic Characterization of Interlayer Contaminants within van der Waals Heterostructures

JEFFREY SCHWARTZ (Presenter), Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, MD 20742, United States, HSUN-JEN CHUANG, MATTHEW R. ROSENBERGER, BEREND T. JONKER, Naval Research Laboratory, Washington, D.C. 20375, United States, ANDREA CENTRONE, Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD 20899, United States — Van der Waals heterostructures (vdWHs) leverage the characteristics of disparate 2D material building blocks to create a myriad of structures with unique and desirable properties. A common fabrication strategy relies on polymeric stamps to assemble layers of 2D materials into vertical stacks. However, the properties of structures produced in this way frequently are degraded by contaminants, typically of unknown composition, trapped between the constituent layers. This contamination impedes the study and application of intrinsic heterostructures requiring pristine interfaces. Here, we use a photothermal induced resonance technique to obtain nanoscale infrared spectra and maps of the contamination with ~20 nm spatial resolution. Heterostructures comprised of WS₂, WSe₂, and hBN layers were found to contain significant amounts of polydimethylsiloxane and polycarbonate, corresponding to the stamp materials used in their construction. Additionally, we validate spectroscopically a previously reported “nano-squeegee” technique as an effective means of locally removing contaminants. These insights into the chemical makeup and sources corrupting vdWHs provide guidance for devising mitigation strategies and enhance capabilities for producing materials with precisely engineered properties.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V14 DMP: 2D Materials (Metals, Superconductors, and Correlated Materials) -- Heterostructures and Twisted Graphene

BCEC 153C - Young Jun Chang, University of Seoul - Tag(s): Focus

2:30PM V14.00001: Coulomb drag between graphene and LaAlO$_3$/SrTiO$_3$ heterostructures* QING GUO (Presenter), JIANAN LI, JEN-FENG HSU, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin–Madison, PATRICK IRVIN, Department of Physics and Astronomy, University of Pittsburgh, BRIAN R D’URSO, Department of Physics, University of Montana, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — Vertical stacking of heterostructures that combine layered materials offer new ways of combining interesting properties of dissimilar electronic materials. Over the past few years we have been integrating graphene with complex-oxide heterostructures, specifically, the LaAlO$_3$/SrTiO$_3$ system. Furthermore, conducting nanostructures can be written under graphene, producing interesting interactions between the two systems. Here we report Coulomb drag measurements between single-layer graphene and a conductive LaAlO$_3$/SrTiO$_3$ interface. The observed Coulomb drag resistance is non-monotonic and increases for temperatures below 20 K. The temperature dependence is also non-monotonic, showing a notable departure from quadratic scaling, as expected from Fermi-liquid theory. Coulomb drag experiments between the graphene and LaAlO$_3$/SrTiO$_3$ layers show strong coupling in both the normal and superconducting state of the LaAlO$_3$/SrTiO$_3$.

*This research was supported by N00014-16-1-3152 (JL, BD), and N00014-15-1-2847 (JL). The work at University of Wisconsin-Madison was supported by the National Science Foundation under DMREF Grant No. DMR-1629270, AFOSR FA9550-15-1-0334 and AOARD FA2386-15-1-4046.

2:42PM V14.00002: Polarity of Coulomb drag signal in carbon nanotube-graphene heterostructures LAUREL ANDERSON (Presenter), AUSTIN K CHENG, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, PHILIP KIM, Harvard University — Coulomb drag is an inter-conductor interaction in which current in one conductor induces a current in a proximate conducting object. This electron-electron coupling can transfer momentum or energy between isolated conductors, creating inter-conductor electronic responses without particle exchange. Coulomb drag has been extensively studied as a probe of interactions in low-dimensional systems. We report measurements of 1D-2D drag resistance between a carbon nanotube and graphene separated by a thin boron nitride insulating layer. The carrier densities of the nanotube and graphene can be separately tuned to access different regimes of drag response. The polarity of the observed drag signal is inconsistent with inter-conductor momentum transfer, suggesting it is a possible signature of energy drag or hydrodynamic electron transport in graphene.
DONGHAN SHIN
3:18PM V14.00005: Electron pairing by remote-phonon scattering in oxide-supported graphene junction, akin to light bending at interfaces between mismatched media.

Our results provide evidence of coherent refraction of electrons passing through graphene that can be controlled on an atomic level, and is thus an ideal candidate for investigating light-like behavior of molecules arranged on a copper surface so as to confine the electrons to a honeycomb lattice, is an artificial form of molecules analogous to the focusing of light by optical instruments. Molecular graphene, consisting of carbon monoxide, suggests the possibility of constructing devices, such as Veselago lenses, that can focus electron wavefunctions in a manner analogous to the focusing of light by optical instruments. Molecular graphene, consisting of carbon monoxide molecules arranged on a copper surface so as to confine the electrons to a honeycomb lattice, is an artificial form of graphene that can be controlled on an atomic level, and is thus an ideal candidate for investigating light-like behavior of Dirac fermions. We report experiments that probe the behavior of electrons incident upon a graphene junction through quasiparticle interference measurements of a molecular graphene system in a low-temperature, ultra-high vacuum Dirac fermions. We report experiments that probe the behavior of electrons incident upon a graphene junction through quasiparticle interference measurements of a molecular graphene system in a low-temperature, ultra-high vacuum scanning tunneling microscope. Our results provide evidence of coherent refraction of electrons passing through the junction, akin to light bending at interfaces between mismatched media.

MORGEN BRUBAKER (Presenter), Physics, Stanford University, YI-TING CHEN, Applied Physics, Stanford University, ALISON DAY, Stanford University, HARI MANOHARAN, Physics, Stanford University — One of the many interesting features of graphene is the light-like behavior of its electrons near the Dirac points, characterized by a massless dispersion relation. This behavior suggests the possibility of constructing devices, such as Veselago lenses, that can focus electron wavefunctions in a manner analogous to the focusing of light by optical instruments. Molecular graphene, consisting of carbon monoxide molecules arranged on a copper surface so as to confine the electrons to a honeycomb lattice, is an artificial form of graphene that can be controlled on an atomic level, and is thus an ideal candidate for investigating light-like behavior of Dirac fermions. We report experiments that probe the behavior of electrons incident upon a graphene junction through quasiparticle interference measurements of a molecular graphene system in a low-temperature, ultra-high vacuum scanning tunneling microscope. Our results provide evidence of coherent refraction of electrons passing through the junction, akin to light bending at interfaces between mismatched media.

MORGAN BRUBAKER (Presenter), Physics, Stanford University, YI-TING CHEN, Applied Physics, Stanford University, ALISON DAY, Stanford University, HARI MANOHARAN, Physics, Stanford University — One of the many interesting features of graphene is the light-like behavior of its electrons near the Dirac points, characterized by a massless dispersion relation. This behavior suggests the possibility of constructing devices, such as Veselago lenses, that can focus electron wavefunctions in a manner analogous to the focusing of light by optical instruments. Molecular graphene, consisting of carbon monoxide molecules arranged on a copper surface so as to confine the electrons to a honeycomb lattice, is an artificial form of graphene that can be controlled on an atomic level, and is thus an ideal candidate for investigating light-like behavior of Dirac fermions. We report experiments that probe the behavior of electrons incident upon a graphene junction through quasiparticle interference measurements of a molecular graphene system in a low-temperature, ultra-high vacuum scanning tunneling microscope. Our results provide evidence of coherent refraction of electrons passing through the junction, akin to light bending at interfaces between mismatched media.

HARALD TOPOLOG AND JENS NORDMANN, Physics, University of Basel — Edge states have recently attracted a lot of attention due to their appearance at surfaces of topological materials and quantum Hall systems. Here we study quantum Hall edge states formed in a GaAs 2D electron gas using a tunnel-coupled quantum wire [1]. We use momentum-conserving tunneling spectroscopy to distinguish spatially overlapping states with different momenta. The tunneling conductance is proportional to the overlap between the edge state and the wire mode wave functions. Because of the varying shape of wire wave functions, their overlaps with edge states will also vary, resulting in a distinct sequence of tunneling conductance intensity patterns for different wire modes. We use self-consistent calculations to obtain the electrostatic potential at zero magnetic field and employ a Schrödinger solver to get the wave functions of the Landau level edge states and wire modes at a finite field. Conductance maps obtained using simulated wave functions agree very well with the measured data, thus confirming the calculated wave functions.


*Supported by Swiss NSF, NCCR QSIT, SNI, European Microkelvin Platform (EMP), NSF, EPIQS, MRSEC.

HIROYUKI TAKENAKA (Presenter), Department of Physics, University of Texas at Austin, MASSIMO V FISCHETTI, Department of Materials Science and Engineering, University of Texas at Dallas, ALEXANDER DEMKOV, Department of Physics, University of Texas at Austin — Using first principles calculations (density functional theory) we find that placing graphene on an (111)-oriented perovskite SrTiO₃ (STO) surface provides a convenient doping mechanism. Moreover, further theoretical analysis suggests that coupling of electrons in graphene to interfacial hybrid plasmon/optical modes via remote-phonon scattering may result in an effective attractive electron-electron interaction that, in turn, could lead to electron pairing and superconductivity. Specifically, we consider the graphene sheet supported by the STO and also gated. Using the full RPA dynamic polarizability of the whole system (including the hybrid mode arising from the coupling of the graphene plasmons to the optical phonons of the STO substrate and gate insulator), we estimate the superconductive transition temperature in both the weak- and the (Eliashberg) strong-coupling limits and also by solving the gap equation.

HIROYUKI TAKENAKA (Presenter), SHANE SANDHOEFNER, ALEXEY E KOVALEV, EVGENY Y TSYMBAL, University of Nebraska - Lincoln — The appearance of topological states in antiferromagnetic (AFM) materials has recently aroused considerable attention, resulting in the emergent field of topological AFM spintronics. Here, we theoretically explore the effect of voltage-controlled AFM order in chromia (Cr₂O₃) on the emerging topological states in graphene coupled across the Cr₂O₃/graphene interface. Chromia is a magnetoelectric AFM insulator exhibiting surface magnetization, intrinsically coupled to the Néel vector, which can be switched by an electric field. We find that the proximity effect leads to the broken time-reversal symmetry and the Rashba spin-orbit coupling in graphene, producing the topologically nontrivial band gaps. The resulting topological states and the quantum anomalous Hall effect in graphene are switchable by voltage with the Néel vector in chromia. Interestingly, the band gaps near the K and K' points in graphene are different due to the staggered coupling on the two sublattices, resulting in the non-vanishing valley current and the valley-polarized anomalous Hall state. The switchable Néel vectorpotentially produces a topological phase transition in graphene.
Fractional Chern insulators in graphene heterostructures

ERIC SPANTON (Presenter), ALEXANDER ZIBROV, HAOXIN ZHOU, JOSHUA ISLAND, XIAOMENG CUI, FANGYUAN YANG, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, MICHAEL ZALETEL, University of California-Santa Barbara, ANDREA YOUNG, University of California, Santa Barbara — Graphene is a highly tunable platform for studying the effects of electron-electron interactions in two dimensions. Encapsulation with a 2D dielectric (hexagonal boron nitride, hBN), and more recently the use of single-crystal graphite top and bottom gates have decreased the electronic disorder to a level suitable for the study of fragile and exotic strongly correlated states. Additionally, control of twist angle between closely-matched crystal lattices allows for unique control of electronic properties, leading to the “Hofstadter butterfly” and more recently unconventional superconductivity. I will describe the first experimental observation of a class of states in nearly aligned hBN/graphene heterostructures called fractional Chern insulators, a close relative of the fractional quantum Hall effect. In graphene, fractional Chern insulators arise in the presence of electron-electron interactions, high magnetic fields, and a long wavelength ‘moiré’ superlattice formed by close alignment between hBN and graphene lattices. Twist angle between graphene and hBN, electron density and perpendicular electric field tune the underlying single-particle bands to realize different types of fractional Chern insulators. The realization of fractional Chern insulators opens the door for the study of novel topological phase transitions and exotic defect states.

Normal state transport in superconducting twisted bilayer graphene

HRYHORIY POLSHYN (Presenter), YUXUAN ZHANG, University of California, Santa Barbara, MATTHEW YANKOWITZ, SHAOWEN CHEN, Department of Physics, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, DAVID E GRAF, National High Magnetic Field Laboratory, CORY R DEAN, Department of Physics, Columbia University, ANDREA YOUNG, University of California, Santa Barbara — Twisted bilayer graphene (tBLG) near the flat band condition is a versatile new platform for the study of correlated physics in 2D. Resistive states have been observed at several commensurate fillings of the flat miniband, along with superconducting states near half filling. To better understand the electronic structure of this system, we study electronic transport of graphite gated superconducting tBLG devices in the normal regime. At high magnetic fields, we observe full lifting of the spin and valley degeneracy. The transitions in the splitting of this four-fold degeneracy as a function of carrier density indicate Landau level (LL) crossings, which tilted field measurements show occur between LLs with different valley polarization. Similar LL structure measured in two devices, one with twist angle θ=1.08° at ambient pressure and one at θ=1.27° and 1.33GPa, suggests that the dimensionless combination of twist angle and interlayer coupling controls the relevant details of the band structure. In addition, we find that the temperature dependence of the resistance at B=0 shows linear growth at several hundred Ohm/K in a broad range of temperatures. We discuss the implications for modeling the scattering processes in this system.

Fabrication and measurement procedures for magic angle graphene devices

ORIOL RUBIES-BIGORDÀ (Presenter), YUAN CAO, DANIEL RODAN LEGRAIN, VALLA FATEMI, Massachusetts Institute of Technology, SHIANG FANG, Physics, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, EFTHIMIOS KAXIRAS, Physics, Harvard University, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Understanding the behavior of strongly correlated materials, such as unconventional superconductors, has been a challenge for decades. Graphene has turned out to be a new platform to study these phenomena. In particular, we have observed unconventional superconductivity and correlated insulating states by stacking two graphene layers and twisting them at a small angle, of about 1.1°. In this talk, we will focus on the fabrication procedures leading to reproducibly achieving high quality and low disorder ‘magic angle’ twisted bilayer graphene devices, with maximum critical temperatures over 2K and critical fields over 100mT. Such achievements with graphene further contribute to an emerging field, commonly referred to as ‘twistronics’, where other 2d –materials can be twisted to give rise to new correlated systems.

This work has been primarily supported by the National Science Foundation (DMR-1809802) and the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4541 for device fabrication, transport measurements, and data analysis. ORB acknowledges support from Fundació Privada Cellex.
Systematic analysis of superconductivity in magic-angle twister bilayer graphene nanodevices

DANIEL RODAN LEGRAIN (Presenter), YUAN CAO, ORIOL RUBIES-BIGORDA, VALLA FATEMI, Department of Physics, Massachusetts Institute of Technology, SHIANG FANG, Department of Physics, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University, PABLO JARILLO-HERRERO, Department of Physics, Massachusetts Institute of Technology — Superconductivity and correlated insulating states have recently been observed in ‘magic-angle’ twisted bilayer graphene heterostructures at twist angles close to 1.1 degrees, featuring nearly-flat bands owing to strong interlayer coupling. We here perform a systematic study of superconductivity and correlated phenomena in more than 10 different superconducting devices with angles comprised between 0.99 degrees and 1.19 degrees. Angle dependence of critical temperature and field, together with the interplay between superconductivity and insulating states, are examined. Higher quality devices allow us to extend the analysis to superconductivity when doping the twisted bilayer system with electrons. This 2D superconductor, based on graphene moiré superlattices, offers a uniquely tunable, clean and relatively simple platform for the investigation of strongly correlated physics.

*This work has been primarily supported by the National Science Foundation (DMR-1809802) and the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant GBMF4541 for device fabrication, transport measurements, and data analysis. DRL acknowledges support from Obra Social “la Caixa” Fellowship.

Transport Properties of a Few-layer Rhombohedral-stacked Graphene

YANMENG SHI (Presenter), YAPING YANG, SERVET CANOZDEMIR, SEOK-KYUN SON, SHUIGANG XU, JUN YIN, SERGEY SLIZOVSKIY, ARTEM MISHCHENKO, School of Physics and Astronomy, University of Manchester — Recently, two-dimensional systems that host flat bands have been extensively investigated experimentally and theoretically, due to the intriguing correlation effects as a result of large density of states. In a few-layer rhombohedral-stacked graphene, the dispersionless flat band localised at the outer surfaces is a promising candidate to realise such strong correlation physics. In this talk, I will present our preliminary data on the electrical transport in a few-layer rhombohedral-stacked graphene. We found that a gap is opened at the surfaces when a displacement field exceeds a threshold value. In a magnetic field we found robust quantum oscillations suggesting the high electronic quality of the observed flat-band surface states.

Quantum Hall effect in a monolayer graphene magnetized by an antiferromagnet

YINGYING WU (Presenter), GEN YIN, LEI PAN, University of California, Los Angeles, ALEXANDER GRUTTER, NIST, KANG L. WANG, University of California, Los Angeles — We experimentally demonstrate the quantum Hall effect in a monolayer graphene magnetized by an underlying layer of an antiferromagnet. When interfacing with the AFM, the π bond formed by the p orbitals of carbon is found to sufficiently overlap with the Cr atoms in the AFM layer, and therefore experiences a sizeable Hund's-rule exchange energy. Through field-cooling, the change in the antiferromagnetic order modifies the spin splitting, and thereby shifts quantum Hall plateau, as well as the SdH oscillation. This transport behavior is then used to quantitatively estimate the spin split energy (about several hundreds of meV).

Anomalous drag in double bilayer graphene quantum-Hall superfluids

ALLAN MACDONALD (Presenter), MING XIE, Department of Physics, University of Texas at Austin — Semiconductor double-layers in the quantum Hall regime tend to have superfluid exciton condensate ground states when the total filling factor is an odd integer, provided that the Landau orbitals at the Fermi level in the two layers have the same orbital character. Since the $N = 0$ Landau level of bilayer graphene contains states with both $n = 0$ and $n = 1$ orbital character, the physics of double bilayers falls outside previously studied cases. We show that the superfluid phase stiffness vanishes in double bilayer graphene when $n = 0$ and $n = 1$ orbitals states are degenerate in one of the layers, even though the gap for charged excitations remain large, and speculate that this property is behind the recent discovery of strong anomalous drag near a $n = 0/1$ degeneracy point.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V15 DMP: 2D Materials (Semiconductors) -- Emerging Materials II

Radboud University - Tag(s): Focus
2:30PM V15.00001: Kinetic Pathways Towards Mass Production of Single Crystalline Stanene on Topological Insulator Substrates

LIYING ZHANG (Presenter), School of Physics and Engineering, Zhengzhou University; International Center for Quantum Design of Functional Materials (ICQD), Hefei National Laboratory for Physical Science at the Microscale, WEI QIN, LEIQIANG LI, International Center for Quantum Design of Functional Materials (ICQD), Hefei National Laboratory for Physical Sciences at the Microscale, and Synergetic Innovation Center of, SHUNFANG LI, School of Physics and Engineering, Zhengzhou University, PING CUI, International Center for Quantum Design of Functional Materials (ICQD), Hefei National Laboratory for Physical Sciences at the Microscale, and Synergetic Innovation Center of, YU JIA, School of Physics and Engineering, Zhengzhou University, ZHENYU ZHANG, International Center for Quantum Design of Functional Materials (ICQD), Hefei National Laboratory for Physical Sciences at the Microscale, and Synergetic Innovation Center of — As a highly appealing new member of the two-dimensional materials family, stanene was first epitaxially grown on three dimensional topological insulator of Bi₂Te₃; yet to date, a standing challenge is to drastically improve the overall quality of such stanene overlayers for various potential applications. Here we use first-principles approaches to explore the atomistic growth mechanisms of stanene on different Bi₂Te₃(111)-based substrates. We fist show that, when grown on the experimentally studied Te-terminated Bi₂Te₃, stanene would follow an unusual partial-layer-by-partial-layer growth mode, characterized by short-range repulsive pairwise interactions of the Sn adatoms; the resultant stanene overlayer is destined to contain undesirable grain boundaries. More importantly, we find that stanene growth on Bi₂Te₃(111) pre-covered with a Bi bilayer will follow a highly desirable nucleation-and-growth behavior, strongly favoring single crystalline stanene. Interestingly, the latter system also provides new opportunities for potential realization of topological superconductivity in 2D heterostructures. The novel kinetic pathways revealed here will be instrumental in achieving mass production of high-quality stanene with emergent physical properties of technological significance.

*NSFC

2:42PM V15.00002: First principles studies of 2D transition metal dichalcogenides on 3D magnetic oxides

ELIZABETH PETERSON (Presenter), Physics, University of California, Berkeley, JEFFREY B NEATON, Lawrence Berkeley National Laboratory — Monolayer transition metal dichalcogenides are desirable for new high-speed, low-power and miniaturized valley optoelectronics. One way to create valley polarization is via magnetic proximity coupling, facilitated by interfacing single-layer TMDs and magnetic substrates; this approach has recently been shown to generate significantly larger valley splitting than applied magnetic fields. However, the reported valley splitting is still relatively small and the details of the interface between TMDs and magnetic substrates are poorly understood. Using first principles and model calculations, we explore the structure of the TMD-oxide interface, and predict the magnitude of the valley splitting generated by proximity to magnetic substrates. We examine the most critical attributes of this interface and develop general design principles that connect the structure of TMD-oxide interfaces to functionality relevant for valleytronics.

*We acknowledge funding from the Air Force Office of Scientific Research Hybrid Materials MURI under award number FA9550-08-1-0480 and NERSC for computing resources.

2:54PM V15.00003: Tunable band alignment in 2D ferroelectric In₂Se₃ based van der Waals heterostructures

ZHE WANG (Presenter), WENGUANG ZHU, University of Science and Technology of China — Van der Waals heterostructures with the advantages of atomically sharp interfaces, digitally controlled layered components, and no lattice parameter constraint, have been attracted substantial research interests in recent years due to their great potentials in electronic and optoelectronic applications and such properties critically depend on the band alignment between the constituent layers. Here we, based on first-principles calculations, demonstrate that by taking advantage of a recently discovered 2D ferroelectric material In₂Se₃ its van der Waals heterostructures with other known 2D materials have the ability to tune their band alignment between different types of semiconductor junctions or the Schottky barrier height by switching the orientation of the electric polarization of the ferroelectric In₂Se₃ layer with an external electric field. This work provides a generic guideline for the application of the 2D ferroelectric In₂Se₃ in tuning the electronic properties of van der Waals heterostructures.
The two-dimensional ferroelectric material GaTeCl monolayer*  
SHI-HAO ZHANG (Presenter), BANG-GUI LIU, Institute of Physics, Chinese Academy of Sciences — Searching for new ferroelectric atomic-thick materials is an important issue in the condensed matter physics. Through first-principles investigation we proposed a new two-dimensional ferroelectric material GaTeCl monolayer which can be exfoliated from pre-existing GaTeCl bulk. The calculated in-plane ferroelectric polarization reaches 578 pC/m. The energy barriers per formula unit of the ferroelastic 90-degrees rotational and ferroelectric reversal transitions are 476 meV and 754 meV respectively. A tensile stress of 4.7 N/m perpendicular to the polarization can drive the polarization to rotate by 90 degrees. The second harmonic generation susceptibility calculations reveal that the GaTeCl monolayer has giant optical second harmonic generation with the intensity being strongly anisotropic. These ensure the great potential of GaTeCl monolayer in high-performance multifunctional applications.

*This work is supported by the Nature Science Foundation of China (No. 11574366), by the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB07000000), and by the Department of Science and Technology of China (Grant No. 2016YFA0300701).

Injection current in single-layer group IV-monochalcogenides*  
SUMAN PANDAY (Presenter), BENJAMIN M. FREGOSO, Physics, Kent State University — Single-layer group-IV monochalcogenides GeS, GeSe, SnS, SnSe are two-dimensional ferroelectrics predicted to exhibit giant second harmonic generation and photovoltaic shift current. Using density functional theory methods, we show that these materials also exhibit giant injection current (circular photogalvanic effect). The magnitude can reach values up to $10^{11}$ A/V²S in the visible spectrum which is two orders of magnitude larger than that of prototypical nonlinear semiconductor CdS. We discuss the correlations between injection current, density of states and electric polarization using analytical and numerical methods. The injection current varies nonmonotonically with polarization reaching a maximum at an optimal polarization but is not correlated with the density of states. Our results establish GeS, GeSe, SnS, SnSe as versatile nonlinear materials suitable for optoelectronic applications.

*NERSC-DOE contract No. DE-AC02-05CH11231.

ABSTRACT WITHDRAWN

Tuning band structures and electronic properties of few-layer InSe by uniaxial strain  
CHAOYU SONG (Presenter), FENG-REN FAN, NINGNING XUAN, SHENYANG HUANG, GUOWEI ZHANG, CHONG WANG, ZHENGZONG SUN, HUA WU, HUGEN YAN, Fudan University — Atomically thin InSe joins the family of 2-dimensional materials recently with the advantage of high carrier mobility and layer-dependent bandgap. In this work, we engineer the band structures of few-layer InSe by uniaxial tensile strain. Prominent redshifts (90-100 meV per 1% strain) of photoluminescence peaks were observed in 4- to 8-layer samples. Density functional calculations well reproduce the observed strain effect and reveal that the shift rate decreases with increasing layer number for few-layer InSe, which can be understood based on the strain-induced change of the inter-layer interactions. In addition, resonant Raman spectroscopy was employed to study the vibrational properties of few-layer InSe. Sizable strain-induced redshifts of first order phonon modes and resonance effect were observed.

Ab initio Carrier Mobility of Two-Dimensional Indium Selenide*  
WENBIN LI (Presenter), SAMUEL PONE, FELICIANO GIUSTINO, Department of Materials, University of Oxford — Owing to its exceptionally high electron mobility, indium selenide (InSe) is emerging as one of the most promising layered semiconductors for two-dimensional electronics and optoelectronics. However, the intrinsic carrier mobility of InSe in the monolayer limit and the corresponding carrier scattering mechanisms remain unknown. By performing ab initio calculations of the intrinsic carrier mobility of InSe in the Boltzmann transport formalism, we find that the electron carriers in InSe are predominantly scattered by the coupling to longitudinal-optical phonons, namely the Fröhlich interaction. We also find that the carrier mobility of InSe exhibits strong layer dependence. At 300 K, the electron mobilities of InSe are found to be 120, 220, and 1060 cm²V⁻¹s⁻¹ for monolayer, bilayer and bulk, respectively, in good agreement with transport measurements.

*Leverhulme Trust (Grant RL-2012-001), UK EPSRC (grant No. EP/M020517/1), Graphene Flagship (Horizon 2020 Grant No. 785219 - GrapheneCore2), Marie Sklodowska-Curie grant (agreement No. 743580), the University of Oxford ARC facility, PRACE DECI resource Abel based in Oslo.
4:06PM V15.00009: First-principles studies on electronic band structure of PdSe₂ with GW approximation

HANYU KIM (Presenter), HYOUNG JOON CHOI, Department of Physics, Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University, Seoul 03722, Korea (the Republic of). — We studied the electronic band structure of PdSe₂ using the density functional theory (DFT) and the GW method. It is known that PdSe₂, a material with stacks of pentagonal layer structure, has a semiconducting band structure experimentally. However, DFT calculations show that bulk PdSe₂ has a semi-metallic band structure because of DFT underestimation of the band gap of the material. To obtain the band gap of PdSe₂ correctly, we calculated the quasiparticle band structure of bulk PdSe₂ using the one-shot GW method and obtained a band gap which is consistent with experimental results. Then we calculated the electronic structure of two-dimensional PdSe₂ to investigate the layer-number dependence on the energy gap. We discuss band-to-band transition energies and other physical properties obtained from band structures of PdSe₂.

*This work is supported by the NRF of Korea (Grant No.2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2017-C3-079).

4:18PM V15.00010: Scalably-nanomanufactured atomically-thin piezoelectric semiconductor for ubiquitous electronics and smart sensors

[Invited] WENZHUO WU (Presenter), Purdue University — The reliable production of atomically-thin crystals is essential for exploring new science and implementing novel technologies in the 2D limit. In this talk, I will discuss our recent discovery of a new 2-D piezoelectric semiconductor, tellurene, synthesized by a substrate-free solution process. The tellurene crystals exhibit process-tunable thicknesses from a monolayer to tens of nanometers, and lateral sizes ~ 100 mm. Our prototypical tellurene transistor device, which is air-stable, shows an excellent all-around figure of merits compared to existing 2D materials. We further carry out the first experimental exploration of piezotronic effect in tellurene and systematically investigate the piezotronic transport properties. The fundamental understanding of piezotronic coupling in tellurene is expected to provide insights for the development of 2-D material piezotronics and electronics, leading to the realization of “smarter” electronics for a multitude of emerging technologies, e.g., wearable electronics, soft robotics, medical prosthetics, and human-machine interface.

*W. Z. W. acknowledges the College of Engineering and School of Industrial Engineering at Purdue University for the startup support. W. Z. W. was partially supported by the National Science Foundation under grant CMMI-1762698.

4:54PM V15.00011: ABSTRACT WITHDRAWN

5:06PM V15.00012: Study of dipolar excitons in TiS₃ double layer

ROMAN KEZERASHVILI (Presenter), Physics Department, New York City College of Technology, City University of New York — The most studied layered semiconductors to date are the transition metal dichalcogenides and nowadays there is a flurry of effort to study the transition metal trichalcogenides (TMTC) with MX₃ composition (M is a metal X is a chalcogen) that have highly anisotropic crystal structure. We present the results of study of the formation of dipolar excitons in a TMTC double layer in the framework of a Wannier-Mott model for the indirect excitons that takes into account the anisotropic effective masses. The energy spectrum and wave functions for a single dipolar exciton are obtained and binding energies are calculated within the harmonic oscillator approximation for the Rutova-Keldysh and Coulomb potentials. In the framework of the Bogoliubov approximation spectrum of collective excitations for the dilute weakly interacting Bose gas of dipolar excitons si studied and the mean field critical temperature for the superfluidity is obtained. It is demonstrated that as a result of the strong in-plane anisotropy, superfluidity is vastly differ in different crystalline directions. The calculations are performed for a direct band gap semiconductor TiS₃ that is a prototypical representative of TMTC materials.

*This work is supported by U.S. Department of Defense under Grant No. W911NF1810433
5:18PM V15.00013: Van der Waals charge-transfer interfaces* YUTA KASHIWABARA (Presenter), MASAKI NAKANO, YUJI NAKAGAWA, YUE WANG, HIDEKI MATSUOKA, YOSHIHIRO IWASA, Department of Applied Physics, The University of Tokyo — The creation of functional interfaces between different materials has often led to a discovery of a unique electronic property and functionality that is missing in the constituent materials, providing an invaluable material platform in modern science and technology. 2D materials are suitable compounds for construction of such an interface due to existence of the van der Waals gap that enables creation of an atomically-abrupt interface, and in fact various types of heterostructures named ‘van der Waals heterostructures’ have been more and more developed for the last few years. However, those researches have mainly focused on electrical transport across the interface, while lateral transport properties along the interface have been less studied so far. In this presentation, we will demonstrate emergence of electrical conduction at the interface between insulating 2D materials fabricated by molecular-beam epitaxy with our growth recipe [1]. [1] M. Nakano, et. al., Nano Lett. 17, 5595 (2017).

*This work was supported by Grant-in-Aid for Scientific Research (No. 25000003) from the Japan Society for the Promotion of Science.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V16 DCOMP: Quantum Manybody Systems: Theory and Computation II

2:30PM V16.00001: Off-Diagonal Expansion Quantum Monte Carlo* ITAY HEN (Presenter), TAMEEM ALBASH, LALIT GUPTA, University of Southern California — I will discuss a novel, parameter-free Trotter error-free, quantum Monte Carlo technique designed to tackle a very broad range of physical models within a single unifying framework. The method builds on a series expansion of the canonical partition function around its classical component. The expansion further allows for a group-theoretical abstraction of the QMC algorithm. Some results showcasing the capabilities of the algorithm will be presented.

*The computing resources were provided by the USC Center for High Performance Computing and Communications. The research is based upon work supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.

2:42PM V16.00002: Finite-temperature Auxiliary-Field Quantum Monte Carlo: Recent Developments and Applications* YUAN-YAO HE (Presenter), CCQ, Flatiron Institute, Simons Foundation, MINGPU QIN, Department of Physics, College of William and Mary, HAO SHI, CCQ, Flatiron Institute, Simons Foundation, ZHONG-YI LU, Department of Physics, Renmin University of China, SHIWEI ZHANG, CCQ, Flatiron Institute, Simons Foundation — We present a highly accurate auxiliary-field quantum Monte Carlo (AFQMC) method to study finite-temperature properties of correlated fermion systems. This approach eliminates the minus sign problem by introducing constraints in auxiliary-field space. Building on earlier ideas [1] and incorporating the latest developments in zero-temperature methods, we introduce a self-consistent formalism [2] to improve the constraint in the finite-temperature framework. This with several other algorithmic advances leads to a more accurate, more efficient, and numerically more stable approach for finite-temperature calculations. We carry out systematic benchmark study in the 2D Hubbard model. Temperatures as low as T=1/80 (in units of hopping) are reached. The finite-temperature method is exact at high temperatures, and approaches the result of the zero-temperature constrained-path AFQMC as temperature is lowered. The benchmark shows that systematically accurate results are obtained for thermodynamic properties. The properties of the 2D doped Hubbard model as functions of temperature will be presented and discussed.


*We acknowledge the support from NSF and Simons Foundation.
ANISH BHARDWAJ (Presenter), Florida State University Tallahassee FL USA; National High Magnetic Field Laboratory, EFSTRATIOS MANOUSAKIS, University of Athens, Panepistimiopolis, Zografos, Athens, Greece; Florida State University, Tallahassee, FL, USA; National High Magnetic Field Laboratory — A diagrammatic expansion for the pair distribution can be derived by starting from the many-body path-integral and using the idea of cluster expansion. The expansion is written as a sum of nodal and non-nodal diagrams. The sum of all the nodal diagrams can be expressed in terms of the non-nodal diagrams using the hypernetted equation technique. The sum of the non-nodal diagrams, which are irreducible diagrams in momentum space, are written as a perturbation expansion in powers of the particle density. Our approach is analogous to the well-known many-body perturbation expansion of the n-body Green's function. The approach was tested on a system of distinguishable particles and our results agree very well with those obtained from the path-integral Monte Carlo.

ZHENGQIAN CHENG (Presenter), CHRIS MARIANETTI, Columbia University — We formulate a general method for constructing a variational expression of the total energy based on two projective ansatz from the weak and strong coupling limits. These two ansatz are then combined according to individual and mutual interactions of low and high energy degrees of freedom. We apply our approach to the single band Hubbar model, where the theory yields the double occupancy and the nonlocal single-particle density matrix. We compare to exact results for $d=1$ and $d=\infty$. For $d=1$, the insulating state is properly obtained at infinitesimal $u$; in addition to an accurate prediction of the ground state energy over a broad range of $t/U$. In infinite dimensions, we properly find a finite-U metal-insulator transition with reasonable quantitative accuracy across all parameter space. Our approach has a negligible computational cost as compared to dynamical mean field theory and could be highly applicable in the context of total energies for strongly correlated materials and molecules.

Johan Nilsson (Presenter), Uppsala University — We discuss some new methods for truncating and closing the equations of motion for composite operators. Our formalism automatically generates a physical theory in the sense of having positive spectral weights. Another important advantage of our methods is that (for judiciously chosen set of operators) all averages necessary to close the formalism can be calculated self-consistently from within the theory itself. We discuss how the method can be applied to the Hubbard model in both fermionic and bosonic sectors.

Fernando Reboredo (Presenter), Oak Ridge National Laboratory — An approach to evaluate a family of semi-local observables from the fixed-node ground state will be discussed. The celebrated importance-sampling diffusion Monte Carlo (DMC) method by Ceperley and Alder is a real space approach. Therefore, beyond the calculation of the total energy of the fixed-node ground state, DMC facilitates the evaluation of observables that are local in real space such as the density, albeit pure estimators or extrapolations are required. The evaluation of semi-local observables is expected to be more involved. It can be shown, however, that the DMC algorithm carries additional information of the fixed-node solution. DMC results for semi-local operators will be compared with exact results, in the hydrogen atom and the harmonic oscillator. The perspectives, computational cost, and potentials problems of this approach when applied to realistic many-body systems will be discussed.

*Supported by the Materials Science and Engineering Division, Basic Energy Sciences, Office of Science, Department of Energy.

ABDULGANI ANNABERDIYEV (Presenter), CODY MELTON, MICHAEL BENNETT, GUANGMING WANG, LUBOS MITAS, North Carolina State University — We present high accuracy total energies of pseudo-atoms, i.e., atoms with effective core potentials (ECP). The pseudo-atoms considered are the 1st, 2nd and 3rd-row elements with correlation consistent effective core potentials (ccECP) we constructed. For each element, we perform configuration interaction, coupled-cluster, and quantum Monte Carlo calculations with systematically eliminated/improved errors. We carry out FCI/CCSDT(Q) calculations with aug-cc-pVnZ (n=3-6) basis set extrapolated to complete basis set limit to obtain highly accurate energies. For these methods, the achieved accuracy in the 1st row is typically 0.1-0.3 mHa, the 2nd row is 0.1-0.2 mHa, and 5-10 mHa in the 3rd row. Wherever possible, we included the kinetic energies obtained from FCI calculations to estimate the smoothness/curvature of the particle density. These accurate total energies will serve as a benchmark for independent calculations as well as the assessment of systematic and methodological errors.
3:54PM V16.00008: Compton Profile of Solid and Liquid Lithium from Quantum Monte Carlo* YUBO YANG (Presenter), University of Illinois at Urbana-Champaign, MARKUS HOLZMANN, Physics, Laboratoire de Physique et Modélisation des Milieux Condensés, DAVID M CEPERLEY, University of Illinois at Urbana-Champaign — Compton scattering cross section is directly related to the electronic momentum distribution and provides an important check of many-body theory. We computed the Compton profile of solid and liquid lithium using quantum Monte Carlo (QMC) and compared with recent experiments obtaining excellent agreement. Importantly, we find it necessary to explicitly include the core electrons for quantitative accuracy. To account for lattice effects, we sampled finite-temperature configurations using molecular dynamics (MD), then performed pseudopotential diffusion Monte Carlo (DMC) simulations on each configuration. We used Slater-Jastrow wavefunction and twist-averaged boundary condition. QMC pseudopotential correction was derived from an all-electron DMC simulation of the perfect crystal. Our calculations provide the first all-electron QMC benchmark for the Compton profile of lithium under both liquid and solid conditions.

*This work made use of the Blue Waters sustained-petascale computing project and the Illinois Campus Cluster, supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993), the state of Illinois, the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.

Yubo Yang and David Ceperley were funded by DOE 0002911.

4:06PM V16.00009: Prediction of the singlet-triplet excitation energy for the spinel, MgTi2O4 via downfolding approach combined with first-principles Quantum Monte Carlo* BRIAN BUSEMEYER (Presenter), GREG MACDOUGALL, LUCAS WAGNER, University of Illinois at Urbana-Champaign — The spinel, MgTi2O4 undergoes a transition into a dimerized state at low temperatures that is expected to be a spin singlet. However, no signature of a singlet-triplet transition as been discovered, in part due to the difficulty of predicting the energy of the transition from theory. Using high-accuracy first-principles quantum Monte Carlo combined with a novel model-fitting approach, we predict the singlet-triplet gap to be 350(50) meV, a higher energy than previous experimental observations have considered. Confirmation of our prediction would suggest that our approach should enable calculation of other excitation energies on the basis of first-principles quantum Monte Carlo combined with effective model calculations.

*This research is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.

4:18PM V16.00010: An Efficient Calculation of the Total Energy Variation in DFT+DMFT Implemented using Orthogonal Basis sets BENNY WAH (Presenter), HYOWON PARK, University of Illinois at Chicago — Calculations of the total energy variation in density functional theory plus dynamical mean field theory (DFT+DMFT) with respect to the structural change are important for atomic force and stress computations for strongly correlated materials. In this talk, we will show that the energy variation of DFT+DMFT implemented using orthogonal basis sets such as Wannier functions can be computed efficiently using analytic formula since the potential energy variation can be exactly cancelled out and the DMFT self-energy itself or its variation does not need to be explicitly accounted. We will use DMFT with the Continuous-Time Quantum Monte Carlo (CTQMC) impurity solver to compute its total energy variation of the two-dimensional one-band Hubbard model with respect to changes of hopping parameters and compare to the results of its analytic energy derivative formula to verify their quantitative agreement. We will also compare the potential energy contributions sampled directly from CTQMC and computed using the Migdal-Galitzki formula. The application of our formula to the calculations of forces and stress in DFT+DMFT will be also discussed.

4:30PM V16.00011: Systematic corrections to the Thomas-Fermi approximation without a gradient expansion JUN HAO HUE (Presenter), THANH TRI CHAU, MARTIN-ISBJÖRN TRAPPE, BERGE ENGLERT, National University of Singapore — We improve on the Thomas–Fermi approximation for the single particle density of fermions by introducing inhomogeneity corrections. Rather than invoking a gradient expansion, we relate the density to the unitary evolution operator for the given effective potential energy and approximate this operator by a Suzuki–Trotter factorization. This yields a hierarchy of approximations, one for each approximate factorization. For the purpose of a first benchmarking, we examine the approximate densities for a few cases with known exact densities and observe a very satisfactory, and encouraging, performance. As a bonus, we also obtain a simple fourth-order leapfrog algorithm for the symplectic integration of classical equations of motion.
4:42PM V16.00012: Approximate States of the Hubbard Model from Heisenberg’s Equation* ROGER HAYDOCK (Presenter), University of Oregon — Operators which add electrons with definite energies to states of interacting electrons are solutions of the time-independent Heisenberg equation. Expanding the operators in the number of electron-hole pairs generated to screen each added electron provides systematic approximations for the energies of these operators. This is illustrated for the simplest Hubbard model on a cubic lattice by relations between the energies and electron densities of ground states.

*Snyder Gift to University of Oregon

4:54PM V16.00013: Bond energies of molecules using strictly-correlated-electron (SCE) limit of Density-Functional-Theory* KSHITEEJ DESHMUKH (Presenter), KAUSHIK DAYAL, Civil and Environmental Engineering, Carnegie Mellon University — Standard Kohn-Sham DFT starts from a mean-field approximation: the kinetic energy is modeled exactly, while the electron-electron interactions are modeled through a split into a mean-field term, and corrections from the exchange-correlation term. The SCE limit starts from the opposite limit: the electron-electron interactions are assumed to dominate over the kinetic energy, and hence it is a semi-classical limit. It is hence well suited to study strongly-correlated situations, e.g. bond breaking. While the SCE limit includes many-body interactions, it can be identified as a problem from Optimal Transport theory with Coulomb cost function. Hence it can be solved by a nested optimization in its dual (Kantorovich) formulation. We incorporate the Kantorovich solution within the KS-DFT framework and solve using Finite Element Method.

*AFSOR MURI

5:06PM V16.00014: Correlated states in magnetic quantum dots with multiple occupancy TIAGO DE CAMPOS (Presenter), University at Buffalo, The State University of New York, JAMES PIENTKA, Physics, ST. BONAVENTURE UNIVERSITY, ALEX MATOS ABIAIGUE, Department of Physics and Astronomy, Wayne State University, JONG E HAN, IGOR ZUTIC, University at Buffalo, The State University of New York — The motivation to magnetically dope semiconductor quantum dots comes from the possibility for an enhanced control of magnetic ordering as compared to their bulklike counterparts. Unlike in the bulk structures, adding a single carrier in a magnetic QD can have important ramifications. An extra carrier can both strongly change the total carrier spin and the temperature of the onset of magnetization[1]. While QDs have been recognized for correlation effects, inherent in the analog of Wigner crystals referred to as Wigner molecules (WMs), the modification of underlying correlated states with magnetic doping is largely unexplored[2]. By focusing on Mn-doped II-VI QDs[3] we show correlated states, which can be viewed as a generalization of WMs, can be studied using exact diagonalization and conditional probability density. We explain how the formation of a shell structure in these Mn-doped QDs and magnetic frustrations are altered by the changes in strength of the Coulomb interaction.


5:18PM V16.00015: Resilience of the Mixed State Wigner Function ALBERT MATERDEY, Roxbury Community College, THOMAS MATERDEY (Presenter), University of Massachusetts Boston, ALEXANDER MATERDEY, Quantum FC, Inc. — Solution of the quantum Vlasov equation shows the phase space dynamics of a mixed-state Wigner function is more resilient against changes in external electric and magnetic fields than a pure-state Wigner function. A particle in a mixed-state is harder to follow and localize, but the freedom to access a range of pure states increases its inertia against changes in external conditions. This could explain the electron’s stability in the Shrodinger’s atomic orbital model and perhaps provides a way to preserve the information of a qubit sufficiently long for quantum computing.

Thursday, March 7, 2019 2:30 PM - 5:18 PM

Session V17 DCOMP: Matter in Extreme Environments: Warm Dense Matter BCEC 156A - Paul Loubeyre, CEA de Bruyeres-le-Chatel - Tag(s): Focus
**2:30PM V17.00001: Modeling Materials at Extreme Conditions for High Energy-Density Science** [Invited]  STEPHANIE HANSEN (Presenter), TAI SUKE NAGAYAMA, ANDREW BACZEWSKI, ATILLA CANGI, THOMAS GOMEZ, Sandia National Laboratories — Modern High Energy-Density experimental facilities study inertial confinement fusion, laboratory astrophysics, and extreme states of matter by compressing energy in space and time to produce hot, dense, and strongly coupled plasmas. In such extreme environments, changes in electronic and ionic structure impact the material equation-of-state, transport properties, and observable signatures that inform both hydrodynamic simulations and interpretations of experimental data. This talk will survey experimental programs in HED science and describe an ongoing effort to develop a highly constrained, fully self-consistent atomic-scale model of material at extreme conditions. Generating equations of state, transport properties (thermal and electrical conductivities, opacities, stopping powers) and diagnostic signatures (X-ray Thomson scattering, spectroscopic line shifts and broadening) from a single, consistent core model helps to constrain simulations and improve the reliability of data interpretation from complex experiments.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. This work was supported by the U.S. Department of Energy, Office of Science Early Career Research Program, Office of Fusion Energy Sciences under FWP-14-017426.

**3:06PM V17.00002: A Stochastic approach to thermal DFT**  YAEL CYTTER (Presenter), Department of Chemistry, Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Israel, DANIEL NEUHAUSER, Department of Chemistry and Biochemistry, University of California Los Angeles, USA, ERAN RABANI, Department of Chemistry, University of California Berkeley and Lawrence Berkeley National Laboratory, USA, ROI BAER, Department of Chemistry, Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Israel — Despite progress in observational astronomy, some elements such as the internal composition of planets are still not well-understood. A root cause is our limited understanding of matter under extreme conditions (MEC) - pressures in the GPa-TPa range and temperatures (T) up to 10^5 K. Due to the difficulty in preparing MECs, the experimental input is limited, and ab initio calculations are sometimes the only source of information. The Kohn-Sham density functional theory (KS-DFT) seems as a reliable and useful tool for obtaining information on MEC. Calculations in finite temperatures, however, are expensive due to the large number of fractionally occupied KS orbitals involved. A stochastic method developed recently[1],[2], appears to be a fitting approach to this problem. By performing a stochastic trace, the KS Hamiltonian is directly obtained from the density, resulting in a scaling of O(T^{-1}). I will introduce the convergence and errors involved in calculations of the canonical free energy. In addition, a stochastic approach to calculate the Kubo-Greenwood conductivity will be presented.


**3:18PM V17.00003: A new capability for large-scale linear scaling Kohn Sham DFT calculations for materials at high temperatures.**  SEBASTIEN HAMEL (Presenter), Physics and Life Sciences, Lawrence Livermore Natl Lab, MANDY BETHKENHAGEN, Physics, University of Rostock, JOHN PASK, BABAK SADIGH, Physics and Life Sciences, Lawrence Livermore Natl Lab, PHANISH SURYANARAYANA, School of Civil and Environmental Engineering, Georgia Tech — We developed a new capability for the accurate and efficient quantum simulation of material properties across an extreme range of densities, pressures and temperatures. This code, SQDFT, enables the use of full Kohn-Sham quantum molecular dynamics from the condensed matter regime, through the warm dense matter regime and into the plasma regime, well beyond the previous state-of-the-art which was restricted to temperatures below approximately 100 000 Kelvins. We demonstrate this new capability by calculating the Hugoniot curve of different materials up to millions of degrees Kelvin and Gigabar of pressure and investigating the structural and transport properties of the materials under these extreme conditions. We also present a performance study of our SQDFT code on various supercomputing platforms. SQDFT scales linearly with system size which allows us to run full Kohn-Sham QMD simulations with several thousand of atoms.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. We gratefully acknowledge support from the Laboratory Directed Research and Development Program.
SCAN-L extended to an exchange-correlation free-energy density functional for extreme conditions

Daniel Mejia-Rodriguez (Presenter), Sam B Trickey, University of Florida — The predictive potential of density functional theory (DFT) for simulation of systems under extreme conditions of temperature and pressure depends crucially on having an exchange-correlation (XC) free-energy functional that is accurate for such state conditions. Distinct from zero-temperature XC functionals, the XC free-energy functional must have an explicit temperature dependence. Recently, that has been achieved for the local density approximation ["KSDT", Phys. Rev. Lett. 112, 076403 (2014)] and generalized-gradient approximation ["KDT16", Phys. Rev. Lett. 120, 076401 (2018)].

By use of the systematic construction scheme of the KDT16 GGA, we extend the recent SCAN-L ground-state orbital-free meta-GGA XC functional [Phys. Rev. A 96, 052512 (2017), Phys. Rev. B 98, 115161 (2018)] to a semilocal XC free-energy functional. This completes the ladder of computationally efficient orbital-free free-energy XC functionals. The accuracy of the new SCAN-LF in the warm dense matter regime is assessed and compared to KSDT and KDT16.

*DMR and SBT were supported by U.S. DOE grant DE-SC-000139

Fast First-Principles Predictions for Warm Dense Matter with Orbital-free Free Energy Density Functional Theory

Kai Luo (Presenter), University of Florida, Valentin Karasiev, Laboratory for Laser Energetics, Sam B Trickey, University of Florida — Warm dense matter encompasses the phase-space region between ordinary condensed matter and plasmas. That poses inconvenient challenges for theory. Conventional Kohn-Sham density functional theory (KS-DFT) is computationally demanding due to a large number of thermally occupied bands involved at high temperature. Meanwhile, path-integral Monte Carlo (PIMC) has intrinsic difficulties for the low-temperature scenario. In contrast, orbital-free free energy density functional theory (OF-FEDFT) is a consistent approach spanning the whole T range. The key to OF-FEDFT usage is good approximate functionals. Here we extend the recent LKT ground-state generalized gradient approximation (GGA) non-interacting kinetic energy density functional (KEDF) (Phys. Rev. B 98, 041111(R) (2018)) to a semi-local free energy functional. In tests on hydrogen at elevated T, it outperforms the previously best single-point free energy functional, VT84F (Phys. Rev. B 88, 161108(R) (2013)) for the equation of state (EOS). For deuterium, it is roughly comparable to KS-DFT and PIMC in accuracy.

*KL and SBT were supported by U.S. DOE grant DE-SC-0002139. VVK was supported by U.S. DOE NNSA award DE-NA0001944.

Approach to Orbital-Free DFT with Englert-Schwinger model

Jouko Lehtomäki (Presenter), Olga Lopez-Acevedo, Department of Applied Physics, Aalto University — Orbital-free density functional theory (OFDFT) is a variant of DFT which tries to circumvent construction of Kohn-Sham orbitals in order to efficiently scale to larger system sizes. Most of the research on OFDFT is on improving the accuracy of the non-interacting kinetic energy density functional (KEDF) as a direct functional of density, which requires use of pseudopotentials. Instead of density functionals, we focus on potential functional formalism. This formalism allows us to sidestep use of pseudopotentials and directly use atomic orbitals alongside orbital-free functionals. We assess the self-consistent performance of potential functionals by Englert and Schwinger[1].

Specifically we compare the Englert-Schwinger model to Kohn-Sham and Thomas-Fermi-Dirac-Weizsäcker models self-consistently on small systems, especially atoms showing that the potential functionals by Englert and Schwinger are a viable alternative to the non-interacting kinetic energy density functionals. We also present the augmentation of this model with Kohn-Sham orbitals, which allow us to explore OFDFT solution without the use of pseudopotentials.

WILLIAM NELLIS (Presenter), Harvard University — An equation of state at extreme conditions in Warm Dense Matter (WDM) is needed for exoplanets and Inertial Confinement Fusion. Development of theory for WDM is problematical because of the need for experimental data for verification. At shock pressures 0.5 - 20 TPa (200 Mbar) measured Hugoniot data of fluid metals [1] are essentially co-linear in U_S (U_P), where U_S and U_P are shock and particle velocity, respectively, essentially independent of material. Calculated shock temperatures of those data range from a few thousand K up to a million K. Those shock-compressed fluids are WDM with Minimum Metallic Conductivity (MMC) [2]. The linear fit to 40 measured data points is known as the Universal Hugoniot of Fluid Metals (UHFM), which is possible verification data for WDM theory. TFD is Thomas Fermi theory for ionized atoms, Fermi-Dirac statistics for electrons, and electron correlation [3]. A possible theory for why co-linear fit is universal might be a common electron correlation function in TF theory that yields the UHFM for Al, Cu, Fe, Mo, Kr, Gd_3Ga_5O_12, etc.


THOMAS SCHENKEL (Presenter), SVEN STEINKE, QING JI, JIANHUI BIN, STEPAN BULANOV, JAEHONG PARK, WIM PIETER LEEMANS, Lawrence Berkeley National Laboratory — We use the BELLA petawatt laser [1] to accelerate ions to multi-MeV energies at a repetition rate of up to 1 Hz [2]. Ion acceleration is now routinely conducted at BELLA in parallel to laser-plasma acceleration of electrons. For laser intensities in the 10^19 W/cm^2 regime, we find ion intensities up to 10^12 ions/shot with low divergence. When transported to a second target, ion pulses can drive the formation and annealing dynamics of defects and they can uniformly heat materials to temperatures of 1-10 eV, well into the warm dense matter regime [3]. Ion intensities can be tuned for materials processing at selected temperatures to form desired defect structures or to drive desired phase-transitions. We present results from ion acceleration and target heating campaigns, including color center synthesis for spin qubits in diamond.


*This work was supported by the US DOE under contract DE-AC0205CH11231 and by LaserNetUS through the US DOE Office of Science, Office of Fusion Energy Sciences.

ANDREW KRYGIER (Presenter), Lawrence Livermore Natl Lab, USA, MARION HARMAND, IMPMC, Université Pierre et Marie Curie, France, BRUNO ALBERTAZZI, LULI, Ecole Polytechnique, France, EMMA MCBRIDE, SLAC National Accelerator Laboratory, USA, KAREN APPEL, European XFEL, Germany, KOHEI MIYANISHI, NORIMASA OZAKI, Institute for Laser Engineering, Osaka University, Japan, GUILLAUME FIQUET, IMPMC, Université Pierre et Marie Curie, France — Earth's core is composed of Fe mixed with small amounts of light elements like Si, O, and C. Determining the properties of high-pressure liquids, the melting curve, and solid phase relations of Fe and derivative alloys is important for understanding the cores of Earth and terrestrial exoplanets. High pressure and temperature conditions can be achieved with high power lasers, but the states are highly transient, and the inherently high strain rate introduces physics not expected to occur in planetary interiors. The recent advance of facilities with high-power lasers coupled to XFELs enables characterization of shocked states with the powerful suite of X-ray techniques used by the static community. Here we present results from recent ultrafast X-ray diffraction measurements of shocked Fe alloys at the coupled XFEL-optical laser facilities using the EHS end station at the SACL laboratory (Japan) and the LCLS end station MEC at SLAC National Accelerator Laboratory (USA).

*This work is supported by the French Agence Nationale de la Recherche with the ANR IRONFEL 12-PDOC-0011, the ERC PLANETDIVE, and under the auspices of the Lawrence Livermore National Security, LLC, (LLNS) under Contract No. DE-AC52-07NA27344
4:42PM V17.00010: Thermal conductivity and equation-of-state measurements in warm dense matter* [Invited]
YUAN PING (Presenter), Lawrence Livermore Natl Lab — Thermal conductivity is one of the most fundamental physical properties of matter. It determines the heat transport rate and has an enormous impact on a variety of mechanical, electrical, chemical, and nuclear systems. Thermal conduction is important in high energy density (HED) matter such as laboratory fusion plasmas, planetary cores, compact stars, and other celestial objects. Examples are in the ablation and instability growth in inertial confinement fusion (ICF) capsules, in energy loss from ICF hot spot, and in the evolution of Earth's core-mantle boundary. Despite the importance of thermal conductivity in HED systems, experimental measurements under relevant conditions are scarce and challenging. We have developed a method of differential heating for thermal conductivity measurements. In this talk, experimental designs will be described for two different platforms: proton heating and x-ray laser heating. Data from various facilities on amorphous carbon, aluminum and iron will be presented and comparison with models will be discussed.

*This work was performed under DOE contract DE-AC52-07NA27344 with support from OFES Early Career program and LLNL LDRD program.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V18 DCOMP: Electronic Structure Methods II BCEC 156B - Rajendra Zope

2:30PM V18.00001: Bringing Electronic Structure Codes into the Modern Software Ecosystem
RAN ADLER (Presenter), Rutgers University, New Brunswick, ANDREY KUTEPOV, Brookhaven National Laboratory, GABRIEL KOTLIAR, Rutgers University, New Brunswick — We propose a novel framework (“Portobello”) for assimilating Electronic Structure codes into the modern software ecosystem and facilitating an efficient software development process. First we discuss some of the pitfalls of Fortran / Python - centric paradigms, which often lead to flawed design and unwieldy code. We identify a culprit to be the lack of high-level abstraction, which prevents reuse of components, obscures developers' intent, and hinders collaboration. Our new object-oriented framework facilitates all steps of the software developments life-cycle, and is applicable to Fortran-based systems, as well as ones written in C/C++.

Next, we demonstrate how the framework provides a concrete way to address important questions in the physics of Correlated Electronic Structure, as well as implement and test new ideas. Following this approach, we combine A. Kutepov's Fortran-based FlapwMBPT (Full potential LAPW Many-Body Perturbation Theory) with a C++ implementation of CTQMC and Materials Project Pymatgen (crystal and symmetry code) to create a Pythonic charge-self-consistent toy DFT+DMFT program. We demonstrate the calculation of correlated electronic structure, as well as calculation of transport properties, and discuss how the program can be used and extended.

2:42PM V18.00002: ComDMFT: a Massively Parallel Computer Package for the Electronic Structure of Correlated-Electron Systems*
SANGKOOK CHOI (Presenter), PATRICK SEMON, BYUNGKYUN KANG, ANDREY KUTEPOV, GABRIEL KOTLIAR, Brookhaven National Laboratory — ComDMFT is a massively parallel computational package to study the electronic structure of correlated-electron systems (CES). Our approach is a parameter-free method based on ab initio linearized quasiparticle self-consistent GW (LQSGW) and dynamical mean field theory (DMFT). The non-local part of the electronic self-energy is treated within ab initio LQSGW and the local strong correlation is treated within DMFT. In addition to ab initio LQSGW+DMFT, charge self-consistent LDA+DMFT methodology is also implemented, enabling multiple methods in one open-source platform for the electronic structure of CES. This package can be extended for future developments to implement other methodologies to treat CES

*This work was supported by the U.S Department of Energy, Office of Science, Basic Energy Sciences as a part of the Computational Materials Science Program
3:30PM V18.00003: Hubbard interactions from density-functional perturbation theory  IURI TIMROV (Presenter),
MATTEO COCCOCCIONI, NICOLA MARZARI, EPFL STI IMX THEOS, Ecole polytechnique federale de Lausanne — DFT+U+V is a novel
and powerful tool to model systems containing partially-filled manifolds of localized states. However, there is a history of
treating Hubbard parameters semi-empirically, which is unsatisfactory. Conceptual methods to determine e.g. Hubbard U
from first principles have nevertheless been introduced long ago, based either on the constrained random-phase
approximation or on linear response theory. Still, these approaches are often overlooked due to their cost or complexity.
Here, we introduce a computationally inexpensive and straightforward approach [1] to determine on-site U and inter-site
V Hubbard parameters, bypassing the need to use supercells. By recasting linear-response susceptibilities in the language of
density-functional perturbation theory we substitute monochromatic perturbations to supercells, and allow for a fully
determined automation of Hubbard parameters in primitive cell calculations. Such developments provide the
community with a robust and reliable tool to calculate consistent values of U and V for any system at hand, while opening
the way for deployment in high-throughput studies. The approach is showcased with applications to the vibrational
spectra of selected transition-metal compounds.

3:06PM V18.00004: RESPACK software to derive ab initio effective low-energy Hamiltonians and its extension to
treat materials with strong spin-orbit interaction.* MAXIME CHARLEBOIS (Presenter), YUSUKE NOMURA, Department of
Applied Physics, University of Tokyo, YOSHIHIDE YOSHIMOTO, Department of Computer Science, University of Tokyo, TERUMASA
TADANO, Materials Science, National Institute for Materials Science (NIMS), MASATOSHI IMADA, Department of Applied Physics,
University of Tokyo, KAZUMA NAKAMURA, Quantum Physics Section, Department of Basic Sciences, Kyushu Institute of Technology —
RESPACK [1] is an open source library that allows to calculate electron correlation effects and to derive effective low-
energy Hamiltonians starting from the density functional theory (DFT). The downfolding to low-energy Hamiltonians is
achieved by combining maximally localized Wannier functions [2] and full (or constrained) random phase approximation. It
can be interfaced with both Quantum ESPRESSO [3] and xTAPP [4]. Here, we present an extension of RESPACK to treat
materials with strong spin orbit effects and application to various test materials.
[1] https://sites.google.com/view/kazuma7k6r

*This work was supported by Fonds de recherche du Québec - Nature et technologies (FRQNT) and by a Grant-in-Aid for
Scientific Research(No. 16H06345) from Ministry of Education, Culture, Sports, Science and Technology, Japan

3:18PM V18.00005: Full-potential relativistic four-component Dirac–Kohn–Sham method for periodic systems using
Gaussian-type functions* MARIUS KADEK (Presenter), MICHAL REPISKY, KENNETH RUUD, Hylleas Centre for Quantum
Molecular Sciences, University of Tromso — I will present a new full-potential all-electron Kohn–Sham theory for obtaining
fully-relativistic band structures of spin–orbit-coupled solids. Our method is based on the four-component Dirac–Coulomb
Hamiltonian, and all operators are represented compactly in real space using Gaussian-type orbitals (GTOs). The local
nature of GTOs allows for explicit handling of one-, two-, and three-dimensional periodic systems avoiding the need to
introduce vacuum layers. In combination with a variational treatment of spin–orbit coupling, this makes the method
suitable for studying two- and three-dimensional topological insulators as well as spin–orbit-induced splittings of bands.
The GTO-based methodology makes no assumptions about the electronic density in the vicinity of nuclei, and can be used to
calculate core-related properties, such as nuclear magnetic resonance parameters. Large-scale relativistic calculations
of solids containing thousands of heavy atoms in the simulation supercell are possible due to the use of quaternian
algebra for the time-reversal-adapted basis and employment of fast-multipole methods.[1]
[1] M. Kadek, M. Repisky, and K. Ruud (to be published)

*This work was supported by Research Council of Norway, grant numbers 179568, 262695, and 214095, and NOTUR grant NN4654K.

3:30PM V18.00006: Density-functional theory for noncollinear magnetism: exact and approximate results on small
Hubbard chains* EDWARD PLUHAR (Presenter), CARSTEN ULLRICH, University of Missouri — We apply a class of orbital-
dependent exchange-correlation functionals (exact exchange and Singwi-Tosi-Land-Sjoelander exchange-correlation) to
two-electron systems on small Hubbard chains in the presence of noncollinear magnetic fields. We compare these
approximations with benchmark results obtained from exact diagonalization and inversion of the Kohn-Sham equation via
a conjugate-gradient optimization. In general, good agreement is found for total energies, densities and magnetizations
over a range of interaction strengths. Exchange-correlation torques, on the other hand, are more subtle and can be
difficult to approximate, especially for strong correlations.

*This work was supported by Research Corporation and by DOE Grant No. DE-SC0019109
3:42PM V18.00007: Metals: Automatic k-point generation for a 60% speed-up of total energy calculations*  
GUS HART (Presenter), WILEY S MORGAN, JEREMY JORGENSEN, RODNEY W. FORCADE, Brigham Young University — A generalized regular k-point grid generation method (more general than the traditional Monkhorst-Pack method) leads to a 60% speed-up for total energy calculations of metallic systems. Generalized regular grids can be generated using the JHU k-point server: http://muellergroup.jhu.edu/K-Points.html. We have developed a new algorithm that can generate these same grids on the fly so that a web request is not necessary. The algorithm relies on group theoretical ideas that connect the concepts of lattices and integer matrices to yield extremely fast grid generation, enabling scans over thousands of candidate grids and select one with the highest efficiency (best k-point symmetry reduction).

*Supported by the Office of Naval Research (MURI N00014-13-1-0635).

3:54PM V18.00008: Get 10 materials for the price of 1: computationally efficient DFT*  
JEREMY JORGENSEN (Presenter), THOMAS W. SEDERBERG, GUS HART, Brigham Young University — We have developed a numerical algorithm that will allow us to run density functional theory (DFT) computations ten times faster. Our improvements in efficiency result from accelerating the convergence rate of the band energy calculation by employing local polynomial interpolation and adaptive mesh refinement. Tests of the algorithm on 2D toy pseudopotentials show an order of magnitude improvement over the rectangular method, the method currently implemented in DFT programs. Our tests demonstrate two counterintuitive results: 1) accurately approximating the Fermi surface is critical to accurately calculate the band energy, and 2) band crossings are inconsequential. Implementing our algorithm in DFT programs will accelerate both the growth of theoretical materials databases and the discovery of materials.

*Authors acknowledge funding from ONR (MURI N00014-13-1-0635).

4:06PM V18.00009: Band Unfolding Made Simple*  
SARA GARCÍA MAYO (Presenter), JOSE M. SOLER, Departamento de Física de la Materia Condensada, Univ. Autónoma de Madrid — We present a simple point of view on band unfolding of the energy bands obtained from supercell calculations that relies on the relationship existing between the local density of states in reciprocal space (qLDOS) and the fully unfolded band structure of a system. This new concept provides an intuitive and valid approach not only for periodic, but also for non-translationally symmetric systems, as well as a way to recover the conventional band structure by doing a refolding back into the primitive Brillouin zone of the pristine crystal. We implemented this algorithm in the Siesta package and tested some of its potential applications on silicon-based systems, such as defective crystals, surfaces and amorphous structures.

*Funded by Spain’s MINECO grant FIS2015-64886-C5-5-P

JASON MUNRO (Presenter), VINCENT LIU, VENKATRAMAN GOPALAN, ISMAILA DABO, Pennsylvania State University — The nudged elastic band (NEB) method is an effective approach for calculating minimum energy pathways of kinetic processes. However, the final paths obtained by the algorithm rely heavily on the initially chosen path. This often necessitates running multiple calculations with different initial conditions in order to obtain reliable results. Recently, this problem has been reformulated using the language of distortion symmetry, which consists of combining static spatial symmetries with a new operation called distortion reversal, and has the property of only being conserved or raised by the NEB optimization [1]. Using this knowledge, symmetry-adapted perturbations to an initial path can be generated and used to systematically lower its symmetry. By doing so, the exploration of other low-energy pathways that may exist is enabled. The group and representation theory details behind this new approach are presented and implemented in standalone software (DiSPy). The algorithm is then demonstrated by applying it to the calculation of ferroelectric switching pathways in LiNbO3. Previously reported pathways are recovered, with new paths that involve a higher degree of atomic coordination also being discovered.

**4:30PM V18.00011: Evaluation of self-energy matrix for electrode based on real-space pseudopotential method**  
SHIGERU IWASE (Presenter), TOMOYA ONO, Department of Physics, University of Tsukuba  
— Evaluation of self-energy matrix for electrode is one of the bottleneck parts of the first-principles transport calculation. Over the past years, several methods have been developed to reduce the computational cost, however calculation is still slow especially when the real-space pseudopotential method is employed because the Hamiltonian matrix of the unit cell becomes very large. We present a method to evaluate the self-energy matrix especially for real-space pseudopotential method. The method combines the partitioning technique [1] with singular value decomposition, which transforms the Hamiltonian matrix of a unit cell into the maximally contracted form. Because of the simplicity of the method, typical methods such as quick decimation method [2] and semi-analytical method [3] can be used for the contracted Hamiltonian without large modification. We applied this method for several examples and validated the accuracy and efficiency of the method.


**4:42PM V18.00012: On the δ-function broadening in Kubo-Greenwood equation**  
PAVLO BULANCHUK (Presenter), Physics, Pennsylvania State University  
— We propose a solution to a long-standing issue in the calculation of Kubo-Greenwood DC conductivity in finite-sized quantum systems. The Kubo-Greenwood equation contains a sum of delta-functions, which are usually broadened. The estimate of the DC conductivity depends significantly on the type of broadening applied, making the estimate ambiguous. We eliminate the ambiguity by mapping the broadening onto a specific way of introduction of the electric field and making a correction based on Drude equation. We also consider the influence of delta-function broadening on conductivity averaged over disorder. We demonstrate the influence can be reduced to a convolution of the average conductivity with the broadening function over the frequency. Even though in finite systems the average conductivity is an oscillatory function of frequency, if convolved with a slowly varying function, it behaves similarly to a Lorentzian. We propose a procedure of extracting the parameters of the Lorentzian by extrapolation similarly to a single system.

**4:54PM V18.00013: Minimizing Reflections in Electronic Structure Calculations**  
GREGORY BENESH (Presenter), Department of Physics, Baylor University, ROGER HAYDOCK, Department of Physics, University of Oregon  
— In electronic structure calculations, large aggregates of atoms are usually approximated by model systems containing far fewer atoms—introducing artificial boundaries that do not occur in the original system. These boundaries ordinarily produce reflected waves that interfere with outgoing solutions of the Schrödinger equation. Depending on the degree of interference, computational results from model calculations may differ widely from the characteristics of the real physical system. Examples of computational studies exhibiting this interference effects abound in many areas of physics. One approach to eliminating the reflection problem is to choose Schrödinger solutions that minimally reflect at the artificial boundary of the model system. These so-called Maximum Breaking of Time-Reversal Symmetry (MBTS) solutions come in pairs that maximally carry current in opposite directions. In effect, by using MBTS solutions, the boundary becomes transparent or nearly-transparent to traveling waves. The MBTS formalism and results for several model systems will be presented.

**5:06PM V18.00014: Long-wavelength density-functional perturbation theory**  
MASSIMILIANO STENGEL (Presenter), ICMAB-CSIC and ICREA  
— Density-functional perturbation theory (DFPT) is nowadays the method of choice for the accurate computation of linear and non-linear response properties of materials from first principles. A notable advantage of DFPT over alternative approaches is the possibility of treating incommensurate lattice distortions with an arbitrary wavevector, \( \mathbf{q} \), at comparable computational cost as the lattice-periodic case. In this talk, I will show that \( \mathbf{q} \) can be formally treated as a perturbation parameter, and used in conjunction with established results of perturbation theory (e.g. the \( 2n + 1 \) theorem) to perform a long-wave expansion of an arbitrary response function in powers of the wavevector components. This provides a powerful, general framework to accessing the physical response to the spatial gradient of an arbitrary external field (electric, magnetic, strain or atomic displacement), with a computational cost that is comparable to that of a standard linear-response calculation. As applications of the method, I will discuss the flexoelectric tensor (the polarization response to a gradient of the strain field) and on the "dynamical quadrupoles" (a higher-order multipolar generalization of the Born effective charge tensor).
5:18PM V18.00015: Tight Binding Molecular Dynamics Study of the Cu-Ag Binary Noble Metal System SWABIR SILAYI (Presenter), DIMITRIOS A PAPACONSTANTOPoulos, George Mason University, MICHAEL MEHL, US Naval Academy — The Naval Research Laboratory tight-binding (NRL-TB) method has been quite successful in accurately describing the electronic and mechanical properties of many systems from semiconductors and simple metals to transition and noble metals. We used the NRL-TB method with parameters determined from a fit to reproduce the electronic structure and total energy versus volume values of first-principles Augmented Plane Wave (APW) calculations to study the Cu-Ag noble metal binary system. The parameters were fit to the structures B1(NaCl), B2(CsCl), L12 (Cu3Au), and C1 (Fluorite) and the NRL-TB method reproduced the APW ordering of these structures and the ground-state structure of the system to be the CsCl. Other structural properties such as bulk moduli and electronic densities of states and energy bands were reproduced as well. We also performed molecular dynamics simulations to determine the energies for vacancy formation, temperature dependence of the coefficient of thermal expansion and the mean squared displacement. The TB parameters are demonstrated to be robust for calculating additional static and dynamical properties which had not been fitted.

Thursday, March 7, 2019 2:30 PM - 5:18 PM

Session V19 DMP: Computational Materials Design and Discovery -- High Throughput Computing and Data Mining BCEC 156C - Geoffroy Hautier, Université catholique de Louvain - Tag(s): Focus

2:30PM V19.00001: Polymer Genome: An Informatics Platform for Rational Polymer Dielectrics Design and Beyond [Invited] RAMAMURTHY RAMPRASAD (Presenter), Georgia Institute of Technology — The Materials Genome Initiative (MGI) has heralded a sea change in the philosophy of materials design. Here, we highlight the importance of computational data generation and screening, targeted synthesis and characterization, polymer fingerprinting, machine-learning prediction models, and the creation of an online Polymer Informatics platform (https://www.polymergenome.org) to guide ongoing and future polymer discovery and design. We lay special emphasis on the fingerprinting of polymers in terms of their genome or constituent atomic and molecular fragments, an idea that pays homage to the pioneers of the human genome project who identified the basic building blocks of the human DNA. By scoping the polymer genome, we present an essential roadmap for the design of polymer dielectrics, and provide future perspectives and directions for expansions to other polymer subclasses and properties.

3:06PM V19.00002: High-throughput computational design of electrode-electrolyte interface for solid-state Li-ion batteries* CHUHONG WANG (Presenter), TIM MUELLER, Materials Science and Engineering, Johns Hopkins University — All-solid-state lithium-ion batteries have attracted significant interest for their enhanced safety compared with conventional batteries employing an organic liquid electrolyte. However the interfacial reaction between electrodes and electrolyte can hinder the transport of charge carriers, thus degrading the battery performance. In this work, we present a systematic high-throughput screening method to identify coatings to maintain interface stability during battery operation. Promising coating materials are rapidly selected from computational databases containing a vast collection of inorganic materials. Material candidates found in this work consist of known electrode coatings as well as a list of promising compounds for further testing. We demonstrate that our approach is an efficient way to predict and evaluate functional coatings for a high performance solid state battery design.

*Toyota Motor Corporation

3:18PM V19.00003: New Olivine-Based Cathode Materials HONG FANG (Presenter), PURUSOTTAM JENA, Physics, Virginia Commonwealth University — Olivine-type lithium transition metal orthosilicates, considered as promising cathode materials for the next-generation lithium-ion batteries, have attracted considerable interest in recent year. This is due to their low cost, good safety, and high theoretical capacity. However, great challenges still remain regarding their relatively low practical capacity, phase instability during charge/discharge, and low electronic conductivity. Here, combining data mining with state-of-the-art first-principles calculations, we present a comprehensive study of new olivine-based materials that can meet the above challenges and serve as ideal candidates for cathode materials of next-generation batteries.
3:30PM V19.00004: High-throughput workflow for discovery of multiferroic materials based on ab initio calculations

STEPHANIE MACK (Presenter), University of California, Berkeley, SINEAD MAGELLA GRIFFIN, TESS SMIDT, JEFFREY B NEATON, Lawrence Berkeley National Laboratory — Expanding the catalogue of multiferroics has thus far mostly relied on finely tuning complex perovskite oxides through strain engineering and chemical substitution. While this has been a successful strategy yielding over a dozen new bulk oxide multiferroics, few new classes of multiferroics have been discovered as typical strategies rely on knowledge of structural motifs of known multiferroics. Prior work [1] has developed a high-throughput workflow to screen the Materials Project database for ferroelectrics based on space group symmetry requirements and ab initio calculations. We extend this strategy and develop a workflow to search for candidate polar insulating materials with magnetic order and switchable polarization. Analysis of the trends identified through the search will be discussed.


*Funding provided by DOE, and computational resources provided by NERSC

3:42PM V19.00005: High-throughput analysis of large heterogeneous and dynamic data spaces with signac

CARL SIMON ADORF (Presenter), VYAS RAMASUBRAMANI, BRADLEY DICE, SHARON GLOTZER, University of Michigan — High-throughput generation and analysis of vast data sets offers enormous opportunities for accelerated scientific discovery, but also requires prudent strategies for the management of computational resources and data spaces. This is especially critical when researchers work with heterogeneous and possibly highly dynamic data. The signac framework enables researchers to maintain well-formed and reusable data spaces from early exploration all the way to production runs on supercomputing scales. This is achieved through a transparent data and workflow model as well as a simple and unobtrusive programmatic interface that scales well between preliminary prototyping and concluding stages of a particular computational investigation. Here, we demonstrate the framework's efficacy and versatility by showcasing examples of how signac is applied across various research projects and disciplines.

*Development and deployment supported by UM and MICCoM, as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Subcontract No. 6F-30844. Project conceptualization and early implementation supported by the National Science Foundation, Award # DMR 1409620.

3:54PM V19.00006: High-throughput First-principles Screening of the Layered Magnetic Double-Perovskites Cs₄MSb₂X₁₂

TAO ZHANG (Presenter), DAN HAN, DEYAN SUN, SHIYOU CHEN, East China Normal University — Compared to the three-dimensional halide perovskites, the layered perovskites can exhibit better air-stability and more flexible optoelectronic properties. Among them, Cs₄CuSb₂Cl₁₂ attracted our attention due to its supreme properties such as suitable bandgap, high conductivity, high photo- and thermal-stability in photovoltaic devices. We investigated a series of <111> layered double-perovskites which can be derived from Cs₄CuSb₂Cl₁₂ through the elemental substitution. High-throughput first-principles calculations identified three stable layered double-perovskites Cs₄MnSb₂Cl₁₂, Cs₄CuSb₂Cl₁₂ and Cs₄ScSb₂Br₁₂. The ground state structure of Cs₄MnSb₂Cl₁₂ has the R-3m symmetry and exhibits antiferromagnetic(AFM) ordering, while the Cs₄CuSb₂Cl₁₂ and Cs₄ScSb₂Br₁₂ favor the C2/m symmetry and show AFM ordering. Our calculated results are consistent with the experimental observations, i.e., the ground state structures of Cs₄MnSb₂Cl₁₂ and Cs₄CuSb₂Cl₁₂ have R-3m and C2/m symmetry and they both exhibit AFM behavior, showing that our high-throughput calculation is valid for searching the thermodynamically stable <111> layered magnetic double-perovskites. A new layered double-perovskite Cs₄ScSb₂Br₁₂ is predicted for the first time and it may be synthesized experimentally in the future.
High-throughput Computational Search for Ternary Oxypnictide Mixed Anion Materials

JIAHONG SHEN (Presenter), VINAY I HEGDE, JIANGANG HE, CHRISTOPHER WOLVERTON, Materials Science and Engineering, Northwestern University — Mixed anion, or heteroanionic materials (HetMs), have seen a recent resurgence in interest owing to their intriguing properties for a wide range of applications, including photocatalysts, thermoelectrics and transparent conductors. Though HetMs present more degrees of freedom for materials design, only a relatively small amount of HetMs have been reported comparing to single anion materials. By means of high-throughput density functional theory (HT-DFT) computations, combined with the Open Quantum Materials Database (OQMD), new HetMs and their thermodynamic stabilities can be predicted across a wide range of compound chemistries. In this work, HetMs MOX (M is periodic table elements; X=N, P, As) are studied and several promising stable HetMs are found. Both experimentally observed and hypothetical new compounds (in total 438 compounds) are calculated, and analyzed for thermodynamic ground state stability. Phase diagrams with respect to anion chemical potentials are constructed for these potential candidates to provide constraints on the gas-phase temperature and pressure conditions under which these compounds are stable, guiding future experimental synthetic efforts.

Computational Exploration of Stable Heteroanionic Compounds ABOX (A and B are metal; X=S, Se, and Te)

JIANGANG HE (Presenter), VINAY I HEGDE, Northwestern University, ZHENPENG YAO, Department of Chemistry and Chemical Biology, Harvard University, S. SHAHAB NAGHAVI, Department of Physical and Computational Chemistry, Shahid Beheshti University, KYLE BUSHICK, CHRISTOPHER WOLVERTON, Northwestern University — Compared with single anion compounds, such as oxides, chalcogenides, and fluorides, compounds with multiple anions (heteroanionic or mixed-anion) are less explored[1]. Many of the known heteroanionic compounds have been found to have compelling properties and promising applications. High-throughput ab initio screening is an efficient approach for new materials discovery and can significantly accelerate the experimental synthesis by pointing out promising candidates. In this talk, we will demonstrate the use of high-throughput ab initio calculations combined with the Open Quantum Material Database (OQMD) of formation energies to discovery hundreds new synthesizable ABXO (X=S, Se, and Te) compounds. Crystal structures, dynamical stabilities, and promising applications of these oxysulfides compounds for thermoelectric, transparent conductors, and ionic conductors have been explored within first principles framework as well.


AFLOW-XTAL-MATCH: Automated method for quantifying the structural similarity of materials and identifying unique crystal prototypes

DAVID HICKS (Presenter), CORMAC TOHER, DENISE FORD, CARLO DE SANTO, OHAD LEVY, Duke University, MICHAEL MEHL, United States Naval Academy, STEFANO CURTAROLO, Duke University — The rapid development of computational materials-property databases has generated an abundance of compounds exhibiting various geometries. As materials are continuously added, distinguishing unique structures from duplicates is a growing challenge. We introduce a crystal comparison module – AFLOW-XTAL-MATCH – that quantifies the similarity between structures, independent of the unit cell representation. Employing the misfit criteria from Burzlaff [1], the routine identifies structurally unique or duplicate crystals. To accommodate automatic workflows, the program's infrastructure can analyze numerous structures simultaneously, performing all necessary comparisons. The tool is integrated into the AFLOW framework [2], with functionality to compare compounds to entries in the AFLOWLIB repository and the library of AFLOW prototypes [3]. The algorithm i) elucidates materials with similar properties, ii) determines distinct crystal prototypes, and iii) guides the discovery of unexplored materials.

Herein, a new module is presented for autonomous thermodynamic stability analysis implemented within the open-source AFLOW framework. Powered by the AFLUX Search-API, AFLOW-CHULL leverages data of more than 1.8 million compounds and can be employed locally from any UNIX-like computer. The module integrates a range of functionality: the identification of stable phases and equivalent structures, phase coexistence, measures for robust stability, and determination of decomposition reactions. As a proof of concept, thermodynamic characterizations have been performed for more than 1300 binary and ternary systems, enabling the identification of several candidate phases for synthesis - including 17 promising C15b-type structures and 2 half-Heuslers. An interactive, online web application has been developed showcasing the results of the analysis and is located at aflow.org/aflow-chull.

4:54PM V19.00011: Novel functionalities in chemically-modified quasi-2D clay minerals.* PRIYA GOPAL (Presenter), MARTA GUSMAO, ILARIA SILOI, Department of Physics, University of North Texas, Denton, TX, STEFANO CURTAROLO, Materials Science and Engineering, Center for Materials Genomics, Duke University, Durham, NC, MARCO FORNARI, Department of Physics and Science of Advanced Materials, Central Michigan University, Mt. Pleasant, MI, MARCO BUONGIORNO NARDELLI, Department of Physics, University of North Texas, Denton, TX — Clays are among the most common, cheap, non-toxic and abundant materials found in nature with an inherent \textit{quasi-2D} crystal structure that can be chemically modified to obtain novel functionalities. In this work, we used our High-Throughput infrastructure, \textit{(AFLOW + PAOFLOW),} to compute the electronic structure and related properties for minerals in the clay family: lizardite \textit{(Mg$_3$(Si$_2$O$_5$(OH)$_4$)}, talc \textit{(Mg$_3$(Si$_2$O$_5$)$_2$(OH)$_2$)}, kaolinite \textit{(Al$_2$(Si$_2$O$_5$)(OH)$_4$)} and pyrophyllite \textit{(Al$_2$(Si$_2$O$_5$)$_2$(OH)$_2$)}. We studied the effect of chemical substitutions on the mechanical, optical, electronic and magnetic properties in these four prototypes. We found that Ni-substituted kaolinite \textit{(Ni$_3$(Si$_2$O$_5$)(OH)$_4$)} is structurally stable and is a promising candidate for spintronic applications.

*We acknowledges collaboration within the AFLOW Consortium (www.aflow.org) under the sponsorship of DOD-ONR (Grants N000141310635 and N000141512266).

5:06PM V19.00012: A Map of the Inorganic Ternary Metal Nitrides* WENHAO SUN (Presenter), Materials Sciences Division, Lawrence Berkeley National Laboratory, CHRISTOPHER BARTEL, University of Colorado, ELISABETTA ARCA, SAGE BAUERS, BETHANY E MATTHEWS, National Renewable Energy Laboratory, BERNARDO ORVANANOS, Massachusetts Institute of Technology, BOR-RONG CHEN, MICHAEL F TONEY, LAURA SCHELHAS, SLAC National Accelerator Laboratory, BILL TUMAS, National Renewable Energy Laboratory, JANET TATE, Oregon State University, ANDRIY ZAKUTAYEV, National Renewable Energy Laboratory, AARON M HOLDER, University of Colorado, GERBRAND CEDER, Materials Sciences Division, Lawrence Berkeley National Laboratory — Exploratory synthesis in novel chemical spaces is the essence of solid-state chemistry. However, uncharted chemical spaces can be difficult to navigate, especially when materials synthesis is challenging. Nitrides represent one such space, where synthesis challenges have limited the exploration of this important class of functional materials. Here, we employ a suite of computational materials discovery and informatics tools to construct a large stability map of the inorganic ternary metal nitrides. Our map highlights hundreds of promising new ternary nitride spaces for experimental investigation, from which we experimentally realized 7 new Zn- and Mg-based ternary nitrides. The map further visualizes broad overarching relationships between nitride chemistry and thermochemical stability. To rationalize these stability trends from their underlying chemical origins, we extract the mixed metallicity, ionicity, and covalency from the DFT-computed electron density—revealing the fascinating and complex interplay between chemistry, composition, and solid-state bonding in governing the stability of ternary nitride materials.


Thursday, March 7, 2019 2:30 PM - 5:06 PM

Session V20 DMP: Hybrid Perovskites -- Optical, Structural Properties and more BCEC 157A -

Laura Herz, University of Oxford
First-principles evidence of strong radiative recombination in hybrid perovskites

XIE ZHANG (Presenter), JIMMY SHEN, WENNIE WANG, CHRIS VAN DE WALLE, University of California, Santa Barbara — Understanding the origin of the high solar conversion efficiency of hybrid perovskites is one key research focus in the field. A number of research groups attributed the high efficiency to low radiative recombination due to strong Rashba spin-orbit coupling. In this work, we perform first-principles calculations to explicitly compute the radiative recombination coefficient in the prototypical hybrid perovskite, CH$_3$NH$_3$PbI$_3$. We demonstrate that the radiative recombination in hybrid perovskites is actually strong, and that spin-orbit coupling has only a minor impact on radiative recombination. The computed radiative recombination coefficient is around $10^{-10}$ cm$^3$s$^{-1}$, which is as high as in typical direct-gap semiconductors. However, our first-principles calculations of nonradiative rates show that strong Auger recombination may suppress efficiency. Fortunately, our insights into the origins of the strong Auger recombination indicates potential avenues for engineering the Auger coefficient.

*This work was supported by DOE.

Nonlinear optical properties of organic-inorganic hybrid perovskite

WENSHEN SONG (Presenter), Physics, Washington University in St. Louis, SU HUANG, Electrical & Systems Engineering, Washington University in St. Louis, GUANG-YU GUO, Physics, National Taiwan University, LAN YANG, Electrical & Systems Engineering, Washington University in St. Louis, LI YANG, Physics, Washington University in St. Louis — Nonlinear optical properties of materials play important roles in lasers, frequency conversion, electro-optic modulators, etc. Here we explore the nonlinear optical properties of hybrid CH$_3$NH$_3$MX$_3$ perovskites (M= Ge, Sn, Pb; X=Cl, Br, I), which are widely studied in photovoltaic areas. Using first-principles approaches, different phases of hybrid perovskites have been studied, and we find considerably large second harmonic generation (SHG) in some of them. Interestingly, large non-diagonal SHG tensors appear in certain structures, which are fairly useful for real-world applications, such as tuning the directions of lasers. All calculations are implemented in our self-developed package aiming for large-scale parallel calculations of nonlinear optical properties.

Second Order Nonlinear Optical Study on The Polar Order in MAPbI$_3$

XIANGPENG LUO (Presenter), WENCAN JIN, Department of Physics, University of Michigan, SUNEEL JOGLEKAR, LINGJIE JAY GUO, Department of Electrical Engineering and Computer Science, University of Michigan, LIUYAN ZHAO, Department of Physics, University of Michigan — Hybrid organic-inorganic methylammonium (MA) lead-halide perovskite MAPbI$_3$ has shown record-breaking photovoltaic conversion efficiency and demonstrated great potential in solar cell applications. Its unusual long carrier lifetime has drawn much research interest, yet its origin remains a debated subject. Whether or not the tetragonal phase of this material is polar is key to resolve the ongoing debates. In this talk, we present clarifying evidence to show the absence of spatial inversion symmetry in single-crystalline MAPbI$_3$ bulk over a wide temperature range starting from 300 K down to 80K, using rotational anisotropy (RA) second harmonic generation (SHG) spectroscopy. We will further discuss the tetragonal to orthorhombic structural phase transition, by analyzing the temperature-dependence of SHG susceptibility tensors. Finally, we will discuss how this non-centrosymmetric phase response to ultrafast optical excitations, from the time-resolved RA SHG measurement results.

*This work was supported by NSF CAREER Award No. DMR-1749774.

Ultrafast Amplified Spontaneous Emission Dynamics in Hybrid Perovskites

KENAN GUNDOGDU (Presenter), North Carolina State University — Methylammonium lead iodide (MAPI) has received significant interest due to high performance of this material in photovoltaic applications. MAPI is also now known to be an efficient light emitter, due in part to its high mobility and long carrier diffusion lengths, which make it a good solar cell. Specifically at reduced temperatures, the light emission process is quite interesting. Specifically at low temperatures due to coexistence of multiple crystal phases, energy and charge transfer dynamics play a significant role in light emission process. At room temperature the crystal structure is tetragonal, whereas at low temperatures material goes through a phase change to orthorhombic crystal structure. However even below the phase transition temperatures, the thin films exhibit tetragonal domain inclusions. Since the tetragonal phase has lower bandgap, most excitations diffuse to these low energy sites and recombine. In this work we studied exciton and charge relaxation dynamics that lead to amplified spontaneous emission (ASE) in MAPI. Our results indicate that reveal the duration of the ASE process and the dynamics that limits ASE in MAPI thin films.

*NSF DMREF Award Number:1729383
3:18PM V20.00005: Waterproof perovskite-hexagonal boron nitride hybrid nanolasers with low lasing thresholds and high operating temperature  HAORAN YU (Presenter), YU YE, LUN DAI, School of physics, Peking University — Solid-state perovskites have recently emerged as promising coherent light sources. Realization of an electrical perovskite-based laser diode still remains challenging due to the heat management and intrinsic instability of the perovskites. Here, we demonstrate waterproof perovskite-hexagonal boron nitride (hBN) hybrid nanolasers with low lasing thresholds and high operating temperature. After capping with the hBN flake which possesses superb and anisotropic thermal conductivity, heat dissipation of the hybrid nanolaser is accelerated, resulting in the significant reduction of lasing thresholds, and clear lasing behavior under a temperature as high as 75.6 °C. Moreover, hBN with high environmental stability can effectively protect the perovskite from the polar solvents. The hBN encapsulated CsPbI₃ nanolasers can incessantly lase in water for an hour, and the lasing behavior can be retained even after 24-hour immersion in water. The reduction of lasing threshold, improved heat removal, and higher temperature tolerance of the hybrid nanolaser marks a major step towards CW-pumped perovskite laser at room temperature, while also allowing perovskites to be integrated into high power density optoelectronic devices and future electrically driven lasers.

3:30PM V20.00006: Shifting the Thermodynamics of Polymorph Transitions in Metal-Halide Perovskites  XIAOQING KONG, Chemical Engineering and Materials Science, Stevens Institute of Technology, KAMRAN SHAYAN, STEFAN STRAUF, Physics, Stevens Institute of Technology, STEPHANIE LEE (Presenter), Chemical Engineering and Materials Science, Stevens Institute of Technology — We demonstrate nanoconfinement as a strategy to stabilize high-temperature cubic phases of metal-halide perovskites and prevent humidity-induced degradation. A combination of temperature-dependent x-ray diffraction and photoluminescence experiments were employed to track polymorph transitions in the range of 4 – 373 K. For methylammonium lead triiodide (MAPbI₃) confined within the nanopores of anodized aluminum oxide templates, the tetragonal-to-cubic phase transition shifted from T = 300 K to T = 170 K. These crystals were stable for a period of at least two years of storage in air, compared to unconfined crystals that degrade into perovskite precursors within two weeks of air exposure. For nanoconfined cesium lead triiodide (CsPbI₃), the tetragonal-to-cubic phase transition, which typically occurs at 583 K, was absent to temperatures as low as 4 K. We hypothesize that nanoconfinement introduces lattice strain into the crystals, shifting the relative free energies of the respective polymorphs and increasing energy barrier to polymorph transitions. In both systems, the cubic phase represents the smallest band gap polymorph, with important implications for solar cell device operation and efficiency.

3:42PM V20.00007: Anisotropic heat conduction in the metal-organic framework perovskites*  DHARMENDRA SHUKLA (Presenter), NARAYAN PRASAI, Physics, University of Miami, THOMAS M. CARLINO, MERCEDES M. A. MAZZA, AMY M. SCOTT, Chemistry, University of Miami, JOSHUA COHN, Physics, University of Miami — We report thermal conductivity (κ) measurements on single crystals of the metal-organic framework perovskite compounds [C(NH₂)₃]X(HCOO)₃ (X=Cu, Zn) in the temperature range 5K ≤ T ≤ 300K. The directionality of N-H---O bonds and their stretching due to the Jahn-Teller distortion in the Cu compound are identified as mechanisms underlying differences in κ(T) behavior for the two compounds and its anisotropy. For heat flow along a direction preferentially transverse to the N-H---O bonds, κ = 0.6 W/mK near 300 K, approaching the theoretical minimum value. A possible magnetic contribution to the heat flow in the Cu compound will also be discussed.

*This material is based upon work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under grant No. DE-SC0008607, and by the Univ. Miami CAS Convergence grant.

3:54PM V20.00008: Halide perovskite thin films for thermoelectrics*  TIANJUN LIU (Presenter), OLIVER FENWICK, School of Engineering and Materials Science, Queen Mary, University of London — Halide perovskites have emerged as promising candidates for photovoltaics and light-emitting diodes. Recently, promising thermoelectric performance has been reported for single nanocrystals of a halide perovskite, but there is not yet a good understanding of how thermoelectric performance can be optimised in these materials, especially in thin films where a diverse range of structures and morphologies are accessible. In this presentation I will report a record thermoelectric figure of merit (ZT) for halide perovskites, using the example of CsSnI₃ thin films. This result is in part due to the ultralow thermal conductivity of our films (0.38 W/mK at room temperature), as well as high electrical conductivity enabled by self-doping of the films through controlled Sn oxidation. I will also discuss the potential role of mixed-halide films in developing these materials further. Finally I will demonstrate how thin film morphology and composition can be used to further reduce the thermal conductivity in vapour- and solution-deposited CH₃NH₃PbI₃.

*Royal Scociety University Research Fellow
China scholarship council
4:06PM V20.00009: Origin of Pressure-Induced Phase Transition and Metallization in Hybrid Halide Perovskites
JUNG-HOON LEE (Presenter), JEFFREY B NEATON, University of California, Berkeley — Hybrid halide perovskites are promising optoelectronic materials due to their favorable electronic properties and low cost. Here we investigate the effects of high pressure on the structural and electronic properties of (MA)PbI3 (MA = CH3NH3+) using first-principles density functional theory (DFT) calculations. Our calculations predict that with increasing external pressure, the cubic high-pressure Im-3m phase becomes more energetically favorable for the MA cations than the orthorhombic low-pressure Fmmm phase, leading to a predicted phase transition at 0.22 GPa, in good agreement with the experiment (~0.3 GPa). With increasing pressure we also find severe octahedral tilting occurs at 6 GPa, introducing I 5p – I 5p* antibonding and Pb 6p – Pb 6p bonding character into the valence band maximum (VBM) and the conduction band minimum (CBM) states, respectively. This leads to a different trend in the VBM and CBM energies under compression compared to their behavior below 6 GPa. Our DFT calculations show that this trend eventually leads to metallization at significantly higher pressures.

4:18PM V20.00010: Pb-free halide double perovskites: Computational materials design and surface properties*
GEORGE VOLONAKIS (Presenter), FELICIANO GIUSTINO, Department of Materials, University of Oxford — Halide double perovskites have been investigated extensively as lead-free alternatives to lead halide perovskites. Since our theoretical predictions, four crystals have successfully been synthesized: Cs2BiAgCl6, Cs2BiAgBr6, Cs2SbAgCl6, and Cs2InAgCl6. These compounds exhibit low carrier effective masses, and Cs2BiAgBr6 has a band gap of 1.9 eV, well within the visible range. Hence, these are candidates for opto-electronic applications such as photovoltaics, sensors, and photo-catalysts. In this talk, we will briefly present the computational design principles that lead to the synthesis of these compounds. In addition, we will focus on the structural and electronic properties of the four synthesised compounds and their surfaces. We will show that based on first-principles calculations, double perovskites Cs2BiAgCl6 and Cs2BiAgBr6 might be promising compounds for photo-catalytic water splitting. For all compounds it is shown that their energy levels, hence their photocatalytic properties, strongly depend on the surface termination. Our computational findings expand the range of potential applications of Pb-free double perovskites.

*Graphene Flagship (Horizon 2020 Grant No. 785219-GrapheneCore2), Leverhulme Trust (Grant RL-2012-001), UK EPSRC (grant No. EP/M020517/1),

4:30PM V20.00011: Structural relationships and relative stability of different ABX3 phases of inorganic halide perovskites with B=Ge*
SANTOSH KUMAR RADHA (Presenter), WALTER RL LAMBRECHT, Case Western Reserve University — Pb-free halide perovskites have recently attracted interest. In Phys.Rev.Mat.2,063605(2018) we proposed the use of Si & Ge as B sites cation and found that these perovskites undergo an off-centering of the group-IV atom leading to a rhombohedrally distorted perovskite with band structure similar to those of the cubic ones. However, for some of these materials, like RbGeX3, a monoclinic structure has been found experimentally.

In this work, we show that the monoclinic structure and the rhombohedral ferroelectric structure are closely related. In fact, if one considers these structures as GeX3 tetrahedrons rather than corner sharing octahedrons, we find that the monoclinic and rhombohedral structure to have parallel and oppositely oriented tetrahedral units. Thus the monoclinic structure can be understood as an anti-ferroelectric arrangement of the GeX3 dipoles. They have a completely different band topology with a wide band gap compared to that of the cubic ones yet are energetically close to each other. We understand this energy difference using a spin-1/2 hamiltonian for dipole interactions, favouring the antiferroelectric alignment of the GeX3 dipoles, and additional Ge-X bonding due to parallel tetrahedron orientation causing the ferroelectric alignment.

*Supported by DOE-BES

4:42PM V20.00012: Effect of water on structural, optical and hot carrier cooling properties of MASnI3 perovskite
MOHAMED EL-AMINE MADJET (Presenter), ALI KACHMAR, GILIBJON BERDIYOROV, Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha, Qatar — Understanding the stability, carrier transport and relaxation of Sn based perovskites CH3NH3SnI3 are of high interest to develop lead free perovskite solar cells. In this study, we performed first principles and non-adiabatic molecular dynamics simulations to address the electronic, optical, and hot carrier relaxation dynamics of the pristine CH3NH3SnI3 and its monohydrated phase CH3NH3SnI3.H2O. Our results show that the water molecule interacts strongly with the organic cation by forming hydrogen bonding, while having also an interaction with the iodide ions. Our study also indicates that the water molecule has in general a negative impact on the optical properties of perovskite materials. In fact, the water molecule reduces the absorption of the system mostly in the visible range of the solar spectrum, and it leads to a faster hot-carrier cooling and to an increase in the polarization of the material.
Investigation of charge dynamics and photoinduced charge transfer in metal halide perovskite/carbon nanotube composites by vibrational spectroscopy*

KATALIN KAMARAS (Presenter), LEILA BADEEB, MEHMET DERYA ÖZEREN, ARON PEKKER, Wigner Research Centre for Physics, SEHAM KAMAL ABDEL-AAL, AHMED SABRY ABDEL-RAHMAN, Physics Department, Cairo University, PAVAO ANDRICEVIC, LASZLO FORRO, ENDRE HORVATH, Laboratory of Physics of Complex Matter, Ecole Polytechnique Federale de Lausanne — Composites formed from metal halide perovskites and semiconducting carbon nanotubes show a fast photoinduced charge diffusion and a slow structural rearrangement due to ionic movement. To understand this latter, phonon-related mechanism, we performed a study of vibrational spectra on various perovskites and composites, changing the central ion of (Pb, Sn, Co and Cu) and the halide (I, Br and Cl). We measured the temperature dependence, followed the phase transitions, and investigated the photoinduced changes by both infrared and Raman spectroscopy. As the structural rearrangement is accompanied by Fermi level alignment and thus modifies the optical gap, our results are useful for fine-tuning the optical properties in solar cell applications of perovskites and perovskite/carbon nanostructure composites.

*Swiss National Science Foundation ERC Advanced Grant Picoprop (670918). European Commission and Hungarian Government VEKOP-2.3.2-16-2016-00011 NKFIH NN 127069 (Hungary) Hungarian Academy of Sciences - Academy of Scientific Research and Technology, Egypt collaboration

Thursday, March 7, 2019 2:30 PM - 5:18 PM

Session V21 DMP: Nanostructures and Metamaterials -- Active Systems

Control of Emission and Energy Transfer with Metamaterials, Plasmonic Structures and Cavities*

SAMANTHA KOUTSARES, Norfolk State University, SRUJANA PRAYAKARAO, University of Kansas, DEVON COURTWRIGHT, SANGEETA ROUT, Norfolk State University, MONIKA BIENER, ZHEN QI, Lawrence Livermore National Laboratory, CARL E BONNER, MIKHAIL NOGINOV (Presenter), Norfolk State University — Metamaterials, plasmonic structures and cavities have been shown to enable and control scores of spontaneous emission, stimulated emission, and energy transfer phenomena. The recent findings of our group in this research area will be discussed at the conference.

Acknowledgments: NSF HBCU-RISE grant # 1646789, NSF EiR grant # 1830886, AFOSR grant # FA9550-18-0417, DoD grant # W911NF1810472.

Mechanisms of GaN quantum dot formation during nitridation of Ga droplets*

HONGLING LU (Presenter), CALEB REESE, SUNYEOL JEON, Materials Science and Engineering, university of Michigan, YAMING FAN, EMILY RIZZI, YUQUN ZHUO, Tsinghua University, LIANG QI, RACHEL GOLDMAN, Materials Science and Engineering, university of Michigan — GaN-based quantum dots (QDs) have been proposed for a variety of optoelectronic devices. Typically, QD formation is driven by a Stranski-Krastanov growth mode transition. Alternatively, the nucleation and conversion of metal droplets to QDs via nitridation, known as droplet epitaxy (DE), has emerged as a promising approach to achieve strain-free QDs. To date, GaN DE has been described as a liquid-phase epitaxy-like and/or a surface-diffusion driven process. Here, we investigate the formation mechanisms for DE GaN QDs using a combined computational-experimental approach. Our first-principles calculations of activation barriers suggest that N is immobile while Ga has a relatively high surface diffusivity, independent of the starting surface structure and chemistry. We consider the temperature and substrate dependence of the size distributions of droplets and QDs, and report on two competing mechanisms mediated by Ga surface diffusion, Ga droplet coarsening with QD formation via impinging N atoms and Ga droplet out-diffusion with QD nucleation at absorbed N surface sites. We also discuss the relative roles of nucleation and coarsening dominant growth, as well as the phase selection, on various substrates.

*National Science Foundation (NSF) under Grant No. DMR-1120923, DMR-1410282.
**3:30PM V21.00004: Harnessing Evanescent Waves by Metasurfaces: An All-Optical Analogue of On-Chip Control of Smith-Purcell Emission**

LIN LI, Department of Mechanical and Industrial Engineering, Northeastern University, KAN YAO, Department of Electrical and Computer Engineering, Northeastern University, ZUOJIA WANG, School of Information Science and Engineering, Shandong University, YONGMIN LIU (Presenter), Department of Mechanical and Industrial Engineering, Northeastern University —

The exponentially decaying nature of evanescent waves renders it difficult to capture, extract and engineer the wealth of energy and information that they can carry. Utilizing the out-of-plane electric dipoles and in-plane magnetic dipoles produced by a C-aperture metasurface, in this work we show that we can mold evanescent waves on demand. Specifically, we demonstrate an all-optical analogue of manipulating Smith-Purcell emission, in which the evanescent waves are produced by attenuated total reflection rather than moving electrons, and subsequently tailored by the designer metasurfaces. The phase, beam profile and polarization state of the Smith-Purcell emission can be controlled via the orientation of C-aperture nanostructures. Our work opens a new avenue for metasurfaces to work in the critical near-field region to efficiently harness evanescent waves, and promises many potential applications, including on-chip free-electron light sources, tabletop particle detectors and near-field energy harvesting.

**3:42PM V21.00005: Radiative spontaneous decay enhancement near an ultrathin plasmonic film**

HAMEZ MOUSAVI (Presenter), IGOR BONDAREV, Math and Physics, North Carolina Central University, USA — We develop a quantum electrodynamics theory for the spontaneous decay process of a point dipole emitter near a thin metallic film. It was previously shown that the strong vertical electron confinement causes the film plasma frequency to become spatially dispersive[1], resulting in a (confinement induced) nonlocal dielectric response of the film[2]. Using this fact we calculate the electromagnetic Green's function and the emitter-to-surface distance dependence for the dipole spontaneous decay rate near the metallic film of finite thickness. We show that the confinement induced dielectric response nonlocality of the ultrathin films can result in a two-order-of-magnitude radiative decay rate enhancement relative to vacuum. The effect can be qualitatively understood in terms of the interacting image dipoles and can be controlled by varying the material composition, the thickness and the surroundings of the film. The inelastic electron scattering diminishes the effect. These are the universal peculiarities of the light-matter interactions in close proximity to ultrathin plasmonic nanostructures. --


*US DOE DE-SC0007117(H.M.), US NSF DMR-1830874(I.B.)
4:06PM V21.00007: Yagi-Uda nanolithographic antennas on a Si photodiode for infrared detection*  WILLIAM RIEGER (Presenter), JEAN HEREMANS, Physics, Virginia Tech, HANG RUAN, YUHONG KANG, RICHARD CLAUS, NanoSonic Inc., TIGRAN ASRYAN, Physics, Virginia Tech — Nanoscale Yagi-Uda antennas were fabricated on a metal-semiconductor-metal rectifying photodetector to enhance detector efficiency. A new approach for characterizing the nanolithographic optical antennas was based on a direct electrical measurement obviating the need for an ITO coating or back contact. The measurements demonstrate control of directivity and wavelength selectivity in an array of 400 nanoantennas. With incident light nearly aligned to the center lobe of the Yagi-Udas, resonances in measured photocurrent were observed at 1110 nm and 1690 nm. These correspond to scaled effective wavelengths of 388 nm and 776 nm, respectively, in agreement with plasmonic theory. Estimated quantum efficiencies are 5.1% and 3.1% at 1110 nm and 1690 nm, respectively, representing a fourfold increase over a device lacking the antenna array. The spatial dependence of the contribution of individual antennas in the array has been investigated to determine the process whereby resonant plasmons contribute to the photocurrent. Associated finite element modeling results will be discussed, aimed at predicting resonances in plasmonic structures with similar geometries.


*U.S. Navy N68335-13-C-0184, NASA NNX17CC63P

4:18PM V21.00008: Theoretical Investigation of Plasmonic Properties of Quantum-Sized Silver Nanoparticles  MASOUD SHABANINEZHAD NAVROOD (Presenter), Physics, Western Michigan University, RAMAKRISHNA GUDA, Chemistry, Western Michigan University — Metallic nanoparticles (NPs) can strongly absorb the incident light and produce enhanced localized electric field when the frequency of the incident light is in phase with coherent oscillation of conduction electrons in them. This characteristic feature of metallic NPs can be tuned by changing parameters such as size, shape, polarization direction of incident light and refractive index of medium. Although plasmonic properties of larger size nanoparticles are extensively investigated, little has been done on smaller sized particles in the size range of 3 to 10 nm. By reducing the size, band structure of the metallic particles discretizes, leading channeling plasmon properties of the NPs from classical to quantum regime. In this work, plasmonic properties of the spherical silver (Ag) NPs in the size range of 3 to 20 nm has been investigated using both quantum and classical model. We performed theoretical calculations using normal Mie theory, and studied size and surrounding medium effects on the absorption efficiency, LSPR energy peak shift and field enhancement of the samples. The results indicate that the quantum model is able to predict blue shift of LSPR peak with decreasing size of the samples from 10 to 3 nm while the classical model fails to observe this effect.

4:30PM V21.00009: Networks of helical, braided quantum wells  ALEXANDRA COURTIS (Presenter), University of California, Berkeley — Architectures with complex and reconfigurable topologies present in a series of naturally occurring systems that have precise nanoscale organization and that execute efficient, rapid, and scalable information transfer. Artificial nanosystems explicitly engineered to probe and mimic these networks hold promise for fundamental studies on energy transfer alongside for the design of new architectures to store and convert information. Here, topological networks comprised of atomically precise, colloidal quantum wells are presented. The experiment highlights structural properties and establishes design strategies for preparing controlled hierarchies of low-dimensional, quantum confined materials distinguished by a high degree of organizational complexity. The discussion addresses the findings in the context of understanding and controlling some properties of atomically precise nanosystems in the limit of jammed, frustrated environments.

4:42PM V21.00010: Metasurfaces to control the quantum dynamics of color centers in hexagonal boron nitride  PANKAJ JHA (Presenter), GHZALEH KAFAEI SHIRMANESH, HAMIDREZA AKBARI, ARUN NAGPAL, BENJAMIN VEST, CORA WENT, WEI-HSIANG LIN, RUZAN SOKHOYAN, HARRY ATWATER, California Institute of Technology — Photonic metasurfaces have revolutionized optical designs by enabling the realization of virtually flat optics via the replacement of bulky optical components with ultrathin planar elements, which possess ease-of-fabrication advantages. However, majority of the application-oriented research in this field has been limited to classical regime and it remains an open question if these metasurfaces can be used for single-photon applications. Here, we perform theoretical and experimental studies to quantify the role of metasurface induced tailored environment to control the quantum dynamics of color centers in hexagonal boron nitride. These color centers in semiconductors have garnered great interest because they can serve as single-photon sources, which are the building blocks for photonic quantum technologies. We investigate the fundamental properties of color centers in hexagonal boron nitride, such as saturation count, life-time etc. and investigate how these characteristics can be manipulated with metasurfaces.
**4:54 PM V21.00011: Effects of Nanostructured Plasmonic Environment on Electrochromic Polymer Switching**

MOHAMMAD SHAHABUDDIN (Presenter), CARL E BONNER, NATALIA NOGINOVA, Center for Materials Research, Norfolk State University — Strong modification of local environment associated with plasmonic nanostructures provides possibilities to control various processes, including charge transfer processes and chemical reactions. In this work, we explore the opportunities to enhance electrochromic polymer performance using plasmonic metasurfaces, and study the origin of this enhancement. Electrochromic polyaniline (PANI) films deposited onto gold metasurfaces demonstrate non-monotonous coloration behavior at low voltages, step-like color-change and much faster saturation in color with the increase in voltage in comparison with polyaniline films deposited on flat gold. The additional small voltage peak in the cyclic voltammogram in nanomesh/PANI cell and the asymmetric and nonlinear I-V characteristics of the sandwich nanomesh/PANI/flat gold structure indicate a possible formation of Schottky-like interface between polyaniline and nanostructured gold, whereas the Ohmic contact is observed for the flat gold-PANI system. The results are discussed in terms of the modified work-function of nanostructured gold, interface charging and threshold-like charge transport. Possibility to engineer optical and charge transport properties of electrochromic materials via nanostructured interfaces can bring niche applications.

*NSF

**5:06 PM V21.00012: FRET Enhancement using Surface Plasmon Modes on Gold Nanogratings**

JENNIFER STEELE (Presenter), CHAE RAMNARACE, Physics and Astronomy, Trinity University, WILLIAM R FARNER, Astrophysics, Drexel University — The plasmonic properties of structured metal surfaces can be engineered to enhance the output of nearby quantum emitters through the manipulation of the local density of optical states (LDOS). Although metal enhanced fluorescence (MEF) has been well understood for decades, the influence of plasmonic modes in Förster resonance energy transfer (FRET) is still a debated issue. Gold nanogratings provide a unique plasmonic substrate to study the effects of altering the LDOS on FRET efficiencies. Gratings support narrow plasmon resonances at a range of wavelengths, allowing for the comparison of FRET efficiencies by increasing the LDOS at donor and acceptor emission wavelengths on a single substrate. In this work, the increase in efficiency was found to be greatest when the surface plasmon modes overlapped the acceptor emission spectrum. Furthering the understanding of the application of MEF to FRET will aid developing methods for the enhancement of FRET, expanding its use in biological systems, photosynthesis, and photovoltaic devices.

*This work was supported by an award from the Research Corporation for Science Advancement and from the W.M. Keck Foundation Undergraduate Education Program.

**Thursday, March 7, 2019 2:30 PM - 5:30 PM**

**Session V22 DCOMP DMP: Electrons, Phonons, Electron-Phonon Scattering and Phononics VII** BCEC 157C - Athanasios Chantis

**2:30PM V22.00001: Materials selection rules for optimum power factor in 2-dimensional thermoelectrics**

ADITHYA KOMMINI (Presenter), ZLATAN AKSAMIJA, Electrical and Computer Engineering, University of Massachusetts, Amherst — Thermoelectrics (TE) can improve the efficiency of power sources to meet ever-growing energy demand by converting waste heat into electricity. With the advent of new 2D materials and the knowledge of their material properties, the ability of these materials for future TE use need to be studied. Studies have predicted the stability of around 2000 van der Waals materials that can be exfoliated into 2D atomic films. Here, the distinct features of 2D materials like effective mass, density of states, and electron-phonon scattering deformation potentials are used to formulate simple material selection rules that can optimize TE power factor. These parameters are widely available in material databases or computationally inexpensive to calculate. Our simulations show that when inelastic scattering with optical phonons is dominant in a material, the TE power factor is highest with phonon energy of 5 kT. Further enhancement is possible with larger height in the step-like 2D density of states, lower effective mass, and higher degeneracy for the conduction band valley that participate in the transport. Employing these material selection rules help in identifying future thermoelectric materials that can have applications in thermal harvesting, thermal sensors, and electronic cooling.
2:42PM V22.00002: Theory of generation and conversion of phonon angular momentum*  MASATO HAMADA
(Presenter), SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology — Mechanical rotations in solids can be converted to magnetization and spin current via the spin-rotation coupling. Recently, in general solids, the phonon angular momentum has been formulated as the microscopic local rotation in the lattice. However, it usually cancels between phonon modes. In this talk, we propose the two ways of generation of phonon angular momentum in non-magnetic and magnetic insulators. In nonmagnetic insulators without inversion symmetry, a heat current induces the phonon angular momentum, in analogy with the Edelstein effect [1]. In magnetic insulators preserving the product of the inversion and time-reversal symmetries, the electric field can induce the phonon angular momentum, in analogy with the magnetoelectric effect. We also discuss microscopic mechanisms how the microscopic local rotations of atoms, i.e. the phonon angular momentum, is converted into electronic spins.


*This work was supported by a Grant-in-Aid for Scientific Research on Innovative Area, “Nano Spin Conversion Science” (Grant No. 26103006), and also by JSPS KAKENHI Grant No. JP17J10342.

2:54PM V22.00003: Impact of Quartic Anharmonicity on Lattice Thermal Transport in SnSe  YI XIA (Presenter),
CHRISTOPHER WOLVERTON, Materials Science and Engineering, Northwestern University — Layered SnSe has demonstrated exceptional thermoelectric properties with record high energy conversion efficiency, majorly owning to the ultralow lattice thermal conductivity. However, a fundamental understanding of the lattice dynamics and thermal transport properties is still lacking, particularly for the high temperature phase. The theoretical challenge originates from the second-order phase transition from low-temperature Pnma to high-temperature Cmcm phases between 700-800~K, wherein the Cmcm-SnSe displays lattice instability and imaginary phonon frequencies. To overcome this limitation, we go beyond harmonic approximation by further incorporating anharmonic phonon renormalization due to quartic anharmonicity. Moreover, both three- and four-phonon scatterings are accounted for in solving Phonon Boltzmann transport equation. We apply this strategy to perform a comparative study of lattice dynamics and thermal transport properties of SnSe at 300~K (Pnma) and 800~K (Cmcm). We reveal in detail the impacts of quartic anharmonicity on lattice stability, phonon quasiparticle energies and lattice thermal conductivities of both Pnma- and Cmcm-SnSe. Our theoretical calculations are in good agreement with experimental measurements performed on SnSe single crystals.

3:06PM V22.00004: Optoacoustic spectrum of GaP: experiment and theory  ANDREY BAYDIN (Presenter), RUSTAM GATAMOV, HALINA KRZYZANOWSKA, Vanderbilt University, CHRISTOPHER J STANTON, University of Florida, NORMAN H TOLK, Vanderbilt University — GaP is an important indirect band gap material with variety of applications in optics ranging from LEDs to possible applications in GaP/Si based solar cells. We investigated the spectral dependence of the opto-acoustic response of GaP using time-domain Brillouin scattering. We found that the amplitude of the Brillouin oscillations varies significantly near the direct transition at Γ point. The developed theoretical model quantitatively explains the experimental data and shows that one can use coherent phonon spectroscopy to provide detailed information about electronic structure and optical transitions in indirect band gap materials. The results for GaP are also compared to GaAs and Si.

3:18PM V22.00005: Electronic properties of IV-VI semiconductors obtained with G0W0 including off-diagonal corrections*  PABLO AGUADO-PUENTE (Presenter), PIOTR CHUDZINSKI, TCHAVDAR TODOROV, JORGE KOHANOFF, School of Maths and Physics, Queen's University Belfast, STEPHEN B FAHY, Department of Physics, University College Cork, MYRTA GRÜNING, School of Maths and Physics, Queen's University Belfast — The computation of electronic properties of IV-VI semiconductors constitutes a challenge for traditional density functional theory (DFT) methods. The underestimation of the bang gap by DFT can lead, in these materials, to a spurious band gap inversion that hinders the characterization of their electronic properties, and therefore the modeling of their thermoelectric performance. In addition, the G0W0 approach often used to correct the DFT band structure also fails because of its perturbative nature, making necessary to improve the starting wavefunctions (e.g. using hybrid DFT) or to use more sophisticated approaches such as quasiparticle self-consistent GW. Here instead we use traditional DFT+G0W0 with corrections from the relevant off-diagonal elements of the self-energy in order to obtain the band structure of some of these materials, e.g. PbTe. This method, which does not require adjustable parameters, is utilized to extract from first principles band structure characteristics necessary for the calculation of transport coefficients. Band gaps, effective masses and deformation potentials are obtained in good agreement and at a fraction of the computational cost of more sophisticated methods.

*Funding from SFI-DfE NI, grant 15/IA/3160. Computational resources provided by ARCHER.
3:30PM V22.00006: Temperature dependent electronic transport in concentrated solid solutions of the 3d-transition metals Ni, Fe, Co and Cr from first principles.* GERMAN SAMOLOYUK (Presenter), SAI MU, ANDREW MAY, Oak Ridge National Laboratory, SEBSTIAN WIMMER, SERGIY MANKOVSKY, HUBERT EBERT, Department Chemie/Physikalische Chemie, Ludwig-Maximilians-Universitat Munchen, BRIAN CRAIG SALES, GEORGE MALCOLM STOCKS, Oak Ridge National Laboratory — An approach to the calculation of transport coefficients is applied to the calculation of transport properties of fcc alloys of Ni, Fe, Co, Cr. The coherent potential approximation used to treat chemical disorder, temperature induced magnetic moment fluctuations and lattice vibrations via the alloy analogy. For the nonmagnetic alloys, Ni20Cr, and NiCoCr the combined effects of chemical disorder and lattice vibrations result in a monotonic increase in the resistivity as a function of temperature from an already large residual resistivity. For magnetic NiCo, NiFe, NiFeCo, additional electron scattering from magnetic fluctuations results in a rapid increase of the resistivity with temperature. The electronic part of the thermal conductivity in Ni20Cr, and NiCoCr, monotonically increases with temperature. In the magnetic alloys, electron scattering from magnetic fluctuations leads to an initial rapid decrease in thermal conductivity until this is overcome by an increasing number of carriers.

*This work was supported as part of the Energy Dissipation to Defect Evolution, an EFRC funded by the US DOE, Office of Science, BES under Contract DE-AC05-00OR22725; Office of Science, BES, Materials Sciences and Engineering Division; Deutsche Forschungsgemeinschaft Priority Program SPP 1538.

3:42PM V22.00007: Bonding Hierarchy Induced High Thermoelectric Performance in Layered Zintl Compound BaAu2P4 KOUISKHI PAL (Presenter), JIANGANG HE, CHRISTOPHER WOLVERTON, Northwestern University — The search for new thermoelectric materials has gained rapid progress in recent years as thermoelectric technology offers the potential for environmentally friendly and sustainable energy conversion methods from waste heat to electricity. Using first-principles calculations based on density functional theory we show that bonding hierarchy gives rise to high thermoelectric performance in BaAu2P4, a layered Zintl compound with a small band gap. BaAu2P4 exhibits crystallographic heterogeneity in which rigid [Au2P4]2− units are separated by layers of Ba2+ cations, which are bonded relatively weakly to the lattice through electrostatic interactions. While the covalently bonded chains of phosphorus atoms facilitate large electrical conductivity, the presence of multiple bands near the Fermi level gives rise to an enhanced Seebeck coefficient. On the other hand, the loosely bound Ba along with the heavy Au atoms strongly scatter the heat carrying acoustic phonons, inducing a very low lattice thermal conductivity along the stacking direction. As a consequence of this coexisting rigid and fluctuating sublattices, BaAu2P4 exhibits a large power factor and low lattice thermal conductivity, which results in a high thermoelectric figure of merit (zT).

3:54PM V22.00008: Emergent localized states in twofold PT-symmetric ladder lattice.* JUNG-WAN RYU (Presenter), SANG-JUN CHOI, SUNGJONG WOO, ARA GO, Institute for Basic Science, NOJOON MYOUNG, Chosun University, HEE CHUL PARK, Institute for Basic Science — We have investigated the localized states at the interface of intertwined PT-symmetric systems which are robust against external pumping and damping. The intertwinement induces an additional PT-symmetry and interface exceptional points (EP) emerge and play the role of new critical points of non-Hermitian phenomena with bulk exceptional point. There are two distinct regimes possessing solidly localized states even though balanced gain and loss is increased. We obtain analytic expressions for the localization length and exceptional points in terms of tight-binding formalism. This theory is demonstrated by numerical calculation of eigenenergies and wave functions on quasi 1D ladder lattice and 2D bi-layered square lattice.

*This work was supported by Project Code (IBS-R024-D1).

4:06PM V22.00009: Local thermal current from cold to hot in a classical harmonic system with multi-path geometry PALAK DUGAR (Presenter), CHIH-CHUN CHIEN, University of California, Merced — The second law of thermodynamics forbids an overall flow of heat from a cold object to a hot one. However, it does not rule out a local heat flow from cold to hot in a multi-path geometry. We show an atypical, local steady-state thermal current from cold to hot emerge in a classical harmonic system of Hookean springs and masses driven by two Langevin Reservoirs at different temperatures. The simulations were performed by the standard molecular dynamics, and physical quantities such as the thermal current were averaged over random realizations in the steady-state regime. Our results show that the atypical thermal current depends explicitly on the system-reservoir coupling, in addition to the spring constants and masses. Including non-linear on-site potentials which models the system-substrate coupling further tunes the regime where the atypical local thermal current can survive. Our theoretical framework is universal and applies to classical systems following Newtonian dynamics. If we consider possible realizations using nano-mechanical systems, the device with a tunable local thermal current may function as a thermal switch or memory element.
4:18PM V22.00010: Activated lone-pair electrons lead to low lattice thermal conductivity: a case study of boron arsenide

GUANGZHAO QIN (Presenter), MING HU, University of South Carolina — Due to the ability of firsthand solid-state conversion to electrical power from thermal energy, thermoelectrics have attracted a lot of attention for the valuable applications in reusing waste resources and thus may make crucial contributions to the crisis of environment and severe energy problems. Reducing the thermal conductivity is an efficient way to boost the thermoelectric performance. In this talk, I would like to introduce an effective way to realize low thermal conductivity by introducing lone-pair electrons or making the lone-pair electrons stereochemically active through bond nanodesigning. With proper bond nanodesigning, the intrinsic thermal conductivity of BAs is largely lowered, which thus would benefit its applications in thermoelectrics with further nanostructuring. Fundamental insight is gained for the underlying mechanism of the reduction of thermal conductivity. Similar approach can also extended to other semiconductor systems, such as silicon and gallium nitride. The approach for realizing low thermal conductivity and the underlying mechanism uncovered in this talk would largely benefit the design of thermoelectric devices with improved performance, especially in future researches involving novel materials for energy applications.

4:30PM V22.00011: Anderson localization of surface plasmon polaritons in engineered disorder*

RUWEN PENG (Presenter), WEN-BO SHI, R. H. FAN, Nanjing University, XIAN-RONG HUANG, Argonne National Laboratory, MU WANG, Nanjing University — In this work, we experimentally demonstrate Anderson localization of surface plasmon polaritons (SPPs) at visible regime in metallic nanogratings with short-range correlated disorder. By increasing the degree of disorder, the confinement of SPPs is significantly enhanced, and the effective SPP propagation length dramatically shrinks. Strong localization of SPPs eventually emerges at visible regime, which is verified by the exponentially decayed fields and the vanishing autocorrelation function of the SPPs. Physically, the short-range correlated disorder induces strong interference among multiple scattered SPPs and provides an adequate fluctuation to effective permittivity, which leads to the localization effect. Our study demonstrates a unique opportunity for disorder engineering to manipulate light on nanoscale and may achieve various applications in random nanolasing, solar energy, and strong light-matter interactions.


*This work is supported by the MOST of China and the NSF of China.

4:42PM V22.00012: Bipolaron insulators and polaron liquids in high-temperature superconductors Ba$_{1-x}$K$_x$BiO$_3$

SHAOZHI LI (Presenter), Department of Physics and Astronomy, University of Michigan, STEVEN JOHNSTON, Department of Physics and Astronomy, Univ of Tennessee, Knoxville — The Su-Schrieffer-Heeger (SSH) type electron-phonon (e-ph) coupling, arising from the modulation of the atomic overlap integrals, has been proposed as a driving mechanism formation of an insulating state in the high-temperature superconducting bismuthates Ba$_{1-x}$K$_x$BiO$_3$. However, this e-ph interaction has not been well studied in dimensions greater than one due to a lack of suitable numerical techniques. In this talk, we present a determinant quantum Monte Carlo (DQMC) method for simulating the SSH-type e-ph interaction in a three-orbital model defined on a two-dimensional Lieb lattice. At half-filling, we observe a bipolaron insulating phase characterized by a long-range dimerized distortion, where the ligand oxygens collapse and expand about alternating Bi atoms creating a bond-disproportionated state. This state is robust against moderate hole doping but is eventually suppressed at large hole concentrations, leading to a metallic polaron-liquid-like state with fluctuating patches of local dimerized distortions. Our result suggests that the polarons are highly disordered in the metallic state and freeze into a periodic array across the metal-to-insulator transition. Moreover, our results have broad implications for many perovskite materials, where the bond phonons are essential.
4:54PM V22.00013: Lattice dynamics and superionic transition in ceria from first principles* SERGEI SIMAK
(Presenter), Linkoping University — We show how lattice dynamics in high-temperature ceria, CeO₂, can be studied beyond the quasiharmonic approximation [1]. The results indicate that the previously proposed precursor for the transition to the superionic phase is an artifact of the failure of the quasiharmonic approximation. We further directly observe the superionic transition at high temperatures [2] in our ab initio molecular dynamics simulations and find that it is initiated by the formation of oxygen Frenkel pairs. The Frenkel pairs are shown to form in a collective process involving simultaneous motion of two oxygen ions.


*The support from Swedish Research Council (VR) (Project No. 2014-4750) and the Swedish Government Strategic Research Area in Materials Science on Functional Materials at Linkoping University (Faculty Grant SFO-Mat-LiU No. 2009 00971) are acknowledged. The computations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at the PDC Centre for High Performance Computing (PDC-HPC), the National Supercomputer Center (NSC).

5:06PM V22.00014: Kinetic Theory of Rectified Motion in a Smarticle Gas* ZACHARY JACKSON (Presenter), WILLIAM C SAVOIE, SHENGKAI LI, KURT A WIESENFELD, DANIEL GOLDMAN, Georgia Institute of Technology — Smarticles are battery powered, self-deforming, three link robots that undergo a repeated prescribed gait. When a small number are confined inside an untethered ring the system undergoes undirected (isotropic) diffusion. Upon deactivation of one of the smarticles, the system displays directed diffusion, with speed and direction which depend on the mass of the confining ring. We present a collisional model that accurately predicts the directed motion.

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5:18PM V22.00015: Phase Stability of Dynamically Disordered Solids from First Principles JOHAN KLARBRING (Presenter), SERGUEI I SIMAK, Linkoping University — The study of phase stability in solid materials containing dynamic disorder, eg. solids with rotating molecular units, or superionic conductors, is a challenging problem in theoretical materials science. This is mainly due to the failure of the standard picture of atoms vibrating around fixed equilibrium positions, which makes theoretical phonon schemes inapplicable. Superionic conductors are dynamically disordered solid materials with exceptionally high rates of ionic conductivity, which makes them very promising solid electrolytes for fuel cells and solid-state batteries.

Here, we present a method to study the phase stability of dynamically disordered materials [1]. The method is based on a stress-strain thermodynamic integration on a deformation path that connects the dynamically disordered phase to a stable variant. We apply the method to study the phase stability of superionic Bi₂O₃. The phase transformation from the low temperature ground state α-phase to the heavily disordered superionic δ-phase is well reproduced, with the critical temperature and the (very large) transition enthalpy closely matching the experimental values.


Thursday, March 7, 2019 2:30 PM - 4:18 PM

Session V23 GIMS: Low Temperature Instrumentation BCEC 158
2:30PM V23.00001: Compact Telescoping Sample Manipulator for Ultra-High Vacuum*  
ROBERT TURNER (Presenter), CHRISTIAN MATT, JENNIFER HOFFMAN, MOHAMMAD H HAMIDIAN, Department of Physics, Harvard University — Scanning tunneling microscopes (STMs) are used to resolve the morphology and electronic structure of a material surface with atomic resolution. Key factors to achieve state of the art STM measurements are stability (i.e. decoupling from external noise sources), low temperatures (<10K) and ultra-high vacuum (UHV) conditions, which usually require a long sample transfer mechanism. However, such a long manipulator is a pendulum that acts as an antenna for acoustic and vibrational noise in the lab and couples the noise into the STM. Here we show the design, construction, and performance of a compact telescoping manipulator attached to an STM system. Our compact manipulator reduces noise coupling both by decreasing the oscillation amplitude and by increasing the resonant frequency and shifting it away from typical ambient noise frequencies (typically 10s of Hz) and resonances of the vibration isolation systems (typically 1 - 3 Hz). In addition, our telescoping arm would be a useful tool for any UHV precision measurement system in a confined space.

*MHH was funded by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4536. CEM is supported by the Swiss National Science Foundation under fellowship P2EZP2_175155

2:42PM V23.00002: Design and development of a low temperature, inductance based 3.5 MHz ac susceptometer.*  
SEAN GIBLIN (Presenter), EDWARD RIORDAN, School of Physics and Astronomy, Cardiff University, FREDRIK AHRENTORP, RISE, GEORGINA M KLEMENCIC, DANIEL MARGINEDA, School of Physics and Astronomy, Cardiff University, CHRISTIAN JONASSON, CHRISTER JOHANSSON, JAKOB BLOMGREN, RISE — We discuss the development of an induction based, low temperature high frequency ac susceptometer capable of measuring at frequencies up to 3.5 MHz and at temperatures between 2 K and 300 K, in applied magnetic dc fields of up to 9 T. Careful balancing of the detection coils and calibration have allowed a sample magnetic moment resolution of 5x10^{-10} Am^2 at 1 MHz. We will discuss the design and characterization of the susceptometer, and explain the calibration process and the applicability of the system to existing cryostat designs. We also include some example measurements on the spin ice materials, iron oxide based nanoparticles and superconductors to describe functionality to illustrate functionality.

*EPSRC, grant number EP/L019760/1.

2:54PM V23.00003: A Modular Design for Ultra-High Vacuum Millikelvin STM Systems*  
KEVIN P NUCKOLLS (Presenter), DILLON WONG, MYUNGCHUL OH, SANGJUN JEON, ALI YAZDANI, Princeton University — We describe the unique modular design of an ultra-high vacuum (UHV) STM system, capable of reaching dilution-refrigerator temperatures (10 mK) and equipped with a vector magnetic field. The goals of our design are to separate the UHV needs of STM instrumentation from the typical non-UHV construction of a dilution fridge system, and to make the STM head module interchangeable. To accomplish this, a custom-built dilution refrigerator surrounds a cooled UHV tube chamber, which houses our STM, with specially designed electrical connections at low temperatures to connect to an interchangeable STM head module. For diagnostic purposes, the microscope can also be used at room temperature in the UHV preparation chambers that are integrated with the low-temperature UHV tube system. The microscope exchange can be done at any time without compromising cryogenics or vacuum. The system works with a 240L liquid He cryostat, with a vector magnet (9T-1T-1T), that has a 10-day hold time. Our current microscope head design features multiple contacts to perform STM on gated structures and simultaneous low-temperature transport measurements on devices. Microscope designs, instrument construction, and preliminary data will be discussed.

*We acknowledge funding from the Moore Foundation for this project.
3:06PM V23.00004: Scanning probe microscopy at ultra-high magnetic fields* LISA ROSSI, High Field Magnet Laboratory (HFML-EMFL), Radboud University, JAN W. GERRITSEN, Institute for Molecules and Materials, Radboud University, LIJNIS NELEMANS, ALEXANDER A. KHAJETTOORIANS, BENJAMIN BRYANT (Presenter), High Field Magnet Laboratory (HFML-EMFL), Radboud University — Up to now, low temperature scanning probe microscopy (SPM) has been limited to a magnetic field strength of around 20 T, as most designs have been based on superconductor magnets. For some experimental applications – for example fractal spectra in graphene superlattices, the room temperature quantum Hall effect and some metamagnetic transitions – higher fields are required. Static fields of more than 30 T can be generated in dedicated high-field facilities by water-cooled, resistive Bitter magnets or hybrid resistive-superconducting magnets. However, implementing SPM in a Bitter magnet is a major challenge, due to the high level of vibrational noise produced by the turbulent cooling water, in addition to the space constraints resulting from the small magnet bore.

We present a novel cryogenic scanning tunnelling microscope (STM) designed to operate inside a 38 T water-cooled Bitter magnet. The performance of the STM is demonstrated through Landau level tunnelling spectroscopy of graphite, at 4.2 K in magnetic fields up to 34 T. Additionally we show the design of a highly compact atomic force microscope (AFM) for operation at cryogenic temperatures in an extremely high magnetic field. We show preliminary imaging data on the frustrated spinel CdCr2O4 at up to 30 T.

*HFML-RU/FOM

3:18PM V23.00005: Achieving µeV resolution in scanning tunneling spectroscopy at mK temperatures in Al-Al SIS junctions JOHANNES SCHWENK (Presenter), SUNGMIN KIM, National Institute of Standards and Technology, JULIAN BERWANGER, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, WILLIAM G CULLEN, STEVEN R BLANKENSHIP, National Institute of Standards and Technology, YOUNG KUK, Center for Quantum Nanoscience, Ewha Womans University, Seoul, Korea, FRANZ J GIESSIBL, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, JOSEPH A STROSCIO, National Institute of Standards and Technology — Improved energy resolution in spectroscopic measurements is one of the main motivations for conducting Scanning Probe Microscopy (SPM) experiments at temperatures of tens of mK using a dilution refrigerator (DR). However, SPM instruments at these temperatures have not always achieved an energy resolution consistent with the DR temperature due to electrical noise coupling into the tunnel junction. Here, we present Scanning tunneling spectroscopy measurements of an Al-Al Josephson junction using an Al thin film grown in situ, together with an Al probe tip. The improved performance is achieved by optimizing our SPM operating in ultra-high vacuum (UHV) inside a DR with a base temperature of 10mK and magnetic field up to 15T [1]. Home built Radio Frequency (RF) powder filters located at the mixing chamber shield the tunnel junction from room temperature RF noise. Further RF filtering at the UHV chamber room temperature feedthroughs, together with attention to grounding, lead to an order of magnitude improved resolution over previous measurements. We demonstrate an energy resolution in the low ueV range and discuss the trials and tribulations to achieve this resolution and the causes of the residual intrinsic energy broadening that is observed.

[1] Song et al., RSI 81, 121101 (2010)

3:30PM V23.00006: Josephson-junction-based bolometer* ROOPE KOKKONIEMI (Presenter), JOONAS GOVENIUS, VISA I VESTERINEN, QCD Labs, Aalto University, RUSSELL LAKE, Boulder, NIST, ANDRAS GUNYHO, KUAN YEN TAN, QCD Labs, Aalto University, SLAWOMIR SIMBIEROWICZ, LEIF GRÖNBERG, JANNE LEHTINEN, MIKA PRUNNILA, JUHA HASSEL, OLLI SAIRA, QTF Centre of Excellence, VTT Technical Research Centre of Finland, IIRO SALLINEN, DIBYENDU HAZRA, QCD Labs, Aalto University, ANTTI LAITINEN, PERTTI JUHANI HAKONEN, NANO, Aalto University, MIKKO MÖTTÖNEN, QCD Labs, Aalto University — We recently introduced a calorimeter capable of detecting packets containing 200 8.4-GHz photons, or 1.1 zJ of energy. Now we report a record low noise equivalent power (NEP) of 50 zW/rtHz, which is reduced to 20 zW/rtHz by introducing a Josephson parametric amplifier to the readout circuitry. The lower NEP value suggests energy resolution of $h \times 480$ GHz. Sensitivity of the detector can be further increased by decreasing the heat capacity of the absorbing element. To this end, we have experimentally studied graphene as an absorber, which is promising material due to its two-dimensional structure. Our preliminary results suggest energy resolution of $h \times 60$ GHz, bringin resolution of thermal detectors close to the qubit-based detectors while maintaining superior detection bandwidth.

*We acknowledge funding from the European Research Council under Consolidator Grant No. 681311 (QUESS) and under Proof of Concept Grant No. 727305 (SNABO), the Academy of Finland through grant nos 312300, 312059, 312294, 314447, 314449, 276528, 305237, 308161, and 314302, the Vilho, Yrjö and Kalle Väisälä Foundation, the Technology Industries of Finland Centennial Foundation, the Jane and Aatos Erkko Foundation, and the Finnish Cultural Foundation.
3:42PM V23.00007: Temperature sensing via photoluminescence lifetimes of Rhodamine B*  JOHN COLTON, Brigham Young University, KATE WATSON (Presenter), Arkansas State University — Non-invasive temperature probes have use in many settings where conventional thermometers may not be suitable or as efficient. An optical temperature probe is a material whose optical properties, such as photoluminescence (PL) or PL lifetime, are known as a function of temperature. We present results of PL lifetime studies of the organic dye Rhodamine B, which is a good candidate for use in temperature probes due to its large PL emission. We have measured PL lifetimes using time correlated single photon counting (TCSPC). The lifetimes were measured from temperatures of 15 K to 330 K. The lifetimes appear to be non-monotonic: they increase with temperature to a point, then decrease again. It is uncertain what is causing this unexpected trend, and we are in the process of verifying these lifetime measurements as well as studying other possible luminescent materials such as semiconductor quantum dots for application as temperature probes.

*Research was performed at BYU as part of the NSF REU program, grant no. 1757998.

3:54PM V23.00008: Single cell temperature measurement with a thin-film thermocouple array  FAN YANG (Presenter), SHENG-YONG XU, Key Laboratory for the Physics & Chemistry of Nanodevices, and Department of Electronics, Peking University — Single cell temperature measurement is an important fundamental issue. A full picture of the temperature distribution and thermal response of a single cell under different conditions is very helpful for answering fundamental biology questions in cell thermogenesis and thermal regulation. However, a reliable method for precise cellular temperature measurement remains a technical challenge.

In this work, we developed high-performance Pd/Cr micron thin-film thermocouple (TFTC) arrays and double-stabilized system with a stability of ±5 mK for single cell temperature measurement. We have obtained frequent temperature increments of 10-60 mK and a maximum up to 200-300 mK for cultured HepG2 cells1. Recently, we have reduced the stripe width of TFTC down to 170 nm, and fabricated 10×10 TFTC arrays on 100×100 µm² Si₃N₄ suspended platforms. We aim to realize the real-time 2D mapping of local temperature distribution for a single live cell with our nano-sized TFTC arrays and double-stabilized measurement system. The measurement results may shed some light on further investigation in determining the absolute temperature distribution of individual cultured live cells, both outside and inside of the cells, in a more precise way.


4:06PM V23.00009: Development of a New Dark Matter Detector that Uses Liquid He and Field Ionization*  DAVID OSTERMAN (Presenter), HUMPHREY J MARIS, GEORGE M SEIDEL, DEREK STEIN, Physics, Brown University — We discuss a new method of dark matter detection[1] that involves He atoms evaporated from a cold surface and their detection using field ionization. When a dark matter particle collides with a liquid He atom it produces phonons and rotons. When these excitations make it to the surface of the liquid He they evaporate a He atom, which can then be detected by ionization in a strong electric field. The >1 meV binding energy of a He atom to the surface opens the door for the detection of dark matter particles with a mass as low as 1 MeV/c². We will discuss the design of the proposed detector as well as the results of preliminary experiments on field ionization. We will also discuss the future of such experiments

*NASA Rhode Island Space Grant

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V24 DAMOP: General Atomic, Molecular, and Optical Physics II: Photonics and New Platforms for Topological States  BCEC 159 - Stojan Rebic, American Physical Society APS
Aharonov-Bohm cages in photonic lattices  
SEBABRATA MUKHERJEE, Heriot-Watt University, MARCO FEDELE DI LIBERTO (Presenter), Université Libre de Bruxelles, PATRIK ÖHBERG, ROBERT R. THOMSON, Heriot-Watt University, NATHAN GOLDMAN, Université Libre de Bruxelles — We report on the experimental realization of a uniform synthetic magnetic flux and the observation of Aharonov-Bohm cages in a rhombic photonic lattice of optical waveguides. In the regime where half a flux quantum is realized in each plaquette, all the energy bands collapse into nondispersive (flat) bands. The resulting localized eigenstates are then probed by studying the propagation of light in the bulk and at the edge of the photonic lattice. Our photonic lattice constitutes an appealing platform where the interplay between engineered gauge fields, frustration, localization, and topological properties can be finely studied. We further theoretically explore the localization properties of this system in the presence of interparticle mean-field interactions, which appear in photonic lattices as optical nonlinearities when increasing the light beam power. Surprisingly, we find that there still exist caged solutions and their nonlinear dynamics is accompanied with a breathing motion of the particle density reminiscent of a bosonic Josephson junction. Our results open an interesting route towards the characterization of nonlinear dynamics in flat band systems.


Role of long-range interactions in one-dimensional non-Hermitian topological photonic systems*  
BOXIANG WANG (Presenter), CHANGYING ZHAO, Shanghai Jiao Tong University — We study topological phonon polaritons (TPhPs) in one-dimensional dimerized silicon carbide nanoparticle chains. While the topological property of longitudinal modes is like the conventional Hermitian Su-Schrieffer-Heeger (SSH) model, for transverse modes, we find a topological phase transition at a substantially large lattice constant, due to the presence of long-range non-Hermitian interactions in an infinitely long chain. On the other hand, in the finite chain, due to these interactions, the edge and bulk modes become hybridized. In this situation, the non-Hermitian skin effect, i.e., the emergence of localized bulk modes over the edges, leads to the breakdown of bulk-boundary correspondence. By considering this effect and subsequently proposing a modified complex Zak phase for a finite chain, the topological behavior of the conventional SSH model is still recovered. Our study provides profound implications to the fields of non-Hermitian topological physics and quantum mechanical models with long-range interactions.

*National Natural Science Foundation of China (Grants No. 51636004, No. 51476097, No. 51521004), Shanghai Key Fundamental Research (Grants No. 18JC1413300 and No.16JC1403200), and National Postdoctoral Program for Innovative Talents (Grant No. BX20180187).

Optical Information Processing with Entangled Topological States*  
DAVID SIMON (Presenter), Physics and Astronomy, Stonehill College, SHUTO OSAWA, ALEXANDER SERGIENKO, Boston University — Topological quantities such as winding number or Chern number have become important tools for solid state physics, and more recently for photonic systems. These topological numbers are highly stable against external perturbations, which makes them attractive for encoding qubits in a robust manner. But they are difficult to determine by local measurements, especially in photonic systems, where the relevant information is often carried by a single photon that is destroyed in the measurement. Here, we use linear optical multiports as a means of constructing systems in which winding number and polarization are jointly entangled. This leads to a reduction in bit flip errors, due to the topological stability of the winding number, while the linkage to polarization simplifies the process of measuring the topological variable. This opens a new range of possible quantum information processing applications. We examine topologically-entangled bulk and boundary states, and outline several applications, such as the construction of topologically-protected photonic memory registers and of entangled memory registers.

*This research was supported by the National Science Foundation EFRI-ACQUIRE Grant No. ECCS-1640968, AFOSR Grant FA9550-18-1-0056, and by the Northrop GrummanNGNext.
3:06PM V24.00004: Near-field levitated optomechanics with a photonic crystal cavity* SUNKUN HONG, LORENZO MAGRINI (Presenter), Faculty of Physics, University of Vienna, RICHARD NORTE, Kavli Institute of Nanoscience, Delft University of Technology, RALF RIEDINGER, Faculty of Physics, University of Vienna, IGOR MARINKOVIĆ, Kavli Institute of Nanoscience, Delft University of Technology, DAVID GRASS, UROS DELIC, Faculty of Physics, University of Vienna, SIMON GROEBLACHER, Kavli Institute of Nanoscience, Delft University of Technology, MARKUS ASPELMEYER, Faculty of Physics, University of Vienna — Optically levitated dielectric particles has recently emerged as a new system in quantum optomechanics. It offers excellent mechanical coherence under high vacuum and a possibility to optically configure potential landscapes. An outstanding problem is the lack of methods to manipulate the particle at the quantum level. Here we introduce a nanophotonic interface that addresses this challenge. By optically trapping a 150 nm silica particle and placing it in the near field of a nanofabricated photonic cavity, we achieve a single-photon optomechanical coupling of up to \( g_0/2\pi = 9 \text{ kHz} \). Combined with an efficient guiding of light through the nanophotonic structure, we demonstrate a 'per-photon' displacement sensitivity increased by two orders of magnitude compared to previous experiments using far-field detection. I will discuss future outlook of the work, including several room-temperature quantum experiments that can be performed.

*This project was supported by the European Research Council (CoG QLev4G and StG Strong-Q), the Austrian Science Fund under the projects F40 (SFB FOQUS), P28172, the Foundation for Fundamental Research on Matter Projectruimte grant (15PR3210) and by the Netherlands Organisation for Scientific Research, as part of the Frontiers of Nanoscience program.

3:18PM V24.00005: Electromagnetically induced transparency in disordered and bidirectional chiral waveguide quantum electrodynamics* IMRAN MIRZA (Presenter), Physics, Miami University, OH, JOHN C SCHOTLAND, University of Michigan — Emitters coupled to nanophotonic waveguides architectures have gained a lot of attention due to the possibility of chiral (unidirectional) couplings between the emitters and the waveguide field [Nature, 541, 473-480 (2017)]. Till date most of the work on many emitter-waveguide quantum electrodynamics has focused on the scenario in which emitters are periodically placed and are symmetrically coupled with the waveguide. I will present single-photon transport problem in a one-dimensional disordered lattice of three-level emitters coupled to a waveguide [JOSA B, 35, 5 (2018)]. In particular, I'll consider Λ-type three-level emitters capable of exhibiting electromagnetically induced transparency and separately consider disorder in the atomic positions and transition frequencies. The question I'll address is how chiral emissions can impact the formation of spatially localized states. This work has possible applications to quantum networks and quantum communications.

*I. M. would like to acknowledge support from Miami University Ohio college of arts science startup funding.

3:30PM V24.00006: Light localization in disordered medium by scattering dislocation sites* FARBOD SHAFIEI (Presenter), The University of Texas at Austin, TOMMASO ORZALI, MAN HOI WONG, SEMATECH, GENNADI BERSUKER, The Aerospace Corporation, MICHAEL C DOWNER, The University of Texas at Austin — Threading dislocation defects at mismatch interfaces between III-V and Si substrate, act as light scattering sites in this disordered medium. Light get localized within the semiconductor film due to multiple scattering by these sites. We had studied the signature of such localizations in nonlinear regime (to avoid the dominating surface linear reflection). Localization signatures are observed in the series of optical measurements using a fiber scanning probe microscope that allows to analyze the light–matter interaction at these atomic irregularities in the material stacks.

*Welch Foundation
Disordered photonic bandgap materials, from functional device design to self-assembly progress.*

BOWEN YU (Presenter), BRANDON GUNN, ZHENNAN FENG, Physics and Astronomy, San Francisco State University, REMI DREYFUS, CNRS, WEINING MAN, Physics and Astronomy, San Francisco State University — Disordered photonic band gap materials are not limited to crystalline symmetries, hence offering unprecedented freedom for functional-defect designs, an inherent advantage associated with the isotropy of the structure. Beyond our previous works in disordered photonic structures, we made further progresses in both functional device designs and self-assembling attempts. We designed hyperuniform-disordered wall-networks for coupling 1.55-micron waves effectively in and out thin Silicon slabs. We systematically studied how various design parameters can be optimized for the best total efficiency, the best directional coupling and the broadest angle coupling. This can be potentially useful for integrated photonic circuits, and large-area and wide-angle light emitters and sensors. Microscopic disordered patterns with different degrees of hyperuniformity can be experimentally realized by driving colloidal suspensions out of equilibrium in a flow with different degrees of shearing. We found a clear correlation between the easiness (minimum required index-contrast) in opening photonic bandgap with the transition of displacement amplitude. This may open new routes for bottom-up self-assemblies of functional photonic materials.

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Chiral transport and localization in a bosonic analogue of the Kitaev-Majorana chain

ALEXANDER MCDONALD (Presenter), University of Chicago, TAMI PEREG-BARNEA, McGill University, AASHISH CLERK, University of Chicago — We study a bosonic system whose real-space Hamiltonian has a form analogous to the celebrated Kitaev chain model of a 1D p-wave superconductor [1]. The system is a 1D chain of non-interacting bosonic cavities which are subject to nearest-neighbour parametric driving. With a suitable choice of drive phases, the system has a number remarkable properties. It exhibits phase dependent chirality: photons propagate and are amplified in a direction that is determined by the phase of the initial drive or excitation. Further, we find a extreme sensitivity to boundary conditions which could serve as a potential quantum sensor. We show that many of these properties can be connected to the dynamics and topology of effective non-Hermitian models (despite our system being fully Hermitian). Our model could be realized in several different superconducting microwave circuits setups (e.g. [2,3]) or silicon photonic platforms (e.g. [4]).


Topological bands and triply-degenerate points in non-Hermitian hyperbolic metamaterials*

JUNPENG HOU (Presenter), ZHITONG LI, XIWANG LUO, QING GU, CHUANWEI ZHANG, University of Texas at Dallas — Hyperbolic metamaterials (HMMs), an unusual class of electromagnetic metamaterials, have found important applications in various fields due to their distinctive properties. A surprising feature of HMMs found recently is that even continuous HMMs can possess topological edge modes. However, previous studies based on equal-frequency surface (analogy of Fermi surface) may not correctly capture the topology of entire bands. Here we develop a topological band description for continuous HMMs that can be described by a non-Hermitian Hamiltonian formulated from Maxwell's equations. We find two types of three dimensional photonic triply-degenerate points with topological charges ±2 and 0 induced by chiral and gyromagnetic effects that break spatial inversion and time-reversal symmetries, respectively. Because of the photonic nature, the vacuum band plays an important role for topological edge states and bulk-edge correspondence in HMMs. The topological band results are numerically confirmed by direct simulation of Maxwell's equations. Our work presents a general nonHermitian topological band treatment of continuous HMMs, paving the way for exploring interesting topological phases in photonic continua.

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ARO (W911NF-17-1- 0128)
4:18PM V24.00010: Large Stark Tuning of InAs/InP Quantum Dots  SHAHRIAR AGHAEIMEIBODI (Presenter), CHANG-MIN LEE, MUSTAFA ATABEY BUYUKKAYA, CHRISTOPHER RICHARDSON, EDO WAKS, University of Maryland, College Park — Quantum dots are excellent sources of single-photon emission and are among the most promising candidates for scalable quantum photonic circuits. However, geometric differences in each quantum dot lead to slightly different emission wavelengths and hinders the possibility of generating multiple identical quantum emitters on the same chip. Stark tuning is an efficient technique to overcome this issue by controlling the emission energy of individual quantum dots. InAs/InP quantum dots are bright single-photon emitters in the telecommunication wavelength band. Stark tuning of these quantum dots has been previously limited to shifts below 1 nm due to the introduction of additional charges. Here, we demonstrate up to 8 nm of Stark tuning in the emission wavelength of InAs/InP quantum dots. Moreover, the single-photon nature and narrow linewidth of the quantum dot emission is preserved under the applied electric field. This result is an important step toward implementing multiple identical quantum emitters at telecom wavelengths, which is crucial for realizing complex quantum photonic circuits for quantum information processing.

4:30PM V24.00011: A nanomechanical-circuit QED analogue of the Unruh effect  HUI WANG (Presenter), MILES BLENCOWE, ALEXANDER J RIMBERG, Physics & Astronomy, Dartmouth College, CHRISTOPHER WILSON, Institute for Quantum Computing, University of Waterloo — In the Unruh Effect (UE), a uniformly accelerating detector is predicted to 'see' thermal photons in the vacuum. A longstanding challenge is to demonstrate the UE in tabletop experiments. However, impractically high accelerations are required in order to produce a measurable thermal photon signal. An alternative approach is to consider condensed matter analogues, where the governing quantum dynamics closely maps onto that of the genuine UE, but which are more easily realised in experiment. We consider a feasible UE analogue involving two coupled superconducting circuit microwave resonators, one playing the role of the photon detector, the other the vacuum cavity. The coupling is via a GHz mechanically oscillating film bulk acoustic resonator, with its fundamental dilatational frequency matching the microwave resonators' fundamental frequencies, functioning effectively as a non-degenerate parametric amplifier with mechanical pump. We show how the resulting photon pair production from vacuum can be verified through available quantum limited linear detection techniques.

4:42PM V24.00012: Experimental design and theoretical model building for higher-order topological insulators  RONNY THOMALE (Presenter), University of Wurzburg — Higher-order topological states establish a new complexity class of topological matter. The contemporary challenge is to devise experimental scenarios in which such exotic states of matter can unfold. We report on a synthetic topological matter realization of a quadrupolar topological insulator in a topolectrical circuit array [Imhof et al., Nature Physics 14, 925 (2018)]. Transcending from specific realizations of this phenomenon, we attempt to draw a line to previous observations of dimensional edge mode hierarchies [Sessi et al., Science 354, 1269 (2016)] before the field's terminology first emerged in 2017.

*The work was supported by ERC-StG-Thomale-336012 and by DFG-SFB 1170, project B04.

4:54PM V24.00013: Measurement of fractional corner charges in rotationally symmetric crystalline topological insulator metamaterials  CHRISTOPHER PETERSON (Presenter), University of Illinois at Urbana-Champaign, WLADIMIR BENALCAZAR, Pennsylvania State University, TIANHE LI, TAYLOR HUGHES, GAURAV BAHL, University of Illinois at Urbana-Champaign — Topological crystalline insulators (TCIs) with bulk dipole and higher multipole moments can host quantized fractional charges at their boundaries. Recently, it was shown that rotationally symmetric TCIs with vanishing bulk electric moments can also host quantized fractional electric charges at their corners. We used arrays of coupled microwave frequency resonators to experimentally investigate the local density of states (LDOS) in C3- and C4-symmetric crystalline topological lattices. We find that the LDOS is indeed fractionally quantized, in an analogous way as what is expected for the corner charge in their fermionic counterparts. Moreover, we show experimentally that these fractional LDOS are associated with corner-localized states that, although initially may be hidden within bulk energy bands, can be pulled out of them and be spectrally isolated. When these arrays are transitioned into their topological trivial phase, on the other hand, no fractionalization is observed, and consequently, corner-localized states cannot be isolated.

*We acknowledge support from the US National Science Foundation and the US Office of Naval Research.
Weyl exceptional rings in a lossy magnetically biased plasma

KUNAL SHASTRI (Presenter), FRANCESCO MONTICONE, Cornell University — Weyl exceptional rings are closed contours in momentum space along which both energy eigenvalues and eigenvectors of a system coalesce. These rings emerge in Weyl semimetals subject to non-Hermitian perturbations. We report the existence of Weyl exceptional rings in the electromagnetic dispersion of a lossy plasma in the presence of an external magnetic field. We describe the conditions under which topologically protected surface states can be preserved or destroyed by changing losses in the system. Increasing losses changes the size of the exceptional rings and anisotropic losses at certain angles relative to the external magnetic field can cause two rings of opposite charge to annihilate each other. This system offers a window to study the rich physics of exceptional rings in a range of plasmonic materials including the optical response of magnetically biased metals and semiconductors.

Microwave shielding of ultracold polar molecules

TIJS KARMAN (Presenter), Institute for Theoretical Atomic, Molecular and Optical Physics (ITAMP), Harvard-Smithsonian Center for Astrophysics, JEREMY M. HUTSON, Department of Chemistry, Durham University — Use microwaves to engineer repulsive long-range interactions between ultracold polar molecules [1]. The resulting shielding suppresses various loss mechanisms and provides large elastic cross sections. Hyperfine interactions limit the shielding under realistic conditions, but a magnetic field allows suppression of the losses to below $10^{-14}$ cm$^3$ s$^{-1}$. The mechanism and optimum conditions for shielding differ substantially from those proposed by Gorshkov et al. [Phys. Rev. Lett. 101, 073201 (2008)], and do not require cancelation of the long-range dipole-dipole interaction that is vital to many applications.


Session V25 DPOLY GSOFT DBIO: Polymer-Mediated Structural Transitions in Soft Materials

2:30PM V25.00001: Rouleaux formation: polymer induced Red Blood Cells aggregates [Invited] CHRISTIAN WAGNER (Presenter), Saarland University — Plasma proteins such as fibrinogen induce the aggregation of red blood cells (RBC) into rouleaux, which are responsible for the pronounced shear thinning of blood, control the erythrocyte sedimentation rate (ESR) — a common hematological test — and are involved in many situations of physiological relevance such as structuration of blood in the microcirculation or clot formation in pathological situations. Confocal microscopy is used to characterize the shape of RBCs within rouleaux at equilibrium as a function of macromolecular concentration, revealing the diversity of contact zone morphology. Three different configurations that have only been partly predicted before are identified, namely parachute, male-female and sigmoid shapes, and quantitatively recovered by numerical simulations. Stable polymer induced clusters in capillary flow are also observed in-vivo in a mouse model by use of intravitral epillumination microscopy and in-vitro in a microfluidic device, wherein the protein or the macromolecule concentration can be freely varied. The interaction energies between the cells are determined by use of single cell force spectroscopy and optical tweezers. Numerical simulations of flowing cells show again a good agreement with the experimental observations.

3:06PM V25.00002: Extracellular polymers control bacterial biofilm expansion and material properties JING YAN (Presenter), BONNIE BASSLER, NED WINGREEN, HOWARD A STONE, Princeton University — Biofilms, surface-attached communities of bacterial cells, are a concern in health and in industrial operations because of persistent infections, clogging of flows, and surface fouling. In this talk, I will explore the consequences to biofilm growth and robustness when the biofilm matrix functions as a material that is responsive to environmental perturbations such as changes in osmotic pressure. Using Vibrio cholerae as the model organism, we showed that matrix production enables biofilm-dwelling bacterial cells to establish an osmotic pressure differential between the biofilm and the external environment. The pressure difference promotes colony biofilm expansion on nutritious surfaces, controls growth of submerged biofilms, and enables matrix-producing cells in biofilms to exclude non-matrix-producing cheaters and to resist invasion by planktonic cells. Furthermore, we discovered how extracellular polysaccharides, proteins, and cells function together to define biofilm mechanical and interfacial properties.
3:18PM V25.00003: Glass transition temperature of poly(lactic-co-glycolic acid) particles YIQING YANG, QINGRUI JIANG, STEVEN HERRERA, KATHLEEN MCENNIS (Presenter), New Jersey Institute of Technology — Poly(lactic-co-glycolic acid) (PLGA), is a commonly used biodegradable biomaterial used to make many different biomedical products including drug delivery particles. The glass transition temperature ($T_g$) of a polymer particle can have a profound effect on its behavior \textit{in vivo} such as aggregation behavior and drug release profile. Bulk PLGA has a $T_g$ of approximately 40°C. Since normal body temperature is 37°C, it is assumed that PLGA particles will remain in their solid, glassy state during \textit{in vivo} experiments. However, many factors can affect the $T_g$ of a particle, such as thermal history. The method used to produce the PLGA particle will therefore affect its $T_g$. Most experiments are done with polymer samples in the bulk form that have been annealed to erase thermal history. In this work, PLGA particles are made by nanoemulsion, nanoprecipitation, and electrohydrodynamic jetting and the $T_g$ of the particles is measured using the first heating scan of a modulated differential scanning calorimetry to run the determination of the role of processing conditions on the $T_g$ of PLGA particles.

3:30PM V25.00004: Polyelectrolyte-Mediated Colloidal Interactions at the Interfaces of Liquid Crystals MICHAEL TSUEI (Presenter), YOUNG KI KIM, Chemical and Biomolecular Engineering, Cornell University, HAO SUN, Department of Chemistry, Northwestern University, XIN WANG, YU YANG, Chemical and Biomolecular Engineering, Cornell University, NATHAN C. GIANNESCHI, Department of Chemistry, Northwestern University, NICHOLAS L. ABBOTT, Chemical and Biomolecular Engineering, Cornell University — Nematic liquid crystals (LCs) are complex fluids within which molecules exhibit long-range orientational order leading to an anisotropic elasticity. When introduced into a LC host, colloidal particles (microcargo) elastically strain the LC and generate topological defects. Consequently, the microcargo experience strong repulsive forces near interfaces of LCs (e.g., LC-aqueous, LC-air interfaces). In this presentation, we will show that formation of polyelectrolyte and polyelectrolyte-surfactant complexes at a LC interface modulates the interactions of colloidal microcargo with that interface. We will describe elastic and electrical double layer interactions occurring at these interfaces and how the interplay of the two interactions is modulated by the formation of complexes of polyelectrolytes and surfactants. We will also illustrate how this competition of interactions can be used to trigger the release of microcargo from the LC.

3:42PM V25.00005: Phase behavior and structure of polyelectrolyte-nanoparticle complex assemblies E NEILSEN (Presenter), SAMANVAYA SRIVASTAVA, Chemical and Biomolecular Engineering, University of California, Los Angeles — Numerous examples of complex assemblies comprising oppositely charged polyelectrolytes and nanoparticles (or proteins) in aqueous environments exist in natural and synthetic systems. The structure and stability of these complex assemblies are dictated by numerous factors including solution conditions as well as polyelectrolyte and nanoparticle properties and are far from being fundamentally understood and controlled. In this work, we examine the effect of polyelectrolyte and nanoparticle concentrations, polyelectrolyte size, flexibility, charge density and degree of ionization, nanoparticle size and effective charge density and the pH and ionic strength of the solution on the structure and phase behavior of model nanoparticle-polyelectrolyte complex assemblies comprising negatively charged silica nanoparticles and diverse polycations. Conditions that lead to destabilization and phase separation of the complexes will be identified through turbidimetric and light scattering studies. Furthermore, X-ray and light scattering investigations on the structure and morphology of phase separated and the "soluble" stable complexes will be presented.

3:54PM V25.00006: Polymer mediated interaction between colloids and their role in the formation of colloidal aggregates* ALEXANDER CHERVANYOV (Presenter), Institute of Theoretical Physics, WWU Munster, Munster, Germany — We theoretically study the polymer mediated (PM) interactions between colloids immersed in different host polymer systems such as (i) semi-dilute polymer solutions; (ii) polymer melts; (iii) polymer blends; (iv) rubber materials. A significance of the effect of attractive polymer-colloid (P-C) and polymer-polymer (P-P) interactions on the effective forces acting between colloids immersed in a polymer melt is shown to drastically depend on the colloid-to-polymer size ratio. For the case of colloids immersed in polymer blends we predict a novel mechanism of the PM interactions caused by non-uniformities in the local composition of the polymer blend induced by these colloids. This mechanism, specific to polymer blends, is shown to play a dominant role in the PM interactions. As a practical application of the developed approach, we study the polymer mediated aggregation of colloids immersed in the above host polymer systems. In addition, we discuss several practical examples showing how the effective interactions between colloids induced by polymers are used to drive thermodynamic, mechanical, and electrical properties of the selected polymer-colloid composites.

*Financial support of Deutsche Forschungsgemeinschaft (DFG) through Grant No. CH 845/2-1, is gratefully acknowledged.
4:06PM V25.00007: Dielectric virial expansion of polarizable dipolar spheres  
HUADA LIAN (Presenter), Department of Materials Science and Engineering, Stanford University, JIAN QIN, Department of Chemical Engineering, Stanford University — Predicting the static dielectric permittivity for composites with polarizable components remains a theoretical challenge. The typical Maxwell-Garnett mixing rule or its variant approximates the composite permittivity with a linear average of inclusion’s polarizability, which neglects the inter-particle interactions. A systematic density expansion is developed to predict the composite permittivity that includes the contribution from interactions of multiple polarizable particles. The lowest order term in such expansion reduces to the Maxwell-Garnett rule. Including the second order term results in a parameter-free prediction, which matches the independently measured values for a set of seven polymer-nanoparticle composites.

4:18PM V25.00008: Co-assembly of anisotropic colloids and diblock copolymer mixtures  
JAVIER DIAZ (Presenter), Centre for Computational Physics, University of Lincoln, ROY SHENHAR, Institute of Chemistry, The Hebrew University of Jerusalem, MARCO PINNA, Centre for Computational Physics, University of Lincoln, IGNACIO PAGONABARRAGA, Departament de Fisica Fonamental, Universitat de Barcelona, ANDREI ZVELINDOVSKY, Centre for Computational Physics, University of Lincoln — Block copolymers are excellent candidates to template the localisation of colloids, in order to create ordered arrays of nanoparticles, with uses in optical and electrical applications. The co-assembly of block copolymer nanocomposite materials can lead to highly ordered systems in the mesoscale. Computer simulations have been used to address the complex assembly of anisotropic rod-like colloids. The crossover between the block copolymer intrinsic length scales and the shape and orientation of anisotropic nanoparticles leads to a rich variety of phase behaviors, both in terms of polymeric morphologies and colloidal organisation. Rod-like nanoparticles have been found to form side-to-side configuration in block copolymer ultrathin films. SEM images are compared with a hybrid Cell Dynamic/Brownian Dynamic computational method which is used to characterise the assembly of anisotropic nanoparticles in diblock copolymers.

4:30PM V25.00009: Predicting chi for polymers with different chain architectures using simulation*  
SHREYA SHETTY (Presenter), MILENA MARIE ADAMS, ENRIQUE D GOMEZ, SCOTT MILNER, Pennsylvania State University — The Flory Huggins interaction parameter chi governs phase behavior in polymer blends and block copolymers. Chain architecture affects how chains pack in the melt, which can significantly influence chi. To explore this, we investigate chi for two different architectures of flexible bead-spring chains, using molecular dynamics simulations and our recently developed “morphing” method to compute the excess free energy of mixing. In the first case, we consider an idealized bead-spring model of polyethylene and polypropylene, in which all beads have the same interactions, but polypropylene chains have a side bead on every other backbone bead. In the second case, we examine blends in which both chain species have the “polypropylene” bead-spring structure, but one species has beads with a slightly weaker interaction – either the side beads (case 1), main chain beads (case 2) or branch point beads (case 3). We use our method to find c for all three cases, for which random mixing models would give identical results. Finally, we compare our values with predictions from PRISM, with correlation functions from simulations as input, as a purely simulation-based test of PRISM.

*Financial support from the National Science Foundation under Award DMREF-1629006 is acknowledged.

4:42PM V25.00010: Novel Dynamical behaviors of charged Macromolecules in a crowded environment*  
DI JIA (Presenter), MURUGAPPAN MUTHUKUMAR, Department of Polymer Science and Engineering, University of Massachusetts Amherst — The phenomenon of “ordinary-extraordinary” dynamical transition in salt-free polyelectrolyte solutions is well known. We report the emergence of additional dynamical mode at higher molecular weights of the polyelectrolyte. We find that the key variable Cp/Cs, which is normally used in describing the onset of the ordinary-extraordinary transition (fast and slow modes), is inadequate in describing the dynamics of polyelectrolyte solutions. For concentrated solutions of sodium polystyrene sulfonate of higher molecular weights, we observe a third intermediate mode. The emergence of the new mode depends crucially on the polymer molecular weight and the concentration of the added salt. We find that Cp/C* (where C* is overlap concentration) is a key variable in addition to Cp/Cs.

*National Science Foundation (DMR-15 04265)
4:54PM V25.00011: Similarity of Crambin Lattice Protein Homologues in the Semi-flexible H0P Model*  
ZEWEN ZHANG (Presenter), ALFRED FARRIS, GUANGJIE SHI, Center for Simulational Physics, University of Georgia, THOMAS WUEST, Scientific IT Services, ETH Zürich, DAVID P LANDAU, Center for Simulational Physics, University of Georgia — The semi-flexible H0P lattice protein model is an extension of the HP model with an extra kind of “neutral” monomer and an energetic term for “bends”. Crambin (a 46 amino acids protein) has been mapped onto the H0P model and studied by replica-exchange Wang-Landau sampling. From the obtained density of states, thermal properties of the lattice protein are extracted at all temperature. With further study by multicanonical sampling, ground state degeneracy as well as the temperature-dependence of structural quantities are measured with high resolution. In this study, we examine five H0P lattice protein homologues of Crambin, i.e. proteins with similar sequences and structures in nature. Our results show that, at low temperature, thermal properties of these H0P-modeled homologues are close to those of Crambin itself, all showing two significant conformational changes. However, results also show that the previous value for the bending energy can lead to high degeneracies for some low excited states of the homologues. Therefore, a slight change has been made to this term, to keep the degeneracies of all tested homologues low and stable.

*The computing sources are provided by Georgia Advanced Computing Resource Center; and Texas Advanced Computing Center under XSEDE Grant No. PHY130014.

5:06PM V25.00012: Is there a universal equation of state for flexible polymers beyond the semi-dilute regime?*  
JAROSLAW PATUREJ (Presenter), JENS-UWE SOMMER, TORSTEN KREER, Leibniz Institute for Polymer Research Dresden — We reconsider the isothermal equation of state (EoS) for linear homopolymers in good solvents, \( p = p(c, T) \), which relates the osmotic pressure, \( p \), of polymers with the bulk concentration, \( c \), and the temperature, \( T \). The classical scaling theory predicts the EoS in dilute and semi-dilute regimes. We suggest a generalized EoS which extends the universal behavior of polymer solutions up to the highly concentrated state and confirmed it by molecular dynamics simulations and using available experimental data. Our conjecture implies that properties of polymer chains dominate the EoS in the presence of many-body interactions. Our theoretical approach is based on a viral expansion in terms of concentration blobs leading to a superposition of two power laws in the regime of concentrated solutions.

*Polish Ministry of Science and Higher Education Grant (IP 2015 059074)

5:18PM V25.00013: Gelation of hydrogel films and coatings induced by substrate swelling.*  
DAVID MOREAU, Centre des Matériaux, Mines ParisTech, CAROLINE CHAUVET, FRANÇOIS ETIENNE, FRANÇOIS P RANNOU, INSERM UMR S1124, Université Paris Descartes, LAURENT CORTE (Presenter), Centre des Matériaux, Mines ParisTech — Hydrogel films used as membranes or coatings are essential components of devices interfaced with biological systems. Their design is greatly challenged by the need to find mild synthesis and processing conditions that preserve their biocompatibility and the integrity of encapsulated compounds. Here, we report an approach to produce hydrogel films spontaneously in aqueous polymer solutions [1]. This method uses the solvent depletion created at the surface of swelling polymer substrates to induce the gelation of a thin layer of polymer solution. Using a biocompatible polymer that self-assembles at high concentration (poly(vinyl alcohol)), hydrogel films are produced within minutes to hours with thicknesses ranging from tens to hundreds of micrometers. A simple model predicts how the solution composition, substrate geometry and swelling properties govern film growth. We also demonstrate the potential of this technique by incorporating other solutes to fabricate ceramic-hydrogel coatings for bone anchoring of osteo-articular implants and matrices for cell-encapsulation.


*Financial support from Mines-ParisTech, ESPCI Paris and Institut Carnot Mines (HAP-Process 2012) as well as French Research Agency (ANR-14-CE15-0019) is acknowledged.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V26 DQI: Superconducting Qubits: Control Hardware and Methods  
Abdo, IBM Thomas J. Watson Research Center
**2:30PM V26.00001: Integration of classical electronics for quantum computing tasks in superconducting qubit systems**

ANTONIO CORCOLES (Presenter), MAIKA TAKITA, KEN INOUE, SCOTT LEKUCH, ABHINAV KANDALA, JAY GAMBETTA, JERRY M. CHOW, IBM Thomas J. Watson Research Center — The acts of controlling and measuring superconducting qubits for quantum information processing rely on classical electronic systems. Although metrics primarily associated to the quantum system, such as qubit coherence time and gate fidelity, are typically quoted as benchmarks for quantum processor quality, the integration of classical hardware and associated software with the quantum device plays a critical role both in these metrics and in the overall performance of a quantum computer.

In this talk we will discuss some important details of this architecture for superconducting quantum processors, touching on current limitations and future outlook.

*This work is supported by IARPA under contract W911NF-16-1-0114.

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**2:42PM V26.00002: Evaluating the performance of classical electronics for quantum computing tasks in superconducting qubit systems**

MAIKA TAKITA (Presenter), ANTONIO CORCOLES, KEN INOUE, SCOTT LEKUCH, ABHINAV KANDALA, JAY GAMBETTA, JERRY M. CHOW, IBM Thomas J. Watson Research Center — We present and discuss quantum protocols for near-term superconducting quantum processors for which quantum feedback or feedforward plays a key role. These protocols hinge heavily on classical electronics for qubit control and signal processing, which makes them ideal candidates for evaluating the performance of NISQ devices in the present and near future. We will discuss, in addition, ways in which these quantum protocols can be used for benchmarking systems exposed to errors that reach beyond quantum noise and coherent errors in qubit control.

*This work is supported by IARPA under contract W911NF-16-1-0114.

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**2:54PM V26.00003: Atomic flux pulses for a superconducting quantum processor, part 1: real-time corrections and repeatability of flux pulses**

FILIP MALINOWSKI (Presenter), MICHIEL ADRIAAN ROL, LIVIO S CIORCIARO, BRIAN M TARASINSKI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, YVES SALATHE, NIELS HAANDBAEK, JAN ŠEDIVÝ, Zurich Instruments AG, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — We present the calibration and characterization of atomic, repeatable flux pulses compatible with a flexible Quantum Instruction Set Architecture (QISA). The flux pulses take advantage of distortion corrections realized by real-time filtering in the arbitrary waveform generator as the sequence of pulses is executed, rather than conventional pre-distortion of the waveform shape in software. We combine the corrections with the net-zero waveform shape and quantify the repeatability of flux pulsing. The phases acquired by the qubit in each of two consecutive flux pulses match within 1 deg, independent of the delay between them.

*This research is supported by Intel Corporation and IARPA (U.S. Army Research Office grant W911NF-16-1-0071).

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MICHIEL ADRIAAN ROL (Presenter), FILIP K MALINOWSKI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, FRANCESCO BATTISTEL, QuTech, Delft University of Technology, BRIAN M TARASINSKI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, BARBARA TERHAL, QuTech, Delft University of Technology, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — We use a novel pulse shape, named net-zero, to realize a coherence limited, codeword-triggered, and repeatable conditional-phase (CZ) gate between transmon qubits in a circuit QED processor. We characterize the performance of both conventional and net-zero CZ flux pulses and quantify specific error sources such as leakage, dephasing, relaxation, non-markovianity, and coherent errors. We compare experimental results to simulations that include realistic modeling of these effects.

*This research is supported by IARPA (U.S. Army Research Office grant W911NF-16-1-0071), Intel Corporation and ERC grant EQEC No. 682726.
3:18PM V26.00005: Superconducting qubit control electronics - Part 1/2: system overview and control hardware

AMIT VAINSENCHER (Presenter), Google Inc - Santa Barbara, BEN CHIARO, Physics, University of California, Santa Barbara, ROBERTO COLLINS, Google Inc - Santa Barbara, BROOKS FOXEN, Physics, University of California, Santa Barbara, EVAN JEFFREY, ERIK LUCERO, Google Inc - Santa Barbara, MATTHEW MCEWEN, Physics, University of California, Santa Barbara, DANIEL SANK, JOHN M MARTINIS, Google Inc - Santa Barbara — The need for numerous analog control lines presents a unique challenge in building control systems for large quantum processors. In the context of superconducting Josephson qubits, particular requirements for the control lines include phase matching across all channels, low noise, and minimal drift. In this talk, we discuss the design, implementation, and challenges encountered in building our next generation modular control system. Using this system in a configuration with 256 DACs, 84 IQ mixers, 24 ADC, and 16 microwave sources, we will show preliminary measurements on Bristlecone, our 72-qubit processor.

3:30PM V26.00006: Superconducting qubit control electronics - Part 2/2: dispersive measurement

DANIEL SANK (Presenter), ROBERTO COLLINS, EVAN JEFFREY, ERIK LUCERO, AMIT VAINSENCHER, Google Inc - Santa Barbara, BROOKS FOXEN, BEN CHIARO, Physics, UCSB, JOHN M MARTINIS, Google Inc - Santa Barbara — Dispersive measurement of transmon-type qubits requires a microwave receiver with nearly 100 dB gain and ~100 mK system noise temperature. Recent increases in qubit number have introduced a new set of requirements on our receivers. These constraints include the need for smaller parts at cryogenic and room temperature stages, higher reliability, lower cost, and uniformity across multiple systems to ensure agreement between staging and production systems. In this talk, we discuss the design and implementation of our dispersive measurement system that meets our integration needs while maintaining performance, with particular focus on the room temperature electronics. We present preliminary results on our latest chips.

3:42PM V26.00007: Superconducting Qubit Control with Single Flux Quantum Pulses in A Multichip Module: Part I – Fabrication and Pulse Driver*

CHUAN-HONG LIU (Presenter), EDWARD M LEONARD, MATTHEW A BECK, Physics, University of Wisconsin-Madison, KENNETH DODGE, ANDREW L BALLARD, CALEB HOWINGTON, VITO M IAIA, JJ NELSON, Physics, Syracuse University, ALEX KIRICHENKO, DANIEL T YOHANNES, IGOR VERNIK, JASON WALTER, OLEKANDR CHERNYASHEVSKYY, OLEG MUKHANOV, Hypres Inc, BRITTON L PLOURDE, Physics, Syracuse University, ROBERT F MCDERMOTT, Physics, University of Wisconsin-Madison — Superconducting qubits are an attractive candidate for quantum information. However, existing control techniques do not scale well to large-scale qubit arrays processing. A promising candidate for scalable control is the Single Flux Quantum (SFQ) digital logical family. In an initial implementation, the fidelity of SFQ-based qubit gates was limited by quasiparticle (QP) poisoning of the qubit induced by the dissipative SFQ pulse driver. Here we introduce a quantum-classical multichip module (MCM) where the SFQ driver and the qubit are segregated onto separate chips in order to suppress QP poisoning. We describe the design, fabrication, and thermalization of the MCM. Finally, we discuss the operation and characterization of the SFQ pulse generator and qubit.

*This work was supported by the U.S. Government under Grant W911NF-15-1-0248.

3:54PM V26.00008: Superconducting Qubit Control with Single Flux Quantum Pulses in A Multichip Module: Part II Qubit and Quasiparticle Measurement

KENNETH DODGE (Presenter), ANDREW BALLARD, CALEB HOWINGTON, VITO M IAIA, JJ NELSON, Syracuse University, CHUAN-HONG LIU, EDWARD M LEONARD, MATTHEW A BECK, Univ of Wisconsin, Madison, ALEX KIRICHENKO, DANIEL T YOHANNES, IGOR VERNIK, JASON WALTER, OLEKANDR CHERNYASHEVSKYY, OLEG MUKHANOV, Hypres Inc, ROBERT F MCDERMOTT, Univ of Wisconsin, Madison, B.L.T. PLOURDE, Syracuse University — We demonstrate coupling of a Single Flux Quantum (SFQ) driver on a classical control chip to a superconducting qubit on a quantum chip in a multi-chip module package. A DC-SFQ driver on the classical chip emits quantized pulses that are capacitively coupled to the qubit island of a transmon on the quantum chip, allowing subharmonic driving of qubit rotations. We examine the effects of on- and off-resonant SFQ pulses on the state of the qubit and the response of the read-out cavity. Quasiparticle (QP) excitations created from the operation of the SFQ circuitry can be a source of decoherence and temporal instability in the qubit. QP contribution to the qubit admittance are examined by monitoring how relaxation and dephasing times correlate with QP creation. Mitigation strategies for QP poisoning will be discussed.
4:06PM V26.00009: Reciprocal Quantum Logic Compatible SFQ-to-CMOS Amplifiers for High-Speed Data Transmission ELIAS GALAN, MARIE MCLAIN (Presenter), MICAH STOUTIMORE, ANDREW MIKLICH, KURT PLEIM, RATZ PAUL, DAVID MCGUIRE, OLIVER OBERG, ZACHARY KYLE KEANE, Northrop Grumman — We have developed an amplifier for use in transmitting high-speed reciprocal quantum logic signals to CMOS digital circuitry at room temperature. The amplifier uses an integrated digital latch to convert the normally return-to-zero (RZ) format of a single flux quantum (SFQ) signal to non-return-to-zero (NRZ) format with a simple and space-efficient design. The NRZ format provides more signal power per unit bandwidth than RZ, and is easier to interface with CMOS circuitry. The output voltage is provided by a series of inductively isolated asymmetric DC superconducting quantum interference devices (SQUIDs). The power efficiency is estimated to be 32±9%. The DC SQUIDs are designed in-line with a 50 Ohm transmission line to reduce high frequency oscillation and improve output signal integrity. Experimentally, the output amplifier demonstrated a bit error rate of better than 9.5E-8 at 1 Gb/s; extrapolations to the optimal operating point project a bit error rate of 1E-37.

4:18PM V26.00010: Engineering cryogenic setups for 100-qubit scale superconducting circuit systems* SEBASTIAN KRINNER (Presenter), SIMON STORZ, PHILIPP KURPIERS, PAUL MAGNARD, JOHANNES HEINSOO, RAPHAEL KELLER, JANIS LUETOLF, CHRISTOPHER EICHLER, ANDREAS WALLRAFF, Department of Physics, ETH Zurich — A robust cryogenic infrastructure in form of a wired, thermally optimized dilution refrigerator is essential for solid-state based quantum processors. In this talk, we present a cryogenic setup, which minimizes passive and active heat loads, while guaranteeing rapid qubit control and readout. We review design criteria for qubit drive lines, flux lines, and output lines used in typical experiments with superconducting circuits. The passive heat load of stainless steel and NbTi coaxial cables and the active load due to signal dissipation are measured, validating our robust and extensible concept for thermal anchoring of attenuators, cables, and other microwave components. Our results are important for managing the heat budget of future large-scale quantum computers based on superconducting circuits.

*This work is supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office grant W911NF-16-1-0071 and by ETH Zurich.

4:30PM V26.00011: Scalable instrumentation for general purpose quantum computers GLENN JONES (Presenter), DEANNA ABRAMS, STEPHAN BROWN, LAUREN CAPELLUTO, SCHUYLER FRIED, SABRINA HONG, BLAKE JOHNSON, ROB LION, ADAM MOCARSKI, MIKE PELSTRING, CHAD RIGETTI, DAMON RUSSELL, MICHAEL RUST, COLM RYAN, DIEGO SCARABELLI, RODNEY SINCLAIR, PRASAHNT SIVARAJAH, CHLOE SONG, ALEXA N STALEY, JOHN STEVENSON, MARK SUSKA, NIMA TAIE-NOBARI, CELENA TANGUAY, NIKOLAS TEZAK, STEFAN TURKOWSKI, Rigetti Quantum Computing — As quantum computers grow to increasing numbers of qubits, it becomes advantageous to use specialized or customized hardware to generate the microwave pulses that control the qubits. We present an FPGA-based system for controlling qubits that demonstrates a number of advantages over commercially available test equipment. The system has been optimized to minimize the noise sources to which the qubits are most susceptible, enabling high fidelity quantum gates. The overall architecture is designed to support hybrid quantum-classical algorithms. Optimized processor cores control the microwave signal generation and provide arbitrary control flow, allowing gates to be applied conditioned on a measurement result. Gate parameters, such as rotation angle, can also be dynamically computed, or loaded from classical shared memory, and applied in real-time. We present results from a straightforward usage of this capability: actively resetting a qubit to its ground state.

4:42PM V26.00012: Scaling the input/output architecture of quantum processors to kQbit, and beyond, size in the NISQ era DAAN KUITENBROUWER, WOUTER BOS, KIEFER VERMEULEN, KELVIN LINDEBOG, RIEMER SORGEDRAGER, VIVIEN THINEY, JAKOB KAMMHUBER, SAL BOSMAN (Presenter), Delft Circuits — Most quantum computing hardware in the NISQ era is designed to support hybrid quantum-classical algorithms. Optimized processor cores control the microwave signal generation and provide arbitrary control flow, allowing gates to be applied conditioned on a measurement result. Gate parameters, such as rotation angle, can also be dynamically computed, or loaded from classical shared memory, and applied in real-time. We present results from a straightforward usage of this capability: actively resetting a qubit to its ground state.
4:54PM V26.00013: Optimizing readout hardware for large scale quantum computers  THEODORE WHITE (Presenter), Google Inc - Santa Barbara, BEN CHIARO, BROOKS FOXEN, U.C. Santa Barbara, JOHN M MARTINIS, Google Inc - Santa Barbara — In a superconducting quantum computer, each microwave readout line requires low noise parametric amplifiers, circulators, and filters. These are expensive resources, not only in cost but also in weight and size. In larger systems it is increasingly necessary to use frequency multiplexed readout tones such that many qubits can be measured with a single line. This in turn requires superconducting parametric amplifiers that operate with broad bandwidth and high saturation power, while maintaining near quantum limited noise performance. In this talk we will compare several different varieties of amplifier from the perspective of device performance, fabrication difficulty, yield, and wiring complexity. We will also report on performance metrics for these architectures in our superconducting qubit processors.

5:06PM V26.00014: Scalable FPGA-based qubit control hardware*  GANG HUANG (Presenter), YILUN XU, LAWRENCE DOOLITTLE, Lawrence Berkeley National Laboratory, UNPIL BAEK, IRFAN SIDDIQI, Physics, University of California, Berkeley — As quantum computing technology evolves from research laboratories to potential industrial applications, the scalability and synchronization of classical control hardware becomes a limiting factor in the development of intermediate-scale (50-100) qubit systems. We introduce a novel FPGA-based architecture comprised of multiple qubit control boards, interconnected by a fiber-based synchronization system, to implement basic operations such as qubit control and readout. Our hardware represents a cost-effective alternative to commercial test and measurement style AWGs and detectors, and can be readily scaled up for intermediate-scale quantum processors with low latency and synchronization among all channels to a common clock cycle. Having assembled a prototype system with commercial evaluation boards, we present results from bench testing of the hardware and initial tests demonstrating qubit control. Customized hardware with higher channel density is under development.

*This work was supported by the Department of Energy.

5:18PM V26.00015: An FPGA-based quantum feedback system for real-time qubit control*  UNPIL BAEK (Presenter), Physics, University of California, Berkeley, YILUN XU, GANG HUANG, LAWRENCE DOOLITTLE, Lawrence Berkeley National Laboratory, IRFAN SIDDIQI, Physics, University of California, Berkeley — Measurement-based quantum feedback is highly sought after due to its potential for quantum error correction and preserving quantum coherence. However, measurement-based quantum feedback has been difficult to achieve due to the limited lifetime of qubits as compared to the longer time required for readout and feedback signal processing. We present a new FPGA-based qubit control architecture that integrates the qubit readout, state recognition, and feedback response together to minimize latency. Using our initial hardware, we demonstrate real-time quantum feedback on superconducting qubits and apply this technology to a multi-qubit superconducting quantum processor.

*This work was supported by the Department of Energy.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V27 DQI: Quantum Foundations I BCEC 160C - Mordecai Waegell, Chapman University - Tag(s): Focus

2:30PM V27.00001: Wigner's friend as a rational agent*  [Invited]  CASLAV BRUKNER (Presenter), Institute for Quantum Optics and Quantum Information — In 1961 the physicist Eugene Wigner proposed the “Wigner’s friend” thought experiment in which an observer, Wigner, observes another observer, his friend, who performs a quantum measurement on a physical system. I will first derive a no-go theorem for observer-independent outcomes (directly observable “facts” such as “detector clicks”) which would be common both for Wigner and the friend. The outcomes then are to be understood as relational in the sense that their determinacy is relative to an observer. I will then discuss a situation where the rationale is to force Wigner's friend to depart from “standard rules of quantum mechanics” when updating her degrees of belief.

*I acknowledge the support of the Austrian Science Fund (FWF) through the project I-2906 . This research was funded by John Templeton Foundation, grant number 60609. The opinions expressed in this publication are those of the authors and do not necessarily reflect the views of the John Templeton Foundation.
3:06PM V27.00002: Contextuality without access to a tomographically complete set* MATTHEW F. PUSEY (Presenter), Department of Computer Science, University of Oxford, LIDIA DEL RIO, BETTINA MEYER, Institute for Theoretical Physics, ETH Zürich — The operational approach to contextuality due to Spekkens requires finding operationally equivalent preparation procedures. Previously these have been obtained by demanding indistinguishably under a set of measurements taken to be tomographically complete. That is, it is taken for granted that the experimenter has access to the full dimension of the system of interest. However, there may in fact be other measurements in the true tomographically complete set, which could break the operational equivalences and hence eliminate the putative contextuality. Here we design tests of contextuality that are immune to this effect for a given number of unknown measurements in the tomographically complete set, allowing contextuality to be demonstrated with weaker assumptions.

*LdR acknowledges support from ERC AdG NLST, EPSRC grant DIQIP, Perimeter Institute for Theoretical Physics (PI), and the Institute for Quantum Computing at University of Waterloo. MP acknowledges PI and the Royal Commission for the Exhibition of 1851. Research at PI is supported by the government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Economic Development & Innovation. This work was partially supported by the COST Action MP1209.

3:18PM V27.00003: Symmetric Informationally Complete Measurements Pinpoint the Essential Difference between Classical and Quantum Probability Theories BLAKE STACEY (Presenter), University of Massachusetts Boston — I describe a general procedure for crafting a purely probabilistic representation of the Born Rule by means of a reference measurement: a minimal informationally-complete quantum measurement (MIC) and a set of linearly independent post-measurement quantum states. It follows that the Born Rule is a consistency condition between probabilities assigned to the outcomes of different, mutually exclusive experiments. The difference between quantum and classical physics is the way their physical assumptions augment bare probability theory: Classical physics corresponds to a trivial augmentation— one just applies the Law of Total Probability between the scenarios—while quantum theory makes use of the Born Rule expressed in one or another of the forms of our general procedure. To mark the essential difference between quantum and classical, one should seek the representations that minimize the disparity between the expressions. Using a symmetric informationally-complete measurement (SIC) minimizes this disparity, according to a large family of optimality criteria. This work complements recent studies in quantum computation where the deviation of the Born Rule from the LTP is measured in terms of negativity of Wigner functions.

(Joint work with J. B. DeBrota and C. A. Fuchs, arXiv:1805.08721)

3:30PM V27.00004: A Volume-Maximizing Map from Quantum States to the Probability Simplex, with Applications to QBism* JOHN DEBROTA (Presenter), University of Massachusetts Boston — In this talk, I make use of a recent formulation of quantum theory in terms of minimal informationally complete quantum measurements (MICs) to promote the idea that probability is more central to quantum theory than either state vectors or operators. One advantage of this formulation is that it permits a direct comparison of classical statistical physics with quantum theory via a standard reference measurement. Classically, the possibility of perfect knowledge of a system's phase space point means any vector in the reference probability simplex is an allowable state of knowledge. By contrast, the image of quantum state space under a MIC is necessarily a proper subset of the simplex. This suggests we could take the size of the allowable subset under a given MIC to be a measure of the representation's deviation from classicality. I report work from arxiv:1805.08721, where we prove that this deviation is minimized if and only if the MIC is chosen to be a symmetric informationally complete quantum measurement (SIC)—that is, the SIC representation minimizes the deviation from classicality. Finally, I speculate that this grants the SICs a unique foundational significance. (Joint work with C. A. Fuchs and B. C. Stacey)

*JBD and CAF were supported in part by grant FQXi-RFP-1612.
Noncontextuality inequalities are usually derived from the distinguishability properties of quantum states, i.e. their orthogonality. Here, we show that antidistinguishability can also be used to derive noncontextuality inequalities. Briefly, a set of states can be antidistinguished if there exists a measurement on the basis of which one can exclude one of the states as definitely not having been prepared. The Yu-Oh 13 ray contextuality inequality can be rederived and generalized as an instance of our antidistinguishability method. For qubit systems subjected to unitary gates and projective measurements, we prove that any strategy in our game can be mapped to a strategy in the CHSH game, which implies that Tsirelson's bound also holds in our setting. More generally, we show that the optimal success probability depends on the reversible or irreversible character of the gates, the quantum or classical nature of the system and the system dimension. We analyse the bounds obtained in light of Landauer's principle, showing the entropic costs of the erasure associated with the game. This shows a connection between the reversibility in fundamental operations embodied by Landauer's principle and Tsirelson's bound, that arises from the restricted physics of a unitarily-evolving single-qubit system.
4:30PM V27.00009: Contextuality and the Fundamental Theorems in Quantum Mechanics*  MARKUS FREMBS
(Presenter), Imperial College London — Contextuality is a key feature of quantum mechanics, as was first properly brought to
light by the Kochen-Specker theorem. Isham and Butterfield put contextuality at the heart of their topos-based formalism
and gave a reformulation of the Kochen-Specker theorem in the language of presheaves. Here, we broaden this
perspective considerably (partly drawing on existing, but scattered results) and show that apart from the KS theorem, also
Wigner's theorem, Gleason's theorem and Bell's theorem relate fundamentally to contextuality. The language of
presheaves serves as a useful tool in this and allows to give reformulations of the theorems with a topological-geometric
flavour. Moreover, we show in a mathematically exact way how much of the structure of a quantum system is encoded by
contextuality, and also what is missing.

*This work is funded through a studentship in the Centre for Doctoral Training on Controlled Quantum Dynamics at
Imperial College London funded by the EPSRC.

4:42PM V27.00010: Rank of contextuality  KAROL HORODECKI, Institute of Informatics, National Quantum Information Centre,
Department of Physics, Mathematics and Informatics, University of Gdansk, JINGFANG ZHOU (Presenter), University of Tokyo, PAWEL
HORODECKI, Faculty of Applied Physics and Mathematics, Gdansk University of Technology, ROBERT RAUSSENDORF, Department of
Physics & Astronomy, University of British Columbia, RYSZARD HORODECKI, Faculty of Applied Physics and Mathematics, National
Quantum Information Centre, Gdansk University of Technology, RAVISHANKAR RAMANATHAN, Laboratoire d’Information
Quantique, Universite Libre de Bruxelles, EMILY TYHURST, University of Toronto — We propose a new measure of statistical
Kochen-Specker contextuality, called rank of contextuality. The rank of contextuality is the minimal number of
noncontextual boxes (input-output devices admitting a non-contextual hidden variable model) that are needed to switch
between in order to simulate a contextual box. We show that the logarithm of the rank of contextuality is additive, faithful
measure of contextuality, monotonous under simple wirings. We also provide a construction of contextual boxes with
arbitrary high rank of contextuality, exhibiting thereby extremely high logical contradiction.

4:54PM V27.00011: Perturbative expansion of entanglement negativity*  JESSE CRESSWELL, ILAN TZITRIN (Presenter),
AARON GOLDBERG, Physics, University of Toronto — A common way to quantify entanglement in bipartite systems is through
entanglement negativity. Because negativity is a non-analytic function of a density matrix, existing methods used in
physics literature are insufficient to compute its derivatives. To this end we develop novel techniques in the calculus of
complex, patterned matrices and use them to conduct a perturbative analysis of negativity in terms of arbitrary variations
of the density operator. The result is an easy-to-implement expansion that can be carried out to all orders. On the way we
provide new and convenient representations of the partial transposition map appearing in the definition of negativity. Our
methods are well-suited to study the growth and decay of entanglement in a wide range of physical systems, including the
generic linear growth of entanglement in many-body systems, and have broad relevance to many functions of quantum
states and observables.

*This work is financially supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) and an
Ontario Graduate Scholarship.

5:06PM V27.00012: Near-100% two-photon-like coincidence-visibility dip with classical light and the role of
complementarity  SIMANRAJ SADANA, DEBADRITA GHOSH, KAUSHIK JOARDER, NAGA LAKSHMI A, Raman Research
Institute, BARRY SANDERS, University of Calgary, URBASI SINHA (Presenter), Raman Research Institute — The famous Hong-Ou-
Mandel two-photon coincidence-visibility dip (TPCVD), which accepts one photon into each port of a balanced beam
splitter and yields an equal superposition of a biphoton from one output port and vacuum from the other port, has
numerous applications in photon-source characterization and to quantum metrology and quantum computing.
Exceeding 50% two-photon-coincidence visibility is widely believed to signify quantumness. In this talk, we show
theoretically that classical light can yield a 100% TPCVD for controlled randomly chosen relative phase between the two
beam-splitter input beams and experimentally demonstrate a 99.635 +/- 0.002% TPCVD with classical microwave fields.
We show quantumness emerges via complementarity for the biphoton by adding a second beam splitter to complete an
interferometer thereby testing whether the biphoton interferes with itself: Our quantum case shows the proper
complementarity trade-off whereas classical microwaves fail.
Out-of-time-ordered-correlator quasi-probabilities for the quantum kicked top* JOSE RAUL GONZALEZ ALONSO (Presenter), Chapman University, NATHAN SHAMMAH, RIKEN, SHAHNAWAZ AHMED, Chalmers University of Technology, FRANCO NORI, RIKEN/University of Michigan, JUSTIN G. DRESSEL, Chapman University — The cumulative nonclassicality of the quasi-probability distribution (QPD) behind the out-of-time-ordered correlator (OTOC) exhibits different time scales that have been conjectured to be useful for distinguishing integrable and nonintegrable Hamiltonians (arXiv: 1806.09637). We further investigate the QPD for a quantum kicked top, and use the time scales of its nonclassicality to understand the relationship between entanglement and chaos for different parameter regimes.

*Fellowship from the Grand Challenges Initiative at Chapman University and Army Research Office (ARO) grant No. W911NF-18-1-0178

Thursday, March 7, 2019 2:30 PM - 5:06 PM

Session V28 DQI: Quantum Measurement with Amplifiers and Photon Detectors BCEC 161 -

2:30PM V28.00001: Achieving the Heisenberg limit in quantum metrology using quantum error correction* [Invited] LIANG JIANG (Presenter), Yale Univ — Quantum metrology has many important applications in science and technology, ranging from frequency spectroscopy to gravitational wave detection. Quantum mechanics imposes a fundamental limit on measurement precision, called the Heisenberg limit, which can be achieved for noiseless quantum systems, but is not achievable in general for systems subject to noise. We study how measurement precision can be enhanced through quantum error correction, a general method for protecting a quantum system from the damaging effects of noise. We find a necessary and sufficient condition for achieving the Heisenberg limit using quantum probes subject to Markovian noise, assuming that noiseless ancilla systems are available, and that fast, accurate quantum processing can be performed. When the sufficient condition is satisfied, a quantum error-correcting code can be constructed that suppresses the noise without obscuring the signal; the optimal code, achieving the best possible precision, can be found by solving a semidefinite program.

*We acknowledge support from the ARL-CDQI, ARO, AFOSR, NSF and Packard Foundation.

3:06PM V28.00002: Broadband Amplification and Squeezed Light Generation with Dispersion Engineered Josephson Metamaterial* JACK YANJIE QIU (Presenter), Massachusetts Institute of Technology, KEVIN O’BRIEN, University of California, Berkeley, Massachusetts Institute of Technology, ARNE GRIMSMO, University of Sydney, BHARATH KANNAN, YOUNGYU SUNG, PHILIP KRANTZ, Massachusetts Institute of Technology, GREG CALUSINE, VLADIMIR BOLKHOVSKY, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, Massachusetts Institute of Technology, IRFAN SIDDIQI, University of California, Berkeley, SIMON GUSTAVSSON, Massachusetts Institute of Technology, WILLIAM D OLIVER, MIT Lincoln Laboratory, Department of Physics, Massachusetts Institute of Technology — The generation of highly-squeezed states using superconducting amplifiers is a valuable tool for quantum optics and quantum metrology in the microwave domain. The high saturation power of these devices makes them promising candidates for generating highly squeezed states. In this talk, we present our latest results for operating in non-degenerate four wave mixing with dual dispersion engineered Josephson traveling wave parametric amplifier (JTWPA) and discuss our investigations of the JTWPA squeezing performance.

*This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.
Ideal two-mode phase sensitive quantum amplifier: theory

ANJA METELMANN (Presenter), Dahlem Center for Complex Quantum Systems and Department of Physics, Free University Berlin, OLIVIA LANES, TZU-CHIAO CHIEN, XI CAO, GANGQIANG LIU, CHENXU LIU, DAVID PEKKER, Department of Physics and Astronomy, University of Pittsburgh, JOSE AUMENTADO, Boulder, National Institute of Standards and Technology, MICHAEL HATRIDGE, Department of Physics and Astronomy, University of Pittsburgh, AASHISH CLERK, Institute for Molecular Engineering, University of Chicago — Quantum-limited amplifiers are crucial for the processing of sensitive quantum information in the microwave world. The textbook (phase-sensitive) quantum-limited amplifier is a degenerate parametric amplifier with just a single mode, which comes with the disadvantage of having a fixed gain-bandwidth product and of no separation between input and output ports. One would think that adding a second mode to get separation between these ports would always be detrimental, as one introduces an extra degree of freedom and therewith extra noise. Here, we show this is not the case: one can have a two-mode phase-sensitive amplifier that is ideal with respect to a number of metrics: it has distinct input and output ports, no reflection gain, is quantum-limited and it does not suffer from a gain-bandwidth limit. Consequently it is more robust to pump-depletion effects. In addition, the here presented phase-sensitive amplifier produces squeezed output light with an enhanced bandwidth compared to single-mode squeezing setups. The proposed setup could easily be implemented in a range of different superconducting circuit architectures.

Ideal Two-Mode Phase Sensitive Quantum Amplifier: Experiment*

OLIVIA LANES (Presenter), TZU-CHIAO CHIEN, XI CAO, GANGQIANG LIU, CHENXU LIU, DAVID PEKKER, University of Pittsburgh, ANJA METELMANN, Physics, Freie Universitaet Berlin, AASHISH CLERK, Molecular Engineering, Institute for Molecular Engineering at the University of Chicago, JOSE AUMENTADO, NIST Boulder, MICHAEL HATRIDGE, University of Pittsburgh — Josephson parametric amplifiers, although nearly quantum limited, typically operate in reflection and have a fixed gain-bandwidth product. Recently, there have been both theoretical and experimental efforts to address these shortcomings by combining multiple parametric processes within a single multimode device. In this presentation, we focus on using multiple parametric processes to couple two modes of a Josephson Parametric Converter. We will present data which uses paired, detuned gain processes as well as two separate methods of combining gain and photon conversion, all in the same physical device. All three schemes avoid the fixed gain-bandwidth product of a singly pumped JPC. We will examine their relative bandwidth, efficiency, and saturation power, as well as the prospects for adding further couplings to a third mode to generate directional amplification.

How Hamiltonian non-linearities limit the performance of Josephson parametric amplifiers*

CHENXU LIU (Presenter), TZU-CHIAO CHIEN, MICHAEL HATRIDGE, DAVID PEKKER, Department of Physics and Astronomy, University of Pittsburgh — The implementation of a Josephson Parametric Amplifier with a large saturation power is an essential ingredient in achieving efficient signal detection in superconducting quantum computing circuits. Using numerical evolution of the classical non-linear equations of motion that describe a single non-degenerate gain process in a Josephson Parametric Converter (JPC), we analyze the factors limiting its performance. We demonstrate that the 3rd order coupling between the signal, idler and pump modes effectively generates a complex cross-Kerr term coupling the signal and idler modes, which can limit device saturation. By comparing properties of the full-nonlinear description of the JPC to descriptions truncated at third, fourth, and higher orders we identify which terms limit the device performance and how to optimize them.

Lumped, Single-ended Josephson Parametric Converters for Hamiltonian Engineering*

TZU-CHIAO CHIEN (Presenter), University of Pittsburgh, KATARINA CICAK, FLORENT LECOCQ, NIST-Boulder, OLIVIA LANES, XI CAO, CHENXU LIU, GANGQIANG LIU, DAVID PEKKER, University of Pittsburgh, JOSE AUMENTADO, NIST-Boulder, MICHAEL HATRIDGE, University of Pittsburgh — Quantum-limited parametric amplifiers have become a crucial tool for quantum information processing. However, they have limited bandwidth and saturation power and operate in reflection. We present a design and implementation of a lumped single ended design for the Josephson Parametric Converter (JPC) whose inductance is dominated by the central Josephson Ring Modulator (RM). Implementation of the JPC as a lumped circuit was facilitated by fabrication in a Nb/Al-AlOx/Nb tri-layer process incorporating a low-loss amorphous silicon dielectric. This design allows us to more easily engineer the device's Hamiltonian to control the amplitude of the JRM's three wave mixing terms which provide gain, and control higher order terms to enhance the saturation power and simplify operation as a directional multi-parametric amplifier.

*Work supported by ARO, NSF, and the Kauffman foundation.
4:06PM V28.00007: Quantum nonlinear dynamics of non-degenerate parametric amplification beyond the stiff-pump approximation  SAEED KHAN (Presenter), Princeton University, A. METELMANN, Physics, Freie Universität, HAKAN TURECI, Princeton University — In circuit QED, non-degenerate parametric amplification is commonly realized using Josephson Parametric Converter (JPC) based nonlinear circuits. While such systems are often studied within a linear stiff-pump approximation, their nonlinear dynamics become important for strong input signals, nonlinearity strengths, and large gain operation. We present a theoretical analysis of non-degenerate parametric amplification going beyond this stiff-pump approximation, in particular accounting for the quantum dynamics of the pump mode. Within a regime of weak quantum fluctuations, strongly amplified input signals dominate the depletion of the pump, and the associated compression of amplifier gain is characterized analytically. By further allowing for fluctuations in the pump mode, we find that interactions between the idler-signal subspace and the common pump mode in the nonlinear regime can strongly modify the noise properties of the amplifier. Finally, we analyze nonlinear dynamics in the regime of strong quantum fluctuations. Employing a reduced nonlinear two-mode description enables full quantum simulations in this regime where pump depletion can be strongly influenced by amplified vacuum fluctuations, leading to additional gain compression and added noise.

4:18PM V28.00008: Microwave photo-multiplication based on inelastic Cooper-pair tunneling  ROMAIN ALBERT (Presenter), FLORIAN BLANCHET, CEA Grenoble, DIBYENDU HAZRA, University of Aalto, JUHA LEPPÄKANGAS, Karlsruher Institut für Technologie, SALHA JEBARI, University of Oxford, MAX HOFHEINZ, University of Sherbrooke — When a Josephson junction is embedded in a low impedance circuit Cooper pair transport is usually elastic and the DC voltage across the junction has to be zero to allow for tunneling through the junction. By coupling a DC voltage-biased junction to a microwave circuit, the light-charge interaction enables inelastic charge transport with photon emission or absorption. The nonlinearity of this light-charge interaction can be tuned via the characteristic impedance of the microwave circuit and makes it possible to design sources of non-classical microwave radiation [Westig17, Grimm18], parametric amplifiers [Jebari18] or in our case, a photon multiplier [Leppäkangas18].

By designing particular high impedance electromagnetic environments, processes involving 3 or more photons can become dominant. In this case, we can show that the energy of a tunneling Cooper pair can be used to convert an incoming single photon state into a n-photon Fock state in a different mode. By cascading two of these multiplication stages followed by linear amplification, this device can discriminate itinerant single photon state from vacuum without dead time.


4:30PM V28.00009: A Superconducting Single Microwave Photon Detector Enabled by Dissipation Engineering - Theory*  EMMANUEL FLURIN (Presenter), Quantronics, CEA Saclay, RAPHAEL LESCANNE, LPA, Ecole Normale Superieure, SAMUEL DELEGLINE, LKB, Sorbonne Universités, ZAKI LEGHTAS, centre automatique et systèmes, Mines ParisTech — Superconducting circuits carry microwave photons five orders of magnitude lower in energy than photons of visible light. For their detection, one must bridge the gap between these low energy excitations and signals measurable by standard microwave electronics. In this work, we develop a new class of detectors, based on dissipation engineering, that perform quantum non demolition measurements of travelling microwave wavepackets. We fabricated and measured a single microwave photon detector that imprints on a transmon qubit the passage of a single photon without destroying it. The key advantage of this scheme is its intrinsic robustness against the main decoherence mechanisms found in these circuits, leading to both low dark counts, high detection efficiency and continuous operation, paving the way towards applications in quantum sensing and computing.

*Junior Research Chairs, LabEx ENS ICFP.
A Superconducting Single Microwave Photon Detector Enabled by Dissipation Engineering -
Experiment*  RAPHAEL LESCANNE (Presenter), LPA, Ecole Normale Superieure, EMMANUEL FLURIN, Quantronics, CEA Saclay, SAMUEL DELEGLISE, LKB, Sorbonne Université, ZAKI LEGHTAS, Centre Automatique et Systèmes, Mines ParisTech —
Superconducting circuits carry microwave photons five orders of magnitude lower in energy than photons of visible light. For their detection, one must bridge the gap between these low energy excitations and signals measurable by standard microwave electronics. In this work, we develop a new class of detectors, based on dissipation engineering, that perform quantum non demolition measurements of travelling microwave wavepackets. We fabricated and measured a single microwave photon detector that imprints on a transmon qubit the passage of a single photon without destroying it. The key advantage of this scheme is its intrinsic robustness against the main decoherence mechanisms found in these circuits, leading to both low dark counts, high detection efficiency and continuous operation, paving the way towards applications in quantum sensing and computing.

Detecting single-Infrared-photon by graphene Josephson junction*  KIN CHUNG FONG (Presenter), BBN Technologies, EVAN WALSH, MIT, GIL-HO LEE, POSTECH, DMITRI K. EFETOV, ICFO, WOO-CHAN JUNG, POSTECH, KO-FAN HUANG, Harvard University, THOMAS A OHKI, BBN Technologies, PHILIP KIM, Harvard University, DIRK R. ENGLUND, MIT — Single-photon detector is a key enabling technology in quantum information processing, cryotography, and deep space communication. However, detecting low frequency photons is challenging because of their vanishingly small energy. Here we will present the concept of a graphene-based Josephson junction single-photon detector that can potentially perform in a wide electromagnetic spectrum. We will focus on our experimental results of the Josephson junction switching induced by single-infrared-photon. We will conclude by its applications in quantum information science, radio astronomy, as well as dark matter detection.

Thursday, March 7, 2019 2:30 PM - 5:30 PM
Session V29 DQI: Hybrid Systems: Coupling to Ensembles and Single Electrons in Helium

Broadband electron spin resonance spectroscopy with a superconducting resonator, Part 1: Theory*  JEROME BOURASSA (Presenter), Département des Sciences de la Nature, Cégep de Granby, GREGORY BROOKES, Institut quantique and Département de Physique, Université de Sherbrooke, DANY LACHANCE-QUIRION, Research Center for Advanced Science and Technology, The University of Tokyo, DAVID ROY-GUAY, RAPHAËL LAFOND-MERCIER, Institut quantique and Département de Physique, Université de Sherbrooke, LÉO DESORMIERS, VINCENT BONNEAU, Département des Sciences de la Nature, Cégep de Granby, MICHEL PIORO-LADRIERE, Institut quantique and Département de Physique, Université de Sherbrooke — Electron spin resonance (ESR) spectroscopy is a useful tool for characterizing spin defects relevant to quantum technologies. Typical ESR systems are based on a resonant exchange interaction between the spins and a high-Q resonant cavity or resonator. While sensitive, the small magnetic-dipole coupling strength limits the ESR detection bandwidth in the dispersive regime and alternative coupling strategies must be used. One such strategy is to rely instead on a longitudinal interaction where the spin magnetization directly influences the resonator frequency, irrespective of the spin transition frequency.

In this talk, we show how we can realize such broadband spectroscopy of spin systems using high-kinetic-inductance superconducting resonators. We demonstrate that the longitudinal interaction is dominated by spins close to the resonator surface and discuss how the coupling strength and detection sensitivity can be optimized. This analysis paves the way towards a broadband ESR spectrometer suitable for novel quantum materials, as well as numerous other applications in chemistry, biology and material sciences.

*This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund and the Institut Transdisciplinaire de Recherche en Information Quantique.
We report experimental evidence of this longitudinal spin-resonator interaction where the resonator is affected by the spins polarization for detunings between the spin and the resonator larger than 1 GHz, where the contribution of the dispersive interaction is vanishing. In the specific implementation, numerical simulations show that the main contributions come from near-surface spins. This novel coupling can lead to new characterization tools and methods of quantum defects, complex quantum materials and many other paramagnetic systems.

*This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund and the Institut Transdisciplinaire de Recherche en Information Quantique.

References

Superradiant emission from colour centres in diamond

Superradiance is a fundamental collective effect where radiation is amplified by the coherence of multiple emitters. Superradiance plays a prominent role in optics (where it enables the design of lasers with substantially reduced linewidths) and quantum mechanics, and is even used to explain cosmological observations such as Hawking radiation from black holes. Superradiance plays a prominent role in optics (where it enables the design of lasers with substantially reduced linewidths) and quantum mechanics, and is even used to explain cosmological observations such as Hawking radiation from black holes.5. Resonators coupled to spin ensembles are promising future building blocks of integrated quantum devices that will involve superradiance. As such, it is important to study its fundamental properties within such devices. Although experiments in the strong-coupling regime have shown oscillatory behaviour in these systems, a clear signature of Dicke superradiance has so far been missing. Here we explore superradiance in a system composed of a three-dimensional lumped element resonator in the fast cavity limit inductively coupled to an inhomogeneously broadened ensemble of nitrogen–vacancy centres. We observe a superradiant pulse being emitted a trillion times faster than the decay for an individual nitrogen–vacancy centre. This is further confirmed by the nonlinear scaling of the emitted radiation intensity with respect to the ensemble size. Our work provides the foundation for future quantum technologies including solid-state superradiant masers.
4:06PM V29.00006: Electron spin hyperpolarization via radiative cooling  BARTOLO ALBANESE (Presenter), SEBASTIAN PROBST, VISHAL RANJAN, DENIS VION, EMANUEL FLURIN, DANIEL ESTEVE, Quantronics, SPEC, CEA-Saclay, JOHN MORTON, University College London, GENGLI ZHANG, REN-BAO LIU, Chinese University of Hong Kong, PATRICE BERTET, Quantronics, SPEC, CEA-Saclay — Electron spin resonance (ESR) spectroscopy is widely employed for the detection and characterization of paramagnetic species [1]. A high degree of spin polarization is essential to maximize the signal. Here, we are interested in increasing the polarization beyond thermal equilibrium. Techniques such as optical pumping are available only for systems with special electronic structures. In the present work we give a proof of principle of a new universal hyperpolarization scheme based on the coupling of the electron spins to a colder electromagnetic bath via Purcell-enhanced radiative relaxation. A superconducting micro-resonator is used in order to reach the regime in which radiative relaxation constitutes the dominant mechanism of spin thermalization [2]. The spin system under study is an ensemble of bismuth donors implanted into a host silicon crystal. The sample is installed at the 800 mK stage of a dilution cryostat while the resonator is coupled via a switch either to a 10 mK or to a 800 mK thermal source. When the switch is connected to the colder black body, the electronic spins are cooled via radiative relaxation while the silicon crystal remains at 800 mK. [1] A. Schweiger and G. Jeschke, Oxford University Press (2001) [2] A. Bienfait et al., Nature 531, 74-77 (2016)

3:54PM V29.00006: Coherent spin-wave excitations in an optically cooled nuclear ensemble  DORIAN GANGLOFF (Presenter), GABRIEL ETHIER-MAJCHER, CONSTANTIN LANG, University of Cambridge, EMIL VOSMAR DENNING, Photonics Engineering, Technical University of Denmark, JONATHAN BODEY, DANIEL JACKSON, CLAIRE LE GALL, METE ATATURE, University of Cambridge — Collective excitations of isolated many-body systems offer the opportunity to control complex quantum dynamics. A simple quantum system, such as a central spin, can act as a probe and a control over a larger and more complex quantum system in ways otherwise intractable, and can help us perform spectroscopy and engineering over its quantum dynamics. Driving the central spin can stimulate exchange of energy with its surrounding spins, and thus modify the mean-field state of its own environment. In this work, we engineer this very interaction between an InGaAs quantum dot electron spin and its isolated ensemble of nuclear spins in a driven-dissipative regime to remove entropic heat from the ensemble, and so vastly reduce the mean-field state uncertainty tied to its thermal fluctuations. Having cooled the system, we reveal an absorption spectrum of transitions between many-body states that are collectively-enhanced by the creation of single spin-wave excitations – nuclear magnons. Resonantly driving such a transition, we stimulate coherent exchange of single magnons between the electron and the nuclear spin ensemble, which is consistent with the controlled creation of entanglement among all constituent particles.

4:06PM V29.00006: High-Q Superconducting Mm-wave Cavities for Rydberg Cavity Quantum Electrodynamics.*  AZIZA SULEYMANZADE (Presenter), ALEXANDER ANFEROV, MARK STONE, JONATHAN SIMON, DAVID SCHUSTER, University of Chicago — We will outline our progress towards a cryogenic hybrid experimental system for engineering strong interactions between single optical and mm-wave photons using Rydberg atoms as an interface. Bulk 3D cavities in the microwave regime routinely reach quality factors above 10^7 at single photon powers and even in some case as high as 10^10. At the same time there has been far less study of resonators at millimeter wave frequencies close to 100GHz. We present experimental results of superconducting fundamental mode niobium cavities at 100GHz, with quality factors exceeding 10^7. We will also present experiments showing tuning the cavity frequency in-situ, to be able to exactly match Rydberg transitions.

*MURI, MRSEC

4:18PM V29.00008: Accessing Nonlinearity in Superconducting Millimeter Wave Coplanar Resonators*  ALEXANDER ANFEROV (Presenter), AZIZA SULEYMANZADE, JONATHAN SIMON, DAVID SCHUSTER, University of Chicago — Current superconducting quantum systems rely on ultra-cold temperatures to reduce sources of noise and quantum decoherence. While many advances have been made in the purification and refinement of quantum devices in the low microwave frequency range, millimeter frequencies have been far less explored. Using higher energy photons as a building block could potentially allow quantum experiments to be run faster, at higher temperatures, and easily access other high frequency quantum systems, such as Rydberg atoms. We use superconducting thin film materials to fabricate resonators with planar geometries to ensure scalability and direct compatibility with other elements in the superconducting quantum toolbox, while gaining a natural increase of kinetic inductance based nonlinear effects with frequency. Here, we present and characterize low-loss millimeter wave resonators with planar geometries exhibiting nonlinear behavior, demonstrating a scalable core component for a new generation of high frequency quantum devices.

*This work was supported by ARO Grant No. W911NF-15-1-0397
Support was provided by the Chicago MRSEC, which is funded by NSF through grant DMR-1420709
**4:30PM V29.00009: Coupling a single electron on helium to a superconducting resonator**

GERWIN KOOLSTRA (Presenter), GE I YANG, DAVID SCHUSTER, University of Chicago — Electrons on helium is a unique two-dimensional system on the interface of superfluid He-4 and vacuum. Both the motional state and spin state of a single electron on helium have been proposed as candidates for long-lived qubits. To trap a single electron on helium, we use a small electrostatic trap located at the voltage anti-node of a superconducting microwave resonator. By adjusting the trap potential we are able to consistently load between one and four electrons and detect their spectroscopic features through the resonator. In particular, in the single electron regime a large resonator frequency shift reveals when the electron motional frequency is resonant and allows us to extract an electron-photon coupling of ~ 10 MHz. I will highlight our latest experiments leading towards the development of an electron on helium qubit.

*Support was provided by the Chicago MRSEC, which is funded by NSF through grant DMR-1420709 and the DOE Office of Basic Energy Sciences*

**4:42PM V29.00010: Thermopower based hot electron thermometry of helium surface states at 1.6 K**

ETHAN KLEINBAUM (Presenter), STEPHEN APLIN LYON, Princeton University — Inelastic scattering processes are crucial for understanding and describing a wide variety of phenomena observed in surface state electrons (SSE) on helium including non-linear transport and microwave absorption line shapes. Further interest in inelastic scattering has been motivated by the relevance to coherence times of Rydberg state based SSE qubits. Despite their fundamental importance, relatively little experimental work have examined inelastic processes which can be attributed to challenges associated with electron thermometry of hot SSE.

We have developed a method to probe SSE temperature using the Seebeck effect. We demonstrate the use of this technique by measuring SSE temperature as a function of applied power at a bath temperature of 1.6 K in a microchannel device with 0.6 μm deep helium. We compare our measurements to the predictions for both vapor atom and 2-ripplon scattering in the single electron regime. Our measurements demonstrate a strong qualitative agreement with the predictions and we attribute small quantitative discrepancies to many body effects. We conclude that this technique provides a reliable and flexible measure of electron temperature.

*This research was supported by the NSF (Grant No. DMR-1506862).*

**4:54PM V29.00011: Phase transitions in a strongly interacting electron system under confinement**

NIYAZ BEYSENGULOV (Presenter), Michigan State Univ, DAVID G REES, Cryogenic Ltd., London, United Kingdom, MIKHAIL ZAKHAROV, Institute of Physics, Kazan Federal University, Kazan, Russia, YURIII LYSOGORSKIY, ICAMS, Ruhr-Universitat Bochum, Bochum, Germany, KIMITOSHI KONO, Department of Electrophysics, National Chiao Tung University, Hsinchu 300, Taiwan, DMITRII TAYURSKII, Institute of Physics, Kazan Federal University, Kazan, Russia — Phase transition in a two-dimensional lattice is described by a Berezinskii-Kosterlitz-Thouless (BKT) mechanism. At low temperatures the ground state of strongly interacting 2D electron system is a Wigner solid, which was experimentally observed in a many experiments with electrons on the surface of liquid helium. A well controlled system of electrons on liquid helium provide an excellent platform to investigate a many-body phenomena. Here we investigate the influence of a quasi-one-dimensional confinement on the structural order and melting of electrons on helium experimentally and by numerical simulations. In the experiments electrons are confined by electrostatic potential in a microchannel structures. By tuning voltages on gate electrodes we were able to demonstrate the control of number of electron rows (from a single chain up to 25 rows). We show that for small number of rows gamma parameter (the ratio of Coulomb energy to thermal energy) is suppressed, while for large number of rows a BKT theory prediction is recovered. We compare the results with molecular dynamics simulations. The temperature dependence of topological defects density, translational correlation function and structure factor were calculated and discussed in the context of BKT transition.
5:06PM V29.00012: Transport measurements of electrons above shallow helium-filled microchannels

ABRAHAM ASFAW (Presenter), ETHAN KLEINBAUM, STEPHEN APLIN LYON, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, USA — The spins of electrons floating on superfluid helium constitute a promising platform for quantum computation. Quantum devices for electrons on helium, such as electrostatically defined quantum dots, require gate electrodes that are patterned beneath thin helium films. This can be particularly challenging at helium depths below 1 μm, since the electrons can be trapped by potential fluctuations on the surface of the gate electrode resulting from surface roughness and variations in the work function.

In this talk, we report transport measurements of electrons on helium in a microchannel device where the channels are 200 nm deep and 3 μm wide. The channels are fabricated above amorphous metallic TaWSi, which has surface roughness below 1 nm and minimal variations in work function across the surface due to the absence of polycrystalline grains. We are able to set the electron density in the channels using a ground plane, obtaining electron densities as high as $2.56 \times 10^9$ cm$^{-2}$. We also demonstrate control of the transport using a barrier which enables pinchoff at a central microchannel connecting two reservoirs. The mobility of electron transport through the central microchannel is at least 300 cm$^2$/Vs.

*This research was supported by the NSF (Grant Nos. DMR-1506862 and DMR-1420541).

5:18PM V29.00013: Acoustoelectric transport of electrons on helium

HEEJUN BYEON (Presenter), KOSTYANTYN NASYEDKIN, JUSTIN LANE, NIYAZ BEYSENGULOV, REZA LOLOEE, JOHANNES POLLANEN, Michigan State Univ — We report on the acoustoelectric transport of electrons on helium induced by coupling to piezoelectric surface acoustic waves (SAWs). In our device, the SAWs propagate along the surface of a lithium niobate piezoelectric crystal that is submerged beneath a thin layer of superfluid $^4$He. Electrons are deposited onto the superfluid and float ~10 nm above its surface. When SAWs propagate along the lithium niobate substrate, electrons are trapped in the moving electric potential of the SAW and transported across the device at the speed of the piezoooustic wave. Electrodes positioned beneath the lithium niobate capacitively couple to the electrons and are used to detect acoustoelectric transport. We have performed time and frequency domain measurements and analysis to characterize the electric current dragged along by the SAW. To our knowledge, these measurements constitute the first demonstration of acoustoelectric charging pumping of electrons on helium.

**This work is supported by the NSF (Grant no. DMR-1708331).

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V31 DCP: Surfaces and Adsorbates (SA) BCEC 203 - Silvina Gatica, Howard University - Tag(s): Focus

2:30PM V31.00001: TBD [Invited] SVETLANA MINTOVA (Presenter), University of Caen, France — TBD

3:06PM V31.00002: Methane Adsorption on Zeolitic Imidazolate Framework -8 (ZIF-8) DINUKA HAR GALLABA (Presenter), ALDO DANTE MIGONE, Department of Physics, Southern Illinois University Carbondale — Zeolitic Imidazolate frameworks (ZIFs) are porous Metal Organic Framework materials that have zeolite-like structures. ZIF -8 has shown structural transition when adsorbing gas molecules, this leads to increment in loading. This has been previously observed with N$_2$, CO, O$_2$ and Xe adsorption. Adsorption studies of energy related gasses are great significant to the petroleum and automotive industries. Among those gasses methane is a good alternative to petroleum based fuels. We present the results of an experimental study of methane sorption in ZIF-8. We measured isotherms at five different temperatures between ~ 85 K and 107 K. We have observed three sub-steps in each of the isotherms. The intermediate sub-step had not been observed experimentally in previous studies of this system. We measured a sharp increase in the equilibration times at loadings corresponding to the intermediate sub-step in the isotherms. We have explored the isosteric heat of adsorption, and its dependence on sorbent loading, for this system.
3:18PM V31.00003: Improving the Adsorption Selectivity of CO₂/CH₄ by Strength, Shape and Kinetics*  
SILVINA GATICA (Presenter), Physics and Astronomy, Howard University — Gas separation by adsorption can be accomplished by three basic physical mechanisms: equilibria, kinetics, and steric effects. Equilibrium mechanisms rely on the strength of attraction between gas molecules and their substrate. For example, the interaction of CO₂ with a substrate is usually stronger than methane-substrate. As a result, the equilibrium mechanism presents a plausible strategy to separate carbon dioxide from mixtures. We have studied the adsorption of CO₂/CH₄ mixtures on various substrates by Monte Carlo and Molecular Dynamics simulations. Our findings show that on substrates including MOFs, carbon nanohorns and graphene, the selectivity of adsorption of CO₂/CH₄ at room temperature is low (near 1). We explore the kinetics and steric effects on the selectivity, finding that the combination of the three above-mentioned mechanisms can significantly boost the CO₂/CH₄ separation at 300K. In this talk, I will present a review of the various cases studied.

*This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

3:30PM V31.00004: Hydrogen Adsorption on Pt(111) Revisited from Random Phase Approximation  
LEI YAN (Presenter), Institute for Solid State Physics, The University of Tokyo, YANG SUN, Global Research Center for Environment and Energy Based on Nanomaterials Science, National Institute for Materials Science, YOSHIYUKI YAMAMOTO, SHUSUKE KASAMATSU, Institute for Solid State Physics, The University of Tokyo, IKUTARO HAMADA, Global Research Center for Environment and Energy Based on Nanomaterials Science, National Institute for Materials Science, OSAMU SUGINO, Institute for Solid State Physics, The University of Tokyo — It is generally believed that H is predominantly adsorbed on the fcc site of Pt(111), as supported by the calculations using density functional theory (DFT) within generalized gradient approximation (GGA). Experiments, however, observe the signal from the top site. Similar problem exists in CO/Pt(111), where GGA is known to wrongly predict the fcc site as the most stable site, for which a correct answer was given recently using a more advanced correlation functional called random phase approximation (RPA). Here we attack this H/Pt(111) problem using DFT-RPA [1]. By using DFT within the exchange-correlation functionals of different level, we evaluate the stability of fcc adsorption site relative to the top site. The most advanced one based on the RPA, is found to revise our knowledge so far derived from the conventional functionals. Two adsorption sites are hereby found to compete sensitively depending on lattice spacing of the surface, mass of the hydrogen isotope, and hydrogen coverage. The revised knowledge provides natural explanation for the controversy regarding the electrochemical and spectroscopic data, giving impact on the research on the fuel-cell reaction mechanism.


3:42PM V31.00005: ADSORPTION OF PHENOL IN ZEOLITES: MULTI-TECHNIQUE MODELING  
HICHAM JABRAQUI (Presenter), University of Lorraine, GUILLAUME MAURIN, Institut Charles Gerhardt Montpellier (ICGM), Université de Montpellier, SÉBASTIEN LEBÈGUE, University of Lorraine, IBRAHIM KHALIL, KARINE THOMAS, FRANCOISE MAUGÉ, Université de Caen Normandie, MICHAEL BADAWI, University of Lorraine — Protonated zeolites were explored as effective adsorbent materials for removing phenol from biofuels using multi-scale modeling. Here, we used a powerful combination of the multiple modeling techniques: i) Density Functional Theory (DFT) [1],[2] allows to determine binding energies of several configurations of guest molecule in zeolites ii) Grand Canonical Monte Carlo (GCMC) [3],[4] shows how much molecules can zeolite hold, i.e. the adsorption capacity as intermolecular interactions at high loading, iii) ReaxFF Molecular Dynamics (RFF-MD) [5] allows knowing both the mobility of molecules within the zeolite framework, and the structure of molecule-loaded faujasite. The obtained results are compared with those measured by different experimental tools (Infrared Spectroscopy, breakthrough curves, and desorption experiments). We will show that USY zeolites provide a good regenerability of the zeolites as a high adsorption capacity.

References
3:54PM V31.00006: Adsorption and Separation of CO2 and CH4 Gas Mixture in a Graphene Layer and a Graphite Surface* HIND ALJADDANI (Presenter), SILVINA GATICA, Howard University — The goal of this work is to predict the selective adsorption of CO2 from a mixture with CH4 on a graphene/graphite substrate. The substrate consists on a layer of graphene with slits suspended on top of graphite at a distance of 10 Å. Molecular dynamics was used to simulate this adsorption. In this system, methane is modeled as a single, spherical atom with one Lennard-Jones site. Carbon dioxide is modeled as a linear rigid body with three Lennard-Jones sites and three partial charges. The slits in graphene are made by deleting carbon atoms from the lattice within a region of specified width. Graphite is modeled as a 10-4-3 wall. We run the simulations at 300K and compare the selectivity of CO2/CH4 on the substrate to test the capability of the graphene/graphite to separate CO2 from CH4. The result shows that the selectivity is higher for narrow slits.

*This work is supported by King AbdulAziz University.

4:06PM V31.00007: Impact of nuclear vibrations on van der Waals interactions and radiative heat transfer in graphene PRASHANTH VENKATARAM (Presenter), Princeton University, JAN HERMANN, University of Luxembourg, TEERIT VONKOVIT, Princeton University, ALEXANDRE TKATCHENKO, University of Luxembourg, ALEJANDRO RODRIGUEZ, Princeton University — We apply a recent theoretical framework describing thermal and quantum electromagnetic phenomena arising from the coupling of photons and phonons in molecular systems, including van der Waals interactions and radiative heat transfer, to interactions among parallel sheets of neutral graphene and metallic substrates. In particular, we show that atom-scale features as well as contributions of phonons to the response of graphene, as captured in ab-initio density functional theory calculations, along with long-range retarded electromagnetic fields, are of utmost importance to describing its van der Waals interactions and radiative heat transfer over a broad range of length scales; interactions no longer behave as simple power laws in terms of surface separation and show noticeable temperature sensitivity at separations well below the micron-scale radiative thermal wavelength. The contributions of phonons and atom-scale effects to the response are largely neglected in continuum treatments of the electromagnetic response of neutral graphene, which typically consider only the electronic contributions to the response derived from a tight-binding model; consequently, we observe significant differences in the predictions of our microscopic framework from such macroscopic treatments.

4:18PM V31.00008: Pseudo-Palladium alloys for catalytic applications* MIKAEL RÅSANDER (Presenter), J. ANDREAS LARSSON, Department of Engineering Sciences and Mathematics, Luleå University of Technology — Palladium is a commonly used catalyst for the formation of C-C, C-O and C-N bonds in pharmaceutical manufacturing. However, Palladium is expensive which results in high production costs. In this project, we have used computational modelling based on density functional theory to search for possible combinations of elements which mimic the behavior of Palladium in order to lower the cost of production. We have investigated both bulk as well as nanoparticles of, e.g., Rh0.5Ag0.5, Pd1-xCu x and Pd1-xAgx alloyed systems and found that these systems have Palladium-like electronic properties and are therefore expected to have similar catalytic properties as pure Palladium. The Pd1-xCu x and Pd1-xAgx systems have Palladium-like electronic structures up to about 25% Cu or Ag, respectively.

*This work was supported by Eli Lilly and Company through the Lilly Research Award Program. We also acknowledge support from the KAW and Kempe foundations, as well as computational resources provided to us by the Swedish National Infrastructure for Computing (SNIC).

4:30PM V31.00009: Influence of inter-crystalline space on diffusion in zeolites: A molecular dynamics investigation* ANGELA THOMAS (Presenter), YASHONATH SUBRAMANIAN, Indian Institute of Science — Understanding the difference in diffusivities of guest molecules in zeolites obtained from different techniques has always been a challenge. The diffusivity values, $D_{\text{P}}$, measured using methods like uptake or PFG-NMR are often smaller by several orders of magnitude than those measured using methods like QENS or MD simulations. In order to understand the underlying reason for this reduction in $D_{\text{P}}$, molecular dynamics simulations of xenon atoms have been carried out in zeolite systems where an inter-crystalline space is introduced along the x-axis. It is seen that the $D_{\text{P}}$ in these systems are significantly altered by the presence of the inter-crystalline space and the value is smaller compared to the other axes, which reduces the total effective $D_{\text{P}}$ when compared to a purely intra-crystalline diffusion. Interestingly, in the intercrystalline space, $D_{\text{P}}$ along y- and z-axes are higher and exhibit ballistic motion. Diffusion measurement techniques of shorter timescales (QENS or MD) generally obtain $D_{\text{P}}$, which are higher as the guest molecules sample intra-crystalline space during these timescales, while in longer timescale methods (e.g., PFG-NMR or uptake) guests manage to sample both the intra- and inter-crystalline space leading to lower values for diffusivities.

*TUE-CMS by DST, India
4:42PM V31.00010: Theoretical Studies of Activation Energies and Pre-Exponential Factors of Alcohol Dehydrogenation on Cu*  WEI CHEN (Presenter), ROBERT J. MADIX, CYNTHIA M. FRIEND, EFTHIMIOS KAXIRAS, Harvard University — We study the thermodynamic and kinetic processes involved in the anhydrous dehydrogenation of linear-chain alcohols on the Cu(110) surface using multiscale approaches. We determine the kinetic barriers for the two dehydrogenation steps, namely, the O–H and the subsequent C–H bond-breaking on Cu. The reaction of methoxy-to-formaldehyde has a rather high-energy transition state, in contrast to that of alkoxide-to-aldehyde in the longer-chain systems. This difference qualitatively explains the lower production efficiency of formaldehyde on Cu. We also use a Monte Carlo sampling to calculate the entropies of initial and transition states. The estimated pre-exponential factors, beyond the harmonic approximation, are found to have a molecular size dependence.

*This work was supported by the Integrated Mesoscale Architectures for Sustainable Catalysis, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0012573.

4:54PM V31.00011: Kinetics of ligands mediated ultra-small silver cluster formation. MOHSEN FARSHAD (Presenter), DYLAN SUVLU, JAYENDRAN C RASAIAH, University of Maine — We discuss a kinetic mechanism that predicts different average size distributions of silver clusters with peak diameters around 0.7 nm and 1.2 nm in solution depending on the initial conditions in a redox reaction. Nanoparticle growth occurs through ligand addition and elimination followed by irreversible dimerization and reversible ligand-monomer addition to the seed cluster. We have also incorporated the coalescence of clusters which can dominate the growth of silver nanoparticles in the presence of a strong reductant. Our calculations provide further insight into the mechanistic details of ultra-small silver cluster formation from an atomic perspective.

5:06PM V31.00012: Boron-doped silicene as a promising anode for Li-ion batteries* ALEX CHEN (Presenter), XUAN LUO, National Graphene Research and Development Center — Two-dimensional (2D) materials as electrodes are the trend for future Li-ion battery technology. By using first-principles calculations, we investigate the adsorption of Li-ions on boron-doped silicene as a potential electrode material. We identified the most stable adsorption sites and their corresponding adsorption energies for the adsorption of Li adatoms on the doped silicene. Then, we increase the ion concentration to examine the impact of Li-ions on the stability and structure of the material. With Bader charge analysis, we confirm the charge transfer from the Li-ion to doped silicene and use that to calculate a high specific capacity for the B-doped silicene. We then used the nudged elastic band method to analyze the energy barriers of Li-ion diffusion along the surface and through the hexagonal hollow of the monolayer. Our findings reveal the potential application of B-doped silicene as an electrode material in lithium batteries.

*This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

5:18PM V31.00013: Direct Determination of the Thermodynamic Properties of Melting for Amino Acids* YEONG ZEN CHUA (Presenter), AMIR ABDELAZIZ, DZMITRY ZAITSAU, SERGEY VEREVKIN, University of Rostock, CHRISTOPH HELD, TU Dortmund University, CHRISTOPH SCHICK, University of Rostock — The properties of melting are used for the prediction of solubility of solid compounds. Unfortunately, by using the conventional DSC or adiabatic calorimetry direct determination of the melting enthalpy and melting temperature is often not possible for biological compounds due to the decomposition during the measurement. The apparent activation energy of decomposition is at least one order of magnitude smaller than that of melting. This allows shifting of the decomposition process to higher temperature without seriously disturbing the melting by applying very high heating rates. High scanning rates up to 2×10^4 K s^{-1} are utilized with fast-scanning calorimeter Mettler Toledo Flash DSC1, which employs thin film chip sensors with sub µJ K^{-1} addenda heat capacities. With the help of this technique the melting parameters for a series of amino acids were successfully determined. The ultra-fast cooling of the melted samples allows the studied compounds to retain in the liquid state and to determine for the first time its glass transition temperatures. The results are in reasonable agreement with the simulated PC-SAFT values.

*Deutsche Physikalische Gesellschaft CH1922/1-1

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V34 FIAP: Innovations from Industry BCEC 205A - Steven Lambert, American Physical Society - Tag(s): Careers, Industry, Invited, Undergraduate
2:30PM V34.00001: Innovations from Texas Instruments Inc. DLP® Products Division: M7 – MEMS Mirrors Moving in Many Modes for a Multitude of Markets [Invited] PATRICK ODEN (Presenter), DLP(R) Products Division, Texas Instruments Inc. — For nearly a quarter century of commercial manufacturing, the Microelectromechanical Systems (MEMS)-based micro-mirrors produced by Texas Instruments Inc. have, by necessity, needed to innovate to stay relevant to various market demands. The highlights of which will be addressed here as well as a discussion of potential innovations to come. I will also share my thoughts on how Physicists trained in solid-state, surface-science, like myself, can contribute to the future of this technology.

3:06PM V34.00002: Next Generation Technology from Google AI Quantum [Invited] ALAN HO (Presenter), Google Inc., Santa Barbara — Alan Ho, product manager from Google AI Quantum, will provide an overview of recent hardware, algorithms, and software developments at Google. He will first provide an overview of Google's superconducting qubits, and highlight the differences between its digital and analog computing architectures. For software, Alan will give an overview of its recent progress on its open source packages - Cirq and OpenFermion, and how physicists can get started to programming a quantum computer.

Alan will also review collaboration research and funding opportunities at Google. He will provide an overview of recent academic partnerships and government partnerships, and the research that has resulted from it. He will also discuss funding opportunities at Google including Ph.D fellowships, internships, Faculty and Focus Award grants. Finally, he will then provide information on how physicists can get access to Google’s experimental hardware.

3:42PM V34.00003: The Economic Impact of Industrial Physics on the U.S. Economy: What value we physicists bring to economic activity [Invited] JOHN RUMBLE (Presenter), R&R Data Services — The American Physical Society, with support from the American Institute of Physics, recently sponsored an in-depth analysis of the impact of industrial physics on the U.S. economy. This report attempts to provide quantitative answers to the specific question: How does industrial physics impact the economy of the United States? Posing the question this way allows us to consider the four major ways that physics contributes to the economy: (1) The direct hire of college-trained physicists of all degrees; (2) Physics as an essential element in the training of scientists and engineers who work in industry; (3) The use of physical principles in the technology that creates products and services; and (4) The emergence of new physics that drives disruptive changes to the economy. The study shows that in 2016 an estimated 12.6% of the U.S. economy (2.3 trillion dollars) with direct employment of about 11,500,000 people can be ascribed directly to the practice of industrial physics. In this talk, the complete results are presented with a discussion of economic analysis methodology and the assumptions made. We provide concrete data on the creation of jobs, investments in the future, and the impact on tax receipts in the period from after World War II to the present day (2016). We present evidence of the creativity that physics brings to industry and the economy, as well as draw conclusions on why this has happened. The data confirm what we inherently know from our knowledge of modern physics – that since the end of World War II, physics discoveries of the twentieth century have been transformed by industrial physicists into incredible products and services. The flow of physics into industry is neither stopping, nor even slowing down as new disruptive products and services continue to emerge. We provide recommendations for academia, industry, government funding agencies and APS itself about how they can support industrial physics in the future.

4:18PM V34.00004: How IBM Research is Enabling the Internet of Things [Invited] HEIKE RIEL (Presenter), Thomas J. Watson Research Center, IBM — TBD
Invited] ALEXANDER JOHN MAJEWSKI (Presenter), United Technologies Research Center — A career path in industry focuses on various products and applications and requires an in-depth knowledge of physics as well as system phenomenology. One topical area of particular interest in industry is sensors. Optical sensors are a broad class of devices for detecting light amplitude, intensity and/or phase. These sensors can range from simple devices (detectors) for threshold detection or a highly complicated system for detecting single photons, measuring the phase variation (wave-front) of an optical system, or a spectrometer used in characterizing the spectral signature of a material.

Optical sensing can encode photons – either through intensity and/or phase, in a temporal and/or spatial manner; e.g. interferometers. These optical sensors and sensing techniques are used in various optical systems with widespread applications in instrumentation, signal processing, spectroscopy, and imaging. They present many design and performance challenges: knowledge of optical, material, and environmental properties that effect sensor performance.

Optical sensors range from micro-probes to large devices used for standoff monitoring and operate across a vast region of the electromagnetic spectrum, from THz to X-rays and are deployed on systems operating in environments from ground to space. An overview of optical sensors and systems with an example of THz chemical detection spectrometers will be presented.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V35 DQI: Materials and Fabrication for Superconducting Qubits

2:30PM V35.00001: A New Technique to Measure Microwave Dielectric Material Loss* KAICHEING LI (Presenter), CHRISTOPHER J AXLINE, LUKE BURKHART, BENJAMIN CHAPMAN, CHAN U LEI, VIJAY JAIN, LEV KRAYZMAN, PHILIP REINHOLD, LUIGI FRUNZIO, ROBERT J SCHOELKOPF, Yale Univ — Qubit coherence time is essential in quantum computation, since, in tandem with gate speed, it governs the number of coherent operations one can eventually perform on a quantum computer. In the field of circuit quantum electrodynamics, a qubit is often formed by the non-linearity of a Josephson junction fabricated on a dielectric substrate. Therefore, any dielectric loss in the substrate can be an important contribution to qubit coherence. Indeed, recent studies suggest that among different qubit loss channels dielectric loss may be a substantial one. In this talk, we describe a sensitive method to selectively measure microwave dielectric substrate loss and present preliminary measurements with the technique.

*This research is supported by US Army Research Office grant W911NF-18-1-0212 and W911NF-16-1-0349, and Air Force Office of Scientific Research grant FA9550-15-1-0015.

2:42PM V35.00002: Atomic defects in silicon compared with standard two-level defects LIUQI YU (Presenter), Laboratory for Physical Sciences, College Park, MD, Y. J. ROSEN, Lawrence Livermore National Laboratory, Livermore, CA, KEVIN DANIEL OSBORN, Laboratory for Physical Sciences, College Park, MD — Atomic two-level systems (TLSs) in materials affect the performance of superconducting quantum devices and new fundamental studies are needed to better understand them. It was found\(^1\)\(^2\) that the TLS bath, initially saturated by the microwave field excitations, can undergo adiabatic transitions when an additional sweeping fields is applied. Although more TLSs would remain in the ground state, the overall rate of TLSs absorbing the microwave field, increases as the sweep rate is increased due to the increase in TLS crossings in the standard distribution. It leads to a universal plateau in non-equilibrium loss equal to the intrinsic linear dielectric loss at the low power limit. Here, we extend the measurements by using a new dielectric which is important in light of qubit substrates and semiconductor qubit devices: amorphous silicon. Quite surprisingly, the loss tangent reveals a second increases in loss with increasing bias rate. The data will be compared to previous data which fit the standard TLS model. We plan to verify the phenomenon with further studies.

2:54PM V35.00003: Atomic Layer Deposition of Titanium Nitride for Quantum Circuits* ABIGAIL SHEARROW (Presenter), GERWIN KOOLSTRA, SAMUEL WHITELEY, NATHAN D EARNEST, PETER BARRY, University of Chicago, JOSEPH HEREMANS, Argonne National Laboratory, DAVID AWSCHALOM, ERIK SHIROKOFF, DAVID SCHUSTER, University of Chicago — High kinetic inductance thin films are of great interest for superconducting detectors, coupling to hybrid systems, and novel superconducting qubits. We demonstrate that titanium nitride thin films grown via plasma-enhanced atomic layer deposition support superconducting microwave resonators with internal quality factors up to 1.0 million at single photon powers, and find that the dominant loss mechanism in these resonators is likely due to two-level systems. Utilizing nanowire geometries, we realize characteristic impedances greater than a resistance quantum with $Z \approx 28 \, \text{k}\Omega$ while maintaining low losses and a compact device footprint ($8 \times 8 \, \mu\text{m}^2$). The corresponding increase in zero point voltage fluctuations makes this material an excellent candidate for integration into hybrid quantum systems and quantum sensing.

*This research was supported by the Army Research Office under contract W911NF-17-C-0024. Support was provided by the Chicago MRSEC, which is funded by NSF through grant DMR-1420709.

3:06PM V35.00004: Fabrication of Sn-Cu alloy superconducting films for filled superconducting through-silicon vias* GO FUJII (Presenter), MASASHI UKIBE, KAZUMASA MAKISE, MUTSUO HIDAKA, SHUICHI NAGASAWA, HIROTKE YAMAMORI, KUNIHIRO INOMATA, TAKAHIRO YAMADA, SHIRO KAWABATA, National Institute of Advanced Industrial Science and Technology — Quantum annealing (QA) is one of quantum computers to solve combinatorial optimization and sampling problems. We have developed new three-dimensional (3D) packaging structure, which obtain a scalability and a flexibility in the circuit size to realize customized circuits for solved problems by stacking qubit-chip, interposer, and package-substrate as much as necessary. In the 3D packaging, superconducting TSVs are necessary because generating heat in through-silicon vias (TSVs) used to connect the qubit and the package-substrate is a big problem. So far, we have fabricated superconducting TSVs with pure Sn, however, fabrication yield of the TSVs was low because it was difficult to fill the Sn in deep holes by electroplating process (EP). In this work, we have changed the material from the Sn to Sn-Cu alloy to solve the above problem. A Sn$_9$-Cu alloy film fabricated by the EP exhibited transition temperature ($T_c$) of 2.4 K. Although the $T_c$ of the Sn$_9$-Cu alloy is about 30 % lower than that of the pure Sn, it is sufficient for our QA machine system.

*This is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO). A part of this work was conducted in Waseda University, supported by Nanotechnology Platform Program.

3:18PM V35.00005: Fabrication of superconducting qubits using free-standing mineral masks* IOANNIS TSIOUTSIOS (Presenter), KYLE SERNIAK, ZHIXIN WANG, SHYAM SHANKAR, LUIGI FRUNZIO, ROBERT SCHOELKOPF, MICHEL H. DEVORET, Applied Physics, Yale University — Over the last years there has been a significant improvement on the energy relaxation properties of superconducting qubits. State-of-the-art transmon and fluxonium qubits exhibit energy relaxation times in the order of hundreds of microseconds and few milliseconds respectively. Progress in their design has resulted in minimizing losses coming from the dielectric environment and radiation into the electromagnetic environment, in addition to gains due to better understanding and control of their inductive losses. However, advancements on reducing dielectric losses associated with organic residues produced by traditional fabrication techniques have been modest. In this talk, we will propose a new fabrication technology for planar superconducting circuits that replaces the commonly used resist-based lithography masks with free-standing mineral masks. Furthermore, we will present preliminary results on the energy relaxation properties and reproducibility of transmon qubits that are fabricated using this new method.

*ARO, ONR, NSF, AFOSR, and YINQE

3:30PM V35.00006: MBE grown AlN-TiN heterostructures for superconducting quantum circuits CHRISTOPHER RICHARDSON (Presenter), ASHISH ALEXANDER, CHRISTOPHER WEDDLE, Laboratory for Physical Sciences — Superconducting transition metal nitrides are a family of superconductors that have been used to produce high internal quality factor superconducting coplanar waveguide (CPW) resonators. Plasma assisted molecular beam epitaxy (MBE) is used to grow both superconducting nitrides and wide-bandgap nitride bilayer heterostructures. This combination of nitride materials provides sufficient degrees of freedom that synthesis of an epitaxial Josephson junction may be possible. Here early stages of this approach are evaluated through measurement of the single photon loss of aluminum nitride that is explored as both an overlayer and underlayer of TiN superconducting CPW resonators.
3:42PM V35.00007: Suspended trace air-gap resonators for superconducting circuits  MICHAEL FANG (Presenter), ANDREW J KELLER, OSKAR PAINTER, Caltech — Quantum memories and networks for distributed quantum information processing require links between the microwave, mechanical, and optical domains. Coherent integration of long-lived superconducting qubits (SCQs) with optomechanical and photonic devices (OMPDs) remains an outstanding challenge. We present a step towards coherent integration using a suspended trace air-gap resonator (STAR): a superconducting resonator on a silicon-on-insulator (SOI) substrate with the center trace suspended by silicon tethers above and between galvanically connected ground metal planes. As a result, the electric field energy is closely confined within the microwave structure, yielding lower crosstalk compared to conventional coplanar waveguides (CPW). Field participation in bulk dielectrics, a dominant source of loss in previous measurements of aluminum CPW resonators on SOI, is reduced to the point where the dominant loss factor is at the metal-air interface. The loss factor of the metal oxide can be reduced by several factors with choice of superconductor. Most importantly, STAR fabrication is compatible with Josephson junction and air-bridge evaporation for integration of SCQs and OMPDs.

3:54PM V35.00008: Microwave loss in amorphous silicon for coherent superconducting technologies  WILLIAM KOEHL (Presenter), STANLEY F STEERS, MOE KHALIL, JON COCHRAN, DANIEL ROBERT QUEEN, JUSTIN HACKLEY, KHYOUTH LIM, JIM KELLIHER, AUSTIN DOYLE, PATRICK WARNER, MONICA LILLY, MICAH STOUTIMORE, Northrop Grumman — Efforts to design superconducting quantum technologies have generated an interest in understanding the materials mechanisms responsible for microwave photon loss in coherent devices. While a desire for long coherence times has driven many groups to pursue devices fabricated on crystalline substrates, close study of loss in deposited dielectrics has also played an important role in the development of the field. Recent efforts at 3D integration suggest that a more complete understanding of the relationship between loss and defectivity in amorphous films is still needed. We discuss current microstructural models of defectivity in amorphous silicon (a-Si), a material commonly used in the semiconductor and solar industries, and relate these concepts to microwave photon loss in superconducting resonators fabricated on a-Si films deposited under growth conditions targeting low defect incorporation. Experimental data from cryogenic quality factor measurements will be presented and coupled to structural information derived via TEM and other materials spectroscopies.

4:06PM V35.00009: Optical Direct-Write Lithography of Shadow Mask Josephson Junctions*  JONATHAN MONROE (Presenter), KATER MURCH, Washington University, St. Louis — We have developed a technique to fabricate Josephson junctions with a direct-write laser lithography system, enabling fast writing of large-area patterns. Using standard Niemeyer-Dolan bridge shadow deposition techniques, we create relatively large junctions (0.5 um^2) suitable for array-based parametric amplifiers. We explore fabrication techniques to create low critical current junctions for superconducting qubits. We present results on reproducibility and performance of Josephson parametric amplifiers and transmon qubits utilizing these junctions.

*This work was supported the ONR Grant No. 12114811 and the NSF Grant No. PHY-1607156

4:18PM V35.00010: Surface Loss Characterization and Comparison in Aluminum, Niobium, and Titanium Nitride Superconducting Resonators*  ALEXANDER MELVILLE (Presenter), GREG CALUSINE, WAYNE WOODS, EVAN GOLDEN, JOVI MILOSHI, ARJAN SEVI, JONILYN L YODER, WILLIAM D OLIVER, MIT Lincoln Lab — Uniquely characterizing loss from two-level systems (TLS) at metal-substrate, metal-air, and substrate-air interfaces and in a dielectric substrate is challenging due to the nearly proportional scaling of the dielectric participations in response to changes in geometry and anisotropic trench depth. We developed a technique utilizing isotropic etching to assign a specific loss tangent to each dielectric, and use that to determine the dominant dielectric losses for a specific fabrication process, enabling targeted geometry and process changes to maximize performance. In this talk, we characterize the loss from high quality factor resonators (Q>1M) for aluminum, titanium nitride, and niobium, and demonstrate the technique's application by targeting specific defect layers to alter the dielectric losses specifically from these defect layers.

*This material is based upon work supported in part by the Intelligence Advanced Research Projects Activity (IARPA) and in part by the Department of Defense under Air Force Contract No. FA8721-05-C-0002 and/or FA8702-15-D-0001. Any opinions, findings, conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of IARPA, the Department of Defense, or the US Government.
4:30PM V35.00011: Study of atomic two-level defects within a Josephson junction proxy

CHIH-CHIAO HUNG (Presenter), NEDA FOROUZANI, KEVIN DANIEL OSBORN, LPS - ESPCI- use #1304 — In superconducting qubits, thermally grown aluminum oxide is generally used as the barrier between two superconducting electrodes to form the S-I-S Josephson junction (JJ). This oxide is amorphous and is known to contain random, atomic-sized two-level systems (TLSs) which are a source of decoherence in superconducting qubits. Here, we present a study of TLSs in parallel plate capacitors mimicking a JJ (Al/AlOx/Al), but where the dielectric layer is 20 nm and therefore block the tunneling supercurrent. In this JJ proxy, the defects near the in AlOx and near the interface of Al/AlOx can be studies using a new analysis method only demonstrated before with a different dielectric. Using a resonator device with a four-arm bridge capacitor, one can tune the frequency of TLSs by applying a DC electric field, and observe individual TLSs reach degeneracy with the resonator in a demonstration of cavity QED with TLS. The transmission versus applied electric field would give us the TLS dipole moment's z-component. We will study these resonators in an effort to better understand TLSs within typical JJs.

4:42PM V35.00012: Microwave Properties of Exfoliated Hexagonal Boron Nitride*

ABHINANDAN ANTONY (Presenter), Columbia University, MARTIN V GUSTAFSSON, GUILHEM RIBEILL, Raytheon BBN Technologies, MITALI BANERJEE, Columbia University, THOMAS A OHKI, Raytheon BBN Technologies, JAMES HONE, Columbia University, KIN CHUNG FONG, Raytheon BBN Technologies — Interfacial and bulk dielectric losses in superconducting qubits are some of the key factors limiting device coherence. We investigate the microwave properties of thin flakes of hexagonal boron nitride (h-BN), which have the potential to serve as low-loss elements in superconducting transmon qubits. The flakes, which are exfoliated from high-quality single-crystals to thicknesses of a few tens of nanometers, have atomically flat interfaces and low defect densities. Our process allows them to be coated with superconducting layers on both sides, thus forming parallel-plate capacitors. By embedding these capacitors in superconducting microwave resonators, we can determine the dielectric constant and loss tangent of h-BN under conditions relevant for qubit operation. Apart from the promise of improved coherence, the parallel-plate geometry would enable qubits to be designed with drastically reduced footprints and cross-talk compared to planar devices.

*We acknowledge funding support from ARO's quantum computing program (W911NF18C0044). AA thanks the sponsor of NSF's QISE-NET program (award number 1747426).

4:54PM V35.00013: Operating a Quantum Processor with Material Defects [Invited]

PAUL KLIMOV (Presenter), Google AI Quantum — A challenge in operating a quantum processor is mitigating computational errors from material two-level-system defects. Defects cause qubit-performance metrics to fluctuate in frequency, time, and between nominally identical qubits [1]. In frequency-tunable qubit architectures, it is possible to mitigate defect-related performance fluctuations in-situ by judiciously picking qubit operating frequencies. The defect avoidance problem thus maps to an optimization problem with a high-dimensional, non-convex, and time-dependent objective whose parameters are defined by defects' physical properties. In this talk, I will discuss recent research towards understanding defect properties, the defect avoidance problem, and related benchmarks.


Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V36 DAMOP: Experimental Realizations of Many-Body Localization and Simulation

BCEC 205C - Alex (Ruichao) Ma, University of Chicago - Tag(s): Invited

2:30PM V36.00001: Generating many-body localization in a trapped ion quantum simulator* [Invited]

PAUL HESS (Presenter), Middlebury College — Levitated crystals of trapped atomic ions are a versatile platform for realizing interacting quantum spin models and studying quantum nonequilibrium phenomena. In this talk, I will discuss how programmable laser-induced disorder can be used to generate a many-body localized (MBL) state in a long-range interacting trapped ion crystal. This technique for generating MBL was also applied in concert with a time-periodic Hamiltonian to explore how MBL can help stabilize discrete time crystalline states of matter. The experiment's single spin resolved measurements and controllable interactions allow us to characterize the MBL state's properties in ways not accessible to other atomic or condensed matter systems.

*This work was supported by the ARO Atomic and Molecular Physics Program, the AFOSR MURI on Quantum Measurement and Verification, the IARPA MQCO and LogiQ programs, and the NSF Physics Frontier Center at JQI.
3:06PM V36.00002: Exploring the many-body localization transition in two dimensions* [Invited] JAE-YOON CHOI
(Presenter), Physics, KAIST — Non-equilibrium dynamics in a closed quantum system has become a central theme in modern statistical mechanics, where experimental studies are accessible via cold atoms, trapped ion, and NV-center spin system. Many-body localization (MBL) is one example of non-trivial quantum phases of matter in non-equilibrium, where initial state information can persist for infinitely long time, violating fundamental hypothesis of classical statistical physics. In this talk, I will introduce a recent experiments of the MBL phase in two dimensions using ultra cold atoms in optical lattice. We prepare a far out-of-equilibrium state and trace its dynamical evolution under disorder potential. We observe the system does not thermalize above a non-zero disorder and verify the interaction effect. Finally, I will present a effect of finite thermal bath on the MBL phase, which can shed light on the stability of the MBL system in higher dimensions.

*We acknowledge funding by Max-Planck-Gesellschaft, Deutsche Forschungsgemeinschaft, the European Union (UQUAM and Marie curi fellowship).

3:42PM V36.00003: Engineering Trapped-Ion Systems for Large Scale Quantum Simulation* [Invited] GUIDO PAGANO
(Presenter), ANTONIS KYPRIANIDIS, HARVEY B KAPLAN, WEN LIN TAN, PATRICK M BECKER, KATE S COLLINS, ALEXEY GORSHKOV, University of Maryland, ZHEXUAN GONG, Colorado School of Mines, ANIRUDDHA BAPAT, University of Maryland, STEPHEN P JORDAN, Microsoft Research, JIEHANG ZHANG, University of Maryland, PAUL HESS, Middlebury, CHRISTOPHER ROY MONROE, University of Maryland — Laser cooled trapped ions offer unprecedented control over both internal and external degrees of freedom at the single-particle level. They are considered among the foremost candidates for realizing quantum simulation and computation platforms that can outperform classical computers at specific tasks. In this talk I will show how linear arrays of trapped $^{171}$Yb$^+$ ions can be used as a versatile platform for studying quantum dynamics of strongly correlated many-body quantum systems. In particular I will describe how to realize time-crystalline phases in a Floquet setting, where the spin system exhibits persistent time-correlations under many-body-localized dynamics. I will also present our observation of a new type of out-of-equilibrium dynamical phase transition in a spin system with over 50 spins. Moreover I will show our latest efforts towards scaling up the trapped-ion quantum simulator using a cryo-pumped vacuum chamber where we can trap more than 100 ions indefinitely. The reliable production and lifetime of large linear ion chains enabled us to investigate quasiparticle excitations showing confinement in the quench dynamics and the implementation of Quantum Approximate Optimization Algorithms (QAOA) with up to 40 spins.

*This work is supported by the ARO and AFOSR Atomic and Molecular Physics Programs, the AFOSR MURI on Quantum Measurement and Verification, the IARPA LogiQ program, the ARO MURI on Modular Quantum Systems, the ARL Center for Distributed Quantum Information, the IC Postdoctoral Fellowship Program, and the NSF Physics Frontier Center at JQI.

4:18PM V36.00004: Signatures of the Many-Body Localized Regime in Two Dimensions* [Invited] THORSTEN WAHL
(Presenter), University of Oxford — Lessons from Anderson localization highlight the importance of dimensionality of real space for localization due to disorder. More recently, studies of many-body localization have focussed on the phenomenon in one dimension using techniques of exact diagonalization and tensor networks. On the other hand, experiments in two dimensions have provided concrete results going beyond the previously numerically accessible limits while posing several challenging questions. We present the first large-scale numerical examination of a disordered Bose-Hubbard model in two dimensions realized in cold atoms, which shows entanglement based signatures of many-body localization. By generalizing a low-depth quantum circuit to two dimensions we approximate eigenstates in the experimental parameter regimes for large systems, which is beyond the scope of exact diagonalization. A careful analysis of the eigenstate entanglement structure provides an indication of the putative phase transition marked by a peak in the fluctuations of entanglement entropy in a parameter range consistent with experiments.

*TOPNES, EPSRC grant number EP/I031014/1
European Commission under the Marie Curie Programme
**Session V37 GMAG DCMP DMP: Spin Ice: Kagome, Artificial, and Theory**

2:30PM V37.00001: Dynamic kagome ice state [Invited]  
ELSIA LHOTEL (Presenter), Institut Néel, CNRS, SYLVAIN PETIT, LLB, CEA Saclay, MONICA CIOMAGA HATNEAN, University of Warwick, JACQUES OLLIVIER, ILL, ERIC RESSOUCHE, INAC, CEA Grenoble, MARTIN LEES, GEETHA BALAKRISHNAN, University of Warwick — Coulomb phases form a novel exotic state of matter which, because of frustration, lacks long range order, yet is described by a local organizing principle. Spin ice is the emblematic example of this physics: in a lattice where magnetic ions occupy the vertices of corner sharing tetrahedra (pyrochlore lattice), the combination of strong Ising anisotropy along local <111> axes with ferromagnetic interactions leads to the so called ice rule (2 spins point in and 2 spins point out in each tetrahedron). Kagome ice is another example, in 2 dimensions, with a lattice made of corner sharing triangles. In this case, the organizing principle is the kagome ice rule, 2 spins pointing into each triangle, and 1 out, or vice versa. The pyrochlore and kagome lattices are intimately related: along the [111] direction, the pyrochlore lattice can be viewed as a stacking of kagome layers separated by the apical spins. Applying a magnetic field along [111] in spin ice freezes out the apical spins, decouples the kagome layers and operates a dimension reduction. In this context, we report here the effect of a [111] magnetic field on Nd$_2$Zr$_2$O$_7$. In this pyrochlore compound, classical spin ice physics is considerably modified by the existence of transverse terms in the Hamiltonian: spin ice signatures are transferred in the excitation spectrum, taking the form of a flat spin ice mode [1]. Correspondingly, we show that above 0.25 T, a flat dynamic kagome ice mode forms in the excitation spectrum, featuring a “dynamic kagome ice” state [2]. Mean-field calculations using the XYZ Hamiltonian [3] account qualitatively for our observations, although some discrepancies point to the existence of more complex processes. More generally, our study highlights the key role of transverse terms in the physics of pyrochlore magnets.

ZHILING DUN, XIAOJIAN BAI (Presenter), School of Physics, Georgia Institute of Technology, JOSEPH PADDISON, Churchill College, University of Cambridge, EMILY HOLLINGWORTH, School of Physics, Georgia Institute of Technology, FRANZ DEMMEL, ISIS facility, Rutherford Appleton Laboratory, NICHOLAS BUTCH, NIST Center for Neutron Research, CLARINA DELA CRUZ, MATTHEW BRANDON STONE, TAO HONG, Neutron Scattering Division, Oak Ridge National Laboratory, MARTIN MOUG, School of Physics, Georgia Institute of Technology, HAIYAN ZHOU, Department of Physics and Astronomy, University of Tennessee — A promising route to realize entangled magnetic states combines geometrical frustration with quantum tunneling effects. Spin-ice materials are canonical examples of frustration, and Ising spins in a transverse magnetic field are the simplest many-body model of quantum tunneling. Here, we show that the tripod kagome lattice material Ho3Mg2Sb3O14 unites an ice-like magnetic degeneracy with quantum-tunneling terms generated by an intrinsic splitting of the Ho3+ ground-state doublet, realizing a frustrated transverse Ising model. Using neutron scattering and thermodynamic experiments, we observe a symmetry-breaking transition at 0.32 K to a remarkable quantum spin-fragmented states with strongly reduced ordered/local moment. Using exact diagonalization and mean-field calculation, we demonstrate that whereas the transverse field tends to drive the system into a spin-liquid state with zero on-site moment, the hyperfine interaction helps to stabilize the fragmented local moments. Our results establish that Ho3Mg2Sb3O14 realizes a quantum spin-fragmented state on the kagome lattice.

*The work at Georgia Tech was sponsored by the Department of Energy under grant DE-SC-0018660.

KAI-HSIN WU (Presenter), Department of Physics, National Taiwan University, YI-PING HUANG, Max Planck Institute for the Physics of Complex Systems, YING-JER KAO, Department of Physics, National Taiwan University — We study the spin-1/2 kagome Heisenberg XYZ Hamiltonian model in the so-called quantum kagome ice regime[1]. From our recent topological entanglement entropy and thermal entropy studies, we find that the system does not show a Z2 topological order down to β=48, while the thermal entropy down to β=200 is consistent with the residual entropy of a classical kagome ice in a magnetic field [2]. Using degenerate perturbation theory (DPT) out of the classical ice manifold, we derive an effective model which shows an intricate competition between the ring-exchange and diagonal processes. Here, we perform exact diagonalization on the effective Hamiltonian. By tuning the weight of the diagonal term, we find that the competition can lead to a quasi-degenerate energy spectrum, consistent with the Quantum Monte Carlo simulation results.


*This work was supported by the Ministry of Science and Technology (MOST) of Taiwan under Grants No. 105-2112-M-002-023-MY3, and 104-2112-M-002-022-MY3

JUSTIN WOODS (Presenter), BARRY W FARMER, University of Kentucky, YONGLEI WANG, Physics, Nanjing University, WAI-KWONG KWOK, Material Science Division, Argonne National Laboratory, JEFFREY T HASTINGS, LANCE DE LONG, University of Kentucky — We study the ordering of magnetic charges in honeycomb artificial spin ice (ASI) having distortions created by applying an aperiodic Fibonacci sequence of binary digits mapped onto short (d1) and long (d2) 2D lattice parameters. Patterned Permalloy (Ni,Fe) thin films were deposited on Si3N4 using standard electron beam lithography (EBL) to create samples with a range of distortion ratios d2/d1 = 1.00, 1.15, 1.30, 1.45 and 1.62.

The lengths of disconnected segments and their location around three-fold honeycomb vertices were modified by these distortions. Two pattern types were studied: 1) Varied segment length; 2) Varied segment distance to vertex. In both cases, the values of d1 and d2 uniquely determine the positions of the pattern vertices.

The magnetic charge distribution of each pattern was imaged using standard magnetic force microscopy (MFM) techniques before and after the system is annealed into a low-energy ASI state. The magnetic charge distributions are then analyzed to determine the effect of the distortions on frustration of the magnetic textures, and relation to the coercive fields measured by SQUID magnetometry.

*Research was supported by U.S. Department of Energy Grant Nos. DE-SC0016519 and DE-AC02-06CH11357 (Argonne Center for Nanoscale Materials).
Degenerate Ground States in Vertex-Frustrated Artificial Spin Ice*  

**3:42PM V37.00005:** Degenerate Ground States in Vertex-Frustrated Artificial Spin Ice*  

XIAOYU ZHANG (Presenter), Applied Physics, Yale Univ, YUYANG LAO, Physics, University of Illinois, NICHOLAS S. BINGHAM, Applied Physics, Yale Univ, JOSEPH SKLENA, Physics, University of Illinois, AYHAN DUZGUN, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, JUSTIN WATTS, Physics, University of Minnesota, JOSEPH BATLEY, Chemical Engineering and Materials Science, University of Minnesota, RAJESH V CHOPDEKAR, Lawrence Berkeley National Laboratory, CHRIS LEIGHTON, Chemical Engineering and Materials Science, University of Minnesota, CRISTIANO NISOLI, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, PETER E SCHIFFER, Applied Physics, Yale Univ — Artificial spin ice systems (ASI) are two-dimensional arrays of interacting single-domain ferromagnetic nano-islands, with uniaxial anisotropy. With careful consideration of the lattice geometry, some ASI systems can have degenerate ground states that include excited vertices, so called vertex-frustrated systems, and these can manifest a wealth of different emergent behavior in the collective dynamics of the magnetic moments. In one example of a vertex-frustrated system, the Santa Fe lattice, the ground state degeneracy changes with the strength of interactions and the excited vertices whose fluctuations control the low energy kinetics of the moments. To examine the ground state behavior of Santa Fe ASI, we performed Photoemission Electron Microscopy measurements as a function of lattice spacing and island moment after a thermal annealing treatment, and we observed a range of novel behavior. The results show a notable change in the possible ground state configurations across different lattice parameters, demonstrating that Santa Fe ASI is an excellent candidate for studying novel order induced by vertex frustration.

*Work is funded by the US Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division. Work at UMN supported by NSF DMR.

Magnetotransport of Vertex Frustrated Artificial Spin Ice Structures*  

**3:54PM V37.00006:** Magnetotransport of Vertex Frustrated Artificial Spin Ice Structures*  

ELYSIA SHARMA (Presenter), Physics, Imperial College London, DAAN M ARROO, Physics, University College London, NIRAT RAY, Indian Institute of Technology Gandhinagar, LESLEY COHEN, WILL BRANFORD, Physics, Imperial College London — Artificial spin ice (ASI) systems are 2D analogues of pyrochlore spin ice, which exhibit frustrated magnetism and magnetic monopole-like defects [1]. ASI is commonly studied in honeycomb or square lattices, but other geometries which exhibit frustration are of growing interest. Previous magnetotransport studies have observed an asymmetric Hall signal and postulated this is related to the phase transition to the chirally ordered state in the kagome lattice [2]. Due to the possible effect of exchange bias [3] and the breakdown of the macrospin approximation for cobalt ASI systems below 50K [4] this has continued to be a topic of much interest and debate. The comparison of the response of different geometries could provide insight which could clarify the origin of this effect. Here we present an investigation of the Longitudinal and Hall resistivity, in the range 2K<T<290K, for non-conventional ASI geometries. Samples consist of permalloy nanowires in 5 geometries: kagome, square, Shakti, brickwork and tetris.


*The authors thank the EPSRC for funding.

Imaging the stray field of chiral artificial spin ice with scanning nanoSQUID-on-tip  

**4:06PM V37.00007:** Imaging the stray field of chiral artificial spin ice with scanning nanoSQUID-on-tip  

MARCUS WYSS (Presenter), DENIS VASYUKOV, University of Basel, SEBASTIAN GLIGA, Physics, University of Glasgow, LORENZO CECCARELLI, GIULIO ROMAGNOLI, University of Basel, ROBERT L. STAMPS, Physics, University of Glasgow, MARTINO POGGIO, University of Basel — We use a scanning nanometer-scale superconducting quantum interference device (nanoSQUID) [1] to image the stray field of an artificial spin ice, which displays structural chirality. Experiments are carried out in a series of magnetic fields at 4.2 K. The "chiral ice" [2] is a 2D arrangement of lithographically patterned permalloy nanomagnets. Each stadium-shaped nanomagnet is much thinner than its in-plane dimensions, producing a strong shape anisotropy that favors a single-domain magnetization configuration [3]. Nevertheless, scanning nanoSQUID measurements, backed by micromagnetic simulations, show that the magnetization in the nanomagnets is not uniform, displaying a bending at the edges of the nanostructures. The results show that the number of degrees of freedom in artificial spin ice can be much larger than typically captured in dipolar models. These additional degrees of freedom contribute to the field-induced dynamics and may be used to create reprogrammable magnonic crystals [4].

4:18PM V37.00008: Simulation of electron holography of pyrochlore spin ice  ANKUR DHAR (Presenter), Okinawa Institute of Science and Technology, LUDOVIC JAUBERT, LOMA, CNRS, University of Bordeaux, NICHOLAS SHANNON, TSUMORU SHINTAKE, Okinawa Institute of Science and Technology — A major topic in frustrated magnetism is emergent magnetic monopoles in spin ice [1]. These low-energy excitations are effective classical analogues of Dirac monopoles and have only been seen indirectly thus far [2]. Electron holography could allow for direct observations due to its high sensitivity to magnetic fields. Electron holography has achieved 3D spatial imaging of spin phenomena with nanometer resolution [3]. This makes the technique uniquely suited for directly imaging spin ice monopoles. I have developed computational methods to predict how an electron wave would propagate through the spin ice’s magnetic structure. The dipole arrangement of pyrochlore spin ice thin films was generated with the help of Monte Carlo simulation [4]. From there I calculate the magnetic vector potential around the spin ice, and its resulting effect on electron phase. These simulated results enable us to show for the first time what a monopole would look like if imaged using electron holography, and what it would take to achieve in experiment.


4:30PM V37.00009: Zone center physics in magnetic diffuse neutron scattering  MIKAEL TWENSTROM (Presenter), Physics, Royal Institute of Technology, LAURA BOVO, Innovation and Enterprise, University College London, PATRIK HENELIUS, Physics, Royal Institute of Technology, STEVEN T. BRAMWELL, London Centre for Nanotechnology, Physics and Astronomy, University College London — Probing physical quantities using neutron scattering is crucial in many areas of physics. Magnetic neutron scattering measures a generalized magnetic susceptibility, but which susceptibility is actually measured as the scattering vector \( Q \rightarrow 0 \)? We consider the case of spin ice, which lends itself well to such a study as it obeys both the static approximation of neutron scattering, the classical fluctuation-dissipation theorem and it also has an extremely large paramagnetic susceptibility. By comparing a direct magnetic measurement using a SQUID magnetometer and a neutron scattering measurement near a Brillouin zone center, we show that the external susceptibility is recovered rather than the intrinsic one. Theoretically we investigate this result by Monte Carlo simulations of the spin ice Hamiltonian with different boundary conditions. Our conclusion is that when measuring the paramagnetic structure factor for a Brillouin zone center point in Fourier space, a demagnetizing transformation may be needed in order to recover the intrinsic susceptibility of a magnetic material.

4:42PM V37.00010: Spectroscopy of spinons in quantum spin ice  SIDDHARDH MORAMPUDI (Presenter), CHRISTOPHER LAUMANN, Physics, Boston University, FRANK WILCZEK, MIT — We calculate the effect of the emergent photon on spectroscopic cross-sections of spinons in quantum spin ice which realizes an emergent phase of QED at low energies. We show that the photon drastically modifies threshold cross-sections of spinons from a naive density of states analysis resulting in effects such as an analogue of the Sommerfeld enhancement. We point out signatures in neutron scattering and Raman spectroscopy and show that this explains some recent numerical and experimental results.

4:54PM V37.00011: Hopfions in lattice dimer model*  GRIGORY BEDNIK (Presenter), Physics, University of California Santa Cruz — In this talk I consider hopfions in 3D lattice dimer model, i.e. topological defects, which can be characterized by 3D topological Hopf invariant. More specifically, I consider 3D bipartite lattice dimer model, define its configurations as equivalent if they can be transformed into each other by a set of local flips, and derive, that they preserve Hopf number. In this way, Hopf invariants answer the question of ergodicity in bipartite lattice dimer model. Furthermore, I consider the case of non-bipartite lattice dimer model, and by using neural networks, demonstrate that its topological phases are characterized by \( \mathbb{Z}_2 \) topological invariant. Since the lattice dimer model is known to describe classical spin ice, my work can be viewed as a proposal to search for hopfions in spin ice materials.

*NSERC of Canada
5:06PM V37.00012: Frustrated Spin Ice Nanomagnets Probed by Superconducting Vortex Dynamics.* JOSE VICENT (Presenter), University Complutense, Spain, VICTOR ROLLANO, IMDEA-Nanociencia, Spain, ALVARO MUNOZ-NOVAL, University Complutense, Spain, ALICIA GOMEZ, CSIC-INTA, Spain, FERNANDO VALDES-BANGO, MARIA VELEZ, JOSE MARTIN, University Oviedo, Spain, MANUEL OSORIO, DANIEL GRANADOS, IMDEA-Nanociencia, Spain, ELVIRA GONZALEZ, University Complutense, Spain — We have studied the superconducting vortex dynamics on hybrid superconducting/magnetic samples. The samples are connected Co nanomagnets with honeycomb structure which are embedded in Nb superconducting film. The samples are patterned in a cross-shaped bridge for magnetotransport measurements. Superconducting vortex lattice motion detects distinct magnetic states of the honeycomb array. These states are governed by the topology of the Co honeycomb which frustrates in-plane magnetic configurations which must follow spin ice rules. Furthermore, in the honeycomb array, each vertex consists of two charged Néel walls. This hybrid system can be set easily in magnetic configuration corresponding to Ice II or Ice I states. We will show that the superconducting vortex flow is sensitive to subtle changes in the magnetic state of the spin ice and remarkably the as-grown state is not fully demagnetized; that is, this spin ice presents remanent magnetization in all the possible magnetic configurations.

*We thank Spanish FIS2016-76058 and CM S2013/MIT-2850. IMDEA Nanociencia acknowledges the 'Severo Ochoa' Program (SEV-2016-0686). DG thanks RYC-2012-09864, S2013/MIT-3007 and AG and DG thank ESP2015-65597.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V38 GMAG DMP: Spin Glasses and Disordered Magnetic Systems BCEC 206B - Zhenzhong Shi, Duke University - Tag(s): Focus

2:30PM V38.00001: A dynamic probe of finite-size effects near the spin-glass transition temperature* GREGORY KENNING (Presenter), Physics, Indiana University of Pennsylvania, DANIEL TENNANT, QIANG ZHAI, Physics, University of Texas, DAVID HARRISON, E. DAN DALHBERG, Physics, University of Minnesota, RAYMOND ORBACH, Physics, University of Texas — Using a high sensitivity dual DC SQUID magnetometer, we have measured the growth of the spin glass correlation length, through the aging and end of aging effects. Measurements were made on bulk CuMn5% and a CuMn12% thin film multilayer with CuMn layer thicknesses of 4.5 nm. As the glass temperature Tg is approached (0.9Tg < T<0.96Tg) in the bulk sample, we find that the waiting time effect (as measured by the time associated with the inflection point of the decay) as a function of increasing temperature, shifts to shorter timescales. For T >0.96Tg, there is no waiting time effect (end of aging) on the magnetization decay, and all decays collapse onto a single decay curve indicating an end of aging even for long waiting times (tw = 10,000s). For the thin film, all effects due to the waiting time disappear at around 0.89Tf, where Tf is the freezing temperature marking the onset of irreversibility. The end of aging results are interpreted in terms of the spin glass correlation length saturating due to finite size effects.

* This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under Award DE-SC0013599. The IUP dual dc SQUID magnetometer was built under an NSF MRI, Award No. 0852643.

2:42PM V38.00002: Seeking the spin-glass state in a field through windows DILINA PERERA (Presenter), Department of Physics and Astronomy, Texas A&M University, A. PETER YOUNG, Department of Physics, University of California, Santa Cruz, HELMUT KATZGRABER, Microsoft Quantum, Microsoft — Although the presence of a finite-temperature transition in the three-dimensional Ising spin-glass is well established in zero field, the behavior in the presence of an external magnetic field has been a matter of long-standing controversy. For the infinite-range Sherrington-Kirkpatrick spin glass, mean-field theory predicts a transition line known as Almeida-Thouless (AT) line that separates the paramagnetic and spin-glass phases in the temperature-field plane. Despite extensive numerical efforts, no consensus has been reached with regard to the presence of an AT line in short-range systems, mostly due to strong corrections to finite-size scaling. Here we investigate the transition in a three-dimensional system via a method in which we perform population annealing Monte Carlo simulations for a large system, but only consider the thermodynamic properties of the system restricted to a small window. By computing the wave-vector-dependent spin-glass susceptibility for the individual windows, as well as for the whole system, we investigate the effects of finite-size corrections to the two-point correlation function.
Evidence of transition between Heisenberg and Ising-like phases in mesoscale Ge:Mn spin glass

SAMARESH GUCHHAIT (Presenter), Department of Physics and Astronomy, Howard University, Washington, DC 20059 — The glassy dynamics of vector spin glasses in presence of a weak uniaxial anisotropy has been a subject of longstanding controversy. It has been predicted that in presence of such anisotropy Heisenberg-like spin glass system first undergoes longitudinal moment freezing, followed by a transverse moment freezing at even lower temperature. Evidence of such phase transition is seen in the temperature chaos experiments in thin film Ge:Mn spin glass. Here the sample temperature is increased from the quench temperature after the correlation length has reached its thickness. For large enough positive change of temperatures the maximum barrier height increases monotonically, which is consistent with a phase change of lower temperature Heisenberg-like phase to higher temperature Ising-like phase.

Study of longitudinal fluctuations of the Sherrington-Kirkpatrick spin glass

LEOPOLDO SARRA (Presenter), Max Planck Institute for the Science of Light, Erlangen, LORENZO TALAMANCA, SV IBI UPNAE, EPFL, G. PARISI, Dipartimento di Fisica, Sapienza Università di Roma — Spin glasses are disordered systems with a complex behavior, caused by the very high degeneracy of low energy states. They have a phase transition between a paramagnetic phase and a spin glass phase, in which the ergodicity is broken in a hierarchical organization of states. This implies many peculiar properties such as aging, remanence and memory effect. In our work, we study finite-size corrections to the mean field model, the Sherrington-Kirkpatrick spin glass, whose solution is well-known. The behavior of these corrections in the low temperature phase has been debated for several years. Because of the complicated form of the theory around the mean field solution and of the difficulty to perform a numerical estimate, no final value has been found so far. We investigate the role of longitudinal fluctuations, neglecting the transverse contribution. Since they can be calculated directly into the full-replica symmetry breaking ansatz, it is easier to obtain a prediction for their behavior.

Chaotic Behavior in CuMn_{13.5} Multilayer Thin Film Spin Glasses

QIANG ZHAI (Presenter), RAYMOND ORBACH, The University of Texas at Austin, DAVID HARRISON, University of Minnesota Twin Cities — The zero field cooled (ZFC) and field cooled (FC) magnetizations of an 11 nm CuMn_{13.5} multilayer thin film spin glass was measured using a superconducting quantum interference device (SQUID) over the time scale where the correlation length has grown to the film thickness, i.e. for time scales where the thin films crossover from 3D to 2D. Temperature chaos, the vulnerability of the quasi-equilibrium state to temperature perturbations, was studied by a series of temperature drops after the crossover time. We find the ZFC and FC magnetization responses are sensitive to temperature changes after crossover. Both reversible and chaotic behavior, the latter characterized as rejuvenation, are observed. The traditional interpretation using a characteristic length for chaos, and the concept that chaos is “driven by rare events,” are discussed in comparison with experimental results.

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award DE-SC0013599.

Experimental Observation of Room-temperature Anomalous Hall Mobility and Positive Magnetic Hysteresis in Amorphous Fe-Dy-O Thin Films

KRISHNA KOIRALA (Presenter), Department of Physics and Astronomy, University of Tennessee, Knoxville, ANIRUDDHA DEB, Department of Chemistry, University of Michigan, Ann Arbor, RITESH SACHAN, Materials Science Division, Army Research Office, DEEPAK SAPKOTA, Department of Physics and Astronomy, University of Tennessee, Knoxville, VENKATANARAYANA P SANDIREDDY, Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, JAMES E PENNER-HAHN, Department of Chemistry, University of Michigan, Ann Arbor, RAMKI KALYANARAMAN, Department of Material Science and Engineering, University of Tennessee, Knoxville — Fe-Dy-Tb-O thin film system was recently reported with very high transparency, conductivity and room temperature ferromagnetism driven by partially filled d- and f- subshells. Here, we have synthesized and studied the Fe-Dy-O thin films. The thin film system was prepared by e-beam evaporation and its structural, transport, magnetic and optical characterizations were performed. The as-grown films were amorphous, as evidenced by transmission electron microscopy and X-ray scattering. X-ray absorption spectra revealed a progressive oxidation of thin films on reducing the dimension. The films showed highly (\sim 10 \text{cm}^2/\text{V-s}) and anomalous (\sim 10^2 \text{cm}^2/\text{V-s}) Hall mobility with n-type semiconducting behavior. Cryogenic magnetic behaviors evinced the existence of spin-glass-like transition at 79 K. Positive hysteretic loop and transverse magneto-resistivity up to 4% in the magnetic field of 5 T were observed at room temperature. Room-temperature optical studies showed the existence of a band gap of 2.42 eV in the visible range. These unique set of properties make the system a rich toolbox for not only understanding condensed matter behavior but also realizing multifunctional devices.

*R K and K P K acknowledge support by NSF grant ECCS-1607874.
By quenched-randomly mixing local units of different spatial dimensionalities, we have studied Ising spin-glass systems on hierarchical lattices continuously in dimensionalities $1<d<3$. The global phase diagram in temperature, antiferromagnetic bond concentration, and spatial dimensionality is calculated. We find that, as dimension is lowered, the spin-glass phase disappears to zero temperature at the lower-critical dimension $d_c=2.431$. Our system being a physically realizable system, this sets an upper limit to the lower-critical dimension in general for the Ising spin-glass phase. As dimension is lowered towards $d_c$, the spin-glass critical temperature continuously goes to zero, but the spin-glass chaos fully sustains to the brink of the disappearance of the spin-glass phase. The Lyapunov exponent, measuring the strength of chaos, is thus largely unaffected by the approach to $d_c$ and shows a discontinuity to zero at $d_c$.


*Academy of Sciences of Turkey (TUBA)

**Trimer Magnet Ba$_4$Ir$_3$O$_{10}$**

**Luttinger Quantum Paramagnet from Dimensional Recombination in the Frustrated Spin-1/2 System**

HENGDI ZHAO (Presenter), HAO ZHENG, YIFEI NI, YU ZHANG, Department of Physics, University of Colorado, Boulder CO 80309, FENG YE, XIAOPING WANG, CHRISTINA HOFFMANN, Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37381, USA, MINHYEA LEE, ITAMAR KIMCHI, MICHAEL A HERMELE, GANG CAO, Department of Physics, University of Colorado, Boulder CO 80309 — We report a highly frustrated spin state persisting down to 0.2 K in the monoclinic Ba$_4$Ir$_3$O$_{10}$ with Ir$^{4+}$($5d^5$) ions, which consists of Ir$_3$O$_{12}$ trimers of face-sharing IrO$_6$ octahedra and wavy two-dimensional Ir-O sheets. This iridate conspicuously avoids any long-range magnetic order down to 0.2 K despite strong antiferromagnetic interaction with Curie-Weiss temperature $-766$ K. The corresponding frustration ratio reaches an astonishing value of 3830. This frustrated spin state is further evidenced by a sizable, linear heat capacity, indicating substantial residual entropy even at milli-Kelvin temperatures. It is equally striking that a mere 2% nonmagnetic Sr substitution for Ba readily lifts frustration and precipitates a long-range antiferromagnetic order at 130 K, suggesting proximity to a quantum critical point potentially with emergent random spin nucleation.

This work was supported by the National Science Foundation via grant DMR-1712101.

**Weird scaling for 2-D avalanches: curing the faceting, and scaling in the lower critical dimension**

L. X. HAYDEN (Presenter), ARCHISHMAN RAJU, JAMES PATARASP SETHNA, Cornell University — The nonequilibrium random-field Ising model (NE-RFIM) is very well studied and yet there are outstanding questions. In two dimensions, power law scaling approaches fail and the critical disorder is difficult to pin down. Additionally, the presence of faceting on the square lattice creates avalanches that are lattice dependent at small scales. We propose two methods which we find solve these issues. First, we perform large scale simulations on a Voronoi lattice to mitigate the effects of faceting. Secondly, the form of the nonlinear functions necessary to perform scaling collapses can be directly determined using our recent normal form theory of the Renormalization Group. This method has proven useful in cleanly capturing the complex behavior which occurs in both the lower and upper critical dimensions of systems and well describes the NE-RFIM in two-dimensions. The obtained scaling collapses span over a range of a factor of ten in the disorder and a factor of 10$^4$ in avalanche size. They are consistent with a critical disorder at zero and with a lower critical dimension for the model equal to two.

This material is based upon work supported by the National Science Foundation under Grant No. DMR-1719490.

**Critical behavior of the Ising model on a lattice with fractional space dimension**

CHAO FANG (Presenter), Physics and Astronomy, Texas A&M University, MAOXIN LIU, Beijing Computational Science Research Center, HELMUT KATZGRABER, Microsoft Quantum, Microsoft — Disorder can have a drastic effect on the critical behavior of a magnetic system. The Harris criterion states that if the critical exponent of the correlation length $\nu$ fulfills the inequality $\nu \geq 2d$, with $d$ the space dimension, disorder does not affect the universality class of the magnetic systems. A recent study reported a violation of this criterion for a two-dimensional three-state Potts model on a Voronoi lattice. To better understand the effects of disorder on the critical behavior of magnetic systems on disordered lattices, we study the critical behavior of a two-dimensional Ising ferromagnet on the largest component of a percolating cluster on a two-dimensional square lattice. There are two possible scenarios: In the weak universality scenario the disordered structure of the underlying lattice slowly changes the critical exponents, whereas in the strong universality scenario the critical exponents are not affected by the fractional space dimension of the system. Our results suggest a strong universality scenario with weak (logarithmic) corrections.
4:30PM V38.00011: Maximally Random Discrete-Spin Systems with Symmetric and Asymmetric Interactions and Maximally Degenerate Ordering* A NIHAT BERKER (Presenter), Kadir Has U, MIT, BORA ATALAY, Kadir Has U, Sabanci U — Discrete-spin systems with maximally random nearest-neighbor interactions that are symmetric or asymmetric, ferromagnetic or antiferromagnetic, including off-diagonal disorder, are studied for q=3,4 states in d dimensions, using renormalization-group theory exact for hierarchical lattices and approximate (Migdal-Kadanoff) for hypercubic lattices. For all d>1 and non-infinite temperatures, the system eventually renormalizes to a random single state, signaling q×q degenerate ordering, which is maximally degenerate ordering. For high-temperature initial conditions, the system crosses over to this highly degenerate ordering after many renormalization-group iterations near the disordered infinite-temperature fixed point. Thus, a temperature range of short-range disorder in presence of long-range order occurs, as previously seen in underfrustrated Ising spin-glasses. The calculated entropy behaves similarly for ferromagnetic and antiferromagnetic interactions and shows a derivative maximum at the short-range disordering temperature. The system is disordered at all temperatures for d=1.


*Academy of Sciences of Turkey (TUBA)

4:42PM V38.00012: Direct Observation of Magnetic Long-range Order in Ammann-Beenker Artificial Quasicrystals* LANCE DE LONG (Presenter), BARRY W FARMER, University of Kentucky, JOHN UNGURIS, NIST Gaithersberg, JUSTIN WOODS, University of Kentucky — Magnetic long-range order (LRO) in 3D Ammann-Beenker tilings (ABT) has been modeled in simulations1,2, but has yet to be experimentally observed3. We fabricated artificial ABT composed of a connected wire network of elongated Permalloy film segments that mimic classical Ising spins interacting via long-range dipolar and short-range exchange interactions. Our MC analysis of ABT (NN interactions) generated a magnetic ground state built upon distinct sublattices, similar to fivefold Penrose tilings4,5. High-resolution images of the in-plane magnetization of ABT were acquired with scanning electron microscopy with polarization analysis (SEMPA). An annealing protocol that yielded improved agreement with the MC ground state. We developed a novel cluster covering that introduces frustration among neighboring clusters, and suggests low-energy, long-range interactions are required for full LRO, and provides a possible explanation for the non-existence of magnetic LRO in atomic quasicrystals.

2) S. Thiem, J. T. Chalker, EPL 110 (2015) 17002

*Research supported by NSF Grant 1506979

5:06PM V38.00014: Study of a generalized XY model using the correlation length*  
NUI XUAN DUONG, Faculty of Mechanics and Civil Engineering, Vietnam National University of Forestry, TUAN LE, School of Engineering Physics, Hanoi University of Science and Technology, KIEN DUC-TRUNG NGUYEN, HUY THANH PHAM, Advanced Institute for Science and Technology, Hanoi University of Science and Technology, HUNG DANG (Presenter), Thanh Tay Institute for Advanced Study, Thanh Tay University, VIET XUAN DAO, Advanced Institute for Science and Technology, Hanoi University of Science and Technology — The correlation length is examined in a generalized XY model where, together with the usual ferromagnetic interaction between spins, there is an additional nematic interaction that allows for half-vortices. The power of the correlation length is demonstrated in distinguishing different phases, thus fully reconstructing the phase diagram of the model. Moreover, it allows for further investigation of the tricritical region in the phase diagram where the paramagnetic, the nematic and the quasi-long-ranged phases meet. It shows that the Ising-type transition between the nematic and the quasi-long-range ordered phases stops at the tricritical point. Starting from this tricritical point, there is an intermediate range of different physics separates the two regions corresponding to the Ising-type and the Berzinskii-Kosterlitz-Thouless-type transitions.

*The research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under Grant No. 103.02-2011.38.

5:18PM V38.00015: Dangerously Irrelevant Field at Clock Models - A study with the Monte Carlo Based RG Flows*  
HUI SHAO (Presenter), Center for Advanced Quantum Studies, Beijing Normal University, WENAN GUO, Physics Department, Beijing Normal University, ANDERS W SANDVIK, Boston University &IOP-CAS Beijing — The phase transitions between the paramagnetic phase and the \( Z_q \) symmetry-breaking phase in the three dimensional XY model with \( Z_q \)-anisotropic field is now well accepted as belonging to the 3D XY universality class for \( q > q_c \), with the \( Z_q \)-anisotropic field being irrelevant at the critical point. However, when \( T < T_c \) it is always relevant as the symmetry is broken discretely. This is “dangerous” because it leads to a larger length scale \( \xi' \) than the normal correlation length \( \xi \), which, by definition, governs the crossover behavior from \( U(1) \) to \( Z(q) \) symmetry breaking. While RG theory has provided generic pictures of the RG flow in coupling space, we here construct a quantitative Monte Carlo based RG flow using corresponding physical observables, where not only the crossover behaviors can be observed explicitly but also the critical exponents \( \nu \) and \( \nu' \) can be extracted accordingly. For this purpose, we have firstly restudied the anisotropy order parameter and confirm that its scaling dimension at the critical point is the same as that of the \( Z_q \) field. We also clarify unsettled issues in several recent studies of this quantity.

* A.W.S. was funded by the NSF under Grants No. DMR-1710170, and by the Simons Foundation.

Thursday, March 7, 2019 2:30 PM - 4:54 PM

Session V39 GMAG DMP: Magnetism in Rare Earth Materials  
BCEC 207 - Brian Kirby, National Institute of Standards and Technology - Tag(s): Focus

2:30PM V39.00001: Controlling magnetism and magneto-structural phase transformation in rare earth containing materials*  
DURGA PAUDYAL (Presenter), Ames Laboratory — In rare earth element based materials the alloyed p-block elements provide chemical formation and stability, and control magnetism exhibited by rare earths. We report here two examples of how non-magnetic elements substitution pinpointed enhanced and controlled magnetism and phase transformation. First example is Eu2In, in which the Eu 5d states strongly hybridize with the In 5p states exhibiting large exchange splitting in ferromagnetic configuration. This unexpectedly high exchange splitting is the root cause of the sharp paramagnetic to ferromagnetic transition [1]. The other example is scandium substituted Gd2Ge4. Total energy calculations show that Sc favors the Gd atoms located inside the slabs and predict a stable ferromagnetic ground state with the 20 atomic % Sc substituted Gd2Ge4. The predicted phase is Pu5Rh4-type which is intermediate between the Sm2Ge4-type and Gd2Si4-type. The delocalized 3d electronic states of Sc strongly hybridize with delocalized 5d electronic states of Gd, thus promoting indirect interslab 4f-4f exchange interactions [2].


*The Ames Laboratory is operated for the USDOE by Iowa State University under contract No. DE-AC02-07CH11358. This work is supported by the DOE, Office of BES, MSED.
Spin dynamics in magnetic reorientation transitions
MASAMICHI NISHINO (Presenter), Research Center for Advanced Measurement and Characterization, National Institute for Materials Science, SEIJI MIYASHITA, Department of Physics, The University of Tokyo — The Nd-Fe-B magnet is known as a permanent magnet with strong coercive field and commercially used for motors and generators, etc. It shows a magnetic reorientation transition at around 150 K (magnetic Tc is 600–700 K) [1]. The origin of the reorientation transition is higher order magnetic anisotropy constants, which causes a tilted spin state at low temperatures. We study the temperature dependence of ferromagnetic resonance frequency of an atomistic spin model of the magnet. We estimate the power spectrum by using the stochastic Landau-Lifshitz-Gilbert equation [2]. We find non-monotonic temperature dependence of the peak position of the frequency. We analyze the cause of this phenomenon and show that this non-monotonicity is universal for this type of magnetic reorientation transitions.


Magnetic Neutron Scattering Study of Rare-Earth Titanates
SAJNA HAMEED (Presenter), School of Physics and Astronomy, University of Minnesota, SAMI EL-KHATIB, Chemical Engineering and Materials Science, University of Minnesota, JOSEPH JOE, School of Physics and Astronomy, University of Minnesota, KARL OLSON, Chemical Engineering and Materials Science, University of Minnesota, MASAAKI MATSUDA, SONGXUE CHI, TAO HONG, DANIEL PAJEROWSKI, TRAVIS J WILLIAMS, Oak Ridge National Laboratory, JOHN BARKER, NIST Center for Neutron Research, CHRIS LEIGHTON, Chemical Engineering and Materials Science, University of Minnesota, MARTIN GREVEN, School of Physics and Astronomy, University of Minnesota — The Mott-insulating rare-earth (R) titanates (RTiO3) are known to host ferromagnetic-antiferromagnetic transitions in solid-solution systems such as Y1-xLaxTiO3, as well as metal-insulator transitions in charge carrier-doped systems such as Y1-xCa_xTiO3. Neutron scattering studies have been largely restricted to the undoped YTiO3 and LaTiO3. Here, we report on our neutron scattering work on the magnetic order and excitations in the doped systems Y1-xLaxTiO3 and Y1-xCa_xTiO3, using triple-axis spectrometry and small-angle neutron scattering (SANS). We find a strong reduction in the transition temperature and ordered magnetic moment, but accompanied by very little change in the spin-wave dispersion in the Y1-xLaxTiO3 system as we approach the critical doping x~0.3. SANS results suggest a rotation of the easy axis with substitution, development of magnetic inhomogeneities on ~10 nm scales, and distinct changes in critical scattering as the magnetic crossover is approached. These results suggest significant changes in the magnetic ground state as one approaches the crossover. Initial studies on the Y1-xCa_xTiO3 system will also be reported.

*Work supported by the Department of Energy through the University of Minnesota Center for Quantum Materials under DE-SC0016371.

Phase diagram of emergent orders of rare-earth nickelates
MINJAЕ KIM (Presenter), GABRIEL KOTLIAR, Rutgers University, New Brunswick, ANTOINE GEORGES, College de France — Phase diagram of Rare-earth nickelates, thin films and heterostructures, is a paradigmatic problem of strongly correlated material having strong coupling in between spin, orbital, lattice degrees of freedom. [1] Recently, there have been suggestions on possible new emergent orders includes antiferromagnetism. [2] In this talk, based on low energy hamiltonian of eg manifold, [3] we discussed possible emergent orders of Rare-earth nickelates includes superconductivity, charge disproportionation, and magnetism. These emergent orders would be accessible by tuning material parameters such as interaction strength and effective crystal field.

ALEXANDER HAMPEL (Presenter), CLAUDE EDERER, Materials Theory, ETH Zurich — Rare-earth nickelates exhibit a metal-insulator transition (MIT) accompanied by a structural distortion that breaks the symmetry between formerly equivalent Ni sites. The quantitative theoretical description of this coupled electronic-structural instability is extremely challenging. Here, we address this issue by simultaneously taking into account both structural and electronic degrees of freedom using a charge self-consistent combination of density functional theory and dynamical mean-field theory, together with screened interaction parameters obtained from the constrained random phase approximation. Our total energy calculations show that the coupling to an electronic instability towards a charge disproportionated insulating state is crucial to stabilize the structural distortion, leading to a clear first order character of the coupled transition. Decreasing octahedral rotations across the series suppress this electronic instability weakening the correlation effects responsible for the MIT. Our approach allows to obtain accurate values for the structural distortion and thus facilitates a comprehensive understanding of the complex interplay between structural properties and electronic correlation effects across the nickelate series.

STEPAN FOMICHEV (Presenter), MONA INESA BERCIU, University of British Columbia, GINHYAT KHALULLIN, Max-Planck-Institut FKF, Stuttgart — We study the magnetic order appearing in the rare-earth nickelates at low temperatures, the exact nature of which is still debated vigorously in the literature. While there is an established link between the metal-insulator transition and lattice distortions in the nickelates, to our knowledge there has been little work on the impact of lattice distortions on the magnetic order, e.g. whether they favor some orders over others. To address this, we consider a two-band Hubbard model for the nickelates, coupled to the lattice distortions (which are treated semiclassically), and use the Hartree-Fock approximation to find the resulting phase diagram. Aside from quantitatively demonstrating how lattice distortions drive bond disproportionation, we find that a variety of 4-site magnetic orders are self-consistent within the model, including both collinear and non-collinear orders. However, in our model a magnetic order can only couple to the lattice distortions if there is an asymmetry in average charge occupation of neighbouring sites. As a result, we find that coupling to the lattice distortions broadly favors the collinear 1-o-1-o order in large sectors of the parameter space.

XINWEI LI (Presenter), Department of Electrical and Computer Engineering, Rice University, MOTOAKI BAMBA, Department of Materials Engineering Science, Osaka University, NING YUAN, Department of Physics, Shanghai University, QI ZHANG, Argonne National Laboratory, YAGE ZHAO, Department of Physics, Rice University, MAOLIN XIONG, KAI XI, ZUANMING JIN, WEI REN, GUOHONG MA, SHIXUN CAO, Department of Physics, Shanghai University, DMITRY TURCHINOVICH, Fakultät für Physik, Universität Duisburg-Essen, JUNICHIRO KONO, Department of Electrical and Computer Engineering, Rice University — Dicke cooperativity is a many-body effect in quantum optics describing the process of N oscillators in a photonic cavity developing macroscopic coherence amongst themselves by interacting with a single light field, while exhibiting a $N^{1/2}$ enhancement of the light-matter coupling rate. Here, we have discovered that cooperatively enhanced coupling similar to this canonical light-matter interaction effect occurs in a magnetic solid in the form of matter-matter interaction. We studied an ErFeO$_3$ single crystal with terahertz magnetospectroscopy at low temperatures and high magnetic fields, and discovered that the exchange coupling of the paramagnetic Er$^{3+}$ ions with a Fe$^{3+}$ magnon field within the crystal quantitatively follows the scaling behavior expected by the Dicke cooperativity effect. This scaling behavior also enables quantitative determination of the Er$^{3+}$-Fe$^{3+}$ exchange coupling coefficients. Our finding provides a novel route for understanding, controlling, or predicting new phases of condensed matter using concepts and tools available in quantum optics.

JASON WHITE, KISHAN SINHA, XIAOSHAN XU (Presenter), University of Nebraska - Lincoln — We have studied crystal structure and magnetic properties of Sc-doped rare earth ferrites R$_1$-xScFeO$_3$ (R=Ho, Er, Yb). For R=Ho, pure structural phases, orthorhombic, garnet, and bixbyte, were observed for $x=0$, $0.5$, and $1$ respectively. Pure garnet phase was also found for $x=0.5$ and R=Er. In contrast, when $x=0.5$ and R=Yb, mixed phases dominated with hexagonal and garnet were observed. Magnetic properties of Ho$_{0.55}$Sc$_{0.5}$FeO$_3$ show incomplete magnetic compensation, with a magnetization minimum at a temperature lower than the compensation temperature of the undoped Ho-Fe-O garnet. These results indicate that Sc atoms occupy both Fe and rare earth sites due to the intermediate atomic radius.

*This work was supported by the NSF DMR-1454618.
**4:06PM V39.00009: Optimizing the intrinsic magnetic properties of REFe₁₂₋ₓMₓ phases**

HEIKE HERPER (Presenter), OLGA VEKILOVA, OLLE ERIKSSON, Uppsala University — Collecting energy from renewable resources, using e.g. wind power plants has become important and goes hand in hand with a growing demand for new permanent magnets (PM) with magnetic performance comparable to Nd-Fe-B magnets. A key task is to identify new PM with less rare earth (RE). Systems with ThMn₁₂ structure are of special interest. They have the lowest RE concentration of all known phases. However, Fe-based 1:12 systems with light RE need a phase stabilizer which goes on the Fe sites. Two types have been studied, (Nd₁₋ₓYₓ)Fe₁₂₋ₓTiₓ and SmFe₁₂₋ₓVₓ, using state of the art density functional theory methods (VASP; FP LMTO RSPt). The phase stability and the magnetic properties were calculated depending on the Ti and V concentration. Aiming to reduce the RE amount the performance depending on the Nd/Y ratio was monitored. We find that the Nd-Y (Sm) system is stable down to y = 0.5 (y=1) which leads to an increase of the magnetization by 17% compared to the commonly used concentrations of Ti (V). In view of the MAE a replacement of Nd by Y turned out to be preferable over a reduction of Ti. MAE values of 1.3 MJ/m³ ((NdY)Fe₁₁Ti) and 1.7 MJ/m³ (SmFe₁₁V) are predicted. The latter could be verified in recent experiments.

*Support by NOVAMAG (EU686056) and VR (SE), STandUP (SE).

**4:18PM V39.00010: Nanoscale characterization of magnetic microstructure in Gd₃Fe₅O₁₂**

SAMUEL MARKS (Presenter), Materials Science and Engineering, University of Wisconsin - Madison, DANNY MANNIX, MAX IV, Lund, Sweden, STEPHAN GEPRÄGS, Walther Meißner Institute, Munich, Germany, PAUL G EVANS, Materials Science and Engineering, University of Wisconsin - Madison, DINA CARBONE, MAX IV, Lund, Sweden — A key barrier to the understanding of magnetic phenomena and design of functional magnetic materials is the limited scope of nanoscale characterization of magnetic microstructure. We utilize scanning x-ray diffraction microscopy to image the magnetic domain morphology in rare-earth iron garnets as a function of temperature using an x-ray wave plate and zone plate focusing optics to generate a 100 nm beam of circularly polarized synchrotron light. Rare earth iron garnets such as Gd₃Fe₅O₁₂ are magnetic systems that can exhibit spin Seebeck effect (SSE) voltage generation with an efficiency that could depend on the morphology of the magnetic domain structures. We have obtained linear and circular x-ray magnetic dichroism maps of the micron- to submicron-scale distributions of magnetic domains recorded in a prototype SSE device composed of epitaxial layers of Gd₃Fe₅O₁₂ capped with 10 nm of Pt for temperatures ranging from 4 K to 250 K. These results bring insight into the relationship between the temperature-dependent magnetic domain morphology and the efficiency of SSE devices based on rare-earth iron garnets.

**4:30PM V39.00011: Large magneto-crystalline anisotropy in strain-tuned epitaxial BiYIG thick films**

RAVINDER KUMAR (Presenter), BISWANATH SAMANTARAY, ZAKIR HOSSAIN, Physics, Indian Institute of Technology Kanpur — Bi-doped Yttrium Iron Garnet (Bi:YIG) with large Magneto-optical (MO) activity and low optical losses still needs to get probed for its magnetization dynamics. The fact that the ablation laser fluence strongly affects the lattice constant of the films, was used to grow two sets of BiYIG/GGG(111) samples with different strain states. The set-A films with lower thicknesses (10.2, 37.0, and, 92.5 nm), grown using ∼ 1 J/cm² laser fluence, show large magnetocrystalline anisotropy (MCA) due to larger rhombohedral distortion induced strain. The set-B films with larger thicknesses (120 and 150 nm) grown using higher laser fluence of ∼ 2 J/cm² show large strain irrespective of film thicknesses and large magnitude of MCA, comparable to the value of a film as-thin-as ∼ 37 nm from Set-A. Interestingly, the substitution of strong spin orbit coupling Bi³⁺ ions enhances the magnetoelastic coupling (MEC) but weakly affects the precessional damping (∼ 9.7×10⁻⁴). Coexistence of two mutually exclusive parameters i.e., low precessional damping and strong MEC, combined with large MO activity and large MCA in BiYIG films may provide a possible material platform for light dependent magnonics and other spintronics applications.

*IIT Kanpur*
Magnetic and Magnetocaloric Properties of (Nd$_{1-x}$Ce$_x$)YFe$_{15}$ Alloys* BISHNU DAHAL, PARASHU KHAREL (Presenter), THOMAS OTT, Physics, South Dakota State University, WENYONG ZHANG, Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE, United States, SHAH VALLOPPILLY, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE, United States, YUNG MOO HUH, Physics, South Dakota State University, RALPH SKOMSKI, DAVID SELLMYER, Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE, United States — Magnetocaloric materials exhibiting a second-order phase transition (SOP) near room temperature have attracted much attention because these materials are free from magnetic and thermal hysteresis, and may show large cooling efficiency and moderate magnetic entropy change. We have investigated (Nd$_{1-x}$Ce$_x$)YFe$_{15}$ (x = 0 - 1) alloys prepared by arc melting and vacuum annealing. The x-ray diffraction patterns analyzed using the Rietveld method shows that the samples crystallized in the rhombohedral Th$_2$Zn$_{17}$-type structure with space group R-3m. The thermomagnetic curves $M(T)$ measured at $\mu_0H = 1T$ show smooth SOP with Curie temperatures near 300 K. The values of peak magnetic entropy change ($\Delta S_M,\text{max}$) and relative cooling power (RCP) measured at 3 T increase with increasing Nd concentration reaching 4.20 Jkg$^{-1}$K$^{-1}$ and 285 Jkg$^{-1}$ for (Nd$_{0.7}$Ce$_{0.3}$)YFe$_{15}$. The measured $\Delta S_M$ and RCP values are relatively high as compared to those of other Gd-free compounds showing magnetocaloric effect due to SOFT near room temperature. This suggests that the (Nd$_{1-x}$Ce$_x$)YFe$_{15}$ alloys have potential for room temperature magnetic refrigeration.

*Research at Nebraska is supported by USDOE (DE-FG02-04ER46152), NSF (NNCI-1542182), and NCMN-NRI.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V40 GMAG DMP DCOMP: Magnetic Oxides: Theory BCEC 208 - David Mandrus, Oak Ridge National Lab -
Tag(s): Focus

2:30PM V40.00001: Intertwined orbital and magnetic order in 5d$^1$ and 5d$^2$ Double Perovskite Mott Insulators* [Invited] MOHIT RANDERIA (Presenter), Ohio State University — In this talk I summarize our work on understanding the unusual properties of Mott-insulating double perovskites $A_2BB'O_6$ where the B' sites are 5d magnetic ions with either 1 or 2 electrons in t$_{2g}$ orbitals and the B sites are non-magnetic. Our theory is motivated by several experimental puzzles, including: (i) Why do almost all cubic 5d$^1$ materials exhibit ferromagnetic (FM) order, rare in Mott insulators, while all the 5d$^2$ materials have antiferromagnetic (AFM) ground states? (ii) Why is only partial (log 2) entropy recovered above the magnetic transition, rather than the expected log 4 for $j = 3/2$, in cubic 5d$^1$ materials? (iii) Why do the cubic 5d$^1$ materials exhibit a high temperature magnetic susceptibility that deviates from a Curie-Weiss form? We derive and analyze low-energy effective Hamiltonians for these systems that include spin-orbit coupling, superexchange, inter-site Coulomb interactions and Hund's coupling. We predict that novel orbital order sets in at a high temperature $T_0$ and strongly constrains the non-collinear magnetic order that appears at a much lower $T_c$. Our results allow us to understand all the puzzles noted above and make predictions for new experiments. This research was done in collaboration with W. Zhang, C. Svoboda, P. M. Woodward and N. Trivedi.

*Supported by the Center for Emergent Materials, an NSF MRSEC, under Award Number DMR-1420451.

3:06PM V40.00002: Entangled spin orbital order in 5d$^1$ and 5d$^2$ Double Pervoskite Mott Insulators* NANDINI TRIVEDI (Presenter), WENJUAN ZHANG, CHRISTOPHER SVOBODA, MOHIT RANDERIA, Department of Physics, The Ohio State University — We theoretically investigate the unusual properties of Mott-insulating double perovskites $A_2BB'O_6$ where the magnetic B' ions have 1 or 2 electrons in the 5d shell and the B sites are non-magnetic. We derive a low-energy effective Hamiltonian that includes spin-orbit coupling, super-exchange, inter-site Coulomb interactions and Hund's coupling, and analyze it within mean field theory. We show that orbital order sets in at a high temperature $T_0$ and strongly constrains the non-collinear magnetic order that appears at a much lower $T_c$. Our results give insight into several experimental puzzles. The prediction of orbital ordering well above $T_c$ explains the puzzle of the missing entropy above the magnetic transition. Orbital order is also responsible for the deviations of the high temperature magnetic susceptibility from a Curie-Weiss form. Finally, we show why cubic 5d$^1$ materials most often exhibit canted ferromagnetism, which is rare in Mott insulators, while the 5d$^2$ and distorted 5d$^1$ materials are all antiferromagnetically ordered.

*This research is supported by the Center for Emergent Materials, an NSF MRSEC, under Award Number DMR-1420451.
3:18PM V40.00003: Deterioration of Spin-Orbit Transitions in Mott Insulating CoO  PAUL SARTE (Presenter), Chemistry, University of Edinburgh, ROGER A COWLEY, Physics, University of Oxford, KA HOU HONG, Chemistry, University of Edinburgh, MANILA SONGVILAY, Physics, University of Edinburgh, RUSSELL A EWINGS, ISIS Facility, Rutherford Appleton Laboratory, DHARMALINGAM PRABHAKARAN, Physics, University of Oxford, ZAHRA-SADAT YAMANI, WILLIAM J L BUYERS, Chalk River Laboratories, JOHN PAUL ATTFIELD, Chemistry, University of Edinburgh, CHRIS STOCK, Physics, University of Edinburgh — Despite a myriad of measurements spanning several decades, the low energy magnetic excitations of the classical Mott insulator CoO in the Néel regime are still poorly understood. As a result of the strong molecular-field induced entanglement of various $j_{\text{eff}}$ manifolds, the establishment of a clear model for the low energy magnetic excitation spectrum of this deceptively simple monoxide has proven intractable using conventional spin wave approaches so far. Having extracted estimates for the exchange constants via the dilute monoxide Co$_{0.03}$Mg$_{0.97}$O (Sarte et al. PRB 98, 024415 (2018)), we have employed a random phase-type approximation in the method of Green's functions to model the rich low energy magnetic excitation spectrum of antiferromagnetically ordered CoO. The multi-level spin wave model successfully accounts for the temporally sharp spin-orbit transitions consistent with orbital ordering observed near the magnetic zone center. However, the model fails to account for higher energy transfers, where well-defined spin waves are replaced by energy and momentum broadened excitations, characterized by steeply dispersive columns of scattering. The failure of the model and breakdown of spin-orbit excitations are discussed in terms of coupling to a higher energy process.

3:30PM V40.00004: Hund nodal line semimetals: The case of twisted magnetic phase in the double-exchange model*  RICHARD GEILHUFÉ (Presenter), NORDITA, Nordic Institute for Theoretical Physics, Stockholm University and KTH, Stockholm, Sweden, FRANCISCO GUINEA, Imdea Nanoscience, Madrid, Spain, VLADIMIR JURICIC, NORDITA, Nordic Institute for Theoretical Physics, Stockholm University and KTH, Stockholm, Sweden — In this talk, we discuss a class of topological metals, which we dub Hund nodal line semimetals, arising from the strong Coulomb interaction encoded in the Hund’s coupling between itinerant electrons and localized spins [1]. We consider a particular twisted spin configuration, which is realized in the double exchange model describing the manganite oxides. As we show, the resulting effective tetragonal lattice of electrons with hoppings tied to the local spin features an antiunitary non-symmorphic symmetry that in turn, together with another non-symmorphic but unitary glide mirror symmetry protects crossings of a double pair of bands along a high-symmetry line on the Brillouin zone boundary. We also discuss the stability of Hund nodal line semimetal with respect to symmetry breaking from various perturbations of the twisted phase. Our results motivate further studies of other realizations of this state of matter, for instance in different spin backgrounds and properties of its drumhead surface states.


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3:42PM V40.00005: Structural and electronic properties of doped NiO from density functional theory and quantum Monte Carlo simulations*  OLLE HEINONEN (Presenter), HYEONDEOK SHIN, Argonne National Laboratory, JARON KROGEL, PANCHAPAKESAN GANESH, Oak Ridge National Laboratory, FRIEDERIKE WROBEL, ANAND BHATTACHARYA, Argonne National Laboratory, PAUL KENT, Oak Ridge National Laboratory — NiO is a prototypical strongly correlated oxide. According to band filling, it should be a metal, but correlations drive the ground state to an antiferromagnetic insulator. The general question of how doping affects the electronic – and chemical – structure of correlated oxides is of great fundamental interest, but also important for the realization of electronics,“Motttronics”, based on correlated materials. We are studying hole- and electron-doped NiO using density functional theory (DFT) methods and much more accurate quantum Monte Carlo simulations and compare our results directly with experimental results on high-quality thin films grown by molecular beam epitaxy. One surprising result is that DFT in all flavors we have used fails to properly account for the K-O bond distance, and underestimates it by over 0.3 A compared to analysis based on extended X-ray absorption fine structure. Preliminary results using QMC show much better agreement with experiments, indicating that correlation effects beyond DFT have a dramatic effect on the energy landscape around the dopant.

*Supported by the U.S. DOE, Office of Science, BES, Materials Sciences and Engineering Division, as part of the Comp. Materials Sciences Program and Center for Predictive Simulation of Functional Materials.
3:54PM V40.00006: First Principles Electronic Structure Study of Ca$_2$CuO$_2$Cl$_2$  MATTHEW MATZELLE (Presenter), Northeastern University, CHENG HU, Chinese Academy of Sciences (CAS), CHRISTOPHER LANE, ROBERT MARKIEWICZ, Northeastern University, JIANWEI SUN, Tulane University, XINGJIANG ZHOU, Chinese Academy of Sciences (CAS), ARUN BANSIL, Northeastern University — We discuss Density Functional Theory (DFT) based results on the oxychloride cuprate Ca$_2$CuO$_2$Cl$_2$ (CCOC), which are obtained by using the recently constructed Strongly-Constrained-and-Appropriately-Normed (SCAN) functional. Theoretical results are compared and contrasted with the corresponding angle-resolved photoemission (ARPES) measurements. Previous first-principles DFT studies have found the ground state of the half-filled CCOC to be metallic in sharp disagreement with the experimentally observed insulating state. Although the insulating behavior can be captured by introducing an empirical Hubbard U parameter in first-principles computations, that reduces the predictive power of the theory. In sharp contrast, the SCAN functional yields the antiferromagnetic insulator phase with a gap in good agreement with optical conductivity studies without the need to invoke the Hubbard U. We also discuss how the electronic structure of CCOC evolves with hole doping.

4:06PM V40.00007: Strange metallicity in the doped Hubbard model EDWIN HUANG (Presenter), RYAN SHEPPARD, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford University — Strange or bad metallic transport, defined by its incompatibility with conventional quasiparticle pictures, is a theme common to strongly correlated materials and ubiquitous in many high temperature superconductors. The Hubbard model represents a minimal starting point for modeling strongly correlated systems. Here we demonstrate strange metallic transport in the doped two-dimensional Hubbard model using determinantal quantum Monte Carlo calculations. Over a wide range of doping, we observe resistivities exceeding the Mott-Ioffe-Regel limit with linear temperature dependence. The temperatures of our calculations extend to as low as 1/40 the non-interacting bandwidth, placing our findings in the degenerate regime relevant to experimental observations of strange metallicity. Our results provide a foundation for connecting theories of strange metals to models of strongly correlated materials.

4:18PM V40.00008: A two-pronged approach to the cuprate pseudogap: A comparison of mode-coupling and first-principles (SCAN) results ROBERT MARKIEWICZ (Presenter), CHRISTOPHER LANE, Northeastern, YUBO ZHANG, JAMES FURNESS, Tulane, BERNARDO BARBIELLINI, Lappeenranta/Northeastern, ARUN BANSIL, Northeastern, JIANWEI SUN, Tulane — Density functional theory using the new SCAN exchange-correlation functional has successfully described the antiferromagnetic ground states of undoped cuprate superconductors. In YBa$_2$Cu$_3$O$_7$ (YBCO$_7$), the energy landscape involves a competition between many different nearly degenerate states – a mixture of antiferromagnetic and stripe states[1]. The organizing principle of these states remains Mott-like: the lower-energy phases tend to have a larger planar copper magnetic moment. In particular, all these phases have substantially lower energy than the nonmagnetic Fermi liquid phase found in most previous DFT calculations, showing that it can play no role in the low-energy properties of YBCO$_7$. The contrasting behaviors of YBCO$_6$ and YBCO$_7$ are reminiscent of the Mott-Slater crossover found in a mode-coupling model of the cuprates[2]. I will demonstrate how these two approaches illuminate each other, leading to a picture of the pseudogap as a gapped paramagnetic metal with only short-range order (SRO) over a broad temperature range. This work provides a realistic model for the cuprate pseudogap phase with implications for superconducting pairing.


4:30PM V40.00009: Tunable band gaps from anion ordering and octahedral tilting in oxyfluorides* RICHARD J SABALLOS (Presenter), JAMES M RONDINELLI, Northwestern University — Heteroanionic materials are currently receiving increased interest because they may support superior functionality than single-anion materials [1]. In perovskite structures, anion ordering combined with octahedral tilting provides new degrees-of-freedom (DOFs) from which to manipulate the chemical, physical and electronic properties. This control has been shown to tune the band gap in oxynitrides, but oxyfluorides remain underexplored [2,3]. Here we discuss the results of first-principles calculations on the experimentally known wide-bandgap semiconductor, KNaNbOF5 [4], and show that octahedral tilting and anion ordering can be used to tune the band gap. We show how the combination of these DOFs make it possible to decrease the band gap so it resides in the visible range. Finally, these results will be used to propose a design strategy for creating novel photovoltaic materials.


*This work was supported by the National Science Foundation’s MRSEC program (DMR-1720139.) at the Materials Research Center of Northwestern University.
Four-spin ring interaction as a source of unconventional magnetic orders in orthorhombic perovskite manganites. Natalya Fedorova (Presenter), Amadé Bortis, Christoph Findler, Nicola Spaldin, ETH Zurich — We use ab initio electronic structure calculations and Monte Carlo simulations to investigate the magnetic and ferroelectric properties of bulk orthorhombic HoMnO₃ and ErMnO₃. Our goals are to explain the inconsistencies in the measured magnetic properties of the orthorhombic perovskite manganites (o-RMnO₃) with small rare-earth (R) cations or Y, as well as the contradictions between the directions and amplitudes of the electric polarizations reported by different experimental groups. We find that several unconventional magnetic orders (so-called w-spiral, H-AFM and I-AFM) can be stabilized in these materials due to strong four-spin ring exchange interactions. We show that the presence of these orders resolves the contradictions in the measured magnetic and ferroelectric properties of o-RMnO₃.

*Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund, for support of this research under contract 56764-UNI10.

Spin-orbital-entangled \( J_{\text{eff}} = 1/2 \) state in 3d transition metal oxide CuAl₂O₄. Choong Hyun Kim (Presenter), Hwanbeom Cho, Santu Baidya, Center for Correlated Electron Systems, Institute for Basic Science & Seoul National University, Vladimir Gapontsev, Sergey Streltsov, M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Daniel Khomskii, Universität zu Köln, Je-Guen Park, Center for Correlated Electron Systems, Institute for Basic Science & Seoul National University, Ara Go, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Hosub Jin, Ulsan National Institute of Science and Technology — We show that CuAl₂O₄ spinel can host a spin-orbital-entangled \( J_{\text{eff}} = 1/2 \) state. During the long history of the 3d transition metal study, spin-orbit coupling has never been a dominating energy scale. Here we propose on the CuAl₂O₄ as the first example of a \( J_{\text{eff}} = 1/2 \) Mott insulator in 3d transition metal compounds. From single crystal X-ray diffraction data, our CuAl₂O₄ is confirmed to have cubic structure without Jahn-Teller distortion and it is consistent with first-principles total energy calculations. Density functional theory combined with dynamical mean field theory calculations reveal that the \( J_{\text{eff}} = 1/2 \) state survives the competition with the orbital-momentum-quenched \( S=1/2 \) state with the help of strong electron correlation.

*This work was supported by Institute for Basic Science (IBS) in Korea (Grant No. IBS-R009-D1 (CHK, SB), IBS-R024-D1 (AG), IBS-R009-G1 (HC, JGP)), the Basic Science Research Program of the National Research Foundation (NRF) of Korea under Grant No. 2016R1D1A1B03933255 and 2017M3D1A1040828 (HJ).

Multi-loop contributions in the pseudo-fermion functional renormalization group for quantum spin systems: implementation and consequences. Tobias Müller (Presenter), Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, Yasin Iqbal, Indian Institute of Technology Madras, Johannes Reuther, Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Ronny Thomale, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg — We extend the pseudo-fermion functional renormalization group (PFFRG) treatment of quantum spin systems by including diagrammatic higher loop contributions into the renormalization group flow. This allows us to consistently account for all contributions of parquet-type diagrams in the two-particle vertex and self-energy derivatives within the two-particle truncated PFFRG flow. We will discuss the impact of these corrections in different quantum spin models within PFFRG, especially in the light of the Mermin-Wagner theorem.

*We acknowledge funding through ERC-StG-TOPOLECTRICS-336012 and DFG-SFB 1170 Project B04.
2:30PM V41.00001: Reservoir Computing with Random Skyrmion Fabrics [Invited] DANIELE PINNA (Presenter), Johannes Gutenberg University — The topologically protected magnetic spin configurations known as skyrmions offer promising applications due to their stability, mobility and localization. Thanks to their many nanoscale properties, skyrmions have been shown to be promising in many applications ranging from non-volatile memory and spintronic logic devices, to enabling the implementation of unconventional computational standards such as Stochastic computing. In this talk we will discuss how a random skyrmion \``fabric`` composed of skyrmion clusters embedded in a magnetic substrate can be effectively employed to implement a functional Reservoir Computing device for recognizing and predicting spatio-temporal events. This is achieved by leveraging the nonlinear resistive response of the individual skyrmions arising from their current dependent anisotropic magneto-resistance effect (AMR). Complex time-varying current signals injected via contacts into the magnetic substrate are shown to be modulated nonlinearly by the fabric’s AMR due to the current distribution following paths of least resistance as it traverses the geometry. By tracking resistances across multiple input and output contacts, we show how the instantaneous current distribution effectively carries temporally correlated information about the injected signal. This in turn allows us to numerically demonstrate simple pattern recognition. We argue that the fundamental ingredients for such a device to work are threefold: i) Concurrent probing of the magnetic state; ii) stable ground state when forcings are removed; iii) nonlinear response to input forcing. Whereas we demonstrate this by employing skyrmion fabrics, the basic ingredients should be general enough to spur the interest of the greater magnetism and magnetic materials community to explore novel reservoir computing systems.

3:06PM V41.00002: Rare Earth-Transition Metal Alloys as Promising Materials for Small Skyrmions and Ultrafast Chiral Spin Texture Dynamics LUCAS CARETTA (Presenter), MAXWELL MANN, FELIX BUETTNER, KOHEI UEDE, CAN AVCI, ETHAN ROSENBERG, JACKSON BAUER, Massachusetts Institute of Technology, BASTIAN PFALU, CHRISTIAN GÜNThER, PIET HESSING, Max-Born-Institut, ALEXANDRA CHURIKOVA, Massachusetts Institute of Technology, CHRISTOPHER KLOSE, MICHAEL SCHNEIDER, DIETER ENGEL, Max-Born-Institut, COLIN MARCUS, DAVID BONO, Massachusetts Institute of Technology, BASTIAN PFAU, CHRISTIAN GÜNTHER, PIET HESSING, Max-Born-Institut, ALEXANDRA CHURIKOVA, Massachusetts Institute of Technology, CHRISTOPHER KLOSE, MICHAEL SCHNEIDER, DIETER ENGEL, Max-Born-Institut, COLIN MARCUS, DAVID BONO, Massachusetts Institute of Technology — Spintronics aims to understand and control spins on the nanoscale and should enable next-generation data storage and logic devices. One technological and scientific key challenge is to stabilize small spin textures and to manipulate them efficiently with high speeds [1-3]. Inspired by hard disk materials, research has primarily focused on ferromagnetic materials, but these materials show fundamental limits for speed and size [4-6], calling for radically different ideas [4-7]. Here, we demonstrate that compensated ferrimagnets are not affected by these limits. We realize a current-driven domain wall velocity of over 1 km/s near the angular momentum compensation temperature (T_A) and room-temperature stable skyrmions with minimum observed diameters approaching ~10 nm near magnetic compensation (T_M). We present theory explaining these observations and demonstrate that high-speed, high-density spintronics devices based on current-driven spin textures can be realized using materials where T_A and T_M are close together.

Skyrmion lattice with a giant topological Hall effect in a frustrated triangular-lattice magnet Gd$_2$PdSi$_3$*  

TAKASHI KURUMAJI (Presenter), Physics, MIT, TARO NAKAJIMA, MAX HIRSCHBERGER, AKIKO KIKKAWA, RIKEN Center for Emergent Matter Science, YUICHI YAMASAKI, University of Tokyo, HAJIME SAGAYAMA, HIRONORI NAKAO, KEK, YASUJIRO TAGUCHI, RIKEN Center for Emergent Matter Science, TAKAHISA ARIMA, University of Tokyo, YOSHINORI TOKURA, RIKEN Center for Emergent Matter Science — Frustrated magnets provide abundant opportunities for discovering complex spin textures, which sometimes yield unconventional electromagnetic responses in correlated electron systems. It is theoretically predicted that magnetic frustration may also promote a topologically nontrivial spin state [1], i.e., magnetic skyrmions. Empirically, however, skyrmions are essentially concomitant with noncentrosymmetric lattice structures or interfacial symmetry-breaking heterostructures [2]. Here, we report the emergence of a Bloch-type skyrmion state in a frustrated centrosymmetric triangular-lattice magnet Gd$_2$PdSi$_3$ [3]. We identified the field-induced skyrmion phase via a giant topological Hall response, which is further corroborated by the observation of in-plane spin modulation probed by resonant x-ray scattering. Our results exemplify a new platform of magnetic frustration for producing topological spin textures endowed with emergent electrodynamics in centrosymmetric magnets.


*This research was supported in part by JSPS Grant-in-Aid No. 24224009, No. 17K14351, and No. 16H05990, and by PRESTO No. JPMJPR177A from JST.

Observation of topological Hall effect in amorphous Fe/Gd heterostructures with asymmetric Bloch-type domain wall chirality population.

SERGIO MONTOYA (Presenter), Space and Naval Warfare Systems Center Pacific, JORDAN J CHESS, BENJAMIN J MCMORRAN, Physics, University of Oregon, ERIC FULLERTON, Electrical and Computer Engineering, University of California San Diego — The non-trivial topological nature of chiral magnetic spin textures results in novel electromagnetic properties, such as the topological Hall effect (THE) which commonly appears as an anomaly in the Hall resistivity. So far, the THE has been primarily observed in magnetic crystals lacking inversion symmetry (e.g. MnSi [1], MnGe [2], SrRuO$_3$-SrIO$_3$[3]). In these systems, the magnetic spin textures possess a single Bloch- or Néel-type chirality that is set by either a bulk or an interfacial antisymmetric exchange interaction, commonly known as Dzyaloshinskii-Moriya interaction.

We report the observation of a THE in amorphous rare-earth transition-metal heterostructures with perpendicular magnetic anisotropy that possess a coexistence of left and right chiral Bloch-type domain walls with unequal population distribution. A combination of real-space observations by Lorentz TEM, magnetometry and transport measurements reveal one can engineer amorphous thin-film materials with a controllable THE, as will be discussed, based on temperature dependent studies on several heterostructures.


Single magnetic skyrmion creation, detection, and dynamics within a magnetic tunnel junction*  

NICHOLAS PENTHORN (Presenter), RAJAPAKSAYALAGE N RAJAPAKSE, Physics & Astronomy, University of California, Los Angeles, XIAOJIE HAO, ZIHUI WANG, YIMING HUAI, Avalanche Technology, HONGWEN JIANG, Physics & Astronomy, University of California, Los Angeles — We experimentally demonstrate the deterministic creation of a stable topological spin texture in the free layer of a magnetic tunnel junction at cryogenic temperatures. Through simultaneous measurements of tunnel magnetoresistance and spin-polarized current-induced magnetic resonance, we find that the spin texture is characterized by a field-dependent intermediate junction resistance and a unique magnetic resonance signature. Comparing our findings to micromagnetic simulations, we confirm that the spin texture transition is best described by the nucleation of a single Bloch-type skyrmion in the free layer, aided by a spatially nonuniform stray field from surrounding magnetic layers. We subsequently identify the skyrmion breathing mode in the resonance spectrum and obtain an estimate for the skyrmion diameter at zero field of 75 nm. This result is the first confirmation that magnetic tunnel junctions are viable candidates for skyrmion-based memory and logic architectures could lead to non-invasive, on-chip skyrmion measurement and detection.

*This work is supported by the NSF under grant # DMR-1809155 and by FAME, a STARnet center.
3:54PM V41.00006: Sluggish steady flow of skyrmion lattice in a confined geometry  TAKURO SATO (Presenter), WATARU KOSHIBAE, AKIKO KIKKAWA, TOMOYUKI YOKOUCHI, RIKEN Center for Emergent Matter Science (CEMS), HIROSHI OIKE, The University of Tokyo, YASUJIRO TAGUCHI, NAOTO NAGAOSA, YOSHINORI TOKURA, FUMITAKA KAGAWA, RIKEN Center for Emergent Matter Science (CEMS) — An aggregate of magnetic skyrmions\textsuperscript{1,2}, topologically protected particlelike objects, is an emerging exotic fluid that flows under electric current\textsuperscript{3,4}. From a hydrodynamics point of view, the skyrmion fluid is peculiar in that its steady flow does not necessarily require a closed-loop skyrmion circuit. However, it remains largely unclear how this peculiarity is involved in the skyrmion steady-flow dynamics. Here, we show that the skyrmion steady flow dramatically slows down when the influence of system edges is not negligible. In the micrometre-sized MnSi, the steady-flow velocity is anomalously slow, as evidenced by the observation of resistance narrow-band noise with 10–10\textsuperscript{4} Hz, and its temperature evolution suggests that the steady flow entails thermally activated processes, which are due most likely to the skyrmion creation and annihilation at the edges. Moreover, numerical simulations reveal that the edges limit the skyrmion motion. Thus, our findings capture a vital role of the edges on the skyrmion steady flow, especially in a microstructure.


4:06PM V41.00007: Visualizing the dynamics of sub-100 nm Néel Skyrmions in Multilayer Nanowires* ANTHONY K C TAN (Presenter), Atomic, Mesoscopic and Optical Physics (AMOP) Group, Cavendish Laboratory, University of Cambridge, PIN HO, LISEN HUANG, JAMES LOUREMBAM, SARJOOSING GOOLAUP, ANJAN SOUMYANARAYANAN, Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR) — The emergence of room temperature skyrmions in technologically-relevant multilayers has intensified efforts towards realizing these topologically stable, nanoscale spin structures for next generation technologies, in particular, neuromorphic computing, Internet of Things. Of great interest is the lateral manipulation of skyrmions on a Racetrack, which builds on their deterministic response to current-induced spin torques in nanowires. Thus far, a clear understanding of the factors governing the dynamics of small (sub-100 nm) skyrmions in granular films remains to be established. Here we utilize magnetic force microscopy to investigate the collective dynamics of a dense skyrmion array with individual speeds up to 24ms\textsuperscript{-1}, in 2um-wide Pt/Co/MgO nanowires. By examining \textasciitilde 2x10\textsuperscript{4} instances of skyrmion motion, we observe several emergent behaviours including the interplay of edge confinement and skyrmion Hall effect, which is crucial to understanding edge-induced skyrmion pinning in Racetrack architectures. In this work, we also detail the effects of skyrmion size, skyrmion-skyrmion interactions and pinning on skyrmion dynamics. The rich dynamics of skyrmions uncovered in our study will potentially fast-track the realization of skyrmion-based Racetrack devices.

*A*STAR Pharos Fund of Singapore

4:18PM V41.00008: Skyrmion Clustering and Dynamics in Strong Pinning or with Strong Magnus Force Dispersion CHARLES REICHHARDT (Presenter), CYNTHIA REICHHARDT, Los Alamos National Laboratory — We show that skyrmions can exhibit density phase separation when driven over strong pinning. This occurs due to the Magnus force interaction, which creates regions of differing effective skyrmion Hall angle, combined with a density dependence of the skyrmion velocity, which is similar to the density dependent velocity observed at clustering transitions in active matter systems. We also investigate the effect of introducing a dispersion in the Magnus force experienced by individual skyrmions, which could arise if different skyrmion species or sizes coexist in a single sample. In this case, we find that the motion of the different species is locked at low drives, but as the drive increases, a disordering transition occurs when the species begin to slide past each other. At higher drives there is a transition to a species phase separated state in which skyrmions with the same Magnus force cluster together. These transitions are associated with signatures in the skyrmion structure, transport response, and velocity fluctuation spectra.
Skyrmion Dynamics under the Influence of Defects from DFT to ASD

JONATHAN CHICO (Presenter), IMARA LIMA FERNANDES, STEFAN BLUEGEL, SAMIR LOUNIS, 1Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Julich & JARA — Any potential skyrmionic application must be able to handle the impact of defects on the skyrmion motion. Until now, most approaches focus on large skyrmions using phenomenological schemes in the micromagnetic regime. Using a combination of first-principles calculations and atomistic spin dynamics, the complex motion of technologically more relevant small skyrmions in Pd/Fe/Ir(111) with 3d and 4d single-atomic defects is studied. Recently, it was shown that such defects can either repel or pin skyrmions [1]. It can be observed that the current threshold needed to overcome the energy barriers, resulting from the impurities, depends on their chemical nature. The obtained dynamical behaviour is richer and goes beyond the expected from the Thiele equation. The complexity of the different motion regimes is revealed and compared with what is known for larger skyrmions. The present study also shines light on how one can engineer defects-based pathways for controlled skyrmion motion.


*Funding provided by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 — DYNASORE).

Anisotropic magnetoresistance in epitaxial FeGe thin films

ADAM AHMED (Presenter), BRENDAN MCCULLIAN, TAO LIU, ROLAND KAWAKAMI, P CHRIS HAMMEL, Ohio State University — The advent of skyrmion imaging and electrical detection is an exciting avenue of research as skyrmions hold promise for next-generation magnetic storage. Presently, in B20 materials, electrical measurements have focused on the detection of non-trivial topological spin textures via topological Hall effect. To further our understanding of transport properties in non-centrosymmetric materials that host skyrmions, we have performed angular-dependent magnetoresistance (ADMR) in the saturated magnetic phase. We have grown epitaxial B20 FeGe/Si(111) films by molecular beam epitaxy. Several features appear in the vicinity of the Curie temperature of 280 K that also persist well above this temperature. Additionally, these features are highly magnetic field dependent. At low temperatures, the signal is dominated by the anisotropic magnetoresistance (AMR) contribution. However, as we approach the magnetic ordering temperature, a strong six-fold symmetric contribution appears. This term, reflecting the crystal symmetry, possibly originates from the magneto-crystalline anisotropy. Curiously, this feature continues to grow in magnitude up to 14 T. We discuss possible origins of these effects above and below the Curie temperature.

*This research was supported by DARPA Grant No. D18AP00008.

Controlling Skyrmion Hall Angle by engineering mixed skyrmions with stray fields

HAMED VAKILITALEGHANI (Presenter), YUNKUN XIE, JIANHUA MA, AVIK GHOSH, University of Virginia — Skyrmions, topologically protected quasi particles in magnetic materials, are widely explored as candidate excitations to store and transmit information. The dynamics of an isolated skyrmion on a racetrack is limited by the Magnus force for a Neel skyrmion and damping force for a Bloch skyrmion. For identical parameters, Neel and Bloch skyrmions tend to move perpendicular to each other. This orthogonality can be understood by the fact that Neel and Bloch skyrmions can be continuously deformed into each other by a 90 degree rotation in parameter space, which can also be seen as a 90 degree rotation of a frame of reference fixed on a point on the boundary of the skyrmion. Accordingly for a mixed skyrmion it is possible to achieve a movement parallel to the drive current with zero spin Hall angle, which is ideal for controlled skyrmion motion in racetrack applications. The mixed skyrmion can be engineered by a combination of the interfacial DMI, which favors the Neel skyrmion, and the stray field which favors the Bloch skyrmion, without the use of synthetic antiferromagnetic multilayer structures.

*This work is supported by the DARPA-Texitronics program and NSF-SHF-1514219.
5:06PM V41.00012: Temperature dependent skyrmion Hall angle in ferrimagnets*  
MICHAEL VOGEL (Presenter), Materials Science Division, Argonne National Laboratory, XIAO WANG, Department of Physics, Bryn Mawr College, PAVEL N. LAPA, Department of Physics, University of California, San Diego, JOHN E. PEARSON, Materials Science Division, Argonne National Laboratory, XUEMEI CHENG, Department of Physics, Bryn Mawr College, AXEL F. HOFFMANN, SUZANNE GABRIELLE TE VELTHUIS, Materials Science Division, Argonne National Laboratory — Analogous to the Hall effect where electronic charges moving in the presence of a magnetic field acquire a transverse velocity, magnetic solitons with non-zero topological charges (i.e. skyrmions and chiral domains walls) exhibit the skyrmion Hall effect, which opens up new possibilities for manipulating the trajectories of these quasiparticles. The skyrmion Hall effect has been theoretically predicted to vanish for antiferromagnetic skyrmions because of the cancelation of opposite topological charges. We present a study of current driven domain wall dynamics in artificially ferrimagnetic multilayers: Ta(4 nm)/Pt (5 nm)/[Co (0.5 nm)/Gd (1 nm)/Pt(1 nm)]10/Al (2 nm). The magnetic texture in different layers of the multilayer films are coherent and antiferromagnetically aligned. Here we experimentally investigate the current driven magnetization dynamics from room temperature down to temperatures below the compensation point at around 100 K.

*Work at Argonne was supported by the US-DOE, Office of Science, MSED. Use of the Center for Nanoscale Materials was supported by the US-DOE, Office of Science, BES, under contract no. DE-AC02-06CH11357. The work at Bryn Mawr is supported by NSF DMR #1708790.

5:18PM V41.00013: Chiral fluctuation driven topological Hall effect in two-dimensional ferromagnets*  
WENBO WANG (Presenter), Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854, USA, MATTHEW W DANIELS, Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, MD 20742, ZHAOLIANG LIAO, National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, 230026 Anhui, People's Republic of China, JUN WANG, GERTJAN KOSTER, GUUS RIJNDERS, MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, the Netherlands, DI XIAO, Department of Physics, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, USA, WEIDA WU, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854, USA — Topological Hall effect (THE) is a real space Berry phase phenomenon originated from the non-coplanar spin texture[1]. Recently THE has been associated with the formation of skyrmions in chiral magnets[2][3]. Although chiral fluctuation driven topological charges have been predicted in chiral magnets, the resultant THE has not been observed yet[4]. Herein, we report a surprising observation of THE around ferromagnetic transition temperature $T_C$ in the ferromagnetic SrRuO$_3$ thin films. The temperature, magnetic field, and thickness dependence of THE are in good agreement with our Monte-Carlo simulations, which provides compelling evidence of the emergence of net topological charges due to chiral fluctuation.

References:

*This work is supported by DOE BES under award # DE-SC0018153

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V43 DCMP: Pairing and Nematicity in Half-filled Landau Levels  
BCEC 210B - Raymond Ashoori, Massachusetts Institute of Technology - Tag(s): Invited
2:30PM V43.00001: The role of electron-electron interactions in the paired-to-nematic transition* [Invited] NOAM BERNSTEIN (Presenter), Naval Research Laboratory — The problem of the ground state of a two-dimensional electron gas at half-filled Landau levels has been a remarkably interesting one. Depending on the number of filled Landau levels, besides the Fermi liquid ground state there are two well-known ordered phases: paired fractional quantum Hall states in the second Landau level and the electronic nematic (or stripe) phases in high Landau levels. Nonetheless, the presence of both of these ordered phases and therefore a transition between them did not seem possible in the absence of an externally applied symmetry breaking field favoring the nematic. This state of affairs has changed recently with the observation a pressure-driven quantum phase transition between the ν=5/2 fractional quantum Hall state, a paired state, and the nematic phase. Here we provide evidence of a similar quantum phase transition at filling factor ν=7/2 and discuss the role of the hydrostatic pressure in driving the transition. Our work highlights universal aspects of the competition of pairing and nematicity present in various condensed matter systems as well as in very clean two-dimensional electron gases. Work done in collaboration with Katherine Schreiber, Nodar Samkharadze, Y. Lyanda-Geller, G. Gardner, M.J. Manfra, L.N. Pfeiffer, and K.W. West.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences, under Award number DE-SC0006671, Gordon and Betty Moore Foundation Grant No. GBMF 4420, and the National Science Foundation MRSEC Grant No. DM-1420541.

3:06PM V43.00002: Even-denominator fractional quantum Hall states in bilayer graphene [Invited] CORY DEAN (Presenter), Columbia University — TBD

3:42PM V43.00003: Competing correlated phases in orbitally mixed half-filled Landau levels [Invited] JOSEPH FALSON (Presenter), Max Planck Institute for Solid State Research — An astounding array of correlated phases have been experimentally realized in high quality two-dimensional electron systems (2DES). By exploiting the quantizing effects of a magnetic field, these systems form an ideal platform for studying the competition between compressible, incompressible and nematic liquids owing to a tunable Landau level index (N) which influences the nature of the ground state. Here, I will present data taken on state-of-the-art MgZnO/ZnO heterostructures that offer the ability to tune N while remaining at a constant Landau level filling. By rotating the sample within a magnetic field, it is possible to selectively decouple the Zeeman and cyclotron energy terms and induce a level crossing between opposing spin branches of the neighboring N=1 and 0 levels. In contrast to the naive expectation of a first-order spin flop transition, an unexpectedly complex cascade of phases is resolved as we incrementally shift the spin and orbital polarization of carriers between levels while remaining at v=5/2 filling. Transport signatures associated with two instances of incompressibility are observed, in addition to two compressible phases and an unanticipated anisotropic phase which breaks rotational symmetry. Our experiments indicate that the depolarization process is gradual and complex. In addition to level polarized states, the unexpected incompressible and anisotropic phases observed in the orbitally mixed regime open questions concerning the possibility of novel interlevel coherence occurring at fractional fillings in systems with strongly mixed levels.

4:18PM V43.00004: Competing charge density waves probed by non-linear transport and noise in the second and third Landau levels [Invited] GUILLAUME GERVAIS (Presenter), McGill University — Competing quantum ground states are ubiquitous in strongly-interacting many-body systems. One prime example is the competition between Wigner crystallization and fractional quantum Hall (FQH) liquids that occurs deep in the first Landau level (LL) of the two-dimensional electron gas (2DEG). In higher LLs, the situation is much more complex, where charge density waves (CDWs) in the form of stripe and bubble phases are also competing with incompressible FQH liquids. In this talk, I will present our results [1] concerning the competition of CDWs and FQH in the second and third LL of an ultra-high mobility GaAs/AlGaAs 2DEG, as probed by both non-linear electronic transport and noise measurements. These measurements were performed in a Corbino geometry to ensure that only bulk properties of the 2DEG were probed, thereby precluding any contribution coming from edge states. Sliding transport of CDWs was revealed by narrow-band noise in re-entrant quantum Hall states of the second LL identified by the Csathy group [2], as well as in pinned CDWs of the third LL. The combining of noise data with maps of conductivity versus magnetic field and bias voltage revealed a complex competition occurring between various quantum phases in the form of stripes, pinned CDWs and fractional quantum Hall liquids, and is consistent with recent results from the Manfra group for the stripe phase suggesting a transition between a smectic and nematic phase at finite temperatures [3].

4:54PM V43.00005: Energy, Momentum, and Spin-resolved tunneling spectra of quantum Hall systems* [Invited]

HEUN MO YOO (Presenter), JOONHO JANG, Massachusetts Institute of Technology, LOREN PFEIFFER, KIRK BALDWIN, KENNETH WEST, Princeton University, RAYMOND ASHOORI, Massachusetts Institute of Technology — Tunneling spectroscopy has an unique power in probing strong electronic correlations of many-body states in a solid. Here, we introduce a novel contactless pulsed tunneling technique that can visualize the energy, momentum, and spin-resolved electronic structure of a quantum Hall effect system. Unlike conventional planar tunneling that requires in-plane conductivity of the system, the pulsed tunneling method functions on strongly insulating systems at exact integer or fractional quantum Hall states. Furthermore, through use of pulses that drive tunneling in the extremely short time intervals, the technique eliminates perturbations such as heating effects or photo-excited defects that commonly occur in other methods. Using the pulsed tunneling technique, we visualize the evolution of discrete quantization of energy levels as well as the effect of electron-optic phonon interactions in energy-momentum space [1]. In addition to momentum and energy resolution, we performed spin-resolved tunneling that probes the ground-state spin polarization of the fractional quantum Hall states in a wide range of magnetic fields and filling factors. Moreover, we can detect the spin-dependent high energy states arising from the strong pair interactions. From these high energy features, we measure Haldane's pseudopotentials that enabled us to directly determine the stability of the composite Fermi sea in a half-filled Landau level. These results illustrate the potentially broad applicability of the pulsed tunneling technique for studying the correlated electronic phases in a variety of two-dimensional materials.


*Funded by BES Program of the Office of Science of the US DOE, contract no. FG02-08ER46514, and the Gordon and Betty Moore Foundation, through grant GBMF2931

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V44 DCMP: Topological Magnons BCEC 210C - Nandini Trivedi, Ohio State University - Tag(s): Invited

2:30PM V44.00001: Topological magnon bands in ultra-thin film pyrochlore iridates and iron jarosites* [Invited]

GREGORY FIETE (Presenter), Department of Physics, Northeastern University — We describe recent theoretical efforts of our group aimed at exploring two-dimensional magnetic systems described by local moment models that possess topological band structures of the low-energy spin fluctuations. We study two systems: (1) Ultra-thin film pyrochlore iridates grown along the [111] direction and (2) the iron jarosites. For the thin film pyrochlore iridates, we consider a bilayer and trilayer and find that in the trilayer case the ground state is the all-in–all-out (AIAO) state, whereas the bilayer has a deformed AIAO state. For range of parameters the lowest magnon band in the trilayer and bilayer case has a nonzero Chern number. We calculate the magnon Hall response for both geometries, finding a striking sign change as a function of temperature. For the iron jarosites, we study magnetic and topological properties of antiferromagnetic kagome spin systems in the presence of both in- and out-of-plane Dzyaloshinskii-Moriya interactions. The in-plane interactions stabilize a canted noncollinear “umbrella” magnetic configuration with finite scalar spin chirality. We derive expressions for the canting angle and use the resulting order as a starting point for a spin-wave analysis. We find topological magnon bands, characterized by nonzero Chern numbers. We calculate the magnon thermal Hall conductivity and propose the iron jarosites as a promising candidate system for observing the magnon thermal Hall effect in a noncollinear spin configuration. We also show that the thermal conductivity can be tuned by varying an applied magnetic field or the in-plane Dzialoshinskii-Moriya strength. In contrast to previous studies of topological magnon bands, the effect is found to be large even in the limit of small canting.


*Work done in collaboration with Pontus Laurell. We gratefully acknowledge funding from the NSF, ARO, and the Simons Foundation.
3:06PM V44.00002: Topological spin excitations in a three-dimensional antiferromagnet* [Invited] WEILIANG YAO, CHENYUAN LI, LICHEN WANG, SHANJIE JUE, YANG DAN, International Center for Quantum Materials, Peking University, KAZUKI IIDA, KAZUYA KAMAZAWA, Comprehensive Research Organization for Science and Society, Japan, KANGKANG LI, JIANGPING HU, CHEN FANG, Institute of Physics, Chinese Academy of Sciences, YUAN LI (Presenter), International Center for Quantum Materials, Peking University — The recent discovery of topological semimetals, which possess distinct electron-band crossing with non-trivial topological characteristics in the bulk, has stimulated intense research interest. By extending the notion of symmetry-protected band crossing into one of the simplest magnetic groups, namely by including the symmetry of time-reversal followed by space-inversion, we predict the existence of topological magnon-band crossing in three-dimensional antiferromagnets [1]. The crossing may take the forms of Dirac points and nodal lines, in the presence and absence, respectively, of the conservation of the total spin along the ordered moments. In a concrete example of a Heisenberg spin model for a “spin-web” compound, Cu3TeO6, we theoretically demonstrate the presence of Dirac magnons over a wide parameter range using linear spin-wave approximation [1]. Inelastic neutron scattering experiments have been carried out to detect the bulk magnon-band crossing in a single-crystal sample [2]. The highly interconnected nature of the spin-1/2 lattice suppresses quantum fluctuations and facilitates our experimental observation, leading to remarkably clean experimental data and very good agreement with the linear spin-wave calculations. The predicted topological magnon Dirac points are confirmed. Further studies will be discussed, including determination of non-collinear spin canting in the ground state with neutron diffraction, and search for topological magnon surface states with inelastic neutron scattering.


*This work is supported by the NSFC and the MOST of China.

3:42PM V44.00003: Topology of magnons: classification and application to honeycomb Kitaev magnets* [Invited] YUAN-MING LU (Presenter), Ohio State University — Compared to their electronic counterparts in topological band theory, much less is known about the topology of spin wave excitations in a general magnetic order. Here we provide a generic theory framework to classify and compute the topology of magnons, by mapping an arbitrary linear spin wave into a local free-fermion Hamiltonian with exactly the same spectrum, symmetry implementation and band topology. This allows us to achieve a full classification and calculation on any topological properties of magnon bands. We apply this fermionization approach to honeycomb Kitaev magnet α-RuCl3, and show the existence of topologically protected magnon band crossings, and field-induced magnon Chern bands under small magnetic fields.

*This work is supported by the Center for Emergent Materials, an NSF MRSEC, under award number DMR-1420451; by NSF under award number DMR-1653769 and in part by NSF PHY-1607611.

4:18PM V44.00004: Discovery of coexisting Dirac and triply degenerate magnons in a three-dimensional antiferromagnet* [Invited] JINSHENG WEN (Presenter), Nanjing University — Topological magnons are emergent quantum spin excitations featured by magnon bands crossing linearly at the points dubbed nodes, analogous to fermions in topological electronic systems. In this talk, we show direct spectroscopic evidence for the coexistence of symmetry-protected Dirac and triply degenerate nodes, the latter involving three-component magnons beyond the Dirac–Weyl framework, by measuring spin excitations of a three-dimensional antiferromagnet Cu3TeO6 with inelastic neutron scattering. Our theoretical calculations show that the observed topological magnon band structure can be well described by the linear-spin-wave theory based on a Hamiltonian dominated by the nearest-neighbor exchange interaction J1. As such, we showcase Cu3TeO6 as an example system where Dirac and triply degenerate magnonic nodal excitations coexist, demonstrate an exotic topological state of matter, and provide a fresh ground to explore the topological properties in quantum materials.

*Work at Nanjing University was supported by National Natural Science Foundation of China with Grant Nos. 11674157, 11774152, 11374138, 11674158 and 11525417, National Key Projects for Research & Development of the Ministry of Science and Technology of China with Grant No. 2016YFA0300401, and Fundamental Research Funds for the Central Universities with Grant No. 020414380105. The research at Oak Ridge National Laboratory’s Spallation Neutron Source was sponsored by the US Department of Energy, office of Basic Energy Sciences, Scientific User Facilities Division.
The surprising usefulness of magnons at intermediate and high energies: from frustration to topology

RODERICH MOESSNER (Presenter), MPI-PKS Dresden — Magnons are among the oldest known elementary excitations, yet very recent developments have yielded plenty of surprises. This talk will cover three aspects of magnons in frustrated magnets -- (i) their topological properties, (ii) their survival at intermediate energies, as well as (iii) their unexpected utility in an S=1 spin liquid state.


Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V46 DMP GMAG: 4d/5d Transition Metal Systems -- New Phases

Magnetic interactions and possible quantum paraelectricity in spin liquid candidate H₃LiIr₂O₆

SHUAI WANG, Peking University, LONG ZHANG, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, FA WANG (Presenter), Peking University — H₃LiIr₂O₆ was recently synthesized and found to be potentially a quantum spin liquid. We studied the crystal structure and magnetic interactions of this material by first principles calculations, and further studied the resulting phase of the obtained pseudospin model by exact diagonalizations. We found that the dominant magnetic interaction of this material is ferromagnetic Kitaev interaction, but residue (further neighbor) Heisenberg interactions would still produce a zigzag magnetic order. We then studied the quantum effect of the hydrogen ions(protons), and found that the electric dipoles of O-H-O “hydrogen bonds” are disordered by strong quantum fluctuations. The electric dipole fluctuations can renormalize the magnetic interactions and potentially lead to a Kitaev spin liquid state in this material. We thus propose that H₃LiIr₂O₆ is a quantum spin liquid promoted by quantum paraelectricity.

RIXS studies of the low-energy magnetic excitations in double perovskite iridates La₂BIrO₆ (B=Co, Ni, Zn)

WENTAO JIN (Presenter), SAE HWAN CHUN, Department of Physics, University of Toronto, Canada, JUNGHO KIM, DIEGO M CASA, Advanced Photon Source, Argonne National Laboratory, USA, CHOONGJAE WON, KYUNGDONG LEE, NAMJUNG HUR, Department of Physics, Inha University, Korea, YOUNG-JUNE KIM, Department of Physics, University of Toronto, Canada — Ordered double perovskite (DP) materials [1-3], A₂BB'₆O₆, where B is a 3d and B’ is a 4d or 5d transition metal ion, respectively, provide a rare opportunity to study the interaction between the intriguing magnetic behaviors of 5d systems and the better understood 3d magnetism, which is important for developing potential applications of these novel magnetic systems. Using resonant inelastic x-ray scattering (RIXS) measurements at Ir L₃ edge, we have investigated the low-energy magnetic excitations in a series of La₂BIrO₆ single crystals, where B is Co, Ni and Zn, respectively. In La₂CoIrO₆ and La₂NiIrO₆, clear magnetic excitations with a large magnon gap ~ 40 meV were revealed, indicating an extremely large magnetic anisotropy in the magnetic interaction in these two compounds containing magnetic 3d ions. In contrast, the low energy magnon mode was absent in La₂ZnIrO₆ in which the 3d ions are non-magnetic, suggesting the importance of 3d-5d hybridization in the magnetic properties of DP iridates.


This work is supported by Natural Science and Engineering Research Council of Canada through Discovery Grant and CREATE program.
2:54PM V46.00003: Effect of charge doping in Os-based double perovskites with strong spin-orbit coupling  
ERICK GARCIA (Presenter), RONG CONG, Brown University, PHUONG TRAN, PATRICK WOODWARD, Department of Chemistry, The Ohio State University, VESNA F. MITROVIC, Brown University, SAMUELE SANNA, Department of Physics and Astronomy, University of Bologna — The combined effects of strong electronic correlations and spin-orbit coupling (SOC) leads to a plethora of emergent novel quantum states. However, predicting such emergent properties is complicated by the fact that spin is not a good quantum number in the presence of SOC. Therefore, experimental studies by local probes are highly sought to guide theoretical descriptions of this new physics. Double perovskite structures are particularly interesting cases of materials with such novel quantum states. Here, we investigate the effects of charge doping via the Na+/Ca++ partial substitution on the magnetic ground state of Ba$_2$NaOsO$_6$, a double perovskite with strong SOC. Ba$_2$NaOsO$_6$ is a 5d$_1$ Mott insulator that displays an exotic canted two-sublattice ferromagnetic state believed to be driven by the staggered quadrupolar order [L. Lu et al. *Nature Comm.* 2017], while Ba$_2$CaOsO$_6$ is a 5d$_2$ compound which displays an antiferromagnetic phase [C.M. Thompson et al. *J. Phys. Cond. Matter* 2014]. We present zero field μSR measurements on powder samples of the compound Ba$_2$Na$_{1-x}$Ca$_x$OsO$_6$ for 0 < x < 1 to investigate the interplay between spin, orbital, and charge degrees of freedom, which are believed to govern novel quantum states of compounds with strong SOC.

3:06PM V46.00004: EDRIXS: an open source toolkit for simulating resonant inelastic x-ray scattering spectrum based on exact diagonalization  
YILIN WANG (Presenter), Department of Condensed Matter Physics and Materials Science, Upton, New York 11973, USA, Brookhaven National Laboratory, XUERONG LIU, School of Physical Science and Technology, Shanghai 201210, China, ShanghaiTech University, MARK DEAN, GABRIEL KOTLIAR, Department of Condensed Matter Physics and Materials Science, Upton, New York 11973, USA, Brookhaven National Laboratory — In this work, we present an open source toolkit called “EDRIXS” to simulate the resonant inelastic x-ray scattering (RIXS) spectrum based on exact diagonalization (ED) of a model Hamiltonian. It can deal with single atom, cluster models with the parameters being obtained by DFT+Wannier90 calculation, and Anderson impurity models obtained from a converged DFT+DMFT calculation. A very efficient parallel ED solver based on arpack library is implemented and RIXS spectrum is calculated by Krylov subspace technique. These key components are written by Fortran90 and a Python interface is designed to prepare the inputs and setup the calculations. We apply this toolkit to study two 5d materials. First, we perfectly reproduce the dimer excitations observed in the experimental RIXS spectrum of Ba$_5$AlIr$_2$O$_{11}$ based on a two site Ir-Ir model and it directly confirms the existence of dimer orbital in this material. Second, we simulate the measured RIXS spectrum in Ba$_2$YOsO$_6$ based on an Anderson impurity model from a DFT+DMFT calculation, and based on this simulation we found that the energy scale of spin-orbit coupling (SOC) and Hund's coupling is comparable and the effective SOC effects in this 5d$_3$ compound is still significant so that it cannot be described by a pure spin-3/2 state.

3:18PM V46.00005: Interplay of novel magnetism and structural symmetry in Ba$_2$NaOsO$_6$ as a function of magnetic field and temperature revealed via resonant and non-resonant x-ray scattering  
ZAHIRUL ISLAM (Presenter), Advanced Photon Source, Argonne National Laboratory, KRISTIN WILLA, ULRICH WELP, Materials Science Division, Argonne National Laboratory, JACOB P.C. RUFF, Advanced Photon Source, Argonne National Laboratory, ZHU DIAO, Physics and Engineering, Halmstad University, ANDREAS RYDH, Physics, Stockholm University, RITESH K. DAS, Advanced Photon Source, Argonne National Laboratory, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, IAN R FISHER, Applied Physics, Stanford University — We studied correlation of lattice symmetry and magnetism in Ba$_2$NaOsO$_6$ (BNOO) showing that it was tetragonal (T) even at 300K, with a transition into an orthorhombic (O) phase near a "ferromagnetic" transition at $T_c$~6.9K . Fluctuations of O-phase seem to appear well above $T_c$, and calorimetric data, concurrently recorded with scattering, indicates a T-to-O transition at $T>T_c$. At $T<T_c$, a commensurate order at $q=(1,0,0)$ (a is the shortest axis of O phase) is observed. In a magnetic field normal to $q$, this staggered order saturates, indicating a coherent rotation of ordered magnetic domains to align with field direction as well as revealing some qualitative differences with bulk M(H) data. Due to structural twins, bulk measurements are susceptible to effects of field applied along all three directions simultaneously, while scattering uniquely probes magnetic order within individual twins. This field evolution of $q$-satellite along with its angular, polarization, and azimuthal properties of resonant scattering is indicative of a novel orbital-ordered phase with quantization (or principal) axis confined to the orthorhombic $bc$-plane.

*This research at the Advanced Photon Source is operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.
Spin-orbit entanglement and \( j=1/2 \) state in \( \text{CuAl}_2\text{O}_4^* \)

SERGEY STRELTSOV (Presenter), Institute of Metal Physics, SERGEY NIKOLAEV, IGOR SOLOVYEV, National Institute for Materials Science, ANDREY IGNATENKO, Institute of Metal Physics, SANTU BAIDYA, Department of Physics and Astronomy, Seoul National University, VALENTIN IRKHIN, Institute of Metal Physics, DANIEL KHOMSKII, University of Cologne, JE-GUEN PARK, Department of Physics and Astronomy, Seoul National University — Spin-orbit (SO) Mott insulators are regarded as a new paradigm of magnetic materials, whose properties are largely influenced by the SO coupling and featured by highly anisotropic bond-dependent exchange interactions, as manifested in 4d and 5d systems. We show that a very similar situation can be realized in cuprates, when the \( \text{Cu}^{2+} \) ions reside in a tetrahedral environment. A special attention will be paid to \( \text{CuAl}_2\text{O}_4 \), which was experimentally found to retain cubic structure and does not show any long-range magnetic order down to \( T=0.5 \) K. These are the strong Coulomb correlations and the spin-orbit coupling, which conspire to suppress the Jahn-Teller distortions in \( \text{CuAl}_2\text{O}_4 \). The spin-orbit-entangled \( j_{\text{eff}}=1/2 \) state is then naturally realizes in the situation of \( t_{2g}^5 \) configuration and degenerate \( t_{2g} \) subshell. This in turn explains unusual magnetic properties of \( \text{CuAl}_2\text{O}_4 \). Using first-principles calculations, we construct a realistic spin model and show that the magnetic properties of this compound are largely controlled by anisotropic compass-type exchange interactions that dramatically modify the magnetic ground state by lifting the spiral spin-liquid degeneracy and stabilizing a commensurate single-q spiral.

*Russian Science Foundation, the project 17-12-01207

Dirac Nodal Lines and Density-Functional Prediction of a Large Spin Hall Effect in 6H-perovskite Iridate \( \text{Ba}_3\text{TiIr}_2\text{O}_9 \)

SAYANTIKA BHOWAL (Presenter), SASHI SEKHAR SATPATHY, University of Missouri — Topological semi-metals have received considerable attention recently due to their nontrivial band structure protected by symmetry, resulting in a number of emerging quantum phenomena such as Fermi arcs, anomalous Hall effect, spin Hall effect (SHE), etc. While the Dirac and Weyl semi-metals, the typical examples of 3D topological semi-metals, are well studied in the literature, currently an interest has been emerging in the Dirac nodal line semi-metals (DNLS) because they are good candidates for SHE. Here, based on the density-functional calculations, we predict a new iridate material \( \text{Ba}_3\text{TiIr}_2\text{O}_9 \) with nodal lines present in the band structure, which with the introduction of SOC become gapped along certain high symmetry directions in the Brillouin zone, but not along the other directions, being protected by the non-symmorphic symmetry of the crystal structure. The latter type of nodal lines are characterized by the quantized Berry phase \( \pi \), while the former kind of nodal lines are responsible for a strong SHE. The magnitude of the SHE is calculated using a tight-binding fit to the DFT band structure. Our work suggests \( \text{Ba}_3\text{TiIr}_2\text{O}_9 \) as a potential SHE material for spintronics applications and motivates experimental work on the system.

Covalency-driven collapse of strong spin-orbit coupling in face-sharing iridium octahedra*

MAI YE (Presenter), HEUNG SIK KIM, JAE-WOOK KIM, Rutgers University, New Brunswick, CHOONG-JAE WON, Max Planck POSTECH/Korea Research Initiative, Pohang University of Science and Technology, KRISTJAN HAULE, DAVID VANDERBLIT, SANGWOOK CHEONG, GIRSH E BLUMBERG, Rutgers University, New Brunswick — We report ab-initio density functional theory calculation and Raman scattering results to explore the electronic structure of \( \text{Ba}_5\text{CuIr}_3\text{O}_{12} \) single crystals. This insulating iridate, consisting of face-sharing \( \text{IrO}_6 \) octahedra forming quasi-one-dimensional chains, cannot be described by the local \( j_{\text{eff}}=1/2 \) moment picture commonly adopted for discussing electronic and magnetic properties of iridate compounds with \( \text{IrO}_6 \) octahedra. The shorter Ir-Ir distance in the face-sharing geometry, compared to corner- or edge-sharing structures, leads to strong covalency between neighboring Ir. Then this strong covalency results in the formation of molecular orbitals (MO) at each Ir trimers as the low-energy electronic degree of freedom. The theoretically predicted three-peak structure in the joint density of states, a distinct indication of deviation from the local \( j_{\text{eff}}=1/2 \) picture, is verified by observing the three-peak structure in the electronic excitation spectrum by Raman scattering.

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Spin-orbit coupled ground state of mixed valence iridate Ba$_2$AlIr$_2$O$_9$*  VAMSHI MOHAN KATUKURI (Presenter), C3MP, IPHYS, École Polytechnique Fédérale de Lausanne, Switzerland, XINGYE LU, Center for advanced quantum studies and Department of physics, Beijing Normal University, China, THORSTEN SCHMITT, Laboratory of Synchrotron Radiation, Paul Scherrer Institute, Switzerland, OLEG YAZYEV, C3MP, IPHYS, École Polytechnique Fédérale de Lausanne, Switzerland — Interplay of electronic correlations and spin-orbit interactions in Ir$^{4+}$ and Ir$^{5+}$ oxides results in insulating $J_{\text{eff}} = 1/2$ and $J_{\text{eff}} = 0$ ground states, respectively. By now, this has been well understood theoretically and established experimentally. However, in compounds where the dimerisation of Ir$^{4+}$ and Ir$^{5+}$ ions is structurally more favourable, the microscopic understanding of the local electronic structure is lacking. For example, a direct overlap of the Ir $d$-orbitals within the dimers may lead to significant bonding-antibonding splittings, which diminishes the role of spin-orbit mixing, considerably modifying the local electronic picture. With Ba$_2$AlIr$_2$O$_{11}$ as an example, we show that the direct $d$-$d$ hybridisation effects are relatively weak, while electronic correlations (configuration mixing) and spin-orbit coupling play a dominant role. Using a combination of ab initio many-body wave function quantum chemistry calculations and resonant inelastic X-ray scattering experiments, we elucidate the electronic structure of Ba$_2$AlIr$_2$O$_{11}$. Our investigation shows that the two Ir ions (Ir$^{4+}$ and Ir$^{5+}$) in Ir$_2$O$_9$ dimer units preserve their local $J_{\text{eff}}$ ground states close to 1/2 and 0, respectively.

*We acknowledge funding from Swiss National Science Foundation Sinergia project 171003.

Magnetic field tuning of non-reciprocal and achiral spin waves in antiferromagnetic Ba$_3$NbFe$_3$Si$_2$O$_{14}$*  CHRIS STOCK (Presenter), MANILA SONGVILAY, University of Edinburgh, JOSE A RODRIGUEZ, NIST Center for Neutron Research, PAOLO G. RADAELLI, LAURENT CHAPON, Physics, University of Oxford, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University — Reciprocity, in the context of optics and scattering, is defined as invariance when a source and detector are swapped indicating that the motion of an object in one direction being the same as that in the opposite. We investigate the magnetic field tuning of non-reciprocal spin waves in antiferromagnetic langasite Ba$_3$NbFe$_3$Si$_2$O$_{14}$ using neutron spectroscopy. Applying a time reversal symmetry breaking magnetic field that also breaks a two-fold symmetry of the underlying structure, different spin wave energies are observed when the sign is reversed for either the total momentum +/- $Q$= +/-($G$ +/- $q$) or applied magnetic field +/- $\mu_0H$. We discuss the scaling of this effect with field and suggest it microscopically originates from spin-orbit coupling mediated through antisymmetric exchange.

*We are grateful for funding from the EPSRC, the Carnegie Trust for the Universities of Scotland, the STFC and through the NSF (DMR-09447720).

New insight into the low temperature phase of Ca$_3$Ru$_2$O$_7$*  DANILO PUGGIONI (Presenter), JAMES M RONDINELLI, Northwestern University — Despite the countless theoretical studies on the Ruddlesden-Popper ruthenate Ca$_3$Ru$_2$O$_7$, the structure and physics of its low temperature phase (T < 48 K) remains unclear. Here, using first principle calculations, we shed light on this phase, reconciling several disparate experimental results with a model based on band theory and static correlations. Our results suggest that an accurate description of the strong interplay among electronic correlation, magnetic ordering, spin-orbit interaction, and structural degrees of freedom are necessary to understand the properties of the low temperature phase of Ca$_3$Ru$_2$O$_7$.

*Support from Army Research Office under Grant No. W911NF-15-1-0017

Electric Field-Tuned Electronic Structure Revealed by Time- and Angle-Resolved Photoemission Spectroscopy  SHAOHUA ZHOU (Presenter), CHANGHUA BAO, YANG WU, SHUYUN ZHOU, Department of Physics, Tsinghua University — External electric field can easily modify the electronic structure of materials and create novel or useful quantum states. Such electric field tunable electronic structure is difficult to be probed by angle-resolved photoemission spectroscopy (ARPES) experiment because the electric field will deflect the photoelectrons. Here I will present our experimental results on electric field-tunable electronic structure by using a new strategy which can obtain the transient electronic structure under a tunable electric field, based on time- and angle-resolved photoemission spectroscopy (TrARPES).
4:54PM V46.00013: Low temperature thermal conductivity measurement of magnetic delafossite PdCrO$_2$  
SEITA ONISHI (Presenter), SEUNGHYUN KHIM, ANDREW MACKENZIE, ELENA HASSINGER, Max Planck Institute for Chemical Physics of Solids — Ultrapure delafossite metals are remarkably distinct from conventional metal oxides with their high electrical conductivity (some even exceeding that of noble metals) [1]. Thermal conductivity has previously been studied in PdCoO$_2$ [2] but never in the magnetic partner compound PdCrO$_2$. Here, we present such a study, down to sub-Kelvin temperatures. The high conductivities of delafossites necessitate samples with high aspect ratios to reach low temperatures with a reliable temperature gradient and minimal sample heating. I will discuss how this was achieved in our experiments.


5:06PM V46.00014: Structural Study of the Multiferroics Perovskite Sr$_{1-x}$Ba$_x$Mn$_{1-y}$Ti$_y$O$_3$  
KAMAL CHAPAGAIN (Presenter), BOGDAN DABROWSKI, OMAR CHMAISSEM, STANISLAW KOLESNIK, HAUMOD SOMALI, DENNIS BROWN, Northern Illinois University — The structural and magnetic properties of unique single-ion manganese-based multiferroic perovskites Sr$_{1-x}$Ba$_x$Mn$_{1-y}$Ti$_y$O$_3$ (SBMTO) were investigated by XRD. For compounds near $x = 0.45$–0.65 and $y = 0$–0.1, a cubic to non-centrosymmetric tetragonal transition takes place below $\sim 430$ K on heating and at $\sim 60$ K lower temperature on cooling. Ferroelectric (FE) distortions $c/a$ that are larger than the $P4mm$ distortions of nonmagnetic BaTiO$_3$ have been observed with maximum estimated polarization of $\sim 29 \, \mu C/cm^2$ at $\sim 220$ K. At lower temperatures, the polarization is suppressed by $\sim 40\%$ due to development of antiferromagnetic (AFM) phase, indicating very strong coupling between FE and AFM. The FE phase is rapidly suppressed by hydrostatic pressure.

5:18PM V46.00015: Emergent quantum criticality from spin-orbital entanglement in d$^8$ Mott insulators: the case of a diamond lattice antiferromagnet  
FEI-YE LI (Presenter), GANG CHEN, Fudan University — Motivated by the recent activities on the Ni-based diamond lattice antiferromagnet NiRh$_2$O$_4$, we theoretically explore on a general ground the unique spin and orbital physics for the Ni$^{2+}$ ions with a 3d$^8$ electron configuration in the tetrahedral crystal field environment and on a diamond lattice Mott insulator. The superexchange interaction between the local moments usually favors magnetic orders. Due to the particular electron configuration of the Ni$^{2+}$ ion with a partially filled upper $t_{2g}$ level and a fully filled lower $e_g$ level, the atomic spin-orbit coupling becomes active at the linear order and would favor a spin-orbital-entangled singlet with quenched local moments in the single-ion limit. Thus, the spin-orbital entanglement competes with the superexchange and could drive the system to a quantum critical point that separates the spin-orbital singlet and the magnetic order. We further explore the effects of magnetic field and uniaxial pressure. The non-trivial response to the magnetic field is intimately tied to the underlying spin-orbital structure of the local moments. We discuss the future experiments such as doping and pressure, and point out the general correspondence between different electron configurations under tetrahedral and octahedral crystal field environments.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V47 DMP: Thermoelectrics -- Emerging Materials and Devices  
BCEC 213 - Daryoosh Vashaee,  
North Carolina State University - Tag(s): Focus
2:30PM V47.00001: 2D Metal-Organic Frameworks as a New Class of Thermoelectric Material**

RYUICHI TSUCHIKAWA (Presenter), Department of Physics and Astronomy, University of Utah, NABAJIT LAHIRI, Department of Chemistry, University of Utah, NEDA LOTFIZADEH, SHUWAN LIU, MACKENZIE LACH, CELINE SLAM, Department of Physics and Astronomy, University of Utah, JANIS LOUIE, Department of Chemistry, University of Utah, VIKRAM DESHPANDE, Department of Physics and Astronomy, University of Utah — Organic materials are desired in many fields of thermoelectric applications due to material abundance, light weight, and flexibility. Electrically conductive 2D metal-organic frameworks (MOFs) are a new class of organic material, and the two dimensionality and nanopores have a potential to realize a comparable thermoelectric figure of merit in 2D MOFs. As such, we measured thermal conductivity, electrical conductivity, and Seebeck coefficient of Copper Benzenehexathiol (Cu-BHT), an electrically conductive 2D MOF, in a mesoscopic device scale. We found that phonon mean free path is of the order of the length scale associated with nanopores and interlayer distance and it is responsible for the observed low thermal conductivity of 0.25 W/mK at room temperature. This result ensures low thermal conductivity in any 2D MOFs without artificially imposing nanostructures. Electronic transport and Seebeck coefficient measurements revealed that the charge carrier is n-type and the electronic transport is governed by the degree of polycrystallinity. However, unlike conductive polymers, each domain retains a definite crystal structure, resulting in an electronic band in each domain. This leads to a possibility of enhancing Seebeck coefficient by band engineering.

**Funded by ACS PRF and USTAR

2:42PM V47.00002: High thermoelectric properties of As-based 122-Zintl compounds Ba$_{1-x}$K$_x$Cd$_2$As$_2$

HARUNO KUNIOKA (Presenter), KUNIHIRO KIHOU, HIROTAKA NISHIATE, National Institute of Advanced Industrial Science and Technology, HIDETOMO USUI, KAZUHIKO KUROKI, Osaka University, CHUL-HO LEE, ATSUSHI YAMAMOTO, National Institute of Advanced Industrial Science and Technology, TSUTOMU IIDA, HARUHIKO OBARA, Tokyo University Of Science — 122-Zintl phase is well known as a high performance thermoelectric (TE) material. For the past decade, Sb-based 122-Zintl compounds have been found that the dimensionless figure-of-merit exceeds the value of 1. In contrast, there are only few studies on As-based Zintl compounds. Lighter atomic mass of As than Sb discourages exploring As-based compounds because the lattice thermal conductivity ($k_L$) usually becomes higher with lighter atoms. Recently we have found that Ba$_{1-x}$K$_x$Zn$_2$As$_2$ exhibits low $k_L$ of 0.8 W/mK and high $ZT$ of 0.67 at 900 K [1]. This discovery demonstrates that the As-based 122-Zintl compounds also have a potential for a high performance TE material.

Being based of the first principle calculation, we decided to examine TE properties of As-based 122-Zintl compounds Ba$_{1-x}$K$_x$Cd$_2$As$_2$. Polycrystalline samples of Ba$_{1-x}$K$_x$Cd$_2$As$_2$ was synthesized by the solid reaction method. The power factor of Ba$_{1-x}$K$_x$Cd$_2$As$_2$ reached to 1.3 mW/mK$^2$ at $T = 773$ K. $k_L$ was 0.5 W/mK at $T = 773$ K. Consequently, $ZT$ reached to 0.81 at 773 K, which is the highest $ZT$ value at As-based 122-Zintl compounds [2].


2:54PM V47.00003: Cold Spray Additive Manufacturing of Thermoelectric Generators*

HARRY RADOUSKY (Presenter), ALEXANDER A. BAKER, Lawrence Livermore National Laboratory, RICHARD THUSS, TTEC LLC, ELISSAIOIS STAVROU, JOSEPH MICHAEL ZAUG, SCOTT MCCALL, Lawrence Livermore National Laboratory — Thermoelectric generators (TEGs) provide a pathway to recovering and converting thermal energy directly into electricity. Adoption of the technology has often been limited due to the difficulty of manufacturing TEGs that can be incorporated into industrial environments where waste heat is prevalent. To address this shortcoming an additive manufacturing technique has been developed for the fabrication of arbitrary shape Bi$_2$Te$_3$ based (and other semiconductors) thermoelectric generators, promising greater design flexibility to harvest low grade waste heat. We have demonstrated that cold-spraying of powdered material yields near-full density parts, without significant loss of thermoelectric properties in the operating window of ~100 C. A systematic study is presented of the structural characteristics for the deposited material, correlated with thermal and electrical transport measurements to allow further understanding of the thermoelectric efficiency in the cold-sprayed samples. In particular cold spraying allows deposition on curved geometries such as copper pipes, and produces thermoelectric materials with Seebeck coefficients comparable to the bulk starting material.

*Prepared by LLNL under Contract DE-AC52-07NA27344.
3:06PM V47.00004: Interplay between flexoelectric and thermoelectric effects in bismuth telluride thin films*  
BRUNO LORENZI (Presenter), SVETLANA BORISKINA, Mechanical Engineering, Massachusetts Institute of Technology, AKIHIRO KOBAYASHI, MASAYUKI TAKASHIRI, Department of Materials Science, Tokai University, GANG CHEN, Mechanical Engineering, Massachusetts Institute of Technology — Flexoelectricity is a phenomena for which a strain gradient induces an internal polarization in semiconductor and dielectric materials. This effect can be used to enhance thermoelectric properties, and to enable the collection of photo-generated carriers without the need of a p-n junction. In this context, flexoelectricity was claimed to be the reason behind the variation of Seebeck coefficient in bismuth telluride (Bi$_2$Te$_3$) thin films deposited on different substrates, and was shown in many materials under illumination. However, a clear explanation of the relation between the applied strain and the detected signal is still missing, along with a comprehensive theoretical and experimental analysis.

We will present the experimental demonstration of flexoelectric effect in Bi$_2$Te$_3$ thin films deposited on flexible substrates, by magnetron sputtering. We will show and discuss how the open circuit voltage in our samples can be varied as a function of applied strain, temperature, and illumination level. Our results help to shed light on the relation between applied strain, material polarization, and the thermo/photoelectric performance, revealing new possible applications of the flexoelectric effect in low-gap materials.

*This work was supported in part by Marie Sklodowska-Curie grant 745304

3:18PM V47.00005: Superionic diffusion and anharmonic lattice dynamics in AgCrSe$_2$*  
JINGXUAN DING (Presenter), Mechanical Engineering and Materials Science, Duke University, JENNIFER L NIEDZIELA, Oak Ridge National Laboratory, DIPANSHU BANSAL, Indian Institute of Technology Bombay, ANDREW MAY, GEORG EHLERS, DOUGLAS L ABERNATHY, Oak Ridge National Laboratory, YANG REN, AYMAN SAID, Argonne National Laboratory, OLIVIER DELAIRE, Mechanical Engineering and Materials Science, Physics, Duke University — Superionic conductors exhibit promising thermoelectric properties due to their ultralow thermal conductivity. The fundamental mechanisms have long been debated between the anharmonicity or the breakdown of transverse acoustic (TA) phonons, where the shearing vibrational degrees of freedom are lost, as in a liquid state. We report on neutron/x-ray scattering and first-principles studies on the lattice dynamics and ionic diffusion of AgCrSe$_2$. Our momentum-resolved measurements on single-crystals clearly establish the persistence of long-wavelength TA phonons in the superionic phase, whereas the shorter wavelength, non-dispersive portions of the TA branches severely broaden reflecting extreme anharmonicity. Further, we find a strong repulsion between Ag neighbors, affecting the diffusion mechanism. Our studies of atomic dynamics and diffusion will help rationalize the emergence of ultralow thermal conductivity for thermoelectrics and facilitate the design of high-performance solid-state electrolytes.

*INS/IIXS measurements supported by the S3TEC EFRC, DOE BES Award #DESC0001299. First-principles modeling supported by the US DOE BES Early Career Award #DESC0016166. Sample synthesis supported by the US DOE BES, Materials Sciences and Engineering Division.

3:30PM V47.00006: Fabrication and Measurement of the Physical and Thermoelectric properties of Ca$_{3-x}$Dy$_x$Co$_{4-y}$Fe$_y$O$_{9+p}$ systems*  
IFEANYI IFEDUBA (Presenter), ROBERT M CATCHINGS, Howard University, DAVID MCKEOWN, Vitreous State Laboratory, WINNIE WONG-NG, NIST, XUEYAN SONG, University of West Virginia — The properties and performance of Cobalt oxide material as a p-type semiconductor for commercial use depends on its stability at high temperature region and its excellent physical and thermoelectric properties. Here in, we substitute (dope) and study the effects of magnetic ions (Dy, Fe) for (Ca, Co) in polycrystalline Ca$_3$Co$_4$O$_9$. A series of Ca$_{3-x}$Dy$_x$Co$_{4-y}$Fe$_y$O$_{9+p}$ samples was synthesized using the sol-gel combustion method. After preparations, the samples were subjected to heat treatment at different temperature. X-ray diffraction analysis indicates the partial substitution of Dy in the Ca site and Fe in the Co site. It also confirmed the formation of single phase compound, as well as changes in the structure of the materials depending on the sintering temperature. The obtained values of the electrical resistivity for all samples falls within the range of a semiconductor. The thermopower values are all positive, indicating that the majority carrier are holes.

*The Support of the Materials Measurement Division at the National Institute of Standard and Technology (NIST) is greatly appreciated.
3:42PM V47.00007: Axis Dependent Transport Properties of Single Crystal Re₄Si₇*  BIN HE (Presenter), MIKE SCUDDER, YAXIAN WANG, WOLFGANG E WINDL, JOSHUA E. GOLBERGER, JOSEPH P C HEREMANS, Ohio State University — We measured the thermoelectric transport properties of Re₄Si₇ along different axis and prove Re₄Si₇ to have axis dependent carrier polarity. In the cryostat measurement, we observe electrical conductivity and thermopower both increasing with temperature. In-plane Hall effects shows the crystals we obtained has a carrier density around 2*10¹⁹/cm³, while the Hall coefficient in-plane and cross-plane have opposite signs. Thermal conductivity measurement shows an isotropic lattice thermal and Nernst measurement shows a small Nernst coefficient and eliminates the possibility of two carrier system. High temperature thermoelectric properties measurement shows the resistivity keeps decreasing at high temperature. The thermopower of the cross-plane direction reaches 300 µV/K and turns flat at high temperature, which may come from a thermal smearing effect. With an estimate of the thermal conductivity, we propose a promising ZT over unity for future optimization.

*Primary funding is supported by NSF EFRI 1433467
Partially supporteb by OSU Center for Emergent Materials: an NSF MRSEC under Award DMR-1420451

3:54PM V47.00008: Spin Effects Making zT > 1  DARYOOSH VASHAEE (Presenter), Department of Electrical and Computer Engineering, North Carolina State University, MD MOBARAK HOSSAIN POLASH, Department of Materials Science and Engineering, North Carolina State University, VLADISLAV PERELYGIN, Department of Chemistry, North Carolina State University, MORTEZA RASOULIANBOROUJENI, Department of Developmental Science, Marquette University, YUANHUA ZHENG, Department of Mechanical and Aerospace Engineering, The Ohio State University, TIANQI LU, NING LIU, Chinese Academy of Sciences, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, MICHAEL MANLEY, RAPHAEL HERMANN, Materials Science and Technology Division, Oak Ridge National Laboratory, ALEX I SMIRNOV, Department of Chemistry, North Carolina State University, JOSEPH P C HEREMANS, Department of Mechanical and Aerospace Engineering, The Ohio State University, HUAIZHOU ZHAO, Chinese Academy of Sciences, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics — Recent studies of thermoelectric properties of the antiferromagnetic MnTe:Li have revealed the existence of a strong spin effect that extends across a broad range of temperature leading to zT>1 [1,2]. While carrier mobility and heat capacity were strongly affected by spin contributions near the Neel temperature, T_N=307K, the thermopower demonstrated robust spin effects extending up to 900K. Spin contribution to those properties below T_N has been attributed to the magnon-drag effect [3]. A recent study [2] attributed the thermopower enhancement to paramagnon-drag effect originated from the mid or short-range magnetic ordering above T_N. Neutron scattering study showed an agreement to that theory to some extent while some competing theories such as the spin-fluctuations and spin entropy can also explain thermopower enhancement in magnetic materials [1,4]. The objective of this work is to show the agreements and disagreements of different spin-based theories in describing the transport properties of MnTe:Li and to compare similar material systems to gain better insight to the underlying physics.


4:06PM V47.00009: Thermal transport and thermoelectric effects at solid-melt interfaces in semiconductors:
Underlying physical phenomena that give rise to Thomson heat in semiconductors* SADID MUNEER, Electrical and Computer Engineering, University of Connecticut, Storrs, CT 06269, USA, GOKHAN BAKAN, Electrical and Electronics Engineering, Attilim University, Ankara, Turkey, NATHAN HENRY, HELENA SILVA, ALI GOKIRMAM (Presenter), Electrical and Computer Engineering, University of Connecticut, Storrs, CT 06269, USA — Partial melting in self-heated nanocrystalline silicon microwires via fast pulses show a drastic asymmetry in melting profiles, where half of a wire may be melted and recrystallized while the other half remain in solid state. This asymmetry, in the direction of the electrical current, point to the significance of Thomson heat close to the solid-melt interfaces in semiconductors. The diffusion of the electron-hole pairs away from the melted regions cause thermal transport via (i) increased electronic convective heat flow and (ii) recombination of the excess carriers away from the melted region. In presence of an electric field a non-equilibrium non-isothermal condition is achieved. Generation (G) of electrons and holes, transport (T), and recombination (R) of the minority carriers downstream, GTR¹, lead to a strong asymmetry in thermal profiles at melt-solid interfaces in semiconductors.


KORNELIUS NIELSCH (Presenter), Institute of Metallic Materials, Leibniz IFW - Dresden — Micro-thermoelectric modules are of potential use in fields such as energy harvesting, thermal management, thermal imaging and high spatial-resolution temperature sensing. In particular, micro-thermoelectric coolers (μ-TECs) – in which the application of an electric current cools the device based on the Peltier effect – can be used to manage heat locally on a micrometer spot in microelectronic circuits, optoelectronic devices and microfluidic channels. However, a cost-effective μ-TEC device that is compatible with the modern semiconductor fabrication industry has been developed. N-type BiTeSe and p-type pure Te were electrochemically deposited at room temperature into microstructured photoresist patterns. A comprehensive study the electrochemically synthesis if thermoelectric chalcogenide materials is presented [1]. The material quality is every high, that even fundamental aspect like topological surface states can be demonstrated in these chalcogenide film by transport measurements.

The final device performance of μ-TECs in terms of transient responses, cycling reliability and cooling stability has not been adequately assessed. Here we report the fabrication of μ-TECs that offer a rapid response time of 1 ms, reliability of up to 10 million cycles and a cooling stability of more than one month at constant electric current. The high cooling reliability and stability for our μ-TEC module [2] can be attributed to a design of free-standing top contacts between the thermoelectric legs and metallic bridges, which reduces the thermomechanical stress in the devices.

Ref:

**MATTHIAS AGNE (Presenter), Northwestern University, PENGFEI QIU, XUN SHI, SIC CAS, JEFF SNYDER, Northwestern University — The possibility of decomposition in superionic mixed ionic-electronic conductors (MIEC) has limited their engineering applications. Specifically, high efficiency MIEC thermoelectric materials have not been utilized due to decomposition under large electronic currents and large temperature gradients. Herein, we derive the critical condition for decomposition, which corresponds to a critical chemical potential difference defined from linear non-equilibrium thermodynamics. This analysis leads to the conclusion that voltage, not current density, is the relevant design parameter. Consequently, the decomposition condition is independent of the geometry of the device; whereby, a strategy is presented for improving stability in devices subjected to electrical and temperature gradients. By using a series of electronically conducting, but ion-blocking barriers to reset the chemical potential it is possible to keep the material below the threshold for decomposition. Experimentally, the thermodynamic theory is validated in the Cu2-dSe MIEC system.

**NASA Science Mission Directorate's Radioisotope Power Systems Thermoelectric Technology Development program

RINKLE JUNEJA, TRIBHUWAN PANDEY, ABHISHEK SINGH (Presenter), Indian Institute of Science — Silicon-based thermoelectric materials would be of great significance due to the huge dependence of electronic industry on silicon. Bulk silicon is not a good thermoelectric material due to its very high thermal conductivity, thereby limiting its thermoelectric efficiency. Nanostructuring and alloying are alternative solutions to reduce thermal conductivity, but the techniques involved are complex and costly. Recently, a silicon-based chalcogenide Si$_2$Te$_3$ has been experimentally synthesized. Si$_2$Te$_3$ exhibits layered structure, in which Te atoms form hexagonal sub-lattice and Si atoms can occupy any of the octahedral voids. Due to uncertainty in Si positions, previously unknown ground state structure of Si$_2$Te$_3$ was obtained using the Wyckoff positions of space group P-31c. The minimum energy configuration exhibits combination of desirable electronic and transport properties. In particular, n-doped Si$_2$Te$_3$ has an unprecedented figure of merit of 1.86 at 1000 K, which is comparable to some of the best state-of-the-art thermoelectric materials. Hence, n-doped Si$_2$Te$_3$ can be a long-sought silicon-based thermoelectric material which could be integrated to the existing electronic devices.

5:18PM V47.00013: Enhanced Cross-plane Thermoelectric Transport of Rotationally-disordered SnSe$_2$ via Se Vapor Annealing* JIHAN CHEN (Presenter), University of Southern California, DANIELLE HAMANN, University of Oregon, DAVID CHOI, University of Texas, Austin, NIRAKAR POUTDEL, LANG SHEN, University of Southern California, LI SHI, University of Texas, Austin, DAVID JOHNSON, University of Oregon, STEVE CRONIN, University of Southern California — In this talk I will review our recent progress in cross-plane thermoelectric measurements of SnSe and SnSe$_2$ films grown by the modulated element reactant (MER) approach. The initially grown SnSe films have relatively low cross-plane Seebeck coefficients due to significant unintentional doping originating from Se vacancies. By performing post-growth annealing at a fixed Se partial pressure, a transition from SnSe to SnSe$_2$ is induced. This results in a 16-fold increase in the cross-plane Seebeck coefficient (from -38.6 to -631μV/K) after Se annealing due to both the SnSe to SnSe$_2$ transition and the mitigation of unintentional doping by Se vacancies. The power factor $S^2σ$ increased by 44X after Se annealing. We believe that these results demonstrate a robust method for mitigating unintentional doping in a promising class of materials for thermoelectric applications.1


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NSF Grant DMR1710214.
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Thursday, March 7, 2019 2:30 PM - 4:18 PM

Session V48 DFD GSOFT GSNP: Drops III BCEC 251 - A Hirsa, Rensselaer Polytech Inst - Tag(s): Focus

2:30PM V48.00001: The Effect of Detaching Force on the Droplet Residue on a Fiber NEDA OJAGHLOU (Presenter), Department of Chemistry, Virginia Commonwealth University, HOOMAN TAFRESHI, Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, DUSAN BRATKO, ALENKA LUZAR, Department of Chemistry, Virginia Commonwealth University — The adherence to, and removal of droplets from cylindrical fibers underlie applications from fog harvesting, oil-water, and water transport in fuel cells. When the droplets are forcibly removed from hydrophilic fibers, the ease of detachment strongly depends on droplet volume and the rate of the process controlled by the applied force. In the present work, we study the mechanism of water droplet detachment and retention of residual water on smooth hydrophilic fibers using nonequilibrium molecular dynamics simulations. We extract scaling relations that allow extrapolation of our findings to larger length scales that are not directly accessible by molecular models. Our studies of the droplet breakup uncover a strongly nonmonotonic influence of external force, with the amount of residual water maximized under the intermediate force strengths whereas a complete or near-complete detachment of the droplet can be achieved in both extremes, with the applied force only slightly, or considerably exceeding the minimal force of detachment. The strength of this force decreases with the size of the drop, while the maximal residue increases with the droplet volume, V, sub-linearly, in proportion to the V$^{2/3}$.

2:42PM V48.00002: Effects of surfactant transport on the electro-deformation of viscous prolate drops HERVE NGANGUIA (Presenter), Indiana University of Pennsylvania, ON SHUN PAK, Mechanical Engineering, Santa Clara University, YUAN-NAN YOUNG, Mathematical Sciences, New Jersey Institute of Technology — We report quantification of effects of surfactant transport on a viscous prolate drop under a DC electric field, focusing on characterization through the dimensionless Peclet number. Our findings reveal distinct equilibrium deformations that depend on the type of drops (leaky dielectric versus conducting) and the transport regime (convection or diffusion).
The mode of deformation, described by the flow circulation in a leaky dielectric drop, also contributes to the non-trivial deformation. For counter-clockwise circulation, we found leaky dielectric drops consistently yield larger deformation compared to perfectly conducting drops. The deformations result from the non-linear coupling between surfactant concentration and transport: higher surfactant concentrations yield larger (smaller) deformation with strong convective (diffusive) flows. For clockwise circulation, the deformation decreases (increases) with increasing surfactant concentration when convection (diffusion) dominates. We show that in this case conducting drops can yield larger deformations compared to leaky dielectric drops at moderate to high surfactant concentration. Finally, we look at the transient evolution of the drop shape, and discuss novel findings that have yet to be disseminated.
2:54PM V48.00003: Migration of droplets on a conical fiber  CARMEN LEE (Presenter), KARI DALNOKI-VERESS, McMaster University — In arid climates, nature has developed an efficient method of harvesting water from the air. Organisms, like cacti, are covered in a multitude of needle-like conical spines. Water droplets that condense on the tip of the fiber are spontaneously driven toward the base by Laplace pressure. The changing curvature of the conical shape is the mechanism responsible for the motion. We examine the effect of geometry on the droplet movement and compare the motion of multiple droplets on a conical glass fiber to that of a single droplet.

3:06PM V48.00004: Preliminary observations of bursting of molten steel thick films in a steel plate irradiated by a high energy laser*  MARY LANZEROTTI (Presenter), Physics and Nuclear Engineering, United States Military Academy, KENNETH BRAKKE, Department of Mathematical Sciences, Susquehanna University, KENNETH ALLEN, JOHN HARTKE, Physics and Nuclear Engineering, United States Military Academy — This talk presents preliminary observations of the bursting of films of molten steel following illumination of a thin vertical steel plate by a 1075-nm continuous-wave 1000W Ytterbium fiber laser. Molten steel formed in the illuminated region persists as a molten disk for several seconds before a hole forms. Gravity is responsible for the formation of a dimple in the upper part of the molten disk and a bulge in the lower part. After several seconds, a hole appears at the dimple. Hole enlargement is quite sudden, like a soap film popping. Following this, a molten drop forms and falls under the influence of gravity below the laser beam, leaving behind a hole in the plate. Images of the initial hole captured by a high speed digital camera show that the hole forms first in the top portion of the molten disk, not in the center.

The molten steel is modeled as liquid contained within a hoop with size of the final hole. 3D images produced by Surface Evolver, an interactive program for modelling liquid surfaces, indicate the presence of a dimple within the molten region near the location of first appearance of the hole, and a bulge in the molten region near the lower portion for a liquid with density and surface tension taking on values near the melting point of iron.

*Army JTO, ARO

3:18PM V48.00005: Mechanism of Contact between a Droplet and an Atomically Smooth Substrate  HAU YUNG LO (Presenter), YUAN LIU, LEI XU, Physics Department, Chinese University of Hong Kong — When a droplet gently lands on an atomically smooth substrate, it will most likely contact the underlying surface in about 0.1 s. However, theoretical estimation from fluid mechanics predicts a contact time of 10–100 s. What causes this large discrepancy, and how does nature speed up contact by 2 orders of magnitude? To probe this fundamental question, we prepare atomically smooth substrates by either coating a liquid film on glass or using a freshly cleaved mica surface, and visualize the droplet contact dynamics with 30-nm resolution. Interestingly, we discover two distinct speed-up approaches: (1) droplet skidding due to even minute perturbations breaks rotational symmetry and produces early contact at the thinnest gap location, and (2) for the unperturbed situation with rotational symmetry, a previously unnoticed boundary flow around only 0.1 mm/s expedites air drainage by over 1 order of magnitude. Together, these two mechanisms universally explain general contact phenomena on smooth substrates. The fundamental discoveries shed new light on contact and drainage research.

3:30PM V48.00006: Manipulating drop shapes in a microchannel  ROCIO NAVARRO (Presenter), ALEXANDER ZINCHENKO, ROBERT DAVIS, Chemical and Biological Engineering, University of Colorado Boulder — We use a boundary-integral algorithm that simulates the motion of a freely suspended, three-dimensional deformable drop in a plane-parallel microchannel at small Reynolds number, large Peclet number, and moderate capillary number. The drop size is comparable to the channel height, which is much smaller than the channel depth. In this problem, the final shape of the drop is extremely dependent on the channel shape, flow ratios and time, so we have studied a variety of conditions. By changing the number of inlet and outlet channels, as well as the physical geometry of the channel and the drop properties, we are able to create a diverse set of droplet shapes, including shapes with interesting geometric properties such as deltoids, dumbbells and oblate spheroids. In principle, desired shapes could subsequently be “frozen” by a temperature-induced or flow-induced phase change, to yield particles with desired geometries and properties for drug delivery, tissue scaffolds, etc. This presentation will describe the simulation method and present example results of how different shapes may be achieved.
FRANK RILEY (Presenter), SHREYASH GULATI, Rensselaer Polytechnic Institute, JUAN MANUEL LOPEZ, Arizona State University, A HIRSA, Rensselaer Polytechnic Institute — In the ring-sheared drop, a liquid drop is constrained by two contact rings, where the rings differentially rotate. This differential rotation generates a flow in the bulk primarily through surface shear viscosity. Numerical predictions of bulk flow and mixing within ring-sheared drops were recently reported. The previous work assumed that the surface shear viscosity, non-dimensionalized by the size of the drop, is large. However, in many cases, especially for large drops, which can be studied in microgravity, the dimensionless surface shear viscosity can be arbitrarily small but still able to affect the bulk flow. Computations reveal that an increasing Reynolds number correlates to an increase in sensitivity to the effects of changing surface shear viscosity. Furthermore, upon decreasing surface viscosity, the coupling between the surface and the bulk flows strengthens. The system is then driven towards solid-body rotation. 

*Supported by NASA grant NNX13AQ22G

3:54PM V48.00008: Droplet Motion on Superhydrophobic Surfaces  
ALEXANDER SMITH (Presenter), REBECCA SUTTON, KEONI MAHELONA, SHAUN C HENDY, University of Auckland — In this talk, molecular dynamics simulations are used to investigate the roles of droplet size and surface geometry on the equilibrium velocity of droplets moving down superhydrophobic surfaces. An extension of prior theoretical descriptions, accounting for interfacial slip, is used to interpret these results. This approach yields three limiting cases for the drop's steady-state velocity, where energy losses are dominated by viscous dissipation, surface friction or contact line friction respectively. We find that for droplets on ideal textured high-slip surfaces, contact line dissipation dominates droplet motion, with droplet velocity increasing with radius. At droplet radii larger than the capillary length, we retrieve the usual viscosity-dominated motion.

4:06PM V48.00009: Numerical Investigation of Hypoxic Effects on the Biodegradation of Oil Microdroplets  
GEORGE KAPELLOS (Presenter), Chemical Engineering, Massachusetts Institute of Technology, NICOLAS KALOGERAKIS, Environmental Engineering, Technical University of Crete, PATRICK DOYLE, Chemical Engineering, Massachusetts Institute of Technology — We present an extended compound particle model for the biodegradation of solitary oil microdroplets moving through a seawater column. The compound particle is of the core-shell type and consists of an oily core that is successively surrounded by an ultrathin bioreactive skin of oleophilic microbes and another bioreactive biofilm shell. The extended model accounts for the counter transport of dissolved oxygen and multiple oil components of varying bioavailability and toxicity within the biofilm that covers and degrades the oily droplet. The governing advection-diffusion-bioreaction PDEs are solved numerically to calculate the droplet shrinking rate as a function of the drifting speed, the non-linear microbial kinetics, the biofilm thickness, and other key parameters. A system of coupled ODEs is also formulated for the evolution of the compound particle dimensions. The impact of hypoxic and inhibitory conditions on the droplet biodegradation rate is quantified and critically discussed in connection with the potential for the - very slow, but feasible-anaerobic hydrocarbon degradation in oxygen-depleted marine waters and sediments.

*EU Horizon 2020 MSCA Grant 741799 - "OILY MICROECOSM"

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V49 GSOFT GSNP: Mechanics of Materials Processing  
BCEC 252A - Frederick Gosselin, Ecole Polytechnique de Montreal - Tag(s): Focus
Plastic instabilities, mechanochemistry, and a bag of (metal) chips*  [Invited]  KOUSHIK VISWANATHAN (Presenter), Indian Institute of Science — Soft and highly strain hardening metals like Ni, Al, Ta and stainless steels, are notoriously difficult to cut, earning them the moniker “gummy”. This difficulty is well-known for its commercial implications, yet its origins have remained largely mysterious. This talk presents high-speed in situ investigations of this problem in two parts. In the first, we unveil the occurrence of a highly unsteady plastic flow mode, termed sinuous flow, as the cause of this difficulty. Sinuous flow arises due to a surface plastic buckling instability and is characterized by repeated material folding, large local strains (>10) and energy dissipation. The physics of this flow, its dependence on material properties, and manifestation across metals are directly observed. In the second part, we demonstrate how sinuous flow can be perturbed using mechanochemistry. A suitable chemical medium applied to the metal surface causes a local ductile-to-brittle transition by coupling plastic instabilities with interface energetics. Consequently, surface buckling and sinuous flow are replaced by a periodic fracture instability in the presence of the medium, with near absence of defects on the cut surface and significantly lower energy dissipation (~80%). The transition in flow is also reflected in the morphologies of the resulting metal chips. This mechanochemical effect is controllable and largely material agnostic, with many chemical media working equally well across different metal systems. Additionally, the benign nature of the media presents exciting opportunities for fundamentally enhancing deformation processing of metals in industrial settings.

*Financial support from the Indian Institute of Science, US Army Research Office (Award W911NF-15-1-0591) and NSF (Awards CMMI1562470, DMR1610094) is gratefully acknowledged.

Mechanics of bilayers: What soft matter physics can teach us about shot peen forming of aircraft wing skins*  FREDERICK GOSSELIN (Presenter), PIERRE FAUCHEUX, MARTIN LEVESQUE, Laboratory for Multiscale Mechanics, Ecole Polytechnique de Montreal — Peening treatments (e.g., shot, laser, and cavitation peening) are ubiquitous when designing metallic parts against fatigue failure: by introducing compressive surface residual stresses that oppose crack initiation and growth, they can significantly increase the fatigue strength of treated parts. Peening induced stresses also cause distortions. Although usually seen as an unwanted side effect, these distortions can be controlled to form thin-walled structures into complex contours—a process referred to as peen forming. In this talk, we focus on modeling shot peen forming (a variant that consists in bombarding the parts with small hard shot). By analogy with thin bilayer actuated systems usually encountered in the fields of smart structures, soft robotics, and composite manufacturing, we investigate the shape and stability of peen formed parts. We also present a procedure to generate peening patterns required to form initially flat plates into a desired shape, alongside experimental validation.

*The authors gratefully acknowledge financial support from Airbus, the Rio Tinto group through a graduate scholarship, and the Canada Research Chairs program.

Cutting as a Tool for Investigating Crack-Blunting-Involved Soft Fracture*  BINGYANG ZHANG (Presenter), CHENG-SHEN SHIANG, SHELBY HUTCHENS, University of Illinois at Urbana-Champaign — During tearing of soft elastomers, large deformation occurs due to crack-blunting. The incorporated material nonlinearity alters the fracture response, resulting in a measured fracture energy value higher than the prediction from network binding energy [Lake and Thomas, 1967]. To understand the dependence of fracture energy on the nonlinear constitutive response, we control the crack tip geometry via cutting. A Y-shaped cutting geometry, inspired by Lake and Yeoh (1978), uses two separate “legs” to form a cutting notch that minimizes contact friction. A blade aligned with the notch imposes its radius during cutting. We find that cutting fracture energy increases nonlinearly with large blade radii. The radius sensitivity reflects the strain-stiffening constitutive response governing crack-blunting during tearing. However, as the blade radius decreases, the effect of nonlinearity is minimized and the cutting energy plateaus to a constant that appears to scale with elastic modulus. We evaluate the potential of cutting as a method for characterizing “intrinsic” fracture energy and provide insight into the microstructural origin of the plateauing transition using cutting tests from idealized, end-linked polydimethylsiloxane (PDMS) networks.

*National Science Foundation (no.1562766)
3:30 PM V49.00004: Stable and collision-free manipulation of an elastic rod using multiple grippers* ANDY BORUM (Presenter), Department of Mathematics, Cornell University — Despite the widespread adoption of robots in manufacturing, many tasks that involve handling and assembly of deformable objects are still completed manually. Automating these tasks requires reasoning about deformations, instabilities, and self-contact experienced by the deformable objects. As a canonical example of such a task, I will discuss the problem of deforming a slender elastic rod into a desired configuration using two or more robotic grippers that grasp the rod at multiple points. In the case when the grippers are required to grasp the rod at fixed arc lengths, I will show that the set of all equilibrium configurations of the rod that are stable is path-connected. If the grippers are allowed to slide along the rod, I will show that the set of all equilibrium configurations that are both stable and non-self-intersecting is path-connected. The proofs of these two results are constructive and provide analytical solutions that can be exploited when designing algorithms for automated handling of slender structures.

*This work was supported by NSF Grant No. DMS-1645643.

3:42 PM V49.00005: Pleat formation and the geometry of pure bending TIAN YU (Presenter), JAMES HANNA, Virginia Tech — We will discuss our recent attempts towards understanding the mechanics of pleat forming in soft textile sheets. This is an elastic-plastic bending process that we formulate as a variable-arc-length multi-point boundary value problem for an inextensible rod, with a moment-curvature constitutive relation as input. To determine this moment-curvature relation, we have developed a linkage mechanism that can impose an exact pure bending (constant curvature) state up to high curvatures. A simpler approximate mechanism that nearly matches the exact boundary conditions is nonetheless shown to result in significant curvature variations. Our approach is relevant to recent studies of crease formation in polymers that can inform models of folded deployable structures.

3:54 PM V49.00006: Mechanistic Insights into Mixed Surfactant-Biosurfactant Self-Assembly, Rheology and Surface Properties SAMIUL AMIN (Presenter), LIANGCHEN XU, YAO ZHOU, Department of Chemical Engineering, Manhattan College — The global surfactant market is expected to reach $44.9 billion by 2022, of which 67% of the demand is from the personal care and detergents market. Due to consumers’ increasing awareness on product sustainability, the microbially produced biosurfactants are increasingly gaining the interest of the personal care industry as potential alternatives for traditional petroleum derived and chemically synthesized surfactants. However, prior to that, an understanding of how performance criteria such as rheology and interfacial properties are affected by substitution of traditional surfactants with biosurfactants is required. In this study, the effect of rhamnolipid and sophorolipid biosurfactants on the rheological response and interfacial properties of traditional surfactants such as sodium laureth sulfate and cocamidopropyl betaine is explored utilizing a range of advanced characterization techniques. Diffusing Wave Spectroscopy based Optical Microrheology is specifically carried out to gain insights into the short time dynamics in these systems and is also utilized for extracting wormlike micelle structural parameters such as contour lengths and persistence lengths. These insights are utilized to develop unique formulation design rules for biosurfactant based products.

4:06 PM V49.00007: Scratching viscoelastic liquids* ASHEESH SHUKLA (Presenter), NICOLAS CHANUT, Civil and Environmental Engineering, Massachusetts Institute of Technology, ROLAND JM PELLENQ, Civil and Environmental Engineering, MIT / CNRS, FRANZ-JOSEF ULM, Civil and Environmental Engineering, Massachusetts Institute of Technology, THIBAUT DIVOUX, Civil and Environmental Engineering, MIT / CNRS — Viscoelastic materials are ubiquitous in our everyday life: from skin tissue to butter or bitumen, we are surrounded by materials that display both a viscous and an elastic response under external deformation. Beyond the linear deformation regime, such materials often exhibit complex flow profiles, from spatially heterogeneous ductile flow to crack and fractures. In this presentation, we focus on the latter category of materials and show that a scratch technique, which has been extensively applied for determining the resistance to fracture of solids, can be successfully applied to viscoelastic materials. Using a Rockwell diamond probe of conical shape mounted on a micro scratch tester (Anton Paar), we perform direct measurements of the fracture toughness of various type of bitumen samples at ambient temperature. We show that the fracture toughness of bitumen increases as a power-law of the horizontal scratch speed, independently of the vertical loading rate. The power-law exponent is characteristic of the sample and increases for decreasing penetration grade. Finally, we use the scratch test to quantify the impact of various additives (polymer, glass beads, etc.) on the fracture toughness of bitumen samples.

*Ditecsesa/Ferrovial
We use classical microfluidics flow-focusing technique to synthesize concentrated emulsions, based on a difunctional acrylic monomer, as constitutive “atoms” of size ~50μm. Then, using in situ photopolymerization, the emulsions turn into soft colloidal particles that interact with each other to form soft colloidal-based gels. We vary the rheological properties of these emulsions by regulating conditions for photopolymerization. Using conventional optical microscopy, we also use a microfluidics-based test cell to hydraulically fracture these soft gels at controlled flow rates and examine both micro-cracking and plastic events, i.e. the local irreversible displacements around the crack tip.

*We like to thank the Institut Pierre Gilles de Gennes (IPGG), ANR-10-EQPX-34, and ESPCI Paris.

**3D printing by tailored extrusion of carbon nanotube inks**

CRYSTAL OWENS (Presenter), GARETH MCKINLEY, JOHN HART, Massachusetts Institute of Technology — 3D printing through direct-ink writing builds objects by layerwise deposition of material; and the properties of the final object are governed both by the ink and by the hierarchical organization within and across layers. In extrusion 3D printing of thermoplastics, strength and thermal stability can be improved by addition of rod-like fillers such as carbon nanotubes (CNTs) or carbon/glass microfibers. However, the mechanical properties of 3D printed objects are far from those achieved by spinning of continuous fibers out of the same material. We study the flow-mediated structure evolution of rigid rod-like particle-based inks using single-walled carbon nanotubes (SWCNTs) at high concentrations from 0.7-1%wt. We report the influence of processing parameters such as the flow rate, rate of elongation, and rate of reaction or diffusion on the strength, conductivity, and dimensions of the extruded filament, and of printed test artifacts. Our results suggest that 3D printing processes for architected materials can be improved by incorporating key principles of fiber spinning.

*The authors acknowledge funding from a National Defense Science and Engineering Graduate Research Fellowship (NDSEG) and from NASA STRI 2017.

**Electrospinning Polyelectrolytes from Complex Coacervates**

XIANGXI MENG, SARAH PERRY, JESSICA SCHIFFMAN (Presenter), Chemical Engineering, University of Massachusetts Amherst — Electrospun fibers are canvases that can be tailored towards a wide variety of applications. However, traditional electrospinning often involves organic solvents that can cause cytotoxicity concerns. Here, I will highlight our revolutionary fibers that form using only water and salt. Polyelectrolyte complexes (PECs) form due to the electrostatic complexation between oppositely-charged polymers. We have recently demonstrated that by exploiting the salt-driven plasticization of PECs, we can enable the electrospinning of ultra-stable solid fibers from an aqueous solution containing a pair of strong polyelectrolytes and salt. Electrospun PEC fiber mats are stable over a wide range of pH values, ionic strength conditions, and many organic solvents. To address the challenge of delivery, we encapsulated a library of dyes into the coacervate phase and subsequently, achieved highly-loaded electrospun fibers. Finally, I will propose a mechanistic understanding of the design rules for electrospinnable coacervates by correlating polymer chain length, with coacervate phase behavior, and as-spun fiber morphology. The overall goal of the talk is to illustrate our recent findings and how these results can guide the green engineering of multifunctional fiber mats.

*NSF CMMI-1727660*
4:54PM V49.00011: Modeling of shot peen forming using non-Euclidean plate theory* VLADISLAV SUSHITSKII (Presenter), Mechanical Engineering, Ecole Polytechnique de Montreal, GUY LEVASSEUR, Aerosphere Inc., WILLEM MARINUS VAN REES, Mechanical Engineering, Massachusetts Institute of Technology, MARTIN LEVESQUE, FREDERICK GOSSELIN, Mechanical Engineering, Ecole Polytechnique de Montreal — Shot peen forming is a versatile technique for shaping large thin panels by impacting them with thousands of high-velocity millimeter-sized shots. The process is widely used in aerospace, notably to form wing skins. Two main factors hinder the process' efficiency: the lack of accurate and simple modeling tools and the lack of automation. Without modeling, the process' setup relies on a lengthy trial and error procedure. Our project is intended to fill this gap and to provide the industry with a reliable and efficient modeling software. The software is based on innovative theoretical framework of non-Euclidean plate theory relying on Riemannian geometry. This theory was initially developed to describe growth-induced reconfiguration of thin organic tissues, and in terms of mechanics these processes share many similarities with peen forming. It is the incompatibility between local stretching and curvature induced by different mechanical processes that is viewed as the reason of reconfiguration. The accuracy and performance of our software were examined in laboratory conditions by comparing simulations with experimental results for the case of large 1x1m aluminum plates submitted to peen forming.

*The authors acknowledge the financial support from Aerosphere Inc., FRQNT and REGAL.

5:06PM V49.00012: A deep learning approach to solving the peen forming inverse problem WASSIME SIGUERDIDJANE (Presenter), FARBOD KHAMENEIFAR, FREDERICK GOSSELIN, Mechanical Engineering, Ecole Polytechnique Montreal, GUY LEVASSEUR, AeroSphere Inc. — Peen forming is a cold forming process where surface plastic deformations are created by high-velocity projectile impacts. The resulting local expansions of the treated surface lead to local curvature variations. The effect of the peening treatment can be represented as a thermal expansion on a bi-layered plate, making this problem identical to bilayers in soft material physics. The motivation for this work is the development of automated robotic peen forming, which will increase the repeatability, accuracy, and efficiency of the process. With our goal being full process automation, we are interested in solving the inverse problem of calculating the required peening trajectories to form a part into the desired shape. To achieve this, we present an efficient method using deep learning to recognize patterns linking deformed plates to the required peening trajectories. The proposed model is trained on a large dataset to infer the required peening trajectories. Our results show that the predicted patterns create deformed shape deviations in the order of 100 microns. We consider that this approach can be used as part of a feedback loop to achieve full process automation.

5:18PM V49.00013: The effect of cryogenic thermal cycling on potential energy states and mechanical properties of metallic glasses NIKOLAI PRIEZJEV (Presenter), Mechanical & Materials Engineering, Wright State University — The structural relaxation, potential energy states, and mechanical properties of a model glass subjected to thermal cycling are investigated using atomistic simulations. We study a non-additive binary mixture which is annealed with different cooling rates from the liquid phase to a low temperature well below the glass transition. The thermal treatment is applied by repeatedly heating and cooling the system at constant pressure. We find that poorly annealed glasses are relocated to progressively lower levels of potential energy over consecutive cycles, whereas well annealed glasses can be rejuvenated at sufficiently large amplitudes of thermal cycling. The structural transition to different energy states is accompanied by collective nonaffine displacements of atoms that are organized into clusters, whose typical size becomes larger with increasing cooling rate or temperature amplitude. We show that the elastic modulus and the peak value of the stress overshoot exhibit distinct maxima at the cycling amplitude, which corresponds to the minimum of the potential energy. The simulation results indicate that the yielding peak as a function of the cycling amplitude for quickly annealed glasses represents a lower bound for the maximum stress in glasses prepared with lower cooling rates.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V50 DPOLY: Ion Transport Mechanisms in Ionic Liquid/Polymer Hybrids BCEC 252B -

Lisa Hall, Ohio State University - Tag(s): Focus
Influence of Side-chain Chemistry on Structure and Ionic Conduction Characteristics of Polythiophene Derivatives: A Computational and Experimental Study

BAN DONG (Presenter), Institute for Molecular Engineering, University of Chicago, CHRISTIAN NOWAK, School of Chemical and Biomolecular Engineering, Cornell University, JONATHAN ONORATO, Department of Materials Science and Engineering, University of Washington, FERNANDO A ESCOBEDO, School of Chemical and Biomolecular Engineering, Cornell University, CHRISTINE LUSCOMBE, Department of Materials Science and Engineering, University of Washington, PAUL F NEALEY, SHRAYESH PATEL, Institute for Molecular Engineering, University of Chicago

While extensive efforts have been devoted to understand electronic transport in conjugated polymers, little is known about their ionic conduction characteristics in relation to polymer chemistry and morphology. This work presents a combined computational and experimental study on morphology and ion transport in thin film blends of polythiophene derivatives and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI). Using molecular dynamics (MD) simulation, we show that in the amorphous phase, a polythiophene derivative P3EGT bearing oligoethylene glycol side-chains with an oxygen directly attached to the thiophene rings possesses lower Li⁺ ion conductivity compared to its analog P3MEGT that has a methyl spacer between the oxygen and the thiophene rings. Structural characterization of P3EGT- and P3MEGT-LiTFSI thin films indicates that LiTFSI preferably resides in the amorphous domain especially at high LiTFSI concentrations. Ionic transport measured by impedance spectroscopy is found to occur in amorphous domain, and ionic conductivity in P3MEGT is always higher than in P3EGT, consistent with prediction from simulation. Our work provides a platform to predict and study the influence of polymer chemistry on ionic conductivity of conjugated polymers.

Ion-Transport Properties of Nanothin Film Dry Polymer Electrolytes

BAN DONG, PAUL F NEALEY, SHRAYESH PATEL (Presenter), Institute for Molecular Engineering, University of Chicago

Polymer electrolytes have demonstrated promise as dry electrolyte materials to enable lithium-metal batteries. However, majority of studies have focused only on thick samples (100's of microns). However, interfaces play a critical role on the performance of batteries, thus investigating polymer electrolyte in the context of nanothin films (5-100 nm) will lead to better understanding of the role of interfaces on charge transport properties. Here, we report on ion transport characteristics of nanothin films of PEO and LiTFSI blends as a function of salt concentration, temperature and film thickness. Ion transport measurements were successfully performed using impedance spectroscopy on films fabricated on custom-designed nanofabricated interdigitated electrode (IDE) devices. Importantly, thickness dependence study of ion transport shows a monotonic decrease in ionic conductivity upon decreasing film thickness from 250 nm to ca. 10 nm, and the effect is stronger at low salt concentrations. The decrease of ionic conductivity at thinner films originate from the increasing fraction of the immobilized layer near the polymer/substrate interface. Our results suggest that using nanothin film configuration is a promising strategy to probe interfacial effects on ion conducting properties.

Proton transport through acid aggregates in a hydrated precise sulfophenylated polyethylene

BENJAMIN PAREN (Presenter), University of Pennsylvania, LIONEL PICARD, LITEN-DEHT-SCGE-LM, CEAtch, PATRICE RANNOU, MANUEL MARECHAL, Univ. Grenoble Alpes, CNRS, CEA, INAC-SYMMES, WILLIAM NEARY, AARON KENDRICK, JUSTIN G KENNEMUR, Florida State University, AMALIE FRISCHKNECHT, Sandia National Labs, KAREN WINEY, University of Pennsylvania

Hydrated acid aggregates in a precise sulfophenylated polyethylene exhibit high proton conductivity. This study focuses on a new precise polymer, synthesized by ring-opening polymerization, that has a polyethylene backbone with a sulfonated phenyl group pendant on every 5th carbon, p5PhSA. The structure of p5PhSA is characterized with X-ray scattering and the proton conductivity is characterized with electrical impedance spectroscopy. Both experiments are performed as a function of relative humidity and temperature. Sorption measurements determined the water uptake in p5PhSA as a function of humidity as well. Atomistic molecular dynamics simulations are used to elucidate the structure of the acid aggregates in the amorphous polymer matrix and are directly compared to absolute X-ray scattering data. At 40°C and 90% relative humidity, the proton conductivity of p5PhSA is 0.17 S/cm, exceeding that of Nafion. At room temperature, interaggregate distance nearly doubles from 1.8 nm at 0% relative humidity, to 3.4 nm at 100% relative humidity. The swelling of these ordered acid aggregates with water is reversible, and facilitates the proton transport through p5PhSA.

Proton transport through acid aggregates in a hydrated precise sulfophenylated polyethylene

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3:06PM V50.00004: Mesoscale Organization and Dynamics in Ionic Liquids* [invited] JOSHUA SANGORO (Presenter), Chemical and Biomolecular Engineering, University of Tennessee — The impact of mesoscale organization on transport and dynamics in ionic liquids is investigated by broadband dielectric spectroscopy and dynamic mechanical spectroscopy as well as x-ray and neutron scattering techniques, complemented by computational approaches. Signatures of slow, sub-α dynamics are identified in the dynamic-mechanical and dielectric spectra and employed to probe lifetimes and dynamics of mesoscale aggregates in ionic liquids. It is found that the dynamics of mesoscale aggregates dominate many physicochemical properties such as the static dielectric permittivity and viscosity. By using mixtures of ionic liquids to tune composition-dependent evolution of the morphology, it becomes possible to realize ionic liquids with enhanced physicochemical properties that are otherwise inaccessible in neat systems. This talk will discuss the role of mesoscale organization and dynamics on macroscopic physical properties of ionic liquids.

*Financial support from the National Science Foundation, the Division of Chemistry through No. CHE-1753282 is gratefully acknowledged.

3:42PM V50.00005: Diffusion of Ions in Diblock Copolymers: Understanding the Molecular Weight Effect Through Coarse-Grained Modeling* YOUNGMI SEO, LISA HALL (Presenter), Ohio State University — Diblock copolymers in which one microphase is mechanically robust while the other solvates and allows conduction of ions are of interest as solid battery electrolytes. The transport of ions through the conducting microphase is generally slower than through the analogous homopolymer, and is thought to depend on the distribution of ions within the conducting phase, among other factors. To understand these effects, we use coarse-grained molecular dynamics simulations and consider a wide range of systems with various ion-polymer and ion-ion interaction strengths. Our model reproduces the experimental trend of increasing ion transport with copolymer molecular weight, and this trend is more dramatic as ions are solvated in one polymer block more strongly or as the ion-ion interactions get stronger. The degree to which ions are locally concentrated, quantified by their average number of nearest ion neighbors out to a distance of approximately three diameters, is a good predictor of the ion diffusion constant. Specifically, systems whose ions are more locally aggregated (have more ion neighbors) have a reduced diffusion constant.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0014209

3:54PM V50.00006: Study of Segmental Dynamics in Polymer-Ceramic Composite Electrolytes using Quasi-elastic Neutron Scattering* CHELSEA CHEN (Presenter), NARESH OSTI, ROBERT L SACCI, NANCY J DUDNEY, Oak Ridge National Laboratory — Composite solid electrolytes consisting of a polymer electrolyte and an ion-conducting ceramic electrolyte have potential in achieving high ionic conductivity, high mechanical modulus and good processability to enable higher energy density technologies. In this work we fabricated composite electrolyte consisting of poly(ethylene oxide) (PEO), lithium trifluoromethanesulfonate (LiTf), and a lithium-conducting glass ceramic (LICGC) from Ohara corporation. We discovered that thermal history has a profound impact on the PEO segmental dynamics, resulting in drastically different conductivities below the melting point of PEO in the first heating and cooling cycles. The average relaxation time of PEO chains decreased with the presence of LICGC. However, the enhanced segmental motion contradicts the decrease in the ionic conductivity of the composite electrolyte. The relationship between ionic conductivity, segmental motion, crystallinity and tortuosity in the composite electrolyte will be discussed.

*This work was sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering. Neutron scattering experiments were performed at Spallation Neutron Source.

4:06PM V50.00007: Analyzing Ion Conductivity in Block Copolymer Electrolytes from Molecular Dynamics Simulations with an Applied Electric Field KUAN-HSUAN SHEN (Presenter), LISA HALL, William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University — Salt-doped block copolymers can be created with one microphase that is mechanically robust and another that solvates and conducts ions. A variety of polymer and ion types can be chosen, and molecular simulations can show how these choices impact ion motion to guide design of new materials. One strategy to increase conduction is to tune dielectric constant to reduce the degree of correlation of cation and anion motion, which can be significant in salt-doped copolymers. However, it is difficult to assess such a strategy in simulations, which often calculate self-diffusion constants of ions and estimate conductivity using the Nernst-Einstein equation (neglecting ion correlations). Conductivity can be directly calculated, including effects of correlated ion motion, from equilibrium simulations. However, this approach introduces a large statistical uncertainty. We aim to calculate conductivity from ion mobilities under an applied electric field. We ensure the field is low enough that the systems are in the linear response regime while still allowing for mobility high enough to measure accurately in the timescale of the simulation. We then compare conductivity of various systems as a function of Coulombic and polymer-ion interactions.
In this study, the diffusion coefficient of lithium salt through a polystyrene-poly(ethylene oxide) block copolymer (SEO) was investigated using time-resolved Fourier Transform infrared - attenuated total reflectance (FTIR-ATR) spectroscopy. FTIR-ATR directly measures change of concentration in response to a concentration gradient, which is relevant for battery operation. FTIR-ATR is simpler and faster than electrochemical measurements, such as restricted diffusion, that require calibration and assumption about how cell potential relates to concentration gradient. Since the measurements are made in the absence of other driving forces, such as applied potential, the diffusion coefficient is independent of ionic conductivity and transference number. We studied the effect of salt concentration on the diffusion coefficient above the melting temperature of the electrolyte. Our results indicate that the diffusion coefficient is concentration-dependent, but not monotonic.

*This work was supported by funding from LG Chem.

We investigate the influence of doping on the conductivity of high molecular weight, crystalline PEO₆ based solid polymer electrolytes (SPEs). Polyethylene oxide (PEO) based SPEs are an attractive alternative to the flammable liquid/gel electrolytes currently used in rechargeable lithium ion batteries. But, SPEs suffer from low ionic conductivity. The conductivity is linked to PEO segmental motion; in order to increase the segmental motion, we must reduce the glass transition temperature $T_g$. Unfortunately increase in polymer dynamics reduces mechanical strength of SPE. PEO₆-LiClO₄ complex is a tunnel like PEO/salt co-crystal which conducts Li⁺ based on a mechanism that decouples conductivity and segmental motion of the polymer. Inspired from ceramics, we dope small amounts of anions or cations to disrupt the PEO₆-LiClO₄ lattice. We vary the size of the anion, and cation to create defects in the crystal lattice. We observe up to 900% increase in the conductivity of doped samples even with small amount dopant (1%). Interestingly, the increase in conductivity is not correlated with the decrease in $T_g$ of the SPEs. With wide angle X-ray scattering, we observe transition from single crystalline phase to mixed phase morphology with increase of the dopant concentration.

In recent work [ACS Macro Lett. 2018, 7, 1149-1154], we explored the role of polymer host polarity on ionic conductivity using the Stockmayer model of polar fluids applied to a coarse-grained Kremer-Grest polymer. In this model, a freely rotating electric dipole moment is embedded in each monomer bead. We found that the ionic conductivity maximized at some intermediate host polarity, as measured by the monomeric point dipole moment strength. We demonstrated that this maximization arises from a tradeoff between reduced ionic aggregation and slowed segmental dynamics as the host polarity increased. In this work, we investigate the influence of salt concentration, temperature, and host molecular weight on ionic conductivity and the nonmonotonic variations with the polarity of the host polymer medium.

*The authors acknowledge the Welch Foundation and the National Science Foundation for funding this work.

We developed a coarse-grained molecular dynamics simulation model incorporating a dynamic bonding scheme to study the transport properties of associated particles in polymeric melts. In order to mimic the hopping of lithium ions in polymer electrolytes, a probability of breaking a dynamic bond between an associated particle and an active bead along polymer chains, $P_{\text{break}}$, was introduced to tune the activation energy between bound and unbound states. Both static (Kuhn length of solvated polymer chains, radial distribution functions, and connectivity of associated particles) and dynamic (mean squared displacement, and diffusion coefficient) properties of two classes of macromolecules were studied: a linear chain system with various bending rigidity and a brush system with various architectures. Simulation results show that the diffusion coefficient of associated particles is linearly proportional to $P_{\text{break}}$ and scales with the diffusion coefficient of polymer chains as $D_{\text{assoc}} \sim D_{\text{poly}}^{3/2}$. These results provide insight in understanding the design rules of polymeric materials for solid-state lithium-ion batteries.
5:06PM V50.00012: Dissolution of Lithium Metal in Poly(ethylene oxide)*  
MICHAEL GALLUZZO (Presenter), WHITNEY LOO, NITASH BALSARA, University of California, Berkeley — Salt doped poly(ethylene oxide) (PEO) has been studied extensively as a model polymer electrolyte system for lithium metal battery applications. In this study, we examine the widely accepted assumption that a stable interface forms between lithium and PEO above the PEO melting temperature by studying lithium symmetric cells. Using Li7 NMR, we show that a lithium species dissolves from the lithium electrode and diffuses into the bulk of initially neat PEO. Impedance spectroscopy is used to demonstrate that the lithium species contributes to ionic conductivity, and small angle X-ray scattering demonstrates that the dissolution also occurs in a PEO containing block copolymer, resulting in a significant increase (>20°C) of the order-to-disorder transition temperature. The results indicate that the lithium/PEO interface is not stable at elevated temperatures and there are clear implications for lithium metal batteries using PEO-based electrolytes.

*Primary funding for the work was provided by the Electron Microscopy of Soft Matter Program from the Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 (KC11BN).

5:18PM V50.00013: Designing efficient polymer electrolytes via end-group controls  
HA YOUNG JUNG (Presenter), GYEONG-CHAN KANG, MOON JEONG PARK, Pohang University of Science and Technology — There has been an increasing demand for the development of high-conductivity solid-state polymer electrolytes (SPEs) to be used in lithium batteries by replacing liquid electrolytes. The most widely studied SPEs are based on poly(ethylene oxide) (PEO) and its derivatives owing to PEO's high solvating capability for lithium salt and low glass transition temperature. Given that lithium ion conduction occurs through the segmental motion of PEO chains, high mobility of lithium ion was feasible in amorphous phases. This prompted extensive research efforts to suppress PEO crystallinity by various physical and chemical approaches. In the present study, we investigate PEO-based polymers incorporated with various terminal functional groups as an effective means of controlling crystallinity of PEO phases. Further, by attaching various di-functional groups to the end of PEO chains, it has been revealed that morphology, ionic conductivity, and lithium transference number of PEO electrolytes are fine-tunable, attributed to the alteration of inter- and intramolecular interactions within.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V51 DBIO DPOLY: Protein Liquid-Liquid Phase Separation  
BCEC 253A - Xiaoqin Zou, University of Missouri - Tag(s): Invited

2:30PM V51.00001: Physical Basis of Protein Liquid-Liquid Phase Separation* [Invited]  
HUAN-XIANG ZHOU (Presenter), Department of Physics and Department of Chemistry, University of Illinois at Chicago — Intracellular membraneless organelles, corresponding to the droplet phase upon liquid-liquid phase separation (LLPS) of mixtures of proteins and possibly RNA, mediate myriad cellular functions [Qin & Zhou 2017 Curr Opin Struct Biol]. Cells use a variety of biochemical signals such as expression level and posttranslational modification to regulate droplet formation and dissolution. Our study focuses on elucidating the physical basis of phase behaviors associated with cellular functions of membraneless organelles, using three complementary approaches. First, we use colloids and polymers, respectively, as models for structured and disordered proteins, to investigate both the common basis for protein phase separation and the unique characteristics of structured and disordered proteins in LLPS [Zhou et al 2018 Trends Biochem Sci]. Disordered proteins are characterized by both extensive attraction throughout the sequence and low energetic cost from steric repulsion, contributing to easy observation of phase separation. Second, we use multi-component patchy particles to investigate the wide range of effects of regulatory components on the droplet formation of driver proteins [Nguemaha & Zhou 2018 Sci Rep]. Third, we have developed a powerful computational method called FMAP for determining liquid-liquid phase equilibria [Qin & Zhou 2014 J Chem Theory Comput; 2016 J Phys Chem B]. By using fast Fourier transform to efficiently evaluate protein-protein interactions, FMAP enables an atomistic representation of the protein molecules. Application to g-crystalins reveals how minor variations in amino-acid sequence, similar to those from posttranslational modifications and disease-associated mutations, lead to drastic differences in critical temperature. These studies contribute to both qualitative and quantitative understanding on the phase behaviors of membraneless organelles and their regulation and dysregulation.

*Supported by NIH Grant GM118091.
3:06PM V51.00002: Identifying sequence-determinants of protein liquid-liquid phase separation using molecular simulations
[Invited] JEEATN MITTAL (Presenter), Chemical and Biomolecular Engineering, Lehigh University — In this talk, I will describe ongoing efforts in my group aimed at developing an accurate simulation model to study the liquid-like assemblies of disordered proteins. We use a "top-down" approach for constructing a Cα-based (one interaction site per amino acid) protein model, which involves comparisons with experimental data available from the recent literature as well as comparisons with atomistic single-chain simulations. The resulting model is found to be of enormous help in decoding the role of specific features of the protein sequence that control their liquid-liquid phase separation. We will demonstrate this with a combination of simulation and experiment data for several protein systems such as Laf-1, FUS, TDP-43.

3:42PM V51.00003: Atomic details of protein/RNA liquid-liquid phase separation by experiment and simulation
[Invited] NICK FAWZI (Presenter), Brown University — Phase separation of RNA-binding proteins via multivalent interactions between aromatic/polar-rich disordered domains contributes to the formation of functional cytoplasmic granules and nuclear puncta, which have been shown to behave as liquids -- flowing, fusing, and returning to spherical shape -- within live cells. These domains have also been identified as the nucleators of cytoplasmic inclusions associated with amyotrophic lateral sclerosis (ALS) and frontotemporal dementia (FTD). We use atomic resolution nuclear magnetic resonance spectroscopy approaches to visualize low complexity domain structure and interactions along the pathway from monomer, to liquid-liquid phase separated state, to static aggregates and hydrogels. We show that the low complexity domains of RNA-binding protein Fused in Sarcoma (FUS LC, associated with ALS and FTD) and hnRNP A2 (associated with ALS and IBM) remain disordered even within liquid phase separated puncta (Burke et al. Molecular Cell, 2015). FUS LC also recruits unphosphorylated RNA-polymerase II C-terminal domain into the liquid phase separated state, adding a potential explanation for FUS LC transcriptional activation in cancer. Importantly, phase separation is reversible and is modulated by interaction with RNA, distinguishing these assemblies from static inclusions that can arise from missense mutations in the LC regions. In contrast, we show that liquid-liquid phase separation of TDP-43 is mediated in part by structured α-helical assembly and extension (Conicella et al. Structure, 2016). Some ALS-associated mutations disrupt helix-helix interaction inhibiting liquid-liquid phase separation while leading to enhanced aggregation. Our current work aims to evaluate the potential of post translational modification to alter assembly and hence disrupt pathological interactions of these disordered domains (Monahan and Ryan et al. EMBO J 2017).

4:18PM V51.00004: Features and consequences for transcriptional activity of transcription factor condensation*
[Invited] XAVIER SALVATELLA (Presenter), Chemistry and Molecular Pharmacology, ICREA and Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology — Transcription activation relies on weak, transient interactions between the activation domains of transcription factors, general transcription factors, transcriptional co-regulators and RNA Pol II. Characterizing these interactions is important to understand the physical principles that govern this important process and, also, to identify opportunities for therapeutic intervention, especially in oncology. We are interested in characterizing how this type of interactions regulate the transcriptional activity of a specific transcription factor, the androgen receptor (AR) - the main therapeutic target for prostate cancer - and in perturbing them with small molecules. In this communication we will provide a characterization of the interactions established by the activation domain of AR [1–3] as well as evidence that the activation domain forms condensates [4] stabilized by hydrophobic interactions between partially structured motifs that are important for transcriptional activity. Finally we will put forward the hypothesis that the multivalent nature of these interactions is in part responsible for AR condensation at the initiation of transcription.


*AGAUR (2017 SGR 324), Marató TV3 (102030), MINECO (BIO2012-31043 and BIO2015-70092-R) and the European Research Council (CONCERT, contract number 648201). IRB Barcelona is the recipient of a Severo Ochoa Award of Excellence from MINECO (Government of Spain).
YING WANG (Presenter), Chemistry and Biochemistry, University of North Carolina Wilmington — Liquid-liquid phase separation (LLPS) is a well-known phenomenon in the field of colloid physics. In the past few decades, LLPS has been reported for various protein solutions. Remarkably, LLPS of protein solutions was observed in living organisms, from “cold cataract” in the eye lenses of fish to the recently reported intracellular segregation of signal protein complexes.

One interesting question is whether LLPS is a ubiquitous phenomenon for proteins or just a serendipitous observation in isolated cases? Theoretically, metastable LLPS can be expected for the particles with short-range interactions. However, LLPS of protein solutions is rarely observed, largely due to freezing of solutions and competition from crystallization and aggregation. In this talk, I will show that LLPS can be induced for many proteins and peptides using a simple experimental method. With the ability to experimentally control LLPS, we were able to explore the phase behavior of various protein systems from large monoclonal antibodies to small lipopeptides. In our studies on the non-spherical proteins, we noticed that the shape of protein molecules has some interesting effects on the phase diagram. Our studies suggest that LLPS in protein solutions is a common phenomenon, and thereby may play important roles in living organisms as well as in practical applications of proteins.

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Session V52 DPOLY: Block Copolymer Thin Films II: Experiment and Application

2:30PM V52.00001: Sequential Infiltration Synthesis – Mechanism and Applications of Metal Oxide Growth within Block Copolymers [Invited] TAMAR SEGAL-PERETZ (Presenter), Technion - Israel Institute of Technology — Sequential infiltration synthesis (SIS) is an emerging technique which harnesses atomic layer deposition (ALD) chemistry for growth of inorganic materials within polymers. The highly selective growth within the polar domains of block copolymers (BCP) makes it an attractive method for fabricating hybrid BCP-metal oxide composite with synergic properties as well as for BCP-templated inorganic nanostructure fabrication. However, complete understanding of SIS mechanism is still missing and exploring its application space has only just began.

Here we investigate the principles that govern SIS growth in homopolymers and block copolymers thin films using a combination of in-situ and ex-situ methods. We characterize the diffusion-limited growth profile within the polymers and show its relationship to the polymer chemistry, precursor chemistry, and SIS process parameters. Judicious selection of the BCP enabled SIS growth of even bulky metalorganic precursor and templating SnO2 porous nanostructure. SIS was also utilized to construct multi-layer BCP-templated Al2O3 membranes with tuned 3D pore structure. Finally, fundamental understanding of diffusion and growth in SIS enabled us to template 3D metal oxide heterostructures, opening a pathway of direct 3D nanofabrication from BCP.

3:06PM V52.00002: Self-Assembly Kinetics Enhancement in Ternary “Wet Brush” Block Copolymer/Homopolymer Blend Thin Films* GREGORY DOERK (Presenter), RUIPAENG LI, MASAFUMI FUKUTO, Brookhaven National Laboratory, ALFREDO RODRIGUEZ, Mechanical Engineering, City College of City University of New York, KEVIN G. YAGER, Brookhaven National Laboratory — In this talk we discuss our recent work investigating the enhanced ordering kinetics in thin film ternary blends of polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) block copolymers with low molecular weight “wet brush” PS and PMMA homopolymers that distribute more uniformly throughout the domains. In lamellar thin films, blending dramatically increases the power law exponent governing the development of long-range order during thermal annealing. For cylinders the impact of blending is more dramatic in films thicker than one monolayer due to rapid early stage ordering and faster domain reorientation with respect to the substrate. This blending strategy is also compatible with solvent vapor annealing, where it is applied to promote rapid self-assembly of ultrahigh molecular weight PS-b-PMMA (> 1000 kg/mol). The robust enhancement in ordering kinetics afforded through wet brush homopolymer blending is attributed to changes in the effective segregation strength.

*Research performed at the Center for Functional Nanomaterials, a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.
Directed self-assembly of block copolymers facilitates the creation of films with highly oriented domains over large areas. However, further enhancing our control over surface design requires the ability to create regions of a desired pattern which could be arbitrarily spaced. We have recently discovered that the utilization of substrates with topographically-defined stripes leads to the formation of different morphologies in the trenches and on the plateaus in ultra-confined block copolymer films. This is explained by the fact that capillary action drives more material to deposit in the trenches than on the plateaus during spin coating. The high sensitivity of the patterns displayed by ultra-confined films to minute differences in film thickness and substrate selectivity gives rise to different patterns in the trenches and on the plateaus. Specifically, we were able to demonstrate the formation of hexagonally packed dots on the plateaus concomitant with featureless appearance of the slightly thicker films in the trenches, owing to the ability of the latter to accommodate lying lamellae. As the widths of the trenches are controlled by the lithographic design, this situation facilitates the creation of patterned domains that are spaced by featureless regions as needed.

Block Copolymer Derived Uniform Mesopores For Supercapacitors

High mass loading and fast charge transport are two crucial but often mutually exclusive characteristics of pseudocapacitors. On conventional carbon supports, high mass loadings inevitably lead to sluggish electron conduction and ion diffusion due to the thick pseudocapacitive layer and clogged pores. Herein from the macromolecular perspective, we revolutionize the design of carbon supports. Utilizing block copolymers that microphase-separate, we synthesize porous carbon fibers (PCFs) with uniform mesopores, which are partially filled with MnO₂. The uniform mesopores and ultrathin MnO₂ enable fast electron/ion transport comparable to carbons in electrical double layer capacitors. The gravimetric and areal capacitances of MnO₂ reach 1148 F/g and 3141 mF/cm², respectively.

*This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0112 through the Young Investigator Program (YIP).

Multi-scale Block Copolymer Coating That Induces Hydrophobic Properties on Inorganic Surfaces

Superhydrophobic surfaces hold promise of a technology with various applications spanning different environments, service conditions and length scales. We demonstrated a cost-effective and robust method for imparting superhydrophobicity to target surfaces through self-assembly of block copolymers (BCPs), while the optical properties of underlying materials are preserved. Our approach involves iterative steps of spin-coating, annealing, and etching of different molecular weight (MW) PS-b-PDMS BCPs into multi-layer hierarchical structure. The resulting periodic pattern introduces necessary nanoscale roughness to trap air and increases hydrophobicity of surfaces, and can be controlled by altering tuning parameters such as MW and composition of BCPs. To understand how superhydrophobicity emerged from multi-layer hierarchical BCP structures, multilayer BCP models were constructed by matching experimental observed dimensions, sweeping through wetting configurations, and calculating externally observed contact angles. The results verified the observed experimental trend, demonstrating superhydrophobicity behavior through modulation of roughness at different layers and formation of air pockets. This technology fulfills a pressing need for superhydrophobicity in optically sensitive settings.

Generalized method for perpendicular orientation of block copolymer microdomains in thin films with surface crosslinking process

By effectively cross-linking the surface of a randomly existing BCPs, the cross-linked BCP layer can be worked as natural-born fraction-tailored neutral brush. The cross-linking method can be directly applied to the poly(styrene-block-methyl methacrylate), poly(styrene-block-dimethylsiloxane) and poly(styrene-block-2-vinylpyridine) films to realize perpendicular orientation from the top surface after thermal/solvent annealing on pristine Si or pre-patterned substrate for chemo-epitaxy directed self-assembly. Also, perpendicular orientation from the bottom interface can be also realized by introducing the new BCP film onto the cross-linked BCP layer.
4:06PM V52.00007: Modification Toward Fluorine-Containing High-$\chi$ Block Copolymers and Orientation Control on Thin Films  SEONJUN JO (Presenter), SEUNGBAE JEON, TAESUK JUN, DU YEOL RYU, Yonsei University — To approach miniaturized patterns such as sub-10 nm, block copolymer (BCP) has emerged as an attractive material to overcome the size limit of the conventional lithography, where Flory-Huggins interaction parameter ($\chi$) plays the key role to control the size. In this study, fluorine-containing high-$\chi$ BCP is newly designed which was synthesized using transesterification method. High-yield conversion was achieved using a polymeric catalyst, where the polymer dispersity remain unchanged during the transesterification. Evaluated $\chi$ was above 0.2 over the entire temperature range which is 8 fold higher than polystyrene-$b$-poly(methyl methacrylate) and the smallest half-pitch feature size was approximately 5 nm from 6.3 kg/mol BCP. Film experiments were demonstrated on a neutralized homopolymer mat substrate where a sub-10 nm perpendicular lamellar morphology was observed in as spun state.

4:18PM V52.00008: Self-organization of Triblock Copolymer Melt Chains Physisorbed on Non-neutral Surfaces* DANIEL SALATTO (Presenter), NAISHENG JIANG, XIAOYU DI, Stony Brook University, CHANG-YONG NAM, MASAFUMI FUKUTO, Brookhaven National Laboratory, MAYA ENDOH, TADANORI KOGA, Stony Brook University — Polymer physisorption is an unavoidable event even when weakly attractive surfaces contact a polymer melt. We report the self-organization process of poly(styrene-$b$-ethylene/butadiene-$b$-styrene) (SEBS) triblock copolymer chains physically adsorbed on a non-neutral surface. The results revealed that the SEBS chains form the two different chain structures on the substrate simultaneously: (i) “flattened chains” with an average height of 2.5 nm, but without forming microdomain structures; (ii) “loosely adsorbed chains” with an average height of 11.0 nm forming perpendicular oriented cylindrical microdomains to the substrate surface. In addition, it was found that the lateral microdomain structures were distorted and the characteristic length of the microdomains varied from the bulk after reaching the quasi-equilibrium state. Furthermore, we highlight the role of the adsorbed chains in the self-assembling process of the entire SEBS thin film: A long-range perturbation propagates into the film interior, overwhelming the free surface effect associated with surface segregation of the lower surface tension of polystyrene blocks.

*This work was supported by the NSF Grant (CMMI-1332499).

4:30PM V52.00009: Fabrication of Dual Nanopatterns at desired area using Block Copolymer Containing Photocleavable Linker* CHUNGRYONG CHOI (Presenter), SOYEONG PARK, YESEONG SEO, JAEYONG LEE, SEONGHYEON AHN, EUNSEOL KIM, JIN KIM, Pohang University of Science and Technology — Block copolymers (BCPs) with various nanodomains, such as spheres, cylinders, and lamellae, have received attention for their nanolithography application. However, those microdomains are determined by the volume fraction of one block. Meanwhile, nanopatterns with multiple shapes are required for the next-generation nanolithography. Although various methods have been reported to achieve dual nanopatterns, all the methods need sophisticated processes using E-beam. Here, we synthesized two kinds of BCP, linear and miktoarm typed BCP, containing o-nitrobenzyl alcohol(ONB) as photo-cleavable linker. In the case of linear BCP, dual nanopatterns consisting of nano-dots and nano-hole were easily fabricated by changing the wavelength of ultraviolet (UV) light. We also fabricated dual nanopatterns consisting of dots and lines at desired regions on a single substrate using miktoarm typed BCP.

*This work was supported by the National Creative Research Initiative Program supported by the National Research Foundation of KOREA(2013R1A3A2042196).

4:42PM V52.00010: Development of Shape-Tuned, Monodisperse Block Copolymer Particles through Solvent-Mediated Particle Restructuring  JAE MAN SHIN (Presenter), YOUNG JUN LEE, MINGOO KIM, KANG HEE KU, JUNHYUK LEE, YONGJOO KIM, HONGSEOK YUN, BUMJOON KIM, KAIST — Controllability of the shape, size, and internal structure of block copolymer (BCP) particles as well as their uniformity is crucial to determine their functionality in the practical applications. Here, we demonstrate the particle restructuring by solvent engineering (PRSE) strategy to produce monodisperse particles using functional BCPs with well-defined structure. Importantly, the advantage of PRSE is the general applicability to various types of functional BCPs including polystyrene-$block$-poly(1,4-butadiene) (PS-b-PB), polystyrene-$block$-polydimethylsiloxane (PS-b-PDMS), and polystyrene-$block$-poly(4-vinylpyridine) (PS-b-P4VP). PRSE starts with producing monodisperse BCP spheres in a wide range of particle size using membrane emulsification, followed by transformation to shape-anisotropic BCP particles by solvent annealing. Monodispersity of particle size was maintained during the PRSE, and the shape transformations to prolate and oblate ellipsoids were successfully achieved. PRSE was also effective in controlling the aspect ratio (AR) of the particles, which was supported by theoretical calculation for describing the particle elongation. Further investigation on the kinetics during the PRSE revealed that the morphology transformation was driven by reorientation of BCP domains.
4:54PM V52.00011: Order-to-disorder transition of block copolymer thin films and its dependence on thickness and preferential interaction  JAEUP KIM (Presenter), DÆSEONG YONG, Ulsan National Institute of Science and Technology, YEONGSIK KIM, DU YEOL RU, Yonsei University — Unlike the phase transitions in the bulk block copolymers (BCPs), the order-to-disorder transition (ODT) in film geometry is influenced by interfacial interactions. An intuitive prediction is that a preferentially selective interaction toward one block promotes microphase separation. Such a prediction is supported by a few theoretical and experimental reports, but a few studies including thermally generated defects or field fluctuation effects suggested an increase in $\chi_N$ value with decreasing film thickness. In this study, we focus on the phase transition behavior of cylinder- and lamella-forming block copolymer films subject to an asymmetric wetting condition. Our self-consistent field theory calculation using a discrete bead-spring model with finite-range interactions exhibits a decrease in $\chi_N$ with decreasing film thickness for both lamella- and cylinder-forming BCP films. This result is consistent with our experiments using PS-$b$-P2VP BCP films with an asymmetric wetting condition that confines the films with selective interactions of the PS/air and P2VP/substrate. For both theory and experiment, the onset of the ODT shift was much thicker for the lamellar case (~20 layers) than for the cylinder case (~10 layers).

5:06PM V52.00012: Directional Alignment of Quasi-Single-Crystalline 2D Dot Array in Diblock Copolymer Thin Films via Epitaxial Cylinder-to-Sphere Transition  YE CHAN KIM (Presenter), SO YOUN KIM, Ulsan National Institute of Science and Technology — Despite the great applicability of block copolymer (BCP) thin films capable of producing dense periodic nanostructures, the difficulty to control the pattern orientation acts as an obstacle to the successful bottom-up lithography of BCPs. The production of guiding pattern on the substrate such as grapho- or chemo- epitaxy has been suggested to create highly ordered nanostructures. However, these methods can be experimentally complicated and expensive, particularly in a large-area.

In this work, we suggest a facile method to fabricate highly aligned quasi-single-crystalline 2D dot array of BCP thin films over large-area (cm²). We utilized the epitaxial morphology transition from BCP cylinders to spheres. First, sphere forming polystyrene-$b$-poly(2-vinyl pyridine) thin films were transformed to cylinders by shear; shear results in the nicely aligned parallel cylinders along the shear direction. Then, the subsequent solvent vapor annealing (SVA) induces a cylinder-to-sphere transition where the dot pattern of BCP spheres is epitaxially grown on the aligned stripe pattern of the cylinders. We found that the increase of d-spacing with SVA is a key factor for the successful generation of highly ordered 2D array, which could compensate the lattice mismatch between dot and stripe pattern.

5:18PM V52.00013: Pore Size Control using Cooperative Assembly with Block Copolymers and Low Volatility Solvents*  MEETA TRIVEDI (Presenter), BRYAN VOGT, Department of Polymer Engineering, University of Akron — Block copolymers (BCPs) provide a facile avenue to the generation of nanoporous materials with well-defined pore geometries. Cooperative assembly of BCPs with functional precursors enables families of materials to be fabricated from a single BCP template. However, the pore size is generally controlled by the BCP, which can be limiting for applications. Here, we demonstrate the ability to effectively tune the pore size (both up and down) through the addition of low volatility solvents during triconstituent co-assembly of carbonizable and silica precursors with a commercial block copolymer (Pluronic F127) that are fabricated by film casting on roll-to-roll equipment. Four different low volatility solvents with varying selectivity were examined. The pore size obtained depends on the hydrophobicity, volatility, and relative amount of solvent added. This enables mesoporous carbon-silica materials with pore sizes ranging from 5 nm to 12.8 nm. The morphology of these materials was elucidated with transmission electron microscopy (TEM) and small angle x-ray scattering (SAXS) to understand how these solvent additives impact the ordered structure.

*This work was financially supported by the National Science Foundation under grant no. CBET-1510612 and CBET-1336057.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V53 GSOFT: Extraordinary Mechanical Properties of Bio-inspired Soft Materials

BCEC 253C - Wouter Ellenbroek, Eindhoven University of Technology - Tag(s): Invited
2:30PM V53.00001: Do bio-inspired metal-coordination crosslink dynamics offer anything new for engineers of hydrogel mechanics? [Invited] NIELS HOLTEN-ANDERSEN (Presenter), Massachusetts Institute of Technology — Efforts to engineer synthetic polymer hydrogel mechanics is increasingly coupled to the design of transient crosslink dynamics. Based on the growing evidence supporting a critical role in desirable material applications in nature, bio-inspired metal-coordinate transient crosslinking might provide unique opportunities in these efforts. Using simple metal-coordinating polymers, we have sought to gain a deeper understanding of whether polymer hydrogel mechanical properties can be controlled over multiple hierarchical time-scales via design of metal-coordinate crosslink structure on multiple length-scales. Specifically, by utilizing metal ion-coordination complexes and metal nanoparticle-coordination junctions as supramolecular crosslink structures, we have obtained easy access to control over network dynamics on the microscopic scale, and thereby unique opportunities to broadly shape the distribution of network stress relaxation on the macroscopic scale. Our findings suggest that bio-inspired metal-coordination crosslink dynamics can indeed be utilized to engineer complex gel mechanics directly via simple design of supramolecular crosslink structure, and could help improve our understanding of and control over spatio-temporal molecular hierarchy in loadbearing biological and bio-inspired materials.

3:06PM V53.00002: Flex your mussels: Harnessing nature's designs to build next-generation materials* [Invited] MEGAN T. VALENTINE (Presenter), University of California, Santa Barbara — Marine mussels create an array of adhesive contacts (the byssus) to secure themselves to rocks, wood, metals and other mussels in the harsh conditions of the intertidal zone. Their superb mechanical and adhesive performance has served as inspiration to create mussel-inspired materials for a wide range of applications ranging from surgical glues to primers and coatings. Historically, much of this success has relied on mimicry of the molecular properties of the mussel's adhesive interfacial proteins. By contrast, the translation of the meso- to macro-scale properties of the natural materials has been comparatively unexplored, providing rich opportunities for further property enhancement to create tough, durable, load-bearing materials. Here, I will present my laboratory's recent work characterizing the properties of natural mussel byssal plaques, and translating these discoveries to enable the design and manufacture of new materials. Experimentally, we observe the dynamics of mussel plaques as they debond from glass using a custom built load frame with integrated dual view imaging capabilities, under monotonic and cyclic loading. We pair these mechanical tests with ultrastructural analysis to understand the molecular origins of strength and toughness. Using insights from the natural materials, we then create high-performance synthetic materials that are extremely strong without compromising extensibility, as well as mussel-inspired 3D structures with tunable stiffness and strength. These innovations open new possibilities for applications of mussel-inspired materials in packaging, soft robotics, and connective tissue repair, and demonstrate the importance of understanding the multiscale, multiphase properties of biological materials.

*This work was supported by the MRSEC Program of the National Science Foundation under Award No. DMR 1720256.

3:42PM V53.00003: Mechanical stresses control the size, shape, and location of phase-separated liquid droplets in polymer networks [Invited] ERIC DUFRESNE (Presenter), Materials, ETH Zurich — Spontaneous phase separation has recently emerged as an essential driver of cytoplasmic organization. With experiments in synthetic materials and living cells, we demonstrate that elastic stresses in polymer networks can regulate phase separation. We apply these insights to the design of photonic materials.

4:18PM V53.00004: DNA-directed hydrogel deformation* [Invited] REBECCA SCHULMAN (Presenter), Johns Hopkins University — DNA polymerization reactions within DNA-crosslinked hydrogels can direct the dramatic shape change of DNA-crosslinked hydrogels, leading of up to 100-fold changes in gel volume. The well-understood kinetics and thermodynamics of these reactions and of DNA transport make it possible to design a myriad of molecular scale reactions and to study the emergent shape-change behavior of these reactions at the millimeter scale. And because DNA molecules can be coupled to molecular sensors, amplifiers, and logic circuits, understanding DNA-directed hydrogel shape change introduces the possibility of building soft devices that respond to diverse biochemical inputs and autonomously implement chemical control programs.

*DOE Early Career 221874
NSF EFRI 1830893
How to toughen polymer gels with entropy-mediated reversible crosslinking* [Invited] NICHOLAS TITO (Presenter), Department of Applied Physics, Eindhoven University of Technology, COSTANTINO CRETON, Laboratory of Soft Matter Science and Engineering, ESPCI ParisTech, CORNELIS STORM, WOUTER ELLENBROEK, Department of Applied Physics, Eindhoven University of Technology — Materials composed of polymers that are permanently crosslinked into a network, such as gels and rubbers, eventually break if strained enough. This is because the network irreversibly ruptures once the local forces acting on the polymers and crosslinks become too large for the bonds to withstand. Recent experiments have revealed that adding *reversible* crosslinks to a gel allows it to be strained to a much larger extent, yet without altering its small-strain elasticity [1]. We are using theory, molecular simulation, and polymer self-consistent field theory for networks, to explore reversible crosslinking as a design paradigm for creating polymer materials that are tough but elastic [2]. Emphasis will be placed on how entropy itself drives reversible crosslinks to toughen the material, while preserving its intrinsic elasticity. Practical guidelines will be outlined to optimise this design in experiment, along with a discussion of key kinetic and timescale considerations.


*This research has been performed within the framework of the 4TU.High-Tech Materials research programme `New Horizons in designer materials' (www.4tu.nl/htm). We are grateful for compute time obtained from the Netherlands Organisation for Scientific Research (NWO) SURFsara Pilot Program (Grant No. 15582).

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V54 DPOLY DBIO: Sequence and Charge Driven Bio- and Bio-inspired Macromolecular Assembly BCEC 254A - Charles Sing - Tag(s): Focus

Theoretical Perspectives on Cellular Compartmentalization by Phase Separation* [Invited] YI-HSUAN LIN, Department of Biochemistry, University of Toronto; and Molecular Medicine, The Hospital for Sick Children, SUMAN DAS, ALAN AMIN, Department of Biochemistry, University of Toronto, ADAM EISEN, Department of Mathematics & Statistics, Queen's University, JULIE D. FORMAN-KAY, Molecular Medicine, The Hospital for Sick Children; and Department of Biochemistry, University of Toronto, HUE SUN CHAN (Presenter), Departments of Biochemistry and Molecular Genetics, University of Toronto — Compartmentalization is essential for many cellular functions. Besides organelles encapsulated by lipid membranes—mitochondria and the nucleus, e.g., dynamic non-membrane-bound compartments also exist in the eukaryotic cell. These include stress granules, germ granules, the nucleolus, and many others. Recent investigations indicate that these bodies behave like mesoscopic liquid droplets. Referred to as “membraneless organelles”, or “biomolecular condensates”, they are underpinned to a significant extent by liquid-liquid phase separation (LLPS) of intrinsically disordered proteins (IDPs) and nucleic acids. Their formation/dissolution is governed largely by the information encoded in the sequences of nucleic acids and proteins. To gain physical insights into this novel phenomenon, we developed analytical theories and simulation models for sequence-specific IDP LLPS. Our effort rationalizes experiments on the DEAD-box RNA helicase Ddx4, elucidates the effect of sequence charge patterns on LLPS, and points to a “fuzzy” mode of molecular recognition by charge pattern matching that likely bears on whether different IDP species remain miscible or demix upon LLPS to serve their biological functions. IDP LLPS depends on temperature and hydrostatic pressure. As a first step toward understanding these behaviors, we show that the trend of such dependence can be qualitatively rationalized by empirical and atomic modeling of elementary hydrophobic interactions.


*This work was supported by CIHR and NSERC of Canada.
3:06PM V54.00002: Transfer Matrix Theory Model of Sequence-Dependent Polyampholyte Phase Separation  JASON MADINIA (Presenter), CHARLES E. SING, University of Illinois at Urbana-Champaign — Intrinsically disordered proteins (IDPs) participate in many critical biological functions within the cell. These proteins lack a well-defined structure and can take on many conformations depending on its sequence and local environment. IDPs can be modeled as polyampholytes and can undergo a liquid-liquid phase separation that is primarily driven by electrostatic interactions. The charge sequence along the polymer is critical to the solution behavior. In this work, we present a Transfer Matrix (TM) model to describe this liquid-liquid phase separation as a function of charge sequence. We show how the TM theory is created for a polyampholyte, and how it can be used to determine the free energy of interaction between the polyampholyte and its local environment. In conjunction with the TM theory, we perform MD simulations of charge-patterned polyampholytes in solution to compare with the model. We find that increasing charge blockiness increases the tendency to undergo phase separation, limiting to the behavior typically seen in polymeric complex coacervates, while alternating positive and negative charges do not exhibit charge-induced phase separation.

3:18PM V54.00003: Impact of complex coacervation on tau amyloid aggregation*  YANXIAN LIN (Presenter), KATE ZENG, YANN FICHOU, YUGE HU, SONGI HAN, University of California, Santa Barbara — Amyloid aggregation of tau protein is implicated in human neurodegenerative diseases. While complex coacervation (CC) of tau and polyanion has shown both biological and pathological significance, its impacts on tau amyloid aggregation is not well understood. We report here recent findings and characterizations of tau-polyanion CC and its relationship with tau aggregation. We first demonstrate that tau can form complex coacervates with almost any polyanion. We found whether tau CC remains fluidic or solidifies towards fibrils is determined by the aggregation propensity of the CC forming constituents, not the CC forming process. Further, we closely examined changes of aggregation kinetics of tau resulting from the CC environment, and found the collision dependence of tau aggregation to be reduced by CC. Finally, we investigated the effect of CC on the fibrillization kinetics and seeding activity by tau fibrils.

*Research reported in this abstract was supported by National Institutes of Health (NIH) http://www.nih.gov (grant number R01AG05605) received by SH and KSK and the Tau consortium http://www.tauconsortium.org received by KSK and SH. The funders had no role in study design, data collection and analysis, decision to publish, or preparation of the abstract.

3:30PM V54.00004: Effect of pH on polymer adsorption and bridging in a two oppositely charged nanoparticle/protein system  RITUPARNA SAMANTA (Presenter), VENKATRAGHAVAN GANESAN, University of Texas at Austin — We discuss the results of molecular simulations of charged particles in presence of oppositely charged, dissociable polymers. The effect of pH on adsorption and bridging characteristics of the polyelectrolyte for both homogeneous and heterogeneously charged particles is studied. We have studied the effect of charge distribution on the particles, charge and size of polyelectrolytes and concentration of polymers on adsorption, bridging and effective interactions between the particles.

3:42PM V54.00005: Tuning interactions between hybrid physical-covalent rigid rods made of computationally designed coiled coils by peptide sequence manipulation  NAIRITI SINHA (Presenter), RAJKUMAR MISRA, Materials Science & Engineering, University of Delaware, DE, RUI GUO, Chemistry, University of Pennsylvania, PA, CHRISTOPHER KLOXIN, Materials Science & Engineering, University of Delaware, DE, JEFFERY G SAVEN, Chemistry, University of Pennsylvania, PA, DARRIN POCHAN, Materials Science & Engineering, University of Delaware, DE — Application of computational design to biomolecular sequence, structure and function prediction provides vast opportunity in artificial biomaterial construction and assembly. Non-natural coiled coils, oligomers of α-helical peptides, can be designed to assemble in solution by computational sequence discovery and manipulation via strategic placement of amino-acids exposed to the solvent. Utilizing a hybrid assembly pathway, computationally designed homotetramer coiled coil bundles are linked in an end-to-end fashion resulting in rigid rods of bundles or “bundlemers”. Transmission Electron Microscopy (TEM) and Small-Angle Neutron Scattering (SANS) confirm that the rods have a 2 nm cross-section commensurate with that of a single bundle. SANS is also used to study inter-rod interactions for peptides that carry increasing net negative charge. Differences in local repulsive interactions between rods is observed due to changes in rod charge density, which is responsive to pH and ionic strength of the solution. Larger percolated clusters of rods which form due to local patchiness of interaction sites is also confirmed. This control of solution structure with fine control of the charged state, length, dispersity and concentration of bundliemer rods will be discussed.
3:54PM V54.00006: Influence of Charge Sequence on the Adsorption of Polyelectrolyte Solution on to Polyelectrolyte Brush*  
VAIDYANATHAN SETHURAMAN (Presenter), MICHAEL P MCGOVERN, DAVID CLARK MORSE, KEVIN DORFMAN, University of Minnesota — We use coarse-grained MD to elucidate the role of charge sequence on the adsorption efficacy of oppositely charged free polyelectrolytes on to a polyelectrolyte brush. We consider four different model systems wherein the free and the brush polyelectrolytes can have either brush or alternating charge sequence. Our model treats the polyelectrolytes in a bath of implicit solvent, excess salt and explicit counterions. Adsorption efficiency is highest when both free and brush polyelectrolytes possess a block charge sequence, and it is lowest when both free and brush polyelectrolytes possess an alternating charge sequence. By computing the free energy, internal energy and entropy of adsorption using umbrella sampling methods, we find that the origin of the differences in adsorption efficiency for different charge sequences is enthalpic. Additionally, equilibrium conformations for different charge sequences reinforce the results obtained from energetic calculations. When the number of brush polymers is more than that of the free polymers, a spatial heterogeneity is observed in the charge distribution within the brush region which is strongly dependent on the charge sequence of free and brush polyelectrolytes.

*Materials Research Science and Engineering Center (MRSEC)  
Award No: DMR-1420013

4:06PM V54.00007: Biomolecules for non-biological things: 1-D and 2-D polymer formation through peptide design and solution assembly*  
DARRIN POCHAN (Presenter), University of Delaware — A new solution assembled system comprised of theoretically designed coiled coil bundle motifs will be introduced. The molecules and nanostructures are not natural sequences and provide opportunity for arbitrary nanostructure creation with peptides. With control of the display of all amino acid side chains (both natural and non-natural) throughout the peptide bundles, desired physical and covalent (through appropriate “click” chemistry) interactions have been designed to produce one and two-dimensional nanostructures. One-dimensional nanostructures span exotically rigid rod molecules that produce a wide variety of liquid crystal phases to semi-flexible chains, the flexibility of which are controlled by the interbundle linking chemistry. The two dimensional nanostructure is formed by physical interactions and are nanostructures not observed in nature. All of the assemblies are responsive to temperature since the individual bundle building blocks are physically stabilized coiled coil bundles that can be melted and reformed with temperature. Additional, novel nanostructures to be discussed include uniform nanotubes as well as the templated growth of metallic nanoparticle on and in peptide nanostructures.

*DOE award #18A01039  
NSF DMREF award # 1235084

4:18PM V54.00008: Engineering protein and polyelectrolyte complexation for cellular applications [Invited] ALLIE OBERMEYER (Presenter), RACHEL KAPELNER, VIVIAN YEONG, NICHOLAS ZERVOUDIS, Columbia University — Oppositely charged polyelectrolytes are known to undergo a liquid-liquid phase separation, termed complex coacervation, under the appropriate solution conditions. Protein polyelectrolytes have also been shown to phase separate with polyelectrolytes. However, protein polymers differ significantly from synthetic polyelectrolytes. Proteins are polyampholytes, have low charge density, and frequently adopt a globular folded structure. These differences impact the complexation and phase separation of proteins with polyelectrolytes. These differences also make protein polymers interesting to study in this context; the charge, charge density, and charge orientation on proteins can be precisely controlled through genetic engineering. Additionally, it has recently been demonstrated that the phase separation of proteins is a fundamental mechanism for eukaryotic cellular compartmentalization. These phase separated membraneless organelles create distinct environments that are essential to cellular processes ranging from cell signaling to gene expression. Many membraneless organelles appear to have the same physical properties as complex coacervates – liquid-liquid phase separated mixtures of oppositely charged polynions. We are motivated to understand protein complex coacervation in order to enable new biological applications of these materials. Toward this end, we have investigated the complex coacervation of engineered proteins with synthetic and biological polynions to determine predictive design rules for protein phase separation. We have also used these design rules to promote phase separation of engineered proteins in vivo.
4:54PM V54.00009: Conditions for complex coacervation of the microtubule-associated tau protein predicted from field theoretic simulations*  JAMES MCCARTY (Presenter), YANXIAN LIN, KRIS T DELANEY, GLENN FREDRICKSON, SONGI HAN, JOAN-EMMA SHEA, University of California, Santa Barbara — The microtubule associated tau protein is a highly charged intrinsically disordered protein (IDP) that has been linked to neurodegenerative diseases including Alzheimer’s disease. Recently, tau has been shown to undergo a liquid-liquid phase transition, leading to speculation about how this process may mediate pathological tau fibrillation. To understand the thermodynamic driving forces of this process, we apply a discrete Gaussian-chain polyelectrolyte model and compute thermodynamic observables using a numerical technique known as field theoretic simulation (FTS). Results from FTS for this coarse-grained tau model reveal how the combination of charge distribution, salt concentration, and temperature-dependent excluded volume determine the observed phase diagram. Our results suggest new avenues for simulation to inform experimental design. Finally, we will comment on extensions of the model and applications to other IDPs.

*This work was partially supported by the MRSEC Program of the National Science Foundation and by a grant from the National Institutes of Health

5:06PM V54.00010: Sequence Effects on Block Copolymer Self-Assembly through Tuning Chain Conformation and Segregation Strength Utilizing Sequence-Defined Polypeptoids*  ANASTASIA PATTERSON (Presenter), SCOTT DANIESEN, BEIHANG YU, EMILY C DAVIDSON, GLENN FREDRICKSON, RACHEL SEGALMAN, University of California, Santa Barbara — Polymers with precise sequence control offer the possibility of tuning segregation strength with comonomer sequence instead of chemical identity. We have synthesized polystyrene-b-polypeptoid block copolymers with different sequences of comonomers in the polypeptoid block, where nonpolar phenyl side chains are incorporated to tune compatibility with polystyrene. Using small-angle X-ray scattering, we see that these materials self-assemble into lamellae with domain spacings and order–disorder transition (ODT) temperatures varying with sequence, despite identical composition. The variation in the ODT suggests that sequence control at the monomer level alters segregation strength, and by comparing domain spacings and SCFT simulations, we find that the main driving force is likely chain conformational effects that localize comonomers at the block–block interface. However, trends seen in the ODT are not captured by SCFT simulations or effective χ parameters (measured in the disordered phase by approximating the copolypeptoid as a uniform block). The disagreement between measured thermodynamic properties and coarse-grained approaches like SCFT and effective χ points to the importance of molecular-scale effects in sequence-defined materials.

*NSF DMR-1608297 and DMR-1822215

5:18PM V54.00011: Kinetics of conformational changes in polyelectrolyte systems*  SWATI SEN, SOUMIK MITRA, ARINDAM KUNDAGRAMI (Presenter), Department of Physical Sciences & Centre for Advanced Functional Materials, Indian Institute of Science Education and Research Kolkata — Equilibrium phase behavior of polyelectrolytes is well-studied in literature. The kinetics of conformational changes in such systems, however, has received sporadic attention, which has increased recently given its relevance to biological problems like protein-folding or biomedical processes like drug-delivery. Our group has been working on studying the time-dependent, inhomogeneous profiles of physical variables, such as mass and charge densities and osmotic stress, related to the swelling kinetics of polyelectrolyte gels. We will present our recent results obtained from the nonlinear theory that uses the expression of osmotic stress as a function of mass and charge densities, and hence is capable of addressing arbitrarily large deformations that are beyond the scope of traditional theories with linear stress-strain relationship. Considering issues like charge-regularization and role of elasticity and electrostatics, the major results we have obtained include estimation of effective elastic modulus, time-dependency of the size, and the relaxation times of charged gels as functions of its charge content, temperature, density of cross-links, and chemical affinity of the polymer and the solvent.

*Ministry of Human Resource Development (MHRD), Government of India

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V55 DPOLY: Polymer Crystallization III: Copolymer Crystallization, Intercrystalline Topology and Mechanical Properties  BCEC 254B - Wenbing Hu, Nanjing University Rufina Alamo, Florida A&M and Florida State University - Tag(s): Focus
2:30PM V55.00001: Statistics of Ties and Loops in Amorphous Regions of Polymer Crystals  SABIN ADHIKARI (Presenter), MURUGAPPAN MUTHUKUMAR, University of Massachusetts Amherst — Polymer crystals grown from melt consist of alternating lamellar crystalline regions and amorphous regions. We study the statistics of ties and loops in the amorphous region. Mechanical properties of crystalline polymers are highly dependent on the relative populations of ties and loops in the amorphous regions. We develop a statistical mechanical formulation to calculate the conformational entropy of ties and loops with consideration of finite chain length and possible association of a chain with multiple lamellae. Results of our numerical calculations show that, the fraction of the tie population relative to loops increases with increasing chain length, and it decreases with increasing the interlamellar separation and the lamellar thickness. The average number of lamellae connected by a chain is also calculated. It is also found to increase with increasing the chain length and to decrease with increasing the amorphous thickness.

2:42PM V55.00002: Tie Molecule Formation in High Density Polyethylene*  SEONG HYUK CHO (Presenter), RICHARD ALAN REGISTER, Princeton University — The mechanical toughness of a semicrystalline polymer, such as polyethylene (PE), originates from tie molecules: polymer chains that span two or more crystalline lamellae. During rapid crystallization, polymers cannot disentangle, so tie molecules form when the size of the polymer coil in the melt, controlled by its molecular weight (M), exceeds the intercrystalline spacing (L) in the solid state, governed by the specimen's crystallization history. Prior studies have yielded some insight into the brittle-to-ductile transition in PE as M is increased, but often for broadly-distributed PE with no measure of L. Here we synthesize a series of narrowly-distributed (dispersity < 1.2), perfectly linear (high density) PEs with targeted M using ring-opening metathesis polymerization of cyclopentene followed by hydrogenation. PEs were either quenched or slow-cooled to vary crystallinity (0.65 - 0.85) and L, measured by differential scanning calorimetry and small-angle x-ray scattering. We investigate the brittle-to-ductile transition of PE by uniaxial tensile testing in relation to its M, end-to-end distance in the melt, and L, and find a relatively abrupt transition in these narrow-distribution PEs.

*NSF Polymers Program (DMR-1402180)

2:54PM V55.00003: Does crystal thickness dictate yield kinetics in polyethylene?  JEVAN FURMANSKI (Presenter), Corporate Strategic Research, ExxonMobil, JONATHAN SCHAEFER, ExxonMobil Chemical Company, LEON GOVAERT, HANS VAN DOMMELEN, Eindhoven Technical University — There has been a longstanding effort to predict the resistance to plastic deformation of polyethylene via crystal plasticity-based micromechanical modeling, deriving the plasticity kinetics from the assumption that the strain carrier is a screw dislocation. This leads to the notion that the yield kinetics are dominated by crystal thickness, or more precisely the chain stem length within the crystal. There is in general a high degree of correlation between the crystallinity and crystal thickness, making it difficult to distinguish between these two microstructural attributes as the driving variable for plasticity. A wide range of crystallinity and stem lengths was obtained by varying crystallization via both cooling rate and various concentrations of short-chain branching, permitting the disentangling of stem length from crystallinity. The rate- and temperature-dependence of yield strengths were fit to a two-term stress-activated Ree-Eyring model. Chain stem length was measured via the Longitudinal Acoustic Mode in low wavenumber Raman spectroscopy. With this material series it was shown that crystallinity drives yield kinetics, rather than stem length. These insights will be placed in the context of a micromechanical model employing stress-activated crystal slip kinetics.

3:06PM V55.00004: Structure and morphology of poly(ethylene)-block-isotactic poly(propylene) di-block copolymers  CLAUDIO DE ROSA (Presenter), ROCCO DI GIROLAMO, ANNA MALAFRONTE, FINIZIA AUEREMMA, MIRIAM SCOTI, Chemical Sciences, University of Napoli Federico II — A study on the structure and morphology of crystalline di-block copolymers (BCP), composed of stereoregular crystallizable polyolefins is presented. In particular, we report a structural characterization of di-block copolymers formed by crystalline PE block linked to crystalline isotactic polypropylene (IPP) block of different block lengths. The dependence of the thin film BCP morphology on the sequential crystallization from the phase separated melt of the crystallizable blocks has been investigated. The BCPs have been epitaxially crystallized onto crystals of a substrate to achieve a better control over the crystallization. Ordered nanostructures where the two blocks are organized in separated alternating lamellar domains guided by the orientation of the crystalline lamellae are obtained. We demonstrate that, tuning the block length and using a specific substrate, it is possible to control the crystallization process and obtain large-sized, well-oriented lamellar microstructures with long range order achieved over the area in contact with the crystalline substrate. Possible applications of these nanostructures are discussed.
Quiescent and flow-induced crystallization of polyolefins studied by a novel low-field RheoNMR combination

KARL-FRIEDRICH RATZSCH, VOLKER RÄNTZSCH, BEGÜM M. ÖZEN, MANFRED WILHELM (Presenter), Karlsruhe Institute of Technology — Combining NMR and rheology has received great attention in the past, as it allows studying the interdependence of macroscopic and molecular properties of soft matter, e.g. polymers, liquid crystals or colloids. Flow profiles (e.g. steady or oscillatory shear) both in the linear and non-linear regime can be applied to monitor and also to modify the (time) evolution of sample properties. Most RheoNMR designs have been realized for high-field NMR spectrometers using only simple shear cells. Here we present a low-field RheoNMR set-up based on a portable 30 MHz NMR unit that was integrated into a commercial strain-controlled rheometer. This unique combination can be employed to simultaneously conduct a full rheological characterization while monitoring molecular dynamics in-situ via $^1$H TD-NMR. Possible applications include the measurement of quantitative composition in crystallizing soft matter (fats, polymers, etc.) and multiphase systems during the application of shear protocols. To display the possibilities of this new technique, studies on the quiescent and flow-induced crystallization of polyolefins are presented. A short time steady-shear protocol was applied to study flow-induced crystallization as a function of different temperatures and flow conditions.

Distribution of Chain Ends in a Crystal-Fixed Polymer Elucidated by Solid-State NMR

SHICHEN YUAN (Presenter), KLAUS SCHMIDT-ROHR, Chemistry Department, Brandeis University — The location of chain ends in the morphology of semicrystalline polymers has recently received renewed attention. In particular, chain ends at the crystal surface can help avoid density anomalies in the noncrystalline surface layers. Here we present a detailed analysis of the distribution of chain ends across the ~ 15 nm repeat unit of semicrystalline poly(ε-caprolactone) (PCL), a crystal fixed polymer of moderate crystallinity. An excellent signal-to-noise ratio and spectral resolution is achieved by isotopic labeling of chain ends via conversion of OH end groups with $^{13}$COO-acetyl groups. Through distinct (an)isotropic chemical shifts and relaxation times, one can distinguish chain ends in the crystalline, interfacial, and amorphous layers. 56% of the chain ends are found in the core amorphous layers, which exceeds the amorphous core fraction. About 20% are immobilized in the crystal lattice; many of these segments are found near the interface, according to fast $^1$H spin diffusion from the amorphous core layer.

The effect of multi-block structure on the crystallization and properties of ethylene/1-octene copolymers from chain shuttling technology.

FINIZIA AURIEMMA (Presenter), CLAUDIO DE ROSA, University of Naples Federico II — The crystallization properties, the morphology at nanometric length scale and the tensile properties of ethylene/1-octene multi-block copolymers (EOBCs) obtained from chain shuttling technology are analyzed. The samples are characterized by a statistical multi-block architecture, where soft and amorphous blocks with high octene concentration (~18.9mol%) alternate with hard and crystalline blocks with low octene concentration (~0.5mol%). A set of samples with similar octene concentration in the hard and soft blocks, fraction of hard blocks and melting temperature of ~120°C, but different average length of the blocks and average number of blocks/chain are selected. We show that the crystallization properties of EOBCs and the structural organization of the chains which develops by effect of crystallization are strongly influenced by the multiblock architecture, the tendency of the hard blocks to crystallize in separated domains, the short and polydisperse length of the hard blocks and the steric constrains imposed by the covalent bonding between the hard and soft blocks. This results in a hierarchical structural organization which is articulated over different length scales, involving the stacking of the chain folded lamellae in separated domains at lamellar length scale, and the relative arrangement of the hard domains in the compliant matrix populated by the soft blocks, at the scale of domain spacing. The block architecture also influences the mechanical properties. The samples, in spite of similar octene concentration, molecular mass and fractional content of hard blocks, show remarkable differences of mechanical properties, which reflect differences in the average block length ad number of block/chain. The achieved properties encompass those of strong elastomers, in the case of samples with low block length and high number of blocks/chain, up to reach those of soft elastomers in the case of samples with high block length and low number of blocks/chain.
4:18PM V55.00008: Contrasting melt memory of homopolymers and random ethylene copolymers using halogen substitution with precision placement or random distribution  STEPHANIE MARXSEN (Presenter), RUFINA ALAMO, Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, Tallahassee, FL — Polyethylenes with Cl or Br atoms placed at an equal distance of 21 or 15 backbone carbons are known to crystallize as homopolymers, accommodating the halogen in layered crystallites. In contrast, analogs with a random distribution display a crystallization path dominated by sequence-length selection. A consequence of the sequence selection of random copolymers is a constrained interlamellar region and broader melting peaks displaced at higher temperatures than systems with the precise placement. Precision and random ethylene-vinyl halides are excellent models to contrast the strong melt-memory behavior observed in random ethylene 1-alkene copolymers with lack of melt-memory seen in linear polyethylene. While precision polyethylenes with Cl or Br placed on each 21st or 15th backbone carbon show negligible deviation in crystallization rate above the observed melting, the increase in crystallization rate of analogs with the random distribution is observed even from melts 60 degrees above the observed melting point. These data give further evidence of the sharp difference of melt-memory behavior between homopolymers and random copolymers.

4:30PM V55.00009: Study on the Thermodynamics of Polymer Crystallization Based on Twin-Lattice Model  NUOFEI JIANG (Presenter), Department of Macromolecular Science, Fudan University — Polymer crystallization is the most important part in determining the performance of polymeric materials. The twin-lattice model originally provided by Lennard-Jones and Devonshire, developed by Pople and Karasz and other researchers, is extended for describing the thermodynamics of polymer crystallization. The positional order of segments and the orientational order of bonds are considered in this model. The free energy of polymers is obtained by further introducing the conformational energy and entropy. We studied two kinds of processes in polymer crystallization, including the process with plastic crystal phase and without any mesophases. The choice of crystallizing process is determined by the magnitude of lattice energy and conformational energy. Considering data reliability, n-paraffins are chosen as the representation of polymers to compare the predictions of the model with experimental observations. We predict the number of carbons beyond which the rotator phase disappears, which is quite in agreement with the experiments. These calculations and results show this model can provide a new understanding to the crystallization of polymers.

4:42PM V55.00010: Crystallization Process with Aggregation of Small Crystallites for Polytrimethylene Terephthalate*  TAKASHI KONISHI (Presenter), DAISUKE OKAMOTO, DAISUKE TADOKORO, YOSHITAKA KAWAHARA, YOSHIHISA MIYAMOTO, Graduate School of Human and Environmental Studies, Kyoto University, KOJI FUKAO, Department of Physics, Ritsumeikan University, — Polymer crystallization mechanism has explained the crystal nucleation and growth mechanism, while the existence of density fluctuations during the initial stage of crystallization has been discussed. In order to clarify the density fluctuations, the isothermal crystallization from the melt state of poly(trimethylene terephthalate) (PTT) has been studied by wide-angle X-ray diffraction (WAXD) and small-angle X-ray scattering (SAXS). Large scattering intensity in the low-q region $I_L(q)$ has been observed by SAXS during the early stage of crystallizations. $I_L(q)$ increases with time, reaches a maximum, and decreases. The results revealed the crystallization mechanism in which the small crystallites cover the entire sample with the aggregation regions[1]. The conclusion quantitatively showed that $I_L(q)$ is due to the correlations among the heterogeneous aggregation regions of the crystallites.


*This work was partially supported by JSPS KAKENHI (JP25800236), and the Kyoto University Foundation.
4:54PM V55.00011: Effects of diffusion barriers on the temperature dependence of polymer crystallization rates*
CAI JUN (Presenter), JIPING WANG, WENBING HU, Nanjing University — Jun Cai, Jiping Wang, Chenghuan Xu, Wenbing Hu*

Department of Polymer Science and Engineering, State Key Laboratory of Coordination Chemistry, Collaborative Innovation Center of Chemistry for Life Sciences, School of Chemistry and Chemical Engineering, Nanjing University, 210023 Nanjing, China.
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We employed kinetic Monte Carlo simulations of bulk lattice polymers to investigate the kinetics of polymer isothermal crystallization in a broad temperature range. Four diffusion barrier parameters were taken into consideration, i.e. the frictional barrier $E_f$ induced by the leaving neighbors of monomers, the diffusion barrier $E_r$ for sliding diffusion of polymers in the crystalline phase, the barriers of the transition from trans to gauche conformation and the reverse transition $E_t$ and $E_g$, respectively. $E_f$ affects the crystallization kinetic greatly at low temperatures. $E_r$ affects less but appears more important at high temperatures than low temperatures. A larger $E_t$ and $E_g$ reduces significantly the crystallization rate at low temperatures. The results shed light onto the comprehension understanding of polymer crystallization kinetics at low temperatures.

*Thanks the financial support from National Natural Science Foundation of China

5:06PM V55.00012: Low-Temperature Crystal Nucleation of Enantiomeric Poly (lactic acids)†
HE YUCHENG (Presenter), Nanjing University, PENGJU PAN, College of Biological and Chemical Engineering, Zhejiang University, WENBING HU, Nanjing University — We employed the commercial chip-calorimeter Flash DSC 1 to investigate the crystal nucleation behaviors of diblock copolymers and blends of half-half enantiomeric poly (lactic acids) at 35°C. The results show that crystal nucleation below the glass transition temperature can accelerates the crystallization rates at higher temperatures. For instance, the crystallization rate of 140°C increases by two orders of magnitude for the diblock copolymer. Such an accelerate can be attributed to the special interactions of stereo-complex crystals, because homo-crystal does not show such effect.

*This work is supported by National Natural Science Foundation of China (Grant No. 21474050 and 21734005)

5:18PM V55.00013: Crystallization Behavior and Kinetics of Blends of PVDF with a Fluorinated Copolymer†
NELAKA DILSHAN GOVINNA (Presenter), Department of Physics and Astronomy, Tufts University, ILIN SADEGHI, AYSE ASATEKIN, Department of Chemical and Biological Engineering, Tufts University, CHRISTOPH SCHICK, Institute of Physics, University of Rostock, PEGGY CEBE, Department of Physics and Astronomy, Tufts University — We present a study on crystallization of poly(vinylidene fluoride), PVDF, blended with a random fluorinated copolymer (FCP) of poly(methyl methacrylate) and 1H,1H,2H,2H-perfluorodecyl methacrylate. These blends are of interest as candidates for use as oil-water separation membranes. The glass transition and crystallization behavior were studied by fast scanning calorimetry using heating and cooling rates from 20 K/s to 4000 K/s. Crystal fraction and crystal formation rate decreased as the fraction of FCP increased in the blends. PVDF, which exhibits crystal polymorphism, crystallizes into β-phase when cooled from the melt at rates faster than 3000 K/s. Cooling rates between 2000 and 3000 K/s resulted in mixed α- and β-phase, while only α-phase occurred at rates slower than 2000 K/s. A series of isothermal melt crystallization experiments was carried out at temperatures in the range 80-120 °C for holding times of 0.1–100 s. It was found that β-phase crystal formation can be completely suppressed even at high cooling rates by generating a sufficient amount of α-phase crystals isothermally. The variation of these isothermal times and temperatures were also studied for the blends to study the effect of FCP in suppressing β-phase.

*NSF DMR 1608125 and Tufts Collaborates seed grant

Thursday, March 7, 2019 2:30 PM - 4:42 PM

Session V56 GSNP: Interactions of Elastic Structures with Fluids and Granular Matter II
BCEC 255 - Douglas Holmes, Virginia Tech
2:30PM V56.00001: Bioinspired soft fluidic channels  MARTIN BRANDENBOURGER, CORENTIN COULAIS (Presenter), University of Amsterdam — Taking inspiration from the lymphatic system, we devise millimetre scale fluidic channels made of soft asymmetric valves. We investigate their non-linear flow response combining experiments, numerics and lubrication theory. We demonstrate that softness, structural asymmetry and geometric nonlinearities govern the fluid-structure interaction, and give rise to a tunable nonlinear flow response. Our work provides a fundamental understanding of how lymphatic system operate and lays the foundation for a novel generation fluidic metamaterials.

2:42PM V56.00002: Hydro-elasto-capillary interactions for programmable microfluidics* HERVE ELETTRO (Presenter), FRANCOIS GALLAIRE, Ecole polytechnique federale de Lausanne — Soft microfibers can be strongly bent by capillary forces and can even be reversibly coiled inside fluid cavities. If present, hydrodynamic forces may compete with capillary forces, uncoil the microfiber and induce its deployment from its original coiled state. Here we fabricate a microfiber coiled within a droplet that is attached on the wall of a microfluidic channel. This is done by photocuring a liquid microjet of hydrogel (PEG-DA) and transporting the resulting soft microfibre to the carefully prepared droplet for adequate coiling. The mechanical response of the hybrid system is then investigated under increasing flow rates. The present results open opportunities to form the building blocks of microfluidic elements with high on-off ratio that may be useful for the design of on-chip tunable circuits for bioengineering applications.

*We acknowledge funding from the Marie Sklodowska-Curie Actions Fellowship, project "El_CapiTun" n°750802.

2:54PM V56.00003: Kirigami fog nets* PIERRE BINTEIN, AXEL CORNU, Physique, trio S lab, ULB, NICOLAS VANDEWALLE, Physique, GRASP, University of Liege, DENIS TERVAGNE (Presenter), Physique, trio S lab, ULB — Fog is harvested in numerous arid coastal regions by nets placed in dominant winds to catch water droplets. We study experimentally how flexible meshes can adapt their shapes to wind and avoid clogging by capillary effects, in order to maintain a good efficiency of fog collection. By considering aerodynamic, capture and drainage requirements together with mechanical constraints, we propose an optimal geometry for kirigami nets of a given material.

*This work was supported by the Fonds de la Recherche Scientifique – FNRS under Grant(s) n° PDR-WISD- 12

3:06PM V56.00004: Capillary stresses in disordered unsaturated porous materials SIAVASH MONFARED (Presenter), TINGTAO ZHOU, Massachusetts Institute of Technology, FARHANG RADJAI, CNRS-Universite de Montpellier, ROLAND JM PELLENQ, FRANZ-JOSEF ULM, Massachusetts Institute of Technology — Capillary condensation in disordered porous materials - specifically, the interplay of spatial distribution of grains/pores, temperature and distribution of capillary stresses - is explored. This is achieved through lattice gas density functional theory and a recently proposed method for computing capillary stresses based on equivalency of lattice and phase field fluid models in the continuum limit. Gaining insights into the distribution of capillary stresses at a given relative humidity and temperature in disordered porous materials pave the way for fluid mixture coupling with solid deformation while enriching current methods for inferring pore size distribution and pore connectivity from adsorption/ desorption experiments.

3:18PM V56.00005: Deformations in the hook and flagellum during bacterial flick motility HENRY FU (Presenter), MEHDI JABBARZADEH, University of Utah — Dynamical bending, buckling, and polymorphic transformations of the thin flagellar filament are known to affect bacterial motility in fluids. The run-reverse-flick motility of monotrichous bacteria also involves the even more flexible hook which connects the flagellum to its rotary motor. First, I will discuss the role of dynamic bending of both the hook and flagellum during the initiation of flicks. We obtain accurate estimates of forces and torques on the hook that suggest that flicks occur for stresses below the (static) Euler buckling criterion, then provide a mechanistic model for flick initiation that requires combined bending of the hook and flagellum. We calculate the triggering torque-stiffness ratio and find that our predicted onset of dynamic instability corresponds well with experimental observations. Second, I will discuss a more efficient numerical treatment of the dynamics of an inextensible filament that will allow modeling of the complete dynamics of the flick as well as recently discovered unconventional bacterial flagellar motility modes.
3:30PM V56.00006: On the unusual swimming gaits of sea-slugs.  
SHANKAR VENKATARAMANI (Presenter), KENNETH YAMAMOTO, University of Arizona — Nudibranchs (sea-slugs) are a family of soft-bodied marine invertebrates. They typically crawl on the sea-floor, but some species (eg. Hexabranchus sanguineus ‘Spanish dancer’) are capable of free swimming. They possess a peculiar swimming gait, which we will argue comes from constraints on their geometry. I will present an analysis of free swimming sea-slugs that touches upon interesting questions in the mechanics of non-Euclidean thin sheets as well as on the interaction of such sheets with a fluid environment. I will also discuss potential applications our analysis to soft robots.

*This work was supported by the Simons Foundation.

3:42PM V56.00007: Buckling Instability to Control the Swimming Direction in Bacterial Flagella
MOHAMMAD KHALID JAWED (Presenter), WEICHENG HUANG, Department of Mechanical and Aerospace Engineering, University of California, Los Angeles, MOJTABA FORGHANI, Department of Mechanical Engineering, Massachusetts Institute of Technology — We analyze the control of a uniflagellar soft robot in low Reynolds fluid. Inspired by the locomotion of bacteria, we consider a robot comprised of a flagellum - a flexible helical filament - attached to a spherical head. The flagellum rotates about the head at a controlled angular velocity and generates a propulsive force that moves the robot forward. When the angular velocity exceeds a threshold value, the hydrodynamic force by the fluid can cause the flagellum to buckle, characterized by a dramatic change in shape. A fluid-structure interaction model that combines Discrete Elastic Rods algorithm with Lighthill's Slender Body Theory is employed to simulate the system. We demonstrate that the robot can follow a prescribed path in three dimensional space by exploiting buckling of the flagellum. The control scheme involves only a single scalar input - the angular velocity of the flagellum. We also show that the complexity of the dynamics can be captured using a deep neural network, from which we identify the input-output functional relationship between the control inputs and the trajectory of the robot. Our study underscores the potential role of buckling in the locomotion of natural bacteria.

*We acknowledge support from HSSEAS, University of California, Los Angeles.

3:54PM V56.00008: Modelling the Transition from Fracture to Granular Flow
JOEL CLEMMER (Presenter), MARK OWEN ROBBINS, Johns Hopkins University — As a brittle solid is loaded, crack growth leads to fracture and fragmentation. The system then transitions to granular flow where these fragments continue to break down into smaller grains in a process known as comminution. To explore this transition, we created a discrete element model of an isotropic, brittle material. The solid is modelled as a disordered packing of locally interacting spheres. Interactions include an attractive and a repulsive pairwise force as well as a three-body angular stiffness. If stretched a critical distance, the attractive and angular interactions will break. The relative strength of interactions can be tuned to control the material's elastic response (Poisson's ratio) as well as the ratio of mode 1 to mode 2 fracture toughness. We use this model to explore how material properties, initial defect density, and strain rate affect both the transition to granular flow and the resulting rheology and comminution. We track the stress response of the system, the spatial and temporal locations of crack growth, and the evolution of the grain size distribution. The grain size distribution shows power-law behavior and with increasing strain rates one can identify a decreasing maximum grain size.

*Support provided by: ARL W911NF-12-2-0022

4:06PM V56.00009: Hydraulically Driven Jamming of Rods
JORDAN KENNEDY (Presenter), LAKSHMINARAYAN MAHADEVAN, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Hydraulically driven flow of filament-like objects has a broad range of natural and industrial applications such as log jams in rivers, or the clogging of an open channel irrigation ditch in agriculture. To investigate the phase space of the jamming of rods in a fluid driven flow, we have performed experiments on buoyant particles over a range of aspect ratios in an open channel flume with a gated restriction, and quantify the results as a function of channel geometry, Froude number and density of logs in the channel.

4:18PM V56.00010: Hydraulic fracturing dynamics in natural and artificial low-permeability porous media
THOMAS COCHARD (Presenter), SEAS, Harvard — Despite the impact that hydraulic fracturing has on the energy sector, the physical mechanisms that control its efficiency and environmental impacts remain poorly understood in part because of the complex heterogeneous structures of the natural low permeability formations. We developed an experimental approach to study the hydraulic fracture propagation in both natural and model low-permeability media. Natural shale sample, thin sections of Mancos Shale, and engineered gels have been hydro-fractured under controlled conditions. The combination of high-speed imaging during the process and X-ray tomography before and after allows us to monitor the fracture propagation and gives insight on how heterogeneities drive hydraulic fracturing dynamics.
Scaling and spatial correlations in the quasibrittle process zone

JARON KENT-DOBIAS (Presenter), JAMES PATARASP SETHNA, Cornell University — We describe a scaling theory for the spatial distributions of damage and stress in the process zone of cracks propagating through quasibrittle materials. Brittle but disordered, these materials are ubiquitous in everyday life, including concrete, shell, and bone. Like in ductile materials, propagating cracks in quasibrittle materials have an extended process zone surrounding the crack surface, but unlike ductile materials this zone is comprised of a large complicated region of microfracture with correlated damage across many length scales. As a result, fracture in these materials exhibits strong sample size and shape dependence whose underlying nature evades standard analysis. Motivated by simulations of disordered fuse networks, our results work towards explaining the way damage and stress are correlated in and around the process zone and use renormalization group ideas first developed by Shekhawat et al. (PRL 110(18), 185505) to grapple with their system size dependence.

Thursday, March 7, 2019 2:30 PM - 5:06 PM

Session V57 GSNP: Mechanical Metamaterials I

2:30PM V57.00001: Sequential Metamaterials [Invited] MARTIN VAN HECKE (Presenter), Leiden University & AMOLF — Ordered sequences of motion govern the morphological transitions of a wide variety of natural and man-made systems, while the ability to interpret time-ordered signals underlies future smart materials that can be (re)programmed and process information. Here we introduce two types of mechanical metamaterials, that either exhibit sequential output or are sensitive to sequential input.

First, we obtain metamaterials that translate a global uniform compression into a precise multistep pathway of reconfigurations.

Second, we introduce the notion of non-commuting metamaterials that are sensitive to a sequence of mechanical inputs. Our work establishes generic principles for infusing metamaterials with sequential input and output.

3:06PM V57.00002: Inverse Kirigami Design* GARY CHOI (Presenter), LEVI DUDTE, L MAHADEVAN, Harvard University — The basic building block of any kirigami pattern is a periodic planar motif with cuts that allow the unit cell to open or close via planar rotations. The tessellations of the plane can take many forms - quads, kagome lattices, and even Islamic tilings. Recent work has explored these geometries in the context of mechanical metamaterials, and focused primarily on the forward problem - given a topology and geometry of the kirigami pattern, how does it deploy and what are the mechanical properties of the structure. In this work, we pose and solve the inverse problem of designing the number, size, and orientation of cuts that allows us to convert a closed, compact regular kirigami tessellation of the plane into a deployment that conforms approximately to any prescribed target shape in two and three dimensions.

*This work was supported in part by the Croucher Foundation (to Gary Choi), National Science Foundation Grant DMR 14-20570 and DMREF 15-33985 (to Levi Dudte and L. Mahadevan).

3:18PM V57.00003: Inverse design of mechanical metamaterials that harness instabilities GIORGIO OLIVERI (Presenter), JOHANNES OVERVELDE, AMOLF — Metamaterials derive their properties from their structure rather than their chemical composition. Their microstructure is specifically designed to create new functionalities not found in nature. Harnessing instabilities is a prominent practice of turning continuous deformations into a discrete response, allowing for sequential transformations, multistability and hysteretic behavior. Despite the complex behavior that these mechanical metamaterials show, their architecture is often surprisingly simple. An iconic example of auxetic material is an elastomeric material patterned with circular pores. While several studies focused on the effects of pore shape and pore distribution, the mechanical properties can only be tuned within limits set by a few geometrical parameters. Our aim is to reverse this paradigm. We introduce a stochastic topology optimization strategy, to inversely design mechanical metamaterials with targeted buckling behavior. Our study, while first focusing on optimizing structure with assigned buckling force, extends at designing structures with predefined post-buckling behavior. This opens up exciting opportunities for the design of soft robots where functionalities can be encoded in the material itself. We complement our results with experimental verification.
3:30PM V57.00004: Bayesian Optimization of Equilibrium States in Architected Elastomers  DAVID YOO (Presenter), CARSON WILLEY, ANDREW GILLMAN, VINCENT CHEN, UES, Inc, ABIGAIL JUHL, PHILIP BUSKOHL, Air Force Research Laboratory — Hyperelastic lattice-based architectures have demonstrated potential for energy absorption and vibration control due to their inherent buckling instabilities, which reconfigure the energy and stiffness distribution of the structure. Multi-resonant vibration isolation can possibly be achieved by tuning the local stiffness properties between the stable equilibrium states. In this study, we develop a design optimization framework to tune the local configuration of the stable equilibrium points and characterize the transition in stiffness through the bistability. We utilize Bayesian optimization to navigate the design space through a balanced approach of exploitation and exploration. The design architecture is parameterized with a Fourier series expansion of the beam geometry, which controls the periodicity and phase of the beam thickness as a function of length. The force-displacement relationship of each design candidate is calculated by the finite element method and segmentation of mono- and bi-stable designs is employed to retain the desired behavior of the response surface. The preliminary results suggest the periodicity of the beam thickness, parameterized by the 1st term in Fourier series, most critically affects the bistability mode.

3:42PM V57.00005: Understanding the Effect of Torsion on Auxetic Behaviors of Three-Dimensional Networks  MENG SHEN (Presenter), The Institute for Molecular Engineering, The University of Chicago, NIDHI PASHINE, SIDNEY ROBERT NAGEL, Department of Physics, The University of Chicago, JUAN DE PABLO, The Institute for Molecular Engineering, The University of Chicago — Bond pruning has recently proved to be an effective method for designing auxetic networks. Previous theoretical work on architected networks includes bond compression terms only, which is a reasonable analog for tenuous systems and frictionless granular packings. For networks made in the laboratory, however, our recent work has shown that the auxetic behavior depends not only on geometry, but also on the interaction parameters, in particular the angle bending term. In three-dimensional networks, the torsion of local connected bonds provides an additional degree of freedom. Here we investigate the effect of torsion on the auxetic behavior of ordered and disordered 3D networks. The research provides insights for the design of 3D networks for the auxetic behavior.

3:54PM V57.00006: Elastic multipole method for describing deformation of 2D solid structures with circular holes and inclusions*  SIDDHARTHA SARKAR (Presenter), Electrical Engineering, Princeton University, MATJAZ CEBRON, MIHA BROJAN, Faculty of Mechanical Engineering, University of Ljubljana, ANDREJ KOSMRLJ, Mechanical and Aerospace Engineering, Princeton University — The analogies between electrostatics and elasticity help us to solve complicated boundary value problems in linear elasticity of 2D solid structures. For example, a hole inside an elastic body is analogous to a perfect conductor in electrostatics in the sense that at the circumference of them the fields, namely the traction force and the parallel component of the electric field respectively, have to be zero. Similarly, an inclusion in an elastic material is equivalent to a dielectric since in both cases the fields have to be continuous at the edge of the inhomogeneity. Furthermore, just like external electric field induces polarization (dipoles, quadrupoles, etc.) of conductive objects, external stress induces elastic multipoles inside holes. Based on this idea, we present a method for obtaining deformations of 2D solid structures with circular holes and inclusions under applied load. We validated the method by comparing the results with table-top experiments. We also utilized the method of image charges from electrostatics to capture the effect of boundaries on the deformed shapes of the holes/inclusions. The excellent agreement with the experimental results shows the power of this intuitive method.

*This work was supported by NSF award DMR-1752100 (CAREER).

4:06PM V57.00007: Homogenisation bounds for micro-architected polymer materials with extreme mechanical properties*  FILIPPO MATTEO AGNELLI (Presenter), ANDREI CONSTANTINESCU, GRIGOR NIKA, Ecole Polytechnique — The aim of this work is the optimal design, additive manufacturing, and testing of micro-architected polymer materials with desired effective mechanical properties. The design process is discussed in terms of homogenisation bounds for composite materials. These bounds define the limits of the space of printable micro-architected materials. The optimal shape design process, uses topology optimisation via a level set method to identify material distribution and track boundary changes within the context of the smoothed interface, allowing us to capture the topological changes that take place within the unit cell. The designed microstructures were printed using stereolithography and mechanically tested. The results are analysed in terms of the overall effective elastic moduli and compared with a series of classical homogenisation bounds for composite materials, e.g. Hashin-Shtrikman, Milton-Kohn, etc. This discussion permits to better define the set reachable elastic coefficients by printing materials with controlled micro-architecture.


*This work is financed by the french-swiss ANR-SNF project MechNanoTruss (ANR-15-CE29-0024-01).
Mechanical failure of disordered networks derived from frictional packings.*

To characterize these networks, we focus on their mechanical stability. We study the uniaxial response of networks with geometry derived from the force chains observed in granular experiments. We perform experiments on samples created by laser-cutting these networks from acrylic sheets. We find that the mean degree of the network is a control parameter of the failure behavior, which ranges from ductile to brittle.

We explain this ductile-brittle transition with rigidity analysis using a frictional (3,3)-pebble game algorithm. We find that the brittle behavior corresponds to the emergence of a percolating rigid cluster occurring at a mean degree close to the isostatic value of a high friction coefficient packing. Finally, we find that for networks close to the transition point, failure events predominantly occur within the floppy regions between the rigid clusters.

*James S. McDonnell Foundation
2:30PM V58.00001: Hyperuniformity and optimal tessellations: structure, formation and properties [Invited] JASNA BRUJIC (Presenter), New York University — After recent breakthroughs in the search for ordered optimal tessellations (for example, including Frank-Kasper phases in copolymer melts), now findings of the optimal properties of amorphous tessellations are emerging, e.g., in biological tissues.

At the same time, there have been intensive studies of amorphous systems with an anomalous suppression of density fluctuations on large length scales, known as hyperuniformity. This geometric concept qualitatively and quantitatively characterizes a hidden-order in amorphous states that allows for unique physical properties--combining those of crystalline and disordered phases. Thus it offers candidates for optimal amorphous tessellations of space.

This session will foster a discourse between these subfields and about the role of hyperuniformity in the search for tessellations that are optimal with respect to geometrical and physical properties. The session will discuss both a theoretical understanding, computational exploration and experimental verification of the temporal evolution of growing or compressed soft cellular entities and the formation of surprising ordered and amorphous phases and their unexpected structures and physical properties. The applications range from functional designer materials to the cell biology of membrane organelles.

3:06PM V58.00002: Disordered Hyperuniform Many-Particle Systems via Tessellations* [Invited] SALVATORE TORQUATO (Presenter), Princeton University — Disordered hyperuniform many-particle systems are exotic amorphous materials characterized by an anomalous suppression of long-wavelength density fluctuations that endows them with novel transport, mechanical and optical properties. I will describe two different tessellation-based procedures that lead to disordered systems that are hyperuniform. Both methodologies convert initially disordered nonhyperuniform systems into disordered hyperuniform ones.

*National Science Foundation

3:42PM V58.00003: Quantifying The Mechanical Energy Landscape of Two-Dimensional Cellular Matter* SASCHA HILGENFELDT (Presenter), University of Illinois at Urbana-Champaign, XAVIER CAUVIN, Mechanical and Aerospace Engineering, Princeton University, SANGWOO KIM, Mechanical Engineering, University of California, Santa Barbara — The local mechanical equilibrium states of cellular materials - consisting of space-filling domains with dominant interfacial energy - are characterized by a spectrum of metastable-state energies on a generally complex landscape. Recent theoretical work quantifies these energies in dramatically simpler ways exploiting geometric and topological statistical information from the structure of the system only, independent of the specific energy functional [1]. We elaborate on and test these theories by analyzing cellular matter samples, particularly in foam monolayer systems, where energies can be directly and independently determined. Two approaches to inferring energies are tested using (i) measured lengths of select boundaries between domains; (ii) the probability distribution of domain sizes and topologies. The experimental results support both theories and elucidate advantages and disadvantages of either approach. It is thus practically demonstrated that the mechanical state of cellular matter is quantifiable by its morphology only, suggesting simple and general diagnostic tools in the study of systems as diverse as biological tissues, foams, or superlattice materials.


*work supported by NSF grant #1504301
Disordered hyperuniform two-phase systems are characterized by anomalous suppression of volume-fraction fluctuations at infinite long wavelengths. They provide fertile ground for fundamental research and have attracted considerable practical interest because they often are endowed with exotic physical properties, including possessing optimal or nearly optimal physical properties. The Hashin-Shtrikman (HS) two-phase multiscale dispersions are derived from special tessellations of space that endow these two-phase systems with the optimal effective transport and elastic properties for given phase properties and phase volume fractions. Using a new tiling formulation that ensures perfect hyperuniformity, we rigorously establish the hyperuniformity of the optimal HS structures. We analytically show that these structures are strongly hyperuniform by deriving the small-wavenumber scaling behavior of their spectral density. We verify these theoretical results numerically in two dimensions by constructing extremely dense polydisperse disk packings. Our work provides insights about the relationship between hyperuniformity in two-phase systems and property optimization.

This work was partially supported by the National Science Foundation under Grant No. CBET-1701843 and DMR-1714722.

General Mechanical Energy Landscape in Two-Dimensional Interacting Systems

Domain systems composed of individual entities, cells, or particles commonly exhibit complex mechanical energy landscape with a plethora of metastable states. Recent studies on a class of domain systems governed by dominant interfacial energy show that an equivalent foam energy (the sum of interfacial lengths), is a strong predictor of metastable state energies, regardless of the exact interfacial energy functionals. The landscape of equivalent foam energies is in turn described accurately by theoretical predictions based either on geometric measures or on statistical measures. Here, we show that this theoretical framework can be extended to systems with particle-based interactions. While the energy of particle-based systems depends on constituent particle positions rather than interfacial structure, the equivalent foam energy of a 2D tessellation generated from particle positions not only yields a strong correlation with the actual energy level but also generates an identical energy landscape. Geometric measures and statistical measures can be obtained from visual information only so this framework can serve as a diagnostic tool for identifying mechanical energy states in a variety of domain systems, including foams, emulsions, granular systems, and confluent tissues.

Nano-Real Space Analysis Takes Dynamics of Colloids Three Decades Closer to the Glass Transition

Glasses are among the most widely used of everyday materials, yet the process by which a liquid's viscosity increases by 14 decades to become a glass remains unclear, as often contradictory theories provide equally good descriptions of the available data. Knowledge of emergent lengthscales and higher-order structure could help resolve this, but this requires time-resolved measurements of dense particle coordinates—previously only obtained over a limited time interval, and a some means of determining local free energy in model glassformers such as hard spheres [1]. Here we present an experimental study of a model colloidal system over a dynamic window significantly larger than previous measurements, revealing structural ordering more strongly linked to dynamics than previously found. Furthermore we find that immobile regions and domains of local structure grow concurrently with density, and that these regions have low configurational entropy [2].


This work was partially supported by the National Science Foundation under Grant No. CBET-1701843 and DMR-1714722.

Experiments on periodically sheared colloidal suspensions with diffusion

Periodically sheared dilute, non-Brownian suspensions explore new configurations through collisions in an otherwise reversible flow. Below a critical strain, the particles remain active until they find a configuration with no collisions and reach an absorbing state. However, in a colloidal system at finite temperature, Brownian motion ensures that no state is ever truly absorbed and simulations by Hexner et. al. have shown that a small amount of diffusion enhances the order of the structures near the critical strain. We built a compact rotational shear cell to drive Brownian colloidal suspensions to explore the effect of diffusion on structures $S(q)$ and dynamics (mean squared displacement) simultaneously using a confocal microscope. From dynamical measurements, we see that the effective diffusion constant is equal to the self-diffusion of the particles below the transition and increases linearly with strain amplitude above. For a 20% volume fraction suspension, we see $S(q)$ at small q in the strain direction drop by a factor of 3 from thermal equilibrium in the strain direction with hyperuniform scaling $S(q) \sim q^{0.5}$ while in the vorticity direction, there is no hyperuniform scaling and $S(q)$ at small q only decreases by 50%.
We show that externally forced particles in a suspension self-organize hyperuniformly in certain directions relative to the force. For this phenomenon to occur, the force-induced coupling between the concentration of particles and their velocity field should satisfy three conditions: (i) it should be long-ranged, decaying with distance $r$ as $1/r^\beta$, with $\beta$ smaller than the dimensionality $d$; (ii) it should have a finite divergence, i.e., the flow of particles should not conserve volume; (iii) it should not be inversion-symmetric. These conditions are fulfilled, for example, for particles which tend to align with the force, or in the presence of a steady concentration gradient. The directions of hyperuniformity depend on the specific coupling. The structure factor for wavevectors $q$ along these directions tends to zero for small $q$ as $q^\alpha$, $\alpha = d – \beta$. We check these analytical results in a simple two-dimensional simulation, showing that they are robust against particle collisions and diffusion.

*Research supported by the Israel Science Foundation (Grant No. 986/18)

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**Complex Spherical Micelle Packings in Aqueous Dispersions of Diblock Polymers**

ASHISH JAYARAMAN (Presenter), Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, DIANA Y ZHANG, McKetta Department of Chemical Engineering, University of Texas at Austin, BETH L DEWING, Department of Chemistry, University of Minnesota, Minneapolis, MAHESH MAHANTHAPPA, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis — Aqueous self-assembly of diblock polymers enables access to a plethora of concentration- and temperature- dependent morphologies including lamellae, hexagonally-packed cylindrical micelles (H), and high-symmetry packings of spherical micelles. Herein, we describe the aqueous lyotropic phase behaviour of poly(ethylene–block–ethylene oxide) using small angle X-ray scattering. The temperature versus amphiphile concentration phase diagram exhibits multiple micellar packings, including well-known body- and face-centered cubic structures as well as the lower symmetry Frank-Kasper (FK) A15 phase. On heating, the A15 phase undergoes a transition into the H-phase. Rapidly quenching this sample from high temperature to 25 °C results in the nucleation and growth of a FK $\sigma$ phase, which contains 30 quasispherical micelles situated at five different symmetry equivalent positions in a tetragonal lattice. We find that the $\sigma$ phase is metastable with respect to A15, and that the metastability strongly depends on the rate of cooling from the H phase and the quench depth. We rationalize our findings based on a subtle energy balance which maximizes interchain cohesion while minimizing both variations in coronal chain stretching and the interfacial penalty for the hydrophobic/hydrophilic contacts.

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**Hyperuniformity of generalized random organization models**

ZHENG MA (Presenter), SALVATORE TORQUATO, Princeton University — Studies of random organization models of monodisperse spherical particles have shown that a hyperuniform state is achievable when the system goes through an absorbing phase transition. Here we investigate to what extent hyperuniformity is preserved when the model is generalized to particles with a size distribution and/or nonspherical shapes. We examine binary disks, disks with a size distribution and hard rectangles of various aspect ratios. We show that the systems are hyperuniform as two-phase media at their respective critical points. This analysis reveals that the redistribution of `mass" of the particles rather than the particle centroids is central to this dynamical process. Our results suggest that general particle systems subject to random organization can be a robust way to fabricate a wide class of hyperuniform states of matter by tuning the structures via different particle-size and -shape distributions. This in turn enables the creation of multifunctional hyperuniform materials with desirable optical, transport and mechanical properties.

*This work was supported by the National Science Foundation under Award Number CBET-1701843.

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**Thursday, March 7, 2019 2:30 PM - 5:30 PM**

**Session V59 GSOFT: Actuation in Soft Matter III** BCEC 257B - Willem Van Rees, Massachusetts Institute of Technology
Mechanics and inverse-design of thin shape-shifting structures

WILLEM VAN REES (Presenter), Massachusetts Institute of Technology, LAKSHMINARAYANAN MAHADEVAN, Harvard University — Recent progress in additive manufacturing and materials engineering has led to a surge of interest in shape-changing plate and shell-like structures. Such structures are typically printed in a planar configuration and, when exposed to an ambient stimulus such as heat or humidity, swell into a desired three-dimensional geometry. Viewed through the lens of differential geometry and elasticity, the application of the physical stimulus can be understood as a local change in the metric of a two dimensional surface embedded in three dimensions. In this talk we present our numerical approach for simulating the elastic response to such a metric change for thin structures. We also show our theoretical contributions on the inverse-design of shape-shifting bilayers, and discuss how these developments have led to the design and experimental realization of a 4D printed lattice that can undergo complex shape changes.

*We thank the Swiss National Science Foundation for support through a postdoctoral grant (WMvR), the American Bureau of Shipping for support through a Career Development Chair at MIT (WMvR), and the National Science Foundation for support from DMR 14-20570 and DMR 15-33985 (LM)

The shape of a rose petal

LAUREN NIU (Presenter), LAKSHMINARAYANAN MAHADEVAN, Department of Physics, Harvard University — The rose petal has a distinctive set of sharp bends along the edges of its outer petals. To understand the origin of this growth pattern, we dissect rose petals to show that the their Gaussian curvature changes from positive to negative toward the outer edges. Using scaling and stability analysis, we show that a curved “sonic” line controls the shape and location of edge buckling, which is itself driven by in-plane growth. We verify our results by numerically solving the nonlinear elastic equations associated with the growing surface. Our analysis suggests a method of designing buckled edge structures with controlled in-plane growth.

Topography Driven Surface Renewal

LUKA POCIVAVSEK (Presenter), University of Chicago, JOSEPH PUGAR, SACHIN VELANKAR, University of Pittsburgh, ENRIQUE CERDA, Universidad de Santiago de Chile — Natural surfaces excel in self-renewal and preventing bio-fouling, while synthetic materials placed in contact with complex fluids quickly foul. We present a novel biophysics inspired mechanism for surface renewal using actuating surface topography, generated by wrinkling. We calculate a critical surface curvature, given by an intrinsic characteristic length scale of the fouling layer that accounts for its effective flexural or bending stiffness and adhesion energy, beyond which surface renewal occurs. The effective bending stiffness includes the elasticity and thickness of the fouling patch, but also the boundary layer depth of the imposed wrinkled topography. The analytical scaling laws are validated using finite element simulations and physical experiments. Our data span over five orders of magnitude in critical curvatures and are well normalized by the analytically calculated scaling. Moreover, our numerics suggests an energy release mechanism whereby stored elastic energy in the fouling layer drives surface renewal. The strategy is broadly applicable to any surface with tunable topography and fouling layers with elastic response.

Differential swelling of boundary-prescribed patterns

CARLOS DUQUE (Presenter), CHRISTIAN SANTANGELO, University of Massachusetts Amherst — Non-Euclidean plates, thin elastic sheets that grow or shrink inhomogeneously, can be thought as geometrically frustrated surfaces that are unable to completely eliminate in-plane stress and are forced to adopt interesting 3D rest configurations as means of reducing their elastic energy cost. We use conformal flattening methods as a natural framework to prescribe isotropic, nonuniform growth patterns on elastic sheets as a way of making them buckle into a given target shape. We tune the ratio of maximal to minimal area distortion required by modifying the planar domain shape and produce 3D patterns that range from ellipsoids and Gaussian bumps to undulating spheres and corroborate the results using finite thickness simulations of growing sheets. Though surfaces with both positive and negative Gaussian curvature behave differently from those with only one sign of Gaussian curvature, we discuss what seems to be a more general composition property of optimal swelling patterns.

*We acknowledge funding through the National Science Foundation grant NSF DMR-1507377.
Twist-induced snapping in a bent elastic ribbon*  TOMOHIKO SANO (Presenter), HIROFUMI WADA, Ritsumeikan University — Snapping a slender structure is utilized in a wide range of natural and man-made systems, to achieve rapid movement without relying on muscle-like elements. Although several mechanisms for elastic energy storage and rapid release have been studied in detail, a general understanding to design such a kinetic system is a key challenge in mechanics. Here we study a twist-driven buckling and flip dynamics of a geometrically constrained ribbon by combining experiments, simulations, and analytical theory. We identify two distinct types of shape transitions; a narrow ribbon snaps, whereas a wide ribbon forms a pair of localized helices. We construct a phase diagram and explain the origin of the boundary determined by geometry. We quantify effects of gravity and timescale dictating the flipping. Our study reveals the unique role of twist-bend coupling on the fast dynamics of a thin constrained structure, which has implications for a wide range of biophysical and applied physical problems.

*We acknowledge the financial support of Grants-in-Aid for Japan Society for the Promotion of Science (JSPS) Fellows (Grant No. 16J05315) and JSPS KAKENHI (Grants No.15H03712, No.16H00815, No.18K13519 and “Synergy of Fluctuation and Structure: Quest for Universal Laws in Non-Equilibrium Systems”).

Self-folded pleated structures in twisted elastic sheets*  ARSHAD KUDROLLI (Presenter), ANDREEA PANAITESCU, Clark University, JULIEN CHOPIN, Physics, Universidade Federal da Bahia — We examine with experiments the post-wrinkling growth of curvature condensation and self-folded structures in thin sheets which are twisted about their axis while held under tension. Using x-ray imaging, we show that the initial sinusoidal wrinkles are found to increasing focus curvature resulting in spontaneous development of pleated structures. Unlike purely tensional wrinkles which decrease in amplitude after an application of a critical strain, the wrinkles are observed to persist and approach a finite value given by the mode number of the primary instability. The number of pleats can be controlled by varying the applied tension and the aspect ratio of the sheet with greater width to length ratios giving rise to more wrinkles and pleats.

*This work was supported by the U.S. National Science Foundation under grant number DMR 1508186.

Instability of an active-elastic chain  TINGYUAN ZHENG (Presenter), MARTIN BRANDENBOURGER, CORENTIN COULAIS, University of Amsterdam — While active materials have drawn an explosion of interest recently, the researches are almost exclusively focused on active fluids. Hereby, we created a simplest form of an active solid: a one-dimensional elastic chain comprising polar self-propelled centimeter scale particles. Combining rapid prototyping and precision desktop experiments, numerical simulations and theory, we report the emergence of the self-oscillating instability in such active chain. We further establish that the bifurcation towards the self-oscillatory dynamics is controlled by the competition between activity and elasticity.

The results provide some key insights into the potential of active solids in mimicking living matter and forming novel materials with far from equilibrium responses.

Dynamics of optical and anisotropic mechanical responses in hydrogels*  C. NADIR KAPLAN (Presenter), Harvard University, PETER A. KOREVAAR, Radboud University, ALISON GRINTHAL, JOANNA AIZENBERG, Harvard University — Materials that perform complex chemical sensing are ubiquitous in living systems, and would transform developments in biomedicine, environmental monitoring, and many other areas. We introduce a continuum mechanical framework that predicts the minimal set of components needed to integrate dynamical signal processing capabilities into simple hydrogels without structural modifications. For a common polyacrylic acid hydrogel, with copper cations and acid as representative chemical stimuli, the theory explains the experimentally observed (i) two-dimensional traveling waves of copper induced blue color selectively indicating a slowly progressing acid stimulus, (ii) anisotropic mechanical responses depending on the direction of acid progression, associated with tilting of an array of embedded passive microplates that report local hydrogel deformations. These results suggest simple hydrogels have a much larger sensing space than is currently made use of.

*This material is based upon work supported by the Department of Energy under Award Number DE-SC0005247.
Active structuring of a particle film on a droplet's surface and examples of its applications

KHOBAB KHOBAB (Presenter), ALEXANDER MIKKELSEN, Faculty of Physics, Adam Mickiewicz University, Poland, ZBIGNIEW ROZYNEK, Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, USA and, Faculty of Physics, Adam Mickiewicz University, Poland — Particle films have a broad range of applications, for instance in smart materials as constituent of strain sensors, actuators, or smart windows. Such films can be assembled and actively controlled by acoustic, magnetic, or electric fields. In this work, we used electric fields to actively compress and stretch particle film monolayers on a droplet interface. Particle manipulation was achieved through the synergetic action of electric field-induced droplet deformation and electrohydrodynamic flows. We studied in detail how droplet deformation and particle structuring are influenced by parameters such as electric field strength, ionic conductivity, and viscosity. We found that the time for particles to compress at the droplet interface was strongly influenced by the electric field, and that it scaled as $E^{-4}$. Moreover, hysteresis effects were observed both in the magnitude of droplet deformation and particle expansion and contraction. Looking towards practical applications, we also demonstrated how particles at droplet interfaces manipulated by electric fields could be used as an active optical lens, a tool for detecting of material encapsulated in particle-covered droplets, or for fabrication of porous materials used in biological applications.

Development of hydrogel-based cell stretching devices as in vitro model of atherosclerotic vessel walls*

QI LU (Presenter), WEIGUO HUANG, Department of Polymer Science and Engineering, University of Massachusetts, Amherst, ARITRA NATH KUNDU, MARIA FERNANDA GENCOGLU, SHELLY PEYTON, Department of Chemical Engineering, University of Massachusetts, Amherst, RYAN HAYWARD, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — Atherosclerosis, the hardening of arteries, is the leading cause of heart attacks and strokes. The disease is worsened by smooth muscle cell (SMC) dedifferentiation, but the cause is difficult to study in vitro because it involves coupling between multiple physical and chemical factors. We sought to improve SMC culture models by creating a device with independent control over substrate stiffness, mechanical stretch and cell attachment. This device was fabricated by embedding micro-heaters under temperature-responsive hydrogel with patterned creases on the surface, and one SMC was seeded between two neighboring creases by photo-lithographically patterned attachment of peptides in desired location. The actuation is achieved by driving the heaters at 1 Hz, which mimics the resting pulse rate, causing the cell to be cyclically stretched and released by the repeatable deepening and relaxation of the creases. The cell is stretched by a strain of 5-10%, which is comparable to the stretch ratio that it experiences in physiological environment. This device can be systematically engineered, avoids macroscopic deformation and can potentially be scaled to high-throughput arrays.

Actuated Fibre Networks to Study Physical Principles of Multicellular Organization*

FAZIL USLU (Presenter), Institute of Mechanical Engineering, Ecole polytechnique federale de Lausanne, CHRISTOPHER D. DAVIDSON, Department of Biomedical Engineering, University of Michigan, Ann Arbor, NIKOLAOUS BOUKLAS, Department of Mechanical and Aerospace Engineering, Cornell University, Ithaca, BRENDON BAKER, Department of Biomedical Engineering, University of Michigan, Ann Arbor, MAHMUT SELMAN SAKAR, Institute of Mechanical Engineering, Ecole polytechnique federale de Lausanne — Cells continuously sense and respond to passive mechanical and topographical properties of the surrounding matrix as well as active forces transmitted through the same matrix. Cell-generated forces in deformable fibrous matrices enable long-range intercellular communication and drive collective cell behavior. Our aim is to quantitatively describe how matrix architecture and mechanics influence transmission of forces, and elucidate principles of physical organization instantiated by remodeling of a fibrillar substrate. We developed a microrobotic manipulation platform along with an experimentally validated finite element modeling framework to systematically manipulate and monitor stress on engineered fibre networks with tunable properties. Our approach allows application of spatiotemporally defined deformations using magnetically controlled microactuators and mapping of stress using simulations of materials, for which we performed measurements using confocal imaging, atomic force microscopy and MEMS force sensors. Preliminary results show that cells do respond to the signals generated by the synthetic actuators and a two-way communication can be established through the fibres using real-time feedback provided by time-lapse microscopy.

*European Research Council ROBOCHIP (714609)
LEYOU ZHANG (Presenter), Department of Physics, University of Michigan, D. ZEB ROCKLIN, School of Physics, Georgia Institute of Technology, LEONARD M SANDER, XIAOMING MAO, Department of Physics, University of Michigan — We present simulation results on fracture mechanics of two lattice models on the verge of mechanical instability. For both models, we show that the fracture and failure mechanism is distinctive from traditional brittle solids: stress does not concentrate on crack tips. In the first model which is a randomly diluted triangular lattice under isostaticity, we observed that nonlinear alignments of fiber chains lead to a steady state in which new load-bearing fiber chains emerge to replace those lost to fracture. We show that the stress concentration is dissipated and eventually prevented when the rigidity of the model decreases to zero. In the second model which is a kagome lattice with topologically protected states of self stress on devised domain walls, we show that stress concentrates on domain walls instead of cracks, leading to delayed catastrophic failure. Suitable boundary conditions for experiments will also be discussed.

*The authors gratefully acknowledge support from the National Science Foundation Grant No. NSF DMR—1609051 and NSF EFMA—1741618.

OCTAVIO ALBARRAN (Presenter), PETER WEIST, EUGENIA BUTKEVICH, RENATA GARCES, Third Institute of Physics, University of Goettingen, CHRISTOPH SCHMIDT, Department of Physics, Duke University — To perform undulatory locomotion, C. elegans nematodes generate forces with their body-wall muscles acting on the surrounding environment and against their own body bending resistance. The knowledge of the passive elastic body response is crucial to understand the dynamic functions of the worm. It has been hypothesized that the worm kinematics can be understood in terms of linear viscoleastic beam theory. However, to date, mechanical studies in the large deformation regime, typical of native undulatory locomotion, are lacking. We here present a micro-needle-based experiment imposing large strains. Living worms were kept straight by clamping their extremities onto agar plates. We laterally displaced the centers of worms with a glass cantilever of known spring constant and directly probed the linear beam model. To separate passive responses from muscle activity, we varied the contraction-relaxation state of the muscles using pharmacological interference. We provide a synthesis of the typical range of magnitudes of the worm's material parameters for different muscles states.

JOSEPH MONTI (Presenter), MARK OWEN ROBBINS, Johns Hopkins University — Disorder at the interface of an amorphous slider on a crystalline substrate leads to vanishing friction for large rigid contacts. The inclusion of elasticity introduces an energetic contribution that competes with the random interfacial potential and allows frictional pinning over a domain with characteristic radius $a_c$. The interfacial force scales linearly with $a_c$, while the elastic restoring force from deformation on the scale of $a_c$ depends upon the dimension of the substrate. For a 2D substrate, the restoring force is independent of $a_c$, while it grows linearly with $a_c$ in 3D. Comparison of the interfacial and elastic contributions shows that the pinning force is proportional to $a_c$ in 2D. The 3D case is marginal because the forces scale with the same power of $a_c$. Extensive simulations are used to test the scaling of friction with disorder strength and system size. In 3D, we find an exponential decrease of the pinning force and increase in $a_c$ with increasing substrate stiffness. In 2D, the expected power law scaling is observed. Substrates of finite thickness show a crossover in scaling with contact size that may be important in understanding solid lubricants with a plate structure.

*Support provided by NSF Grant No. DMR-1411144
5:18PM V59.00015: Global and Local Mechanical Properties of Responsive Microgels Adsorbed to Solid-Liquid Interfaces  
MARIE FRIEDERIKE SCHULTE (Presenter), ANDREA SCOTTI, MONIA BRUGNONI, STEFFEN BOCHENIKE, RWTH Aachen University, AHMED MOURRAN, DWI - Leibniz Institute for Interactive Materials, WALTER RICHTERING, RWTH Aachen University — Microgels are highly interfacial active, although not being amphiphilic. They readily adsorb to liquid/liquid, liquid/air or solid interfaces and deform [1]. We studied microgels with unique internal structures, (i) one with a rigid silica core and a PNIPAM shell, (ii) hollow microgels obtained by dissolving the silica core, and (iii) ultra-low cross-linked microgels. These responsive microgels were investigated at the solid-liquid interface by scanning force microscopy. An important parameter is the size of the probe compared to the dimensions of the microgel [2]. Colloidal probe experiments lead to a compression of the whole microgel and provide information on their global mechanical properties. Changing the probe dimensions, we will demonstrate that indentation experiments using sharp tips lead to a local penetration of the porous swollen microgel network. Therefore, force-distance curve measurements enable to probe the segment density distribution orthogonal to the substrate of adsorbed single microgels.


*The Deutsche Forschungsgemeinschaft (DFG) is acknowledged for financial support within the Sonderforschungsbereich SFB 985 “Functional Microgels and Microgel Systems”.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V60 FPS: The Future of U.S. Nuclear Forces: What Do We Need? BCEC 258A - Frank von Hippel, Princeton University - Tag(s): Invited, Undergraduate

2:30PM V60.00001: Nuclear Modernization, ICBMs, and Launch On Warning [invited] STEVE FETTER (Presenter), University of Maryland, College Park — The US is replacing all three legs of the triad, ballistic missile submarines (SSBNs), bombers, and intercontinental ballistic missiles (ICBMs), at a cost of over $1.2 trillion. The SSBN force is the core of the deterrent because it can survive a Russian attack and deliver a devastating retaliatory strike. The strategic bomber can support conventional missions and the cost of adding a nuclear capability is modest. But silo-based ICBMs are not survivable; they can be destroyed in a first-strike. For this reason, ICBMs are kept ready to be launched on warning of a Russian attack. This forces decisions to be made in minutes and creates the possibility of launch on false warning.

Two arguments are made in favor of retaining a ICBMs. First, ICBMs are a hedge against failures in other legs of the triad. But ICBMs cannot serve as a hedge unless the US commits to launch under attack. Second, without the 400-plus aimspoints provided by ICBMs, Russia might be tempted to strike the small number of remaining targets. Why Russia would take this risk knowing that SSBNs armed with over 700 warheads would remain capable of delivering a devastating retaliatory strike is unclear. The key is the survivability of command, control, and communication capabilities.

3:06PM V60.00002: US Plans for New Nuclear Weapons [invited] LISBETH GRONLUND (Presenter), Union of Concerned Scientists — For decades, the United States produced a stream of nuclear warheads, with new types replacing previous types on an ongoing basis. It did not seriously consider the behavior of aging warheads until it declared a moratorium on nuclear explosive testing in 1992. At that time the United States believed it could not validate new warhead designs without nuclear testing, and that it would therefore have to extend the life of existing warheads. Two warhead types have undergone life extension programs that were straightforward refurbishments. However, the latest plan is to replace—not refurbish—one of the warheads deployed on silo-based missiles. The weapons designers now believe their computer models allow them to validate new designs without explosive testing. I will discuss the rationale for this new warhead and the downsides of deploying it.
3:42PM V60.00003: Current Nuclear Weapons Issues, and Sid Drell’s Contributions to Arms Control and Strategic Stability [Invited] RICHARD L. GARWIN (Presenter), IBM Thomas J. Watson Research Center — 1. The history of the M-X missile, of various bomber programs, and naval ship procurement confirms that one of the great threats to U.S. national security is the aggressive overselling and underpricing of weapon systems. Beware envy of weapons we don't need, in contrast with countering adversary weapon systems by defense, deception, or a combination of electronic warfare and cyber attack, or by the use of alternative (asymmetric) systems. 2. At Sid’s retirement from SLAC 20 years ago, I recounted some of his work in creating and perfecting satellite imagery that greatly improved our knowledge of denied territories. His work, both technical and programmatic, resulted in his being named one of the ten Founders of National Reconnaissance. A separate portion of his efforts was devoted to work on and to the leadership of the strategic military panel of the President’s Science Advisory Committee --PSAC-- with its annual assessment of proposals for U.S. national missile defense. He undertook public analysis of various proposals for land-basing of the 10-warhead M-X missile in Nevada or Utah, and lectured there, and worked within the JASON group for the US Department of Defense to propose a novel and highly unwelcome system for basing four encapsulated M-X missiles alongside each of a fleet of small non-nuclear submarine. In the 1990s, Sid was key to readying the Defense Department and the nuclear weapons elements of the Department of Energy to support a total ban of nuclear explosion testing-- the CTBT-- and to put substance on the Science-based Stockpile Stewardship Program for maintaining U.S. nuclear weapons safe and reliable under the CTBT. In recent decades Sid worked with George P. Shultz, Sam Nunn, Henry A. Kissinger, and William J. Perry toward massive reductions of nuclear weaponry, and with the goal of eliminating nuclear weapons. Sid's energy and warm personality enhanced his effectiveness, making it a pleasure to work with him.

4:54PM V60.00004: Engaging the Physics Community in Nuclear Threat Reduction [Invited] STEWART PRAGER (Presenter), Princeton University — The threat posed by nuclear weapons has been well-known, well-articulated, and well-studied for 70 years. Most importantly, a network of international agreements has slowed proliferation and led to dramatic reduction in the number of warheads in the US and Russia. Despite these advances, the grave threat persists and is arguably getting worse – a result of weapons spread to nine nations, the appearance of non-state actors, the threat of cyber attacks against weapon systems, weapons modernization over the coming decades, withdrawal from treaties, potential new tactical weapons, and government discussions of reducing the threshold for the use of nuclear weapons. Yet, this issue is largely ignored by the public. Physicists have a special relation to nuclear arms and, if organized, can add an influential voice to the effort to reduce the threat. There are many threat reduction steps that the physics community can encourage, such as de-alerting, adoption of policies of no-first-use and no launch-on-warning, reduction of global weapons-usable materials and much more. An initiative is being formulated to engage and activate the US physics community to this end.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V61 GSOFT: Physics and Hydrodynamics of Micro-swimmers' Suspensions BCEC 258B -

Arnold Mathijssen, Stanford University - Tag(s): Focus

2:30PM V61.00001: Swimming bacteria in a Poiseuille flow : the quest for active Bethoven-Jeffery trajectories*

GASPARD JUNOT (Presenter), THIERRY DARNIGE, ESPCI ParisTech, NURIS FIGUEROA MORALES, 508 Wartik Lab, PA 16802, USA, The Pennsylvania State University, ANKE LINDNER, ESPCI ParisTech, HAROLD AURADOU, F-91405, Orsay, France, FAST, Univ. Paris Sud, ERIC CLEMENT, ESPCI ParisTech — Using a 3D Lagrangian tracking technique, we determine the swimming trajectories of E.coli in a Poiseuille flow. We identify many trajectories displaying the qualitative features of an “active Bretherton-Jeffery” model featuring an axi-symmetric self-propelled ellipsoid swimming in a flow. By deriving closed-forms for two phase-portraits involving one spatial and two angular coordinates as well as, the mean angular shift displayed by the families of cycloid trajectories, we show that for a smooth swimmer mutant, a quantitative mapping with the actual experimental trajectories can be made. Furthermore we show that from cycloid trajectories, the effective aspect ratio of the swimmer can be extracted. This analysis also allows to highlight the crucial influence of Brownian rotation noise, on the swimmer trajectories.

*This work was supported by the ANR grant “BacFlow” ANR-15-CE30-0013
2:42PM V61.00002: Characteristics of collective and individual motions of swimming Phytophthora zoospores
QUANG TRAN (Presenter), PHILIPPE THOMEN, CÉLINE COHEN, Institut de Physique de Nice (INPHYNI), Université Côte d’Azur, CNRS UMR 7010, Nice, France, ERIC GALIANA, Institut Sophia Agriobiotech (ISA), Université Côte d’Azur, INRA UMR 1355, CNRS 7254, France, XAVIER NOBLIN, Institut de Physique de Nice (INPHYNI), Université Côte d’Azur, CNRS UMR 7010, Nice, France — Phytophthora diseases cause big threats to agriculture and eco-systems. Spreading is based on rapid dispersion of biflagellate swimming zoospores that once having reached a host initiate plant infection. Understanding their swimming mechanism and their interactions against gradients and surrounding environments becomes important. In this study, we develop a microfluidic system to investigate collective and individual motions of Phytophthora parasitica zoospores, a species that infects a broad range of host plants. Our system has the ability to generate a chemical gradient diffusing to a group of swimming zoospores and observe their swimming motions as well as the changes of the gradient at the same time. Our results show that a group of P. parasitica react differently against different doses of potassium chloride gradients: Low concentration of potassium reduces their speed and lures them away or initiates auto-aggregation, while high concentration (>3mM) causes them to change their swimming pattern to circulating around or stop moving. Moreover, observing a single zoospore swimming in water, we achieved the characteristics of its beating flagella. The correlation between zoospore velocity and its flagella motions helps us explain their reactions against the potassium gradients.

2:54PM V61.00003: Dancing to the swimmers’ beat: Loopy Lévy flights enhance tracer diffusion in active suspensions*
KIYOSHI KANAZAWA, Institute of Innovative Research, Tokyo Institute of Technology, TOMOHIKO SANO, Department of Physical Sciences, Ritsumeikan University, ANDREA CAIROLI (Presenter), Department of Bioengineering, Imperial College London, ADRIAN BAULE, School of Mathematical Sciences, Queen Mary University of London — The diffusion process followed by a tracer in a medium out of equilibrium typically exhibits anomalous diffusion that cannot be modelled by Brownian motion. Prototypical active media are suspensions of swimming microorganisms like algae and bacteria, where the tracer is dragged by the hydrodynamic flow generated by the swimmers. Several experiments have characterised the tracer diffusion in dilute conditions by a greatly enhanced diffusion coefficient, non-Gaussian tails of the displacement statistics, and crossover scaling phenomena. Despite the abundant experimental results, there is so far no comprehensive theory that can describe all these features. Here we present a theoretical framework of the enhanced tracer diffusion from first-principles, by coarse-graining the microscopic tracer-swimmer interactions as a coloured Lévy Poisson process. This theory not only provides the toolkit necessary to characterise theoretically the tracer diffusion but also paves the way to the study of its stochastic thermodynamics.

*This work was funded by Grant-in-Aid for JSPS Fellows (Grant No. 16J05315), JSPS KAKENHI (Grant Nos. 16K16016 and 18K13519), the Research Fellowship of the Royal Commission for the Exhibition of 1851, and the Atoms program of the Yukawa Institute for Theoretical Physics.

3:06PM V61.00004: Active colloidal particles in emulsion droplets: A model system for the cytoplasm
VIVA HOROWITZ (Presenter), Physics Department, Hamilton College, ZACHARY C. CHAMBERS, Department of Physics, Harvard University, IREP GÖZEN, Department of Medicine, University of Oslo, Norway, THOMAS G. DIMIDUK, VINOTHAN N MANOHARAN, Department of Physics, Harvard University — In living cells, molecular motors create activity that enhances the diffusion of particles throughout the cytoplasm, and not just ones attached to the motors. We demonstrate initial steps toward creating artificial cells that mimic this phenomenon. Our system consists of active, Pt-coated Janus particles and passive tracers confined to emulsion droplets. We track the motion of both the active particles and passive tracers in a hydrogen peroxide solution, which serves as the fuel to drive the motion. We first show that correcting for bulk translational and rotational motion of the droplets induced by bubble formation is necessary to accurately track the particles. After drift correction, we find that the active particles show enhanced diffusion in the interior of the droplets and are not captured by the droplet interface. At the particle and hydrogen peroxide concentrations we use, we observe little coupling between the active and passive particles. We discuss the possible reasons for lack of coupling and describe ways to improve the system to more effectively mimic cytoplasmic activity.
Microswimmers can self-organize to a variety of collective geometries and can exhibit spontaneously broken mirror symmetry. This allows for the realization of chiral Beltrami vector fields, which can support inverse energy transport from smaller to larger scales, in contrast to classical 3D turbulence.

We acknowledge support from IdEx (Initiative d'Excellence) Bordeaux and French National Research Agency through Contract No. ANR-13-IS04-0003.

3:18PM V61.00005: Spontaneous chiral symmetry breaking in active fluids* [Invited] JORN DUNKEL (Presenter), Physics, University of Warwick, JORGE ARRIETA, RAMON SALETA-PIERSANTI, IDAN TUVAL, Instituto Mediterraneo de Estudios Avanzados, IMEDEA, Universitat de les Illes Balears-CSIC — Microorganismal motility is often characterised by complex responses to environmental physico-chemical stimuli. Although the biological basis of these responses is often not well understood, their exploitation already promises novel avenues to directly control the motion of living active matter at both the individual and collective level. Here we leverage the phototactic ability of the model microalg Chlamydomonas reinhardtii to precisely control the timing and position of localised cell photo-accumulation, leading to the controlled development of isolated bioconvective plumes. This novel form of photo-bio-convection allows a precise, fast and reconfigurable control of the spatio-temporal dynamics of the instability and the ensuing global recirculation, which can be activated and stopped in real time. A simple continuum model accounts for the phototactic response of the suspension and demonstrates how the spatio-temporal dynamics of the illumination field can be used as a simple external switch to produce efficient bio-mixing.

*We acknowledge the support of the Spanish Ministry of Economy and Competitiveness Grants No. FIS2016-77692- C2-1-P, and CTM-2017-83774-D, and the subprogram Juan de la Cierva No. IJCI-2015-26955.

3:54PM V61.00006: Dial-a-plume: Active Control of Localised Photo-Bio-Convection* MARCO POLIN (Presenter), Physics, University of Warwick, JORGE ARRIETA, RAMON SALETA-PIERSANTI, IDAN TUVAL, Instituto Mediterraneo de Estudios Avanzados, IMEDEA, Universitat de les Illes Balears-CSIC — Microorganismal motility is often characterised by complex responses to environmental physico-chemical stimuli. Although the biological basis of these responses is often not well understood, their exploitation already promises novel avenues to directly control the motion of living active matter at both the individual and collective level. Here we leverage the phototactic ability of the model microalg Chlamydomonas reinhardtii to precisely control the timing and position of localised cell photo-accumulation, leading to the controlled development of isolated bioconvective plumes. This novel form of photo-bio-convection allows a precise, fast and reconfigurable control of the spatio-temporal dynamics of the instability and the ensuing global recirculation, which can be activated and stopped in real time. A simple continuum model accounts for the phototactic response of the suspension and demonstrates how the spatio-temporal dynamics of the illumination field can be used as a simple external switch to produce efficient bio-mixing.

*We acknowledge the support of the Spanish Ministry of Economy and Competitiveness Grants No. FIS2016-77692- C2-1-P, and CTM-2017-83774-D, and the subprogram Juan de la Cierva No. IJCI-2015-26955.

4:06PM V61.00007: Percolation theory of intercellular communication through hydrodynamic trigger waves* ARNOLD MATHIJSSEN (Presenter), Department of Bioengineering, Stanford University, JOSH CULVER, SAAD BHAMLA, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, MANU PRAKASH, Department of Bioengineering, Stanford University — Here, akin to a chain reaction, we present the discovery of hydrodynamic trigger waves in cellular communities of the protist Spirostomum ambiguum, propagating hundreds of times faster than their swimming speed. These cells can contract their body by 50% within milliseconds, equivalent to 14g-forces. A single contraction (transmitter) generates long-ranged vortex flows that trigger neighbouring cells, in turn. We further present a microfluidic device to measure the sensitivity to hydrodynamic signals (receiver). Using percolation theory, a phase transition is revealed that requires a critical cell density to sustain communication. Our results suggest that this signalling could help organise cohabiting communities over large distances, comparable to quorum sensing. Moreover, as contractions release toxins, synchronised discharges could also facilitate the repulsion of large predators, or conversely immobilise large prey. We postulate that beyond protists numerous other freshwater and marine organisms could coordinate with variations of hydrodynamic trigger waves.

*We acknowledge funding from the Human Frontier Science Program (Fellowship LT001670/2017).

4:18PM V61.00008: Gravity induced structures of microswimmers on a surface* ZAIYI SHEN (Presenter), ALOIS WÜRGER, JUHO LINTUVUORI, LOMA, Université de Bordeaux — Microswimmers can self-organize to a variety of collective states. The underlying forces, however, are not well characterized. Besides the electric, magnetic or chemical surface forces, hydrodynamic interactions are believed to play important role on the collective motion of active colloids. In typical experiments of artificial self-propelled colloids, the particles are observed to sediment. We study microswimmer suspensions by lattice Boltzmann simulations, using a squirmer model. We show that hydrodynamic interactions, together with a gravity-like field, lead to tunable collective behaviors of self-propelled spheres near a surface. For example chiral spinners, swarming clusters and living crystals are observed. We rationalize the formation of these structures, in detail, based on hydrodynamic interactions between a pair of swimmers. These interactions depend crucially of the swimming mechanism, pusher or puller, and can be tuned such that they are either directional, leading to the formation of small chiral spinners or mutually attractive, creating large hydrodynamically bound motile aggregates.

*We acknowledge support from IdEx (Initiative d'Excellence) Bordeaux and French National Research Agency through Contract No. ANR-13-IS04-0003.
4:30PM V61.00009: Emergence of phytoplankton patchiness at small scales in mild turbulence  
REBEKKA BREIER, CRISTIAN C LALESCU, MICHAEL WILCZEK, Max Planck Institute for Dynamics and Self-Organization, MARCO G. MAZZA (Presenter), Loughborough University — Phytoplankton often encounter turbulence in their habitat. The spatial distribution of motile phytoplankton cells exhibits patchiness at distances of decimeter to millimeter scale for numerous species with different motility strategies. The explanation of this general phenomenon remains challenging. We combine particle simulations and continuum theory to study the emergence of patchiness in motile microorganisms in three dimensions, by including hydrodynamic cell-cell interactions, which grow more relevant as the density in the patches increases. By addressing the combined effects of motility, cell-cell interaction and turbulent flow conditions, we uncover a general mechanism: the coupling of cell-cell interactions to the turbulent dynamics favors the formation of dense patches.

4:42PM V61.00010: Non-Gaussian limit fluctuations in active swimmer suspensions [Invited]  
DAISUKE MIZUNO (Presenter), TAKASHI KURIHARA, Kyushu University, ZAID IRWIN, Oxford University — Hydrodynamic fluctuations in suspensions of swimming microorganisms (Chlamydomonas and E-coli) exhibit heavily-tailed distribution which is not Gaussian nor Levy, for which both the classical and extended central limiting theories do not apply. In this study, the physical limit distribution, instead of mathematical ones, was derived in an analytical form by summing the general power-law interactions from field sources (here, swimming microorganisms) randomly distributed in general spatial dimensions. The origin of the non-Gaussianity is not just the power-law decay of hydrodynamic fields, but the summing procedure of the fields, which we refer to as the physical limit operation [1].

The non-Gaussian shape of the hydrodynamic fluctuations in active swimmer suspensions obeys the analytic theory concomitantly with independently determined parameters such as the strength of force generations and the concentration of swimmers. Time evolution of the distributions collapsed to a single master curve, except for their extreme tails, for which our theory presents a qualitative explanation. Investigations thereof and the complete agreement with theoretical predictions revealed broad applicability of the formula to fluctuations in active systems [2].

Fluctuations show up differently in different spatial dimensions since dimensionality affects the spatial correlations of fields and the population of field sources as a function of system size. Swimmers that resist to sedimentation or ordinary force-dipolar swimmers confined in 2D generate $1/r$-decaying fields that are long-ranged in the sense that there is no thermodynamic limit. If time permitted, I will discuss the implication of our study for the dimensionality dependence of active fluctuations.


5:18PM V61.00011: Bacterial diodes: Rectified transport of swimming cells in porous media flow  
NICOLAS WAISBORD, JEFFREY GUASTO (Presenter), Tufts University — Directed motility enables swimming microbes to navigate their porous habitats for resources, where self-propulsion competes with fluid flow to affect processes ranging from disease transmission and bioremediation. Despite this broad importance, how directed motility affects the self-transport and dispersion of microswimmers in flow through constricted pores remains unknown. Focusing on magnetotactic bacteria in a microfluidic porous medium, we show that upstream oriented cells, directed by a magnetic field, are localized and trapped in vortical orbits at a constriction. Vortical cell localization results in three distinct regimes of rectified bacterial conductivity through a throat, akin to a ‘bacterial diode’, whereby cells swim upstream, become trapped within a pore, or are advected downstream with increasing flow speed. Langevin simulations reveal that the trapping regime results in near-complete transport suppression, while ephemeral trapping in the downstream regime enhances dispersion. We also show that vortical cell localization persists in three-dimensional flow through a packed microfluidic bed, emphasizing the relevance of this phenomenon in realistic hydraulic networks.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V63 GSOFT: Membranes, Micelles and Vesicles  
BCEC 259A - Anna Wang, Massachusetts General Hospital
2:30PM V63.00001: Electrostatic shape control of a charged molecular membrane from ribbon to scroll* SUMIT KEWALRAMANI (Presenter), CHANGRUI GAO, HONGHAO LI, MONICA OLVERA DE LA CRUZ, MICHAEL J BEDZYK, Northwestern University — Bilayers of amphiphiles can organize into a number of distinct mesoscopic shapes, which interconvert under suitable conditions. The pathway for such transformations is often elusive. We use a charged amphiphile (palmitoyl-lysine, C16-K1) to elucidate the planar nanoribbon to cochleate transition induced by salt (NaCl) concentration (c). In-situ small- and wide-angle X-ray scattering (SAXS/WAXS), atomic force and cryogenic transmission electron microscopies (AFM and cryo-TEM) tracked transformations over Å to µm length scales. AFM reveals that the large length (L) to width (W) ratio nanoribbons (L/W > 10) convert to sheets (L/W ~ 1) before rolling into cochleates. A theoretical model based on electrostatic and surface energies shows that the ribbon to sheet conversion is a first order transition, occurring at a critical Debye length. SAXS shows that the interbilayer spacing (D) in the cochleates scales linearly with Debye length (or c^-1/2). Theoretical arguments that include electrostatic, bending and van der Waals energies explain the membrane rolling and the linearity between D and Debye length. These models suggest that the salt-induced ribbon to cochleate transition should be common to all charged bilayers possessing an intrinsic curvature.

*Doe- BES:DE-FG02-08ER46539

2:42PM V63.00002: A gel based on vesicle-vesicle adhesion induced by polyelectrolyte: from morphology to rheology* RUI CAO (Presenter), DEEPAK KUMAR, IAN TORRES, NARAYANAN MENON, ANTHONY DINSMORE, Physics, University of Massachusetts Amherst — Phospholipid membranes are of great interest for encapsulation due to its outstanding barrier properties. Here we show that one can build an elastic solid with giant vesicles (1-30 mm diameter) that adhere to one another. A slight negative potential on the lipid membrane enables electrostatic attraction with polycations, which induces vesicle-vesicle adhesion. The vesicle adhesion leads to a macroscopic vesicle based gel that is >99% water but has a closed-cell structure. Shear rheology measurements show a low-frequency modulus of a few Pa and linear response extending to very large strains of approximately 0.7. We find that the vesicle adhesion strength and shear modulus can be tuned with polyelectrolyte concentration. We also find that the shear modulus does not scale with vesicle size as long as the adhesion strength is held constant. The vesicle gel system shows great potential as a soft-solid platform for a stimulus-responsive material that can deliver reagents on demand.

*This work was supported by a MURI grant from the U.S. Army Research Office (W911NF-15-1-0568).

2:54PM V63.00003: Controlling the elasticity of lipid membranes with pluronic block copolymers PETER BELTRAMO (Presenter), Chemical Engineering, University of Massachusetts Amherst, SANDRO STUCKI, JAN VERMANT, ETH Zurich — Pluronic triblock copolymers consisting of a hydrophobic poly(propylene-oxide) (PPO) block, flanked by two hydrophilic poly(ethylene-oxide) (PEO) blocks have been widely investigated in drug delivery applications as membrane sealants and plasticizers. However, despite a single pluronic (F68) being FDA approved, there is minimal insight into how block copolymer architecture can be engineered to dictate membrane response. Here, we investigate the influence of the structure of the pluronic on the interaction with artificial biological membranes using the large-area model biomembrane (LAMB) technique. We systematically measured the change in membrane tension and elasticity of a planar, freestanding DOPC membrane upon interaction with several pluronics with with varying PEO and PPO chain lengths and HLB values. Based on the membrane tension - area relationship, the apparent elasticity modulus was calculated. Interestingly, the main factor determining the membrane elasticity is the length of the hydrophilic PEO chain, rather than the hydrophobic PPO block. We also discuss the effect of concentration above and below the cmc on the membrane elasticity. These findings may prove beneficial for future medical applications of pluronics as treatment for membrane-tension mediated maladies.
3:06PM V63.00004: Spontaneous division of model protocell membranes* ANNA WANG (Presenter), Molecular Biology and Center for Computational and Integrative Biology, Massachusetts General Hospital, STEPHANIE ZHANG, Department of Chemistry and Chemical Biology, Harvard University, JACK W. SZOSTAK, Molecular Biology and Center for Computational and Integrative Biology, Massachusetts General Hospital — Prior to the existence of phospholipid membranes, the ancestors of modern day cells likely had membranes consisting of much simpler molecules. On early Earth, these membranes would have provided the function that modern cell rely on proteins for - nutrient transport, growth and division - prompting the question of whether such functions can arise from a lipid-only system.

We show that fatty acids can self-assemble into giant unilamellar vesicles (GUVs) without the need for scaffolding droplets, substrates, or microfluidics. Remarkably, such GUVs are capable of spontaneously dividing upon an increase in surface area to volume ratio, instead of simply forming tubular vesicles. When nucleic acids are encapsulated, the protocells - membranous compartments containing nucleic acids - are able to divide into daughter protocells without apparent loss of content.

We find that the bilayer properties of fatty acid membranes depend on the pH and ionic strength of the surrounding solution, and explore how the differences between fatty acid membranes and the better-studied phospholipid systems enable the unusual self-assembly and morphology changes we see.

*A.W. would like to thank the NASA Postdoctoral Program for support

3:18PM V63.00005: Direct imaging of micelle dynamics with an electron microscope* HIMANAGAMANASA KANDULA (Presenter), YE-JIN KIM, OH-HOON KWON, STEVE GRANICK, Center for soft and living matter, Institute for Basic Sciences — Direct imaging of single micelle dynamics and the kinetics of their assembly is not possible with conventionally used imaging techniques such as transmission electron microscopy (TEM) or cryo-TEM. In this talk, I will discuss our efforts to image the dynamics of simple block copolymer micelles using liquid-phase TEM. By directly visualizing small micellar assemblies in solution, we demonstrate the structure-dependent dynamics of these assemblies, with intriguing surprises.

*Institute for Basic Sciences, South Korea.

3:30PM V63.00006: The role of particle shape in the deformation and disruption of lipid membranes: Experiments with tunable particle shape and adhesion* SARAH ZURAW (Presenter), ANTHONY DINSMORE, University of Massachusetts Amherst, MAHSA SIAVASHPOURI, physics, Brandeis University, ZVONIMIR DOGIC, Physics, University of California Santa Barbara — We seek to understand the effects of DNA origami nano-rods on membrane structure and morphology. We combine giant unilamellar lipid vesicles (GUVs) with a sufficiently high concentration of oppositely charged nano-rods and observe the interactions. The adhesion of the nano-rods to the membrane is a tunable parameter controlled by the lipid composition, and results in three primary behaviors. At weak adhesion strengths, vesicles adhere to one another and form a stable gel, with the nano-rods acting as a glue that holds the gel together. At intermediate adhesion strengths, gel forms but is subsequently destroyed by avid binding of the nano-rods. At higher adhesion strengths, the vesicles are ruptured by the nano-rods without ever forming a gel. These behaviors can be explained respectively by shallow, deep, or complete wrapping of the nano-rods onto the lipid membrane. These results are a robust example of tuning response in a synthetic membrane system and provide a physical understanding of the design principles toward controlled membrane morphologies. These results will lead to a bio-inspired membrane material that is stimuli-responsive, has high surface area and is reconfigurable.

*This work is funded by the NSF Materials Research Science and Engineering Center grant DMR-1420382
Controlling Cargo Trafficking in Multicomponent Membranes

TINE CURK (Presenter), Institute of Physics, Chinese Academy of Sciences, PETER WIRNSBERGER, Department of Chemistry, University of Cambridge, JURE DOBNIKAR, Institute of Physics, Chinese Academy of Sciences, DAAN FRENKEL, Department of Chemistry, University of Cambridge, ANDELA SARIC, Physics, UCL — Biological membranes typically contain a large number of different components dispersed in small concentrations in the main membrane phase, including proteins, sugars, and lipids of varying geometrical properties. Most of these components do not bind the cargo. Here, we show that such “inert” components can be crucial for the precise control of cross-membrane trafficking. Using a statistical mechanics model and molecular dynamics simulations, we demonstrate that the presence of inert membrane components of small isotropic curvatures dramatically influences cargo endocytosis, even if the total spontaneous curvature of such a membrane remains unchanged. Our results suggest a robust and general method of controlling cargo trafficking by adjusting the membrane composition without needing to alter the concentration of receptors or the average membrane curvature. This study indicates that cells can prepare for any trafficking event by incorporating curved inert components in either of the membrane leaflets.

Refs:

Precision measurements of lipid membrane hydrodynamic drag

PHILIP JAHL (Presenter), RAGHUVEER PARTHASARATHY, Physics, University of Oregon — The hydrodynamic drag at a lipid bilayer determines, among other things, the flow properties of suspensions of cells and liposomes. For spherical liposomes or lipid vesicles, the Stokes equation relates the drag coefficient ζ to the radius r and the fluid viscosity η by ζ = Cπηr, where the dimensionless C depends on the hydrodynamic boundary between the sphere and the fluid. For solid spheres C=6 and for liquid spheres C=4. This constant has been assumed to be 6 for lipid membranes, but we have found no direct measurements of it, and given the fluidity of lipid membranes it is not obvious that the solid-sphere value applies. The Stokes-Einstein relationship D = kBT/(Cπηr), where D is the diffusion coefficient, kB is Boltzmann's constant, and T is the temperature allows determination of C provided D can be determined precisely. We use light sheet fluorescence microscopy to image lipid vesicles far from surfaces that complicate application of the Stokes-Einstein relationship. Combined with high-accuracy image localization, this allows us to measure C, finding that it closely matches the C=6 value of a solid sphere. We comment on deviations from C=6 for non-spherical vesicles with thermally driven undulations.

Shape Control of Deformable Nanocontainers by Modulating Surface Tension and Charge Patterning

VIKRAM JADHAO (Presenter), NICHOLAS BRUNK, Intelligent Systems Engineering, Indiana University Bloomington — Shape-reconfigurable polymeric vesicles, micelles and other soft-matter-based nanomembranes have important applications as adaptive drug-delivery carriers that change shape in response to external cues, and as dynamic building blocks for designing reconfigurable materials. The shape of these nanocontainers can be controlled by modulating their surface composition and environment. Molecular dynamics simulations are used to explore the role of surface tension and surface charge patterning in changing the shape of charged, elastic, volume-preserving nanocontainers. For homogeneously charged nanocontainers, sphere-to-rod-to-disk shape transitions are shown to be facilitated by decreasing surface tension; this could be realized by functionalizing the nanocontainer surface with surfactants. For inhomogeneous, hemispherically-charged Janus nanocontainers, transitions to hemispherical shapes are observed. Shape control of nanocontainers with inhomogeneous surface charge patterns characteristic of pH values near the pKa of the charged surface moieties is discussed. Robustness of shape transitions is investigated by including the effects of ions via mean-field models and explicit-ion simulations.

Morphology of toroidal vesicles

YIHAO LIANG (Presenter), Northwestern University, XIANGJUN XING, Shanghai Jiao Tong University, MONICA OLVERA DE LA CRUZ, Northwestern University — The equilibrium shapes of toroidal fluid vesicles have been studied for many years. Recently, a new class of stable nonaxisymmetric circular shapes has been observed both from experiment and simulation. This shape contains a necklace-like main ring, usually accompanied by buds. Using Monte Carlo simulation and theoretical analysis, we investigate the morphology of toroidal vesicle. Based on Delaunay unduloids we give a perturbative estimation of the properties of the main ring.

*This work is supported by the National Science Foundation through Awards 1720625 and 1753182.
4:30PM V63.00011: A  ORRIN SHINDELL (Presenter), Department of Physics & Astronomy, Trinity University, NATALIE MICA, School of Physics and Astronomy, University of St. Andrews, K KELVIN CHENG, Department of Physics & Astronomy, Trinity University, EXING WANG, Department of Cell Systems & Anatomy, University of Texas Health Science Center San Antonio, VERNITA GORDON, Department of Physics, University of Texas at Austin — We report on a complex fingering pattern that forms in an approximately 25μm-diameter circular lipid membrane adhered by biotin-avidin bonds to a solid supported membrane. The experiment involves applying tension to form a tear in the bound circular membrane. The pattern in the torn membrane then evolves as 1μm-scale pores form intermittently on the scale of tens of seconds at the boundary of the tear. As the pores form, the biotin-avidin bonds are laterally compressed. As the density of bonds increases, the width of the pores decreases linearly and the rate of new pore formation decreases exponentially. Finally, when the biotin-avidin bonds are compressed into a solid-like state, the process arrests leaving a complex finger pattern in the membrane. We show that these findings are consistent with a thermodynamic description of tension induced pore formation.

4:42PM V63.00012: Arbitrary Lagrangian–Eulerian finite element method for biological lipid membranes*
AMARESH SAHU (Presenter), YANNICK OMAR, University of California, Berkeley, ROGER SAUER, Aachen Institute for Advanced Study in Computational Engineering Sciences, RWTH Aachen University, KRANTHI K MANDADAPU, University of California, Berkeley — We present an arbitrary Lagrangian–Eulerian (ALE) finite element method for arbitrarily curved and deforming lipid membranes. We provide a formalism to determine the equations of motion governing lipid membrane behavior using an irreversible thermodynamic analysis of curved surfaces. We develop an ALE theory by endowing the surface with a mesh whose in-plane velocity is independent of the in-plane material velocity, and which can be specified arbitrarily. The general isoparametric finite element implementation of the theory, based on an arbitrary surface parametrization with curvilinear coordinates, is used to model lipid membranes in several biologically relevant situations. A new physical insight is obtained by applying the ALE developments to cylindrical lipid membrane tubes: though lipid membrane tubes are stable, in the limit of vanishing bending rigidity (the limiting case of a fluid film) we numerically and analytically find tubes to be unstable with respect to long-wavelength perturbations when their length exceeds their circumference.

* A.S. is supported by the Computational Science Graduate Fellowship from the U.S. Department of Energy.

4:54PM V63.00013: Stretching induced disk-to-ribbon transition of chiral colloidal membranes*
LEROY JIA (Presenter), Brown University, ANDREW J BALCHUNAS, MARK J ZAKHARY, Brandeis University, ZVONIMIR DOGIC, UC Santa Barbara, ROBERT ALAN PELOCVITS, THOMAS POWERS, Brown University — Colloidal membranes are fluid monolayers consisting of rod-like virus particles held together by the depletion interaction. When optical tweezers are used to apply a diametric stretching force, these disks transform into twisted ribbons. We measure the force and pitch as functions of membrane extension and identify three distinct regimes of twisting. Assuming that the bending stiffness of the membrane is large, we also calculate the shape of the membrane as it deforms using a purely geometric theory that effectively incorporates liquid crystal degrees of freedom.

*MRSEC-1420382 and CMMI-1634552

5:06PM V63.00014: Localization of flexural waves in randomly curved membranes  JONATHAN KERNES (Presenter), ALEXANDER JACOB LEVINE, Physics, Univ of California - Los Angeles — We consider the propagation of flexural waves across a thin membrane whose unstressed state has a quenched random geometry. Since the local curvature of the unstressed surface couples the mechanics of in-plane and out-of-plane displacements, flexural waves are scattered by these changes in the local geometry of the unstressed surface. Due to this effect we expect that flexural waves are localized by the random geometry of the surface. We investigate this localization phenomenon using the Donnell-Mushtari-Vlasov theory of membrane elasticity. We show that the energy density associated with flexural waves obeys a diffusion equation at long length and time scales. We observe that local curvature scatters flexural waves anisotropically, leading to a decrease in both the phase coherence length of the waves and the diffusion of their energy. Time-reversed interference corrections, i.e., coherent backscattering, is shown to reduce the diffusion coefficient logarithmically with system size, in agreement with general results for 2D localization. Finally, we consider a self-consistent calculation of the energy diffusion coefficient at high frequencies and use it to estimate the localization length.
FATEMEH AHMADPOOR (Presenter), GUIJIN ZOU, HUAJIAN GAO, School of Engineering, Brown University — Understanding the interaction of 2D materials including graphene-based nano-sheets, boron nitride and MoS2 with biological systems is a growing topic of interest to many applications such as biosensors, drug delivery, gene therapy and nanotoxicity. In this paper, we show that the interaction of 2D materials with cellular membranes at its early stage of approaching is dominantly controlled by entropic factors. Recent experiments indicate that graphene sheets, depending on their size, can either undergo a near-orthogonal cutting or a parallel attachment mode of interaction with cell membranes. Here we perform a theoretical statistical mechanics analysis as well as coarse-grained molecular dynamics simulations to characterize the entropic energy barrier for these modes of interactions. Our results indicate that micro-sized graphene sheets strongly prefer to approach cellular membranes through their sharp corners. In contrast, nano-sized sheets are likely to adhere to the membranesurface, instead of piercing through their sharp corners.

*We gratefully acknowledge financial support from the National Science Foundation through Grant No. CMMI-1562904.

Thursday, March 7, 2019 2:30 PM - 5:30 PM

Session V64 DBIO GSOFT: Robophysics: Robotics Meets Physics II

2:30PM V64.00001: Microrobots as robophysical models for the study of biomechanics and control of small animals

[Invited] ROB J WOOD (Presenter), Harvard University — This talk will highlight our recent work on the development of physical models for the exploration of structure-function relationships in small animals (primarily arthropods), and for the development of robots that exhibit similar capabilities. Examples include centimeter-scale legged robots that help uncover gait strategies for high speed and robust locomotion on planar surfaces and for vertical and inverted climbing; ultra-fast power amplification mechanisms that produce rapid strikes and jumps; and insect-like flapping-wing robots used as a testbed for studies of fluid mechanics and under-actuated flight control. These models are enabled by the use of a multi-scale, multi-material fabrication paradigm, high bandwidth micro actuators, and detailed analytical, numerical, and experimental investigations. Robot complexity (e.g., measured by actuated degrees of freedom) typically decreases with reduced size. Our methods, however, buck this trend and allow us to create fully-actuated physical models that mimic key features of the biomechanics of the organisms in question. Furthermore, these robots serve as platforms for experimentation with novel sensors, computation architectures, and power solutions that all must reconcile strict size, weight, and power limits of these bioinspired devices with the desire to achieve similar capabilities as the organisms they are inspired by.

3:06PM V64.00002: Physics of animal and robot locomotor transitions in complex terrain

RATAN SADANAND OTHAYOTH MULLANKANDY, GEORGE S THOMS, CHEN LI (Presenter), Johns Hopkins University — Robots are still poor at traversing complex terrain like earthquake rubble and construction sites for applications like search and rescue and structural examination. By contrast, animals move through nature by transitioning between different forms of movement. This is largely due to a lack of understanding of the physics of locomotor transitions in complex terrain. Here, we propose locomotion energy landscape as a framework for understanding how macroscopic, self-propelled, legged locomotors physically interact with terrain to probabilistically transition between locomotor modes. By integrating animal and robophysical experiments and physics modeling, we discovered that: (1) Different locomotor modes have different “terradynamic favorability”, measured by the potential energy barrier that must be overcome to traverse using each mode; and (2) Kinetic energy fluctuation from body vibration, induced by seemingly wasteful, oscillatory leg movement, helps animals and robots overcome mode-separating potential energy barriers and transition from less favorable to more favorable modes. Our study is a step in establishing terradynamics of locomotion in complex 3-D terrain. Such physics-based terrain traversal complements geometry-based obstacle avoidance and expands the reaches of robots.
Giving Fish Robots a Pulse: Implementing Bio-inspired Control Algorithms in Fish Robots

STEPHEN HOWE (Presenter), HENRY ASTLEY, Biology, University of Akron — Most fish use undulatory locomotion to control forward swimming and direction change relying heavily on their body and caudal fin to produce the motions. This style of locomotion allows for robust locomotion across aquatic environments. As such they have been models for designing autonomous under water vehicles (AUVs). To date, fish robots have been designed to maneuver using two basic modes of turning. The first is a waveform offset in which the frequency and amplitude of the oscillation remain unchanged, but the entire wave is biased to the right or the left, causing the fish to favor bending in one direction. The second is akin to the C-start maneuver in fish, in which a maximum amplitude deflection is simultaneously applied to all joints of the body to one side, interrupting the typical locomotor body oscillations. We developed a new turning model based on observations from high speed videos of live Giant Danio (*Devario aequipinnatus*). These videos show that maneuvers consist of propagating pulses of curvature. These pulses are independent events and can be modeled as a transient wave with a speed, amplitude, and width. Using a 3D printed robot, we will be evaluating the performance of the pulse model alongside the offset wave and C-start methods.

Classroom Robophysics: Methods for teaching bioinspired design

MARIANNE ALLEYNE (Presenter), AIMO A WISSA, University of Illinois at Urbana-Champaign — In our Bioinspired Design course, students work in interdisciplinary teams to design engineering solutions based on biological analogies. Teams study core physics principles that enable biological functions and build prototypes to mimic these principles for applications in wearable technologies and robotics. Lectures cover current research in the area of bioinspiration, and the different design concepts and tools that can be used for bioinspired design. In this paper, we detail the approach the students undertake to distil the core physics principles and how to use them to create mechanical prototypes. The ultimate goal of the prototypes is to either solve an engineering challenge using lessons from nature, or to use engineering tools to study a biological phenomenon. In the course we present pedagogical tools to help students compare multiple organisms with similar functions but different underlying physics. Students are then asked to brainstorm different embodiments based on learned physics principles. They then apply design evaluation tools to choose the most suitable embodiment to solve the problem they identified at the start of the course. Students use their prototypes to verify that they captured the enabling physics rather than simply copying the superficial function.

Fabricating Autonomous Machines for the Cellular Scale

MARC MISKIN (Presenter), ALEJANDRO CORTESE, ITAI COHEN, PAUL L MCEUEN, Laboratory of Atomic and Solid State Physics, Cornell University — This talk presents a new approach for fabricating cell-sized robots that can explore their environment, be manufactured en masse, and carry the full power of silicon-based information technology. We fabricate 10 to 100 um walking robots that are powered and controlled wirelessly using embedded silicon photovoltaics. Our robots walk using a new class of voltage controllable, electrochemical actuators made from nanometer thick membranes of platinum. These actuators impose low power requirements yet can carry loads ten thousand times their own weight. Moreover, actuation only requires 200 mV signals, facilitating straightforward integration with silicon microelectronics. Combine, these results present a broad platform that can unite mechanical systems, information processing and control into autonomous robots that operate at the cellular scale.

*We acknowledge funding from the army research office (ARO W911NF-18-1-0032), the Cornell Center for Materials Research DMR-1719875, NSF Grant DMR-1435829, Air Force Office of Scientific Research (AFSOR) MURI Grant FA2386-13-1-4118, and the Kavli Institute at Cornell for Nanoscale Science. The work was performed at Cornell NanoScale Facility, a member of the National Nanotechnology Infrastructure Network (NSF Grant ECCS-0335765).*
bacteria. The efficiency of the robot. This model robotic system can potentially help us understand the locomotion of living systems, e.g. resulting from the drag of granular medium. Finally, flagella of different geometrical shapes are explored to optimize the efficiency of the robot. This model robotic system can potentially help us understand the locomotion of living systems, e.g. bacteria.

*We acknowledge support from HSSEAS, University of California, Los Angeles.

4:06PM V64.00007: How to force an army of self-propelled mindless robots to act collectively? ANTOINE DEBLAIS (Presenter), Institute of Physics, University of Amsterdam, THOMAS BAROIS, THOMAS GUERIN, PIERRE-HENRI DELVILLE, REMI VAUDAIN, JUHO LINTUVUORI, JEAN-FRANÇOIS BOUDET, JEAN-CHRISTOPHE BARET, HAMID KELLAY, University of Bordeaux — We study assemblies of rodlike robots made motile through self-vibration. When confined in circular arenas, dilute assemblies of these rods act as a 2D gas of molecules. But above a critical surface fraction, some fraction of the bots line up in one or more tight clusters along the corral boundary while, in the bulk, gaslike behavior is retained. We find that the unified pushing of the cluster bots can drive collective motion: by selecting corrals that are deformable but free to move, we take advantage of surface cluster formation to force the robot army to work together.

KIRSTY WAN (Presenter), Living Systems Institute, University of Exeter, KELIMAR DIAZ CRUZ, YASEMIN OZKAN AYDIN, DANIEL GOLDMAN, Georgia Institute of Technology — Multi-legged animals exhibit several distinctive patterns of limb movements, or gaits. In most cases, rhythmic patterns of limb actuation are generated by neural circuits called central pattern generators (CPGs), which operate in the absence of external timing cues or higher-level input. However, the capacity to coordinate locomotion gaits is by no means a feature exclusive to vertebrates. Indeed, species of micron-sized, pond-dwelling algae were recently discovered to be capable of orchestrating the beating of their four whip-like flagella to produce swimming gaits reminiscent of the motor patterns of quadrupeds (Wan & Goldstein 2016). Here it is thought that coordination is driven by contractile elements within the algal flagellar apparatus, which fulfill the role of the vertebrate CPG. In order to understand this unique intracellular control of motility, we developed robots which modeled quadriflagellate swimming at low-Reynolds number, and systematically evaluated the hydrodynamic performance of distinct gaits, including the trot, pront, and gallop. Our results suggest a novel role of the algal cytoskeleton in providing mechanical stability during active flagellar beating.

*KYW acknowledges funding from the University of Exeter.

4:30PM V64.00009: Body compliance helps snake robots traverse large steps QIYUAN FU (Presenter), CHEN LI, Johns Hopkins University — Snake robots still struggle to traverse complex 3-D terrain such as earthquake rubble and construction sites. By contrast, snakes traverse similar terrain like mountains and forests at ease. In both cases, how well the body engages the terrain is critical to successful traversal. Here, we use robophysical experiments to test the hypothesis that body compliance helps better engage and traverse complex 3-D terrain. We developed a snake robot with one-way wheels capable of traversing a large step using a partitioned gait that we recently discovered in snakes. An adjustable suspension was added to the wheels to vary compliance between the body and terrain. When traversing steps as high as 35 ± 3 % body length (BL), higher compliance allowed the suspension to compress more (from 1.0 ± 0.3 mm to 2.1 ± 0.6 mm) to better maintain contact with ground below and above the step (from 81 ± 8 % to 87 ± 5 % of the body), which increased traversal probability (from 63 ± 19 % to 90 ± 0 %) at the cost of 12 ± 6 % more power consumption (P < 0.05, ANCOVA). For larger step height (40% BL), however, the larger compression increased the chance of the rigid body edges being caught by the step corner. This is a limitation of the discrete robot body and highlights the need for a continuum compliant body.
It is well known in thermodynamics that viscosity-like dissipation external and internal disturbances. We explore the extent to which a learning-based approach can generate strategies that are robust to dynamics of the environment, we posit that the agents can learn transition probabilities to achieve an optimal digging probabilities based on their sensed environmental information. By varying the learning rules that rely on the local tunnel density via contact sensing, the robots can excavate more effectively by adjusting their behavior transition duration and timing of robot-robot contacts correlates with tunnel density. We hypothesize that with the ability to deduce sensing capabilities so that each robot can distinguish different kinds of contact; preliminary results suggest that the tunnels, in which maximal robot activity enables high performance. We have now augmented the robots with contact distribution strategy in mitigating clogs and jams in congested environments. This contrasts with a strategy for spacious swarm experiments and numerical/theoretical models demonstrated the importance of this unequal workload approximately 30% of the workers performed 70% of the digging [Aguilar et al, PNAS 2015]. With data from sidewinders interacting with pegs embedded in sand and a robophysical model, we investigate a peg-snake interaction where the animal forms a static contact with the substrate at an anatomical point anterior to the peg. This interaction mode facilitates "squeezing" the posterior body sections past the peg. Using a copper foil wrapped peg and 7 capacitive sensors along the 14-joint robot, we tested passive and active obstacle-clearing control templates. Early data shows the robot actively clears a peg using an increase in lateral wave amplitude or a reversal turn. When setting the multiphase undulations to produce two wavelengths along the robot's body, the robot passively clears the peg if the peg interacts with a region of the robot's body closest the head. These results will generate hypotheses for control strategies based on muscle activation patterns involved in sidewinding (Jayne, J. exp. Biol. 1988).

Flying insects may achieve energy efficient flight by storing and releasing elastic energy in their thorax and muscle. Similarly, flapping wing micro-aerial vehicles (FWMAVs) may benefit from inclusion of elastic components in their actuation system. Despite significant investigation into the aerodynamics of flapping wings, the actuation of these movements through elastic structures in insects and robots is relatively unexplored. We have developed a dynamically-scaled robophysical experiment to study the dynamics of series-elastic flapping wings, with specific emphasis on discovering the role of linear and nonlinear elastic components in energy efficiency, perturbation resistance, and control. We vary system (elasticity) and actuation (amplitude and frequency) parameters and find that energy storage and recovery by an elastic element is dependent upon the stiffness of the element and upon the driving amplitude, frequency, and stroke profile. System response experiments suggest that the inclusion of series-elastic elements may have a negative overall effect on control capabilities. The results of the project will inform the design of future FWMAVs, providing insight into elastic element selection, power requirements, and control design.

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Viscous friction-like relationship arises from a simple Columb friction locomotion model

Learning Multi-agent Workload Distributions in Confined Excavation

5:18PM V64.00013: Learning Multi-agent Workload Distributions in Confined Excavation* KEHINDE AINA (Presenter), Georgia Institute of Technology, LEWIS CAMPBELL, Morehouse College, HUI-SHUN KUAN, Max Planck, M. BETTERTON, UC Boulder, DANIEL GOLDMAN, Georgia Institute of Technology — Our recent work with collective fire ant tunnel excavation revealed that approximately 30% of the workers performed 70% of the digging [Aguilar et al, Science 2018]. Complementary robot swarm experiments and numerical/theoretical models demonstrated the importance of this unequal workload distribution strategy in mitigating clogs and jams in congested environments. This contrasts with a strategy for spacious tunnels, in which maximal robot activity enables high performance. We have now augmented the robots with contact sensing capabilities so that each robot can distinguish different kinds of contact; preliminary results suggest that the duration and timing of robot-robot contacts correlates with tunnel density. We hypothesize that with the ability to deduce local tunnel density via contact sensing, the robots can excavate more effectively by adjusting their behavior transition probabilities based on their sensed environmental information. By varying the learning rules that rely on the local dynamics of the environment, we posit that the agents can learn transition probabilities to achieve an optimal digging performance. We explore the extent to which a learning-based approach can generate strategies that are robust to external and internal disturbances.

*NSF PoLS
2:30PM V65.00001: Amphiphilic nanoparticles can modify lipid membrane permeability*  
MUKARRAM TAHIR (Presenter), ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Lipid bilayers are the structural foundation of biological membranes and contain a characteristic hydrophobic interior that prevents passive permeation of water and other polar molecules. Proteins embedded in these membranes controllably modify these barrier properties by allowing selecting transport in response to environmental stimuli. Previous work from our group has demonstrated that a certain class of nanoparticles can assume a transmembrane configuration similar to these protein channels, and that charged ligands grafted to these nanoparticles can cross the hydrophobic interior of the membrane at an anomalous rate. In this work, we use molecular dynamics simulations to demonstrate that this ligand flipping behavior is associated with transient water transport across the membrane and can be exploited for altering the permeability of lipid membranes to water and charged solutes. Through a combination of free energy analysis and unbiased simulations, we reveal that this gating ability is sensitive to membrane tension, allowing these nanoparticles to function as synthetic mimics of mechanosensitive membrane channels, and have potential applications ranging from single-cell therapeutics to novel methods of water desalination.

*US DOE CSGF contract DE-FG02-97ER25308.

2:42PM V65.00002: Direct observation of topological turbulence in the oocyte membrane  
JINGHUI LIU (Presenter), TZER HAN TAN, PEARSON WHITEHEAD MILLER, MELIS TEKANT, Physics, Massachusetts Institute of Technology, JOERN DUNKEL, Mathematics, Massachusetts Institute of Technology, NIKTA FAKHRI, Physics, Massachusetts Institute of Technology — Living systems self-organize local interactions into global structures and dynamics. Despite prevalence of such features across biological entities, the underlying self-organization principles have not been fully understood. Here we report on direct observation of a class of biochemical patterns formed during early development in starfish oocytes. The observed patterns maintain long-live structures despite short molecular turn-over times, and each pattern has distinguishing wavelength and orientation in spite of sharing the same local interaction rules. Through field analysis, we find that phase singularity dynamics in the chemical field dominates evolution of observed patterns. The pair interactions between the point singularities drive topological turbulence in phase velocity field. Such topological turbulence shares the same characteristic vortex size across observed patterns, reminiscent of quantum turbulence feature. An Onsager vortex model with pairwise interaction potential captures the essential features of the experimentally observed phase singularity dynamics. We propose topological turbulence in phase velocity field underlies dynamics of the observed self-organized biochemical patterns, propagating order from local molecular to global cellular scales.

2:54PM V65.00003: Physical Models of Proton-Pumping Complexes of Mitochondria Membranes*  
LEV MOUROKH (Presenter), Physics, Queens College of CUNY, MICHELE VITTADELLO, Chemistry, Medgar Evers College of CUNY — The models are proposed for all three proton-pumping complexes. The model for Complex IV includes the electron source, electron drain, and three electron sites in between, as well as proton source, proton drain and three proton sites in between. Electon transport occurs along the inner mitochondria membrane and the protons are transferred across the membrane. The chemical potential of the electron source is larger than that of the electron drain, while the protons are pumped to the higher potential. The middle electron and proton sites are in the close proximity, so their electrostatic interaction facilitates the energy transfer. We suggest that in Complex I the energy exchange is mediated by the conformational changes. In both cases, we use the methods of condensed matter and statistical physics to derive quantum equations of motion for the electron and proton operators in the presence of protein environment and to calculate the electron and proton currents. In the model of the Complex III, we couple the equations of motion to phenomenological Langevin equation describing electron and proton transport by quinons.

*The authors acknowledge AFOSR for funding, grant # FA9550-16-1-0279
**3:06PM V65.00004: Nanovesicles versus Nanoparticle-Supported Lipid Bilayers: Differences in Equilibrium Structures and Properties Unraveled by Molecular Dynamics Simulations**

HAOYUAN JING (Presenter), YANBIN WANG, PARTH RAKESH DESAI, University of Maryland, College Park, KUMARAN RAMAMURTHI, National Cancer Institute, National Institute of Health, SIDHARTH DAS, University of Maryland, College Park — Molecular Dynamics (MD) simulations are conducted to unravel the equilibrium properties of the nanoparticle-supported lipid bilayers (NPSLBs) in atomistic details and the findings are compared with that of the similar-sized nanovesicles (NVs). Three key differences emerge. First, the NV is found to contain significantly larger number of lipid molecules in the outer layer/leaflet, while the NPSBL has equal number of lipid molecules in inner and outer layers. Second, for the NV the lipid molecules in the outer and inner layers showed identical diffusivities, while for the NPSBL the diffusivity of the lipid molecules in the outer layer was more than double than that of in the inner layer. Finally, the nanoconfined water (located in the cavity for the NV, while being present as a few layers between the inner leaflet and the NP core for the NPSBL) showed much lesser diffusivity for the NPSBL as compared to that for the NV. The findings will be key to better understand the structure of this important nanomaterial (namely NPSBL) with applications in a plethora of disciplines ranging from targeted drug and gene delivery to characterization of curvature-sensitive biomolecules.

*University-of-Maryland-National-Cancer-Institute Partnership for Integrative Cancer Research*

**3:18PM V65.00005: Microfluidic Generation of Giant Lipid Vesicles with Membrane Protein Reconstitution**

ANQI CHEN (Presenter), YUTING HUANG, DAVID A WEITZ, Harvard University — Giant unilamellar lipid vesicles (GUV) are clean experimental models to study the biophysical mechanisms of biomembranes and transmembrane proteins from a quantitative point of view. Traditional generation methods of GUVs like rehydration or electroswelling produce vesicles with a wide size and composition distribution. These drawbacks limit experiment accuracy, and thus hinder the capacity of experiments to validate theoretical models in lipid membrane biophysics. Here we present a microfluidic emulsion template method to generate monodispersed lipid vesicles with transmembrane protein reconstitution. Compared to other emulsion-templated methods, our protocol allows a wider range of lipid choices, eliminates the influence of residual solvents, requires a shorter incubation time for solvent evaporation, and supports fabrication of lipid vesicles with more complicated structures. Our method opens up opportunities for more quantitative lipid membrane-related experiments and are also potential candidates in synthetic biology constructions.

*We acknowledge NSF Collaborative Research Grant DMR-1705775 for supporting this project.*

**3:30PM V65.00006: Thermodynamic equilibrium of lipid mixtures on curved substrates**

PIERMARCO FONDA (Presenter), LUCA GIOMI, DANIELA JUTTA KRAFT, MELISSA RINALDIN, Leiden University — It has been known since long that thermodynamic stability of two-dimensional lipid mixtures is influenced by curvature. Inspired by recent experimental results on lipid membranes coated on colloidal scaffolds, we propose a simple and general framework for interpreting the phase diagram of inhomogeneous closed systems. When the critical behaviour of a system is affected by its shape, we further show how new thermodynamic states can arise in the phase diagram, where lipids are in a mixed phase yet exhibit strong lateral segregation. We prove how different types of inhomogeneous couplings must induce qualitatively different phenomena - such as a curvature dependent line tension - and thus provide a way to distinguish different types of curvature interactions.

**3:42PM V65.00007: Numerical simulations of intracellular membranes of high genus**

DAVID YLLANES (Presenter), Chan Zuckerberg Biohub, GEORGE LYKOTRAFITIS, Department of Mechanical Engineering, University of Connecticut, GREG HUBER, Chan Zuckerberg Biohub — Bilayer membranes within eukaryotic cells adopt dynamic geometries of extraordinary complexity and interdependency. Examples include the continuous vesicular traffic of the endocytic and secretory pathways, the layers of the Golgi apparatus, the inner membranes of mitochondria, and the sheets, tubes, and, indeed, the nuclear envelope itself, comprising the endoplasmic reticulum. Some of these have topological genus zero (or near zero) while others have very high genus.

We use a coarse-grained molecular dynamics (CGMD) model to study the mechanics of intracellular membranes with complicated geometries. In particular, we investigate the behavior of pores in sheets, and how junctions of sheets organize and interact.

*Simulations carried out on the Cierzo supercomputer (BIFI-ZCAM, Spain). We acknowledge funding by FIS2015-65078-C2-1-P (MINECO, Spain and FEDER, EU).
3:54PM V65.00008: Simulation of the passive permeation of potassium ion through phospholipid membranes: Thermodynamics and kinetics*  
ARMAN FATHIZADEH (Presenter), RON ELBER, University of Texas at Austin — Here we revisit the problem of passive ion permeation through a phospholipid membrane and find new rich mechanisms that were not captured in earlier investigations by introducing new coarse variables. Numerous experimental and simulation studies have been performed on passive permeation through membranes. Most of simulation studies only consider one reaction coordinate that is the vertical position of the center of mass of the permeant with respect to the center of mass of the membrane. However, when the permeant is positively charged, it interacts strongly with the phosphate groups and permeation is accompanied by significant distortions of the membrane. To model their distortion of the membrane, we introduce two new coarse variables: the minimal distances of the positively charged group from the phosphate groups of each leaflet. We illustrate the efficiency of this new set of coarse variables on permeation of a single potassium ion. Using Milestoning, we were able to calculate free energy landscape, mean first passage time, and the permeability of the ion in the space of the two new coarse variables. The results compared favorably to the available experimental data.

*We acknowledge NIH grants GM 059796, GM 111364, and Welch grant F-1896.

4:06PM V65.00009: Assembly of mechanosensitive channels can regulate whole cell volume*  
SMITHA HEGDE (Presenter), Centre for Synthetic and Systems Biology, School of Biological Sciences, University of Edinburgh, ALEXANDRU PARASCHIV, ANDELA SARIC, Department of Physics and Astronomy, Institute for the Physics of Living Systems, University College London, TEUTA PILIZOTA, Centre for Synthetic and Systems Biology, School of Biological Sciences, University of Edinburgh — E.coli's membrane embedded mechanosensitive channels (MSC) protect them from bursting when the intracellular osmotic pressure increases due to hyposmotic shock. MSC sense an increased membrane tension and respond by opening a large pore to passively let out cytoplasmic solutes. Using epifluorescence microscopy to look at single E.coli cells, we previously demonstrated that upon a hyposmotic shock cells rapidly swell due to water diffusion into the cytoplasm. Subsequently, MSC open to recover cell volume and osmotic pressure by solute efflux which lasted up to few minutes. Our phenomenological model explained the observed dynamics, however, could not capture large cell-to-cell variability. So, we propose a coarse-grained model which considers MSC dynamic aggregation and incorporate into the phenomenological model. Results suggests that MSC cluster at lower membrane tensions and disaggregate at higher membrane tensions, altering MSC's opening probability, which also depends on tension. Additionally, we constructed a hepta-mutant (all 7 MSC genes deleted) and show that upon hyposmotic shock, the mutant swells but fails to recover cell volume; we illustrate the cells' survivability and dynamics of death when they fail to restore internal pressure.

*Darwin Trust of Edinburgh and IBioIC

4:18PM V65.00010: Membranes and Machine Learning: Designing a Model of Antibiotic Activity to Bypass Gram Negative Membranes and Efflux Pumps  
RACHAEL MANSBACH (Presenter), CESAR LÓPEZ, NICOLAS HENGARTNER, Theoretical Biology and Biophysics, Los Alamos National Lab, HELEN ZGURSKAYA, Chemistry and Biochemistry, University of Oklahoma, S GNANAKARAN, Theoretical Biology and Biophysics, Los Alamos National Lab — Due to the growing prevalence of antibiotic-resistant bacteria, there is a pressing need for rapid design of new antibiotics with unique modes of action. Gram negative bacteria in particular pose a thorny problem for antibiotic design due to the combined effects of their impermeable outer membranes and their antibiotic-removing efflux pumps. We employ a combined theoretical and experimental approach to understand the limiting factors on antibiotic efficacy in *P. aeruginosa* and rationally design experiments to rapidly zero in on promising antibiotic candidates. By using machine learning to identify a relevant subset of descriptors produced by simulation and experiment for predicting experimentally-measured minimum inhibitory concentrations of different antibiotic candidates, we are able to learn a self-consistent model of antibiotic retention based on a simple kinetic approximation. We separately employ a Gaussian process regressor to direct a search for antibiotic candidates with optimal experimental and simulated properties. This work leads to heightened understanding of the qualities important to antibiotic retention in Gram negative bacteria and offers a simple way to narrow the experimental design space of antibiotic candidates, allowing for rapid, high-throughput screening.
4:30PM V65.00011: Diffusion Rate of Cholesterol through a Single Lipid Bilayer* YANGMINGYUE LIU, MICHAEL STANFIELD (Presenter), NETI BHATT, ARTHUR RALKO, WONWHA CHO, JUSTIN LORIEAU, URSULA PEREZ-SALAS, University of Illinois at Chicago — Our lab has measured the rate and energetics of the intramembrane diffusion (flip-flop) of the steroid-lipid cholesterol using small angle neutron scattering (SANS) and found that the diffusion rate was much slower (hundreds of minutes) than the accepted value (under a second). Our work showed that the discrepancy was due to artifacts produced by differences between cholesterol and its analogues or by the use of compounds, like cyclodextrin, that, our group argued, disrupts the membrane. Our results were based on measurements in which cholesterol flip-flop within the membrane occurred while cholesterol was also diffusing between different membranes (exchange). So, our team has been taking steps to eliminate exchange from the measurement, thus measuring the flip-flop diffusion rate directly. We used a new method to craft an asymmetric distribution of cholesterol in the lipid bilayers of unilamellar vesicles to measure the rate at which cholesterol diffuses through the bilayer. We used orthogonal cholesterol sensors, nuclear magnetic resonance spectroscopy (NMR), and SANS in order to follow the change of cholesterol’s distribution within the bilayers as a function of time and temperature.

*We thank CAREER award DMR-1753238 and UIC’s LASURI award for funding.

4:42PM V65.00012: Real-time measurements of lipid domain rearrangements, membrane thickness, and intermembrane forces during membrane hemifusion* KAI KRISTIANSEN (Presenter), DONG WOOG LEE, University of California, Santa Barbara, STEPHEN DONALDSON, Physics, Ecole Normale Superieure, NICHOLAS CADIROV, University of California, Santa Barbara, XAVIER BANQUY, Pharmacy, Universite de Montreal, JACOB ISRAELACHVILI, University of California, Santa Barbara — We have developed a Fluorescence Surface Forces Apparatus (FL-SFA), which can fluorescently image the surfaces while measuring interaction forces and distance between surfaces in real-time. Using the FL-SFA, hemifusion of two supported model lipid bilayers was monitored. At the membrane-membrane contact, the localization of liquid disordered phases and depletion of liquid ordered domains are observed during lipid membrane hemifusion. Interaction forces and lipid membrane thicknesses are simultaneously measured together with the fluorescence images of model membranes. The results show that the domain rearrangements decrease the energy barrier to fusion illustrating the significance of dynamic domain transformations in membrane fusion processes. Importantly, the FL-SFA can unambiguously correlate interaction forces and in situ imaging in many dynamic interfacial systems.

*This study was research-supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-87ER-45331.

4:54PM V65.00013: Influence of Pressure-Induced Fluid Flow on DNA Translocation Dynamics in Solid-State Nanopores* KUN LI (Presenter), DEREK STEIN, Brown University — We studied the translocation dynamics of DNA through solid-state nanopores under the influence of an electrokinetic driving force and a pressure-driven fluid flow. Through the use of long, λ-DNA molecules, we sought to probe conformation-dependent translocation modes that were not observable in the pioneering experiments of Lu et al. (Nano Lett. 2013 Jul 10; 13(7): 3048–3052) on short molecules. We fabricated nanopores in 10-nm thick SiN membrane using the controlled dielectric breakdown (CBD) technique, which gave useable nanopores about 90% of the time. Then a pressure difference was applied across the nanopore to provide a drag force to counter the electrokinetic driving force. We monitored the disruptions of the ionic current through the nanopore and studied the influence of the applied pressure on the distribution of translocation times and the integrated charge deficits (ECDs) of λ-DNA translocations. We present the results of measurements with applied pressures ranging from 0 to 300 kPa and a theoretical analysis that models the initial polymer configurations and the fluid and electrokinetic force profiles.

*This work was supported by NSF Grant DMR-1505878.
**5:06PM V65.00014: Improving membrane protein expression by optimizing simulated integration efficiency**

MICHIEL NIESEN (Presenter), Chemistry, MIT, THOMAS MILLER, Caltech — Integral membrane proteins (IMPs) are critical for the transport of information and matter across the cell membrane. However, their study is often hindered by difficulties in obtaining sufficient purified IMP using heterologous overexpression.

Co-translational insertion into the cell membrane via the Sec translocon is a key step in the production of IMPs. However, both experimental and computational studies of this process are difficult due to the role of long-timescale non-equilibrium dynamics during ribosomal translation. We have developed a coarse-grained molecular dynamics (CGMD) approach that is capable of reaching experimentally relevant (i.e. minute) timescales, while retaining the level of detail required to capture the effect of individual amino-acid substitutions.

Using a combination of simulations of IMP integration and experimental quantification of IMP expression levels; we demonstrate a link between the efficiency of IMP integration into the cell membrane and IMP expression, yielding a powerful tool for the rational prediction of sequence modifications that improve expression.

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**5:18PM V65.00015: A Biophysical Model of Intermediate Phases in Developing Cell Plates.**

MUHAMMAD ZAKI JAWAID (Presenter), GEORGIA DRAKAKAKI, DANIEL LEE COX, University of California, Davis — Plant cell cytokinesis is a fascinating process that involves the formation of a cell plate via a homotypic fusion of vesicles. Cell plate formation depends on organized vesicle delivery, accumulation, fusion, and membrane maturation, along with the timely deposition of polysaccharides such as callose, cellulose, and cross-linking glycans. One unanswered question is the role of callose in cell plate formation.

We hypothesize that callose deposition produces an anisotropic driving force that acts along the periphery of the cell plate. A biophysical model based on the Helfrich general shape equation is presented to explain flat regions within the developing cell plate. The increase in callose deposits is reflected in the increase of membrane area and the anisotropic driving force. By postulating a force per callose polymer of 0.25-0.3pN, as well as an osmotic pressure difference of 0.01MPa and a finite surface tension of 0.0014N/m, we can achieve stable disks of radius 80-100nm, in agreement with observed sizes corresponding to intermediate stages of plate development.

References:


*This work was supported by the NSF MCB Grant No.1818219 to G.D., D.L.C., and M.Z.J.*

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**Thursday, March 7, 2019 2:30 PM - 5:30 PM**

**Session V66 DBIO: Microbial and Viral Quantitative Evolution**

BCEC 261 - Ariel Amir, Harvard University - **Focus**

**2:30PM V66.00001: RNA virus evolution and the predictability of next year's flu**

[Invited] RICHARD NEHER (Presenter), Biozentrum, University of Basel — RNA viruses like HIV of influenza virus evolve rapidly and thereby evade human immunity. We have performed whole genome deep sequencing of longitudinal samples spanning 5-10 years from acute to chronic HIV infection. From these data, we estimate the landscape of fitness costs at every nucleotide in the genome and characterize the the complex dynamics of immune escape and reversion. Similarly, influenza viruses change their antigenic properties rapidly and the seasonal influenza vaccine needs to be updated whenever the viruses change antigenically. We show how sequence data can be used predict which influenza virus variants are most likely to succeed and circulate in future seasons. These predictions use theoretical insights into the structure of genealogies of rapidly adapting populations and are provided in near real-time at nextflu.org.
3:06PM V66.00002: Single nucleotide mapping of locally accessible trait space in evolving yeast [Invited]  
YUPING LI, Genetics and Biology, Stanford University, GAVIN SHERLOCK, Genetics, Stanford University, DMITRI PETROV (Presenter), Biology, Stanford University — Tradeoffs constrain the improvement of performance of all traits simultaneously. Such tradeoffs define a Pareto optimality front that represents a set of optimal individuals that cannot be improved in any one trait without reducing performance in another trait. While widely assumed, direct experimental evolutionary approaches often fail to detect tradeoffs with many experiments generating individuals that improve performance in all measured traits. Moreover, even when an improvement in one trait is found to be associated with the loss of performance in another, it is hard to establish that such a negative correlation is not induced by the specific features of sampled mutations and that other possible adaptive mutations cannot escape such apparent tradeoffs. Here we detect tradeoffs and define the Pareto optimality front in the context of short-term evolution of *S. cerevisiae* in glucose-limited media. We have evolved barcoded yeast populations under several conditions, with each condition selecting for improved performance in different parts of the yeast growth cycle. By isolating hundreds of adaptive clones and quantifying their performances in each growth part of the cycle, we defined tradeoffs between performances in fermentation and respiration and respiration and stationary phase. Importantly, due to the large numbers of the studied clones we were able to claim that no single point mutation in the yeast genome can improve the performance beyond either of the defined optimality fronts. We found that in both cases the shape of the optimality front is convex suggesting the possibility of short term evolution to select for generalists. Finally, by sequencing hundreds of adaptive clones, we identified the molecular basis underlying identified trade-offs and revealed novel targets of adaptation.

3:42PM V66.00003: Tracking pathogenetic bacteria at the plasmid, genome, and pan-genomic level.*  
NICHOLAS NOLL (Presenter), RICHARD NEHER, Biozentrum, University Basel — The rapid global increase of multidrug-resistant organisms presents a major global health threat that will dramatically reduce the efficacy of antibiotics and thus constrain the number of effective treatments available to patients. As opposed to analogous efforts in viral epidemiology, accurate reconstruction of the pandemic spread of antibiotic resistance remains intractable for reasonable sample sizes due, in large part, to the high rate of homologous recombination and horizontal gene transfer that prevents the application of traditional phylogenetic approaches. Lastly, complete assemblies are a prerequisite to such quantitative study.

In this talk, I will present a novel computational framework for bacterial evolution that generalizes the traditional linear reference genome to a pan-genomic non-planar graph. Using this framework, I will analyze 120 antibiotic resistant genomes collected in Basel, Switzerland over the course of a decade, sequenced with both ONT and Illumina data. We show that the evolution of antibiotic resistance exhibits a nested doll structure in which genetic transposition, homologous recombination, and clonal expansion occur at similar time-scales.

*University of Basel

3:54PM V66.00004: Investigating the role of hemagglutinin protein stability in influenza A evolutionary dynamics*  
CHADI SAAD-ROY (Presenter), Lewis-Sigler Institute for Integrative Genomics, Princeton University, YIGAL MEIR, Department of Physics, Ben-Gurion University of the Negev, BRYAN T GRENFELL, SIMON LEVIN, Department of Ecology and Evolutionary Biology, Princeton University, NED WINGGREEN, Lewis-Sigler Institute for Integrative Genomics, Princeton University — Influenza A viruses (IAVs) cause a significant burden to human populations. They are notable for their rapid evolution arising from error-prone RNA polymerases in conjunction with selective pressures from hosts. Most host immune responses target the surface protein hemagglutinin (HA) and typically generate lifelong antibodies to seen strains. Thus to survive, IAVs must undergo mutations in HA that allow immune escape, while the HA protein must also satisfy functional constraints. We formulate a mathematical model of IAV evolution and transmission that spans scales from molecular to population processes. We couple models for HA protein thermal stability, mutation, and cross-immunity with a population-level model for the spread of infection, and characterize the effects of stability. Certain residues buried in the core of the HA protein may affect stability but not immunogenicity. We adapt our model to include these "buried" residues, and evaluate their influence on viral diversity, transmission, and evolutionary dynamics.

*We acknowledge funding from National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030), James S. McDonnell Foundation, Bill and Melinda Gates Foundation, and Natural Sciences and Engineering Research Council of Canada.
4:06PM V66.00005: Dynamics of lineage diversity during adaptation to weak antibiotic pressure

MICHAEL MANHART (Presenter), Harvard University and ETH Zurich, JESSE LERNER, WERONIKA JASINSKA, Ben-Gurion University of the Negev, ADRIAN SEROHJOS, University of Montreal, SHIMON BERShteIN, Ben-Gurion University of the Negev —

Tracking low-frequency lineages in large microbial populations is key to fully elucidating their evolutionary dynamics, especially under weak selection pressures and short time scales. However, resolution is often limited by methods for labeling lineages or whole-genome sequencing. To overcome this challenge, we introduce a large library of random DNA barcodes into *E. coli*, allowing us to track lineages down to tens or hundreds of cells. We observe two distinct phases of lineage dynamics during adaptation to low levels of antibiotics. During the first phase, the diversity of lineages undergoes a rapid and predictable drop which is characteristic of the drug and concentration. In particular, we find that low amounts of trimethoprim actually slow down the loss of diversity compared to the absence of drug. This initial loss of diversity appears to be driven by selection on standing genetic variation, leading to groups of lineages rising or falling together both within and between populations. During the second phase of dynamics, new mutations arise on these lineages, leading to clonal interference. Lineage diversity then stabilizes at a low but nonzero level, which appears to be universal across conditions despite the variation in initial dynamics.

4:18PM V66.00006: Testing the Retroelement Invasion Hypothesis for the Emergence of the Ancestral Eukaryotic Cell

GLORIA LEE, NICHOLAS SHERER, NEIL KIM, DAVNEET KAUR, K MICHAEL MARTINI, CHI XUE, NIGEL GOLDENFELD, Physics, University of Illinois at Urbana-Champaign, THOMAS KUHLMAN (Presenter), Physics and Astronomy, University of California Riverside —

Phylogenetic evidence suggests that the ancestral eukaryotic cell emerged as a result of invasion and proliferation of retroelements, selfish mobile genetic elements that copy and paste themselves within a host genome. Here we test this hypothesis by determining the pressures retroelements exert on simple genomes. We transferred two retroelements, human LINE-1 and the bacterial group II intron LL1.LtrB, into bacteria, and find that both are functional and detrimental to growth. We find, surprisingly, that retroelement lethality and proliferation is enhanced by the ability to perform eukaryotic-like nonhomologous end-joining (NHEJ) DNA repair. We show that the only stable evolutionary consequence in simple cells is maintenance of retroelements in low numbers, and that retrotransposition in eukaryotes must be finely tuned to allow proliferation.

*This work was supported by the NSF Center for the Physics of Living Cells (PHY 1430124), the Alfred P. Sloan Foundation (FG-2015-65532), and the Institute for Universal Biology, through partial support by the NASA Astrobiology Institute (NAI) under Cooperative Agreement No. NNA13AA91A. GL is supported by the National Science Foundation Graduate Research Fellowship Program under Grant Number DGE-1144245.

4:30PM V66.00007: Physical Constraints on Epistatic Interactions

KABIR HUSAIN (Presenter), ARVIND MURUGAN, James Franck Institute —

Epistasis, or the context-dependence of mutations, makes evolutionary trajectories difficult to predict. Here, we argue that knowledge of the physics of a system can tame its apparent evolutionary complexity. We focus on proteins, inspired by recent work on low-energy mechanical modes of bio-inspired, functional mechanical networks. Mutations in the sequence of a protein affect its shape, thereby modulating the effect of subsequent mutations; we find epistatic interactions at all probed orders. However, the structure of deformations limits the number of independent epistatic parameters. We find that such constrained epistasis is reflected in the topology of the fitness landscape. In addition to providing a mechanistic basis for experimentally observed epistatic couplings in proteins, we demonstrate how similar considerations may constrain epistasis in other complex systems.

*KH is supported by a James S McDonnell Foundation postdoctoral fellowship; AM acknowledges support from the Simons Foundation.

4:42PM V66.00008: Effects of clonal interference on adaptation in a fixed fitness landscape

YIPEI GUO (Presenter), ARIEL AMIR, Harvard University —

Adaptation in a fixed environment, where as a population evolves its fitness increases, is typically thought of as a hill climbing process on a fitness landscape. On a fitness-parameterized landscape, the fitness trajectory depends on the statistics of mutation effects and how they vary with current fitness ('macroscopic epistasis'). Results on fitness-parameterized landscapes are typically obtained in the strong selection, weak mutation regime, where mutations fix or go extinct sequentially. In a large population, while the phenomenon of clonal interference is known to slow down the rate of evolution, it is unclear how the shape of the fitness trajectory is affected. Here, we investigate the effects of clonal interference on fitness evolution on various fitness landscapes, including ones that explicitly takes into account microscopic epistasis between mutation sites.
Disentangling effects of genetic linkage on estimates of selection in intrahost HIV evolution
MUHAMMAD S SOHAIL, Department of Electronic and Computer Engineering, Hong Kong University of Science and Technology, RAYMOND H Y LOUIE, University of New South Wales, Kirby Institute, MATTHEW R MCKAY, Department of Electronic and Computer Engineering, Hong Kong University of Science and Technology, JOHN BARTON (Presenter), Department of Physics and Astronomy, University of California, Riverside — The evolutionary history of a population contains information about the underlying forces driving population diversity and adaptation. However, it is difficult for current methods to disentangle the effects of individual mutations from complex evolutionary dynamics. Here we describe a method to infer selection from genetic time-series data while also accounting for the confounding effects of genetic linkage, using a path integral approach based in statistical physics. We apply this method to investigate within-host HIV-1 evolution at the half-genome scale. Our approach reveals selective pressures for escape from human immune responses. Due to clonal interference between escape mutants, we find that accounting for genetic linkage is crucial to infer realistic estimates of selection. Our ability to account for genetic linkage is also critical for insight into complex evolutionary scenarios, highlighted by a struggle for dominance between co-infecting strains of the virus in an individual who ultimately develops broadly neutralizing antibodies.

Dynamics of within-host evolution and strain replacement in the human gut microbiome
BENJAMIN GOOD (Presenter), Physics and Bioengineering, University of California, Berkeley, NANDITA R GARUD, Gladstone Institutes, OSKAR HALLATSCHEK, Physics and Integrative Biology, University of California, Berkeley, KATHERINE S POLLARD, Gladstone Institutes — The human gut contains trillions of rapidly reproducing bacteria, making it a potential hotbed of within-host evolution. While the species-level dynamics in the gut have been extensively studied, we currently know very little about the evolutionary dynamics that take place within individual species. In this talk, I will discuss our recent efforts to measure the statistical properties of within-host evolution from a large panel of human gut metagenomes. Our analysis shows that on short timescales, genetic differences are only rarely caused by the invasion of distantly related strains. Resident strains more commonly acquire putative evolutionary changes, in which small numbers of nucleotide variants or gene content differences rapidly sweep to high frequency within a host. However, comparisons of adult twins suggest that strain replacement eventually overwhelms evolution over multi-decade timescales, hinting at fundamental limits to the extent of local adaptation. Together, our results show that gut bacteria can evolve on human-relevant timescales, and they provide key empirical constraints necessary for future modeling efforts.

Tuning Evolution Towards Generalists Through Resonant Environmental Cycling
VEDANT SACHDEVA (Presenter), Graduate Program in Biophysical Sciences, University of Chicago, KABIR HUSAIN, James Franck Institute, University of Chicago, SHENSHEN WANG, Department of Physics and Astronomy, University of California, Los Angeles, ARVIND MURUGAN, James Franck Institute, University of Chicago — Natural environments can present diverse fitness pressures, but some genotypes remain fit across a wide range of challenges. Such 'generalist' genotypes can be hard to evolve because there may be entropic or absolute fitness costs relative to specialist genotypes. Here, we study the conditions under which time-dependent evolutionary protocols stabilize generalists even when static protocols fail. We find that cycling environments on timescales tuned to match fixation times can reliably evolve generalists when the landscape is too rugged, or deleterious selection too adverse, for static protocols to succeed. We discuss 'chirp' protocols that circumvent the need for protocol fine-tuning. Our work reveals regimes in which time-dependent 'seascapes' can find and stabilize populations around genotypes that are fundamentally unstable in any static protocol.

*KH thanks the James S McDonnell Foundation for support via a postdoctoral fellowship.

Thursday, March 7, 2019 2:30 PM - 5:30 PM
Session V69 APS/SPS: Careers in Physics Workshop BCEC 052A - Tag(s): Careers, Undergraduate
2:30PM V69.00001: Careers in Physics Workshop — In this informative workshop, celebrated career coach and author Peter Fiske provides advice and strategies for taking your physics job search to the next level, including tips for self-assessment, network building, resume writing, interviewing, and salary negotiation. Don't miss this great opportunity to get some help with taking your next steps. This workshop is free, but please RSVP (https://goo.gl/xzWa6Z).

Thursday, March 7, 2019 5:45 PM - 6:57 PM
Session W70 APS: Nobel Prize Session BCEC Ballroom East/West - Roger Falcone, APS Past President; Univ of California - Berkeley - Tag(s): Invited, Undergraduate
5:45PM W70.00001: From Nonlinear Optics to High-Intensity Laser Physics [Invited]  DONNA STRICKLAND (Presenter), University of Waterloo — With the invention of lasers, the intensity of a light wave was increased by orders of magnitude leading to new phenomena being observed like violet light coming out when red light went into the material. The laser intensity increased dramatically again with the development of Chirped Pulse Amplification, which created short, intense pulses of light that kicked electrons off their atoms. This new high-intensity laser matter interaction lead to new laser machining techniques that are now commonly used in eye surgery.

6:21PM W70.00002: Passion Extreme Light [Invited]  GERARD MOURO (Presenter), Ecole Polytechnique — Extreme-light laser is a universal source providing a vast range of high energy radiations and particles along with the highest field, highest pressure, temperature and acceleration. It offers the possibility to shed light on some of the remaining unanswered questions in fundamental physics like the genesis of cosmic rays with energies in excess of $10^{20}$ eV or the loss of information in black-holes. Using wake-field acceleration some of these fundamental questions could be studied in the laboratory. In addition, extreme-light makes possible the study of the structure of vacuum and particle production in "empty" space which is one of the field's ultimate goal, reaching into the fundamental QED and possibly QCD regimes. Looking beyond today's intensity horizon, we will introduce a new concept that could make possible the generation of attosecond-zeptosecond high energy coherent pulse, de facto in x-ray domain, opening at the Schwinger level, the zettawatt, and PeV regime; the next chapter of laser-matter interaction.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X01 DCMP: Integer Quantum Hall Effect BCEC 106

8:00AM X01.00001: Landau Velocity for Collective Quantum Hall Breakdown in Bilayer Graphene*  HOLGER GRAEF (Presenter), WEI YANG, Laboratoire Pierre Aigrain, Paris, France, XIAOBO LU, GUANGYU ZHANG, Beijing National Laboratory for Condensed Matter Physics, Beijing, China, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Tsukuba, Japan, ADRIAN BACHTOLD, ICFO, Barcelona, Spain, EDWIN HANG TONG TEO, Nanyang Technological University, Singapore, EMMANUEL BAUDIN, ERWANN BOCQUILLON, GWENDAL FÈVE, JEAN-MARC BERROIR, Laboratoire Pierre Aigrain, Paris, France, DAVID CARPENTIER, ENS Lyon, Lyon, France, MARK OLIVER GOERBIG, Université Paris Saclay, Orsay, France, BERNARD PLAÇAIS, Laboratoire Pierre Aigrain, Paris, France — Breakdown of the integer quantum Hall effect (QHE) is associated with an electric field approaching the inter-Landau-level (LL) Zener field, ratio of the Landau gap and the cyclotron radius. The intrinsic Zener limit, corresponding to critical drift velocity, is reported here [1] using high-mobility bilayer graphene and high-frequency shot noise [2] over a large number of LLs. The steep onset of shot noise at breakdown, exhibiting super-Poissonian Fano factors, shows that collective excitations arising from electron-electron interactions are essential. The breakdown mechanism can be described by a Landau critical velocity limited by the excitation of large momentum magneto-excitons, in analogy with the roton mechanism of superfluids [3]. The fractional QHE counterpart would involve magneto-rotons [4].


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8:12AM X01.00002: Stabilizing a SQUID-based amplifier in high magnetic fields*  VIDHI SHINGLA (Presenter), Purdue University, ETHAN KLEINBAUM, LOREN PFEIFFER, KENNETH WEST, Electrical Engineering, Princeton University, GABOR CSATHY, Purdue University — dc SQUID-based circuits, when connected to sources exposed to strong magnetic fields, are often unstable in their fluxed-locked mode. We present a low noise SQUID-based current amplifier, which is unconditionally stable with a source exposed to magnetic fields up to 10 T.

Stability is achieved by inserting a four-pole low-pass filter between the source and the current amplifier. With this circuit, we demonstrate Johnson noise measurements below 1 K for source impedances in the kΩ range subjected to strong magnetic fields. We also discuss preliminary high-resolution thermal transport data in a two-dimensional electron gas confined in GaAs/AlGaAs.

*The work at Purdue was supported by the NSF grant DMR-1505866. L.N.P. and K.W.W. acknowledge the Gordon and Betty Moore Foundation Grant No. GBMF 4420, and the National Science Foundation MRSEC Grant No. DMR-1420541.

8:24AM X01.00003: Andreev reflection at the interface with an oxide in the quantum Hall regime*  YUSUKE KOZUKA (Presenter), National Institute for Materials Science, ATSUSHI SAKAGUCHI, The University of Tokyo, JOSEPH FALSON, Max-Planck Institute, ATSUSHI TSUKAZAKI, Tohoku University, MASASHI KAWASAKI, The University of Tokyo — Quantum Hall/superconductor junctions have been an attractive topic as the two macroscopically quantum states join at the interface. Despite longstanding efforts, most semiconductors hosting high-mobility two-dimensional electron systems (2DES) usually form Schottky barriers at the metal contacts, preventing efficient proximity between the quantum Hall edge states and Cooper pairs. In this study, we propose another material system for investigating 2DES/superconductor junctions, that is ZnO-based heterostructure. Due to the ionic nature of ZnO, a Schottky barrier is not effectively formed at the contact with a superconductor MoGe, as evidenced by the appearance of Andreev reflection at low temperatures. With applying magnetic field, while clear quantum Hall effect is observed for ZnO 2DES, conductance across the junction oscillates with the filling factor of the quantum Hall states. We find that Andreev reflection is suppressed in the well-developed quantum Hall regimes, which we interpret as a result of equal probabilities of normal and Andreev reflections as a result of multiple Andreev reflection at the 2DES/superconductor interface.

*This work was supported by JST, PRESTO Grant Number JPMJPR1763 and JST, CREST Grant Number JPMJCR16F1, Japan.

8:36AM X01.00004: Graphene in a Uniform Magnetic Field*  ANKUR DAS (Presenter), RIBHU KAUL, GANPATHY N MURTHY, University of Kentucky — We study monolayer graphene in a uniform magnetic field in the absence and presence of interactions. In the non-interacting limit for 1/q flux quanta per unit cell, the central two bands have 2q Dirac points in the Brillouin zone for nearest neighbor hopping. The Dirac points can be gapped out with a 2nd nearest neighbor hopping ($t_2$) and the central two bands pick up large Chern numbers. If we break the inversion symmetry by introducing a staggered potential ($m$) Chern number of the central bands becomes 1. Competition between $t_2$ and $m$ leads to a topological phase transition.

In the case of interacting graphene, there are at least three different competing phases when we consider Hubbard interaction and nearest neighbor spin-spin interaction. In the continuum limit, the theory has been studied before. It has been found that there exist four competing phases namely, ferromagnetic, antiferromagnetic, charge density wave, and Kekule distortion phase[1]. In our study, we attempt to understand all the phases in the lattice model. We investigate if there are phases in the lattice model not found in the continuum limit.


*We thank NSF DMR-1611161 & DMR-1306897
8:48AM X01.00005: Edge excitations in the 2D electron gas at \( v=2 \)

AMARTYA SAHA (Presenter), GANPATHY N MURTHY, University of Kentucky — Edge reconstruction for the 2D electron gas in a magnetic field at \( v=2 \) has been studied by Dempsey, Gelfand, and Halperin[1], who found that when the confining potential is softened the two spin polarized channels spatially separate. In this project we study the collective excitations both in the bulk and the edge at \( v=2 \) using the time dependent hartree fock (TDHF) method. We find that beyond a certain slope of the edge potential both the spin-wave and the charged excitations have instabilities. This analysis is similar to what Franco and Brey[2] did for the \( v=1 \) edge, where they showed that there are other phases (spin textured and charge density wave) with lower energy than the earlier proposed stripe phase by Chamon and Wen[3]. Finally, we will look for translation-symmetry-breaking ground states with lower energy than the one proposed in ref. 1 using Hartree-Fock methods.


9:00AM X01.00006: Boundary critical behavior of the integer quantum Hall transition

MARTIN PUSCHMANN (Presenter), Department of Physics, Missouri University of Science and Technology, PHILIPP CAIN, MICHAEL SCHREIBER, Institute of Physics, Chemnitz University of Technology, THOMAS VOJTA, Department of Physics, Missouri University of Science and Technology — We recently performed a high-accuracy study of the integer quantum Hall transition for a microscopic model of non-interacting disordered electrons: Based on a recursive Green function approach, we investigated the electronic wave functions in the lowest Landau band of a tight-binding model on a simple square lattice. To determine the bulk critical behavior, we employed lattices with the topology of an infinite cylinder [1].
Here, we consider quasi-one-dimensional lattices with the topology of an infinite strip, i.e., open boundary conditions. Edge states can expand along the entire rim of the system. They can undergo a boundary localization-delocalization transition. We investigate its critical behavior in the lowest Landau band and compare it with previous works. Additionally, we study the localization-delocalization transitions in the lowest Landau band of two-dimensional topologically disordered random Voronoi-Delaunay lattices [2].


*This work was supported in part by the NSF under Grant Nos. DMR-1506152 and DMR-1828489.

9:12AM X01.00007: Black Hole Phenomena in Quantum Hall Systems 1: Quasinormal Modes

VARSHA SUBRAMANYAN (Presenter), SURAJ HEGDE, SMITHA VISHVESHWARA, BARRY BRADLYN, University of Illinois at Urbana-Champaign — Point contact geometries in quantum Hall systems have formed excellent probes of quasiparticle scattering. Here, we demonstrate how they can access quasinormal modes – temporally decaying excitations – which are hitherto unexplored in QH settings. On the astronomical scale, quasinormal modes are one of the characteristic signatures of black holes and have played a key role in the recent LIGO detection of black hole mergers. We show how lowest Landau level physics in the presence of a saddle potential, such as at a point contact, can directly simulate the scattering of scalar particles by a black hole spacetime. The S matrix obtained from this scattering problem has poles in the complex plane corresponding to the quasinormal modes. We present the results of Gaussian wavepacket scattering to discern these states in the reflected wavepacket. We also discuss the possible signatures of the quasinormal modes in time-resolved measurements on quantum Hall systems in point contact geometries.

9:24AM X01.00008: Black Hole phenomena in Quantum Hall Systems 2: The Hawking-Unruh effect

SURAJ HEGDE (Presenter), VARSHA SUBRAMANYAN, BARRY BRADLYN, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign — In this talk, we present a parallel between dynamics in quantum Hall systems and the Hawking-Unruh effect associated with black holes. Hawking-Unruh radiation can be looked upon as a thermal distribution that arises from a Bogoliubov transformation generated by the Rindler Hamiltonian, corresponding to accelerated observers. We show that the Rindler Hamiltonian is functionally identical to that of Hamiltonian governing electrons in the lowest Landau level in the presence of a saddle potential. We show that this arises from a deeper connection between the symmetries of the two disparate systems – the isomorphism between the lie algebras of the 2+1D Lorentz group and that of SL(2,R) group of area-preserving transformations. This connection further allows us to see quantum Hall phenomena in the light of Lorentz kinematics.
Quantum tomography of electrical currents

REMI BISOGNIN (Presenter), Laboratoire Pierre Aigrain, Ecole Normale Supérieure - CNRS, BENJAMIN ROUSSEL, Laboratoire de Physique, ENS de Lyon - CNRS, CAMILLE CHAPDELAINE, Laboratoire des signaux et systèmes, Centrale-Supélec CNRS, ARTHUR MARGUERITE, MANOHAR KUMAR, Laboratoire Pierre Aigrain, Ecole Normale Supérieure - CNRS, CLÉMENT CABART, Laboratoire de Physique, ENS de Lyon - CNRS, ALI MOHAMMED-DJAFARI, Laboratoire des signaux et systèmes, Centrale-Supélec CNRS, JEAN-MARC BERROIR, ERWANN BOCQUILLON, BERNARD PLAÇAIS, Laboratoire Pierre Aigrain, Ecole Normale Supérieure - CNRS, ANTONELLA CAVANNA, ULF GENNSER, YOUNG JIN, Centre de Nanosciences et Nanotechnologies, C2N-Marcoussis CNRS, PASCAL DEGIOVANNI, Laboratoire de Physique, ENS de Lyon - CNRS, GWENDAL FÈVE, Laboratoire Pierre Aigrain, Ecole Normale Supérieure - CNRS — Recent developments in quantum nanoelectronics have enabled the realization of electron sources emitting a quantized number of excitations. However, reconstructing all wavefunctions of the elementary excitations embedded in electrical currents was still out of reach. Combining two-electron Hong-Ou-Mandel interferometry [1] with signal processing techniques, we demonstrate a quantum tomography protocol [2, 3, 4] able of extracting from any electrical current the generated electron and hole wavefunctions as well as their emission probabilities. The interferometer is implemented in a 2D electron gas in the integer quantum Hall effect where charges propagate along 1D ballistic edge channels. First we demonstrate the protocol with sinusoidal currents which allow for simple comparison with theoretical predictions. Then we turn to periodic single electron Lorentzian pulses and show that thermal effects lead to the generation of a statistical mixture between two single-electron wavefunctions.


QED-Bloch Theory with Homogeneous Magnetic Fields: Modifications of the Landau Levels and the Hofstadter Butterfly

VASIL ROKAJ (Presenter), MARKUS PENZ, MICHAEL SENTEF, MICHAEL RUGGENTHALER, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter — Probing electronic properties of periodic systems by arbitrary homogeneous magnetic fields has unravelled fundamental new phenomena in condensed matter physics. Much theoretical work has been devoted to describe those systems in different regimes, still a general first principles modeling of such fundamental effects is lacking. Here we propose a solution to the problem of Bloch electrons in a homogeneous magnetic field by including the quantum fluctuations of the photon field. A generalized quantum electrodynamical (QED) Bloch theory from first principles is presented. As an application we show how the well known Landau physics shows up in this framework and we derive quantum corrections to the Landau levels. These quantum corrections have direct implications for the integer quantum Hall effect. Moreover, in the case of a 2D solid in a perpendicular magnetic field, in the limit where the field fluctuations go to zero, we recover the fractal pattern of the Hofstadter butterfly. Further generalizations and modifications of the Hofstadter butterfly will be presented.

A Topological Sum-Rule Causes the Total Suppression of the Hall Response

MICHELE FILIPPONE (Presenter), CHARLES-EDOUARD BARDYN, SEBASTIAN GRESCHNER, THIERRY GIAMARCHI, University of Geneva — We present a topological sum-rule for the transverse polarization valid for out-of-equilibrium quantum states in two-dimensional lattices. Whenever the state equally spreads over all bands at a fixed energy, the topological sum-rule implies the identical suppression of the polarization, regardless of the magnetic field strength. As a remarkable consequence, the Hall response robustly vanishes even in absence of particle-hole symmetry and with arbitrary strong magnetic fields. We show that these out-of-equilibrium states are commonly realized in standard (Landauer) quantum transport settings and we rely on DMRG to show that our results equally apply to strongly interacting regimes.
**10:12AM X01.00012: Andreev edge state in the quantum Hall regime**

LINGFEI ZHAO (Presenter), ETHAN ARNAULT, ANDREW SEREDINSKI, ANNE M DRAELOS, Department of Physics, Duke University, HENGMING LI, TATE FLEMING, BRANDON BELL, Department of Physics and Astronomy, Appalachian State University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, NIMS, FRANCOIS AMET, Department of Physics and Astronomy, Appalachian State University, GLEB FINKELSTEIN, Department of Physics, Duke University — We investigate Andreev reflections in the quantum Hall regime. We study an encapsulated graphene sample contacted by both superconducting and normal electrodes. In the well-quantized regime, we find evidence for Andreev reflections of the QH edge states traveling along the superconducting contacts. The observed spectroscopic features decay to zero with increasing temperature and magnetic field. We attribute them to beating between electron-hole modes hybridized by Andreev reflections. These chiral modes under certain conditions are predicted to be Majorana-Weyl fermions.

*L.Z., A.D. and G.F. were supported by the Office of Basic Energy Sciences, US DoE, Award DE-SC0002765. A.S. and E.A. were supported by ARO Award W911NF-16-1-0122. H.L., T.F., B.B. and F.A. were supported by ARO Award W911NF-16-1-0132.*

**10:24AM X01.00013: Interacting quantum Hall states at integer filling with a non-Abelian twist: a coupled wire description**

PEDRO LOPES, Physics, University of British Columbia, VICTOR QUITO, Physics, Iowa State University, BO HAN, Physics, University of Illinois, Urbana-Champaign, JEFFREY TEO (Presenter), Physics, University of Virginia — We construct a theoretical coupled wire model that describes new many-body interacting quantum Hall states at integer filling. The strongly-correlated states support exotic electric and thermal Hall transport that violate the Wiedemann-Franz law $\nu/c=(\alpha_{xy}/\kappa_{xy})[\pi^2 k_B^2/(3e^2)]T>1$. We focus on strongly-paired states where combinations of pairs of electrons form the fundamental interacting constituents. These bosonic combinations associate to a Kac-Moody current algebra, which is removed from low-energy by the interaction in the 2+1D bulk but is left behind along the 1+1D boundary. We propose a new quantum Hall state at filling $\nu=16$ that supports a bosonic chiral $E_8$ edge current algebra at level 1 and is intimately related to the topological paramagnets in 3+1D. This topological state can be partitioned into two quantum Hall states at filling $\nu=8$, each carries a bosonic chiral $G_2$ or $F_4$ edge current algebra at level 1 and hosts non-Abelian Fibonacci anyonic excitations in the bulk. Moreover, we discover a new notion of particle-hole conjugation, based on the $E_8$ bosons, that switches between the $G_2$ and $F_4$ states.

*National Science Foundation under Grant No. DMR-1653535

**10:36AM X01.00014: Filling-enforced quantum oscillation phase shift anomaly in few-layer graphene**

BISWAJIT DATTA (Presenter), PRATAP CHANDRA ADAK, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, LI-KUN SHI, Institute of High Performance Computing, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, JUSTIN SONG, Division of Physics and Applied Physics, Nanyang Technological University, MANDAR DESHMUKH, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research — Quantum oscillations provide a striking visualization of the Fermi surface of metals: Fermi surface size, shape, and Berry phase naturally manifest in quantum oscillation frequency, field-direction dependence, and phase shift respectively. We report on unconventional magneto-transport of ABA-trilayer graphene, a multiband system comprising a (non-trivial) gapped monolayer graphene (MLG)-like band, nested within a large (trivial) bilayer graphene (BLG)-like band. Detailed field and density maps reveal BLG-like Shubnikov-de Hass (SdH) oscillations shifted by an anomalous non-trivial phase that sharply departs from that expected from the constant and trivial (2n) Berry phase of the BLG-like Fermi surface. The anomalous phase shift switches sharply from $\pi$ to $-\pi$ as density is tuned from below the MLG-like gap to above it. This originates from a strong filling-enforced constraint between the BLG-like and MLG-like Fermi surfaces, enabling the quantum oscillations of one Fermi surface to inherit the phase shifts of the other co-existing Fermi surface. We expect filling-enforced phases in quantum oscillations to arise generically in multi-Fermi-surface metals, and provide a detailed window to map the rich pattern of carrier filling in multi-band topological materials.
10:48AM X01.00015: Taming electronic decoherence in 1D chiral ballistic conductor*  
CLEMENT CABART, Ecole Normale Superieure de Lyon, BENJAMIN ROUSSEL, Advanced Concept Team, European Space Agency, GWENDAL FÈVE, Laboratoire Pierre Aigrain, Ecole Normale Superieure (Paris), PASCAL DEGIOVANNI (Presenter), Ecole Normale Superieure de Lyon —  
Decoherence and relaxation of single-electron excitations induced by strong effective screened Coulomb interactions in Quantum Hall edge channels are an important challenge for the applications of electron quantum optics in quantum information and quantum sensing. We present a complete study of intrinsic single-electron decoherence within an ideal single-electron channel with long-range effective Coulomb interactions to determine the influence of the material and sample properties [Phys. Rev. B 98, 155302 (2018)]. We find that weak-coupling materials characterized by a high velocity of hot-electron excitations such as graphene may offer interesting perspectives for limiting intrinsic decoherence due to electron/electron interactions compared to lower velocity materials such as AlGaAs/AsGa. We discuss quantitatively how extrinsic decoherence due to the coupling with the channel's electromagnetic environment can be efficiently inhibited in specifically designed samples at filling fraction two with one closed edge channel and we propose a realistic geometry for testing decoherence control in a Hong Ou Mandel experiment.

*This work is supported by the ANR grant “1shot reloaded” (ANR-14-CE32-0017) and ERC Consolidator grant “EQuO” (No. 648236).

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X02 DMP: Topological Materials -- New Materials I  
BCEC 107A - Lu Li, University of Michigan - Tag(s):

Focus

8:00AM X02.00001: Observation of topological nodal-loop fermionic state in CaAs3 family*  
MD MOFAZZEL HOSEN (Presenter), GYANENDRA DHAKAL, University of Central Florida, BAOKAI WANG, Northeastern University, KLAUSS DIMITRI, FIROZA KABIR, CHRISTOPHER SIMS, SABIN REGMI, YANGYANG LIU, University of Central Florida, TOMASZ DURAKIEWICZ, National Science Foundation, DARIUSZ KACZOROWSKI, Polish Academy of Sciences, ARUN BANSIL, Northeastern University, MADHAB NEUPANE, University of Central Florida — Nontrivial states in topological semimetals are attracting intense interest driven by their numerous novel properties such as high bulk carrier mobility, Fermi arcs, chiral anomaly, large negative magnetoresistance, and high density of states. Here, using high-resolution angle-resolved photoemission spectroscopy (ARPES) along with first-principles calculations, we report the discovery of a topological nodal-loop (TNL) state in CaAs3 family. Our analysis reveals that surface projections of the bulk nodal-points are connected by surface states. Notably, the observed topological state in CaAs3 family are well separated from other bands in the vicinity of the Fermi level. CaAs3 family thus offers a unique materials realization of a prototype nodal-loop semimetal, and a platform for gaining a deeper understanding of the interplay between TNL and topological insulator physics in semimetals.

*This work is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415 and the startup fund from UCF (M.N.).

8:12AM X02.00002: Prediction of a large-gap and switchable Kane-Mele quantum spin Hall insulator from first-principles simulations*  
ANTIMO MARRAZZO (Presenter), Ecole polytechnique federale de Lausanne, MARCO GIBERTINI, Department of Quantum Matter Physics, University of Geneva, DAVIDE CAMPI, NICOLAS MOUNET, NICOLA MARZARI, Ecole polytechnique federale de Lausanne — Fundamental research and technological applications of topological insulators are hindered by the rarity of materials exhibiting a robust topologically non-trivial phase, especially in two dimensions. Here, by means of extensive first-principles calculations, we propose a novel quantum spin Hall insulator (QSHI) with a sizeable band gap of ~0.5 eV that is a monolayer of jacutingaite [1, 2], a naturally occurring layered mineral first discovered in 2008 in Brazil [3] and recently synthesised [4]. This system realises the paradigmatic Kane-Mele model for QSHIs in a potentially exfoliable two-dimensional monolayer, with helical edge states that are robust and that can be manipulated exploiting a unique strong interplay between spin-orbit coupling, crystal-symmetry breaking and dielectric response [1]. Finally, we give an update on ongoing experimental efforts in the synthesis and characterisation of bulk and monolayer jacutingaite.


*This work was supported by the MARVEL NCCR of the Swiss NSF, the H2020 CoE MaX, the H2020 EPFL Fellows program and PRACE.
Clarification of charge-density wave gap symmetry and topology in bulk 1T-TiSe$_2$*  

SHIN-MING HUANG (Presenter), Physics, National Sun Yat-sen University, SUYANG XU, Department of Physics, Massachusetts Institute of Technology, BAHADUR SINGH, SZU-NUS Collaborative Center and International Collaborative Laboratory of 2D Materials for Optoelectronic Science & Technology, Engineering Technology Research Center for 2D, MING-CHIEN HSU, Physics, National Sun Yat-sen University, CHUANG-HAN HSU, Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, CHENLIANG SU, SZU-NUS Collaborative Center and International Collaborative Laboratory of 2D Materials for Optoelectronic Science & Technology, Engineering Technology Research Center for 2D, ARUN BANSIL, Department of Physics, Northeastern University, HSIN LIN, Institute of Physics, Academia Sinica —

We examine the symmetry of the charge density wave (CDW) phase of 1T-TiSe$_2$ and answer the connection of electronic structures between the normal and the CDW states. Especially, we unravel the consequential irreducible representations (IRs) of electronic states and, more ahead, those of gap functions among bands when the CDW occurs. Normally symmetry-related topology will be achieved directly, so we assert that the theory is valuable and practical for the search of topological CDW insulators.

*SMH is supported by the Ministry of Science and Technology (MoST) in Taiwan under grant No. 105-2112-M-110-014-MY3 and also by the NCTS of Taiwan.

Exotic Topological properties in compensated half-metallic inverse-Heusler systems*  

HYOSUN JIN (Presenter), YOUNG-JOON SONG, Department of Applied Physics, Graduated School, Korea University, WARREN E PICKETT, Department of Physics, University of California, Davis, KWAN-WOO LEE, Division of Display and Semiconductor Physics, Korea University — Recently three-dimensional (3D) topological features mixing with zero-dimensional (0D) band-crossings (Dirac, Weyl, multi-Weyl, and triple-nodal points [TNPs]) have stimulated further interest. An exotic phase, so called nexus fermion, has been expected when a 0D TNP coincides with a 1D nodal line. The nexus fermions are a yet more intricate excitation that have been proposed, but no realistic system has been proposed for such an exotic phase.

In this presentation, we will address a unique topological metallic system displaying simultaneous pure spin WPs, TNPs, nodal loops, and nexus fermions in the absence of (minor) spin-orbit coupling (SOC), in Cr-based inverse-Heusler compensated half-metals with neither inversion nor time-reversal symmetry, using density functional theory-based calculations. This combination gives rise to fully spin polarized nexus fermions, in a system with broken time-reversal symmetry but negligible macroscopic magnetic field. The observed high Curie temperature of 750 K and calculated SOC hybridization mixing of several meV should make these nexus fermions readily measurable.

*This research was supported by NRF Grants No. NRF-2016R1A2B4009579.
Topological materials host various novel quantum phases of electrons which are characterized by band topology and topologically protected surface/edge states. [1] Despite recent progress, intense world-wide research activity in search of new classes of topological materials is continuing unabated. This interest is driven by the need for materials with greater structural flexibility and tunability to enable viable applications in spintronics and quantum computing. We have used first-principles band theory computations to successfully predict many new classes of 3D topologically interesting materials, including Bi2Se3 series, [2] ternary half-Heuslers, [3] TlBiSe2 family, [4] Li2AgSb-class, and GeBi2Te4 family as well as topological crystalline insulator (TCI) SnTe family [5] and Weyl semimetals TaAs, [6,7] SrSi2, [8] (Mo,W)Te2,[9] Ta3S2, and LaAlGe family. [10] I will also highlight our recent work on unconventional chiral fermions in RhSi, [11] cubic Dirac points in LiOsO3, [12], rotaional symmetry protected TCIs [13], and Kramer-Weyl fermions in non-magnetic chiral cyrstals. [14]


Quantum Oscillations in Trigonal PtBi1.6 Single Crystals*

LINGYI XING (Presenter), RAMAKANTA CHAPAI, ROSHAN NEPAL, RONGYING JIN, Louisiana State University — Transition-metal dichalcogenide PtBi2 is known to form multiple structures with extreme large magnetoresistance (XMR). We have successfully grown high-quality PtBi1.6 single crystals with the trigonal structure. In addition to the XMR effect, the magnetization exhibits de Haas–van Alphen (dHvA) oscillations at low temperatures. Through Fourier transformation, we identify two oscillation frequencies $F_\delta = 4$ T and $F_\alpha = 39$ T with the sign of Zeeman splitting. Using Lifshitz–Kosevich (LK) formula to fit experimental data, we obtain the effective masses ($m^*_\delta = 0.092m_0$ and $m^*_\alpha = 0.189m_0$) and Berry phases ($\Phi_{B\delta} = (0.82 + 2\delta)\pi$ and $\Phi_{B\alpha} = (0.86 + 2\delta)\pi$) for both $\delta$ and $\alpha$ bands. The results indicate the trigonal PtBi1.6 has non-trivial topological properties.

*This work is supported by DOE through DE-SC0016315.

Crystal Structure determination of Ge2Sb2Te5 and Se-doped Ge2Sb2Te5 material

ZHENYANG XU (Presenter), JOHN SCHNEELOCH, KEESONG PARK, DESPINA LOUCA, Physics, University of Virginia — The [GeTe]n[Sb2Te3]m layered materials have been widely used as component of data storage devices and electronic memories. Ge2Sb2Te5 is a well-known phase change material that exhibits three phases: an amorphous phase, a rock-salt NaCl-type metastable phase and a hexagonal stable phase. To obtain the amorphous phase in bulk samples, we synthesized Ge2Sb2Te5-xSex where we replaced Te with Se. At about 90 % of Se, the system becomes amorphous by quenching. The Se atom function as a stabilizer of the amorphous phase and helps to trigger the local displacements of the Sb and Ge atoms within the unit cell, thus breaking the long-range order and render the system into an amorphous one. The rich physics within this transition will be discussed. Moreover, Ge2Sb2Te5 is associated with naturally occurring stacking faults and a topological phase transition depends sensitively on the distribution of these faults. It has been proposed theoretically that depending on the stacking sequence, GST can undergo a topological phase transition from the low temperature topological insulating phase with the so-called Kooi structure to the high temperature Weyl semi-metal phase with the Ferro structure. We synthesized the Kooi structure and the results from the DFT calculations will be discussed.
Topological properties are not protected in unstable crystal structures

(ALEX ZUNGER (Presenter), GUSTAVO DALPIAN, XINGANG ZHAO, University of Colorado Boulder, OLEKSANDR MALYI, University of Oslo, Norway, HANNES RAEBIGER, University of Yokohama, Japan, QIHANG LIU, Southern University of Science and Technology, China — The ability of DFT to reveal the consequences of assumed crystal symmetries on band inversion, band crossing and degeneracy in solids has led to a plethora of predicted compounds that should be topological insulators(TI's), Dirac Semimetals(DSM) and unconventional quasiparticles. Before offering predicted compounds for experimental evaluation, it may be wise to use not only the band structures as design filters, but also the DFT total energy (E_{tot}) of the given crystal. Inspecting E_{tot} one finds: i) the predicted 3D non-symmorphic DSM band crossing of BiO_2 in assumed SiO_2 structure is dynamically unstable and disappears if its structure is allowed to relax to another polymorph; ii) the predicted 8-fold band degeneracy of CuBi_2O_4 in assumed nonmagnetic configuration disappears once energy-lowering spin polarization is allowed; iii) the predicted oxide TI BaBiO_3 with upshifted Fermi level disappears once allowed to lower its energy in response to n-type doping; iv) the predicted unconventional quasiparticle in Ba_4Bi_3 with downshifted Fermi energy is destabilized by the required p-type doping. Thus, although proven bulk topological characteristics lead to protected surface/edge states, nothing protects bulk states from thermodynamic instability.

Giant negative magnetoresistance in a topological hourglass candidate

(PRISCILA ROSA (Presenter), Los Alamos National Laboratory, SATYA K KUSHWAHA, Pulsed Field Facility, NHMFL, MAREIN RAHN, MARC JANOSCHEK, ERIC BAUER, Los Alamos National Laboratory, MUN KEAT CHAN, NEIL HARRISON, Pulsed Field Facility, NHMFL, JOE D THOMPSON, FILIP RONNING, Los Alamos National Laboratory — Non-symmorphic materials have been recently predicted to host protected surface fermions displaying hourglass dispersion [1]. Here we report the physical properties of Eu_5In_2Sb_6 single crystals crystallizing in the non-symmporphic space group Pbam (55) [2]. Our results show that Eu_5In_2Sb_6 is a narrow-gap antiferromagnetic insulator that exhibits giant negative magnetoresistance driven by magnetic polarons. We discuss the potential surface states in Eu_5In_2Sb_6, and the role of magnetic correlations on hourglass fermions.


Properties of Bi_2Se_3 and Bi_xSb_2-xTe_3 grown by MBE

(YANG BAI (Presenter), DAVID FLÖTOTTO, BRIAN MULCAHY, JOSEPH HLEVYACK, XUN ZHAN, TAI-CHANG CHIANG, JIAN-MIN ZUO, JAMES ECKSTEIN, XIANGYU SONG, University of Illinois at Urbana-Champaign — We have studied molecular beam epitaxy growth of Bi_2Se_3 and Bi_xSb_2-xTe_3. We have demonstrated that by using a two-step growth recipe, very flat films of both materials can be obtained. The film quality was confirmed using RHEED oscillations during growth and, post-growth XRD, AFM, and STEM. Under other growth and processing conditions, we have observed a more complicated film morphology in the growth of Bi_xSb_2-xTe_3, which we attribute to compositional phase segregation. Using different substrates strongly impacts the film morphology. By tuning the ratio of Bi to Sb, the carrier type can be tuned from p-type to n-type measured via the Hall effect. The films were also studied by ARPES using a flip-chip cleaving approach in which the film plane at the interface to the substrate is measured after cleaving. The Hall and ARPES results agreed with regard to carrier type.

*This work is supported by the National Science Foundation.
**10:24AM X02.00011: Epitaxial growth of ultrathin Bi$_2$Se$_3$ films as characterized by *in situ* angle-resolved photoemission spectroscopy**

DONGSUNG CHOI (Presenter), NIKE SH KOIRALA, EDOARDO BALDINI, CHANGMIN LEE, NUH GEDIK, Massachusetts Institute of Technology — Combining molecular beam epitaxy with time- and angle-resolved photoemission spectroscopy (MBE-trARPES) provides a powerful way to investigate electronic structures of quantum materials. By using our *in situ* MBE-trARPES system, we measured ultrathin epitaxial films of Bi$_2$Se$_3$ grown on sapphire substrate. In its ultrathin limit, i.e. below 6 quintuple layers (QL), topological surface states are gapped due to hybridization and theory predicts the film to become a two-dimensional topological insulator (2D TI) until 3QL. From 3QL to 2QL, topological phase transition to trivial insulator is expected to occur. Previous ARPES experiments explored this phase transition in ultrathin Bi$_2$Se$_3$ films grown on bilayer graphene on SiC and Si substrate. In this experiment, we investigated various growth methods for ultrathin (2-6 QL) Bi$_2$Se$_3$ film on sapphire substrate: one-step growth, two-step growth, and growth on (Bi$_{0.5}$In$_{0.5}$)$_2$Se$_3$ buffer layer. By measuring ARPES spectra at several positions on the film, we evaluated band structure and uniformity of film. This work provides a guideline for growth of ultrathin Bi$_2$Se$_3$ on sapphire substrate for future experiments exploring topological phase transition in ultrathin Bi$_2$Se$_3$.

*Gordon and Betty Moore foundation, U.S. Department of Energy

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**10:36AM X02.00012: Crystal phase control in an YBiO$_3$ thin film by using a BaBiO$_3$ buffer layer**

ROSA LUCA BOUWMEESTER (Presenter), KIT DE HOND, University of Twente, NICOLAS GAUQUELIN, EMAT, University of Antwerp, GERTJAN KOSTER, ALEXANDER BRINKMAN, University of Twente, JO VERBEECK, EMAT, University of Antwerp — Topological insulating materials are very promising for applications in spintronics and quantum computing. The presently confirmed topological insulators are not suitable for room temperature applications. Perovskite oxides are interesting in this respect, since topological insulating phases have theoretically been predicted with large band gaps. YBiO$_3$ has been predicted to be a topological insulator for the perovskite phase with yttrium and bismuth located at the A-site and B-site, respectively. However, the fluorite phase turns out to be thermodynamically more stable than the perovskite phase. In this work we show that we were able to engineer the perovskite crystal phase of thin film YBiO$_3$ by using a BaBiO$_3$ buffer layer and interval deposition. When the YBiO$_3$ is deposited on top of the BaBiO$_3$, a single oriented perovskite phase is observed with the expected lattice constants. These findings pave a way towards the fabrication of quantum devices for testing the hypothesized topological insulating phase in YBiO$_3$.

*This work is financially supported through a NWO Vici grant. For the work in Antwerp, we acknowledge the financial support of the GOA project “Solarpaint” and the Hercules Fund of the Flemish Government.

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**10:48AM X02.00013: Structure-Property relationships and superconductivity in Single Crystals of Nb$_x$Bi$_2$Ch$_3$, (Ch ≡ S, Se, Te)**

CHRISTIAN PARSONS (Presenter), YANAN LI, PRASENJIT GUPTASARMA, Department of Physics, University of Wisconsin Milwaukee, Wisconsin 53211 — Studies of Topological Insulators, possibly a new quantum phase of matter believed to possess a 2-dimensional Fermi surface, have led to a search for other insulators or semi-metals in which topologically non-trivial properties can be tuned using a chemical, structural, or external thermodynamic parameter. Topological insulators such as Bi$_2$Se$_3$ and Bi$_2$Te$_3$ have attracted much interest due to not just their non-trivial topology, but also due to the appearance of superconductivity upon intercalation or substitution with elements such as Cu, Sr and Nb. Many potentially interesting transition-metal intercalated/doped Bismuth-Chalcogenides have not yet been explored. Here, we discuss our growth and study of Nb$_{0.2}$Bi$_2$Ch$_3$ crystals (Ch = S, Se, Te). We report resistivity measurements and confirm a superconducting transition near 3K for Nb$_{0.2}$Bi$_2$Se$_3$. We also report a possible charge density wave (CDW) transition in Nb$_{0.2}$Bi$_2$Te$_3$. In contrast, Nb$_{0.2}$Bi$_2$S$_3$ was found to be a good conductor with no phase transitions. Detailed fitting of x-ray diffraction shows that all three families of single crystals have a primary phase of Bi$_2$Ch$_3$ and a minor secondary phase of BiNbCh$_3$. We discuss our results together with Raman Spectroscopy, X-ray Diffraction and Electron Diffraction studies of our crystals.

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**Friday, March 8, 2019 8:00 AM - 10:36 AM**

**Session X03 DCMP: Topological Superconductors and Superfluids**

BCEC 107B - Tag(s): Focus
8:00AM X03.00001: Symmetry-protected line nodes and Majorana flat bands in nodal crystalline superconductors
SHINGO KOBAYASHI (Presenter), Nagoya University, SHUNTARO SUMITA, YOUICHI YANASE, Kyoto University, MASATOSHI SATO, YITP, Kyoto University — Over the last few years, the study on node structures in SCs has received renewed interest due to the fact that they are a kind of topological objects. In this context, a line node in time-reversal (TR) invariant SCs is protected by a one-dimensional (1D) topological number and induces a Majorana flat band (MFB) in a surface. The MFBs exhibit a zero-bias conductance peak through the tunneling measurement for TR invariant SCs such as high-$T_c$ SCs and non-centrosymmetric SCs, which gives a conclusive evidence for the bulk topological line nodes.

In this talk, we discuss topology of crystal symmetry protected line nodes in unconventional SCs. We introduced the 1D and 0D topological numbers associated with line nodes, each of which ensures the existence of MFBs and stability of line nodes, respectively. Establishing a relationship between them, we clarified that MFBs are classified into three classes of SCs [1]: (i) odd-parity SCs, (ii) even-parity SCs with pure TR symmetry, and (ii) even-parity SCs with a magnetic translation. These classes are distinguishable through surface sensitive experiments.


8:12AM X03.00002: Full proximity approach to induced gap in topological superconductor junctions
FNU SETIAWAN (Presenter), James Franck Institute, University of Chicago, CHIEN-TE WU, Electrophysics, National Chiao Tung University, KATHRYN LEVIN, James Franck Institute, University of Chicago — Recently, a Josephson junction formed from a two-dimensional electron gas (2DEG) proximitized by two superconductors subjected to an in-plane magnetic field has emerged as a viable platform to realize topological superconductivity [1-3]. In this talk, we address the proximity-induced superconductivity in this setup by studying the full proximity model of a superconductor-insulator-superconductor junction in contact with a spin-orbit-coupled substrate. To this end, we numerically solve the Bogoliubov-de Gennes Hamiltonian of this model and study the effect of spin-orbit coupling and thickness of the substrate on the induced pairing amplitude and energy dispersion. Finally, we will discuss the topological phase diagram of multiband topological Josephson junctions for a thick substrate.


8:24AM X03.00003: Hot electron magnetotransport in the high mobility GaAs/AlGaAs two dimensional electron system below 1K
C.RASADI MUNASINGHE (Presenter), BINUKA GUNAWARDANA, RASANGA SAMARAWEERA, THARANGA NANAYAKKARA, U. KUSHAN WIJEWARDENA, SAJITH WITHANAGE, ANNIKA KRIISA, Physics and Astronomy, Georgia State University, CHRISTIAN REICHL, WERNER WEGSCHEIDER, Laboratorium für Festkörperphysik, ETH Zürich, RAMESH MANI, Physics and Astronomy, Georgia State University — Non-equilibrium hot electron phenomena play a major role in semiconductor transport when, for example, the heat applied directly to the electronic system becomes substantial. The carrier temperature can differ from the lattice temperature, and the carrier temperature results, in the steady state, from a balance between energy gain from the heating source, and energy loss to the lattice from electron-phonon scattering. In this experimental study, we examine heating induced by the small ac-bias current utilized in the low-frequency lock-in based four terminal transport measurements. Since at small bias current, the carrier heating is expected to be small, we have utilized an effect that is associated with a small energy scale to follow the heating effect, namely the spin splitting in the Shubnikov-de Haas effect. The development of fields such as spintronics and spin-based quantum computing have encouraged further studies, such as this one, of the parameters affecting the behavior of electron spin in low dimensional electron systems. Thus, magneto-transport measurements have been carried out below 1K to observe the ac current effect on the characteristic features of the GaAs/AlGaAs system. In this report, we show evidence for a carrier heating effect due to the small ac bias.
8:36AM X03.00004: Topological Phases in Nodeless Tetragonal Superconductors*  
SANTIAGO VARONA (Presenter), LAURA ORTIZ, Departamento de Física Teórica, Complutense University, OSCAR VIVUELA, Department of Physics, Harvard University, MIGUEL ANGEL MARTIN-DELGADO, Departamento de Física Teórica, Complutense University — We compute the topological phase diagram of 2D tetragonal superconductors for the only possible nodeless pairing channels compatible with that crystal symmetry. Subject to a Zeeman field and spin-orbit coupling, we demonstrate that these superconductors show surprising topological features: non-trivial high Chern numbers, massive edge states, and zero-energy modes out of high symmetry points, even though the edge states remain topologically protected. Interestingly, one of these pairing symmetries, $d+i\sigma$, has been proposed to describe materials such as water-intercalated sodium cobaltates, bilayer silicene or highly doped monolayer graphene.

*We acknowledge financial support from the Spanish MINECO grants FIS2012-33152, FIS2015-67411, and the CAM research consortium QUITEMAD+, Grant No. S2013/ICE-2801. The research of M.A.M.-D. has been supported in part by the U.S. Army Research Office through Grant No. W911NF-14-1-0103. O.V. thanks Fundación Ramón Areces and RCC Harvard. S.V. thanks FPU MECD Grant.

8:48AM X03.00005: Fractional Josephson Vortices and Braiding of Majorana Zero Modes in Planar Superconductor-Semiconductor-Superconductor Josephson junctions*  
ADY STERN (Presenter), EREZ BERG, Weizmann Institute of Science — We consider the one-dimensional (1D) topological superconductor that may form in a planar superconductor-metal-superconductor Josephson junction in which the metal is subjected to spin orbit coupling and to an in-plane magnetic field. This 1D topological superconductor has been the subject of recent theoretical and experimental attention. We examine the effect of perpendicular magnetic field and a supercurrent driven across the junction on the position and structure of the Majorana zero modes that are associated with the topological superconductor. In particular, we show that under certain conditions the Josephson vortices fractionalize to half-vortices, each carrying half of the superconducting flux quantum and a single Majorana zero mode. Furthermore, we show that the system allows for a current-controlled braiding of Majorana zero modes.

*ERC project MUNATOP, CRC183, ISF, Micosoft Station Q

9:00AM X03.00006: An Exactly Solvable Interacting Edge Theory for a Weak 2D Topological Superconductor.  
JOSEPH SULLIVAN (Presenter), MENG CHENG, Yale Univ — We study interacting edge states of a 2D weak topological superconductor protected by time-reversal symmetry. Such a system can be viewed as a stack of Majorana/Kitaev chains (class BDI), possessing translation symmetry in the transverse direction. Interestingly, in this model, time-reversal symmetry forbids terms quadratic in fermionic degrees of freedom on the edge, so any edge dynamics must be inherently interacting. We proposed an exactly solvable model for the edge and worked out its phase diagram. It is shown that the edge is either symmetry breaking or gapless as expected from the bulk-boundary correspondence of a topological phase. We then construct a low energy field theory for the model in the gapless phase. We propose that the same field theory describes the edge of an intrinsically interacting fermionic symmetry-protected phase with $Z_4 \times Z_2^T$ symmetry.

9:12AM X03.00007: Majorana corner states in D class*  
XIN LIU (Presenter), XIAO-HONG PAN, KAI-JIE YANG, Huazhong University of Science and Technology — Majorana corner states (MCSS) in D class can naturally form a topological qubit. In this talk, we show that how to realize MCSS in two-dimensional topological insulators in the presence of both superconductivity and magnet. It is noted that there is only one MCS at each corner which is allowed due to the time-reversal symmetry broken. An edge theory is performed to clearly demonstrate the physics behind these results. At last, we study the spin property of MCSS and propose to use spin-resolved scanning tunneling microscope to detect their existence.

*This work is supported by National Key R&D Program of China (Grant No. 2016YFA0401003), NSFC (Grant No.11674114), and Thousand-Young-Talent program of China.
9:24AM X03.00008: Generalized Aubry-André-Harper model with p-wave superconducting pairing  
Qi-Bo Zeng (Presenter), Tsinghua University, Shu Chen, Chinese Academy of Sciences, Institute of Physics, Rong Lu, Tsinghua University —  
We investigate a generalized Aubry-André-Harper (AAH) model with p-wave superconducting pairing. Both the hopping amplitudes between the nearest-neighbor lattice sites and the on-site potentials in this system are modulated by a cosine function with a periodicity of $1/\alpha$. In the incommensurate case ($\alpha = (\sqrt{5} - 1)/2$), due to the modulations on the hopping amplitudes, the critical region of this quasiperiodic system is significantly reduced and the system becomes easier to be turned from extended states to localized states. In the commensurate case ($\alpha = 1/2$), we find that this model shows three different phases when we tune the system parameters: Su-Schrieffer-Heeger (SSH)-like trivial, SSH-like topological, and Kitaev-like topological phases. The phase diagrams and the topological quantum numbers for these phases are presented in this work. This generalized AAH model combined with superconducting pairing provides us with a useful test field for studying the phase transitions from extended states to Anderson localized states and the transitions between different topological phases.

9:36AM X03.00009: Conformal phase transition in topological superconductors  
Flavio Nogueira (Presenter), Jeroen van den Brink, IFW Dresden, Asle Sudbo, Dept. of Physics, Norwegian University of Science and Technology —  
A conformal phase transition (CPT) is a phase transition defining a critical point with a non-power law diverging correlation length, but which nevertheless exhibits a universal jump in some generalized stiffness of the system. A well-known example is the Berezinskii-Kosterlitz-Thouless (BKT) phase transition taking place in two-dimensional superfluids and superconductors when they transition from the low-temperature phase to the normal state, and in the melting transition of two-dimensional crystals. In this talk we will introduce a more subtle type of CPT, one that is driven by a topological term in the effective action in 2+1 dimensions. The main motivation comes from the modification of Maxwell electrodynamics in topological insulators and superconductors. Quite generally, the surface of a topological insulator features an electromagnetic response characterized by a Chern-Simons term in the Lagrangian. We will show in this context that a topological Abelian Higgs model exhibits quantum criticality with BKT scaling when the Hall conductivity lies in a well defined interval where conformality is lost. We explore the physical consequences of this novel quantum critical phenomenon in topological materials.

9:48AM X03.00010: Superconformal Cardy states and entanglement structure of 1D quantum critical points with emergent supersymmetry  
Chun Chen (Presenter), Joseph Maciejko, Physics Department, University of Alberta —  
Condensed matter systems with quantum critical points exhibiting emergent spacetime supersymmetry in the long-wavelength, low-energy limit have attracted much attention recently. In particular, several elements of the N=1 series of superconformal minimal models originally discovered by Friedan, Qiu, and Shenker in 1985 have been realized recently in a variety of 1D quantum lattice models ranging from anyonic spin chains to interacting Majorana chains and boson-fermion mixtures. To better understand the entanglement structure of these exotic quantum critical points, we revisit the problem of the construction of boundary states for the superconformal minimal models and find a new set of Cardy states not previously discussed. As an application of this formalism we present and discuss numerical DMRG results for the entanglement spectrum of the Grover-–Sheng–Vishwanath model as a lattice realization of the tricritical Ising universality class.

10:00AM X03.00011: Majorana Corner Modes in a High-Temperature Platform  
Zhongbo Yan (Presenter), School of Physics, Sun Yat-sen University, Fei Song, Zhong Wang, Institute for Advanced Study, Tsinghua University —  
We introduce two-dimensional topological insulators in proximity to high-temperature cuprate or iron based superconductors as high-temperature platforms of Majorana Kramers pairs of zero modes. The proximity-induced pairing at the helical edge state of the topological insulator serves as a Dirac mass, whose sign changes at the sample corner because of the pairing symmetry of high-Tc superconductors. This sign changing naturally creates at each corner a pair of Majorana zero modes protected by time-reversal symmetry. Conceptually, this is a topologically trivial superconductor-based approach for Majorana zero modes. We provide quantitative criteria and suggest candidate materials for this proposal. [Reference: Phys. Rev. Lett. 121, 096803 (2018)]

*This work is supported by NSFC (Grant No. 11674189). Z. Y. is supported in part by the China Postdoctoral Science Foundation (Grant No. 2016M590082).
10:12AM X03.00012: Zero-energy Andreev bound states from quantum dots in proximitized Rashba nanowires  
CHRISTOPHER REEG (Presenter), OLESIADMYTRUK, DENIS CHEVALLIER, DANIEL LOSS, JELENA KLINOVKAJA, University of Basel
— We study an analytical model of a Rashba nanowire that is partially covered by and coupled to a thin superconducting layer, where the uncovered region of the nanowire forms a quantum dot. We find that, even if there is no topological phase possible, there is a trivial Andreev bound state that becomes pinned exponentially close to zero energy as a function of magnetic field strength when the length of the dot is tuned with respect to its spin-orbit length such that a resonance condition of Fabry-Perot type is satisfied. In this case, we find that the Andreev bound state remains pinned near zero energy for Zeeman energies that exceed the characteristic spacing between Andreev levels but that are smaller than the spin-orbit energy of the dot. Importantly, as the pinning of the Andreev bound state depends only on properties of the dot, we conclude that this behavior is unrelated to topological superconductivity. To support our analytical model, we also perform a numerical simulation of a hybrid system that explicitly incorporates a thin superconducting layer, showing that all qualitative features of our analytical model are present in the numerical results.

References:

10:24AM X03.00013: The survival of topological signatures in the presence of average symmetries*  
YINGYI HUANG (Presenter), Physics, Sun Yat-Sen University, CHING-KAI CHIU, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences — The robust properties in topological states of matter under the effect of disorders is of great theoretical as well as experimental interests. One focus is on the disorders breaking either spatial symmetry or non-spatial symmetry (e.g., time-reversal, particle-hole and chiral symmetry) but restoring it on average. In this work, we consider a quasi-one-dimensional topological superconductor in the presence of disorders preserving average time-reversal symmetry or mirror symmetry. By calculating the transport signatures of multi-chain Kitaev and Majorana models, we show that the survival of the edge modes depends on the form of the disorders.

*C.-K. C acknowledges the funding from the Strategic Priority Research Program of the Chinese Academy of Sciences, Grant No. XDB28000000.
Electronic structure of twin wall/surface intersections in CaTiO$_3$ (001)*

NICHOLAS BARRETT (Presenter), QIANG WU, EKHARD SALJE, Department of Earth Sciences, University of Cambridge, ZIYUAN ZHAO, Department of Materials Science and Engineering, Xi’an University of Technology, CLAIRE MATHIEU, CHRISTOPHE LUBIN, DOMINIQUE MARTINOTTI, CEA-Saclay — Domain wall engineering of functional oxides provides a new paradigm for post-CMOS electronics [1]. Domain walls are potentially the perfect structural discontinuity, maintaining the crystalline phase but defining a change in the functional order parameter.

In CaTiO$_3$ the strain order is defined by the octahedral tilt. At the twin walls the octahedral tilt goes to zero allowing Ti off-centering and the twin wall acquires a ferroelectric polarization [2, 3].

We have studied the intersections between different twin walls and the (001) surface using low energy electron microscopy (LEEM) and molecular dynamics simulations including Landau springs and Coulomb interactions. The domain surfaces develop polarity close to the twin walls. The elastically induced dipoles cause contrast in LEEM, unexpected for nominally non-polar surfaces. The outward and inward twin wall polarity is in good agreement with simulations.


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Nature of the Atomic Structure Underlying the Vortex Polarization Domains in Hexagonal RMnO$_3^*$

HAN ZHANG, SIZHAN LIU, New Jersey Inst of Tech, SUYIN GRASS WANG, YU-SHENG CHEN, Argonne National Laboratory, SANG-WOOK CHEONG, Rutgers University, TREVOR TYSON (Presenter), New Jersey Inst of Tech — Hexagonal phase RMnO$_3$ systems exhibit polarization domains with complex vortex pattern with density depending on the cooling rate from the high temperature paraelectric phase. Structural measurements are used to probe the structure on length scales commensurate with the variations in polarization. Structural measurements reveal variations on the lengthscale of the changes in polarization.

*This work is supported by NSF Grant No. DMR-1809931.

Towards adaptable nano-circuitry - functional domain walls and disorder engineering in improper ferroelectrics [Invited]

DENNIS MEIER, DONALD M. EVANS (Presenter), Materials Science and Engineering, Norwegian University of Science and Technology - NTNU — Oxide materials exhibit a broad range of tunable phenomena, including magnetism, multiferroicity, and superconductivity. Oxide interfaces are particularly intriguing. The low local symmetry combined with the sensitivity to electrostatics and strain leads to unusual physical properties. Recently, ferroelectric domain walls have attracted attention as conducting and spatially mobile interfaces. In order to ultimately design domain-wall-based devices and circuitry, however, additional functionality beyond just conduction is required.

In my talk, I will discuss how improper ferroelectric domain walls can be used to emulate key electronic components. In the first part, I will address domain walls in ErMnO$_3$. The system naturally develops all fundamental types of ferroelectric domain walls, including neutral as well as negatively and positively charged wall configurations. I will show how the electronic domain-wall properties can be controlled and discuss the possibility to use such walls for designing, e.g., 2D digital switches and half-wave rectifiers [1]. In the second part, I will consider domain walls in spin-spiral multiferroics with strong magnetoelastic couplings and additional functionality that arises from the interplay of charge and spin degrees of freedom. Because of the coupling, it is possible to reversibly control the configuration at ferroelectric domain walls by magnetic fields, switching between nominally charged and neutral domain wall states [2,3]. Furthermore, I will present an innovative approach for controlling conductivity and wiring up domain-wall-based devices with nanoscale spatial resolution, bringing us an important step closer to adaptable all-domain-wall circuitry for next-generation nanotechnology.

9:12AM X04.00005: Probing Microwave Dynamics of Ferroelectric Domain Walls* [Invited] KEJI LAI (Presenter), University of Texas at Austin — The past decade has witnessed the emergence and rapid development of domain wall (DW) nanoelectronics, which take advantage of the enhanced electronic conductivity at ferroelectric DWs due to the accumulation of free carriers. For practical high-speed electronics, however, the dielectric dispersion of ferroelectric materials at microwave frequencies has to be taken into account. Using a cohort of imaging techniques such as piezo-force microscopy, conductive atomic-force microscopy, and microwave impedance microscopy, we are able to determine the contribution of both mobile carriers and bound dipoles to the GHz response at ferroelectric domain walls. In LiNbO₃, BiFeO₃, and YMnO₃, the effective microwave conductivity of certain DWs is higher than that at DC by several orders of magnitude, while other walls behave the same at both DC and AC. First-principles and model calculations indicate that the AC-conductive DWs exhibit a localized vibrational mode, which can be excited by the alternating electric fields from the tip. In addition to the DW dynamics, the local electromechanical energy transduction in ferroelectric domains can also be visualized by the microwave probe. Our work opens up a new avenue to explore various phenomena in complex materials and novel devices by near-field electromagnetic imaging.


*This work is supported by NSF DMR-1649490 and DMR-1707372.

9:48AM X04.00006: Microwave Conductivity of Ferroelectric Domain Walls in BiFeO₃ Bulk Crystals LU ZHENG (Presenter), University of Texas at Austin, XIAOCHE FANG, XIANGHAN XU, SANG-WOOK CHEONG, Rutgers University, KEJI LAI, University of Texas at Austin — Domain walls (DWs) in multiferroic materials exhibit novel functionalities that may be utilized for nanoelectronic applications. In recent years, the enhanced DW dc conductivity due to the accumulation of free carriers and ac conductivity due to the excitation of wall vibration have both been reported in various ferroelectrics. Combining piezo-force microscopy and microwave impedance microscopy, we directly probe the nanoscale dielectric response of various DWs in BiFeO₃ bulk crystals at microwave frequencies. Interestingly, regardless of the type of the walls (71-, 109-, or 180-degree), the neutral DWs always display high ac conductivity around 1 GHz, whereas the charged walls do not. In addition, interference of surface acoustic waves can be observed near the 180-degree walls. Our results provide a unified picture to understand the DW dynamics in BiFeO₃, which is crucial for its application in high-speed nano-devices.

10:00AM X04.00007: Thermal effect on domain wall roughness in epitaxial PbZr₀.₂Ti₀.₈O₃ thin films with different as-grow polarization orientations* KUN WANG (Presenter), JINGFENG SONG, LE ZHANG, XUEGANG CHEN, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln — In epitaxial ferroelectric films, the asymmetric boundary condition can lead to strong polarization asymmetry that affects the thermal stability of different polar states. We have carried out piezo-response force microscopy (PFM) studies on the thermal evolution of domain walls (DW) in epitaxial 50 nm PbZr₀.₂Ti₀.₈O₃ (PZT) films grown on (La,Sr)MnO₃ and LaNiO₃ buffered SrTiO₃, which show different as-grown polarization. The correlation function of the DW roughness depends on the distance $L$ along the DW as $L^{2\zeta}$. At room temperature, the roughness exponent $\zeta$ is 0.2-0.3, consistent with 2D DWs in weak random bond disorder. The films were then heated at progressively higher temperatures till approaching $T_C$. The subsequent PFM images show that $\zeta$ gradually increases to ~0.6, evolving to dominant thermal roughening. Both the bottom electrode type and the as-grown polarization orientation affect the $T$-dependence of $\zeta$. We also compare the results obtained from in situ high temperature measurements and rapid thermal quench. Our study provides critical information about the thermal stability and size scaling limit of epitaxial thin films-based ferroelectric devices.

*This work was supported by the US DOE Award # DE-SC0016153.
Giant electroresistance effect in single-crystalline lithium niobate thin films enabled by domain wall control

JAMES MCCONVILLE (Presenter), Centre for Nanostructured Media, Queen's University Belfast, HAILDONG LU, Department of Physics and Astronomy, University of Nebraska-Lincoln, MICHELE CONROY, KALANI MOORE, Department of Physics, University of Limerick, ALEXEY LIPATOV, ALEXANDER SINITSKII, Department of Chemistry, University of Nebraska-Lincoln, ALEXEI GRUVERMAN, Department of Physics and Astronomy, University of Nebraska-Lincoln, URSEL BANGERT, Department of Physics, University of Limerick, MARTY GREGG, Centre for Nanostructured Media, Queen's University Belfast — One of the most prominent features of ferroelectric domain walls (DWs) is their electrical conductivity, which was observed in a number of materials, such as BiFeO₃, Pb(Zr,Ti)O₃, ErMnO₃. We combine scanning transmission electron microscopy (STEM) and local probe techniques to investigate the conduction through charged DWs in the ion-sliced single-crystalline LiNbO₃ thin films with sub-µm thickness. STEM shows large inclination of the electrically-generated 180° DWs away from the polar z-axis (with angles reaching 16°) suggesting the DWs are strongly charged. Using piezoresponse force microscopy (PFM) in combination with conductive atomic force microscopy (CAFM) it was shown that head-to-head DWs have higher conductivity than the tail-to-tail DWs, suggesting an electronic type of conductance. One of the most important findings is a modulation of conductivity by an external voltage. It is demonstrated that the resistance of the LiNbO₃ thin film capacitors can be changed continuously by 5 to 9 orders of magnitude by controlling the DW perimeter allowing development of multi-level resistive switching devices. Resistance states can be altered by exposure to cumulative voltage pulses, suggesting that these domain wall memristors might be useful in the context of artificial synapses.

Dipole-dipole interaction and domain relaxation of ferroelectric triangular lattice

HYE-JIN JIN (Presenter), Ewha Womans University, CHANG JAE ROH, Gwangju Institute of Science and Technology, JANGHYUN JO, JUNSIK MUN, Seoul National University, JONGSEOK LEE, Gwangju Institute of Science and Technology, MIYOUNG KIM, Seoul National University, YOUNG-HAN SHIN, University of Ulsan, WILLIAM JO, Ewha Womans University — In ferroelectric lattices, dipole arrangements are controlled by manipulating structural formation and orientations of ferroelectric thin films are determining factor to control dipole arrangements. Herein, tetragonal PbTiO₃ (PTO) thin films were obtained and triangular lattice is observed in (111)-PTO thin films. We used pulsed laser deposition and compared (001)- and (111)-PTO thin films. To confirm structural characteristics, X-ray diffraction patterns and second harmonic generations were used. In addition, dipole arrangements are investigated by using transmission electron microscopy. In particular, directions of dipoles are gradually changed and vortex-like domain structure is obtained in the (111)-PTO thin films. It is induced by tilting characteristics of polarization axes of the (111)-PTO thin films. To study domain relaxation, temporal change of domain is obtained by using piezoresponse force microscopy and a stretched exponential decay mechanism is applied. In the (111)-PTO thin films, dipole frustration is induced because of poling and redistribution of dipoles occurred to release dipole frustration. During relaxation, dipole-dipole interaction should be addressed and it gives a deep insight to understand fundamental relaxation mechanism of ferroelectric thin films.

Designing ferroic domain states and coupling through low-energy He-irradiation*

ANDREAS HERKLOTZ (Presenter), ROBERT ROTH, KATHRIN DORR, Institute for Physics, Martin-Luther-University Halle-Wittenberg, YOGESH SHARMA, THOMAS WARD, Oak Ridge National Laboratory — The physical properties of ferroic thin films are typically dominated by their domain configurations and the response of domain walls to external fields. Domain engineering has thus developed as a powerful tool to tailor functionalities of oxide thin films. A particularly successful approach has been the use of strain fields through heteroepitaxy.

As an alternative approach we deploy low-energy He implantation to induce out-of-plane strain in epitaxial ferroelectric thin films, while the in-plane strain due to coherent growth on single-crystal substrates remains fixed. We show that this kind of uniaxial strain engineering effectively alters the ratio of ferroelectric and ferroelastic domains in BaTiO₃ and BiFeO₃ films. We also demonstrate that controlling domains by strain doping can provide a direct handle on ferromagnetic metal films magnetoelastically coupled to the interfaced ferroelectric films.

*This effort was supported by the DFG SFB 762 and the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), Materials Sciences and Engineering Division
8:00AM X05.00001: Quasi 1D topological nodal superconducting vortex line state in doped 3D Dirac Semimetals
SHENGSHAN QIN (Presenter), Kavli Institute of Theoretical Sciences, LUN HU, Department of Physics, University of California, San Diego, California 92093, USA, CONGCONG LE, Kavli Institute of Theoretical Sciences, JINFENG ZENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, FU-CHUN ZHANG, Kavli Institute of Theoretical Sciences, CHEN FANG, JIANGPING HU, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We study the vortex bound states in three dimensional (3D) Dirac semimetals with both time reversal symmetry and inversion symmetry. Assuming two Dirac points on the kz-axis and bulk s-wave superconductivity, the results turn out to be strongly anisotropic: if the vortex line is perpendicular to the kz-direction, the bulk superconductor plus a single quantum vortex line is always topologically trivial; if the vortex line is parallel to the kz-direction, the system has a robust quasi 1D topological nodal superconductor phase, for certain range of doping level. The emergence of the nodal superconductor phase is a reflection of the topological property of the Dirac point. Finally, we discuss the possible material realization of such nodal superconducting vortex line state.

8:12AM X05.00002: Finite temperature topological states in a chain of magnetic adatoms on a superconductor*
MACIEJ MASKA (Presenter), ANNA GORCZYCA-GORAJ, University of Silesia in Katowice, TADEUSZ DOMANSKI, Maria Curie-Skłodowska University in Lublin — It is known that magnetic moments of a one-dimensional chain of adatoms on a superconductor self-organize into a spiral magnetic structure, which leads to topologically nontrivial superconductivity. Such a system can host the Majorana quasiparticles near its edges. The interaction between the localized moments is mediated by itinerant electrons. Upon tracing out the fermionic degrees of freedom, one obtains long range temperature-dependent effective interaction between the moments. Using Monte Carlo techniques we calculate the thermodynamic properties of the system. In particular, we demonstrate that with increasing temperature the correlation length of the magnetic order decreases, eventually driving the system to a topologically trivial phase. Using the simulated annealing method we also show, that at low temperature a phase separation can take place in the chain, where only part of the system is in the topologically nontrivial state and the rest of it is in the trivial state.

*This work is supported by the National Science Centre, Poland via Project No. 2016/23/B/ST3/00647

8:24AM X05.00003: Quantum Transport in Nanowires Grown via Template Assisted Selective Epitaxy and Contacted by an s-wave Superconductor*
M A MUEED (Presenter), BENJAMIN MADON, IBM Almaden Research Center, FABRIZIO NICHELE, MARKUS RITTER, IBM Zurich Research Center, NOEL ARELLANO, IBM Almaden Research Center, HEINZ SCHMID, IBM Zurich Research Center, FENNER HARPER, RAHUL ROY, Physics, University of California at Los Angeles, HEIKE RIEL, IBM Zurich Research Center, AAKASH PUSHP, IBM Almaden Research Center — The hybrid system of an s-wave superconductor and a semiconducting nanowire with strong spin-orbit coupling (e.g. InAs, InSb) is a robust platform for realizing Majorana Fermion, a quasi-particle which is considered to be the building block for fault tolerant quantum computation. In our study, we prepare InAs nanowire networks using Template Assisted Selective Epitaxy (TASE) method and contact them using an s-wave superconducting material. The TASE method offers a reproducible way to grow high-quality nanowire in non-trivial device geometries, such as cross and Y-junctions, proposed for braiding operations of Majorana Fermions. Here, we present the quantum transport data measured on TASE-grown InAs nanowires with different device geometries.

*DARPA
8:36AM X05.00004: Enhanced Triplet Pairing in Magnetic Junctions with s-wave Superconductors  
CHENGHAO SHEN (Presenter), University at Buffalo, The State University of New York, THOMAS VEZIN, École Polytechnique, JONG E HAN, IGOR ZUTIC, University at Buffalo, The State University of New York — A common path to Majorana fermions and topologically-protected quantum computing relies on spin-triplet superconductivity[1]. While spin-triplet pairing is elusive in nature and even common spin-triplet candidates, such as Sr2RuO4, could support alternative explanations[2], proximity effects in heterostructures can overcome these limitations. Specifically, a common expectation is that robust spin-triplet superconductivity in magnetic junctions should rely on highly spin-polarized magnets or complex magnetic multilayers[3]. Instead, we predict that the interplay of interfacial spin-orbit coupling and the barrier strength in simple magnetic junctions with s-wave superconductors can lead to nearly complete spin-triplet superconducting proximity effects when magnets have only a small spin polarization. We show that this enhanced spin-triplet regime is characterized by a huge increase in conductance magnetoanisotropy[4], orders of magnitude larger than in the normal state.

We thank P. Högl for valuable discussions.


8:48AM X05.00005: Magnetic coupling between dopant atoms in superconducting doped topological insulators*  
CODY YOUMANS (Presenter), City College of New York, AREG GHAZARYAN, Physics, Institute of Science and Technology, Austria, POUYAN GAHEMI, City College of New York — Doped topological insulators have been shown to exhibit unconventional superconducting phases where novel bound states can occur at defects such as vortices. Recent experimental studies on Niobium-doped Bismuth Selenide have shown that the magnetic properties of dopant atoms can strongly affect the resulting superconducting phase. This effect is mainly due to the development of Yu-Shiba-Rusinov bound-states at the magnetic atoms and the coupling of such states through the superconducting environment. In this talk, we show that the doping level can critically affect the type of magnetic coupling between dopant atoms in superconducting doped topological insulators and thereby influence their magnetic and superconducting properties.

*National Science Foundation CREST Center for Interface Design and Engineered Assembly of Low Dimensional systems (IDEALS), NSF grant number HRD-1547830

9:00AM X05.00006: Superconductor Quasiparticles with Random Curvature, Robust Criticality, and T-Linear Resistivity  
SAYED ALI AKBAR GHORASHI, Physics, College of William & Mary, MATTHEW FOSTER (Presenter), Physics & Astronomy, Rice University — We study quenched random curvature disorder for 2D massless relativistic carriers. This describes a topological superconductor Majorana surface fluid with generic time-reversal invariant dirt. It should also apply to any non-topological Dirac or Majorana system in which the disorder is sufficiently smooth, as could be the case for d-wave quasiparticles in the cuprates with remote dopants.

Random curvature is strongly irrelevant at zero energy, but we show that it profoundly affects the finite-energy states. These are found to exhibit robust, universal criticality (see also Ghorashi, Liao, and Foster, PRL 2018). Our results imply that the local density of states imaged via STM would exhibit minimal spatial structure near zero bias, but robust, static and universal fluctuations over a large finite bias range.

We also consider a speculative connection to the pseudogap regime. Assuming that the superfluid component is quenched by phase fluctuations, we calculate the electrical conductivity. Preliminary results indicate linear-in-T resistivity, attributed to the crossover between ballistic and critical states at zero and finite-energy, respectively.

9:12AM X05.00007: Majorana bound states in magnetic skyrmions imposed onto a superconductor  
STEFAN REX (Presenter), IGOR V. GORNYI, ALEXANDER D. MIRLIN, Karlsruhe Institute of Technology — We consider a two-dimensional superconductor exchange-coupled to the magnetic texture of a close-by chiral magnetic layer. In particular, we study how magnetic skyrmions can induce the formation of Majorana bound states (MBS) in the superconductor, where we focus on realistic skyrmions with winding number one. We show that MBS are supported if a vortex is pinned to the skyrmion core. In addition, we consider a chain of skyrmions, which may host MBS at its ends. In light of recent experimental progress on the manipulation of skyrmions, such systems are promising candidates to achieve direct spacial control of MBS.
9:24AM X05.00008: Development of the Scanning Majorana Microscope*  ERIC GOODWIN (Presenter), MICHAEL GOTTSCHALK, Michigan State University, ALEX LEVCHENKO, University of Wisconsin-Madison, STUART HOLDEN TESSMER, Michigan State University — The Scanning Majorana Microscope (SMM) is being developed to provide novel ways for verification of the existence of Majorana zero modes. Inspired by a variety of scanning probe methods, the SMM consists of an aluminum quantum dot fabricated on the end of a sharp glass tip. By connecting the probe to an ultrasensitive charge-sensing circuit, the counting statistics of electrons entering the quantum dot can be characterized. It has been predicted theoretically that cases with and without Majorana coupling should exhibit qualitatively different full counting statistics of charge tunneling events despite the fact that differential linear conductance might have zero-bias features in both cases. Thus this microscope represents an important tool for detecting Majoranas going beyond existing experimental probes. Fabrication and preliminary measurements of the SMM will be presented.

*This work was supported by the U.S. Department of Energy, Basic Energy Sciences under Award DE-SC0017888.

9:36AM X05.00009: Local Andreev reflection induced by Chiral Majorana Fermions  ZHESHEN GAO (Presenter), KAM TUEN LAW, CHUI-ZHEN CHEN, Department of Physics, Hong Kong University of Science and Technology — When superconductivity is proximity induced into a quantum anomalous system, it is predicted to host Chiral Majorana Edge Modes(CMEMs), which would induce a unique half quantized plateau as its transport signature. This was recently found in the experiments[Science 357, 294 (2017)]. However, it was argued that without superconductivity, disorder alone could also induce such signature. Thus more experimental evidence is called to determine whether superconductivity was the actual factor. Here we proposed to use local tunneling spectroscopy to directly probe the edge state of the hybrid system. We used Non-Equilibrium Green's Function to show that for topological phase with chern number N=±1/2 which hosts 1/2 actual factor. Here we proposed to use local tunneling spectroscopy to directly probe the edge state of the hybrid system.

9:48AM X05.00010: Erasing odd-parity states in a semiconductor quantum dot coupled to a superconductor  PO ZHANG (Presenter), HAO WU, ZHAOEN SU, Department of Physics and Astronomy, University of Pittsburgh, ROK ZITKO, Department of Theoretical Physics, Jozef Stefan Institute, EDUARDO LEE, Department of Condensed Matter Physics, Universidad Autonoma de Madrid, DIANA CAR, Applied Physics, Eindhoven University of Technology, SÉBASTIEN PLISSARD, LAAS CNRS, MOIRA HOCEVAR, Institut NEEL CNRS, SASA GAZIBEgovIC, ROY OP HET VELD, GHADA BADAWY, ERIK P. A. M. BAKKERS, Applied Physics, Eindhoven University of Technology, SERGEY M FROLOV, Department of Physics and Astronomy, University of Pittsburgh — Andreev bound states (ABS) exhibit many similarities to Majorana bound states (MBS). It would be of interest to study ABS in the system where MBS may emerge. The knowledge of ABS in a single dot is also crucial to understand more complicated systems, such as an artificial NbTiN /InSb dot chain that emulates a 1D Kitaev model. Here we study the erasing of odd-parity ABS in a quantum dot with gate-tunable superconducting coupling. The dot is defined in an InSb nanowire/NbTiN superconductor hybrid system. Fine gates are used to tune the coupling, the barrier and the chemical potential. In weak coupling regime, a parity-changing pattern of ABS is observed inside the Coulomb diamonds. In strong coupling regime, the ABS pattern opens a gap and the odd-parity regime is ‘erased’ from the pattern. We study this transition with different source-drain bias, map the phase boundary between even/odd states in magnetic fields and compare it to a finite-size Majorana nanowire.

10:00AM X05.00011: Observing pairs of zero-bias states in three-terminal Superconductor-Semiconductor devices: Part I*  DENISE PUGLIA (Presenter), GIAN-LUCA ANSELMETTI, GERBOLD MENARD, FILIP MALINOWSKI, ESTEBAN A MARTINEZ, University of Copenhagen, JOON SUE LEE, SUKGEUN CHOI, MIHIR PENDHARKAR, University of California Santa Barbara, GEOFFREY C. GARDNER, SERGEI GRONIN, RAY KALLAHER, MICHAEL MANFRA, Microsoft, CHRIS PALMSTROM, University of California Santa Barbara, CHARLES M MARCUS, LUCAS CASPARIS, ANDREW P HIGGINBOTHAM, Microsoft — Majorana zero-energy modes located at the ends of topological superconductors are an appealing platform for topological quantum computing. Zero-bias peaks (ZBPs) are ubiquitously observed in tunneling spectroscopy of hybrid superconductor-semiconductor nanowires, consistent with expectations for Majorana modes. However, the emergence of those zero-energy modes in pairs at the ends of 1D topological superconductors is a central -- and so far untested -- prediction. Enabled by recent materials breakthroughs in selective area growth (SAG), we demonstrate a platform for testing this prediction by probing the conductance matrix of a three-terminal InAs wire proximitized by Al. We introduce the measurement technique and study correlations of sub-gap states at zero field, finding evidence of localized states at the wire ends and delocalized bulk states. Correlated, zero-bias features emerging in finite field at both ends of the device will be presented in Part II.

*This work was supported by Microsoft Project Q, the Danish National Research Foundation and the Villum Foundation.
Observing pairs of zero-bias end states in three-terminal superconductor-semiconductor nanowires, consistent with expectations for Majorana modes. However, the emergence of those zero-energy modes in pairs at the ends of 1D topological superconductors is a central -- and so far untested -- prediction. Enabled by recent materials breakthroughs in selective area growth (SAG), we demonstrate a platform for testing this prediction by probing the conductance matrix of a three-terminal InAs wire proximitized by Al. We perform tunneling spectroscopy independently on both ends of the wire as a function of longitudinal magnetic field and voltage. ZBPs emerge which are correlated and robust for these parameters.

*This work was supported by Microsoft, the Danish National Research Foundation and the Villum Foundation.
Session X06 DCMP: Quantum Phase Stability and Criticality: Theory BCEC 109A

8:00AM X06.00001: Superconductivity from quantum fluctuations of itinerant quantum critical points* YUNCHAO HAO (Presenter), YANG QI, Physics, Fudan University, KAI SUN, Physics, University of Michigan — In the vicinity of a quantum critical point, critical fluctuations can often act as glue for the formation of BCS pairs, which is one important path way towards unconventional superconductivity. Recently, thanks to the development in quantum numerical techniques, such as sign-problem quantum Monte Carlo simulations, new insights and unbiased numerical understanding about this phenomenon become accessible. In particular, the numerical results suggest superconductivity emerged from these quantum critical points are highly diversified and are highly sensitive microscopic details. In this study, we investigate these systems utilizing analytic approach. By exploring different model systems and compare with numerical results, we aim at understanding universal properties behind these diversified behaviors.

*This work is supported by Minstry of Science and Technology of China under grant numbers 2015CB921700, and by National Science Foundation of China under grant number 11874115.

8:12AM X06.00002: Characterizing the quantum critical point between a Dirac spin liquid and an antiferromagnet* ERIC DUPUIS (Presenter), WILLIAM WITCZAK-KREMPA, Universite de Montreal — The spin-1/2 kagome Heisenberg antiferromagnet hosts a putative quantum spin liquid phase for which a candidate ground state is the Dirac spin liquid. At low energies, this state is described by quantum electrodynamics in 2+1 dimensions with 2 Nf = 4 flavors of two-component gapless spinons. We describe a transition to a coplanar antiferromagnetic (AFM) phase by coupling the spinons to a vectorial bosonic order parameter. We find a non-trivial quantum critical point and compute critical exponents using a one-loop d=4-ε expansion. The compactness of the U(1) gauge field allows topological configurations named monopoles which must condense to induce the AFM phase. We classify the monopole operators by their isospin and compute their contributions to the AFM critical behavior. The agreement between our results and other model systems will be discussed.

*This work is supported by Minstry of Science and Technology of China under grant numbers 2015CB921700, and by National Science Foundation of China under grant number 11874115.

8:24AM X06.00003: Quantum Criticality in the Two-Dimensional Periodic Anderson Model* THOMAS SCHAEFER (Presenter), CPHT, Ècole Polytechnique, ANDREY A. KATANIN, Institute of Metal Physics, Ekaterinburg, MOTOHARU KITATANI, ALESSANDRO TOSCHI, KARSTEN HELD, Institute of Solid State Physics, TU Wien — Despite the fascinating phenomena accompanying a quantum critical point, e.g. non-Fermi liquid behavior, a general theory for quantum phase transitions is lacking. In this talk, I will present a step forward by analyzing results from the dynamical vertex approximation, a cutting-edge quantum field theoretical method including temporal as well as spatial correlations. Within this framework, I will analyze the fundamental model of strongly correlated heavy fermion compounds, the periodic Anderson model. By varying the hybridization strength of localized f-electrons and itinerant d-electrons, and a careful analysis of response functions, one can trace the change in the ground state from an antiferromagnet to a paramagnetic Kondo insulating phase, resembling the famous Doniach phase diagram. Eventually, I will show the evolution of the critical exponents of the magnetic susceptibility, which are changing from the one of free spins γ=1 to γ=2 in the quantum critical regime. T. Schäfer, A. Katanin, K. Held, and A. Toschi, PRL 119, 046402 (2017), T. Schäfer, A. Katanin, M. Kitatani, A. Toschi, and K. Held, in preparation.

*This work is supported by Minstry of Science and Technology of China under grant numbers 2015CB921700, and by National Science Foundation of China under grant number 11874115.

8:36AM X06.00004: Quantum critical scaling beyond Ginzburg-Laudau-Wilson paradigm in heavy-fermion metals YUNG-YEH CHANG (Presenter), National Chiao Tung University, STEFAN KIRCHNER, Department of Physics, Zhejiang Institute of Modern Physics, CHUNG-HOU CHUNG, National Chiao Tung University — Within the standard bosonic Ginzburg-Landau-Wilson (G-L-W) theory of phase transitions, the hyperscaling ansatz exists only below the upper critical dimension (d+z < 4) with d being spacial dimension and z being the dynamical exponent. Surprisingly, however, we show that the hyperscaling ansatz can survive above the upper critical dimension (d+z > 4) in an effective field theory of a large-N approach to the Kondo-Heisenberg lattice model, relevant for describing a wide range of heavy-fermion materials. A novel Bose-Fermi effective field theory is constructed beyond our large-N saddle-point solution. Via perturbative renormalization group approach, a nontrivial interacting Gaussian fixed point is discovered due to the presence of a boson-fermion (Yukawa) coupling in our field theory, giving rise to novel hyperscaling relations beyond the G-L-W paradigm. The outstanding open issues on the singular-in-temperature behaviors for the specific heat coefficient and the Gruneisen ratio in the strange metal regime observed in heavy-fermion metal Ge-substituted YbRh2Si2 are well accounted for within our theory. The implications of our results to heavy-fermion quantum criticality, in general, are discussed.

*This work is supported by National Science Foundation of China under grant number 11874115.
8:48AM X06.00005: Exact non-linear I-V curve near two-channel Kondo-Luttinger quantum critical point  CHAO-YUN LIN (Presenter), YUNG-YEH CHANG, Department of Electrophysics, National Chiao-Tung University, Hsinchu, Taiwan, R.O.C., COLIN RYLANDS, NATAH ANDREI, Department of Physics, Rutgers University, Piscataway, New Jersey, U.S.A., CHUNG-HOU CHUNG, Department of Electrophysics, National Chiao-Tung University, Hsinchu, Taiwan, R.O.C. — It has been known since 1990’s that a Kondo impurity coupled to Luttinger liquid wire undergoes an exotic quantum phase transition with decreasing Luttinger parameter $K$ (or increasing electron interactions) from the 1-channel to 2-channel Kondo ground states at $K=1/2$. However, the quantum critical properties near this transition is still not known to date due to lack of controlled theoretical tools to examine the physics near the strong coupling 2-channel Kondo fixed point. In this paper, we address this long-standing issue via bosonization-refermionization approach near 2-channel Kondo state. We overcome the problem by mapping the system at the Toulouse point onto an effective two-lead free fermion model subject to a local tunneling. Remarkably, the non-equilibrium transport of the system is exactly solvable in this limit. An analytic form for the non-linear differential conductance is obtained. Our results offer an unique example of exactly and analytically accessible non-equilibrium transport near a quantum critical point; they are relevant for the recent experiment in a dissipative Kondo dot.

9:00AM X06.00006: Thermodynamic properties of 3D plaquette antiferromagnet  GUANG YU SUN (Presenter), NUSEN MA, Chinese Academy of Science, ANDERS W SANDVIK, Boston University & Chinese Academy of Science, ZI YANG MENG, Chinese Academy of Science — We design a 3D checker-board J-Q model to capture phase transitions between a plaquette-singlet solid with lattice translational symmetry breaking to a 3D Neel phase with spin rotational symmetry breaking. The system is investigated via unbiased large-scale quantum Monte Carlo simulation. We use Binder cumulant to determine the finite temperature phase boundary and measure the specific heat and magnetic susceptibility to reveal the nature of the different phases and their transitions. Our results are closely related with the on-going experimental effort in pressure-induced magnetic phase transitions in Shastry- Sutherland (SS) compound SrCu$_2$(BO$_3$)$_2$.

9:12AM X06.00007: Emergence of non-Fermi liquid dynamics through nonlocal correlations in an interacting disordered system*  SUDESHNA SEN (Presenter), School of Physics, University College Dublin, Ireland, N S VIDHYADHIRAJA, Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, MARK JARRELL, School of Physics and Astronomy, Louisiana State University — We provide strong evidence for a quantum critical point (QCP) associated with the destruction of Kondo screening in the Anderson-Hubbard model for interacting electrons with quenched disorder. The evidence comprises three elements: (a) the identification of an energy scale, that delineates infrared Landau damping from higher frequency non-Fermi liquid (nFL) dynamics; (b) the finding that this crossover scale appears to vanish with increasing disorder; and (c) the concomitant appearance of a finite intercept in a broad distribution of Kondo scales. Our findings indicate a Kondo destruction scenario, albeit distinct from the local QCP picture. The nFL behavior is shown to stem from an interplay of strong electron-electron interactions and the systematic inclusion of short-range dynamical fluctuations induced by the underlying random potential. The results have been obtained through a computational framework based on the typical medium dynamical cluster approximation.

*Irish Research Council Laureate Awards Programme, IRCLA/2017/169

9:24AM X06.00008: U(N)/U(m)U(N-m) nonlinear sigma model: critical behavior and a physical realization*  DA WANG (Presenter), Nanjing University — The nonlinear sigma model defined on the Grassmann manifold U(N)/U(m)U(N-m) is a direct generalization of the widely studied $\mathbb{C}P^{N-1}$ model. In space dimension $2<d<4$, we use 1/N expansion technique to obtain its critical exponents including two-particle ones, which are found to be only functions of $m/N$ up to the first order. As a result, larger $m$ effectively reduces $N$ and thus brings stronger fluctuations. Next, we show such a model is a low energy description of the SU(N) Hubbard model which has been realized in cold atom experiments. With determinant quantum Monte Carlo simulations of the half-filled SU(6) Hubbard model on the square lattice, we have found strong evidences of a continuous quantum phase transition from the antiferromagnetic to valence bond solid states as $U$ increases. Such a phase transition is described by the U(6)/U(3)U(3) nonlinear sigma model.

*NSFC (Nos. 11504164, 11574134)
9:36AM X06.00009: Phase transitions in the "easy plane" JQ model*  NISHEETA DESAI (Presenter), RIBHU KAUL, University of Kentucky — We study the JQ model on the square lattice after adding to it "easy plane" terms that explicitly break the SU(2) symmetry of the original model. The Néel to VBS transition is believed to be continuous for the full SU(2) symmetric model. In the easy-plane limit, this model was shown to have a first order transition between the superfluid and the VBS phases. We use Stochastic Series Expansion Quantum Monte Carlo to investigate the nature of this transition for various strengths of this easy-plane anisotropy. We find that the first order nature of the transition weakens as we weaken the strength of the easy-plane interaction. However, we find no evidence that this transition becomes continuous before the SU(2) symmetric point.

*NSF DMR-1611161, XSEDE DMR-140061

9:48AM X06.00010: Phase diagram of effective model for twisted bilayer graphene at particle-hole symmetric point

YUAN DA LIAO (Presenter), Institute of physics, Chinese Academy of Sciences, XIAO YAN XU, Department of Physics, Hong Kong University of Science and Technology, ZI YANG MENG, Institute of physics, Chinese Academy of Sciences — We study an effective extended Hubbard model on the honeycomb lattice with two orbitals per site at the particle-hole symmetry filling. The tight-binding part of the model is believed to describe the low-energy electronic properties of the twisted bilayer graphene. Using large-scale projection quantum Monte Carlo method, we map out the ground state phase diagram of the model, the novel properties of electrons in the presence of non-local (plaquette) interaction, are revealed with high accuracy.

10:00AM X06.00011: Renormalization group analysis of phase transitions in the two dimensional Majorana-Hubbard model*

KYLE WAMER (Presenter), IAN AFFLECK, Stewart Blusson Quantum Matter Institute and the Department of Physics and Astronomy, University of British Columbia — A lattice of interacting Majorana modes can occur in a superconducting film on a topological insulator in a magnetic field. The phase diagram as a function of interaction strength for the square lattice was analyzed recently using a combination of mean field theory and renormalization group methods, and was found to include second order phase transitions. One of these corresponds to spontaneous breaking of an emergent U(1) symmetry, for attractive interactions. Despite the fact that the U(1) symmetry is not exact, this transition was claimed to be in a supersymmetric universality class when time reversal symmetry is present and in the conventional XY universality class otherwise. Another second order transition was predicted for repulsive interactions with time reversal symmetry to be in the same universality class as the transition occurring in the Gross-Neveu model, despite the fact that the U(1) symmetry is not exact in the Majorana model. We analyze these phase transitions using a modified ε-expansion, confirming the previous conclusions.

*This research was supported by NSERC of Canada and the QuEST Program of the Stewart Blusson Quantum Matter Institute.

10:12AM X06.00012: Imaginary-spin-bond order induced by a magnetic field

MENGXING YE (Presenter), ANDREY CHUBUKOV, University of Minnesota — We show that a 2D fermion system with well separated electron and hole pockets may develop a time-reversal symmetric directional imaginary-spin-bond order. It emerges when some interactions are repulsive and some are attractive. Moreover, we demonstrate that this order is necessarily triggered by a magnetic field, even if the order at zero field is a conventional spin-density-wave state. We show that a finite field linearly couples the bond order to the spin-density-wave order. We also discuss the ways to probe such an order in experiments.

10:24AM X06.00013: Nonthermal states in nonintegrable magnetic models*

NEIL ROBINSON (Presenter), Institute for Theoretical Physics, University of Amsterdam, ANDREW J JAMES, Physics, University College London, GIUSEPPE BRANDINO, exact-lab, ROBERT KONIK, Condensed Matter Physics & Material Science, Brookhaven National Lab — There is a new paradigm emerging for quantum systems: those which are nonintegrable but nevertheless possess nonthermal states embedded throughout their many-body spectrum (whose number is polynomial in the system size). The presence of such states violates a strong version of the eigenstate thermalization hypothesis, and the behaviour expected for generic nonintegrable systems, such as thermalization, can be broken. Why such nonthermal states appear in certain models is currently not understood, although recent works have drawn analogies with the physics of "quantum scars". We show that nonthermal states, extending far into the many-body spectrum, can arise in simple magnetic (continuum and lattice) models that exhibit confinement and the associated formation of "meson-like" excitations. As a result, certain quenches in these models do not lead to thermalization and the nonequilibrium dynamics of local observables can show persistent, long-lived oscillations.

*NJR is supported by the EU Horizon 2020 MSCA grant No. 745944. RMK is supported by the US DOE, Office of BES, under Contract No. DE-SC0012704. AJAJ is supported by the EPSRC, grant no. EP/L010623/1.
10:36AM X06.00014: Spin echoes in disordered Hubbard models  
TASNEEM BIADSY (Presenter), YOAV SAGI, NETANEL LINDNER, Physics Department, Technion - Israel Institute of Technology — We study spin-echo signals in disordered Hubbard models. We numerically show that the spin echo signal is characterized by a timescale which depends non-monotonically on disorder strength through the many-body localization transition. Our results yield a tool for detecting the transition which is based on short time evolution, making it efficient numerically and an attractive tool for experimental implementation.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X07 DCMP: Novel Approaches to Studying Quantum Matter  
BCEC 109B - Laurel Winter, Los Alamos National Laboratory

8:00AM X07.00001: Boson-Fermion Duality in Four Dimensions*  
TAKUYA FURUSAWA (Presenter), YUSUKE NISHIDA, Tokyo Institute of Technology — In this talk, we propose a novel boson-fermion duality in four space-time dimensions by generalizing the lattice construction approach [1], which was applied to derive 3D boson-fermion duality [2]. Our analysis suggests that the Abelian Higgs model of $\theta=\pi$ is equivalent to a free Dirac fermion. The phase transition between topological and trivial insulators on the fermion side is dual to that between Higgs and confined phases on the boson side. Moreover, the Dirac fermion corresponds to a three-body bound state of one Higgs boson and two dyons in the bosonic theory.


*This work was supported by JSPS KAKENHI Grants No. JP15K17727 and No. JP15H05855.

8:12AM X07.00002: Monte Carlo Study of Compact Quantum Electrodynamics at larger Fermion Flavors  
WEI WANG (Presenter), BEIJING NATIONAL LABORATORY FOR CONDENSED MATTER PHYSICS AND INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCE, CHONG WANG, PERIMETER INSTITUTE FOR THEORETICAL PHYSICS, ZI YANG MENG, BEIJING NATIONAL LABORATORY FOR CONDENSED MATTER PHYSICS AND INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCE — Based on our development in quantum Monte Carlo (QMC) technique (arXiv:1807.07574), the compact U(1) lattice gauge theory coupled to fermionic matter at (2+1)D is now accessible with large-scale numerical simulations, and the phase diagram as a function of fermion flavor and the strength of gauge fluctuations is mapped out. Here we focus on the large fermion flavor case ($N_f \geq 8$), where the deconfine-confine phase transition is investigated in detail. In the deconfine phase, fermions coupled to the fluctuating gauge field to form U(1) spin liquid and in the confined phase, fermions are gapped out into valence bond solid. The different behaviors in terms of gauge flux, spectral of gauge-invariant observables as well as the deconfine-confine phase transition (QED3-Gross-Neveu-type) are presented.

8:24AM X07.00003: Exact Results on Itinerant Ferromagnetism and the 15-puzzle Problem*  
ERIC BOBROW (Presenter), KEATON STUBIS, YI LI, Johns Hopkins University — We apply a result from graph theory to prove exact results about itinerant ferromagnetism. Nagaoka's theorem of ferromagnetism is extended to all non-separable graphs except single polygons with more than four vertices by applying the solution to the generalized 15-puzzle problem, which studies whether the hole's motion can connect all possible tile configurations. This proves that the ground state of a $U \to \infty$ Hubbard model with one hole away from the half filling on a 2D honeycomb lattice or a 3D diamond lattice is fully spin-polarized. Furthermore, the condition of connectivity for $N$-component fermions is presented, and Nagaoka's theorem is also generalized to $SU(N)$-symmetric fermion systems on non-separable graphs.

*E. B. and Y. L. are supported by the U.S. Department of Energy, Office of Basic Science, Division of Materials Sciences and Engineering, Grant No. DE-FG02-08ER46544.
**8:36AM X07.00004: The Fermion Bag Approach to Hamiltonian Theories**  
EMILIE HUFFMAN (Presenter), Physics, Perimeter Institute, SHAILESH CHANDRASEKHARAN, Duke University — Quantum Monte Carlo (QMC) methods, when applicable, offer dependable ways to extract the nonperturbative physics of strongly-correlated many-body systems. However, there are some formidable bottlenecks to the applicability of these methods such as the sign problem and algorithmic update inefficiencies. Using the t-V model Hamiltonian, we demonstrate how the fermion bag approach--originally developed in the context of Lagrangian lattice field theories--led to the first sign problem solution for this model. We then show how using fermion bag ideas to develop a new efficient QMC algorithm to study the t-V model allowed us to compute critical exponents for the chiral Ising universality class (involving one flavor of four-component Dirac fermions) that seem to be more reliable than those from previous QMC calculations. Finally, we discuss how the fermion bag approach offers certain advantages to the study of other models involving Dirac fermions and also extends to fermion-spin interactions and $Z_2$ gauge theories.

**8:48AM X07.00005: Fracton and Holography**  
HAN YAN (Presenter), Okinawa Institute of Science and Technology — We propose that the fracton topological order is a class of toy models for holography. The discovery of AdS/CFT correspondence as a concrete construction of holography, and the subsequent developments including the Ryu-Takayanagi formula of entanglement entropy have revolutionized our understanding of quantum gravity, and provided a powerful tool set for solving various strongly-coupled quantum field theory problems. In this work we discuss a classical toy model based on fracton topological order, a class of exotic many-body systems with boundary area law of ground state degeneracy and (partially) immobile excitations. We show that such a model defined on the hyperbolic lattice satisfies some key properties of holographic correspondence. These properties include: the AdS-Rindler reconstruction is realized; the mutual information obeys the Ryu-Takayanagi formula, and a naively defined black hole's entropy scales as its horizon area.

*HY is supported by the Theory of Quantum Matter Unit at Okinawa Institute of Science and Technology, and the Japan Society for the Promotion of Science (JSPS) Research Fellowships for Young Scientists.

**9:00AM X07.00006: Monte Carlo Study of Compact Quantum Electrodynamics with Fermionic Matter: the Parent State of Quantum Phases**  
YANG QI (Presenter), Department of Physics, Fudan University, XIAO YAN XU, Department of Physics, Hong Kong University of Science and Technology, LONG ZHANG, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, FAKHER ASSAAD, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, CENKE XU, Department of Physics, University of California, Santa Barbara, ZI YANG MENG, Institute of Physics, Chinese Academy of Sciences — The interplay between lattice gauge theories and fermionic matter accounts for fundamental physical phenomena ranging from the deconfinement of quarks in particle physics to quantum spin liquid with fractionalized anyons and emergent gauge structures in condensed matter physics. Here we show that the problem of compact U(1) lattice gauge theory coupled to fermionic matter in (2+1)D is possible to access via sign-problem-free quantum Monte Carlo simulations. One can hence map out the phase diagram as a function of fermion flavor and the strength of gauge fluctuations. By increasing the coupling constant of the gauge field, gauge confinement in the form of various spontaneous symmetry breaking phases such as valence bond solid (VBS) and Néel antiferromagnet emerge. Deconfined phases with algebraic spin and VBS correlation functions are also observed. Such deconfined phases are an incarnation of exotic states of matter, i.e. the algebraic spin liquid, which is generally viewed as the parent state of various quantum phases. The phase transitions between deconfined and confined phases, as well as that between the different confined phases provide various manifestations of deconfined quantum criticality.

**9:12AM X07.00007: Hidden SU(2) Symmetries, Symmetry Hierarchy and Emergent Eight-Fold-Way in Spin-1 Quantum Magnets**  
HUI-KE JIN (Presenter), YI ZHOU, JIAN-JIAN MIAO, Physics Department, Zhejiang University — The allowed largest symmetry in quantum spin-1 systems is SU(3) rather than spin rotational SO(3). In this work, we study some SU(2) symmetries as subgroups of the SU(3), which was not bewared in literature to the best of our knowledge. We construct two-body Hamiltonians where these SU(2) symmetries are respected, and explore the ground phase diagram according to the symmetry hierarchy SU(3)/SU(2)×U(1). It is natural to treat the eight generators of the SU(3) symmetry on an equal footing, called eight-fold-way. And possible experimental consequences are discussed as well.

*YZ is supported by National Key Research and Development Program of China (No.2016YFA0300202), National Basic Research Program of China (No.2014CB921201), National Natural Science Foundation of China (No.11774306), the Key Research Program of the Chinese Academy of Sciences (Grant No. XDPB08-4) and the Fundamental Research Funds for the Central Universities in China. J.J.M is supported by Postdoctoral Science Foundation of China (No.119103S284).
9:24AM X07.00008: Numerically study the conformality of Q-state 1+1D quantum Potts model at Q>4  HAN MA  
(Presenter), University of Colorado, Boulder, YIN-CHEN HE, Perimeter Institute — The existence of complex conformal field theory (CFT) is proposed to be a mechanism of weak first order phase transition featuring extremely slow renormalization group flow with approximate scale invariance. We numerically study the simplest platform of this physics — the Q-state 2D Potts model when Q>4. We find that the properties of the phase transition are well captured by the complex CFTs. The central charge and conformal tower are extracted and studied. We also analyze how these data rely on length scale using conformal perturbation theory away from the nearby complex CFT.

9:36AM X07.00009: Slow scrambling in a quantum rotor model with random exchange interactions  DAN MAO  
(Presenter), DEBANJAN CHOWDHURY, SENTHIL TODADRI, Physics, MIT — In recent years, out-of-time-order correlation functions (OTOC) have been used to diagnose the onset of information scrambling in a wide class of problems, ranging from black holes to interacting field theories and lattice models. We study the OTOC for a solvable model of a large number (N) of M-component quantum rotors coupled by Gaussian-distributed random, infinite-range exchange interactions [1]. At a finite temperature above the quantum critical point separating a spin-glass and a paramagnetic phase, there is no exponential growth of the OTOC of the rotor fields. We show that in this large N, M limit, the random rotor model is integrable, and can be described by random matrix theory. The apparent lack of quasiparticle excitations in this limit arises as a result of disorder averaging and not strong interactions. We also compute the leading 1/M contribution to the OTOC of the rotor fields and find a slow exponential growth.

9:48AM X07.00010: Superfluidity without Condensation  ANTHONY HEGG (Presenter), Shanghai Jiao Tong University, WEI KU, Tsung-Dao Lee Institute — The connection between superfluidity and Bose-Einstein condensation (BEC) is well studied in 3D, but it is untenable in 2D due to the lack of condensation in such systems. We develop a new microscopic theory that exhibits low temperature superfluidity on a 2D lattice despite the lack of condensation and show that it has surprising properties. Fluctuations play a key role in the stability of this superfluid, and it is more robust than superfluidity in the presence of a BEC. Finally, we discuss the application of this mechanism to produce superfluidity in a 3D system.

10:00AM X07.00011: Numerically efficient parquet-equations solver for correlated electron systems*  CHRISTIAN ECKHARDT (Presenter), ANNA KAUCH, Institut für Festkörper Physik, TU Wien, GIULIO A.H. SCHOBER, CARSTEN HONERKAMP, Theoretical Solid State Physics, RWTH - Aachen, KARSTEN HELD, Institut für Festkörper Physik, TU Wien — The parquet equations are a set of self-consistent equations for the effective interaction vertex of an interacting many-fermion system [1]. Their numerical solution has, however, been plagued by the extreme memory consumption of the vertex functions, even for small systems. We use the truncated-unity method, previously developed in the context of the functional renormalization group (fRG), to approximate the complex emergent momentum structure of the vertex [2]. There, the full momentum dependence of the vertex is projected onto few formfactors. By these means, we can reduce the memory needed to solve the parquet equations by several orders of magnitude. This makes the parquet-approach a useful tool to calculate two particle properties in the parquet approximation and as nonlocal corrections to Dynamical Mean Field Theory (DMFT) calculations (parquet Dynamical Vertex Approximation)[3]. We will show results for the two-dimensional Hubbard model and comparisons with the ladder-Dynamical Vertex Approximation and fRG methods.


*Fonds zur Förderung der wissenschaftlichen Forschung (FWF) project P 30997

10:12AM X07.00012: ABSTRACT WITHDRAWN —
10:24AM X07.00013: Fibonacci Topological Superconductor  YICHEN HU (Presenter), CHARLES KANE, University of Pennsylvania — In this talk we will present a model of interacting Majorana fermions that describes a superconducting phase with a topological order characterized by the Fibonacci topological field theory. Our theory, which is based on a SO(7)\textsubscript{1}/(G\textsubscript{2})\textsubscript{1} coset factorization, leads to a solvable one dimensional model without parafermions that is extended to two dimensions using a network construction. In addition, we predict a closely related "anti-Fibonacci" phase, whose topological order is characterized by the tricritical Ising model. We will show that Majorana fermions can split into a pair of Fibonacci anyons, and propose an interferometer that generalizes the Z\textsubscript{2} Majorana interferometer and directly probes the Fibonacci non-Abelian statistics.

10:36AM X07.00014: Nonlocal probes for strongly-correlated quantum phases  BARBARA CAPOGROSSO-SANSONE (Presenter), FABIO LINGUA, Clark University, WEI WANG, Max Planck Institute for the Physics of Complex Systems, LIANA SHPANI, Clark University — In this talk, we propose non-local probes to study correlations in lattice bosons. We argue that these probes can be used as an alternative to characteristic quantum phases. We use Path-Integral Monte-Carlo and define the proposed probes in terms of the geometric braiding in world-line configurations. We show that these probes can be used as alternatives to local order-parameters in certain known phase transitions. Further, we describe a framework which links these probes (based on braiding properties of in world-line configurations) to entanglement in hardcore lattice bosons.

10:48AM X07.00015: Effective spin-orbit models using correlated first-principles wave functions*  YUEQING CHANG (Presenter), LUCAS WAGNER, Department of Physics, University of Illinois at Urbana-Champaign — In recent years, spin-orbit effects have been used to design and predict new emergent phases in condensed matter systems. Most of the theory has been done at the level of band structure. It is of high current interest how to extend these ideas to correlated electron systems. We present a new computational technique that uses first-principles quantum Monte Carlo calculations to address spin-orbit effects efficiently while also treating electron correlation accurately. To test this technique, we perform benchmark calculations in atomic systems and monolayer tungsten disulfide. The calculated results of the spin-orbit splittings in these systems agree with the experimentally determined values. This new tool allows us to investigate electron-electron interaction, spin-orbit effects and one-body terms on the same footing in realistic materials, with a cost similar to the standard fixed-node diffusion Monte Carlo.

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

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X08 DCMP: Superconductivity: Odd-Frequency, Non-Centrosymmetric and Other Exotic States  BCEC 150 - Stuart Brown, Univ of California - Los Angeles

8:00AM X08.00001: The Effect of Antisymmetric Spin-Orbit Coupling on the Superconducting Order Parameter in Noncentrosymmetrical Superconducting PbTaSe\textsubscript{2} Single Crystal*  CONG REN (Presenter), Physics, Yunnan University — In superconducting material without an inversion center of symmetry the spin degeneracy of the conducting band is lifted by an antisymmetric spin orbit coupling (ASOC). As a consequence, spin and parity cannot be seperately used to classify the Cooper pairing states. The superconducting order parameter is generally a mixture of spin singlet and triplet pairing states. However, such spin mixture state has rarely been revealed in weakly correlated noncentrosymmetrical superconductors. In this talk, we report a pressure-dependent point contact Andreev reflection measurement on high quality single crystals of the noncentrosymmetrical superconductor PbTaSe\textsubscript{2}. The experimental result reveals the effects of ASOC on the superconducting order parameter of PbTaSe\textsubscript{2}.

*This work is supported by the National Science Foundation of China (11574373, 11774303).
In the normal state, spin current generated by RSOI was studied analytically and found to be proportional to $J^2$. For the electrical spin generation, the Edelstein-effect with Rashba spin-orbit interaction (RSOI) is a representative one. Spin current play an important role and there are several methods to make spin current, for example, spin Hall effect and spin pumping. As for the electrical spin generation, the Edelstein-effect with Rashba spin-orbit interaction (RSOI) is a representative one. In the normal state, spin current generated by RSOI was studied analytically and found to be proportional to $J^2$. And as for non-centrosymmetric superconductors with RSOI, there is a previous theoretical work about Edelstein-effect [2], which is focusing on the temperature region slightly below the superconducting critical temperature and chemical potential well above the band crossing point. Here we study the magnetization and spin current produced by the super current in 2D non-centrosymmetric superconductors with RSOI for the whole region of temperature and chemical potential. We have found the highly efficient spin supercurrent generation when the electron density is small.


8:24AM X08.00003: Occurrence of Non-Centrosymmetric Superconductivity by Tuning the Antisymmetric Spin-orbital Coupling in La(Pt$_x$Si$_{1-x}$)$_2$ Thin Films

YUNBO OU (Presenter), Plasma Science and Fusion Center and Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, JIAN LIAO, Department of Physics, University of Texas at Dallas, CIGDEM OZSOY-KESKINBORA, School of Engineering and Applied Sciences, Harvard University, STEPHAN KRAEMER, Center for Nanoscale Systems, Harvard University, DAVID BELL, School of Engineering and Applied Sciences, Harvard University, XIAOYAN SHI, Department of Physics, University of Texas at Dallas, JAGADEESH MOODERA, Department of Physics, Massachusetts Institute of Technology — The physical properties of solid compounds are governed by the symmetry of their crystal structure. In superconductors, an unconventional mixed-parity pairing which is neither spin singlet nor triplet state can emerge due to Fermi surface splitting caused by the absence of inversion symmetry. The complicated spin structure originating from mixed-parity pairing can cause topologically nontrivial surface or edge states in non-centrosymmetric superconductors. In this work, La(Pt$_x$Si$_{1-x}$)$_2$ thin films have been grown by systematically varying $x$ from 0 to 0.68 by MBE technique. The superconductivity has been observed up to 2.60 K by transport measurement. The increasing concentration of Pt tends to suppress the transition temperature. Furthermore, incorporating Pt without changing the crystal structure can continuously tune the strength of the asymmetric spin-orbital coupling (ASOC) in La(Pt$_x$Si$_{1-x}$)$_2$ thin films, which thereby results in a non-centrosymmetric superconductor with multiple unconventional phases. Our work could facilitate the search for topologically nontrivial surface or edge states in non-centrosymmetric superconductors.

*National Science Foundation (NSF-DMR 1700137), Office of Naval Research (N00014-16-1-2657), and Center for Integrated Quantum Materials (DMR-1231319).

8:36AM X08.00004: Fermi surface instabilities of spin-orbit-coupled metals

TILMAN SCHWEMMER (Presenter), DOMENICO DI SANTE, MARIO FINK, XIANXIN WU, WERNER R HANKE, RONNY THOMALE, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg — The pursuit of novel phases in correlated electron systems, such as possibly topological instances of unconventional superconductivity, must consider multiple energy scales including interaction strength, electronic band width, and, in particular, spin-orbit coupling (SOC). While density functional theory and related ab initio techniques can provide a detailed description of a materials electronic structure that can carefully account for the effects of SOC, it is necessary to additionally refine quantum many body techniques to study Fermi surface instabilities in the presence of SOC. Starting from a picture of itinerant electrons, we study the effect of electronic correlations on the Fermi surface via renormalization group techniques. Combining ab initio electronic structures with perturbative and functional renormalization group calculations, we develop the toolbox to analyse a plethora of symmetry breaking phases arising from the interplay of SOC, fermi surface topology, and electronic correlations.

*This work is supported by ERC-StG-TOPOLECTRICS-336012 and DFG-SFB 1170 (Project B04)

8:48AM X08.00005: Superconducting pairing transition tuned by structural distortions in strong spin-orbit coupled systems

AUSTIN LINDQUIST (Presenter), HAE-YOUNG KEE, Physics, University of Toronto — Strong spin-orbit coupled systems have been gaining increased attention, as they may host exotic phases such as spin liquids and topological superconductors. In particular, Sr$_2$IrO$_4$ has been suggested as a potential candidate for a high temperature d-wave superconductor. However, these materials have strong spin-orbit couplings, and the electronic band structures are sensitive to the structural distortions such as the rotation and tilting of the octahedral cages. Here, we study the effects of these structural distortions on pairing instabilities, and present the transitions between spin-singlet and spin-triplet pairings tuned by structural distortions. Testing our proposals using a series of superlattices is also discussed.
9:00AM X08.00006: Singlet-Quintet Mixing in Superconductors with $j=3/2$ Fermions*  JIABIN YU (Presenter), CHAO-XING LIU, Pennsylvania State University — Recently, a new pairing state with the mixing between s-wave singlet channel and isotropic d-wave quintet channel induced by centrosymmetric spin-orbit coupling has been theoretically proposed in the superconducting materials with $j = 3/2$ electrons. It is the first realistic proposal of the mixing between different spin channels that preserves the inversion symmetry in solid state systems. As physical consequences, the singlet-quintet pairing mixing can give rise to topological nodal-line superconductivity and surface Majorana flat bands. In this talk, the singlet-quintet-mixed state will be reviewed. Moreover, its experimental signatures, including spin susceptibility, upper critical field, disorder effect and surface local density of states, will be discussed.

*We acknowledge the support from the Office of Naval Research (Grant No. N00014-15-1-2675 and renewal No. N00014-18-1-2793) and the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under award No. DE-SC0019064.

9:12AM X08.00007: Odd-frequency pairing in a superconductor coupled to two parallel nanowires  CHRISTOPHER TRIOLA (Presenter), ANNICA M BLACK-SCHAFFER, Department of Physics and Astronomy, Uppsala University — We study the behavior of Cooper pair amplitudes that emerge when a two-dimensional superconductor is coupled to two parallel nanowires, focusing on the conditions for realizing odd-frequency pair amplitudes in the absence of spin-orbit coupling or magnetism. In general, any finite tunneling between the superconductor and the two nanowires induces odd-frequency spin-singlet pair amplitudes in the substrate as well as a substantial odd-frequency interwire pairing. Since these amplitudes are odd in spatial parity, they do not directly impact the local observables. However, in the regime of strong superconductor-nanowire tunneling, we find that the presence of two nanowires allows for the conversion of non-local odd-frequency pairing to local even-frequency pairing. By studying this higher-order symmetry conversion process, we are able to characterize the effect of the odd-frequency pairing in the superconductor on local quantities accessible by experiments. Specifically, we find that odd-frequency pairing has a direct impact on the local density of states of the superconductor and on the maximum Josephson current, measurable using Josephson scanning tunneling microscopy.

9:24AM X08.00008: Odd-frequency spin-triplet superconductivity in two dimensional disordered electron liquid.*  VLADIMIR ZYUZIN (Presenter), ALEXANDER FINKELSTEIN, Texas A&M University — In this work we theoretically study the odd-frequency spin-triplet superconductivity in disordered two dimensional electron liquid. We propose a pairing mechanism based on the interplay of screened Coulomb interaction and the interference of electrons due to the impurity scattering. The mechanism suppresses possible attraction in the singlet part of the Cooper channel, and depending on the ratio of repulsive interaction in the charge and spin channels, it results in attraction between electrons in the odd-frequency spin triplet part of the Cooper channel. Being derived for the metallic phase of the system, it can be relevant for the metal to insulator transition point.

*This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0014154

9:36AM X08.00009: Odd frequency Berezinski pairing and cross junction coherence in Josephson effect.*  ALEXANDER BALATSKY (Presenter), Nordita, SERGEY PERSHOGUBA, Physics, Yale University, CHRISTOPHER TRIOLA, Physics, Uppsala University — Odd frequency or Berezinski pairing state is now claimed to be present in multiple heterjunctions. We now demonstrate the emergence of odd-frequency pair amplitudes as a cross junction Berezinski coherence in conventional Josephson junctions. We considerate both in the absence of a voltage (DC effect) and in the presence of a finite voltage (AC effect). In both cases, we find that Berezinski interlead pairing emerges whenever a Josephson current is expected to flow. Additionally, we show that the interlead spin-susceptibility is directly influenced by the presence of the odd-frequency pair amplitudes. Specifically, we find that the spin-susceptibility is suppressed when the odd-frequency component is the largest. By establishing a novel link between the physics of Josephson junctions and Berezinski pairing, we extend the notion of Berezinski pairing to cross junction coherences and to conventional Josephson effect.

*Work supported by KAW 2013.0096 and Villum Center of Excellence for Dirac Materials.
Study of chiral d-wave superconductor candidate URu$_2$Si$_2$ by using scanning SQUID microscopy

YUSUKE IGUCHI (Presenter), IRENE ZHANG, Department of Applied Physics, Stanford University, Stanford, California 94305, USA, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, KATHRYN ANN MOLER, Department of Applied Physics, Stanford University, Stanford, California 94305, USA — The heavy electron superconductor URu$_2$Si$_2$ has been extensively studied since the transitions of its hidden order and superconducting state were reported by the specific heat measurement in 1985[1]. Recent studies of thermal conductivity[2] and optical Kerr measurement[3] on URu$_2$Si$_2$ have shown evidence of chiral d-wave superconductivity. The chiral d-wave order superconductivity has also been suggested by a theoretical calculation of the magnetic excitation spectrum[4]. A chiral superconductor is expected to show chiral edge current modes analogous to a topological insulator. In order to search for evidence of chiral superconductivity in URu$_2$Si$_2$, we will report a study of the local superconducting and local charge current states of URu$_2$Si$_2$ single crystals using a scanning SQUID microscope.


Ir d-band derived superconductivity in the lanthanum-iridium system LaIr$_3$ system*

NEEL HALDOLAARACHCHIGE (Presenter), Physical Sciences, Bergen Community College, LESLIE SCHOOP, Princeton University, MOJAMMEL ALAM KHAN, Physics, Louisiana State University, WENXUAN HUANG, Department of Mat. Sci. and Eng., Massachusetts Institute of Technology., HUIWEN JI, Princeton University, KALANI HETTIARACHCHILAGE, Physics, The Collage of New Jersey, DAVID P YOUNG, Physics, Louisiana State University — Here, we have reported the synthesis and characterization of LaIr$_3$, which displays superconductivity below $T_c = 3.3$ K.

LaIr$_3$ is a superconductor where the bands near the Fermi surface are dominated by Ir 5 d states that are strongly affected by SOC. Thus, it is one of the few examples of a lanthanide-based superconductor where 5 d electrons play the dominant role in the superconductivity. The superconducting parameters obtained from physical properties measurements of LaIr$_3$ suggest that it is a weakly-coupled BCS-type superconductor. These results motivate future work focused on exploring intermetallic Ir-based superconductors that form in noncentrosymmetric structure types. Strong SOC in these systems would then be antisymmetric, which often leads to exotic and unconventional superconductivity.

*DPY acknowledges support from the NSF through Grant No. DMR-1306392.

Low-Energy Quasiparticle Excitations in Half-Heusler Superconductors with $j = 3/2$ Fermions

KOTA ISHIHARA (Presenter), TAKAAKI TAKENAKA, YIJIE MIAO, YUTA MIZUKAMI, University of Tokyo, OREST PAVLOSIUK, PIOTR WISNIEWSKI, DARIUSZ KACZOROWSKI, Polish Academy of Sciences, TAKASADA SHIBAUCHI, University of Tokyo — In noncentrosymmetric half-Heusler compounds where the strong spin-orbit coupling causes a band inversion, fermions with total angular momentum $j = 3/2$ contribute mainly to the transport phenomena, including the superconductivity. Interestingly, Cooper pairs formed by the $j = 3/2$ fermions can form not only usual singlet and triplet states but also even-parity quintet and odd-parity septet states. Recently, it has been reported that the temperature dependence of magnetic penetration depth shows a power-law behavior in YPtBi, which suggests an unconventional nodal gap structure. Several theories with the quintet or septet pairings have been proposed to explain this result, whereas it is still experimentally unclear whether the reported nodal structure is universal or not in the non-magnetic half-Heusler superconductors with $j = 3/2$ fermions. To study the gap structure in several half-Heusler superconductors, we have measured the magnetic penetration depth on YPtBi, LuPtBi, and LuPdBi with different spin-orbit coupling strength. Our data suggest the existence of gap minima rather than nodes in all the materials, which strongly indicates that the nodal structure is not protected by symmetries. Based on these results, we discuss the pairing symmetry of these half-Heusler compounds.
10:24AM X08.00013: Nonlinear susceptibility of unconventional superconductors* DAMJAN PELC (Presenter), ZACHARY ANDERSON, BIQIONG YU, SAJNA HAMEED, MARTIN GREVEN, University of Minnesota — Nonlinear magnetic response can be used to investigate several important features of superconductors: the pre-pairing regime above $T_c$, the superconducting gap features through the low-temperature nonlinear Meissner effect, and time-reversal symmetry. Based on our work on the superconducting precursor in oxides [1,2], we present complementary experiments on a wide range of conventional and unconventional superconductors. Several characteristic types of behavior are observed, including mean-field Ginzburg-Landau nonlinear response, an inhomogeneity-dominated precursor, and strong fluctuations not described by mean-field theory.


*This work was funded by the DOE through the University of Minnesota Center for Quantum Materials under DE-SC-0016371.

10:36AM X08.00014: Suppression of odd-frequency superconducting pairing by phase-disorder in a nanowire coupled to Majorana zero modes DUSHKO KUZMANOVSKI, ANNICA M BLACK-SCHAFFER, JORGE CAYAO (Presenter), Uppsala University — Majorana zero modes (MZMs) exhibit pure odd-frequency superconducting pairing correlations. Recently, it was reported that a robust odd-frequency superconducting pairing can be induced in a spin-polarized wire due to an array of MZMs, where their coupling to the wire was considered real.

Considering the physically more realistic case of complex coupling strengths that generically appear for varying system parameters, we demonstrate that all superconducting correlations, including odd-frequency, suffer a considerable suppression due to phase-disorder averaging. In the first part we, evaluate the $T$-matrix within the second Born approximation, and demonstrate exponential suppression of the electron-hole pairing with phase-disorder strength. In the second part, we perform numerical calculations on a tight-binding lattice model and study the effects of phase-disorder averaging on the local density of states and superconducting correlations.

We attribute the suppression of superconducting correlations in the wire to the filling of the energy gap by in-gap Andreev Bound States appearing due to phase-matching conditions between spatially-separated MZMs. Our work helps clarify the conditions favorable for practical realization of the proposed odd-frequency superconducting system.

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X09 DCMP: Topological Materials -- Thin Films BCEC 151A - Hang Chi, Massachusetts Institute of Technology - Tag(s): Focus

8:00AM X09.00001: Quantum transport in ultra-thin topological crystalline insulator films STEPHEN D ALBRIGHT (Presenter), Department of Physics, Yale University, FREDERICK J WALKER, CHARLES H AHN, Department of Applied Physics, Yale University — Recent developments have demonstrated the unique properties of conventional topological insulators, such as from dissipation-free transport and the creation of Majorana fermions by interfacing with superconductors, and offered a method for controlling them spatially with magnetic fields. Topological crystalline insulators (TCIs), such as SnTe, offer the same unique properties but an alternate mode of control: crystal symmetry breaking through strain or electric fields. Growth of TCIs thin and uniform enough to access these unique properties is challenging to achieve. This work presents structural and electronic characterization of ultra-thin SnTe films, down to 5nm, grown by molecular beam epitaxy on SrTiO$_3$ substrates. X-ray diffraction and atomic force microscopy reveal that SnTe films are single-domain and uniform, which is critical to realizing controllable topological properties. Quantum transport effects observed in magnetotransport measurements are consistent with the existence of topological states. To better understand their behavior and inform next steps towards their control, we extract details of the topological states by fitting the magnetotransport over a range of film thicknesses.
In topological crystalline insulators the topological conducting surface states are protected by crystal symmetry. Here, we show using scanning tunneling microscopy/spectroscopy that defects that break local mirror symmetry of SnTe suppress electron tunneling over an energy range as large as the bulk band gap, an order of magnitude larger than that produced globally via magnetic fields or uniform structural perturbations [1]. The results reveal the influence of various defects on the electronic properties, including screw dislocations, point defects, and tilt boundaries that lead to dislocation arrays that serve as periodic nucleation sites for pits grown on SrTiO3 [2,3].

Complementary ab initio calculations show how local symmetry breaking obstructs topological surface states as shown by a threefold reduction of the spectral weight of the topological surface states. The findings highlight the potential benefits of manipulating the surface morphology to create devices that take advantage of the unique properties of surface states and can operate at practical temperatures.


GdBi is an antiferromagnetic semimetal which has been proposed to have non-trivial band topology [1,2]. Despite attempts to experimentally observe its topological nature, it is challenging due to the large band overlap between the conduction and valence bands. Here we show via electrical transport measurements that quantum confinement can suppress the band overlap in GdBi thin films. The semimetallicity is lifted below a film thickness of approximately 8 crystallographic unit cells while the antiferromagnetic order is preserved down to our minimum thickness of 5 crystallographic unit cells. This is a step toward realizing a bulk insulating antiferromagnetic topological insulator, which can potentially realize a Chern insulating state in the monolayer limit.


Recent studies have shown that Rare-earth Bismuth (RBi) hosts topologically protected Dirac surface states [1,2]. However, spectroscopic measurements on bulk single crystals thus far have limited to (001) natural cleavage surface of RBi. Here we report the first successful realization and characterization of GdBi (111) films grown on BaF2 substrates with Molecular Beam Epitaxy. GdBi, in a bulk form, is a semimetal with type-II antiferromagnetic (AFM) order below $T_{N,bulk} = 28$ K. With torque magnetometry, we confirm that type-II AFM order is preserved in our films with a Neel temperature $T_{N,film} = 30$ K. From electrical transport measurements, we observe a non-linear Hall effect and non-saturating magnetoresistance, the characteristics of a compensated semimetallic electronic structure. Stabilization of GdBi (111) films enables previously unexplored studies of the interplay of symmetry-breaking and Dirac crossings on the (111) surface of RBi. We further anticipate a possible Chern insulator phase in the ultrathin limit, when quantum confinement lifts semimetallicity while retaining non-trivial band topology. Reference: [1] M. Zeng and C. Fang et al., arXiv:1504.03492 (2015), [2] J. Nayak et al., Nat. Comm. 8, 13942 (2017).
8:48AM X09.00005: Nanoscale Synthesis and Characterization of Topological Materials* [Invited] ILIJA ZELJKOVIC (Presenter), Boston College — Interest in the superconducting proximity effect (SPE) has recently been reignited by theoretical predictions that it could be used to achieve topological superconductivity. However, small proximity-induced gaps ($\Delta_{\text{ind}}$) of ~1 meV have predominantly been obtained so far using select few low-Tc superconductors. In this talk, I will discuss how we use a combination of molecular beam epitaxy and scanning tunneling microscopy/spectroscopy to study topological insulators grown on high-Tc superconductors Fe(Te,Se) and Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$. On the surface of Bi$_2$Te$_3$ grown on Fe(Te,Se), we detect $\Delta_{\text{ind}}$ as high as ~3.5 meV, which is the largest reported gap induced by proximity to an s-wave superconductor to-date. We find that $\Delta_{\text{ind}}$ exponentially decays with Bi$_2$Te$_3$ thickness, but remains finite even after the topological surface states had been formed. By imaging the scattering and interference of surface state electrons, we provide a microscopic visualization of the fully gapped Bi$_2$Te$_3$ surface state due to Cooper pairing. We contrast this observation with the lack of observed superconducting gap in Bi$_2$Te$_3$/Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ heterostructures. We conclude by discussing the roles of various parameters in driving the SPE effect across complex interfaces.

*We gratefully acknowledge the support from the Army Research Office Grant No. W911NF-17-1-0399 and the NSF-DMR Grant No. 1654041.

9:24AM X09.00006: In-situ analysis of MBE-grown ZrTe$_5$ thin films* TIMOTHY PILLSBURY (Presenter), ANTHONY RICHARDELLA, YANAN LI, NITIN SAMARTH, Department of Physics and Materials Research Institute, Pennsylvania State University — Originally of interest for its resistivity anomaly, ZrTe$_5$ has been predicted by recent theoretical work to be a quantum spin Hall insulator (QSHI) with band-gap of ~100meV [PRX 4, 011002 (2014)]. Additionally, bulk measurements of ZrTe$_5$ have shown a variety of states from a strong topological insulator (TI) to a weak TI and even a Dirac Semimetal depending on the experimental methods [Scientific Reports 7, 45667 (2017)]. This makes ZrTe$_5$ also interesting for studying the transition from a weak to strong TI. Since experiments so far have used films exfoliated from bulk crystals, they are complicated by the difficulty of exfoliating large area crystals. Moreover, rapid oxidization of ZrTe$_5$ films prevents thorough analysis of exfoliated thin films. To help elucidate the nature of the topological properties of ZrTe$_5$ and achieve a large band-gap QSHI, we have grown epitaxial thin films under ultra-high vacuum using molecular beam epitaxy (MBE) and performed in-vacuo analysis using ARPES and STM to confirm the growth quality and analyze the band structure, laying the groundwork for future MBE studies that utilize strain engineering to study the strong to weak TI transition and the observation of a large gap QSHI.

*Funded by 2DCC-MIP under NSF Grant No. DMR-1539916.

9:36AM X09.00007: Remote Doping of Sb Quantum Wells with Te RYAN P O’TOOLE, KAUSHINI WICKRAMASINGHE, TETSUYA D MISHIMA, MICHAEL SANTOS (Presenter), University of Oklahoma — Antimony (Sb) has topological surface states, but its bulk band structure is semimetallic. Our goal is to study the transport properties of the topological states by suppressing the bulk conductivity through quantum confinement and enhancing the surface conductivity through remote n-type doping. A series of Sb quantum-well structures was grown by molecular beam epitaxy with Al$_x$Ga$_{1-x}$Sb barrier layers and GaAs (111) substrates. The Sb layer thickness of 4 nm was chosen to be thin enough to open a bandgap in the bulk band structure. To populate the topological electron states in the Sb quantum well, a section of one Al$_x$Ga$_{1-x}$Sb barrier was doped with Te atoms, which act as donor impurities. We report on Hall effect measurements that characterize the effectiveness of our approach in increasing the contribution of topological surface states to the conductivity of the structure.
9:48AM X09.00008: Nanoscale strain induced effects on the optoelectronic properties of monolayer transition metal dichalcogenides. MARKUS TEAGUE (Presenter), JIAQING WANG, WEI-HSIANG LIN, DUXING HAO, CHEN-CHIH HSU, NAI-CHANG YEH, Physics, California Institute of Technology — We perform simulations and scanning tunneling spectroscopic (STS) studies of the strain effects on the optoelectronic properties of monolayer TMDC materials MS₂, where M = Mo and W. We use molecular dynamics to simulate the strain effect on MS₂ by relaxing a (60x60) nm² monolayer MS₂ sheet on top of a 2.5 nm radius semi-sphere gold nanoparticle. We find that the strain tensor component \( \varepsilon_{xy} \) changes between the top S-layer (positive) and bottom S-layer (negative), indicating the top S-layer experiences an effective stretching force whereas the bottom S-layer is compressed. For STS studies, high quality monolayer MoS₂ single crystals with areas to 200x200 nm² are synthesized by CVD and transferred to Si substrates with triangular arrays of nanostructures. Nanostructures are ~20 nm in size with a lattice constant of ~400 nm. Spatially resolved STS studies on the LDOS in MS₂ are carried out to investigate spatial variations resulting from strain and temperature evolution of the local electronic bandgap. Using a variable-wavelength light source, circularly polarized light is also applied to the sample under STS studies, and the spatially resolved LDOS in strained MS₂ are investigated as a function of temperature, optical wavelength and polarization. This work is supported by NSF and ARO.

10:00AM X09.00009: Electrical Transport Study in Wafer Scale Epitaxial WTe₂ Film Grown by Molecular Beam Epitaxy. JASON TRAN (Presenter), JUNXUE LI, JUSTIN HOROWITZ, JING SHI, PENG WEI, University of California, Riverside — WTe₂, a member of the layered transition metal dichalcogenides (TMDs), has recently garnered attention due to its topological properties. Current studies of WTe₂ have mainly focused on samples produced by mechanical exfoliation. Recent success has shown that WTe₂ is able to grow on graphene using molecular beam epitaxy (MBE). As a conducting layer, graphene may weaken or smear any signatures of topological transport in WTe₂. In this talk, we present our electrical transport studies in wafer scale WTe₂ grown on insulating sapphire substrate. The 1T' structural phase of the MBE grown samples is confirmed by in situ reflection high energy electron diffraction (RHEED). Electrical transport studies show a sharply enhanced magnetoresistance (MR) at low temperature. The MR has a clear linear magnetic field dependence over a range of magnetic fields up to 12 Tesla. In the low field regime, we observe signatures of weak antilocalization which suggest the presence of strong spin-orbit coupling. We will also present the effect of varying thickness of WTe₂ on magnetotransport, and discuss potential signatures related to topological order. *This work is supported by the Startup fund from University of California, Riverside.

10:12AM X09.00010: Epitaxial growth and electronic properties of 2D topological insulator 1T WSe₂. CHENHUI YAN (Presenter), HUIMING ZHANG, LIAN LI, Department of Physics and Astronomy, West Virginia University — Monolayer 1T WSe₂ has recently been predicted to be a two-dimensional topological insulator (2D TI) with a larger bulk bandgap than 1T WTe₂, more preferable for practical applications. However, the energetically stable structure of WSe₂ is the 2H phase, and hence the 1T WSe₂ doesn't exist in the bulk. Here, we report the molecular beam epitaxial growth of monolayer 1T WSe₂ on epitaxial graphene/SiC(0001). We find the growth of homogeneous monolayer WSe₂ is strongly dependent on the substrate temperature: while the 1T phase can be grown below 300, a mixed 1T and 1H is obtained with increasing substrate temperature, with a complete 1H phase formation above 400°C. Using scanning tunneling microscopy/spectroscopy and angle resolved photoemission spectroscopy, we determine a bulk bandgap of 130 meV in monolayer 1T WSe₂, almost twice that of 1T WTe₂ (70 meV). We further observe one-dimensional edge states within the bulk bandgap in tunneling spectroscopy, confirming that monolayer 1T WSe₂ is indeed a 2D TI. This research is supported by NSF (DMR-1734017). *This research is supported by NSF (DMR-1734017).
Effect of epitaxial strain on topological properties of LaSb

SHOAIB KHALID (Presenter), Department of Physics and Astronomy, University of Delaware — RARE-EARTH MONO-PNICTIDES DISPLAY INTERESTING PROPERTIES THAT INCLUDE EXTREME MAGNETORESISTANCE AND NON-TRIVIAL TOPOLOGICAL BAND STRUCTURES, YET HAVE SIMPLE CRYSTAL STRUCTURE. FOR INSTANCE, LaSb IS ON THE VERGE OF A TRANSITION FROM TRIVIAL TO NON-TRIVIAL TOPOLOGICAL SEMIMETAL, LABI BEING A NON-TRIVIAL SEMIMETAL, AND LAAS A TRIVIAL SEMIMETAL. SINCE THESE MATERIALS CAN BE EPITAXIALLY GROWN ON III-V SUBSTRATES AND, THEREFORE, EASILY INTEGRATED TO WELL-KNOWN ELECTRONIC MATERIALS, IT IS IMPERATIVE TO UNDERSTAND THE EFFECTS OF EPITAXIAL STRAIN ON THEIR BAND STRUCTURES AND TOPOLOGICAL PROPERTIES. USING DFT WITH THE HSE06 HYBRID FUNCTIONAL, WE STUDY THE EFFECTS OF EPITAXIAL STRAIN ON THE ELECTRONIC PROPERTIES OF THESE RARE-EARTH MONO-PNICTIDES. FOR EXAMPLE, WE FIND THAT AT AROUND 1.5% COMRESSIVE EPITAXIAL STRAIN THERE IS A BAND CROSSING BETWEEN La d band AND Sb p band NEAR THE Z POINT OF THE BCT BRILLOUIN ZONE OF STRAINED LaSb. THIS BAND CROSSING INDICATES A TOPOLOGICALLY NON-TRIVIAL BEHAVIOR OF LaSb UNDER APPLIED EPITAXIAL STRAIN. THESE RESULTS HELP UNDERSTANDING THE NOVEL TRANSPORT AND TOPOLOGICAL PROPERTIES OF EPITAXIALLY GROWN STRAINED THIN FILMS OF THESE RARE EARTH MONO-PNICTIDES.

*This work was supported by the U.S. Department of Energy Basic Energy Science program (DE-SC0014388).

Electric Field Tuned Quantum Phase Transition from Topological to Conventional Insulator in Few-Layer Na3Bi

JAMES COLLINS (Presenter), Department of Physics and Astronomy and Centre for Future Low Energy Electronics Technologies, Monash University, ANTON TADICH, Australian Synchrotron, LIDIA GOMES, JOÃO RODRIGUES, Department of Physics and Centre for Advanced 2D Materials, National University of Singapore, JOHN HELLERSTEDT, CHANG LIU, Department of Physics and Astronomy and Centre for Future Low Energy Electronics Technologies, Monash University, HYEJIN RYU, SHUJIE TANG, Lawrence Berkeley National Laboratory, WEIKANG WU, SHENGYUAN YANG, Singapore University of Technology and Design, SHAFFIQUE ADAM, Department of Physics and Centre for Advanced 2D Materials, National University of Singapore, SUNG-KWAN MO, Lawrence Berkeley National Laboratory, MARK T EDMONDS, Department of Physics and Astronomy and Centre for Future Low Energy Electronics Technologies, Monash University — Na3Bi in bulk is a zero-bandgap topological Dirac semimetal (TDS), but when confined to a few layers it is predicted to be a large-gap (~300 meV) topological insulator. Application of an electric field to few-layer Na3Bi has been predicted to drive a band inversion due to Stark effect and induce a topological phase transition, which could be the basis of a topological transistor. Here we demonstrate the growth of epitaxial few-layer Na3Bi via MBE, and probe its electronic structure and response to an electric field using scanning probe microscopy/spectroscopy (STM/STS) and angle-resolved photoelectron spectroscopy, and compare with results from DFT. Both monolayer and bilayer Na3Bi show bandgaps >300 meV in STS, and the observation of an edge state with exponential decay into the bulk confirms their topological nature, consistent with DFT. With application of an electric field via potassium doping or approach of the STM tip the bandgap can be tuned to semi-metallic and then re-opened to greater than 100 meV. The electric fields required to induce this transition are below the breakdown field of many conventional dielectrics, making the creation of a topological transistor based on a few-layer TDS within reach.

molecules binding to metallo-porphyrins can be probed with STM combined with DFT methods. The experimental STM images in the simulated images. Thus, our study shows that geometric structures of small molecules, binding to metallo-porphyrin on Au(111). We observed square ring, rectangular ring, and center-bright (STM) images at the single molecule level. Here, we present STM images of further systems, di, tri, and quadra-atomic systems such as oxygen delivery, muscle contraction, and synaptic transmission. Their geometrical structures such as reaction between small gas molecules and metallo-porphyrins play crucial roles in functional processes of biological systems such as oxygen delivery, muscle contraction, and synaptic transmission. Their geometrical structures such as tilted binding of NO to metallo-porphyrin have been recently confirmed by high-resolution scanning tunneling microscopy (STM) of metal-free naphthalocyanine (NPC) molecules adsorbed on Ag(111) surfaces. As guided by the theoretical predictions, at elaborately adjusted scanning temperature and bias, STM experiments achieve a direct visualization of the cis-intermediate. This work demonstrates a practical way to directly visualize elusive intermediates, which enhances understanding of the quantum dynamics of hydrogen atoms.

This work was supported by the NKR and DPC (2016YFA0202300, 2018YFA0305800), NNSFC (61390501, 61725107), SPRP of the CAS (XDB30000000), and by the U.S. DOE grant DE-FG02-09ER46554; computations were performed at NERSC.

Imaging Binding Structures of Small Molecules to Metallo-porphyrin Using Scanning Tunneling Microscopy

Minhui Chang (Presenter), Korea University, Yun Hee Chang, Na Young Kim, Kaist, Un Seung Jeon, Howon Kim, Kyung Min Kim, Korea University, Yong-Hyum Kim, Kaist, Se-Jong Kahng, Korea University — Binding reaction between small gas molecules and metallo-porphyrins play crucial roles in functional processes of biological systems such as oxygen delivery, muscle contraction, and synaptic transmission. Their geometrical structures such as tilted binding of NO to metallo-porphyrin have been recently confirmed by high-resolution scanning tunneling microscopy (STM) images at the single molecule level. Here, we present STM images of further systems, di, tri, and quadra-atomic small molecules, binding to metallo-porphyrin on Au(111). We observed square ring, rectangular ring, and center-bright structures for three different small molecules. With the help of density functional theory (DFT) calculations, we reproduce the experimental STM images in the simulated images. Thus, our study shows that geometric structures of small molecules binding to metallo-porphyrins can be probed with STM combined with DFT methods.

Sub-Monolayer Annealed CuPc on Cu(111): Defect Hinderred Dynamic Clusters

William Huxter (Presenter), Jun Nogami, Chandra Veer Singh, Materials Science and Engineering, University of Toronto — Annealed sub-monolayer copper phthalocyanine on Cu(111) was studied with room temperature scanning tunneling microscopy (STM) and density functional theory (DFT). At coverages of 0.25 ML we observed that annealing produces a disordered cluster network of CuPc that attach together by forming C-C bonds across isoindole lobes. At lower coverages we find that smaller CuPc clusters (less than ~20 CuPc in size) are mobile on the Cu(111) surface. This dynamic motion was tracked by repeated STM image scans. Subsequent deposition of CuPc (without annealing) produced a Cu(111) surface covered with highly mobile single CuPc molecules and less mobile CuPc clusters. This enabled resolution of surface defects that were found to immobilize the CuPc clusters through a defect pinning mechanism.

9:24AM X10.00006: Structure and electronic properties of end states of self-assembled 1D covalent molecular chains on Au(111)  
ALEX CAHLIK (Presenter), JOHN HELLERSTEDT, MARTIN SVEC, V M SANTHINI, Institute of Physics, ASCR, v.v.i., SIMON PASCAL, Aix Marseille Université, CNRS, CIaNAM UMR, SIGUIOUR INGÉ ERLINGSSON, School of Science and Engineering, Reykjavík University, KAREL VYBORNÝ, Institute of Physics, ASCR, v.v.i., OLIVIER SIRI, Aix Marseille Université, CNRS, CIaNAM UMR, PAVEL JELÍNEK, Institute of Physics, ASCR, v.v.i. — One-dimensional structures offer a rich ecosystem for realizing quantum states with potential application for advanced information technologies. Surface confined molecular self-assembly is one avenue for creating 1d systems, where the extent structure is controlled by the precursor shape, and functional group interlinking chemistry. Here we study self-assembled 1d chains of zwitterionic molecule bis-bidentate ditopic (DABQDI) on Au(111) in ultrahigh vacuum, measured at 5K using combined scanning tunneling and non-contact atomic force microscopies (STM/ nc-AFM). Submolecular resolution achieved with a CO-functionalized tip offers detailed structural information, specifically regarding the unusual hydrogen bonds linking the precursor units. In-gap electronic states near the Fermi energy are observed via scanning tunneling spectroscopy (STS), strongly localized to the chain ends. We present our latest efforts to understand and simulate the observed structures via density functional theory (DFT) and nc-AFM simulations, and rationalize the observed electronic properties via modelling inspired by the Su, Schrieffer, Heeger (SSH) one-dimensional tight binding model.

9:36AM X10.00007: Long-Range Energy Level Shifts Induced by Single Impurity Molecules in C60 Thin Films  
ERIK MÅRSELL (Presenter), BINGKAI YUAN, KATHERINE COCHRANE, MIRIAM D. DEJONG, DAVID J. JONES, University of British Columbia, MORITZ RIEDE, University of Oxford, SARAH BURKE, University of British Columbia — Organic photovoltaics (OPV) is a promising technology for low-cost, flexible solar cells with low embodied energy. However, the efficiency remains low due to high exciton binding energies. The main driving force behind exciton dissociation is the energy landscape around the donor-acceptor interface. To optimize device efficiency, we therefore need to better understand the pathways of exciton dissociation at interfaces in OPV materials and how they correlate with the energy landscape. We use scanning tunneling microscopy and spectroscopy to study model systems consisting of thin films of C60 with single molecules of pure and fluorinated zinc phthalocyanine (ZnPc, F4ZnPc, and F8ZnPc) added. We measure how a molecule affects the energy levels in the surrounding C60 matrix; they shift by up to 150 meV depending on the degree of fluorination of the impurity molecule. This shift prevails over at least several C60 molecules from the impurity. This large and long-range shift induced by the phthalocyanine, and heavily influenced by the fluorine atoms, opens up new possibilities for controlled design of the energy landscape in the OPV heterojunction to optimize charge transfer efficiency.

NATHANIEL RAIMBAULT (Presenter), MARIANA ROSSI, Fritz-Haber Institute — Anharmonic contributions to vibrational Raman spectra of molecular crystals can be decisive to identify the structure of different polymorphs. In this work we characterise the low-frequency Raman spectral region of different polymorphs of the flexible aspirin and paracetamol crystals. We include anharmonicities through the time-correlation formalism, combining ab initio molecular dynamics and density-functional perturbation theory (DFPT) implemented in a full-potential, all-electron framework [1]. Lattice expansion and anharmonic thermal nuclear motion strongly affect the collective vibrations of the low-frequency region. This effect is much less pronounced at higher frequencies. We obtain excellent agreement with experimental lineshapes, highlighting the necessity of going beyond the harmonic approximation. In order to bypass the cost of DFPT evaluations of the polarizability tensor, we employ different forms of Kernel Ridge Regression (KRR) and discuss their efficiency. Training our models on several hundreds of points, we reproduce Raman spectra that would otherwise require the calculation of tens of thousands of points. This technique is extended to surface-sensitive vibrational sum-frequency generation.

10:00AM X10.00009: Evaluation of Pulay forces due to change in overlap of subspace-projection orbitals in constrained DFT: Application in calculation of reorganization energy of adsorbed molecule*  SUBHAYAN ROYCHOUDHURY (Presenter), DAVID D. O’REGAN, STEFANO SANVITO, Trinity College Dublin — Total energy of a constrained DFT calculation depends on population of subspace(s). When such subspace is defined in terms of orbitals localized on host atoms, ionic translations change the overlap of corresponding projection orbitals generating unconventional Pulay terms. We derive an exact expression for such Pulay terms maintaining non-orthogonality of projection orbitals. The corrected forces are implemented in the linear scaling DFT code ONETEP and, in conjunction with constrained DFT, are used to calculate the reorganization energy of a pentacene molecule adsorbed on a graphene flake. We show that subspace population depends on the choice of projection orbitals centred on a given set of host atoms and that non-orthogonal Wannier functions offer more precise results compared to pseudo-atomic orbitals. Our calculations of reorganization energy, performed by including ensemble DFT, correction for periodic boundary conditions and dispersion corrections show that, in general, reorganization energy of an adsorbed pentacene is lower than that of one in gas phase. This is consistent with effect of steric hindrance.

*We acknowledge funding from European Research Council project QUEST.

10:12AM X10.00010: Impacts of Electrostatic Screening and Interfacial Charge Transfer on Molecular Donor-Acceptor Heterojunctions Studied by Scanning Probe Microscopy/Spectroscopy*  ANDREW TAN (Presenter), PENGPENG ZHANG, Department of Physics and Astronomy, Michigan State University — A common need in organic electronics is the thorough understanding and control of the electronic structures and interfacial properties of molecular thin films on inorganic substrates. However, when donor (D) and acceptor (A) molecular heterojunctions are concerned, the interfacial charge transfer effects can compete with intermolecular charge transfer, which, along with the electrostatic effects from the substrate, exerts a significant substrate perturbation on the heterojunction. Employing archetypal D and A organic molecules and a variety of different supporting substrates, we show that the presence of the substrate, even a weakly interacting one, can still significantly perturb the intrinsic properties of the D-A heterojunction via interfacial charge transfer. Furthermore, substrate electrostatic screening can be modulated by interfacial charge transfer. This study highlights the impacts of the substrate electrostatic environment and the interfacial coupling on molecular electronic structures, an essential aspect in the applications of organic and molecular electronic devices.

*This work is funded by the U. S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0019120, and DE-SC0006400 (Early Career Research Program).

10:24AM X10.00011: Spectroscopic evidence of two-impurity Kondo effect in potassium doped p-sexiphenyl films on Au (111)  YAJUN YAN (Presenter), WEI CHEN, MINGQIANG REN, YILIN ZHANG, TONG ZHANG, DONGLAI FENG, Fudan University — Molecular magnetism is usually observed in organic coordination compounds consisting of transition metals or rare-earth metals, while it is rare in transition metal free or full-shell molecules. In this work, we grow high-quality p-sexiphenyl (PSP) monolayer film on Au (111) substrate, and then doped it with potassium (K) atoms. Various ordered phases are observed, with different structural and electronic properties. For a particular ordered phase, we observe obvious Kondo resonance peaks in isolated/misarranged PSP molecules, but clear splitting of such peaks is observed in PSP dimers. These phenomena share strong similarities to the two-impurity Kondo effect. Combined with theoretical calculation, we find that local spin is induced in PSP molecules by charge transfer from K atoms, leading to the appearance of Kondo resonance and the magnetic interaction of two Kondo impurities. Such two-impurity Kondo effect has only been reported in quantum dot system or dilute adatoms system, but the splitting of the Kondo resonance peak is much smaller than in our PSP system, which is as large as 5 meV. Our study not only provides a new and simple platform for investigating the two-impurity Kondo effect, but also provides a new route to construct a Kondo lattice on metal substrate.

Friday, March 8, 2019 8:00 AM - 10:36 AM

Session X11 DMP DCMP: Transport in Nanostructures -- Nanoscale Transport II  BCEC 152 - Xuan Gao, Case Western Reserve University - Tag(s): Focus
8:00AM X11.00001: Super-geometric transverse electron focusing on the hexagonal Fermi surface of PdCoO$_2$

PHILIP MOLL (Presenter), Ecole polytechnique federale de Lausanne, MAJA D BACHMANN, Max-Planck-Institute for Chemical Physics of Solids, AARON SHARPE, ARTHUR BARNARD, Stanford University, MARKUS KOENIG, Max-Planck-Institute for Chemical Physics of Solids, CARSTEN PUTZKE, Ecole polytechnique federale de Lausanne, SEUNGHYUN KHIM, ANDREW MACKENZIE, Max-Planck-Institute for Chemical Physics of Solids, DAVID GOLDHABER-GORDON, Stanford University — Single crystals of PdCoO$_2$ can be easily synthesized at remarkably high quality. At low temperatures, the mean-free-path of this most conductive oxide exceeds 20μm, reflected by its ultra-low residual resistivity of 8 nΩcm. This high conductivity gives rise to different transport regimes, spanning from ballistic transport to hydrodynamic transport regimes. Its ballistic transport is highly unusual, owing to its peculiar Fermi surface resembling an almost perfect hexagon. We fabricate ballistic structures for transverse electron focusing from as-grown single crystals via focused ion beam machining, and demonstrate magnetic focusing up to 20μm. Compared to typically studied materials with circular Fermi surfaces, the transverse focusing amplitude is strongly enhanced owing to its large parallel sections. We demonstrate this focusing enhancement experimentally, and corroborate it by transport simulations.

8:12AM X11.00002: Direct Growth of Vertically Aligned Carbon Nanotube Arrays on Stainless Steel and Their Field Emission Properties*

ARUN THAPA (Presenter), WENZHI LI, Physics, Florida International University — We report the growth of VACNT arrays on stainless steel (SS) via dc plasma enhanced chemical vapor deposition without the use of a metal catalyst layer. TEM and AFM examinations revealed the occurrence of nano-hills formed on the SS surface during the heating process in an NH$_3$ environment, which is a critical step for the uniform growth of VACNTs. The particles on the tips of most of the VACNTs were found to be single crystalline Fe metal, although a few other VACNTs were found to have alloy of Fe, Ni, Mn, and Cr at their tips. Field emission (FE) performance of a dense array of VACNTs was enhanced by changing the array morphology through a simple water treatment process. The FE performance was further enhanced by coating the exterior of CNTs with a layer of crystalline SnO$_2$ nanoparticles of 4.18 nm in diameter. The enhancement of FE performance was ascribed to the morphological change and mechanical strength reinforcement of VACNTs by the SnO$_2$ coating process. The characteristic features of the sample as the conductive substrate, ohmic contact between the VACNTs and the substrate, and bundled morphology resulted in a lower turn-on and threshold electric field, higher field enhancement, and excellent emission stability.

*This work is supported by the NSF under grant DMR-1506640.

8:24AM X11.00003: The connection between enhanced phonon-exciton interaction next to localization centers and photoluminescence of few-body complexes in tungsten-based transition metal dichalcogenide monolayers.*

DINH VAN TUAN (Presenter), HANAN DERY, University of Rochester — Photoluminescence (PL) experiments in WSe$_2$ show that the neutral-exciton peak X0 in the charge-neutral regime is often accompanied by additional lower-energy peak. The spectral position of the peak is below X0 by one phonon energy. Recently, several groups reported on trion-exciton complexes in encapsulated WSe$_2$ [1,2,3,4,5], where once again, their PL spectra reveal that the peak attributed to the five-particle complex is one phonon energy below that of the biexciton. We show that these PL peaks stem from phonon-assisted recombination of excitons or biexcitons next to localized electrons (i.e., these are not real trions or trion-exciton complexes that can diffuse in the monolayer). We explain why the proposed PL mechanism is prevalent in these monolayers while being absent in absorption-type experiments [6], showing that it supports the observed PL dependences on temperature and background charge density.


*This work is supported by the Department of Energy, Basic Energy Sciences (DE-SC0014349).
8:36AM X11.00004: Synthesis, structure, and physical properties of carbon nanotubes filled with nickel sulfide nanowires*  
YUBA POUDEL (Presenter), WENZHI LI, Physics, Florida International University — We report a novel synthesis of carbon nanotubes (CNTs) filled with continuous nanowires of nickel sulfide via a chemical vapor deposition method. Pyrolysis of thiophene (C₄H₄S) on the nanoparticles of Ni catalyst can induce the simultaneous growth and filling of CNTs which can be well explained by a large volume expansion experienced by the Ni nanoparticles during the sulfidation reaction. Electron microscopy measurements reveal that most of the CNTs are completely filled with single crystalline nickel sulfide nanowires of several micrometers in length. We also validate that there exists a direct relationship between the concentration of catalyst precursor and the dimensions of nickel sulfide filled CNTs within a certain cut-off region. Besides, a simple sonication process can be a quick and reliable method to extract the filled CNTs from the substrate whereas the regrowth of nickel sulfide filled CNTs on the same layer of the catalyst particles ensure the recyclability of the synthesis technique. Fundamental physical properties of the nickel sulfide nanowire filled CNTs will also be presented.

*This work is supported by the National Science Foundation under grant DMR-1506640.

8:48AM X11.00005: Title: Refrigeration and thermometry for millikelvin and sub-millikelvin nanoelectronics.*  
JOSHUA CHAWNER (Presenter), IAN BRADLEY, ANTONY GUÉNAULT, Department of Physics, Lancaster University, DAVID GUNNARSSON, VTT Technical Research Centre of Finland Ltd, RICHARD HALEY, ALEXANDER JONES, YURI PASHKIN, Department of Physics, Lancaster University, JARI PENTTILA, Aivon Oy, JONATHAN PRANCE, Department of Physics, Lancaster University, MIKA PRUNNILA, VTT Technical Research Centre of Finland Ltd, LEIF ROSCHIER, Aivon Oy — Cooling electrons in a nanoelectronic device to a few milikelvin, and further into the microkelvin regime, is a longstanding challenge. Weak electron-phonon coupling at low temperatures creates a bottleneck in traditional cooling techniques [1]. Here we will present our approach to solving the problem: nuclear demagnetization refrigeration of on-chip copper to directly cool the electrons without intervening phonons [2]. Our method has achieved a base electron temperature below 1.3 mK, held for several 1000s. On-chip refrigeration could potentially provide improvements in the operation of quantum simulators, computers and metrology standards, and open a new regime for the study of electron transport in nanostructures and 2D materials. However, it will be necessary to couple the copper refrigerator to the system of interest and to employ non-invasive thermometry techniques. We will discuss our progress towards these goals, including the development of a single-electron thermometer that is measured by RF reflectometry and does not require galvanic connection between the cooled electron gas and the outside world.


*This research is supported by the U.K. EPSRC (EP/N019199/1)

9:00AM X11.00006: Modeling transport in phosphorus δ-doped silicon tunnel junctions*  
LEON MAURER (Presenter), MICHAEL MARSHALL, DEANNA CAMPBELL, LISA A TRACY, TZU-MING LU, DANIEL WARD, SHASHANK MISRA, Sandia National Laboratories — Electrical devices based on Si:P δ layers can be fabricated with atomic precision, which could allow for the fabrication of high-efficiency tunneling field effect transistors (TFETs). While great strides have been made in fabricating nanoelectronics from Si:P δ layers, there is little agreement about the electronic structure of the Si:P δ layers. Furthermore, the transport properties of only a few devices have been modeled. We use a scalable model to study transport in nanoscale tunnel junctions made from Si:P δ layers, and we show that the transport properties of tunnel junctions can provide insight into the electronic structure of Si:P δ layers. We also compare our model to experimental results and find good agreement.

*This work was supported by the Laboratory Directed Research and Development Program and was performed in part at the Center for Integrated Nanotechnologies, a US DOE Office of Basic Energy Sciences user facility. Sandia National Laboratories is managed and operated by National Technology and Engineering Solutions of Sandia LLC, a subsidiary of Honeywell International Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed do not necessarily represent the views of the DOE or the U.S. Government.
9:12AM X11.00007: Effect of electron-phonon interaction on the opto-electronic properties of semiconducting nanoparticles*  
HAN YANG (Presenter), University of Chicago, MARCO GOVONI, Materials Science Division, Argonne National Laboratory, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — We report on the impact of electron-phonon coupling on the opto-electronic properties of semiconducting nanoparticles. We used a newly developed first-principle method [1] based on many-body-perturbation-theory, which efficiently combines electron-electron and electron-phonon interaction without explicitly evaluating virtual electronic orbitals. The method is implemented in the WEST code [2]. In particular we discuss carbon-based nanoparticles and chalcogenide nanostructures.

*This work was supported by MICCoM, as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under contract number DE-AC02-06CH11357.

9:24AM X11.00008: Electronic noise due to temperature differences in atomic-scale junctions: beyond standard thermal and shot noises  
OFIR SHEIN-LUMBROSO, Department of Chemical and Biological Physics, Weizmann Institute of Science, LENA SIMINE, Department of Chemistry, University of Toronto, ABRAHAM NITZAN, Department of Chemistry, University of Pennsylvania, DVIRA SEGAL, Department of Chemistry, University of Toronto, OREN TAL (Presenter), Department of Chemical and Biological Physics, Weizmann Institute of Science — Since the discovery of electronic thermal and shot noise almost a century ago, these two forms of fundamental electronic noise have had an enormous impact on science and technology. Here, we report on a new version of electronic noise that is generated by temperature differences across nanoscale conductors, which we term ‘delta-T noise’. We experimentally demonstrate this noise in atomic and molecular junctions, and analyze it theoretically using the Landauer formalism. The delta-T noise reveals a peculiar combination of characteristics that makes it different from the known thermal noise and voltage-activated shot noise. This noise can be used to detect temperature differences across nanoscale conductors without the need for fabricating sophisticated local probes. Furthermore, delta-T noise should be considered when designing modern nanoscale electronics, since temperature gradients are often generated unintentionally across electronic components.


9:36AM X11.00009: Surface Plasmon Polaritons in Chalcogenides*  
CIGDEM OZSOY KESKINBORA (Presenter), KUNDAN CHAUDHARY, MICHELE TAMAGNONE, Harvard University, YUNBO OU, ARAVIND DEVARAKONDA, TAKEHITO SUZUKI, JOSEPH CHECKELSKY, JAGADEESH MOODERA, MIT, FEDERICO CAPASSO, DAVID BELL, Harvard University — The surface plasmon polaritons is a highly investigated field of research due to their high potential applications for sensors, information technologies, high resolution imaging, to name a few. These collective electron oscillations are common at metal dielectric interfaces. However, they also exist in highly doped semiconductors, conducting oxide systems, and in many other systems with high carrier mobility. This poses the question of whether such resonances can be observed at the insulator interfaces with these novel materials. Chalcogenides, the general name of sulfides, selenides, tellurides can show highly anisotropic crystal structures, that gives them exotic properties such as topological surface state, superconductivity or negative dielectric permittivity. It was shown that Bi₂Se₃ supports Dirac plasmons, but the Dirac state is not the only reason for the existence of plasmon resonance in Bi₂Se₃. This material also has highly anisotropic dielectric properties allowing surface plasmon excitations. It is not the only chalcogenide system that can support them. Here we show the electron energy loss spectroscopy and a finite difference frequency domain study for investigating Bi₂Se₃, and BaNbS.

*Supported by the Center for Integrated Quantum Materials, NSF Grant No DMR 1231319.
9:48AM X11.00010: Room Temperature Phonon Focusing As a Tool for Tuning Thermal Conductivity in Nanostructured Materials  GIUSEPPE ROMANO (Presenter), Department of Mechanical Engineering, Massachusetts Institute of Technology —

Phonon focusing arises from the anisotropy in the phonon dispersions in crystalline materials. This effect has been extensively studied at low temperatures in bulk materials, where relatively low phonon scattering rates lead long mean-free-paths (MFP) with respect to the material’s specimen [1]. Here we investigate this phenomenon at room temperature in Si nanostructured materials. These systems can have a feature size as small as a few nanometers thus are comparable with a large fraction of phonon MFPs. By using the MFP-Boltzmann transport equation [2], we compute heat transport of nanoporous materials with different crystal orientations with respect to the pore lattice, finding a significant variation in the thermal conductivity. These results illustrate a route for tuning thermal transport in nanostructured materials beyond shape optimization.


10:00AM X11.00011: Vertical p-n junction of a thermoelectric material investigated using photoemission technique  JIEUN LEE (Presenter), JINWOONG HWANG, MINHEE KANG, Pusan National University, KYOO KIM, Physics, POSTECH, HYEJIN RYU, KIST, SHUJE TANG, ALS, SUNGLAE CHO, Uwins, SUNG-KWAN MO, ALS, HO-SOON YANG, CHONGYU HWANG, Pusan National University — The thermoelectric materials can generate electricity out of heat when they form a p-n junction, connected to an electric circuit. Typically, such a junction is made of two pieces of a thermoelectric material that are doped by electrons and holes, respectively, and then put together. Here we report one of the plausible ways to prepare the p-n junction via the experimental investigation of the electron band structure of a thermoelectric material using photoemission technique.

10:12AM X11.00012: One-Dimensional Atomic Tellurium Chains in Boron Nitride Nanotubes: Synthesis and Devices  PAI-YING LIAO (Presenter), JINGKAI QIN, MENGWEI SI, Purdue University, SIQI ZHANG, YOKE KHIN YAP, Michigan Technology University, PEIDE (PETER) YE, Purdue University — Tellurium has a unique one-dimensional (1D) helical chain crystal structure. The adjacent tellurium atoms in a single chain are covalently bonded, and different chains interact with each other by van der Waals force to form planar and bulk crystal. As a narrow-bandgap p-type semiconductor, bulk tellurium has a direct bandgap of ~0.35 eV. Here, 1D atomic tellurium chains were grown inside the boron nitride nanotubes (BNNTs) whose inner diameter was only a few nanometers. 1D tellurium crystal was synthesized and grew along the direction of BNNTs due to the natural confinement of the BNNT physical structure. Raman spectroscopy and energy-dispersive X-ray spectroscopy (EDX) were utilized to characterize the tellurium crystal structure and guaranteed the high quality of the Te-BNNT samples. The electrical properties of Te-BNNT devices were studied by current-voltage measurement. The devices were fabricated by transferring Te-BNNTs onto SiO2/p++ Si substrate, Ar-SF6 dry etching, and deposition of metal electrodes on top of the nanotubes. The realization of BNNTs-capsulated tellurium chains enhanced the current capacity of tellurium crystal several times compared to bare tellurium nanowires.

10:24AM X11.00013: Single-molecule rectifiers based on voltage-dependent deformation of molecular orbitals in carbazole oligomers  TATSUHIKO OHTO (Presenter), Graduate School of Engineering Science, Osaka University, KEN ALBRECHT, Laboratory for Chemistry and Life Science Institute of Innovative Research, Tokyo Institute of Technology, RYO YAMADA, KEIGO MINODE, Graduate School of Engineering Science, Osaka University, KIMIHISA YAMAMOTO, Laboratory for Chemistry and Life Science Institute of Innovative Research, Tokyo Institute of Technology, HIROKAZU TADA, Graduate School of Engineering Science, Osaka University — Current-voltage characteristics of single molecule junctions are governed both by the energy level alignment of molecular orbitals with respect to the Fermi level of the electrodes and by the hybridization of electronic structures at the interface between the molecule and the electrodes. While there have been many studies on tuning the former, only a few works intended to control the latter. In the present study, we demonstrate that molecular junctions based on carbazole oligomers showed a current rectification behavior due to asymmetric-symmetric control of electronic hybridization between the molecule and electrodes at both terminals. The carbazole oligomers originally showed an asymmetric molecular orbital and, hence, electronic hybridization with the electrodes because of the electric dipole moment. Symmetric electronic hybridization was achieved when the applied electric field between electrodes deformed molecular orbital to be symmetric. This is a novel way to control charge transport in single-molecule junctions (R. Yamada et al., Nanoscale, in press).

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X12 DMP: Devices from 2D Materials -- Advanced Fabrication  BCEC 153A - Cui-Zu Chang, Pennsylvania State University - Tag(s): Focus
8:00AM X12.00001: Interlayer Excitons in Transition Metal Dichalcogenides Heterostructures* [Invited]  XIAOQIN (ELAINE) LI (Presenter), University of Texas-Austin — In van der Waals heterostructures formed by stacking two monolayers of transition metal dichalcogenides, interlayer excitons with long recombination lifetime represent the lowest energy optical resonances. In heterostructures created by using different material recombinations and different fabrication methods, interlayer exciton properties are drastically different. I will discuss the observation of multiple interlayer exciton resonances with either positive or negative circularly polarized emission in a MoSe$_2$/WSe$_2$ heterobilayer with a small twist angle created using the mechanical exfoliation and stacking method. We attribute these resonances to the ground state and excited states confined within the moiré potential. I will compare these experiments to those observed in a MoSe$_2$/WSe$_2$ heterobilayer created using the chemical vapor deposition method.

*This work is primarily supported by NSF MRSEC program DMR-1720595.

8:36AM X12.00002: Top-down nanopatterning of layered transition metal dichalcogenide heterostructures*  
PUFAN LIU (Presenter), TEODOR STANEV, Northwestern University, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, Japan, NATHANIEL STERN, Northwestern University — Nanostructured materials give rise to useful features such as size-dependent properties, interfacial phenomena, and edge effects, allowing optimization for opto-electronics. Although electron beam lithography has been widely used for top-down fabrication of nanostructures, translating this approach to the emerging class of 2D materials has challenges. Direct electron beam exposure on 2D materials can lead to non-reversible damage and degradation of optical and electronic properties. We show that e-beam damage can be significantly reduced on monolayer transition metal dichalcogenides by covering it with a thin hexagonal boron nitride layer. The reduced damage allows direct negative resist lithographic writing of sub-10nm nanostructure fabrication without impairing the monolayer optical and electrical properties.

*Work supported by the Office of Naval Research (N00014-16-1-3055).

8:48AM X12.00003: Optical Annealing of Graphene Oxide Thin Films*  
SHASHANK RAM NANDYALA (Presenter), JOSEPH MURPHY, MICHAEL A SEAS, VIVEK SANTOSH JAIN, SUBASH KATTEL, JON M PIKAL, PATRICK A JOHNSON, JOHN ACKERMAN, WILLIAM RICE, University of Wyoming — Graphene oxide (GO) can be converted to highly conductive reduced GO (rGO) via photochemical methods, solution chemistry, and high-temperature treatments. Specifically, highly localized, controllable laser-based annealing has been shown to create conductive patterns of rGO. This optically induced thermal transition is characterized by the ratio of $sp^2$-to-$sp^3$-hybridized carbon (using Raman spectroscopy) and electrical conductivity. Here, we show that circuit-like patterns of rGO can be created using a 532 nm laser at intensities of ~6 MW/cm$^2$. Using the integrated ratio of the GO $sp^2$ G-band (~1594 cm$^{-1}$) to $sp^3$ D-band (~1363 cm$^{-1}$), we show that the optically generated GO-to-rGO conversion is slower and more uniform in an argon environment than in vacuum, an observation we attribute to the greater thermal exchange created by the high heat capacity argon gas. We determine the GO-to-rGO transition temperature of our optical process using the ratio of the integrated Stokes to anti-Stokes peaks and find that this temperature is consistent with standard induction furnace rGO annealing. Our findings suggest that optically created circuits of conductive rGO can be reproducibly created from GO films.

*We acknowledge support of the UW School of Energy Resources.
9:00AM X12.00004: One-Dimensional Potential in Graphene  APOORV JINDAL (Presenter), AVISHAI BENYAMINI, Department of Physics, Columbia University in the City of New York, SAI SUNKU, Department of Applied Physics and Mathematics, Columbia University in the City of New York, YIHANG ZENG, Department of Physics, Columbia University in the City of New York, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, JAMES HONE, Department of Mechanical Engineering, Columbia University in the City of New York, CORY R DEAN, DIMITRI BASOV, ABHAY PASUPATHY, Department of Physics, Columbia University in the City of New York — With improvements in fabrication techniques, low-disorder graphene devices have been realized to study a variety of correlated physics including fractional quantum Hall effect, and Mott insulating behavior. One possibility for inducing new electronic phenomena is by the use of nanometer-scale one-dimensional potentials to define narrow channels in graphene sheets. Previous efforts to study such effects in graphene have relied on lithographic fabrication of narrow metal gates. Lithographic methods suffer from edge disorder and a resolution limited to tens of nanometers. In this talk, we describe the engineering of a 1D potential in graphene using a carbon nanotube (CNT) that is a few nanometers from the graphene surface. We will describe cryogenic magnetotransport measurements that indicate the presence of a one-dimensional mode in graphene under appropriate gating conditions from the CNT. Electronic 1D bound states are also predicted to cause plasmonic reflections. These have been observed with cracks, stacking faults, and wrinkles in graphene. Our system provides an ideal platform to probe these reflections with the CNT gate inducing a tunable 1D barrier in graphene. In this talk, we also report near-field optical microscopy measurements probing such plasmonic reflections.

9:12AM X12.00005: Two dimensional SrTiO3 membranes*  WEI GUO (Presenter), AGHAM POSADAS, ALEXANDER DEMKOV, ANUPAM ROY, AMRITESH RAI, OMAR MOHAMMED, SANJAY BANERJEE, KEVIN OLSSON, XIAOQIN (ELAINE) LI, University of Texas at Austin — Perovskite SrTiO3 (STO) exhibits a wide range of exciting phenomena in addition to being a common substrate in epitaxial growth of various oxides like LaAlO3, BaTiO3, etc. There is a growing interest in studying new physical phenomena happens in the oxide materials in the two dimensional limit. We developed an etching method to fabricate free-standing STO membranes. The membranes are typically 5-8 um wide and 10-20 um long with thickness ranging from two to several tens of nanometers. We use Micro-Raman spectroscopy to investigate the STO membranes’ vibrational spectra and compare with that of the bulk STO. To exploit the high dielectric constant of STO, we design and fabricate electronic devices combining STO membranes with other two dimensional materials such as graphene and h-BN.

*This research was partially supported by the National Science Foundation through the Center for Dynamics and Control of Materials: an NSF MRSEC under Cooperative Agreement No. DMR-1720595 and by the Air Force Office of Scientific Research under Grant FA9550-18-1-0053.

9:24AM X12.00006: Lithographically-defined strain control in atomically-thin semiconductors  LEO YU (Presenter), JINGYUAN LINDA ZHANG, Stanford University, SVEN BORGHARDT, Stanford University & Forschungszentrum Jülich, MINDA DENG, GEUN HO AHN, JELENA VUCKOVIC, Stanford University, TONY F HEINZ, Stanford University & SLAC National Accelerator Laboratory — Frontier quantum science calls for a large-scale deployment of solid-state artificial atoms, or quantum dots (QDs). But the progress has been limited due to the lack of simultaneous control of a material's bandgap spatially and in energy. Here, we present a new approach based on lithographically-defined strain to achieve control of both the spatial position and bandgap energy in atomically-thin semiconductors. In our method, we first suspend a monolayer over a nanoscale cavity in the substrate; we then deform the layer using high-pressure gas, atomic force microscopy or thermal molding. With an optimized new process, we have produced localized biaxial strain down to 40-nm widths at defined positions in a WSe2 monolayer and in other atomically-thin semiconductors. Tensile strains up to 3.5% have been achieved appropriate design of the cavity depth and can be maintained without any external pressure or voltage. Because of the strain-induced reduction in the bandgap, these QDs exhibit emission peaks spectrally separated from the intrinsic peaks by more than 100 meV. We discuss potential applications of such localized QD structures in 2D semiconductors.

9:36AM X12.00007: Design of Nanocarbon Electronic Devices for Single-Molecule Measurements  AMIRA BENCHERIF (Presenter), Biomedical Engineering, Universite de Montreal, RICHARD MARTEL, Department of Chemistry, Universite de Montreal, DELPHINE BOULLY, Physics, Universite de Montreal — With the miniaturization of electronics, it is now possible to assemble field-effect transistors (FET) with single-molecule components as channel or gate. Single-molecule FETs have been recently used to study different fundamental mechanisms at the individual molecule scale, such as charge transport, folding and chemical reactions, both for small molecules and complex biological macromolecules. Here, our goal is to use nanocarbon materials (graphene or carbon nanotubes) to design and fabricate FET architectures suitable for single-molecule measurements. First, we report the fabrication of large arrays of FET devices with similar electrical characteristics, built from long carbon nanotubes or large-area graphene synthesized by chemical vapor deposition (CVD). Second, we used electron-beam lithography to pattern high-resolution features (20nm), in order to design nanoconstrictions in the graphene channel, as well as nanofluidic cavities allowing for single-point reaction chemistry. We will present the electrical characteristics of these devices, as well as high-resolution imaging using scanning electron and atomic force microscopy (SEM/AFM). Finally, we will discuss future work in terms of single-molecule functionalization with biological molecules.
In this presentation, the mechanical resonance behaviors of porous graphene resonator used for were studied. The goal of this research is to find an optimal geometric structure of drum-like graphene for with obtaining its mechanical resonance with high frequencies and high Q-factors. Resonance behavior of graphene drums with various periodic hole-patterns has been studied by using finite element modeling simulation. The geometry and number of hole structures on graphene were designed and fabricated according to the simulation modeling. Our simulation results suggest that the resonance frequency of the graphene drum gradually increases and then drops as the number of pores of the graphene increases from 0 to 100. In addition, the porous graphene resonator devices are experimentally realized by transferring a porous graphene membrane on substrate with a trench structure. Experimentally measured resonance frequencies and estimated quality factors of graphene resonator with various pore structures were compared to and analyzed by simulation results.

We have investigated switching characteristics in graphene/semiconducting single-walled carbon nanotube (SWCNT) junction device, so-called graphene/SWCNT barristor. We modulated Schottky barrier between the graphene and the carbon nanotube by using top and bottom gate electrodes, and achieved on-off ratio of $10^8$ and the subthreshold swing of 74 meV/dec with high current density. This all-carbon device can be useful to graphene logic circuit, flexible electronics circuit and memory device.

We present high throughput thermal conductance data at alloy/graphene interfaces as a function of alloy composition and adhesion layer thickness, with a maxima observed at 10 at. % Pd in Ni without an adhesion layer. Graphene contact research has been exclusively limited to pure metals, where the metal/graphene interface inhibits the flow phonons, quantified by the thermal interface conductance. For future electronics to fully capitalize on the revolutionary transport properties of graphene, sufficient heat dissipation at the contact interface is critical to performance. [1]

To make high throughput measurements, metal films with a continuous alloy composition gradient spanning two pure metals were deposited on monolayer graphene on SiO$_2$/Si substrates. Frequency domain thermoreflectance was used to measure thermal interface conductance as a function of metal composition. Future measurements of electrical contact resistance will be done through transmission line measurement structures, in order to determine the optimal alloy concentration for both electrical and thermal transport across the interface.

Quantum point contact in bilayer graphene

HAILONG FU (Presenter), JING LI, YA-WEN CHUANG, Pennsylvania State University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, 1-1 Namiki, Tsukuba 305-0044, JUN ZHU, Pennsylvania State University — Edge state interferometry has been an important tool in probing the charge and statistics of elementary excitations of the quantum Hall and fractional quantum Hall effect of a two-dimensional electron gas. The recent observations of a plethora of fractional quantum Hall states in bilayer graphene, especially a series at even denominators, made this technique all the more appealing. A quantum point contact (QPC) is a key component of an interferometer, the realization of which is difficult in graphene owing to its gapless nature. In bilayer graphene, a pair of aligned top and bottom gates[1, 2] can be used to open a band gap and therefore construct a QPC. Here we report on our effort in fabricating QPC devices using high-quality h-BN encapsulated bilayer graphene. Because of the thin gating profile, the confining potential of the QPC in bilayer graphene is much sharper than what can be achieved in GaAs 2D systems. We observed well-developed quantum Hall states across QPCs with large openings and gate-controlled backscattering of edge states in QPCs with smaller openings. We discuss our fabrication processes, challenges and progress towards a Fabry-Perot interferometer in bilayer graphene.


Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X13 DMP: 2D Materials (General) -- Mechanical Properties and Phases BCEC 153B - Niyaz

Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene

AVANISH MISHRA (Presenter), POOJA SRIVASTAVA, Materials Research Centre, Indian Institute of Science, ABEL CARRERAS, ISAO TANAKA, Department of Materials Science and Engineering, Kyoto University, HIROSHI MIZUSEKI, KIWANG-RYEOL LEE, Computational Science Research Center, Korea Institute of Science and Technology, ABHISHEK KUMAR SINGH, Materials Research Centre, Indian Institute of Science — Oxygen-functionalized MXene, M2CO2 (M = group III-V metals), are two-dimensional (2D) materials with the immense possibility for device applications. Using first-principles calculations, we perform a study on the stability of M2CO2 MXenes. Depending on the position of O atoms, the M2CO2 can exist in two different phases. CB phase, where O at the top of carbon and metal atom. On the other side, O atom can occupy either the site on the top of the metal atom (BB' phase). We found that for M = Sc and Y the CB phase is stable, whereas for M = Ti, Zr, Hf, V, Nb, and Ta the stable phase is BB'. The electron localization function and atom-projected density of states, provide a rational explanation for the relative stability. Instability of BB'- M2CO2 (M = Sc and Y) originates from the weakening of M−C interactions due to the motion of C atom in the−b plane. The insight into the stability of these competing structural phases of M2CO2 is an important step in the direction of identifying the stable phases of these 2D materials and their applications.


*UGC-JRF/SRF fellowship

DFT study of Ni-doped MoS2 as a solid lubricant for space applications

ENRIQUE GUERRERO (Presenter), RIJAN KARKEE, DAVID STRUBBE, University of California, Merced — MoS2 is a layered material with interesting mechanical properties not unlike graphite. The weak Van der Waals forces between MoS2 sheets allow the material to be used as a solid lubricant with application in the low temperature and pressure environment in space, where liquid lubricants fail. Some preliminary studies suggest that doping with transition metals can improve tribology performance by reducing friction and wear. We use density functional theory (DFT) calculations to determine the structure and properties of bulk Ni-doped MoS2, considering formation energy of Ni in different sites as a function of growth conditions, and study the potential energy for sliding to connect to frictional forces measured in atomic-force microscopy (AFM). We calculate vibrations with density-functional perturbation theory (DFPT) for comparison to infrared and Raman spectra in experimental characterization. Our resulting DFT data will be used to parametrize classical force fields for larger-scale reactive molecular dynamics (MD) simulations that can directly address friction and wear.

*Funding from Merced nAnomaterials Center for Energy and Sensing, a NASA-funded research and education center, under award NNX15AQ01
**Effect of net charge on the relative stability of different 2D boron allotropes**

DAN LIU (Presenter), DAVID TOMANEK, Michigan State Univ — We study the effect of electron doping on the bonding character and stability of 2D structures of elemental boron, called borophene, which is known to form many stable allotropes. Our *ab initio* calculations reveal a previously unknown stable 2D \( \varepsilon \)-B structure for the neutral system. We find that the chemical bonding characteristic in this and other boron structures is strongly affected by extra charge. Beyond a critical degree of electron doping, the most stable allotrope changes from \( \varepsilon \)-B to a buckled honeycomb structure. Additional electron doping, mimicking a transformation of boron to carbon, causes a gradual decrease in the degree of buckling of the honeycomb lattice that can be interpreted as piezoelectric response. Net electron doping can easily be achieved by placing borophene in direct contact with the layered \( \text{Ca}_2\text{N} \) electride. In particular, electron doping can be doubled by changing from a bilayer to a sandwich geometry.

*Dan Liu and David Tomanek acknowledge financial support by the NSF/ AFOSR EFRI 2-DARE Grant EFMA-1433459*

**VIBRATIONAL PROPERTIES OF PHOSPHORENE UNDER HIGH PRESSURE**

MANTHILA RAJAPAKSE (Presenter), MEYSAM AKHTAR, CONGYAN ZHANG, MD RAJIB KHAN MUSA, MING YU, Physics and Astronomy, University of Louisville, JACEK JASINSKI, University of Louisville, GAMINI SUMANASEKERA, Physics and Astronomy, University of Louisville — In this study, few layer phosphorene was subjected to high pressure using a Diamond Anvil Cell (DAC) and its vibrational properties were studied via in-situ Raman spectroscopy. Systematic shifting in the Raman frequency of \( A^1_g \), \( B^2_g \), and \( A^2_g \) modes were observed and theoretical calculations were performed to understand the relationship between the strain and the electronic/phononic band structure. The results from computational calculations carried out by employing the density functional theory (DFT) framework, as implemented in the Vienna Ab-initio Simulation Package (VASP) agree well with the experimental data. The results can enable rational engineering of strain towards additional functionalities and device applications of phosphorene and few-layer black phosphorous.

*DOE funded this work.*

**Capillary Origami with Atomically Thin Sheets**

MICHAEL REYNOLDS (Presenter), KATHRYN L MCGILL, Department of Physics, LASSP, Cornell University, MARITHA WANG, Department of Chemistry, Institute for Molecular Engineering, and James Franck Institute, University of Chicago, MARC MISKIN, Department of Physics, LASSP, Cornell University, HUI GAO, Department of Chemistry and Chemical Biology, Cornell University, FAUZIA MUJID, Department of Chemistry, Institute for Molecular Engineering, and James Franck Institute, University of Chicago, KIBUM KANG, Department of Chemistry and Chemical Biology, Cornell University, JIWOONG PARK, Department of Chemistry, Institute for Molecular Engineering, and James Franck Institute, University of Chicago, ITAI COHEN, PAUL L MCEUEN, Department of Physics, LASSP, Cornell University — The paper art of origami has inspired several works in which two-dimensional materials are cut and folded into desired geometries at the micron scale. At this scale, surface energies can easily dominate over bending energies, allowing sheets to be folded with droplets, a technique known as capillary origami. In this talk, we show capillary origami of monolayer molybdenum disulfide (MoS\(_2\)) using droplets in water. By adding rigid panels to the MoS\(_2\), we demonstrate controllable folding of polyhedra. Finally, we show that these shapes can be self-folded by using partially miscible droplets in water. These results provide a new approach for creating pre-patterned three-dimensional devices using two-dimensional materials.

*This work was supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875), the Air Force Office of Scientific Research (MURI: FA9550-16-1-0031), and the Kavli Institute at Cornell for Nanoscale Science. This work was performed in part at the Cornell NanoScale Facility, a member of the National Nanotechnology Coordinated Infrastructure (NNCI), which is supported by the National Science Foundation (Grant NNCI-1542081).*
9:00AM X13.00006: Modeling the dynamics of a single graphene ripple with LAMMPS  JAMES MANGUM (Presenter), PAUL THIBADO, University of Arkansas — In recent years, graphene has shown great promise for a variety of reasons, but most notably for its potential for energy harvesting. Graphene requires ripples to maintain stability. It has been speculated that kinetic energy of the spontaneous flipping of ripples may be converted into electrical energy using vibration energy harvesting technology. The dynamics of larger graphene sheets may be understood by running molecular dynamic simulations with nanoscale sheets that contain a single ripple. Creating single ripples in graphene requires introducing an optimal level of compressive strain, and freezing the molecules on the edge of the sheet. In this talk, we discuss single-ripple graphene dynamics, modeled on LAMMPS. This includes the effect that compressive strain has on flipping time, and equilibrium position. Additionally, videos of the output will be included to elucidate the mechanics of graphene ripple flipping. Our results will be compared to previous results.

9:12AM X13.00007: Organized Brownian Motion in Freestanding Graphene: A New Type of Thermal Motion  PAUL THIBADO (Presenter), PRADEEP KUMAR, SURENDRALAL SINGH, University of Arkansas, MIGUEL RUIZ GARCIA, University of Pennsylvania, ANTONIO LASANTA, LUIS BONILLA, Universidad Carlos III de Madrid — Conversion of omnipresent thermal motion into stored electrical charge has been achieved using vibration energy harvesting technology. Our studies demonstrate that the thermal movement of freestanding graphene produces an alternating electrical current when near a biased metal electrode. The magnitude of this induced electrical current is consistent with a constant-voltage, variable-capacitance power generator. The key mechanism behind this discovery is the spontaneous curvature inversion of ripples, during which thousands of atoms move coherently [PRL 117, 126801 (2016)]. The collective motion of the atoms is a many-body effect and represents a new type of thermal motion with long time correlations enabling energy extraction [PRL 71, 1477 (1993)]. Our results lay the groundwork for a new source of thermal power originating from organized Brownian motion. Circuit details and quantities of energy harvested from this new many-body thermal force will be highlighted in the presentation.

9:24AM X13.00008: Exploring out-of-plane Mechanics of Graphene Membrane by 3D Force Field Spectroscopy on various Nanotubes  MAKOTO ASHINO (Presenter), Department of Electrical and Electronic Engineering, Kanazawa Institute of Technology, ROLAND MARTIN WIESENDANGER, Department of Physics, University of Hamburg — Bending rigidity and Gaussian modulus are key parameters to understand flexibilities of two-dimensional (2D) crystalline membrane embedded in three-dimensional (3D) space. These two parameters of graphene membranes are still unclear because of their difficulties to distinguish purely intrinsic characteristics from others due to thermal fluctuations, consequent local strains and so on. Here we present experimental determinations of those properties by analyzing noncontact interaction between the opposing two atoms of probe-tip apex and convexly-curved graphene folding into various nanotubes. We have quantitatively evaluated the relationship between out-of-plane displacement and elasticity of monolayer graphene by 3D force field spectroscopy at low temperature not only on folded nanotubes with well-defined curvatures but also on unfolded one (i.e. graphene nanoribbon) with unknown curvatures. The quantitative evaluations allow us to determine the smaller and locally different curvatures of unfolded monolayer. Our findings to separate the in-plane and out-of-plane contributions allow us to derive the substantially small bending modulus enough to expect the intrinsic characteristics of negligibly small (zero) modulus for the ultimate 2D membrane without any curvature.

9:36AM X13.00009: Probing the Domain Architecture in 2D α-Mo2C via Polarized Raman*  TIANSHU LI (Presenter), Materials Science and Engineering, Boston University, WEIJUN LUO, HIKARI KITADAI, XINGZHI WANG, XI LING, Chemistry, Boston University — MXenes are a group of two-dimensional (2D) materials with excellent stability and intriguing properties. Here, we conduct a systematic study on the Raman spectra of α-Mo2C and use it to study the unique domain structure of 2D α-Mo2C crystals grown by chemical vapor deposition (CVD). Six experimentally observed Raman modes are assigned with the assistance of phonon dispersion calculated from density functional theory (DFT). Angle-resolved polarized Raman spectroscopy indicates the anisotropy of α-Mo2C in the b-c plane, which is further applied to study the domains of the CVD grown 2D α-Mo2C crystals with different morphologies. Most of the α-Mo2C flakes contain multiple domains and the c-axes of neighboring domains within the same flake tend to form a 60° or 120° angle, indicating the carbon chains in α-Mo2C align along three equivalent directions. This is attributed to weak Mo-C bonds in this interstitial carbide and the low formation energy of the carbon chains along certain directions. Our study demonstrates that polarized Raman spectroscopy is a powerful and effective way to characterize the domain structures in α-Mo2C, which will facilitate the further exploration of properties and applications of α-Mo2C, as well as other MXenes.

*This work is supported by Boston University.
9:48AM X13.0001: On the mechanism for the 2D phase transition in freestanding group-IV monochalcogenide monolayers*  
JOHN VILLANOVA (Presenter), SALVADOR BARRAZA-LOPEZ, University of Arkansas — Group-IV monochalcogenides monolayers MX (M=Ge,Sn ; X=S,Se) are low-dimensional semiconductors which exhibit significant piezoelectric and ferroelectric responses. Monochalcogenide monolayers undergo a structural phase transition from a rectangular unit cell to a square unit cell at a critical temperature. There exist two intriguing descriptions of this behavior: (1) a Landau-Ginzburg effective model and (2) a description of the order-disorder transition based on ab initio molecular dynamics. We explore the phase transition by examining the softening of the phonon modes of SnSe as a function of temperature, in order to shed light on the possible physical mechanism underpinning the transition.

*This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Early Career Award DE-SC0016139. Calculations were performed at Trestles, funded by the National Science Foundation, the Arkansas Economic Development Commission, and the U of A Office of the Vice Provost for Research and Innovation.

10:00AM X13.00011: Delocalization of Impact Energy in Multilayer Graphene Subjected to Supersonic Impact in Vacuum*  
WANTING XIE (Presenter), JAE-HWANG LEE, University of Massachusetts Amherst — We employed vacuum micro-ballistic characterization for the first time to explore the ballistic perforation dynamics of multilayer graphene (MLG). The vacuum level is approximately 1/3,000 of the atmospheric pressure to avoid undesired effects from air, including aerodynamic friction of a projectile or a membrane specimen. 3.7 um diameter silica spheres were accelerated to 300 – 900 m/s as projectiles and a suspended graphene membrane was subjected to projectile's impact. With an ultrafast microscopic imaging system (40 million frames per second), accurate velocities of the projectile before and after penetration were obtained. We studied the residual speed as a function of impact speed. The specific penetration energy of MLG was quantified with respect to projectile's impact speeds and specimen's thicknesses. As a result, MLG demonstrated twice better performance in vacuum compared to that in air, opposite to conventional predictions. The penetration features near the impact region were examined by scanning electron microscopy to uncover the correlations with the energy dissipation.

*This research was supported by the U.S. Army Research Laboratory under contract W911NF-15-2-0024.

10:12AM X13.00012: The governing role of interlayer chemical bonding in polar properties of the van-der-Waals ferroelectric CuInP$_2$S$_6$*  
JOHN BREHM (Presenter), Vanderbilt University, MARIUS CHYASNAVICHUS, SABINE NEUMAYER, NINA BALKE, Oak Ridge National Lab, MICHAEL SUSNER, Air Force Research Laboratory, MICHAEL A MCGUIRE, PANCHAPAKESAN GANESH, PETRO MAKSYMOVYCH, Oak Ridge National Lab, SOKRATES T PANTELIDES, Vanderbilt University — Copper indium thiophosphate (CuInP$_2$S$_6$) is a van-der-Waals (vdW) layered crystal that is ferrielectric below room temperature. It has unusual properties, including a negative longitudinal piezoelectric coefficient whose atomistic origin remains unknown. In this talk, we present the results of density functional theory calculations which show that the potential energy for Cu displacement away from the centrosymmetric position has two distinct minima in each longitudinal direction instead of the usual one, with stable positions within the layer as well as in the vdW gap. The two minima correspond to two structural phases with distinct polarizations, which is corroborated by piezoresponse force microscopy experimental data. The anharmonicity of the potential governing Cu displacements yields a negative piezoresponse in one of the phases. At the same time, the potential is strongly influenced by strain and the corresponding width of the vdW gap, rendering CuInP$_2$S$_6$ a rare example of a uniaxial non-zero-polarization multi-well ferroelectric, with new potential for both fundamental studies and prospective applications.

*U.S. DoE grant DE-FG02-09ER46554.
Basic Energy Sciences, US Department of Energy. Laboratory Directed R&D at ORNL
10:00AM X13.00013: Mechanical and Electrical Studies of Two-dimensional Covalent Organic Frameworks* 
RUOFAN LI (Presenter), Cornell University, MICHIO MATSUMOTO, AMANDA CORCOS, Northwestern University, HALLEH BALCH, University of California - Berkeley, RAGHUNATH DASARI, Georgia Institute of Technology, AUSTIN EVANS, Northwestern University, GREGORY STIEHL, Cornell University, SETH R. MARDER, Georgia Institute of Technology, FENG WANG, University of California - Berkeley, WILLIAM DICTEL, Northwestern University, DANIEL RALPH, Cornell University — Two-dimensional (2D) covalent organic frameworks (COFs) are a promising new class of 2D materials with the potential for highly-tunable chemical, mechanical, electrical, and optical properties. As porous polymers, 2D COFs are predicted to have a combination of low mass density and high mechanical strength. Here we discuss mechanical and electrical measurements on COF thin films. For the mechanical measurements, we have developed a protocol for synthesizing COF films as thin as 1.5 nm at a liquid-liquid interface, lifting and drying them on a PDMS stamp, and then performing a dry transfer onto a prepatterned substrate to make suspended COF films. The transferred films exhibit excellent uniformity, smoothness, and cleanliness. We report results for the 2D Young's modulus and mechanical strength using nanoindentation measurements performed using an atomic force microscope. We will also discuss initial electrical measurements on COF films designed to have small energy gaps.

*This work was supported by the Army Research Office (W911NF-15-1-0447).

10:30AM X13.00014: Buckling of thermalized sheets* 
ALI MORSHEDIFARD (Presenter), Civil and Environmental Engineering, University of California, Irvine, MIGUEL RUIZ GARCIA, Physics, University of Pennsylvania, MOHAMMAD JAVAD ABDOLHOSSEINI QOMI, Civil and Environmental Engineering, University of California, Irvine, ANDREJ KOSMRLJ, Mechanical and Aerospace Engineering, Princeton University — Two dimensional atomically thin membranes (ATMs), such as graphene and transition metal dichalcogenides, display exceptional properties that have been exploited in advanced electronic applications. In this talk, we utilize tools from statistical physics and molecular dynamics simulations to investigate how thermal fluctuation affect buckling of ATMs. Of special interest are ATMs that are larger than the characteristic thermal length scale $l_{th}$, which is a function of temperature and material constants. Both simulations and theory predict that for small sheets of size $L< l_{th}$ the critical buckling load coincides with the classical continuum theory $\sigma \sim L^{-2}$. However, for large sheets of size $L>> l_{th}$ thermal fluctuations effectively stiffen the bending rigidity, which increases the critical buckling load that scales as $\sigma \sim L^{-2+\eta}$. Here $\eta\sim 0.8$ is the universal exponent that is related to the increased bending rigidity. We demonstrate that the critical buckling load scales the same way for both periodic and clamped boundary conditions. These results shed light on fundamental mechanisms that underlie buckling of ATMs and make possible accurate predictions that can be used for design purposes in applications.

*This work was supported by NSF awards DMR-1752100 (CAREER) and CMMI-1826122

10:45AM X13.00015: Friction Anisotropy of MoS2 Investigated via Atomic Force Microscopy 
OGULCAN ACIKGOZ (Presenter), MEHMET BAYKARA, University of California, Merced — Two-dimensional (2D) materials are of particular interest as solid lubricants for nano- and micro-scale devices as traditional fluid-based lubrication schemes fail at such small length scales due to problems including but not limited to surface tension. Among various 2D materials investigated as solid lubricants, MoS2 is of special importance for space applications since its lubricative properties do not degrade but rather improve under vacuum conditions. A particular aspect that has so far not been addressed in detail within this context is the direction dependence, i.e. anisotropy, of the frictional properties of MoS2, which could be an important design parameter for various applications. Here, we perform atomic force microscopy (AFM) measurements on CVD-grown and mechanically-exfoliated MoS2 to investigate the potential occurrence of friction anisotropy. Results indicate that (i) both CVD-grown and mechanically-exfoliated MoS2 exhibit strong friction anisotropy and remarkably, (ii) the periodicity associated with the anisotropy is not exclusively determined by the atomic structure of MoS2, but is a function of the AFM probe employed in the experiments.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X14 DMP DCMP: Devices from 2D Materials -- Twisted bilayers BCEC 153C - Matthew Yankowitz, Columbia University - Tag(s): Focus
8:00AM X14.00001: Bilayer graphene Josephson junctions with induced spin orbit coupling  AVRADEEP PAL
(Presenter), QuTech and Kavli Institute of NanoScience, Delft University of Technology, 2600 GA, Delft, The Netherlands, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan, SRJIT GOŚWAMI, QuTech and Kavli Institute of NanoScience, Delft University of Technology, 2600 GA, Delft, The Netherlands — Interfacial coupling of graphene with transition metal dichalcogenides (TMDs) have emerged as a way to induce enhanced spin orbit coupling in few layer graphene. In our experiment, bilayer Graphene is sandwiched between exfoliated WSe2 (bottom) and h-BN (top) and edge contacted by means of superconducting NbTiN. We report the first study of induced superconductivity in such systems by demonstrating the Josephson effect in a series of samples of varying junction lengths (300nm to 1300nm). All measured devices are found to be in the long junction limit. By means of bottom gating, we access a wide range of densities far away from the charge neutrality point, and trace the product as a function of Thouless Energy (Em). By testing the validity of standard SNS long junction diffusive limit superconducting proximity effect scaling behavior (IcRn = aEm) in spin orbit coupled graphene systems. As expected from theory, a universal scaling of these parameters is observed for all devices, however with a severely reduced a than expected.

8:12AM X14.00002: Electron scattering and thermopower in twisted bilayer graphene  TING FUNG CHUNG
(Presenter), YANG XU, LISHA AN, EVAN WITKOSKE, NA (LUNA) LU, YONG CHEN, Purdue University — Twisted bilayer graphene (TBLG) with a small twist-angle is of particular interest because of its distinct energy band, where recent electrical transport experiments revealed van Hove singularities (VHSs), hybridization gaps, and correlation-induced behaviors. To better understand the effect of VHSs in TBLG, we perform transport experiments in this study. We observe that the temperature-dependent resistivity follows a power-law for carrier density between the main charge neutrality and hybridization gap. The evolution of the temperature exponent with carrier density shows a W-shaped dependence, with minima near the VHSs and maxima toward the hybridization gap. This W-shaped behavior could be attributed to different electron scattering mechanisms. We also study thermopower in TBLG, where we observe multiple sign changes in thermopower near VHSs at low temperatures. Our work may provide more information about the electronic structure and physical process in the TBLG system.

8:24AM X14.00003: Towards a gate-controlled valley-analyzer in bilayer graphene  HAO CHEN (Presenter), JENS MARTIN, Physics, National University of Singapore — The inequivalent valleys K and K' in k-space of 2D-hexagonal materials offer a new valley-degree of freedom similar to spin and controllable via electrostatic gating. In bilayer graphene, the sign of Berry curvature in each valley is determined by the direction of the external electric field whereas the sign of Berry curvature in each valley has opposite sign. Theorists have predicted that at 1D-boundaries at which the sign of Berry curvature changes, counter-propagating valley-polarized 1D-channels emerge. Including spin and sublattice degeneracy, there are 4 quantized conduction channels in each direction. This approach provides a gate-controlled platform for valley-polarizers and analyzers, yet it is technically challenging to build such a nanoscale system. Here, we fabricate such system with four pairs of dual-split gates with optimized geometry and stacking methods. Low temperature measurements show large conductance contrast with a factor of 100 between different gate configurations. In our devices, we achieve conductivity of nearly 4 conduction channels in each valley polarized state, much closer to the ballistic limit than previous work. Ultimately, one pair can be valley polarizer and the subsequent pair could detect the valley polarization and serve as valley analyzer.

8:36AM X14.00004: Magnetotransport of twisted bilayer transition metal dichalcogenides  EN-MIN SHIH (Presenter), Physics, Columbia University, LEI WANG, Physics, Cornell University, AUGUSTO GHIOTTO, DANIEL A RHODES, CHENG TAN, ABHAY PASUPATHY, Physics, Columbia University, JAMES HONE, Mechanics, Columbia University — Two-dimensional van der Waals material has become an exciting field. One of the reason is that this system provides multiple degrees of freedom, including stacking order, interlayer spacing and interlayer twisted angle, to engineer the material band structure. Manipulate these degrees of freedom has led to observation of several emergent phenomena, including the fractal quantum Hall effect, tunable Mott insulators, and unconventional superconductivity. In particular, interlayer interaction in van der Waals heterostructures at a different twisted angle could induce many exotic phenomena. How the interlayer interaction affect the electronic structure of a material is a fundamental question. In this study, we report magnetotransport of twisted bilayer transition-metal dichalcogenides (TMDs) and demonstrate how its band structure vary with twisted angle. These results broaden the application range of van der Waals heterostructure for future electronic devices.
Charge-transfer insulation in twisted bilayer graphene. PAULA MELLADO (Presenter), Universidad Adolfo Ibáñez, LOUK RADEMAKER, Department of Theoretical Physics, University of Geneva — We studied the real space structure of states in twisted bilayer graphene at the "magic angle" θ = 1.08°. The flat bands close to charge neutrality are composed of a mix of "ring" and "center" orbitals around the AA stacking region. An effective model with localized orbitals is constructed, which necessarily includes more than just the four flat bands. Long-range Coulomb interaction causes a charge-transfer at half-filling of the flat bands from the "center" to the "ring" orbitals. Consequently, the Mott phase is a featureless spin-singlet paramagnet. We estimate the effective Heisenberg coupling that favors the singlet coupling to be J = 3.3 K, consistent with experimental values. The superconducting state depends on the nature of the dopants: hole-doping yields p+ip-wave whereas electron-doping yields d+id-wave pairing symmetry.

*P.M. acknowledges Fondecyt Grant No. 1160239.
L.R. is supported by the SNSF by an Ambizione grant.
This research was supported in part by Perimeter Institute for Theoretical Physics. Research at Perimeter Institute is supported by the Government of Canada through the Department of Innovation, Science, and Economic Development, and by the Province of Ontario through the Ministry of Research and Innovation.

Phases of a phenomenological model of twisted bilayer graphene. JOHN DODARO, STEVEN KIVELSON, YONI SCHATTNER, XIAO-QI SUN, CHAO WANG (Presenter), Physics Department, Stanford University — We propose a lattice scale two-band generalized Hubbard model as a caricature of the electronic structure of twisted bilayer graphene. Various possible broken symmetry phases can arise, including a nematic phase (which is a form of orbital ferromagnet) and an orbital-triplet spin-singlet superconducting phase. Concerning the mechanism of superconductivity -- we propose an analogy with superconductivity in alkali-doped C_{60} in which a violation of Hund's first rule plays a central role.

*This work was supported in part by the Department of Energy, Office of Basic Energy Sciences, under contract no. DE-AC02- 76SF00515 at Stanford (JFD, SAK, YS, XQS and CW). YS was also supported by the Zuckerman STEM Leadership Program.

Characterization of atomic scale lattice reconstruction in twisted van der Waals interfaces of layered material [Invited]. PHILIP KIM (Presenter), Harvard University — Control of the interlayer twist of van der Waals (vdW) interfaces has been widely used to engineer an artificial 2-dimensional (2D) electronic systems by the formation of a moiré superlattice. Many exotic physical phenomena occur associated with the incommensurability of the moiré superstructures where the wealth of the nontrivial topology of electronic band structures plays a key role to create exotic physical phenomena. In this presentation, we will discuss the engineered atomic scale reconstruction at twisted vdW interfaces using electron microscopy, optical spectroscopy, and electrical transport. We then will discuss emerging electronic and optoelectronic physics in the vdW interface between homojunctions.

Transport measurements of correlated insulating states in twisted bilayer graphene. AARON SHARPE (Presenter), ELIJ FOX, ARTHUR BARNARD, JOE FINNEY, Stanford University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, MARC KASTNER, DAVID GOLDHABER-GORDON, Stanford University — Twisted bilayer graphene (TBG) has emerged as a prominent platform for strongly correlated electrons. When two sheets of monolayer graphene are stacked at an angle near 1.1°, interactions are expected to break the four-fold spin and valley degeneracy resulting in correlated insulating states and superconductivity near densities corresponding to an integer number of electrons per superlattice unit cell [Cao et al., Nature 556, 43-50 (2018), Cao et al., Nature 556, 80-84 (2018)]. Here we present transport measurements studying these correlated states.

*This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.
10:00AM X14.00009: Dynamic band structure in twisted bilayer graphene near the magic angle* JINHAI MAO (Presenter), YUHANG JIANG, XINYUAN LAI, Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, Piscataway, NJ 08855 USA, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, Piscataway, NJ 08855 USA — A twist between the orientations of superposed 2D crystal structures leads to a moiré superstructure which can significantly alter their electronic properties. In the case of superposed graphene layers with small twist angle, the energy band flattens resulting in a slow-down of the charge carriers until, at certain “magic angles”, they come to a complete halt. In this regime, electron-electron interactions become strong leading to the emergence of new correlated phases and topologically protected ballistic channels. Using STM on gated twisted bilayer graphene samples, we study the band structure and the emergence of correlated states as a function of doping and twist-angle near the first magic angle. Far from the magic angle, we observe two van hove singularity (VHS) peaks whose separation allows us to extract the interlayer coupling. Contrary to expectation we find that the interlayer hopping is a function of the twist angle and doping. Upon approaching the magic angle the VHS merge into a single flat band which straddles the charge neutrality point. We observe a dynamic reconstruction of the band structure with gap-like features at certain fillings and a corresponding unique spatial reconstruction of the electronic wave-function.

*DOE-FG02-99ER45742, NSF DMR 1708158

10:12AM X14.00010: Effect of vacancies on the electronic and optical properties on twisted bilayer graphene* FRANCISCO CULCHAC (Presenter), RODRIGO CAPAZ, Universidade Federal do Rio de Janeiro — We systematically study the effects of a random distribution of vacancies on the electronic and optical properties of twisted bilayer graphene (TBLG), using a tight-binding method. We study the density of states and optical absorption for different concentrations of vacancies and different rotation angle between the layers. The density of states and the optical absorption spectra are calculated by averaging over several vacancy configurations. The increase in the concentration of vacancies increases the number of midgap states near the Dirac point. For large twist angles, it is possible to observe that the intensity of the absorption peaks, typical of TBLG without vacancies, decrease and slightly shift when the vacancy concentration increases. In addition, peaks of lower intensity can be observed at low energies, coming from optical transitions between midgap states. For small rotation angles and for a certain range of vacancy concentrations, the optical absorption peak is eliminated. This occurs when the energy range of the midgap states located at the Fermi level is comparable to the energy of Van Hove singularities where the optical transitions occur in the case of TBLG without vacancies.

*Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro - FAPERJ.

10:24AM X14.00011: Scanning tunneling microscopy of van Hove singularities in small angle twisted bilayer graphene* JEANNETTE KEMMER (Presenter), Watson Laboratory of Applied Physics, California Institute of Technology, 1200 East California Boulevard, Pasadena, California 91125, USA, YOUNGJOON CHOI, Department of Physics, California Institute of Technology, 1200 East California Boulevard, Pasadena, California 91125, USA, HARPREET SINGH ARORA, ROBERT POLSKI, Watson Laboratory of Applied Physics, California Institute of Technology, 1200 East California Boulevard, Pasadena, California 91125, USA, YIRAN ZHANG, Department of Physics, California Institute of Technology, 1200 East California Boulevard, Pasadena, California 91125, USA, HECHEN REN, Watson Laboratory of Applied Physics, California Institute of Technology, 1200 East California Boulevard, Pasadena, California 91125, USA, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305 0044, Japan, STEVAN NADJ-PERGE, Watson Laboratory of Applied Physics, California Institute of Technology, 1200 East California Boulevard, Pasadena, California 91125, USA — Electronic properties of stacked van der Waals bilayers critically depend on the twist angle between the monolayers. A famous example of this effect is the observation of superconductivity and strongly correlated insulating phases in twisted bilayer graphene (TBG) where the two graphene monolayers are twisted by the so-called magic angle (~1.1°). This system supports electronic bands that are almost completely non-dispersive (flat), which gives rise to strong electronic correlation effects. We use scanning tunneling microscopy and spectroscopy to track the positions of van Hove singularities originating from the flat bands in gated TBG for the range of twist angles from 1° to 3°. We find that close to magic angle values the van Hove singularities are strongly modified when the flat bands cross the Fermi level.

*This work was supported by NSF (Partly through grants DMR 1744011 and DMR 1753306). J. K. was supported by the Deutsche Forschungsgemeinschaft (Projektnummer 406557161).
10:36AM X14.00012: Pressure Induced Compression of Flatbands in Twisted Bilayer Graphene* BHEEMA LINGAM CHITTARI, NICOLAS LECONTE, SRIVANI JAVVAJI, JEIL JUNG (Presenter), University of Seoul — We investigate the bandwidth compression due to out of plane pressure of the moiré flatbands near charge neutrality in twisted bilayer graphene for a continuous range of small rotation angles of up to $\sim 2.5^\circ$. The flatband bandwidth minima angles are found to grow linearly with interlayer coupling $u$ and decrease with Fermi velocity. Application of moderate pressure values of up to 2.5 GPa achievable through a hydraulic press should allow accessing a flatband for angles as large as $\sim 1.5^\circ$ instead of $\sim 1^\circ$ at zero pressure. This reduction of the moiré pattern length for larger twist angle implies an increase of the effective Coulomb interaction scale per moire cell by about 50% and enhance roughly by a factor of $\sim 2$ the elastic energy that resists the commensuration strains due to the moire pattern. Application of pressure will hence notably facilitate the device preparation efforts required for exploring the ordered phases near magic angle flatbands. We also discuss the phase diagram of flatbands in other hybrid Dirac materials.

Reference, arXiv:1808.00104

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10:48AM X14.00013: Optical measurements of twisted bilayer transition metal dichalcogenides AUGUSTO GHIOTTO (Presenter), Columbia University, LEI WANG, Cornell University, EN-MIN SHIH, DANIEL A RHODES, CHENG TAN, ABHAY PASUPATHY, JAMES HONE, CORY R DEAN, Columbia University — Two-dimensional Van der Waals material has become an exciting field. One of the reason is that this system provides multiple degrees of freedom, including stacking order, interlayer spacing and interlayer twist angle, to engineer the material band structure. Manipulation of these degrees of freedom has led to observation of several emergent phenomena, including the fractal quantum Hall effect, tunable Mott insulators, and unconventional superconductivity. In particular, interlayer interaction in van der Waals heterostructures at different twist angle could induce many exotic phenomena. How the interlayer interaction affects the electronic structure of a material is a fundamental question. In this study, we report optical measurements of twisted bilayer transition-metal dichalcogenides (TMDs) and demonstrate how its band structure vary with twist angle. These results broaden the application range of van der Waals heterostructure for future optoelectronic devices.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X15 DMP: 2D Materials (Semiconductors) -- Synthesis, Defects, and Strain BCEC 154 -

8:00AM X15.00001: Spinodal Dewetting Instabilities on Graphene and two-dimensional atomic crystals VALERI KOTOV (Presenter), DAVID PETERSON, JUAN VANEGAS, University of Vermont — We demonstrate theoretically, for the first time, the possibility of spinodal dewetting in heterostructures made of light-atom liquids (hydrogen, helium, and nitrogen) deposited on graphene and other 2D substrates. Extending our theory of film growth on 2D materials [S. Sengupta et al., Phys. Rev. Lett. 120, 236802 (2018)] to include analysis of surface instabilities via the hydrodynamic Cahn-Hilliard – type equation, we characterize in detail the resulting periodic patterns. Both linear stability analysis and advanced computational treatment of the surface hydrodynamics show unconventional, micron-sized (generally material dependent) patterns of “dry” regions. The physical reason for the development of such instabilities on graphene can be traced back to the inherently weak van der Waals interactions between atomically-thin materials and atoms in the liquid, causing the arrest of film growth under normal equilibrium conditions and triggering the associated surface instabilities. These phenomena are robust to some mechanical deformations and are also universally present in doped graphene and other 2D materials, such as monolayer dichalcogenides. Thus, two-dimensional materials represent a universal theoretical and technological platform for studies of spinodal dewetting.
Surface functionalization of two-dimensional monolayers can produce materials with different structural and electronic properties as compared to their pure counterparts. The lowest energy phase for molybdenum (Mo) based transition metal dichalcogenides is the semiconducting hexagonal H phase. However, the alternative T phase with Mo atoms in octahedral coordination and the distorted version of the T phase (T’) can be stabilized by intercalation, chemical doping, and charge mediation. In this work, we use density functional theory calculations to demonstrate that H to T phase transition can be achieved in MoX2 monolayer with hydrogenation. We find that the phase stability of the T phase increases as a function of hydrogenation coverage. This phase transition results in the semiconductor to metallic transition in these monolayers. Our results suggest that these MoX2 monolayers with controllable structural and electronic properties can find applications in catalysts and nanodevices.

*This work is supported by National Science Foundation under grant number DMR-1752840.

The ability to control nanoscale electronic properties by introducing macroscopic strain is of critical importance for the implementation of 2D materials into flexible electronics and next generation strain engineering devices. In this work we use scanning tunneling microscopy and spectroscopy (STM/STS) to correlate the atomic-scale lattice deformation and local electronic properties with a systematic macroscopic bending of monolayer molybdenum disulfide (MoS2) films, using a custom-built sample holder. Using this technique, we find a reduction of the quasiparticle band gap with increasing strain. In addition, nanoscale strain relaxation of van der Waals monolayer sheets has been investigated and resulted in 1D ripples and 2D wrinkles which alter the local strain fields as well as the local electronic density of states.

*Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. This work was supported as part of the Center for Complex Materials from First Principles, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Grant No. DE-SC0012575.

In a recent report [1], the present authors demonstrated the existence of quantum-confined states arising from spatially varying band edge energies in a MoS2/WSe2 vertical heterostructure. Here, this system is studied in more detail, combining results from low-temperature scanning tunneling microscopy/spectroscopy (STM/STS) measurements and density functional theory (DFT) calculations. It is experimentally observed that in addition to the band edge shifts, the moiré pattern, which forms due to a 3.7% lattice mismatch, results in spatially varying biaxial strain in the MoS2 of ~2% tension (compression) at the corrugation minima (maxima). Including band edge shifts due to strain and corrugation of the underlying WSe2 leads to a consistent explanation for the observed spatial locations of the quantum-confined states.


*This work was supported in part by the A. von Humboldt Foundation and by the Center for Low-Energy Systems Technology (LEAST), one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by Microelectronics Advanced Research Corporation (MARCO) and Defense Advanced Research Projects Agency (DARPA).
Spin effects at mirror twin grain boundaries in monolayered dichalcogenides

MIGUEL PRUNEDA (Presenter), Theory & Simulation Group, Institut Catala de Nanociencia i Nanotecnologia — First-principles calculations are used to study the origin of the charge density wave observed in 1D inversion domain grain boundaries in monolayered MoSe$_2$. A small structural (Peierls) distortion with the same periodicity observed in the STM experiments can be reproduced. However, an opening of the gap does not require this distortion, which can be obtained with a suitable spin configuration for the edge electronic states. Spin-orbit effects on these peculiar interfacial states are also discussed. Remarkably, similar spin configurations can also be obtained for edge states in zigzag-edged domains.

Work supported by European Union H2020-EINFRA-5-2015 MaX Center of Excellence (Grant No.824143). ICN2 is funded by the Severo Ochoa Centers of Excellence Program under Grant SEV-2013-0295 and the CERCA Program/Generalitat de Catalunya. Funding from Generalitat de Catalunya (Grant 2017SGR1506) and Spanish MINECO (Grant No.FIS2015-64886-C5-3-P) is acknowledged.

Point defects, impurities, and single-photon emitters in hexagonal boron nitride

LEIGH WESTON, Lawrence Berkeley National Laboratory, DARSHANA WICKRAMARATNE, Naval Research Laboratory, MARK E. TURIANSKY, University of California, Santa Barbara, MAZENA MACKOIT, AUDRIUS ALKAUSKAS, Center for Physical Sciences and Technology, Vilnius, Lithuania, CHRIS VAN DE WALLE (Presenter), University of California, Santa Barbara — Hexagonal BN (h-BN) is attracting a lot of attention for two-dimensional electronics and as a host for single-photon emitters. We have studied the properties of native defects and impurities in h-BN using density functional theory with a hybrid functional. Native vacancy and antisite defects have high formation energies. Self-interstitials can have low formation energies, but their low migration barriers render them highly mobile, and they are unlikely to be present as isolated defects. We find that the defect chemistry of h-BN is likely dominated by unintentional impurities rather than native point defects. Substitutional carbon and oxygen, as well as interstitial hydrogen and boron vacancy–hydrogen complexes, are low-energy defects in h-BN. Our results allow us to comment on frequently observed emission lines and on the microscopic origins of single-photon emitters.

Work supported by NSF and DOE.

Localized strain tuning of exciton emissions on suspended two-dimensional materials

HYOWON MOON (Presenter), CHITRALEEMA CHAKRABORTY, GABRIELE GROSSO, DIRK R. ENGLUND, Massachusetts Institute of Technology — Two-dimensional materials can endure extraordinarily large strain which strongly influences its electronic and optical properties. Strain tuning has been reported for free excitons in transition metal dichalcogenides (TMDs) as well as for single photon emissions in TMDs or in hexagonal boron nitrides (hBN). However, strain applied on the entire substrate or over few micrometers has a limited ability to produce or control individual strain-induced quantum emissions in TMDs. Here we demonstrate extremely localized strain tuning of exciton emissions in suspended 2D materials induced by sub-10nm radius tip mechanical probe, which can be potentially used to create and tune nonclassical light sources in atomically thin materials.

4. Chakraborty et al., in preparation
5. Grosso et al., Nature Communications 8, 705 (2017)

This work was supported by NSF EFRI 2-DARE 1542863, ARO MURI, and EFRC:Center for Excitonics funded by U.S. DoE BES DE-SC0001088.
Strain-tunable single-photon emission from an atomically thin semiconductor

Chitraleema Chakraborty (Presenter), Electrical Engineering and Computer Science, MIT, Kumarasiri Konthasinghe, The Institute of Optics, University of Rochester, Hyowon Moon, Dirk R. Englund, Electrical Engineering and Computer Science, MIT, Nick Vamivakas, The Institute of Optics, University of Rochester — One of the most unique mechanical properties of two-dimensional (2D) materials over conventional semiconductors is their high stretchability of more than 20% before fracture. Recently strain induced single photon emitters have been observed in 2D transition metal dichalcogenides. Tuning their emission energy is highly desired for efficient coupling to photonic devices. We demonstrate such tunability by engineering van der Waals heterostructure consisting of graphene/h-BN/WSe2 on a piezoelectric actuator. Application of an electric field across the piezoelectric substrate induces a biaxial strain on the emitters hosted by the monolayer WSe2 in the heterostructure. We have demonstrated a strain tunable energy shift of tens of meV using this approach.


*This work was supported by NSF EFRI 2-DARE 1542863, NSF EFRI EFMA-1542707, NSF CAREER DMR 1553788, AFOSR FA9550-16-1-0020, Army Research Office (ARO W911NF-18-1-0431).

Electrical Control of Defect Assisted Trapped Excitons and trions States in Monolayer MoS2

Pradeepa H L (Presenter), Praloy Mondal, Aveek Bid, Jaydeep K Basu, Physics, IISc Bangalore — Unique optical properties of monolayer MoS2 such as strong binding energy of excitons and trions at room temperature make it a suitable material to study the dynamics of these quasi particles. We report a transition between quasiparticle states using Time resolved Photoluminescence (TRPL) and Photoluminescence (PL) spectroscopy by tuning the carrier concentration of MoS2 monolayer in FET configuration. Since the defect assisted trapping potential is electrically sensitive, we are able to control the trapping states of quasiparticle by applying gate voltage in FET. This control of defect assisted states could influence the exciton exciton annihilation mechanism which is one of the dominant nonradiative decay channel of excitons in two dimensional materials. Our study helps in understanding the exciton dynamics in 2D materials.

*HLP thanks CSIR-UGC for financial support. All the authors thank DST nanomission for funding. The authors thank SERB, India for funding.

Synthesis of large-scale transition metal dichalcogenide films and their applications in hydrogen production

Judy Cha (Presenter), Yale University — Transition metal dichalcogenides (TMDCs) have been studied extensively for their attractive mechanical, electrical, optical, and electrochemical properties. A large scale synthesis of these materials in thin films down to monolayers with thickness control and high crystalline quality remains a major hurdle to utilize them in applications. In this talk, I will discuss our efforts to synthesize centimeter-scale thin films and heterostructures of TMDCs including tellurides such as WTe2 and MoTe2. I will discuss how the morphology and grain size of the thin films is intimately linked to the strain that builds during synthesis and ways to mitigate such strain. With our synthesized films, we explore thermal conductivity of WTe2 thin films and aspects of hydrogen evolution reaction that is often overlooked, such as the Schottky barrier at the interface between the chalcogenide catalyst (for example MoS2) and the electrode and the dielectric substrate effect. Finally, I will discuss the detrimental surface oxidation effect on the transport properties of the TMDCs, which must be overcome for large-scale applications.

*NSF 1749742
DOE DE-SC0014476
10:36AM X15.00012: Strained bilayer WSe2 with reduced exciton-phonon coupling  OZGUR BURAK ASLAN (Presenter), MINDA DENG, MARK BRONGERSMA, TONY F HEINZ, Stanford University — We investigate excitonic absorption and emission in bilayer (2L) WSe2 under tensile strain. We observe a redshift of 110 meV in the energy of the A exciton absorption peak (direct gap) under 2.1% strain. The photoluminescence (PL) spectrum exhibits multiple peaks under 0% strain, corresponding to the indirect and direct gaps. Surprisingly, the spectral linewidth of the A exciton decreases by almost a factor of two under strain, from 70 to 36 meV at room temperature. We explain this effect as the result of suppression of phonon-mediated exciton scattering channels. That suppression is associated with the relative shift under strain of the Q valley in the conduction band (involved in the indirect PL), which is nearly degenerate with the K valley (involved in the A exciton). We analyze the strain-dependent absorption and PL spectra to determine the relative positions of those valleys and to calculate the intervalley scattering rates. Our model describes well the strain-induced linewidth decrease of both monolayer (1L) and 2L WSe2 and help us understand what contributes to the linewidths. The results show that strain tuning can be employed to probe the band structures and the excitonic properties of 1L and 2L TMDCs.

10:48AM X15.00013: Mechanical control of valley magnetization and Berry curvature dipole in monolayer MoS2  JOOLEE SON (Presenter), Department of Physics and Department of Energy Systems Research, Ajou University, KYUNG-HAN KIM, Department of Physics, Pohang University of Science and Technology, YOUNGHWAN AHN, Department of Physics and Department of Energy Systems Research, Ajou University, HYUN-WOO LEE, Department of Physics, Pohang University of Science and Technology, JIEUN LEE, Department of Physics and Department of Energy Systems Research, Ajou University — Monolayer transition metal dichalcogenides (TMDs) are known to have the valley degree of freedom of electrons in momentum space, called K and K'. The control of valley degree of freedom utilizes the valley-dependent Berry curvatures which have the opposite signs at the K and K' valleys. Here we report a new type of valley control using the Berry curvature dipole. By applying strain to monolayer MoS2, we show that Berry curvature distributions about K and K' valleys become asymmetric, leading to the emergence of the Berry curvature dipole. The Berry curvature dipole is manifested by the valley magnetization arising as functions of the Berry curvature dipole and an in-plane electric field. We fabricated several flexible monolayer MoS2 devices and measured the valley magnetization by scanning Kerr rotation microscopy. We will discuss the dependence of the valley magnetization on the direction and magnitude of strain and in-plane electric fields. Our results obtained at room-temperature pave a way for practical valley-based electronic devices and information processing.

Friday, March 8, 2019 8:00 AM - 10:36 AM

Session X17 DCOMP: Matter in Extreme Environments: Dynamic Compression BCEC 156A - Jon Eggert, Lawrence Livermore Natl Lab - Tags: Focus

8:00AM X17.00001: Watching extreme materials through the ultrafast shock compression microscope* [Invited]  DANA DLOTT (Presenter), University of Illinois at Urbana-Champaign — We have developed a microscope that looks into solids and liquids as they are subjected to controlled high velocity impacts. These impacts generate shock waves that propagate a few kilometers per second, creating intense mechanical and thermal effects that can trigger new kinds of chemistry. One of these impacts can create pressures of 200,000 atm and temperatures of 4000K while compressing matter to half its density. I will describe the shock compression microscope and the peripheral high-speed optical diagnostics that measure pressure, temperature, density, composition and structure in real time. A few applications will be discussed: shock initiation and detonation of high explosives, shock attenuation by molecular frameworks, and chemistry in extreme states of water.

*The work described in this presentation was supported by the US Army Research Office and the US Air Force of Scientific Research
8:36AM X17.00002: Results of Rayleigh-Taylor material strength experiments at high pressure and high strain rates on NIF and Omega* 

HYE-SOOK PARK (Presenter), A ARSENLIS, NATHAN R BARTON, CHANNING M HUNTINGTON, JAMES M MCNANEY, BRUCE ALLEN REMINGTON, PHILIP D POWELL, SHON T. PRISBREY, ROBERT RUDD, DAMIAN C SWIFT, CHRISTOPHER WEHRENBERG, Lawrence Livermore Nat’l Lab — We are studying material strength at high pressures (upto 8 Mbar), high strain rates (~10⁷ s⁻¹) and high strains (> 30%) under ramped compression condition using Rayleigh-Taylor instability properties. Understanding plastic deformation dynamics of materials under these extreme conditions is an area of research of high interest to a number of fields, including meteor impact dynamics and advanced inertial confinement fusion designs. We have studied various metals such as tantalum, lead and copper using laser driven high pressure platform. Our studies show that the work hardening dominates in this regime. We will describe the experimental results of the high pressure, high rate plastic deformation dynamics of various metals from Omega and NIF in comparison with the various strength models including Livermore Multiscale Model [2].


*This work was performed under the auspices of the U.S. Department of Energy (DOE) by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

8:48AM X17.00003: In-Situ X-Ray Probes of Water-Saturated Granular Media under Dynamic Compaction* 

RYAN CRUM (Presenter), ERIC B HERBOLD, DOROTHY MILLER, JONATHAN LIND, Lawrence Livermore Natl Lab, RYAN C HURLEY, Johns Hopkins University, MICHAEL ANDREW HOME, Lawrence Livermore Natl Lab, BRIAN JENSEN, Los Alamos Natl Lab, DANIEL E EAKINS, DAVID J CHAPMAN, University of Oxford, MINTA C AFIN, Lawrence Livermore Natl Lab — Granular systems are ubiquitous in our everyday world and influence many scientific problems including mine blasts, projectile penetration, and astrophysical collisions. Despite its significance, a fundamental understanding of granular media's behavior falls short of its solid counterpart, limiting predictive capabilities. Granular response is complex in part to the intricate interplay between numerous degrees of freedom not present in its solid equivalent. To address the role of geophysically relevant water-saturation in granular media, previous studies use VISAR or PDV, diagnostics that focus on the aggregate effect leaving the principal interactions of these multiple degrees of freedom too entangled to elucidate. This study uses a gas gun platform coupled to in-situ X-ray probe diagnostics to probe the role of water-saturation in dynamic compaction. Analyses include evaluating displacement fields, grain fracture, and diffraction profiles. Results herein are directly compared to previous studies that were unable to include in-situ X-ray diagnostics.

*Work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and supported by LLNL's LDRD program under grant 16-ERD-010. Experiments at DCS are supported by DOE / NNSA Award Number DE-NA0002442.

9:00AM X17.00004: Laser-induced Microparticle Impact Experiments on Viscoelastic Gels* 

DAVID VEYSSET (Presenter), YUCHEN SUN, STEVEN E KOOI, Massachusetts Institute of Technology, ALEX J HSIEH, U.S. Army Research Laboratory, ALEXEI MAZNEV, Massachusetts Institute of Technology, SHAWN T. COLE, RANDY A. MROZEK, JOSEPH L. LENHART, U.S. Army Research Laboratory, KEITH ADAM NELSON, Massachusetts Institute of Technology — High-velocity impact testing is used to study fundamental aspects of materials behavior under high strain rates as well as in applications ranging from micrometeorite detection to the development of novel drug delivery platforms. In this work, we study the high-velocity micro-particle impact response of viscoelastic gels, including hydrogels and synthetic polymer gels with non-aqueous solvents. In an all-optical laser-induced projectile impact test, micro-particles are accelerated through a laser ablation process. Depending on the laser energy, particles reach speeds up to 1 km/s in free space. Steel and silica particles are monitored during impact with an ultrahigh-speed multi-frame camera that can record up to 16 images with time resolution of each frame as short as 5 ns. We present images and movies capturing individual particle impact and penetration in gels and discuss the observed dynamics under a typical strain rate of 10⁸ s⁻¹. The results can provide direct input for modeling of high-velocity impact responses and high strain rate deformation in gels and other soft materials.

*This material is based upon work supported in part by the U. S. Army Research Office through the Institute for Soldier Nanotechnologies, under Cooperative Agreement Number W911NF-18-2- 0048.
agreement between the calculations and the experimental densities obtained. In general, there is a good understanding of the shock states in double shocked experiments compared with the as obtained material densities. The Laboratory has given us the opportunity to probe the α-ε phase transition states in cerium metal. A couple of experiments were fielded measuring the in-situ material density of the shocked material. A two-phase model which was developed to apply to experiments to infer the density. Proton radiography allows the direct measurement of density. The under extreme conditions the standard Rankine-Hugoniot jump conditions are applied to experiments to infer the density. Proton radiography allows the direct measurement of density. The non-trivial refractive index distorts interferometry measurements of target-window interface velocity. An accurate optical correction to this distortion is crucial in the determination of isentropes in other experiments. We present a measurement of LiF refractive index for stress up to 825 GPa from a shock-ramp experiment at the National Ignition Facility. We argue that a relationship between true and apparent velocity of the target-window interface is more valuable than refractive index to the EOS community. Finally, we present simulated data of dynamically compressed tin and LiF to demonstrate the propagation of the optical uncertainty from this work to EOS measurements. Simulations in which the tin-LiF interface reaches a peak stress of 825 GPa show that the tin isentrope can be determined up to a peak stress of 1.5 TPa with a 0.2% uncertainty in density due to the optical response of LiF.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

9:24AM X17.00006: Damage mechanics from high-velocity micro-particle impacts on polyethylene tape.* Michael Daniti (Presenter), Yuchen Sun, David Veysset, Mostafa Hassani-Gangaraj, Massachusetts Institute of Technology, Alex J Hsieh, US Army Research Laboratory, Steven E Kooi, Keith Adam Nelson, Massachusetts Institute of Technology — Understanding damage mechanics is important when designing materials that will be exposed to high velocity particle impacts, such as polymer-based erosion coatings for helicopter rotor blades or impact shields for satellites. Here, we investigate the high-velocity impact deformation response of ultra-high molecular weight polyethylene (UHMWPE) tape to determine the fundamental impact dynamics and to evaluate how material processing can modify the tape’s mechanical behaviors. Using a laser-induced projectile impact test, we conduct impact experiments using steel particles (~15-30 μm diameter) against UHMWPE tape with linearly structured fibrals at velocities up to 500 m/s. The particles are monitored pre- and post-impact with an ultra-high-speed 16-frame camera with nanosecond time resolution. Post-mortem damage morphologies are assessed as a function of particle impact speed. Based on real-time and post-mortem observations, we discuss the damage mechanisms of the UHMWPE tape under supersonic micro-particle impacts.

*This material is based upon work supported in part by the U. S. Army Research Office through the Institute for Soldier Nanotechnologies, under Cooperative Agreement Number W911NF-18-2-0048.

9:36AM X17.00007: Dynamic experiments to examine the high-pressure, solid phases of cerium Brian Jensen (Presenter), Frank Cherne, Los Alamos National Laboratory — The ability to understand and predict the response of matter at extremes requires knowledge of a materials equation-of-state including the location of phase boundaries, transition kinetics, and the evolution of material strength. Cerium metal exhibits a rich phase diagram at moderate pressures that continues to attract scientific interest as an ideal material for studies focused on the dynamic multiphase properties of materials. Recent dynamic experiments have provided information on the shock-melt transition, and the Hugoniot that spans two solid phases and the liquid. Despite these efforts, the high-pressure, solid region of the phase diagram remains largely unexplored dynamically. Static data have identified the ε phase which exists up to Mbar pressures along a room temperature isotherm. At higher temperatures (greater than 600 K), a direct α-ε transition has been reported although there are disagreements in both slope and location of the boundary. In this work, double-shock loading was used to access the α-ε region of the phase diagram to obtain equation-of-state (EOS) information, and to determine the location of the epsilon phase boundary for shock loading (LA-UR-18-30153).

9:48AM X17.00008: Proton radiography experiment probing the double shock nature around the α-ε phase boundary of cerium Frank Cherne (Presenter), Brian Jensen, Los Alamos National Laboratory — Traditionally, to understand the density variations in matter at extreme conditions the standard Rankine-Hugoniot jump conditions are applied to experiments to infer the density. Proton radiography allows the direct measurement of density. The reintroduction of the 40-mm powder driven gas gun into the proton radiography facility at Los Alamos National Laboratory has given us the opportunity to probe the α-ε phase transition states in cerium metal. A couple of experiments were fielded measuring the in-situ material density of the shocked material. A two-phase model which was developed to understand the shock states in double shocked experiments was compared with the as obtained material densities. The density comparison with the model and the interpretation of the data will be discussed. In general, there is a good agreement between the calculations and the experimental densities obtained.
10:00 AM X17.00009: Shock compression of additive manufactured metals* DAVID ROBERT JONES (Presenter), SARYU FENSIN, KENDALL JON HOLLIS, BENJAMIN M MORROW, GEORGE T GRAY, Los Alamos National Laboratory — Additive manufacturing allows production of novel structures, not possible with conventional methods. These can take the form of complex geometries, unusual microstructures, or even functionally graded materials. The benefits that these could bring to industries such as aerospace and defense have resulted in a large push to develop AM techniques for structural metals. However, the mechanical response of such parts is often far removed from that of their conventional counterparts. Here, we present results on the shock compression of a range of AM metals, including Ti6Al4V, stainless steel, and tantalum, investigating how they respond to dynamic loading. Comparisons of their equation-of-state and damage tolerance to that of wrought samples will highlight the importance of thorough testing and qualification of AM parts, and reveal some of the challenges that need to be addressed before they can replace traditional methods.

*U.S. Department of Energy: Science Campaigns, LDRD program

10:12 AM X17.00010: Backward and Forward Analyses of Shocked and Ramp-Compressed Metals to 5 Mbars* JEFFREY NGUYEN (Presenter), MINTA C AKIN, Lawrence Livermore Natl Lab, PAUL D ASIMOW, California Institute of Technology — In this report, we present a series of shocked and ramp compressed data on various metals including tantalum and tin. These samples were shocked and ramp-compressed to pressures as high as 5 Mbars with graded density impactors (GDI). To analyze these data, we utilize both backward (characteristics) and forward analyses. The former method does not require a priori knowledge of a pressure drive, and often fails in the presence of strength or phase transition. By using both of these analysis techniques, we can explore the possibility of looking at phase transition and strength during ramp compression. This study also gives us insights into the in-situ properties of GDI during ramp compression. The results are compared to non-destructive ultrasonic scans of GDIs.

*This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

10:24 AM X17.00011: Update on multi-megabar shockless compression at the Z machine* JEAN-PAUL DAVIES (Presenter), JUSTIN BROWN, Sandia National Laboratories — Quasi-isentropic, shockless ramp-wave experiments promise accurate equation-of-state (EOS) data of materials in the solid phase at relatively low temperatures and multi-megabar (100's GPa) pressures. In this range of pressure, isothermal diamond-anvil techniques have limited pressure accuracy due to reliance on theoretical EOS of calibration standards, thus accurate quasi-isentropic compression data would help immensely in constraining EOS models. Multi-megabar shockless compression experiments using the Z Machine at Sandia as a magnetic drive with stripe targets have been performed on many solid materials over the past decade. An update is given on recent results and developments, including experimental techniques, analysis methods, and uncertainty quantification.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X19 DMP: Computational Materials Design and Discovery -- Potential Models and Molecular Dynamics BCEC 156C - Alexander Urban

8:00 AM X19.00001: Deep neural networks to accelerate and reproduce DFT LINDA HUNG (Presenter), Toyota Research Institute, BRIAN ROHR, KRISTOPHER S BROWN, MICHAEL STATT, Chemical Engineering, Stanford University, PATRICK HERRING, ARJUN BHARGAVA, HA-KYUNG KWON, SANTOSH SURAM, MURATAHAN AYKOL, JENS HUMMELSHØJ, Toyota Research Institute — Databases such as the Open Quantum Materials Database and the Materials Project contain the results of density functional theory (DFT) calculations for hundreds of thousands of materials structures. Data at this scale allows us to leverage machine learning models to accelerate DFT computations, or to completely replace them. In this talk we present our recent progress in deep neural network models that can accelerate or reproduce DFT predictions, including energies, band gaps, and electron densities. When training for multiple targets, these networks also generate reduced-dimensional latent space representations that may act as materials fingerprints.
8:12AM X19.00002: MAISE package: Materials prediction accelerated with neural network potentials

ALEKSEY KOLMOGOROV (Presenter), SAMAD HAJINAZAR, ERNESTO D. SANDOVAL, Binghamton University — Our recently released Module for Ab Initio Structure Evolution (MAISE) features an evolutionary algorithm for structure prediction and a neural network formalism for modeling interatomic interactions [1]. The open-source code has a simple interface for parallelized local optimization of crystalline or nanosized structures using a library of neural network or traditional classical potentials. Unique capabilities include a symbiotic evolutionary optimization of nanoparticles and a stratified construction of neural network models for multicomponent systems [2]. This presentation will review confirmed MAISE predictions and illustrate the acceleration of global structure searches with neural network models.


*NSF DMR-1410514

8:24AM X19.00003: Accelerating superalloy discovery using moment tensor potentials

HAYDEN OLIVER (Presenter), BRAYDEN BEKKER, CHANDRAMOULI NYSHADHAM, CARLOS ALBERTO LEON CHINCHAY, GUS HART, Brigham Young University — Superalloys are used in applications where high-temperature strength is necessary. Their extraordinary mechanical properties rely on the formation of the $\gamma'$ – $L1_2$ phase. The discovery of a new superior superalloy will revolutionize the energy and transit industries. Computational methods such as density functional theory (DFT) are used to predict the $\gamma'$ phase, but DFT is expensive and it limits how fast we can discover new superalloys. Moment Tensor Potentials (MTP) create an interatomic potential via machine learning that approximates the quantum mechanical energies of a crystal structure many orders of magnitude faster than DFT. We explore the ternary alloy system Al-Co-W, who's $\gamma'$ phase was discovered experimentally in 2006, and show that MTP correctly predicts this phase. We also explore the ternary alloy system Hf-Ni-Si, which is a superalloy candidate that was found to have a lower formation enthalpy and smaller decomposition energy than Al-Co-W, and report the results of the investigation.

*Authors acknowledge funding from ONR (MURI N00014-13-1-0635)

8:36AM X19.00004: Using machine learning interatomic potentials for finding CoNiTi ternaries

CARLOS ALBERTO LEON CHINCHAY (Presenter), WILEY S MORGAN, GUS HART, Brigham Young University — Superalloys are materials with excellent mechanical properties at extreme temperatures. Superalloys including Co or Ni atoms [1] prompt for a thorough search to improve industry-demanding properties, which requires new computational methods to sweep the huge amounts of possibilities. We search through 200,000 CoNiTi crystal structures to find superalloy phases using machine learning based on interatomic moment tensor potentials (MTP) [2, 3]. We have not only reproduced results reported in the AFLOW database but also predicted stable binary and ternary phases that are not present in the literature. The MTP approach shortens the computational analysis of CoNiTi systems by a factor of 100 compared to a pure DFT methodology. Further analysis will include searching for stable structures at higher temperatures for possible industrial applications.

References

*Authors acknowledge funding from ONR (MURI N00014-13-1-0635).
8:48AM X19.00005: Exploring Materials Space with Machine Learning*  BRAYDEN BEKKER (Presenter), HAYDEN OLIVER, CHANDRAMOULI NYSHADHAM, Brigham Young University, ALEXANDER SHAPEEV, Skolkovo Institute of Science and Technology, GUS HART, Brigham Young University — Electronic structure calculations are too computationally expensive to thoroughly explore the composition space of any system. We use a surrogate model approach that constructs an interatomic potential from a small training set of electronic structure calculations. The surrogate model, called the Moment Tensor Potential (MTP)[1], automates and optimizes the creation of the training set for the interatomic potentials. The potential is then used to explore materials space and predict stable structures including those with new geometries not contained in the training set[2]. We use MTP to study the six promising candidates from a recent high-throughput search for ternary superalloys [3], namely MnNiSb, NiSbTi, NiSbSi, HfNiSi, CoTaV, and CoNbV. We analyze the phase diagram of each ternary system using a pool of 1.2 million structures to show the accuracy of these machine learned surfaces and predict new stable phases at a fraction of the computational time.


*Funding: ONR (MURI N00014-13-1-0635)

9:00AM X19.00006: Combined cluster and atomic displacement expansion for solid solutions and magnetism  KEVIN GARRITY (Presenter), National Institute of Standards and Technology — Finite temperature disordered solid solutions and magnetic materials are difficult to study directly using first principles calculations, due to the large unit cells and many independent samples that are required. In this work, we develop a combined cluster expansion and atomic displacement expansion, which we fit to first principles energies, forces, and stresses. We then use the expansion to calculate thermodynamic quantities at nearly first principles levels of accuracy. We demonstrate that by treating all the relevant degrees of freedom (DOF) explicitly, we can in some cases achieve better convergence than a simple cluster expansion, and we can naturally treat coupling between structural DOF and chemical or magnetic DOF. As examples, we use our expansion to calculate properties of Si1-xGex, magnetic MnO, Al with vacancies, and KxBi1-xTiO3.

9:12AM X19.00007: High-order rotational invariants for structural representations: Application to linearized machine learning interatomic potential*  ATSUTO SEKO (Presenter), ATSUSHI TOGO, ISAO TANAKA, Kyoto University — Machine-learning interatomic potential (MLIP) has been of growing interest as a useful method to describe the energetics of systems of interest. Firstly, we examine the accuracy of linearized pairwise MLIPs and angular-dependent MLIPs for 31 elemental metals [1]. They correspond to generalizations of the embedded atom method (EAM) and modified EAM potentials, respectively. Building the optimal MLIPs for the 31 elemental metals, we show the robustness of the linearized frameworks, the general trend of the predictive power of MLIPs and the limitation of pairwise MLIPs. We also introduce higher-order rotational invariants for improving the accuracy of linearized MLIPs.In this study, a set of rotational invariants up to six-order is derived by the general process of reducing Kronecker products of irreducible representations for SO(3) group. The use of high-order invariants significantly improves the prediction error for a wide range of structures generated from many structure types.


*This study was supported by PRESTO from JST.
9:24AM X19.00008: The second-principles MULTIBINIT software project*  FABIO RICCI (Presenter), ALEXANDRE MARTIN, MARCUS SCHMITT, JORDAN BIEDER, XU HE, ERIC BOUSQUET, MATTHIEU J. VERSTRAETE, PHILIPPE GHOSEZ, Theoretical Materials Physics, Q-MAT, CESAM, Université de Liège, Belgium — Density Functional Theory calculations are limited to relatively small spatial- and time-scales. The purpose of the MULTIBINIT project is to extend the capabilities of first-principles codes to predict properties at the meso-scale, accounting for external constraints (temperature, pressure and fields), while retaining most of the first-principles predictive power and accuracy. MULTIBINIT is distributed within the ABINIT package [1] exploiting first-principles data by a “second-principles” approach. In its initial form, it relies on effective atomic potentials [2] for lattice dynamics, including also explicit coupling with homogeneous strains. Moreover, current developments involve the construction of a spin model and its coupling with the lattice. MULTIBINIT integrates efficient tools for the (i) automatic generation of the models, (ii) automatic fit of the coefficients from first-principles data, (iii) finite temperature simulations and (iv) efficient analysis of results. The power of the method will be illustrated on the full-Heusler Fe2VAl compound to predict finite temperature lattice dynamics and the influence on the thermoelectric properties.


*Work supported by the FEDER project LoCoTED.

9:36AM X19.00009: Structural Deformations in Graphene under Laser Ablation  MOHAMMAD ALAGHemandi (Presenter), MICHELLE Y. SANDER, SAHAR SHARIFZADEH, Boston University — Graphene, with its extraordinary properties, is an excellent compound for a wide range of applications. Moreover, the ability of designing, controlling, and fabricating 3D structures based on graphene would be a breakthrough for manufacturing the new advanced nano-structures. Laser ablation is currently the only technique that allows patterning of free-standing substrates. In this study, we investigate the ablation of a single layer graphene under high energy pulses by using first-principles density functional theory and reactive molecular dynamics (RMD) simulations. To mimic the laser pulse irradiation, we locally heat the selected area of the graphene layer using a Nosé-Hoover thermostat and considered a range of thermally-heated areas with a radius from 2 to 100 Å, and temperature from 1000 to 10000 K. RMD studies indicate that the shape of the ablated area is not only a function of the pulse energy, but also the radius of the pulse beam. When the radius of pulse beam is smaller than 10 Å, no deformation in graphene is observed for pulses with temperature lower than 8000 Å. Additionally, our predicted trends in the size and shape of the ablated areas coincide well with the experimental results carried out using femtosecond laser beams on a micrometer scale.

9:48AM X19.00010: Atomistic investigation of a carbonization process for C/H/O/N-based polymers with use of the reactive potentials: ReaxFF*  MALGORZATA KOWALIK (Presenter), CHOWDHURY M. ASHRAF, ADRI C. T. VAN DUIN, Mechanical Engineering, PSU — During a carbonization process of the raw polymer precursors, the graphitic structures evolve and are responsible for improved mechanical properties of the carbonized carbon fibers. To gain a deeper understanding of a chemistry behind an evolution of these graphitic structures, we perform atomistic simulations using a reactive force field: ReaxFF. We considered three different polymers as a precursor: idealized ladder PAN, proposed oxidized PAN and PBO to understand how underlying molecular details of polymers direct final carbon fibers structure. Since these are C/H/O/N-based polymers, firstly we proposed an improved force field for C/N/H chemistry based on new DFT data. Then, with use of this improved force field, we perform atomistic simulations of the carbonization process for the considered polymers. Based on these simulations we were able to determine small molecules, as well, all carbon rings productions, and analyzed the graphic structures evolutions. We also performed the stress-strain simulations on the initially carbonized samples and were able to assess how a presence of the graphitic structure affects the mechanical responds.

*Work supported by US DoE EERE VTO DE-EE0008195.
10:00AM X19.00011: Molecular Dynamics Investigations of the Mechanical Properties of Heterogeneous Structures Composed of Graphene Sheets, Graphene Ribbons, and Boron Nitride Sheets  CUIYING JIAN (Presenter), NICOLA FERRALIS, JEFFREY C GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — It is well known that monolayer/multilayer graphene possesses ultra-high elastic modulus and critical stress with intrinsic low toughness. In order to explore ways to reduce its brittleness, in this work we employ atomistic modeling to examine the mechanical properties of mono- and multilayers of graphene, nanoribbons, boron nitride and a range of combinations. Regardless of size, edge type exhibits a significant effect on the critical stress/strain, evidenced by the higher mechanical strength of zigzag compared to armchair ribbons, as well as the armchair direction in graphene sheets. Furthermore, our calculations show that with increasing number of layers the mechanical strength of graphene deviates from that of the monolayer sheet, while in contrast multilayer boron nitride sheets preserve the fracture point of the single layer. Based on these results, we explored a range of heterogeneous structures composed of graphene sheets, graphene nanoribbons, and boron nitride sheets. Under tensile stretch, components in these heterogeneous structures show asynchronous cracking behavior helping to improve the overall toughness. By analyzing interfacial binding/sliding between heterogeneous components, the underlying mechanisms are explored and improved compositions can be proposed.

10:12AM X19.00012: Toward Sustainable Asphaltic Materials: A Molecular Dynamics (MD) Investigation of Bio-oil Modified Asphalt*  ISKINDER ARSANO (Presenter), KSHITIJ C JHA, MESFIN TSIGE, The University of Akron — We have investigated the behavior of a novel asphaltic material obtained by adulterating a model asphalt system1 with a rationally selected foreign species of bio-oil. A wide range of systems is modeled by MD simulations featuring a systematic combination of modifier type, modifier concentration, and temperature. The mobility and structural integrity of the proposed materials were investigated in addition to mechanical response prediction by use of moduli calculations. The need to resolve issues of processability such as phase separation of commonly used modifiers, for example scrap tire2, represents an important impetus for the current project. A case is made whereby the molecular observations made in the proposed modified asphalt systems indicate a maintenance of or improvement over essential macro functionalities of pristine asphalt. The replacement of a significant proportion of traditional asphalt by bio-oils constitutes a move toward green construction materials by allowing for less use of bitumen, a byproduct in heavy oil refineries implicated in pollution.

References:

*We acknowledge support from NSF Grant # 1506275

10:24AM X19.00013: Computational design of organic molecules for reducing friction at the nanoscale  JING YANG (Presenter), JON PAUL JANET, FANG LIU, HEATHER J KULIK, Chemical Engineering, Massachusetts Institute of Technology — Computational modeling has the promise to enable atom-by-atom design of nanoscale properties that give rise to essential changes in macroscale properties. In the quest for increasing energy efficiency and resource utilization, energy losses remain an outstanding challenge that can be solved in part through computational materials design. Friction reducers (FRs) are molecular additives that can minimize friction loss in these engines by reducing friction between moving parts at the nanoscale. Traditional FRs contain metals, sulfur, and phosphorus, which can poison exhaust system catalysts and diesel particulate filters. Thus, if suitably designed, organic friction reducers (OFRs) present a promising alternative solution. Here, we apply non-equilibrium molecular dynamics simulations together with density functional theory methods to enable the atom-by-atom design of OFRs. We directly compute the coefficients of friction of OFRs on model engine iron oxide surfaces with varying coverage and temperature, and explore a number of conditions not easily probed during experiments. These studies allow us to build a quantitative structural property relationship for predicting good OFR characteristics, enabling an iteratively improving materials design workflow.
10:36AM X19.00014: Machine-Learning Provides New Insights into the Coil-to-Globule Transitions of Thermosensitive Polymers*  
KARTEEK KUMAR BEJAGAM, YAXIN AN, Chemical Engineering, Virginia Tech, SAMRENDRA SINGH, CNH Industrial, SANKET DESHMUKH (Presenter), Chemical Engineering, Virginia Tech — First of its kind, a temperature-independent coarse-grained (CG) model of poly(N-isopropylacrylamide) (PNIPAM) that can accurately predict its experimental lower critical solution temperature (LCST) in the presence of explicit water model is developed. This extensively validated CG model by conducting MD simulations by changing the radius of gyration of initial structure, the chain length, and the angle between the adjacent monomers of the initial configuration of PNIPAM. The model could retain PNIPAM's tacticity and thereby predict its LCST, which is consistent with experiments and all-atom simulations. A data-driven machine-learning (ML) approach, non-metric multidimensional scaling (NMDS) method, was used to analyze these CG MD simulation trajectories. This analysis suggest that PNIPAM chain undergoes a coil-to-globule transition above the LCST via multiple metastable states. 

*Virginia Tech Start-up Funds

10:48AM X19.00015: Bayesian inference of grain growth prediction via multi-phase-field models*  
HIROMICHI NAGAO (Presenter), SHIN-ICHI ITO, TAKASHI KUROKAWA, TADASHI KASUYA, JUNYA INOUE, University of Tokyo — We propose a Bayesian inference methodology to evaluate unobservable parameters involved in multi-phase-field models with the aim of accurately predicting the observed grain growth, such as in metals and alloys. This approach integrates models and a set of observational image data of grain structures. Since the set of image data is not a time series, directly applying conventional inference techniques that require time series as the input data is difficult. Our key idea is to construct a time series with an appropriate statistic that characterizes static image data of grain structures. The empirical Bayes method estimates not only a probability density function of the parameters but also an initial phase-field, which is generally unobservable in real experiments. The proposed method is confirmed to estimate, from real experimental images of grain structures in a steel alloy, unobservable parameters together with their uncertainties, and successfully selects the initial phase-field that best explains the experimental data from among candidate initial phase-fields.

*This work was supported by the Council for Science, Technology and Innovation (CSTI), the Cross-ministerial Strategic Innovation Promotion Program (SIP) "Structural Materials for Innovation" (Funding agency: JST).
SOC strength is much larger due to the larger charge confinement effect in these materials. The results were confirmed and magneto-electroluminescence (MEL) in the 3D perovskite devices in which MC and MEL with 0.07% magnitude and distortions of the lattice, necessary for high performance solar cells. Nevertheless, fundamental studies on SOC strength of these materials have still been very limited. Here, we present the magnetic field effect (MFE) in light emitting diodes (LEDs) made of the 3D hybrid perovskite CH$_3$NH$_3$PbI$_3$ (MAPbI$_3$) and 2D Ruddlesden-Popper hybrid perovskite (CH$_3$(CH$_2$)$_3$NH$_3$)$_2$(CH$_3$NH$_3$)Pb$_2$I$_7$, where the width and the magnitude of the magnetic response in conductivity and electroluminescence are measures of the SOC strength in the materials. We observed the magneto-conductance (MC) and magneto-electroluminescence (MEL) in the 3D perovskite devices in which MC and MEL with 0.07% magnitude and 250 G half width indicate the strong SOC strength. The absence of the MFE in the 2D perovskite devices indicates that the SOC strength is much larger due to the larger charge confinement effect in these materials. The results were confirmed by our MFE studies on the photocurrent of the devices.

8:36AM X20.00004: Freestanding Crystalline Monolayers of Oxide Perovskites* DIANXIANG JI, SONGHUA CAI, National Laboratory of Solid State Microstructures, and College of Engineering and Applied Sciences, Nanjing University, TULA PAUDEL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, HAOYING SUN, CHUNCHEANG ZHANG, LU HAN, YIFAN WEI, YIPENG ZANG, MIN GU, National Laboratory of Solid State Microstructures, and College of Engineering and Applied Sciences, Nanjing University, YI ZHANG, WENPEI GAO, HUAIXUN HUYAN, Department of Chemical Engineering and Materials Science and Department of Physics and Astronomy, University of California, Irvine, WEI GUO, DI WU, ZHENGBIN GU, National Laboratory of Solid State Microstructures, and College of Engineering and Applied Sciences, Nanjing University, EVGÉNY Y TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, PENG WANG, YUEFENG NIE (Presenter), National Laboratory of Solid State Microstructures, and College of Engineering and Applied Sciences, Nanjing University, XIAOQING PAN, Department of Chemical Engineering and Materials Science and Department of Physics and Astronomy, University of California, Irvine — Two-dimensional (2D) materials like graphene have demonstrated new electronic phases that can emerge when a bulk crystal is thinned down to a mono-layer. As transition metal oxide perovskites host a variety of correlated phases, realizing the analogs with oxide perovskite materials would open the door to a rich spectrum of exotic 2D correlated phases that have not yet been explored. Here we report on the fabrication of freestanding perovskite films with high crystalline quality down to a single unit cell. Using the recently developed method based on water-soluble Sr$_3$Al$_2$O$_6$ as the sacrificial buffer layer we synthesize freestanding SrTiO$_3$ and BiFeO$_3$ ultrathin films by reactive molecular beam epitaxy and transfer them to different substrates such as crystalline silicon wafers and holey carbon films. We find that freestanding BiFeO$_3$ films exhibit an unexpected giant tetragonality and polarization when approaching the ultimate 2D limit. The ability to synthesize crystalline freestanding perovskite films without thickness limitation opens a new field for the 2D correlated electronic phases and interfacial phenomena.

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Optoelectronic properties of layered and 3D hybrid perovskites: recent results

Invited

JACKY EVEN (Presenter), Institut foton, insa

In the past five years, solution-processed organometallic perovskite based solar cells have emerged as a promising thin-film photovoltaic technology with record conversion efficiencies as high as 23.3%. The presentation will review recent optical spectroscopy and diffraction results on 3D halide perovskites, as well as colloidal nanocrystals that also exhibit attractive light emission properties. Presently, the intended optoelectronic applications of this class of 3D materials are in the realm of semiconductors. But they can be described as unconventional semiconductors, because the spin-orbit coupling is giant and shows up in the conduction band. More, the band gap is direct with a critical wavevector located at one of the edges of the reference Brillouin zone, and among others, excitonic and Rashba-Dresselhaus effects, as well as electron-phonon coupling and lattice anharmonicity may play a crucial role. Related 2D multilayered phases, composed of perovskites multilayers sandwiched between two layers of large organic cations, have recently demonstrated improved solar cells photostability under standard illumination as well as humidity resistance, leading to conversion efficiencies in the 10-15% range. In this case, intrinsic quantum and dielectric carrier conﬁnements are afforded by the organic inner barriers and a tunable perovskite layer thickness, which lead to stable Wannier excitons at room temperature. These excitations share some similarities with the ones observed in Van der Waals heterostructures. Solar cell and LED device operations are related to internal exciton dissociation through low energy states in multilayered perovskites, as shown from the investigations of both thin films and small exfoliated single crystals. Multilayered halide perovskites shall lead to extensive chemical engineering in the future.

First-Principles Studies of the Electronic and Optical Properties of Halide Perovskites: From Three to Two Dimensions*

MARINA R FILIP (Presenter), Molecular Foundry, Lawrence Berkeley National Lab, JONAH HABER, Physics, University of California Berkeley, JEFFREY B NEATON, Molecular Foundry, Lawrence Berkeley National Lab

Metal-halide perovskites have emerged in the past six years as a disruptive new class of optoelectronic materials. Solar cells based on 3D lead-halide perovskites have recently reached a record power conversion efficiency of 23.3%. In addition, the 2D variants are gaining momentum as a promising new class of versatile materials for applications in light emission and solar energy conversion [1,2,3]. Despite these developments, fundamental optoelectronic properties of this novel family of layered materials are not yet fully understood. Here, we will explore the role of structural effects on the optoelectronic properties of 2D lead-halide perovskites with DFT and ab-initio many-body perturbation theory. We will examine the effects of various mean field starting points and self-consistency in the GW approximation, while explicitly incorporating spin-orbit interactions. Lastly, we will analyze the importance of electron-hole interactions upon optical excitation, within the Bethe-Salpeter equation, and discuss the optical spectra and photophysics of these complex class of compounds.


*This work is supported by the Department of Energy; computational resources provided by NERSC
Making and breaking the exciton in layered halide hybrid perovskites

MIKAEL KEPENEKIAN (Presenter), BOUBACAR TRAORE, Institut des Sciences Chimiques de Rennes (ISCR), CNRS, JEAN-CHRISTOPHE BLANCON, Department of Chemical and Biomolecular Engineering, Rice University, LAURENT PEDESSEAU, Institut FOTON, INSA Rennes, WANYI NIE, LANL, CONSTANTINOS STOUMPOS, Department of Materials Science and Technology, University of Crete, MERCOURI KANATZIDIS, Department of Chemistry, Northwestern University, JACKY EVEN, Institut FOTON, INSA Rennes, ADITYA D. MOHITE, Department of Materials Science and Nanoengineering, Rice University, SERGEI TRETIAK, LANL, CLAUDINE KATAN, Institut des Sciences Chimiques de Rennes (ISCR), CNRS — Layered halide hybrid organic–inorganic perovskites (LHP) [1] have been the subject of intense investigation before the rise of three-dimensional (3D) halide perovskites and their impressive performance in solar cells. Recently, LHP have also been proposed as attractive alternatives for photostable solar cells [2] and revisited for light-emitting devices. LHP present inherent quantum and dielectric confinements imposed by the organic layers sandwiching the inorganic core, and computational approaches have successfully helped rationalize their properties [4-6].

Here combine theoretical and spectroscopic studies inspect the various ingredients of LHP strong exciton binding energy and the ways to break the electron-hole pair [3,4]. In particular, we propose an elastic model providing design principles for future layered perovskites with optimized properties for photovoltaics or light emission [7].


Rashba Splitting in Hybrid Lead Halide Perovskites probed by Photogalvanic Spectroscopy

XIAOMEI JIANG (Presenter), Physics, University of South Florida, — Hybrid Lead Halide Perovskites (HLHPs) such as MAPbX3 (where MA is methyl-ammonium and X is halogen) have shown unprecedented performance in optoelectronic device applications such as solar cells, photodetectors and light emitting diodes. The recent discoveries of giant Rashba splitting in both bulk (3D) and two-dimensional (2D) HLHPs have raised promise that these compounds may be excellent candidates for spintronic device applications. Using both photogalvanic (PGA) and photoluminescence spectroscopies we evaluate the Rashba splitting value in both polycrystalline and single crystal HLHPs. We have uncovered the morphological influence on the Rashba splitting in these compounds by measuring angular, temperature and excitation dependencies of the PGA. We also report on the influence of defects and grain boundaries on the Rashba splitting in various HLHP crystallographic phases.

Control over ultrafast Rashba splitting dynamics in quasi-2D arrays of 3D hybrid perovskite nanocrystals by the interfacial electric field

YURI GLINKA (Presenter), RUI CAI, Department of Electrical and Electronic Engineering, Guangdong University Key Lab for Advanced Quantum Dot Displays and Lighting, Shenzhen Key Laboratory for Advanced Quantum, JUNZI LI, XIAODONG LIN, TINGCHAO HE, College of Physics and Energy, Shenzhen University, Shenzhen 518060, China, RUI CHEN, Department of Electrical and Electronic Engineering, Guangdong University Key Lab for Advanced Quantum Dot Displays and Lighting, Shenzhen Key Laboratory for Advanced Quantum, XIAO WEI SUN, Department of Electrical & Electronic Engineering, Guangdong University Key Lab for Advanced Quantum Dot Displays and Lighting, Shenzhen Key Laboratory for Advanced Quantum D — Snapshot spectral imaging has been performed with 100 fs steps in delay-times for fully encapsulated quasi-2D arrays of 3D hybrid perovskite MAPbBr3 nanocrystals (~20 nm in size) spin-coated to either the clean sapphire plate or to that initially ALD-coated by a ~30 or ~100 nm thick ZnO layer. The absorption bleaching band for the bare MAPbBr3 nanocrystal arrays reveals a ~200 meV splitting appearing within ~1 ns, which has been assigned to the Rashba splitting effect. However, the splitting unexpectedly disappears for the MAPbBr3/ZnO samples at delay-times longer than ~500-600 fs when the interfacial electric field at the MAPbBr3/ZnO heterointerface develops due to charge separation. The effect has been treated theoretically in the frame of the model taking into account the interfacial-field-induced structural phase transition in MAPbBr3 nanocrystals.
10:12AM X20.00010: Revealing nanocrystal growth within CsPbI$_{2-x}$Br$_{3-x}$ perovskite thin films  LINDSEY GRAY (Presenter), JUNWEI XU, XIAOHENG SEAN YAN, DAVID CARROLL, Wake Forest University, WAYNI NIE, Los Alamos National Laboratory —

Inorganic lead halide perovskites have greatly impacted the optoelectronics field due to their band-tunability and solution-processability in high performance light emitting diodes (LEDs). However, the bulk material is unstable under room temperature which tends to phase segregate under ambient or device operational conditions. Recent breakthrough has successfully demonstrated a stabilized CsPbX$_3$ phase at room temperature by fabricating into nanostructured crystals (NC). Further, photo-physical property enhancement is attributed to the nano-scale structure control which are thus the most promising candidate for the lighting applications. It is therefore critical to systematically understand the structure of the CsPbX$_3$ NC synthesized via controlled approach and connect that with device operation efficiency and stability. In this study, we systematically investigated the synthetic approach to obtain room temperature stabilized mixed halide nanocrystals, focusing on the effect of the molar ratio between Cs source and Pb source on the optical performance in the mixed CsPbI$_2$Br perovskite thin films. The findings revealed the nanocrystal growth mechanism of the in situ processed perovskite layer which enabled us to fabricate bright and efficient red perovskite LEDs.

10:24AM X20.00011: Above-bandgap emission properties of CsPbBr$_3$ as probed by fine-scale photoluminescence excitation spectroscopy* HONG SEON RYU, Physics, Sogang University, CONSTANTINOS STOUMPOS, Materials Science and Technology, University of Crete, KYLE MCCALL, MERCOURI KANATZIDIS, Chemistry, Northwestern University, JOON JANG (Presenter), Physics, Sogang University — Halide perovskites are next-generation materials for solar cells and light emitting diodes. Despite rapid progress in applied perovskite technology, understanding of their basic properties is not complete yet. Especially, it is necessary to clarify the bandgap and the nature of the photoluminescence (PL) process (whether excitonic or electron-hole recombination) for the high performance of the devices. As a case study, we investigated unusual bandgap and recombination behaviors of CsPbBr$_3$ using PL excitation spectroscopy. Significant variation of both shape and intensity of the PL was observed when the excitation wavelength was tuned across the bandgap. Intriguingly, PL emission occurs above the bandgap, which arises presumably from radiative recombination at halide vacancies. Excitation power dependence of the PL shows that the power exponent continuously varies from 2 to 1 and to sublinear with increasing the laser intensity. The rate equation for pulsed excitation was modeled to account for this anomalous effect. Our model implies that the PL arises from electron-hole recombination at room temperature.

*The work was supported by the Basic Science Research Program (2017R1D1A1B03035539) through the National Research Foundation of Korea (NRF), funded by the Korean government.

10:36AM X20.00012: Optical and transport properties of mixed halide all-inorganic quantum dot inkjet-printed films* DYLAN RICHMOND (Presenter), Department of Physics, State University of New York-Oswego, Oswego, NY 13126-3599, THILINI K EKANAYAKA, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588-0299, MASON MCCORMICK, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588-0304, NICOLE BENKER, SYED QAMAR ABBAS, CORBYN MELLINGER, GUANHUA HAO, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588-0299, ALEXANDER SINITSKII, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588-0304, PETER A DOWBEN, ANDREW J YOST, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588-0299, CAROLINA C. ILIE, Department of Physics, State University of New York-Oswego, Oswego, NY 13126-3599 — Inorganic halide perovskite quantum dot inks may have great potential in applications related to the field of inkjet-printed photovoltaics. The photoactive inks are synthesized by a wet chemical reaction and are printed into thin films using a commercial inkjet printer. The inkjet-printed films were then characterized using optical absorption spectroscopy, photoluminescent spectroscopy, X-ray diffraction, X-ray photoemission spectroscopy, and electronic transport measurements. Characterization indicates that interlayer printing, alternating printed layers of CsPbBr$_3$ and CsPbI$_3$, results in a halide exchange producing a high quality (220) CsPbBr$_{2.10,9}$ quantum dot thin film. The repeatable properties of the inkjet-printed thin films suggest high quality, customizable, photovoltaic films are realizable with an inkjet printing method.

*This work was supported by the National Science Foundation (NSF) through the Nebraska Materials Research Science and Engineering Center (MRSEC) (grant No. DMR-1420645) and grant No. CHE-IJ65692, and SUNY Oswego.

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X21 DMP: Nanostructures and Metamaterials -- Nonlinear Effects BCEC 157B - Sui Yang -

Tag(s): Focus
8:00AM X21.00001: Controlling emission and nonlinearity with plasmonic metamaterials* [Invited] VIKTOR PODOLSKIY (Presenter), University of Massachusetts Lowell — Metamaterials encompass a broad class of structures whose electromagnetic response is driven by their geometry in addition to their composition. Plasmonic nanowire metamaterials provide a platform for engineering optical response from dielectric to epsilon-near-zero to strongly anisotropic (hyperbolic) regimes. Importantly, these metamaterials support exotic additional electromagnetic waves. From the effective medium standpoint, these waves can be described by nonlocal (spatially dispersive) permittivity. In this talk we present a theory of nonlocal electromagnetism in nanowire metamaterials and analyze the effect of optical nonlocalities on spontaneous emission and nonlinear optics in these composites. We show that additional electromagnetic modes can drastically increase local density of photonic states, causing significant enhancement of decay rates. We also demonstrate that plasmonic composites can be used to engineer bulk second-order nonlinearities, with amplitude of effective nonlinear polarizability comparable to that in LiNb and KDP. Finally, we show that geometry of nanowire composites can be used as an important parameter to control polarization properties of structural second harmonic generation.

*This research has been partially supported by the US Army Research Office

8:36AM X21.00002: Deterministic modal control of second-harmonic generations in a plasmonic two-wire transmission-line* TZU-YU CHEN, National Tsing Hua University, JULIAN OBERMEIER, MARKUS LIPPITZ, University of Bayreuth, CHENBIN HUANG (Presenter), National Tsing Hua University — A plasmonic two-wire transmission-line supports two modes, one with surface plamon fields strongly confined in the gap, the other loosely guided by the wire perimeters. Using the modal asymmetry provided by the loosely guided mode, we demonstrate a new way to allow second-harmonic generation (SHG). Moreover, we demonstrate both experimentally and theoretically the ability to deterministically control the SHG modes.

*Ministry of Science and Technology in Taiwan under grant MoST 106-2112-M-007-004-MY3.

8:48AM X21.00003: Large diffracted transverse magneto-optic Kerr effect in magnetoplasmonic crystals RAFAEL CICHELEIRO, MIKKO KATAJA, MARIANO CAMPOY-QUILES, GERVASI HERRANZ (Presenter), Institute for Materials Science of Barcelona ICMAB-CSIC — Phase-matching conditions are exploited to enable nonreciprocal optical propagation and enhanced magneto-optic responses in magnetoplasmonic systems [1]. Here we show that exploiting diffraction in conjunction with plasmons adds versatility and flexibility in the design of photonic systems. As a testbed we analysed the transverse magneto-optic Kerr effect (TMOKE) in Au/Co magnetoplasmonic gratings that combined magneto-optics, diffraction and plasmonics. Angular resolved measurements revealed narrow line-shape plasmon resonances, enabling large diffracted magneto-optical activity. We show that exploiting diffraction in magnetoplasmonic crystals allows unexpectedly large TMOKE responses that exceed 3% - one of order of magnitude larger than conventional TMOKE. Our results pave the way towards using magneto-optical modulation of SPPs to build non-reciprocal, active photonic components. We anticipate that our results can be used to design more complex diffractive surfaces, such as plasmonic metasurfaces, with the objective to enable creation of novel non-reciprocal photonic devices.

9:00AM X21.00004: Effects of Spatial Confinement on Nonlinear Light Emission from Plasmonic Nanostructures ROBERT LEMASTERS (Presenter), HAYK HARUTYUNYAN, Emory University — Photoluminescence (PL) from plasmonic nanostructures with spatial inhomogeneities have been demonstrated to exhibit an interesting nonlinear character [1,2]. Previous studies on rough metal films have shown the PL signal to have a wavelength dependent nonlinear scaling exponent which increases linearly with emitted photon energy [2]. This result was attributed to recombination of nonequilibrium electrons within the conduction band mediated by the breakdown of momentum restrictions as a consequence of the spatial inhomogeneities of the surface. However, in these experiments the spatial structures under study were random in nature. Thus, the degree of momentum breakdown and its effect on PL are not obvious from these results. To address this, we use a geometry of Au nanowires separated from Au films by nanometric SiO2 layers via ALD to control the degree of spatial confinement of the resonant gap-mode plasmons. Our results indicate that the PL signal from this nanoprecise system has a nonlinear power law exhibiting two distinct linear regimes, differing from that of rough films. This indicates that the physical mechanism of the nonlinear PL signal originating from thermalized hot electron relaxation needs to be revisited.
9:12AM X21.00005: Bistable shallow arches: a new building block for nonlinear mechanical metamaterials
ELEONORA TUBALDI (Presenter), University of Arizona, GABRIELE LIBRANDI, KATIA BERTOLDI, SEAS, Harvard University — Snap-through instability of shallow arches is a well-known phenomenon and it has been extensively investigated in the literature. However, the mechanics of shallow arches has not been exploited yet for engineering nonlinear mechanical metamaterials. In this study, we use shallow arches as building blocks for realizing snapping-through bistable nonlinear structures. By carefully assembling shallow arches in 2D arrangements, we can engineer fully snapping unit cells, which snap between two equally stable energy configurations. These unit cells can tile a 2D space which will have both bistability and snapping-through behavior. In this 2D array, the snapping of a unit cell triggers the snapping of the neighbor cells allowing the propagation of a "snapping wave" in the whole structure. We also show that it is possible to design snapping unit cell showing different configurations accordingly with the specific type of mechanical applied stimulus (i.e. moments, concentrated forces etc.). We successfully prove that a fully reversible nonlinear mechanical metamaterial by harnessing shallow arches snap-through instability is viable. This anticipates being a promising avenue because its versatility in both the 2D space tessellation and the shallow arch design (i.e. bilayer shallow arches).

9:24AM X21.00006: X-ray creation by relativistic electrons in a nanophotonic vacuum*
NICHOLAS RIVERA (Presenter), Massachusetts Institute of Technology, LIANG JIE WONG, Singapore Institute of Manufacturing Technology, JOHN D JOANNOPOULOS, MARIN SOLJACIC, Massachusetts Institute of Technology, IDO KAMINER, Technion Israel Institute of Technology — The vanishingly small response of matter to light beyond ultraviolet (UV) frequencies makes it challenging to leverage concepts from nanophotonics to manipulate the emission and propagation of light at such frequencies. Here, we show that free-electron based two-quanta processes allow tunable light sources from UV to gamma ray frequencies, without the need for any external electromagnetic fields. We find that the intentional design of vacuum fluctuations by tuning the permittivity of a material at IR frequencies allows one to exert direct control over the spectrum and intensity of output X-ray radiation. The per-electron power of such X-ray emission is comparable with that of synchrotrons employing a 0.1-1 T magnetic field. We find that this powerful emission derives its strength from the strong Casimir-Polder forces in the extreme nanoscale of materials. Fundamentally, our results reveal a way to apply the tools of nanophotonics even at frequencies where materials do not respond. They also constitute a new mechanism by which vacuum fluctuations can be used to generate high frequency light, potentially enabling new concepts such as compact and tunable sources of photons from UV-to-gamma-ray energies.

*N.R. is supported by the DOE Computational Science Graduate Fellowship.

9:36AM X21.00007: Imaging collective behavior in an rf-SQUID metamaterial tuned by DC and RF magnetic fields*
ALEXANDER P. ZHURAVEL, B. Verkin Institute for Low Temperature Physics and Engineering, SEOKJIN BAE, STEVEN ANLAGE (Presenter), Physics Department, University of Maryland, College Park — We examine the collective behavior of two-dimensional nonlinear superconducting metamaterials using a novel imaging technique. The metamaterial is made up of self-resonating microwave oscillators in a strongly coupled 27 x 27 planar array of radio-frequency Superconducting QUantum Interference Devices (rf SQUIDs). By using low-temperature laser scanning microscopy (LSM) we image the photoresponse caused by local heating across the SQUID array, and this corresponds to the strength of oscillation of each meta-atom. Complex collective modes of the metamaterial which are not revealed in global measurements become visible to the LSM. The clustering of active meta-atoms in each collective mode of the metamaterial are imaged. We observe the rearrangement of coherent patterns due to meta-atom resonant frequency tuning as a function of external dc and rf magnetic flux bias. We find that the excited rf SQUID distribution across the metamaterial at zero dc flux and small rf flux reveals a low degree of coherence. By contrast, the spatial coherence heals upon increasing of rf flux amplitude. We discuss possible origins of such coherence variations.

*This work is supported by NSF grant No. DMR-1410712, and DOE grants No. DESC0017931, DESC0018788, and a Volkswagen Foundation grant No. 90284.
9:48AM X21.00008: Towards Room Temperature Plasmonic Lasing from Zn-Doped GaAs Nanowires*  
GYANAN AMAN  
(Presenter), Department of Electrical Engineering and Computer Science, University of Cincinnati, Cincinnati, OH 45221, U.S.A,  
FATEMESADAT MOHAMMADI, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, U.S.A,  
MYKHAYLO LYSEVYCH, HOE TAN, CHENNUPATI JAGADISH, Department of Electronic Materials Engineering, Research School of Physics and Engineering, Australian National University, Canberra ACT, 0200, Australia,  
HEIDRUN SCHMITZER, Department of Physics, Xavier University, Cincinnati, OH 45207, MARTIN FRAENZL, Department of Physics, University of Leipzig, 04103 Leipzig, Germany,  
MARC CAHAY, Department of Electrical Engineering and Computer Science, University of Cincinnati, Cincinnati, OH 45221, U.S.A,  
HANS PETER WAGNER, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, U.S.A — We investigated optically pumped lasing from zinc-doped GaAs nanowires (NWs) on a Au film and from NWs comprising a nominally 10 nm thick Au coating at temperatures ranging from 80 to 295 K. The NWs have an average diameter and length of 200 nm and 2.5 µm, respectively, and possess a 7 nm thin Al₂O₃ spacer layer surrounding the NWs. The NWs were optically excited with 150 fs laser pulses with a center wavelength of 770 nm which were provided by a Ti-Sapphire laser. Due to the shortness of the NWs only one longitudinal lasing mode resonates with the gain spectrum which extends from ~1.48 to 1.52 eV at 80 K. At higher temperature the lasing mode slightly shifts towards lower energy and weakens due to band-gap shrinkage and increasing non-radiative losses at surface states. The lasing output versus excitation power (L-L) plot at 80 and 295 K shows the characteristic “S” shape curve for NWs on Au. The L-L plot for Au coated NWs shows lasing at 80 K but suggests amplified spontaneous emission at 295 K due to higher plasmonic losses. A simulation of the experimental data with FDTD calculations reveals that lasing from NWs on Au is predominantly plasmonic while it has a hybrid photonic-plasmonic character in Au coated NWs.  
*Support from Australian Research Council and URC is acknowledged.

10:00AM X21.00009: Characterization of a Single Quantum Meta-atom for a Superconducting Quantum Transmission Line Metamaterial*  
JINGNAN CAI (Presenter), STEVEN ANLAGE, University of Maryland, College Park — The quantum transmission line (QTL) metamaterial provides a unique opportunity to investigate emergent quantum phenomena, due to the strong coupling between the meta-atoms and the bosonic mode in the resonator as well as the quantum mechanical nature of such interaction. Two designs for QTL are considered in this study: flux and charge qubits embedded in a coplanar waveguide, the latter of which possesses interesting nonlinear coupling between neighboring meta-atoms that depend on the quantum state of the Josephson junction. Here we report the first step towards the realization of QTL metamaterial: the design, fabrication, and characterization of a single flux qubit in the coplanar waveguide. The characterization, which will eventually include vacuum Rabi splitting, Rabi oscillations, and quantum tomography, will be conducted through a microwave transmission measurement.  
*This work is supported by the Department of Energy through grant # DESC0018788

KYOUNGWEON PARK (Presenter), Air Force Research Laboratory, JAKE FONTANA, Naval Research Laboratory, JASON STREIT,  
JAMIE GENGLER, CARL M LIEBIG, RICHARD VAIA, Air Force Research Laboratory — Optical bandpass filters allow or reject a range of wavelengths. Metallic nanorods (NRs) and their assemblies are a promising platform for such components due to their intense light-matter interactions and ability to tune optical cross-section based on the NR’s aspect ratio and volume. Fabrication of arbitrary NR filter design however is challenging due to synthetic limitations on aspect ratio and inherent polydispersity. Herein we demonstrate design and fabrication of arbitrary optical notch filters with a flat top profile using new synthetic strategies combined with wavelength selective particle reshaping. Bandwidth and spectral profile is defined by a collection of NRs with narrow longitudinal plasmon resonances (LSPR) that define absorption and sharp roll-off at the filter edges. Laser irradiation transcribes transmission notches by reshaping a population of NRs in resonance with the LSPR. Furthermore, single or multiple transmission windows across the visible to mid-IR can be fabricated using polydisperse NRs or nanowires. Experimental validation of fabrication models confirm rational design of position, depth, and width of the transmission window, enabling manufacturing of complex optical elements (solutions or solid) not found in natural media.
10:24AM X21.00011: Tailoring Localized Surface Plasmon Resonances in Metallic Nanoarcs for Surface Enhanced Infrared Absorption Spectroscopy*  KUNYI ZHANG (Presenter), ODED RABIN, University of Maryland, College Park — Surface enhanced infrared absorption (SEIRA) takes advantage of the strong localized electromagnetic fields of metallic nanoantennas to amplify the optical absorption of molecules in the infrared region, which provides new opportunities for ultra-sensitive molecule detection. The maximum signal enhancement is predicted when the localized surface plasmon resonance (LSPR) frequency matches with the vibrational band of molecules. In this work, we established an empirical relation between the geometric parameters of gold nanoarcs on silicon wafers and their LSPR frequency. This relation was then utilized to design substrates for SEIRA measurements. The SEIRA signal evolves as the LSPR frequency is scanned from above to below the bond vibrational frequency.

*This work was supported by a grant from the National Science Foundation (DMR-1151614). This research used resources of the Advanced Light Source, which is a DOE Office of Science User Facility under contract no. DE-AC02-05CH11231. We acknowledge the support of the Maryland NanoCenter and its FabLab and AIMLab.

10:36AM X21.00012: Large-scale testing and simulation of nanofabricated thermionic energy converters  PETER SCHERPELZ (Presenter), STEPHEN E CLARK, ARVIND KANNAN, HSIN-I LU, DANIEL MERTHE, Modern Electron — Thermionic energy converters are a potential technology for efficient, direct, and compact heat-to-electricity conversion with no moving parts. We discuss the testing and simulation of devices for thermionic conversion which incorporate a nanofabricated electrostatic lensing system to mitigate space charge. In order to achieve high performance, these devices must minimize loss of the vacuum electrons to the electrostatic grids, which requires precise modeling of electron emission and absorption. We demonstrate the use of a large experimental dataset, encompassing a variety of grid geometries and operating conditions, to validate and improve our model. Specifically, we show that including effects such as dielectric charging provides statistically significant improvements in agreement between experiments and kinetic particle-in-cell simulations. We then use these models to improve device performance, exemplifying the value of experimental validation.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X22 DCOMP DMP: Electrons, Phonons, Electron-Phonon Scattering and Phononics VIII  BCEC 157C - David Broido, Boston Coll - Tag(s): Focus
Computational quest for high-mobility 2D materials

Recently, we identified close to 2000 exfoliable 2D materials from first-principles calculations [1]. The next natural step is to explore their properties and look for novel or improved performance. Here, we are searching for electrostatically-doped 2D semiconductors with superior electronic transport properties.

A first goal is then to develop accurate and systematic workflows to compute phonon-limited mobilities [2]. These workflows identify the pockets of electronic states relevant to transport and the phonons needed to describe all possible scattering events within these pockets. Electron-phonon couplings are computed using density-functional perturbation theory with the appropriate 2D boundary conditions and gates to induce doping [3]. Notably, this comprehensive approach to electron-phonon scattering reveals the consistently large intervalley scattering and the subtle impact of doping on electron-phonon interactions. Finally, mobilities are obtained by solving the Boltzmann transport equation using an iterative scheme, combined with an exact integration of the delta functions associated with energy conservation.

Computing the mobility of all the materials in the database remains impractical. Instead, we learn the key features that characterize a high mobility 2D material from a first in-depth study of a small but diverse selection of materials. Density of states, carrier velocities, number of valleys, phonon energetics as well as intra- and inter-valley electron-phonon interactions all play a role. We then translate these observations into computationally affordable and quantifiable descriptors to identify the best candidates in the database.


Lattice dynamics and thermal conductivity in antiferromagnetic semiconductor MnTe

We discuss electronic, magnetic, vibrational and transport properties of the antiferromagnetic semiconductor MnTe. This work derives physically justified Coulomb repulsion, magnetic structure and exchange parameters from density functional theory and the Heisenberg model. Calculated vibrational density of states, magnon and phonon dispersions compare favorably with literature values and our measurements from neutron scattering experiments. First principles Peierls-Boltzmann phonon transport calculations are also presented and show good agreement with measured values. Our work demonstrates that vibrational and magnetic degrees of freedom do not strongly couple in MnTe.

Thermal conductivity of perovskite KTaO3 and PbTiO3 from first principles

The low thermal conductivity of piezoelectric perovskites is a challenge for high power transducer applications. We report first principles calculations of the thermal conductivity of ferroelectric PbTiO3 and the cubic nearly ferroelectric perovskite KTaO3. The calculated thermal conductivity of PbTiO3 is much lower than that of KTaO3 in accord with experiment. Analysis of the results shows that the reason for the low thermal conductivity of PbTiO3 is the presence of low frequency optical phonons associated with the polar modes. These are less dispersive in PbTiO3, leading to a large three phonon scattering phase space. These differences between the two materials are associated with the A-site driven ferroelectricity of PbTiO3 in contrast to the B-site driven near ferroelectricity of KTaO3. The results are discussed in the context of modification of the thermal conductivity of electroactive materials.

Work at the University of Missouri is supported by the Department of Energy, Basic Energy Sciences, Award DE-SC0019114.
In the presence of disorder, it is possible to reach a point where the phonon wave-packets do not propagate far enough to sample the periodicity of the solid, rendering impossible to attribute them a wave vector or a group velocity. This regime is often described by a harmonic theory introduced by Allen and Feldman [4].

We generalize the Peierls and Allen-Feldman approaches with a unified master equation, which enables reliable first-principles predictions of the thermal conductivity of any insulator, ranging from complex crystals to anharmonic glasses. We showcase this approach with an application to a thermoelectric material that displays ultra-low glass-like thermal conductivity and rattling phonon modes.

9:36AM X22.00007: Orbitally driven low thermal conductivity of monolayer gallium nitride (GaN) with planar honeycomb structure: a comparative study  
ZHENVEN QIN (Presenter), Zhengzhou University, GUANGZHAO QIN, RWTH Aachen University, XU ZUO, Nankai University, ZHIHUA XIONG, Jiangxi Science & Technology Normal University, MING HU, University of South Carolina — Monolayer gallium nitride (ML GaN) with honeycomb structure was successfully fabricated recently in experiments, generating enormous research interest for its promising applications in nano- and opto-electronics. By solving the Boltzmann transport equation (BTE) based on first-principles calculations, we performed a comprehensive study of the phonon transport properties of ML GaN, with detailed comparison to bulk GaN, 2D graphene, silicene and ML BN with similar honeycomb structure. We find that the thermal conductivity (κ) of ML GaN (14.93 W/mK) is more than two orders of magnitude lower than that of graphene and is even lower than that of silicene with a buckled structure. Systematic analysis is performed based on the study of the contribution from phonon branches, comparison among the phonon mode levels and phonon anharmonicity. Further deep insight is gained from the electronic structure. Resulting from the special sp orbital hybridization mediated by the Ga-d orbital in ML GaN, the strongly polarized Ga–N bond and its inhomogeneous distribution could lead to the intrinsic low κ of ML GaN. The unraveled orbitally driven low κ of ML GaN offers fundamental understanding of phonon transport and will shed light on further studies of phonon transport in 2D materials.

9:48AM X22.00008: Anomalous phonons in Pb_{0.5}Sn_{0.5}Te*  
AASHISH SAPKOTA (Presenter), JOHN TRANQUADA, IGOR ZALIZNYAK, YANGMU LI, Brookhaven National Laboratory, BARRY L. WINN, Oak Ridge National Laboratory — The (Pb_{0.5}Sn_{0.5})_{1-x}In_{x}Te system is of current interest because of its potential connection to topological superconductivity [1,2]. Recent inelastic neutron scattering (INS) measurements on powder samples of (Pb_{0.5}Sn_{0.5})_{1-x}In_{x}Te, x = 0 and 0.3, reported unexpected low-energy peaks (in the range of 1 to 2.5 meV) in the phonon density of states, which presently lack theoretical explanation [2]. To further determine the nature of these low-energy phonons, we recently performed an INS measurement on a Pb_{0.5}Sn_{0.5}Te (x = 0) crystal. The results reveal that dispersing longitudinal and transverse phonons are not the contributor. Instead, there exist diffusive phonons with spectral weight in the energy range of 1 to 2.5 meV and characteristics deviating from conventional behavior. This suggests that some localized non-dispersive modes are the source for the anomalous low-energy peaks in the density of states. However, a proper understanding of these diffusive excitations will require further study. [1] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011), [2] K. Ran et al., Phys. Rev. B 97, 220502(R) (2018).

*Work at BNL was supported by Office of BES, U.S. DOE under Contract No. DE-SC0012704. Research conducted at ORNL’s SNS was sponsored by SUFD, Office of BES, U.S. DOE.

10:00AM X22.00009: Unified ab initio thermal transport theory for insulators*  
NAVANEETHA KRISHNAN RAVICHANDRAN (Presenter), DAVID A BROIDO, Boston College — In insulators, heat is carried by phonons. Standard ab initio methods to get the thermal properties of solids rely on the phonon quasiparticles being well-defined, and assume that the lowest order 3-phonon scattering sufficiently describes thermal transport. Here we show that this is not the case for weakly bonded solids, where phonon scattering is so strong that the standard phonon quasiparticle picture can break down, and 3-phonon scattering is insufficient to explain the experiments. To address this issue, we present a novel ab initio method that features an anharmonic many-body renormalization scheme to create well-defined phonon quasiparticles with weakened interactions, and includes both 3-phonon and 4-phonon scattering to obtain thermal transport properties [1]. With this approach, we accurately capture the measured phonon dispersions, thermal expansion and thermal conductivity of both weakly bonded solids like sodium chloride and strongly bonded solids like diamond. Our work presents a unified ab initio framework to accurately predict the thermal properties of solids with varying bond strengths.


*This work was funded by ONR MURI [No. N00014-16-1-2436] & DOE S3TEC-EFRC [No. DE-SC0001299/DE-FG02-09ER46577].
10:12AM X22.00010: First principles investigation of the impact of symmetry and dimensionality on thermal transport* TRIBHUWAN PANDEY (Presenter), CARLOS POLANCO, VALENTINO R. COOPER, DAVID PARKER, LUCAS LINDSEY, Oak Ridge National Laboratory — Symmetry and dimensionality reduction have a profound impact on lattice dynamics, phonon scattering and thermal transport. Here, we will present new insights developed from predictive first principles Boltzmann transport theory in 1D-Ba$_3$N and 2D-InSe and compare them with their bulk counterparts. In particular, for 1D materials new symmetry-based selection rules will be introduced and their effect on thermal conductivity will be assessed. Furthermore, the challenges related to thermal transport modelling in low dimensional materials will be discussed.

*Acknowledgements: This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:24AM X22.00011: Characterization of Analytical Thermal Conductivity Models Through Assessment Against Experiment and Simulation RAMYA GURUNATHAN (Presenter), RILEY HANUS, MAXWELL DYLLA, JEFF SNYDER, Materials Science and Engineering, Northwestern University — The Klemens/Callaway equations [Phys Rev 119 (2), 507-509 (1960)] model lattice thermal conductivity ($\kappa_L$) versus temperature and impurity concentration. This framework highlights the dominant phonon scattering mechanisms in a system, and is used for routine interpretation of experimental trends. The model predictions are often regarded as rough estimates due to the assumption of a monatomic lattice and Debye model dispersion. In this study, the Klemens model is applied to both experimental measurements and first-principles simulations of $\kappa_L$, where imperfections are introduced to scatter phonons. We demonstrate the proper application of this model to materials with complex unit cells, and resolve discrepancies over model inputs that can yield a factor of 2-10 difference in the predicted $\kappa_L$ values. Additionally, the model is demonstrated to provide robust predictions of point defect scattering strength in a wide range of materials, whose dispersion relations are known to deviate significantly from the Debye model. We demonstrate how the dispersion relation dependence of the model is, in practice, lifted, allowing for surprising agreement between analytical theory and experiment. Thus, we provide justification for using this model on systems with arbitrary dispersion relations.

10:36AM X22.00012: Thermal conductivity of wide band gap nitrides from first principles calculations* SAHIL DAGLI (Presenter), KELSEY MENGLE, EMMANOUIL KIOUPAKIS, University of Michigan — Wide band gap nitrides are of interest for applications in deep-UV optoelectronics and power electronics. Materials for these devices must be able to dissipate heat generated from operation, making thermal conductivity an important parameter for high-power applications. We have investigated the thermal conductivity of AlN, GaN, Al$_x$Ga$_{1-x}$N and BN polymorphs with first-principles calculations, with a focus on effects from compositional and isotopic disorder. We use density functional theory to calculate the phonon frequencies and interatomic force constants. This information is used to calculate the thermal conductivity using the solution from the full Boltzmann transport equation calculation. Our results provide understanding on the benefits of using isotopically pure compositions in increasing the thermal conductivity of wide band gap nitrides.

*This work was supported by NSF DMREF program (1534221). Computational resources provided by DOE NERSC (DE-AC02-05CH11231).

10:48AM X22.00013: Thermal transport through GaN-AlN interfaces with mass and force variance from first-principles CARLOS POLANCO (Presenter), LUCAS LINDSEY, Oak Ridge National Laboratory — We present thermal conductance calculations of a GaN-AlN interface using a Landauer formalism with all interatomic force constants (IFCs), including those relaxed at the interface, computed from density functional theory. A thorough convergence study of the conductance value is outlined, focusing on the effects of truncating long-range IFCs from polar materials and properly enforcing various symmetries and invariances. For example, enforcing the simple acoustic sum rule instead of using more advanced methods overestimates the conductance by 7% with a 35% overestimation of the optical phonon contributions. We compare our fully first-principles conductance with those using empirical mixing rules to define interfacial IFCs. Moreover, we contrast our calculations with values inferred from thermal conductivity measurements of GaN-AlN superlattices. Our calculations constitute initial steps towards a fully predictive framework of interfacial thermal conductance.

Nanoelectromechanical systems are highly sensitive to adhered particles, and by using frequency shifts caused by particle adhesion on the surface of the resonator, it is possible to obtain stiffness of the adsorbate in addition to its mass and position on the resonator. In order to conduct our experiments, we fabricated NEMS resonators using top-down fabrication techniques. We have measured their multimode resonance response using electrothermal actuation and piezoresistive detection. Matrix Assisted Laser Desorption and Ionization (MALDI) is implemented to deliver particles towards the resonator. We have detected and characterized, in-real time, 20-nm gold nanoparticles using the first four out-of-plane modes. Simultaneous measurements of multiple modes were accomplished using phase-locked loop circuits running in parallel. By using the frequency shifts of resonance frequencies, we propose a method in which we assume the analytes adhered on the beam are hemispherical to obtain mass and stiffness, size and positions of the analytes. The size and position values for individual nanoparticles obtained were verified with independent characterization under SEM. The measurements provided here confirms the utility of multimode NEMS detection technique with analytes down to 20 nm radius.

Mass and Stiffness Spectrometry of 20-nm Gold Nanoparticles by Nanoelectromechanical Systems

Mary Shultz (Presenter), Joam Marmolejos, Patrick Bisson, Tufts University — Soft interfaces are common in biology, the environment, and technological applications. Probing these, particularly when the interface is buried between two condensed phases presents many challenges. The only current method available for probing such interfaces with molecular specificity is the vibrational spectroscopy, sum frequency generation (SFG). SFG attains surface sensitivity due to its nonlinear nature. Due to nonlinearity, separating overlapping signals is difficult, usually leading to nonunique separation. This problem has long been recognized by SFG practitioners and several methods for determining the complex components of the signal have been devised. None produce an absolute measurement of the complex signal. This contribution reports a nonlinear interferometer, that not only addresses this issue but also complex measurement sensitivity due to its nonlinear nature. Project Mjolnir latest status will be presented.

8:24AM X23.00003: Project Mjolnir: High efficiency real time mass spearator and ion trap

Jason Burke (Presenter), Barbara Alan, Aaron Hellingber, Lawrence Livermore Nat Lab — A low energy mass separator and ion trap for the real time separation and trapping of radioactive isotopes has been developed. The apparatus consists of an ultra-high purity helium buffered electrostatic recoil gas stopper and RF carpet to guide ions from a radioactive source to the exit aperture. A natural helium jet created at the exit imparts momentum to the ions. The ions enter a large acceptance radio-frequency quadrupole ion guide which has a DC gradient applied to it. The ions are cooled in the residual helium buffer gas are damped and collimated and continuously injected into a quadrupole mass separator (QMS). Ions are mass and charge selected in the QMS and exit into another RFQ for further beam collimation before being injected into a linear ion trap. The entire apparatus has been designed to be able to continuously load the ion trap. The ion trap is physically small allowing a large solid angle to be covered by detectors to study of short-lived isomers. Project Mjolnir latest status will be presented.

Effective Realtime Data Processing using LabJack T-Series DAQs

Benjamin Montgomery (Presenter), Paul Nakroshis, University of Southern Maine — The ability to accurately collect and computationally process data from sensors in real time is crucial to many scientific experiments. This generally leads to cost-ineffective solutions from well-known manufacturers, usually tied to proprietary analysis software, or oft-crude home-built alternatives. In light of this issue, we have created an open-source python API for the LabJack T-series of DAQs as a powerful, cost-effective alternative that is extensible and accessible to users with varying backgrounds in programming. We demonstrate the efficacy of this interface in the context of gathering and processing data from a quadrant-cell photodiode used to monitor a torsion pendulum in real time, as well as highlighting a few notable advantages found processing data with the LabJack.

*Funding for the equipment used in this project comes from the University of Southern Maine.
8:48AM X23.00005: Measuring Hall Conductivity Using a Cantilever Torque Magnetometer*  Tiffani Paul (Presenter), Samuel Mumford, Stanford University, Amir Yacoby, Harvard University, Aharon Kapitulnik, Stanford University — We present Hall conductivity measurements of Corbino-disk patterned thin film samples on a cantilever-based torque magnetometer. When a voltage is applied across the sample and a magnetic field is applied through the sample plane, the Hall current provides a magnetic moment that interacts with the external magnetic field and yields a torque on the end of the cantilever. The symmetry of this technique eliminates contributions from longitudinal resistance, making Hall conductivity measurements of previously inaccessible materials possible. Following a demonstration of how we determine the elastic properties of the cantilever system, we discuss various realizations of the technique, including for transverse thermoelectric currents, and show preliminary results on simple electronic systems.

*This work was funded by the Army Research Office grant W911NF1710588, and by the Gordon and Betty Moore Foundation through Emergent Phenomena in Quantum Systems (EPiQS) Initiative Grant GBMF4529

9:00AM X23.00006: Increase the sensitivity of magnetoelastic sensors by modifying the sensor geometry  Paula Gonzalez (Presenter), David Gandia, BCMaterials (Basque Center for Materials, Applications & Nanostructures, Andoni Lasheras, University of the Basque Country, Iban Quintana, Ik4-Tekniker, Jon Gutierrez, Maria Isabel Arriortua, University of the Basque Country, Ana Catarina Lopes, BCMaterials (Basque Center for Materials, Applications & Nanostructures — Magnetoelastic sensors have gained a huge interest during the last years. Due to their change on the resonance frequency in response to a mass load, they present the capacity to detect low amounts of different chemical or biological compounds in a precise, cheap, quick and wireless way. In this work, we present a novel approach to increase the sensitivity of that kind of sensors by changing the sensor geometry and by modifying the percentage of coated surface by a mass load. By this new approach, the sensitivity could increases more than a 1000% with respect to the commonly used rectangular shaped magnetoelastic sensors with an uniformly distributed mass load. This work correlates experimental and theoretical results to develop a new model able to quantify the mass attached to the magnetoelastic ribbons. Moreover, the influence of the sample geometry and coating distribution on different magnetic and magnetoelastic parameters such as the delta E effect, the position of the nodal point or the anisotropy field has been studied and significant differences have been observed.

9:12AM X23.00007: Optimal Optical Systems for Collecting Photoluminescence of Point Emitters  Juan Lizarazo Ferro (Presenter), Rashid Zia, Brown University — Many applications that leverage optics, and explorations in fundamental physics, are limited by the experimenter’s ability to collect luminescence from point emitters embedded in solid state hosts. Here we explore the limitations imposed by the common type of optical systems used for this purpose, and we compare them against proposed alternative designs. In addition to comparing their collection efficiency, these new designs are also analyzed for tolerance in the lateral and axial position of the emitters with respect to reference auxiliary surfaces or alignment guides. Ray-optics and FDTD simulations will be used to quantify the proposed alternatives. Both an objective composed of spherical surfaces and a metalens implementation will be presented.

9:24AM X23.00008: Fast Reflective Optic-Based Rotational Anisotropy Nonlinear Harmonic Generation Spectrometer  Jason Dinh Tran (Presenter), Baozhu Lu, Darius Torchinsky, Department of Physics, Temple University — Rotational anisotropy second harmonic generation (RA-SHG) has emerged as effective probe of structural and electronic symmetry of hard condensed phase systems, as well as a spectroscopic tool for investigating the energy-dependent nonlinear electronic properties of solids. A common implementation of this technique has involved sample rotation to obtain the maximal number of nonlinear susceptibility coefficients, leading to significant challenges in experimental alignment which have recently been overcome by diffractive optic-based approaches. However, the same diffractive optics that have opened up this metrology to a variety of new sample configurations have also restricted the RA-SHG spectrometer in both data acquisition speed and broadband spectroscopic capability. We describe the design and application of an RA-SHG spectrometer based almost entirely upon reflective optics that overcomes the wavelength-dependent shortcomings of current state of the art RA-SHG devices and provide examples of the apparatus’ application to a variety of test samples.
9:36AM X23.00009: Fourier Domain Rotational Anisotropy Second Harmonic Generation  BAOZHU LU (Presenter), DARIUS TORCHINSKY, Department of Physics, Temple University — We describe a novel scheme of detecting rotational anisotropy second harmonic generation (RA-SHG) signals using a lock-in amplifier referenced to a fast scanning RA-SHG apparatus. The method directly measures the $n^{th}$ harmonics of the scanning frequency corresponding to SHG signal components of $C_n$ symmetry that appear in a Fourier series expansion of a general RA-SHG signal. We will present measurements on a GaAs test sample to compare point-by-point averaging with the lock-in based method. We will discuss how, when divided by the $C_\infty$ signal component, the lock-in detected data allow for both self-referenced determination of ratios of $C_n$ components of up to 1 part in $10^4$ and significantly more sensitive measurement of the relative amount of different $C_n$ components when compared with conventional methods.

9:48AM X23.00010: High-Pressure Laser Floating Zone Furnace* JULIAN SCHMEHR (Presenter), MICHAEL ALING, ELI ZOGHLIN, STEPHEN WILSON, University of California, Santa Barbara — The floating zone technique is one of the most established methods in growing single crystals for materials research applications, due to its propensity to produce large, extremely high quality specimens. However, limitations in the ultimate pressures of growth atmospheres in standard furnace designs renders many compounds not suitable for crystal growth employing the floating zone technique, either due to excessive volatility or metastability. Here we demonstrate a high pressure laser floating zone system which pushes the envelope of processing pressure for this technique. Focused laser light allows for extremely sharp heating gradients, uniform radial heating profiles and high processing temperatures. In turn this allows for the implementation of a high strength metal growth chamber, allowing for greatly enhanced processing pressures. We demonstrate successful single crystal growths of a range of oxide compounds up to 10 kpsi applied gas pressures, a more than two-fold increase in processing pressures compared to commercially available floating zone systems.

*We gratefully acknowledge funding from the W.M. Keck Foundation.

10:00AM X23.00011: Advancing Silicon Atomic-Scale Applications* ROSHAN ACHAL (Presenter), MOHAMMAD RASHIDI, JEREMIAH CROSHAW, University of Alberta, DAVID CHURCHILL, CS, Memorial University of Newfoundland, MARCO TAUCER, TALEANA HUFF, University of Alberta, MARTIN CLOUTIER, JASON PITTERS, Nanotechnology Research Centre, ROBERT A WOLKOW, University of Alberta — Dangling bonds (DBs) on the surface of hydrogen-terminated silicon present an attractive basis for next generation atomic scale devices as they possess both ideal electronic properties and high thermal stability. One of the ultimate applications of DBs is the creation of atomic scale logic circuitry, where designs may reduce power consumption by several orders of magnitude. We use a Scanning Tunneling Microscope (STM) to fabricate proto-devices and other DB-based structures. Recent developments in the precise fabrication of DBs have enabled significant progress towards this goal. With these developments, new applications of DBs are also emerging. In one such application we demonstrate the use of DBs to store information at the atomic scale, including the ability to read out the information. Further, we demonstrate the potential to advance site selective chemistry on the surface through the reliable creation of reactive sites.

*NSERC, AITF

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X24 DAMOP: Vortices, Rotation, Spin-orbit Coupling and Artificial Gauge Fields

BCEC 159 - David Feder, University of Calgary
So far, lattices of quantum vortices have been observed in axially symmetric, rotating superfluid 4He or rotating Bose-Einstein condensates (BECs). Vortex configurations in rotating superfluids lacking axial symmetry have been discussed theoretically, but experimental observation of such systems proves to be challenging. Here, we present a study of vortices in microscopic free, prolate superfluid 4He droplets rotating around their short axis. The vortices were doped with Xe atoms and studied via coherent x-ray scattering at the LCLS free-electron laser. It was found that the vortices form a distorted lattice within the droplet. We compare the shapes of classical droplets executing rigid body rotation to rotating prolate superfluid droplets, the angular momentum of which has contributions from quantum vortices and potential flow.

*This work was funded under the NSF grant DMR 1701077.

Recent advent of X-ray free electron lasers (XFEL) has enabled the study of rotation in free isolated superfluid 4He droplets. The work presented here extends our study of rotating quantum fluids to non-superfluid 3He droplets. Sub micrometer sized 3He droplets were obtained from free jet expansion of liquid 3He at temperatures less than 3 K and studied via X-ray scattering at the LCLS XFEL. The obtained shapes and sizes of rotating 4He and 3He droplets have been compared. In contrast to superfluid 4He droplets, 3He droplets (T = 0.15 K) are devoid of quantum vortices. Tracing of quantum vortices inside 4He droplets have been previously achieved by doping with large number of Xe atoms. This work presents the first experimental study of the formation dynamics of atomic clusters in a homogenous, vortex-free quantum fluid.


*NSF - DMR 1701077

Superstripe phases in Bose-Einstein condensates, possessing both crystalline structure and superfluidity, opens a new avenue for exploring exotic quantum matters—supersolids. However, complete detection and exploration of superstripes are still challenging in experiments because of the short period, low visibility and external factors such as magnetic field fluctuations or heating issues. Here we propose a scheme in a spin-orbit coupled BEC which overcomes these obstacles and generates a robust magnetic superstripe phase [i.e., only spin (no total) density modulation] with a long period and high visibility, ready for direct real-space observation. In the scheme, two hyperfine spin states are individually Raman coupled with a largely-detuned third state, which induce a momentum-space separation between two lower band dispersions, yielding an effective spin-1/2 system with tunable spin-orbit coupling and Zeeman fields. Without effective Zeeman fields, spin-dependent interaction dominates, yielding a magnetic superstripe phase with a long tunable period and high visibility. Our scheme provides a platform for observing and exploring exotic properties of superstripe phases as well as novel physics with tunable spin-orbit coupling.

*AFOSR, NSF, and ARO.
Anderson localization in presence of spin-orbit coupling in an atomic Bose gas  
YUCHEN YUE
(Presenter), EMINE ALTUNTAS, FRANCISCO SALCES-CARCoba, ANDiKA PUTRA, CHRIS BILLINGTON, IAN SPIELMAN, Joint Quantum Institute, National Institute of Standards and Technology and the University of Maryland — Anderson localization (AL), describing the absence of diffusion in 1D noninteracting quantum particles in disordered media, is based on multiple scattering processes. Spin-orbit coupling (SOC) is an intrinsic property in many material systems. SOC’s spin-dependent alteration of band structure affects the scattering processes leading to AL. Both disorder and SOC are difficult to tune and control in-situ. Here we describe the interplay of tunable disorder (from optical speckle) and SOC (generated by two-photon Raman coupling) in quasi-1D Bose-Einstein condensates. We show that SOC can significantly decrease the impact of disorder, thereby increasing the conductivity of 1D systems.

Spin-Orbit Coupled Bosons in One Dimension: Entanglement Entropy and Dynamics*  
JUNHYUN LEE (Presenter), WILLIAM COLE, JAY SAU, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park — We study the entanglement and dynamical properties of a spin-orbit coupled Bosons which describe one-dimension ultracold atoms with Raman-induced spin-orbit coupling. The two component spin-orbit coupled Bose liquid was proposed as a platform for studying quantum criticality in itinerant magnets [1]. In the presence of strong spin-independent interactions and spin-orbit coupling, this spinor Bose liquid undergoes an interaction (or density) tuned quantum phase transition similar to those in itinerant magnetic solid state systems. Although the order parameter describes a broken $Z_2$ spin symmetry, the associated phase is qualitatively distinct from the Ising phase transition and has a dynamical critical exponent $z=2$, typical of a Lifshitz transition. We discuss the unusual entanglement and dynamical features of this Lifshitz critical point stemming from its non-integrablility and absence of Lorentz symmetry.


*This work was supported by the JQI-NSF-PFC.

Ground state for trapped two-component Bose-Einstein condensates with synthetic spin-orbit interactions and magnetic fields*  
DAVID FEDER (Presenter), University of Calgary — The experimental realization of synthetic gauge fields in ultracold atomic gases has spurred great interest in the ground state and excitations of multicomponent Bose-Einstein condensates (BECs) in the presence of spin-orbit (SO) interactions and artificial magnetic fields, driven in part by the pursuit of topologically non-trivial states in these systems. While the characteristics of SO-coupled weakly interacting BECs in uniform geometries and in two-dimensional traps are well-understood, for example the existence of stripe phases, little work has been performed for fully three-dimensional harmonic potentials. In this work, the ground state is determined for interacting (effective) two-component BECs in the presence of Raman-induced synthetic SO interactions and magnetic fields, confined in three-dimensional traps. To ensure efficient calculations but also accurate results, the calculations employ a spatial mesh based on a finite element discrete variable representation. The results are compared with previous theory and simulation results and with experimental data where possible.

*This work is supported by the Natural Sciences and Engineering Research Council of Canada.

Rotating sonic black hole from Spin-orbit coupled Bose-Einstein condensate*  
INDERPREET KAUR (Presenter), SANKALPA GHOSH, Department of Physics, Indian Institute of Technology Delhi, New Delhi-110016, India — We show that an analog of rotating black hole namely, BTZ type can be realized in a quasi-2D spin-orbit coupled Bose-Einstein condensate without using any external rotation. In hydrodynamic approximation, the equation for phase fluctuations in the total density modes, that describes the phonon field is similar to the scalar field equation in 2 + 1 dimensions whose space-time metric can be identified with the metric of BTZ black hole. By time evolving the condensate in a suitably created laser-driven potential, we show that the moving condensate forms such rotating black hole in an annular region bounded by inner and outer event horizon as well as elliptical ergo surfaces. We identify the supersonic and subsonic zones and analyze the self-amplifying Hawking radiation that strongly depends on the spin-orbit coupled anisotropy. We calculate the density-density correlation function and show the distribution of the analog Hawking temperature on the event horizon.

Reference:

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Phases and phase transitions of Bose condensed light

VICTOR FLEUROV (Presenter), School of Physics and Astronomy, Tel-Aviv University, ANATOLY KUKLOV, Department of Physics, College of Staten Island — Bose-Einstein condensation of light [1] is characterized by two classical complex fields corresponding to two polarizations of light as well as by the distribution of dye molecules inducing light thermalization through dipolar transition coupled to the thermal bath of molecular vibrations. We emphasize a crucial role of removing the full degeneracy of the dipolar transition in forming algebraic order of the condensate in 2D. The resulting symmetries of the condensate can be characterized by groups $O(2) \times Z_2$, $O(2)$ and $Z_2$ order emerging before $O(2)$. [If the transition is triple degenerate, the symmetry becomes $O(4)$ which excludes the algebraic condensation at any finite temperature]. The main result of this work [2] addresses orientational disorder introduced by local dipolar anisotropy. It can destroy algebraic order in one-photon density matrix while preserving it in the two-photon one. This produces a condensate of photon pairs without any attraction between photons. We call such pairing geometrical.


Fermionic Superfluids in a Ring Trap

YANPING CAI (Presenter), DANIEL ALLMAN, PARTH SABHARWAL, KEVIN WRIGHT, Dartmouth College — Multiply-connected geometries provide a natural setting for studying transport properties of quantum phases of matter. We will report on an all optical approach to create ultracold fermionic superfluids in a ring-shaped trap. The conditions for creating and observing persistent currents in fermionic superfluids are somewhat different than experiments previously conducted with bosonic superfluids. We will report on initial efforts to create and observe persistent flow in a molecular BEC of of $^6$Li atoms. With this new platform for studying transport in dilute fermionic superfluids, we plan to study critical velocities and dissipation mechanisms across the BEC-BCS crossover, and in rings with different dimensionality.

*This research is funded by NSF (1707557)

Linked and knotted synthetic magnetic fields

CALLUM DUNCAN (Presenter), SUPA, Institute of Photonics and Quantum Sciences, Heriot-Watt University, CALUM ROSS, Maxwell Institute for Mathematical Sciences and Department of Mathematics, Heriot-Watt University, NICLAS WESTERBERG, MANUEL VALIENTE, SUPA, Institute of Photonics and Quantum Sciences, Heriot-Watt University, BERND J SCHROERS, Maxwell Institute for Mathematical Sciences and Department of Mathematics, Heriot-Watt University, PATRIK ÖHBERG, SUPA, Institute of Photonics and Quantum Sciences, Heriot-Watt University — We show that the realisation of synthetic magnetic fields via light-matter coupling in the Lambda-scheme implements a natural geometrical construction of magnetic fields, namely as the pullback of the area element of the sphere to Euclidean space via certain maps. For suitable maps, this construction generates linked and knotted magnetic fields, and the synthetic realisation amounts to the identification of the map with the ratio of two Rabi frequencies which represent the coupling of the internal energy levels of an ultracold atom. We consider examples of maps which can be physically realised in terms of Rabi frequencies and which lead to linked and knotted synthetic magnetic fields acting on the neutral atomic gas. We also show that the ground state of the Bose-Einstein condensate may inherit topological properties of the synthetic gauge field, with linked and knotted vortex lines appearing in some cases.

* This work was supported by the National Science Foundation under the grant DMR1720251.

Kaleidoscope vortex lasers possessing orbital angular momentum

TING-HUA LU (Presenter), TENG-DE HUANG, GUAN-YING CHIOU, Department of Physics, National Taiwan Normal University — We propose an efficient and robust method to generate the kaleidoscope vortex beam by employing an astigmatic laser cavity with an extra-cavity cylindrical lens. The kaleidoscope vortex beam is arising from the superposition of Laguerre-Gaussian modes with the longitudinal-transverse coupling effect in the laser cavity. The superposed Laguerre-Gaussian mode leads to the formation of complex phase singularities and implies the participation of different optical orbital angular momentum involved in a single kaleidoscope vortex beam. We experimentally demonstrate that a series of kaleidoscope vortex beams with different symmetry are systematically achieved by using a simple setup. The output power of the laser is dependent on the cavity length. This approach is expected to create high-order optical vortex beams and pave the way for optical entanglement.
10:12AM X24.00012: Imbalanced Fermi gas in antiparallel magnetic fields*  
TAKAAKI ANZAI (Presenter), YUSUKE NISHIDA, Department of Physics, Tokyo Institute of Technology — We study a two-dimensional Fermi gas with the finite density imbalance between two spin components of atoms in antiparallel magnetic fields. The antiparallel magnetic fields act on two different spin components of atoms with same magnitude but opposite directions [1]. It was revealed in the absence of magnetic fields that the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, where the Cooper pairing takes place with nonzero momentum, emerges in the phase diagram of an imbalanced Fermi gas. Therefore, it is an interesting problem to how the antiparallel magnetic fields compete or cooperate with the FFLO state. We investigate the ground-state phase diagram within the mean-field approximation. At the weak-coupling limit, we find that the FF state is stable with compare to the LO state when the chemical potentials of the two components lie right at Landau levels [2].


*This work was supported by JSPS KAKENHI Grants No. JP15K17727 and No. JP15H05855.

10:24AM X24.00013: Unified Spin Electrodynamics of Maxwell Bosons and Dirac Fermions  
FARHAD KHOSRAVI (Presenter), Electrical and Computer Engineering, University of Alberta, TODD VAN MECHelen, ZUBIN JACOB, Electrical and Computer Engineering, Purdue University — Bosons and fermions show similar spin and angular momentum textures. Studies of the spin for the surface plasmon polaritons (SPPs) propagating at the interface of an insulator and a metal, as well as the solutions of the Dirac equation propagating at the interface of a positive and negative fermionic mass media (known as the Jackiw-Rebbi problem (JRP)), show that both photons and fermions in these structures have fully transverse spin and form a momentum-decay-spin triplet. By solving Maxwell equations for bosons and Dirac equation for fermions we have derived these fundamental properties and have shown that they make consistent connection to the experimental results. We have also studied these spin properties in the cylindrical problems of an optical fiber (OF) for bosons, as well as the cylindrical problem of a Dirac wire (DW) for fermions. We have shown that the bosons in OF and fermions in DW show very similar spin and angular momentum textures with longitudinal and transverse spin components that are locked to their respective perpendicular component of the momentum. Our results present an important platform for the study of spin and angular momenta by making accurate predictions about the spin properties of bosons (fermions) by studying the spin of fermions (bosons).

JIN ZHANG (Presenter), University of California, Riverside, JUDAH F UNMUTH-YOCKEY, Syracuse university, JOHANNES ZEIHER, Max-Planck Institute of Quantum Optics, ALEXEi BAZAVOV, Michigan State University, SHAN-WEN TSAI, University of California, Riverside, YANNICK MEURICE, University of Iowa — Analog quantum simulations of lattice gauge theory are a promising direction in understanding high energy physics. We derive a Hamiltonian formulation for the (1+1)-dimensional Abelian Higgs model that is manifestly gauge-invariant. The Hamiltonian formulation of the Polyakov loop can be obtained by the same method, which makes it possible to study this order parameter for the confinement/deconfinement phase transition experimentally. The corresponding quantum simulator is an asymmetric multi-leg ladder of atoms trapped in optical lattices and interacting with Rydberg-dressed interactions, where the required quadratic attractive interactions can be realized. The finite size scaling of the energy gap created by the insertion of a Polyakov loop can be obtained accurately by choosing spin truncations (the number of legs in the ladder) properly, which are cross-checked by tensor renormalization group calculations and Monte Carlo simulations. Phase transitions and quench dynamics also can be studied with this quantum simulator.

*This work was supported in part by the U.S. Department of Energy (DOE) under Award Number DE-SC0010113 (YM) and DE-SC0009998 (JUY) and by the NSF under Grant No. DMR-1411345 (SWT). JZ was supported by MPG and the European Commission (UQUAM).

10:48AM X24.00015: Dynamics of active particles in Bose superfluids  
VISHWANATH SHUKLA (Presenter), Institut de Physique de Nice, Universite Cote d’Azur, France — We investigate the dynamics of active particles in two- and three-dimensional Bose superfluids at finite temperatures. We make use of a minimal model in which particles obey Newtonian dynamics and their equations of motion are self-consistently coupled with the Gross-Pitaevskii equation. We characterize the effective drag force acting on the particles at finite temperatures and study their interaction with vortices in both simple and turbulent environment. In particular, we elucidate the role played by the drag-force, mutual-friction and the Magnus force.

Friday, March 8, 2019 8:00 AM - 10:48 AM
8:00AM X25.00001: Observation of classical dynamical isolation in nonadiabatically modulated photonic cavities*
AVIK DUTT (Presenter), MOMCHIL MINKOV, QIAN LIN, Stanford University, LUQI YUAN, Shanghai Jiao Tong University & Stanford University, DAVID A. B. MILLER, SHANHUI FAN, Stanford University — We experimentally demonstrate the phenomenon of dynamical isolation in harmonically modulated photonic cavities. We achieve this by strongly modulating a fiber ring cavity at a rate much faster than its linewidth. Such a nonadiabatically modulated cavity can show complete suppression of intracavity power even for an on-resonance input, resulting in dynamical isolation of the cavity field from the input light, as predicted in a recent theoretical study by Minkov et al. [APL Photonics 2, 076101 (2017)]. This counterintuitive behavior is strikingly different from the adiabatic regime typically studied in modulated photonic cavities, where the intracavity field is enhanced when the cavity's instantaneous resonance frequency matches the input light's frequency. Our work shows that periodically driven photonic systems can exhibit classical versions of quantum effects such as dynamical decoupling, which rely on modulating an open system at a rate faster than the system-reservoir interaction. Such effects have applications in signal optimization and frequency conversion in integrated photonics.

*Vannevar Bush Faculty Fellowship (Grant No. N00014-17-1-3030) from the U. S. Department of Defense, MURI grant from the U. S. Air Force Office of Scientific Research (Grant No. FA9550-17-1-0002).

8:12AM X25.00002: Floquet quantum critical points in (1+1) dimensions
XUEDA WEN (Presenter), JIE-QIANG WU, Massachusetts Institute of Technology — Given a generic (1+1) dimensional quantum critical points which can be described by conformal field theory (CFT), we propose an analytically solvable setup to study the Floquet dynamics of the CFT, i.e., the dynamics of a CFT subject to a periodic driving. A complete phase diagram in the parameter space can be analytically obtained within our setup. We find two phases: the heating phase and the non-heating phase. In the heating phase, the entanglement entropy keeps growing linearly in time, indicating that the system keeps absorbing energy; in the non-heating phase, the entanglement entropy oscillates periodically in time, i.e., the system is not heated. At the phase transition, the entanglement entropy grows logarithmically in time in a universal way. Furthermore, we can obtain the critical exponent by studying the entanglement evolution near the phase transition. Mathematically, different phases (and phase transition) in a Floquet quantum critical point correspond to different types of Mobius transformations.

8:24AM X25.00003: Entanglement features of Floquet random and fully random unitary quantum circuits
WEI-TING KUO (Presenter), DANIEL AROVAS, YIZHUANG YOU, University of California, San Diego — We study the entanglement dynamics for Floquet random and fully random unitary circuits. The Floquet circuit consists of an on-site Haar random layer alternating with a nearest neighbor interaction layer. In the limit where the local Hilbert space dimension q is large, we show an emergent Ising symmetry and obtain an analytical expression for short time periods via the transfer matrix method. Based on our short time result, we promote the "entanglement feature" to an operator formalism and derive a diffusion equation for the entanglement dynamics at long times. The similar functional form of the corresponding diffusion operators implies a universal thermalization behavior in Floquet random and fully random unitary circuits.


8:36AM X25.00004: Single-photon bound states in atomic ensembles
YIDAN WANG (Presenter), Joint Quantum Institute, MICHAEL GULLANS, Department of Physics, Princeton University, ANTOINE BROWAEYS, Laboratoire Charles Fabry, Institut d'Optique Graduate School, CNRS, Universite Paris-Saclay, JAMES V PORTO, Joint Quantum Institute, DARRICK CHANG, Institut de Ciencies Fotoniques, ALEXEY V GORSHKOV, Joint Quantum Institute — We illustrate the existence of single-excitation bound states for propagating photons interacting with N two-level atoms. These bound states can be calculated from an effective spin model, and their existence relies on dissipation in the system. The appearance of these bound states is in a one-to-one correspondence with zeros in the single-photon transmission and with divergent bunching in the second-order photon-photon correlation function. We also formulate a dissipative version of Levinson's theorem for this system by looking at the relation between the number of bound states and the winding number of the transmission phases. This theorem allows a direct experimental measurement of the number of bound states using the measured transmission phases.
A flow equation approach to periodically driven quantum systems

*This research is supported by JSPS KAKENHI Grant Numbers JP16K13847, JP17H03279, 18K03471, and JP18H032.

8:48AM  X25.00005: Semiclassical Phase Reduction Theory for Quantum Dissipative Nonlinear Oscillators

YUZURU KATO (Presenter), HIROYA NAKAO, Department of Systems and Control Engineering School of Engineering, Tokyo Institute of Technology — The phase reduction theory is a framework for analyzing rhythmic dynamics of weakly perturbed classical limit-cycle oscillators. It has been widely used for analyzing synchronization properties of classical dissipative nonlinear oscillators, but it has not been formulated for quantum dissipative nonlinear oscillators in a general way. Thus, we formulate a phase reduction theory for quantum dissipative oscillators. More specifically, we derive a semiclassical multi-dimensional Langevin equation from a general master equation for quantum dissipative systems exhibiting limit-cycle oscillations, and reduce it to an approximate one-dimensional classical stochastic differential equation describing phase dynamics of the oscillator. The density matrix and power spectrum of the oscillator can be explicitly reconstructed from the reduced phase equation. As an example, we analyze synchronization properties of a quantum van der Pol oscillator with harmonic driving and squeezing. The proposed framework allows us to analyze the dynamics of quantum dissipative nonlinear oscillators by using a simple classical stochastic differential equation under semiclassical approximation.

9:00AM  X25.00006: Achieving transitionless quantum driving in a many-particle system via coupling to an auxiliary many-particle system of opposing statistics

RAFAEL HIPOLITO (Presenter), PAUL M. GOLDBART, Physics, The University of Texas at Austin — Transitionless quantum driving (TQD) in a quantum system driven by a time dependent Hamiltonian, \( H_0(t) \), is in principle always possible via the addition of a counterdiabatic term, \( H_1(t) \), as shown by Berry, and where \( H_1(t) \) is in general nonlocal. Time dependence of \( H_0 \) gives rise to a curvature term in the comoving frame, which can be described via a gauge field, that induces transitions between different states, and whose influence is exactly nullified by \( H_1(t) \). We explore an alternative way of achieving TQD in a many-particle quantum system (composed of either bosons or fermions), where all fields are coupled locally. In lieu of \( H_1(t) \), we locally couple the original system A to a second system B (whose particles carry statistics opposite to A's) via a gaugino field. We explore the relationships between the A and B systems and the gauge and gaugino fields necessary to achieve TQD, and show that these relationships have a SUSY-like character. To illustrate, we explore the suppression of the Schwinger effect in a 1+1 D gas of Dirac electrons coupled to a time-dependent electric field that results from the suitable coupling (via gauginos) to its SUSY like partner.

9:12AM  X25.00007: A flow equation approach to periodically driven quantum systems

MICHAEL VOGL (Presenter), Physics, University of Texas at Austin, PONTUS LAURELL, Physics, Oak Ridge National Laboratory, AARON BARR, GREGORY FIETE, Physics, University of Texas at Austin — We present a theoretical method to generate a highly accurate time-independent Hamiltonian governing the finite-time behavior of a time-periodic system. The method exploits infinitesimal unitary transformation steps, from which renormalization group-like flow equations are derived to produce the effective Hamiltonian. The method has a range of validity reaching into frequency regimes that are usually inaccessible via high frequency expansions. Our approach is demonstrated for many-body Hamiltonians where it offers an improvement over the more well-known Magnus expansion. We show how the method relates to the rotating frame approximation and how it can be used to approximately transform to a rotating frame where the exact transformation isn't tractable because infinitely many couplings are generated in an exact treatment. We compare our approximate results to those found via exact diagonalization.

9:24AM  X25.00008: Driven-dissipative coupled Ising models: a new non-equilibrium universality class

MICHAEL FOSS-FEIG, Army Research Lab, ALEXEY V GORSHKOV, Join Quantum Institute, MOHAMMAD MAGHREBI, Michigan State University — Driven-dissipative systems can potentially exhibit non-equilibrium phenomena that are absent in their equilibrium counterparts. However, phase transitions present in these systems generically exhibit an effectively classical, equilibrium behavior in spite of their non-equilibrium origin. In this talk, I investigate an experimentally motivated model where two Ising-like order parameters interact and form a multicritical point. Using perturbative renormalization group techniques, I show that a pair of inherently non-equilibrium multicritical points emerge. These non-equilibrium multicritical points exhibit a variety of exotic phenomena with no counterpart in equilibrium, including spiraling phase boundaries, the emergence of discrete scale invariance rather than the more familiar continuous scale invariance, and the violation of the fluctuation-dissipation theorem at all length scales, resulting in a system which becomes hotter and hotter at longer and longer wavelengths.
**9:36AM X25.00009: Driven-Dissipative Quantum Phase Transitions**  OSCAR VIYUELA GARCIA (Presenter), Department of Physics, Harvard University, JIASEN JIN, Department of Physics, Dalian University of Technology, ALBERTO BIELLA, CRISTIANO CIUTI, Laboratoire Matériaux et Phénomènes Quantiques, Paris Diderot University, ROSARIO FAZIO, Condensed Matter and Statistical Physics, ICTP, DAVIDE ROSSINI, Department of Physics, Universita di Pisa — In this talk, I will explain how quantum simulators can produce novel phases of matter known as driven-dissipative quantum phases. Just like equilibrium phases of matter, systems out-of-equilibrium display critical behavior when transitioning from an ordered to a disordered phase. However, the appearance of different steady-state ordering is of purely dynamical origin and cannot be reduced to the usual equilibrium results. Within this framework, I will show how a combination of powerful numerical and analytical tools beyond mean-field theory unveils novel phases of matter and quantum many-body physics not present under purely equilibrium conditions. I will also discuss how these effects and phases can be found using state-of-the-art quantum simulators.

**9:48AM X25.000010: Scrambling and Floquet in Conformal Field Theory**  RUIHUA FAN (Presenter), Physics Department, Harvard University, XUEDA WEN, Physics Department, Massachusetts Institute of Technology, YINGFEI GU, ASHVIN VISHWANATH, Physics Department, Harvard University — Scrambling and Floquet are two important subjects in the study of quantum dynamics but hard to describe in general. Conformal field theory provides an ideal platform to get more analytical understanding. My talk will be divided into two parts. In the first part, I will discuss scrambling in the unitary minimal models, by analytically calculating out-of-time-order-correlation functions. In particular I will focus on the early-time and late-time behaviors and how they are related to each other. In the second part, I will talk about Floquet physics for general 2D CFTs. The Floquet driving is implemented with the sine-squared deformation. I will discuss the heating features and their stability.

*R.F and Ashvin Vishwanath acknowledge funding from the Simons Foundation through Ashvin Vishwanath's Simons Investigator grant. R. F. was also supported by the Purcell fellowship. Yingfei Gu is supported by the Gordon and Betty Moore Foundation EPiQS Initiative through Grant (GBMF-4306). Xueda Wen is supported by the Gordon and Betty Moore Foundation's EPiQS initiative through Grant (GBMF-4303).

**10:00AM X25.000011: Random Lindblad Dynamics**  TANKUT CAN (Presenter), Initiative for the Theoretical Sciences, CUNY Graduate Center, SARANG GOPALAKRISHNAN, VADIM OGANESYAN, Physics, CUNY College of Staten Island, DROR ORGAD, Racah Institute of Physics, The Hebrew University of Jerusalem — The Lindblad superoperator is the generator of time translation for the quantum Markov master equation. We ask the question: what dynamics follow from a random Lindblad generator? To answer this, we define an ensemble of Lindblad superoperators using random matrix theory, and study the statistical properties its eigenvalues. In particular, we characterize the spectral gap (a.k.a. dissipative gap) which determines the asymptotic decay rate of typical operators in the Hilbert space. We find that the spectral gap is finite in the limit of infinite Hilbert space dimension, and described by a universal non-monotonic scaling function of the dissipative coupling constant.

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**10:12AM X25.000012: Drive-dependent dissipation in open quantum systems regularized by thermal fluctuations**  RANGEET BHATTACHARYYA (Presenter), Indian Institute of Science Education and Research, Kolkata — We report an alternate formulation of the quantum master equation (QME) to describe the dynamics of a quantum system weakly coupled to a heat bath, in the presence of weak external drive. A key feature of this approach is the introduction of an explicit Hamiltonian to model the thermal fluctuations in the heat bath. We show that the resulting time coarse-grained dynamical equation for the quantum system has dissipators with a natural regulator, which emerges from an ensemble average over the fluctuations. Importantly, such regularized dissipators arise from the second-order contributions of both the external drive as well as the system-environment coupling. We show that the second-order drive terms, regularized to time-scales set by the fluctuations, result in dynamic drive-induced frequency shifts (such as Bloch-Siegert shifts) as well as drive-dependent relaxation phenomena (the Kramers-Kronig pair of the shift terms). We also present the experimental verification of the drive-induced dissipation terms using Nuclear Magnetic Resonance techniques. It is contemplated that such drive-induced dissipation will play important roles in quantum information processing.

10:24AM X25.00013: Dissipation-induced instabilities of two-component Bose-Einstein condensates in optical cavities  EZEQUIEL RODRIGUEZ CHIACCHIO (Presenter), ANDREAS NUNNENKAMP, University of Cambridge — We investigate the dynamics of a gas of ultra-cold spin-1 atoms inside an optical cavity, which is driven transversely by an external laser whose polarization is not aligned with that of the cavity field. By considering the atom population to be equally distributed between the +1 and -1 spin states, we obtain a two-component Dicke model with complex light-matter couplings. We study the effects of cavity losses on the system by computing the steady-state phase diagram and observe the emergence of dynamical instabilities in the form of limit cycles, induced by the interplay between coherent and dissipative processes. We characterize the physical mechanisms behind the unstable behavior and study the role of cavity fluctuations in the system.

10:36AM X25.00014: Low-cost ultrafast eigenstate transition without undergoing an adiabatic process  FATEMEH MOSTAFAVIKHATAM (Presenter), HAMIDREZA RAMEZANI, physics, university of texas rio grande valley — We introduce a class of non-Hermitian Hamiltonians that offers a dynamical approach to have complete population transfer from the ground state of a system to the ground state of a new system in no time. In particular, in our proposed 2×2 Hamiltonians, one eigenvalue is absolutely real and the other one is complex. This specific form of the eigenvalues helps us to exponentially amplify or decay the population in an undesired eigenfunction while keeping the probability amplitude in the other eigenfunction conserved. This provides us with a powerful method to have a diabatic process with the same outcome as its corresponding adiabatic process. In contrast to standard shortcuts to adiabaticity, our Hamiltonian has a much simpler form with a lower thermodynamic cost. Our proposed Hamiltonians not only have application in rapid population transfer but also can be used for tunable mode selection and filtering in acoustics, electronics, and optics.

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X26 DQI: Quantum Optimal Control and Machine Learning BCEC 160B - Daniel Egger, IBM Research - Zurich - Tag(s): Focus

8:00AM X26.00001: Universal Quantum Control through Deep Reinforcement Learning*  MURPHY YUEZHEN NIU (Presenter), Massachusetts Institute of Technology, VADIM SMELYANSKIY, SERGIO BOIXO, HARTMUT NEVEN, Quantum A. I. Laboratory, Google — We discover in this work that deep reinforcement learning (RL) techniques are capable of solving complex multi-qubit quantum control problems robustly against control errors. We propose a control framework to jointly optimize over stochastic control errors and facilitates time-dependent controls over all independent single-qubit Hamiltonians and two-qubit Hamiltonians, thus achieving full controllability for any two-qubit gate. As an essential ingredient, we derive an analytic leakage bound for a Hamiltonian control trajectory to account for both on- and off-resonant leakage errors. We utilize a continuous-variable policy-gradient RL agent consisting of two-neural networks to find highest-reward/minimum-cost analog controls for a variety of two-qubit unitary gates crucial for quantum simulation. We achieve up to a one-order-of-magnitude of improvement in gate time over the optimal gate synthesis approach based on the best known experimental gate parameters in superconducting qubits, an order of magnitude reduction in fidelity variance over solutions from both the noise-free RL counterpart and a baseline SGD method, and two orders of magnitude reduction in average infidelity over control solutions from the SGD method.

*Claude Shannon research fellowship from MIT.

8:12AM X26.00002: Reinforcement learning using AlphaZero to optimize entanglement sythesis in circuit QED  FELIX MOTZOI (Presenter), MOGENS DALGAARD, JENS JAKOB SORENSON, JACOB F SHERSON, Aarhus University — We present an implementation of a reinforcement learning algorithm using deep neural networks and Monte Carlo tree search to demonstrate global optimization of the control landscape of superconducting qubits. Our findings show significant improvement in time and best-found fidelity compared to long established local-climbing methods such as GRAPE. Our research suggests that for increasingly complex quantum control problems (as system sizes and architectures grow), sophisticated machine learning may become a preferable tool for calibrating and optimizing high-performance quantum computing experiments.
Applications of machine learning and related techniques to quantum control problems
Sergio Boixo (Presenter), Murphy Niu, Vadim Smelyanskiy, Hartmut Neven, Google Inc. — NISQ quantum computers require precise quantum control to achieve the necessary high fidelity operations. Machine learning offers tools that can be applied to this task. For example, reinforcement learning is a promising paradigm for universal quantum control. In the case of superconducting qubits, this requires explicit bounds on qubit leakage. To achieve high fidelity operations, quantum control parameters are fine tuned experimentally. Machine learning techniques can be applied in the optimization process. Cross entropy benchmarking is a technique to extract the experimental fidelity for generic operations with high precision, providing the cost function for the optimization loop.

Filtering noise through quantum control in high-dimensional systems
Michael Hush, Harrison Ball, Claire Edmunds, Dennis Lucarelli, Michael Jordan Biercuk (Presenter), Q-CTRL — Engineering-inspired filter functions are a powerful heuristic for the development of noise-robust quantum logic operations. We expand on existing single-qubit approaches and present a generalized, computationally efficient framework to calculate filter functions for operations performed on D-dimensional manifolds such as pairs of interacting qubits (including spectator levels), and qudits. We describe the computational approach and illustrate application in both systems. Filter function predictions for noise susceptibility in Molmer-Sorensen entangling gates are experimentally validated via experiments on trapped ions, showing good agreement with no free parameters.

Fast, high-fidelity single-qubit gates in strongly coupled multi-qubit systems
Xiu Hao Deng (Presenter), Shenzhen Institute of Quantum Science and Engineering, SUSTech, Edwin Barnes, Sophia Economou, Virginia Tech — Increasing the coupling strength between qubits can speed up multi-qubit entangling gates, which is essential for implementing more complex algorithms on a quantum processor. However, there is a tradeoff: It becomes challenging to implement single-qubit gates in the strong-coupling regime because the relevant transition frequencies become strongly dependent on the states of other qubits. In a fixed-frequency processor, this leads to significant gate errors and fidelity loss if this effect is not taken into account. To avoid this issue, most works to date have focused on the weakly coupled regime where individual qubits retain their identity, albeit at the price of slow entangling operations. Even in the weak-coupling case though, errors due to inter-qubit coupling can still accumulate over the course of several gates applied in sequence. Here, we present a novel method to mitigate errors in single-qubit gates due to coupling to a second qubit that involves building the coupling-dependent frequency shifts directly into the gate design. This is achieved through a combination of pulse shaping and pulse sequencing. Our techniques provide a way to speed up two-qubit entangling gates without sacrificing the speed and fidelity of single-qubit gates.

Optimal Control for Robust Atomic Fountain Interferometers
Michael Goerz (Presenter), Paul Kunz, U.S. Army Research Laboratory, Mark Kasevich, Physics Department, Stanford University, Vladimir Malinovsky, U.S. Army Research Laboratory — Atomic fountain interferometers provide precision measurements of gravitational fields with unprecedented sensitivity. This provides a wealth of possible applications, from fundamental science such as testing the equivalence principle, to next-generation inertial navigation systems. Fundamentally, the atom interferometer is implemented by laser pulses driving Bragg-transitions between the momentum states of the atomic cloud. Signal contrast is limited by the ability to realize large-momentum-transfer atomic mirrors and beamsplitters with high fidelity and robustness with respect to laser amplitudes and initial velocity distribution of the atoms. Starting from a pulse scheme based on rapid adiabatic passage, we employ Krotov's method of numerical optimal control and ensemble optimization to find shaped laser pulses that yield an increase in fidelity and robustness by roughly two orders of magnitude.


Research was sponsored by the Army Research Laboratory and was accomplished under cooperative Agreement Number W911NF-17-2-0147.
9:36AM X26.00007: Hamiltonian Amplification  CHRISTIAN ARENZ (Presenter), Frick Laboratory, Princeton University, DENYS BONDAR, Department of Physics, Tulane University, DANIEL BURGARTH, Department of Mathematics, Aberystwyth University, CECILIA CORMICK, Universidad Nacional de Cordoba, HERSCHEL A RABITZ, Frick Laboratory, Princeton University — Speeding-up quantum dynamics is of paramount importance for quantum technology. However, in finite dimensions and without full knowledge of the dynamics, it is easily shown to be impossible. In sharp contrast we show that many continuous variable systems can be sped-up without such knowledge, given that the structure of the underlying Hamiltonian is known. We call the resultant procedure Hamiltonian amplification. The method relies on the application of local squeezing operations allowing to amplify even unknown or noisy couplings and frequencies by acting on individual modes. We discuss the performance, physical realisations, robustness and implications of Hamiltonian amplification. Furthermore, we show how to combine amplification with dynamical decoupling to achieve amplifiers that are free from environmental noise. Finally, a significant reduction in gate times of cavity resonator qubits illustrates one potential use of Hamiltonian amplification.

9:48AM X26.00008: Enhanced superconducting qubit gates via accelerated adiabatic evolution  HUGO RIBEIRO (Presenter), Max Planck Institute for the Science of Light, AASHISH CLERK, Institute for Molecular Engineering, University Of Chicago — Qubit gates based on adiabatic evolution are in principle attractive, as they exhibit in-built robustness: they are in principle insensitive to the amplitude, duration and phase of control pulses used to realize the gate. However, the requirement of adiabaticity makes them extremely slow, and hence impractical in many settings. Here, we show how counter-diabatic driving techniques can be used to design one and two qubit gates that have many of the advantages of purely adiabatic gates, but are at the same time fast. We focus on approaches based on accelerated STIRAP (stimulated Raman adiabatic passage) [1, 2], and on specific implementations in various superconducting circuit architectures (both for transmon style qubits, and for fluxonium style qubits).


10:00AM X26.00009: Optimized Single Flux Quantum Pulse Trains for High-fidelity Qubit Control*  KANGBO LI (Presenter), ROBERT F MCDERMOTT, MAXIM VAVILOV, University of Wisconsin - Madison — The hardware overhead associated with microwave control is a major obstacle to scale-up of superconducting quantum computing. An alternative approach to qubit control involves irradiation of the qubits with trains of Single Flux Quantum (SFQ) pulses, pulses of voltage whose time integral is precisely quantized to the magnetic flux quantum. SFQ pulses can be generated and delivered to the qubit via a proximal classical Josephson digital circuit, offering the possibility of a streamlined, low-footprint classical coprocessor for monitoring errors and feeding back to the qubit array. In this talk, we describe an approach for the derivation and validation of complex SFQ pulse sequences in which classical bits are clocked to the qubit at a frequency that is a factor of a few higher than the qubit oscillation frequency, allowing for variable pulse-to-pulse timing in the qubit control sequence. Optimized sequences allow fast, coherent rotations in the qubit 0-1 subspace while suppressing leakage out of the computational manifold. We present simulation results and demonstrate that the performance of optimized SFQ control sequences is comparable to that of microwave-based sequences, with significantly reduced hardware requirements.

*The Hilldale Fellowship.

10:12AM X26.00010: Minimal Time Robust Control for Superconducting Qubit Devices*  ERAN GINOSSAR (Presenter), JOSEPH ALLEN, Advanced Technology Institute, University of Surrey, ROBERT KOSUT, SC Solutions — Fault tolerant quantum computing requires quantum gates with high delity. Given limitations on the lifetime of the qubits two-qubit gate delities can be coherence limited if the gate times are too long, but decreasing the operation time of two-qubit gates is a non-trivial exercise. Optimal control techniques can be used to decrease the operation time in theory, but generally do not take into account the realistic nature of uncertainty within the system when doing so. We apply robust optimal control techniques to demonstrate that it is feasible to reduce the operation time of the cross-resonance gate in superconducting systems to under 100 ns with two-qubit gate delities of F > 0.999, where this gate delity will not be coherence limited and would thus be achievable in experimental operation. This is while ensuring the pulse is robust to some uncertainty in the system, and having chosen a parameterization that aides in experimental feasibility.

*We acknowledge financial support from the EPSRC grants (Grants No. EP/L026082/1 and No. EP/L02263X/1)
10:24AM X26.00011: Error robust quantum logic for superconducting circuits  HARRISON BALL (Presenter), PER J LIEBERMANN, MICHAEL HUSH, MICHAEL JORDAN BIERCUK, Q-CTRL — Superconducting quantum computers differ substantially in the physical implementation of quantum logic operations, and therefore exhibit divergent error processes across hardware systems. In this talk we describe error modeling identifying dominant error channels in superconducting circuits implementing both parametrically activated and cross-resonance two-qubit gates. We use these insights to derive new classes of error-robust controls which combine modulation of both fields mediating the entangling operation and unitary operations applied to individual qubits. We present both analytic and numerically optimized solutions which are designed to reduce sensitivity to time-varying noise in critical system parameters by orders of magnitude.

10:36AM X26.00012: Geometric formalism for constructing arbitrary single-qubit dynamically corrected gates  JUNKAI ZENG (Presenter), EDWIN BARNES, Virginia Tech — Implementing high-fidelity quantum control and reducing the effect of the coupling between a quantum system and environmental noise is a major challenge in developing quantum information technologies. In recent work, a geometrical pulse-shaping method was introduced to facilitate the design of time-optimized pulses that implement gates while suppressing quasistatic noise errors. This method works for resonant pulses that implement a subset of single-qubit gates corresponding to rotations of the qubit about an axis that is orthogonal to the noise fluctuation term in the qubit Hamiltonian. Here, we show that these earlier findings are a special case of a larger geometrical structure hidden within the time-dependent Schroedinger equation. In this framework, any noise-suppressing single-qubit gate corresponds to a closed three-dimensional space curve, where the driving fields that implement the robust gates can be extracted from the curvature and torsion of the space curves. This provides a systematic approach to obtain all possible driving fields that implement an arbitrary dynamically corrected gate in the presence of quasistatic noise. We show that similar geometrical structures exist for quantum systems of arbitrary Hilbert space dimension.

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X27 DQI: Quantum Foundations II  BCEC 160C - Matthew Pusey, University of Oxford - Tag(s): Focus

8:00AM X27.00001: Quantum theory cannot consistently describe the use of itself* [Invited]  RENATO RENNER (Presenter), DANIELA FRAUCHIGER, ETH Zurich — Can quantum theory be used to consistently describe an agent who herself uses the theory? If quantum theory was a universally valid theory, applicable to arbitrarily complex systems, then this should clearly be the case. To study the question, we consider a setup consisting of four computers that take the role of agents. They are programmed with the rules of quantum theory, which they use to derive statements about the outcome of particular measurements, as well as about the statements that the other computers derived. We then show that the computers sometimes arrive at contradictory statements. This indicates that quantum theory cannot be extrapolated to complex systems, at least not in a straightforward manner.

This talk is based on Frauchiger and Renner, "Quantum theory cannot consistently describe the use of itself," Nature Comm. 9 (2018).

*This project was supported by the Swiss National Science Foundation (SNSF) via the National Centre of Competence in Research “QSSIT”, by the Kavli Institute for Theoretical Physics (KITP) at the University of California in Santa Barbara, by the Stellenbosch Institute for Advanced Study (STIAS) in South Africa, by the US National Science Foundation (NSF) under grant No. PHY17- 48958, by the European Research Council (ERC) under grant No. 258932, and by the European Commission under the project “RAQUEL”.

8:36AM X27.00002: Why QBism is immune to no-go theorems [Invited]  RUEDIGER SCHACK (Presenter), Royal Holloway, University of London — In 2012, Pusey, Barrett and Rudolph published a no-go theorem ruling out a class of ontological models for quantum mechanics. In 2015, the first loop-hole free Bell tests confirmed the assumptions of Bell’s theorem, the most famous of all no-go theorems. In 2018, Frauchiger and Renner published a no-go theorem based on the Wigner’s friend thought experiment. Because each of these no-go theorems, and their many variants, rule out a number of competing interpretations, QBism has emerged significantly strengthened from these developments.

What is the reason QBism is immune to these no-go theorems? It is not that QBism is anti-realist; on the contrary, QBism strongly embraces a form of structural realism. The reason lies in the particular way QBism takes the Born rule to be fundamental. This talk will explain the QBist take on the Born rule and how it resolves the apparent contradictions inherent in some recent versions of the Wigner’s friend paradox.
9:12AM X27.00003: An incompleteness theorem for physics  JOHN MYERS (Presenter), Harvard University, F. HADI MADJID, Consultant — We show how Gödel's incompleteness theorems have an analog in quantum theory. Gödel's theorems imply endless opportunities for appending axioms to arithmetic, implicitly showing a role for an entity that writes axioms as logically undetermined strings of symbols. There is an analog of these theorems in physics, to do with the set of explanations of given evidence. We prove that the set of explanations of given evidence is uncountably infinite, thereby showing how contact between theory and experiment depends on activity beyond computation and measurement—a physical activity of logically undetermined symbol handling.

9:24AM X27.00004: Ambiguity in the branching process of Many-Worlds Theories  KATHRIN GERHARD (Presenter), RENATO RENNER, ETH Zurich — Quantum mechanics correctly predicts measurement results and is therefore considered a useful physical theory. However, in a recently proposed thought experiment by D. Frauchiger and R. Renner, agents use quantum theory to describe how other agents use the theory, and contradictory statements appear.

Among the most popular interpretations of quantum theory that try to circumvent such consistency problems are the many-worlds theories. They provide a collapse-free model of the physical world: The wave function of the universe evolves unitarily in time, and every time a measurement happens, the global state splits into branches. Each branch is taken to correspond to an eigenstate of the measured observable, and in that sense, all measurement outcomes happen, but each one in a different world.

In this talk, we present a theorem stating that none of the existing many-worlds theories can give a consistent model of a physical process. Our argument is independent of commonly raised objections to many-worlds theories such as the preferred basis problem or the meaning of probability. In connection with the Frauchiger-Renner thought experiment, we show that the branching process leads to an ambiguity when judging the reality of worlds.

9:36AM X27.00005: Testing Envariance on Quantum Computers*  LUKASZ CINCIIO (Presenter), WOJCIECH ZUREK, Los Alamos National Laboratory — Born's rule does not need to be postulated – it can be derived from entanglement-induced invariance, the symmetry of entangled quantum states [1]. The same envariance can be used as a foundation of quantum statistical physics, to derive microcanonical and canonical ensembles [2]. We discuss logical circuits needed to test these entanglement symmetries on quantum computers and explore the possibility of using envariance to benchmark quantum computers.


*This research was supported in part by DoE via LDRD program at Los Alamos, J. Robert Oppenheimer fellowship and in part by FQXi "Agency in the Physical World".

9:48AM X27.00006: Small violations of Bell inequalities for multipartite pure random states*  CRISTHIANO SILVA (Presenter), Chapman University, RAPHAEL DRUMOND, Federal University of Minas Gerais, ROBERTO OLIVEIRA, Brazilian Institute for Pure And Applied Mathematics — For any finite number of parts, measurements and outcomes in a Bell scenario we estimate the probability of random N-qudit pure states to substantially violate any Bell inequality with uniformly bounded coefficients. We prove that under some conditions on the local dimension the probability to find any significant amount of violation goes to zero exponentially fast as the number of parts goes to infinity. In addition, we also prove that if the number of parts is at least 3, this probability also goes to zero as the local Hilbert space dimension goes to infinity.

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Hybrid Computation for Consistent Histories* ANDREW ARRASMITH (Presenter), LUKASZ CINCIO, Theoretical Division, Los Alamos National Lab, ANDREW T SORNBORGER, Information Sciences, Los Alamos National Lab, PATRICK J COLES, WOJCIECH ZUREK, Theoretical Division, Los Alamos National Lab — The consistent histories approach to quantum mechanics can be a valuable tool for studying many physical processes, ranging from the stochastic behavior of molecules to the quantum-to-classical transition. This approach resolves seeming paradoxes and allows us to apply classical logic to sequences of quantum events. Unfortunately, this tool has historically been limited to small systems or simple cases as the computational expense involved exponentially grows with both the system size and with the number of times considered on a classical computer, quickly becoming intractable. To remedy this difficulty, we present a hybrid quantum/classical algorithm suited for noisy intermediate-scale quantum computers that allows us to find and study consistent histories. We demonstrate the performance of this algorithm on the IBM and Rigetti quantum computers, and show a simulated demonstration of what will be possible on larger quantum computers. Finally, we discuss some potential future applications of this algorithm.

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- HEP QuantISED program

Observing a Quantum Measurement WALTER LAWRENCE (Presenter), Dartmouth College, University of Chicago — As a model quantum detector system, place a qubit in each path of a Stern-Gerlach apparatus, so that each qubit registers the passage (or not) of the atom along its path. Now, prepare a spin-1/2 atom with spin-up along X, send it through, and bring the paths back together after passing the quantum detectors. The spin qubit and the two detector qubits are now in a GHZ state. Of course to see this, one must (irreversibly) read out the individual detector states and measure the atomic spin with an ordinary “downstream” Stern-Gerlach system. While these all produce random outcomes, the appropriate products are definite, revealing the state. The products correspond to tensor product observables of which the GHZ state is an eigenstate. We can choose three independent, compatible observables to characterize the state. Two of our choices recover the usual Stern-Gerlach collapse scenario that one would get without the quantum detectors. The third detects the coherent superposition of both scenarios, finding the two detectors in a Bell state conditioned on the X-state of the atom's spin. Thus, when observing the detectors along with the atom, "which path" is compatible with “both paths.” Without the quantum detectors, one loses the option of measuring the third observable.
8:00AM X28.00001: Improved implementation of reflection operators* ANIRBAN NARAYAN CHOWDHURY (Presenter), University of New Mexico, YIGIT SUBASI, ROLANDO D SOMMA, Los Alamos National Laboratory — Quantum algorithms for diverse problems, including search and optimization problems, require the implementation of a reflection operator over a target state. Commonly, such reflections are approximately implemented using phase estimation. We provide a method that uses a linear combination of unitaries and a version of amplitude amplification to approximate reflection operators over eigenvectors of unitary operators using exponentially less ancillary qubits in terms of the precision of implementing the reflection. The gate complexity of our method is comparable to that of the phase estimation approach. We then extend our results to the Hamiltonian case where the target state is an eigenvector of a Hamiltonian whose matrix elements can be queried. Our results are useful in that they reduce the resources required by various quantum algorithms in the literature. Our improvements also rely on an efficient quantum algorithm to prepare a quantum state with Gaussian-like amplitudes that may be of independent interest. We prove a lower bound which shows that the implementation of the reflection operator is optimal in terms of the query complexity.

*ANC was supported partly by a Google Reserarch Award. YS and RS acknowledge support from the LDRD program at Los Alamos National Laboratory.

8:12AM X28.00002: Vibronic Molecular Spectra on a Universal Quantum Computer* NICOLAS SAWAYA (Presenter), Intel Labs — Calculating a molecule's vibronic spectrum is a hard problem in theoretical chemical physics, as any ground-state vibrational mode can couple to any excited-state mode via the Duschinsky transformation. Though this problem scales combinatorially on a classical computer, researchers have previously proposed an $O(M^3)$ scaling algorithm that solves the vibronic problem using a Boson Sampling Device. With a wholly different approach that uses the quantum phase estimation algorithm in the standard circuit model, we present a quantum algorithm that scales as $O(M^2)$ both in parallel classical and quantum operations, with linear circuit depth. Besides the scaling improvement, we also present methods that allow for substantial reductions of the number of samples collected. Additionally, because our measurement procedure does not destroy the vibronic state, the final state can be used in further computational analyses. Finally, we show how one would include finite temperature effects with a small cost. Our results are relevant to chemical/materials discovery and to the simulation of bosonic systems on a universal quantum computer.

*This research is funded by Intel Labs, a division of the Intel Corporation.

8:24AM X28.00003: Quantum Circuit and Algorithm Validation With Prove-It* WAYNE WITZEL (Presenter), KENNETH RUDINGER, Center for Computing Research, Sandia National Laboratories, ROBERT CARR, Computer Science, University of New Mexico, MOHAN SAROVAR, Sandia National Laboratories — Validating algorithm implementations is increasingly important, especially to distinguish implementation mistakes from noise inherent to so-called Noisy Intermediate-Scale Quantum (NISQ) technologies. Debugging a quantum computation is problematic because intermediate states cannot be probed without interfering with the computation. We demonstrate formal quantum algorithm verification using our versatile Python software package called Prove-It [1]. Prove-It is designed to be accessible, convenient, and extensible. It supports unlimited expressivity using LaTeX (including quantum circuit expressions), freedom to add and conveniently track axioms, flexibility to prove theorems independently in any order, and extensible automation capabilities.

[1] www.pyproveit.org

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8:36AM X28.00004: Hamiltonian and Lindbladian Parameter Estimation STEFAN KRASTANOV (Presenter), SISI ZHOU, Departments of Physics and Applied Physics, Yale University, STEVEN FLAMMIA, School of Physics, University of Sydney, LIANG JIANG, Departments of Physics and Applied Physics, Yale University — Estimating the parameters governing the dynamics of a system is a prerequisite for its control. We present a simple but powerful new method to estimate the Hamiltonian (or Lindbladian) governing a quantum system of a few qubits. Our method makes efficient use of all measurements taken of the system and it saturates the information-theoretic limits for such an estimator. Importantly, it is inherently robust to state preparation and measurement errors. It is not limited to evaluating only a fixed set of possible gates, rather it estimates the complete Hamiltonian of the system. The estimator is applicable to any Hamiltonian that can be written as a piecewise-differentiable function and it can easily include estimators for the non-unitary parameters as well. At the heart of our approach is a stochastic gradient descent over the difference between experimental measurement and model prediction.
8:48AM X28.00005: Quantum Computation with Quantum Schur Circuits* VOJTECH HAVLICEK (Presenter), Computer Science, University of Oxford, SERGI STRELCHUK, Applied Mathematics and Theoretical Physics, University of Cambridge, KRISTAN TEMME, IBM Research — Many quantum algorithms can be given as reversible classical circuits between a pair of quantum Fourier transformations. Here we study quantum circuits where QFT is substituted by the quantum Schur transform. This is motivated by Permutational Quantum Computing, a restricted computational model believed to capture nonclassical features of quantum computing.

A problem supporting this belief was the efficient approximation of matrix elements of the Young orthogonal matrices. While solvable efficiently with PQC, there was no efficient classical algorithm for this task. We give such algorithm by showing that the relevant PQC computation is a quantum Schur circuit and using symmetries of the Schur transformation.

Efficient classical approximation of transition amplitudes however does not mean that the circuits can be also efficiently sampled. We hence prove that quantum Schur sampling circuits with sparse enough output can be sampled from efficiently classically. Numerical study on a small number of qubits shows that a significant fraction of PQC satisfy this condition, allowing for their efficient sampling.

*V.H. was supported by Keble de Breyne and Clarendon scholarships. S.S. by the Leverhulme Early Career Fellowship. K.T. acknowledges support from the IBM Research Frontiers Institute.

9:00AM X28.00006: Disentangling quantum algorithms using symmetry+ DANIEL GUNLYCKE (Presenter), SEAN A FISCHER, C STEPHEN HELLBERG, STEVEN POLICASTRO, SERGIO TAFUR, United States Naval Research Laboratory — Quantum entanglement is a natural phenomenon in quantum mechanics that has enormous significance in quantum information science, including quantum computing. It enters quantum states in algorithms through the application of multi-qubit quantum logic operations such as the CNOT and Ising gates. While deliberate entanglement adds power and efficiency to algorithms, unintentional entanglement can be undesirable for a variety of reasons. Unintentional entanglement adds complexity, often making the outcome of a given algorithm more difficult to understand, and potentially more sensitive to errors. Furthermore, it can be an indication that an algorithm has not been optimized. If we could transfer entanglement from our algorithms into the bases that define our systems, then we could potentially reduce our algorithms. Such algorithm reductions will be of outmost importance for resource-limited, noisy intermediate-scale quantum (NISQ) computers.

In this presentation, we will demonstrate how such a reduction could be achieved in a small quantum system using symmetry. In addition to reducing the needed resources, our quantum computer calculations show a significant improvement in accuracy.

*This work has been supported by the U.S. Naval Research Laboratory through its Section 219 authority.

9:12AM X28.00007: Finding paths with quantum walks MARK HILLERY (Presenter), Physics and Astronomy, Hunter College of CUNY — Quantum walks, which are quantum versions of random walks, have proven useful in the development of quantum algorithms. They have been used to study searches on different graphs. In most cases, the object of the search is a distinguished vertex. However, a quantum walk can find more general objects with a quantum speedup, e.g. extra edges or subgraphs that break the symmetry of the overall graph. They can also find a path from one marked vertex to another, and an example of that will be presented.

9:24AM X28.00008: Machine learning search for quantum algorithms* JIAN LIN (Presenter), ZHONG YUAN LAI, XIAOPENG LI, Department of Physics, Fudan University — Quantum algorithm design lies in the hallmark of applications of quantum computation and quantum simulation. Recent theoretical progress has established complexity-equivalence of circuit and adiabatic quantum algorithms. Here we utilize deep reinforcement learning methods to search for optimal Hamiltonian path in the framework of quantum adiabatic algorithm. We benchmark our approach in Grover search and 3-SAT problems, and find that the adiabatic algorithm obtained by our reinforcement learning approach leads to improved performance in the final state fidelity and significant computational speedups for both moderate and large number of qubits compared to conventional algorithms. Our approach offers a recipe to design quantum algorithms for generic problems through a systematic search. This approach paves a novel way to automated quantum algorithm design by artificial intelligence.

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Thousand-Youth-Talent Program of China
Adiabatic Grover’s Algorithm and Graph Theory

SAMUEL MENDELSON (Presenter), JAKE FARINHOLT, Naval Surface Warfare Center Dahlgren Division — Adiabatic Grover’s Algorithm generally assumes the problem Hamiltonian is diagonal in the computational basis. In this talk, we will show how to reinterpret Grover’s search algorithm as a Graph Theory problem, and conversely, we will show how to build the problem Hamiltonian for various graph search problems directly from the Graph Laplacian. Finally, we analyze the performance of the adiabatic algorithms under various graph constraints and provide evidence to suggest that the performance improves with the number of edges. We rigorously prove that the graph search algorithm is exactly Grover’s algorithm when the graph is complete.

Many-Body-Localization Transition in a Universal Quantum Circuit Model

ADRIAN CHAPMAN (Presenter), School of Physics, University of Sydney, AKIMASA MIYAKE, Physics and Astronomy, University of New Mexico — We develop both exact and approximate methods to compute out-of-time-ordered correlators for arbitrary universal quantum circuits, taking advantage of the mapping of quantum circuits to the dynamics of interacting fermions in one dimension. In this framework, the out-of-time-ordered correlator can be calculated exactly as a superposition of exponentially many Gaussian-fermionic trajectories in the number of interaction gates. We develop a variationally-optimized, Gaussian approximation to the spatial propagation of an initially-local operator by restriction to the fastest-traveling fermionic modes, in a similar spirit as light-front computational methods in quantum field theory. We demonstrate that our method can detect the many-body localization transitions of generally time-dependent dynamics without the need for perturbatively weak interactions.

Intermediate-Scale Full State Quantum Circuit Simulation by Using Lossy Data Compression

XIN-CHUAN WU (Presenter), Department of Computer Science, University of Chicago, SHENG DI, FRANCK CAPPELLO, HAL FINKEL, YURI ALEXEEV, Argonne National Laboratory, FRED CHONG, Department of Computer Science, University of Chicago — To develop, evaluate, and validate new quantum algorithms or quantum computers, we need tools to assess their correctness and fidelity. This requires the capabilities of quantum circuit simulation. However, the number of quantum state amplitudes increases exponentially with the number of qubits, leading to the exponential growth of the memory requirement for the simulations. In this work, we present our quantum circuit simulation by using lossy data compression. We simulate quantum circuits by full-state update technique, and the lossy data compression is applied to the quantum state vector. Our preliminary results suggest that we should be able to significantly increase the size of quantum simulations beyond 50 qubits for certain algorithms.

Low-depth parallelization of k-local gates and applications

BRYAN O’GORMAN (Presenter), WILLIAM HUGGINS, University of California, Berkeley, ELEANOR RIEFFEL, NASA Ames Research Center, BIRGITTA K WHALEY, University of California, Berkeley — Practical use of near-term quantum computers requires taking their limited connectivity into account when realizing quantum circuits. We address this embedding problem for families of quantum circuits defined by a hypergraph where each hyperedge corresponds to a potential gate. We show that any set of k-local gates on n logical qubits can be ordered and parallelized in O(n^{k-1}) depth using a linear arrangement of n physical qubits. The construction is completely general and achieves optimal scaling in the worst case. We demonstrate benefits of this construction for i) sets of mutually commuting gates, as encountered in the Quantum Alternating Operator Ansatz circuits of the generalized QAOA algorithm, and ii) sets of gates that do not commute but for which compilation efficiency is the dominant criterion in their ordering. We find polynomial speedups in cost with number of spin-orbitals and electrons for Trotterized time-evolution of fermionic Hamiltonians under the Jordan-Wigner transformation.

Low-depth parallelization of k-local gates and applications

B. O’Gorman was supported by a NASA Space Technology Research Fellowship. W. Huggins and K. B. Whaley were supported by the U.S. Department of Energy, Quantum Algorithm Teams Program.
Stationary Phase Method in Discrete Wigner Functions and Classical Simulation of Quantum Circuits

Lucas Kocia (Presenter), NIST, Peter J Love, Tufts University — We apply the periodized stationary phase method to discrete Wigner functions of systems with odd prime dimension using results from \( p \)-adic number theory. We derive the Wigner-Weyl-Moyal (WWM) formalism with higher order \( h \)-bar corrections representing contextual corrections to non-contextual Clifford operations. We characterize the stationary phase critical points as a quantum resource injecting contextuality and show that this resource allows for the replacement of the \( p^2t \) points that represent \( t \) magic state Wigner functions on \( p \)-dimensional qudits by \( \leq p^t \) points. We find that the \( \pi/8 \) gate introduces the smallest higher order \( h \)-bar correction possible, requiring the lowest number of additional critical points compared to the Clifford gates. We then establish a relationship between the stabilizer rank of states and their number of critical points and exploit the stabilizer rank decomposition of two qutrit \( \pi/8 \) gates to develop a classical strong simulation of a single qutrit marginal on \( t \) qutrit \( \pi/8 \) gates that are followed by Clifford evolution, and show that this only requires calculating \( 3^{t+1} \) critical points corresponding to Gauss sums. This outperforms the best alternative qutrit algorithm for any number of \( \pi/8 \) gates to full precision.

Quantum Simulation and Optimization in Hot Quantum Networks

Martin Schuetz (Presenter), Harvard University, Benoit Vermersch, Gerhard Kirchmair, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, Lieven Vandersypen, QuTech and Kavli Institute of NanoScience, TU Delft, Juan Ignacio Cirac, Max-Planck-Institut für Quantenoptik, Mikhail Lukin, Harvard University, Peter Zoller, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences — We propose and analyze a setup based on (solid-state) qubits coupled to a common multi-mode transmission line, which allows for coherent spin-spin interactions over macroscopic on-chip distances, without any ground-state cooling requirements for the data bus. Our approach allows for the realization of fast deterministic quantum gates between distant qubits, the simulation of quantum spin models with engineered (long-range) interactions, and provides a flexible architecture for the implementation of quantum approximate optimization algorithms.


Manuel H. Muñoz-Arias, Pablo Poggi (Presenter), Ivan Deutsch, University of New Mexico — We study the implementation of a measurement-based feedback scheme to realize quantum nonlinear dynamics. We specifically study the Quantum Kicked Top (QKT), a standard paradigm of quantum chaos, in the context of an ensemble of spins. The scheme uses a sequence of (not-so) weak measurements of a collective spin variable and global rotations conditioned on the measurement outcome. We show that the resulting dynamics, ensemble averaged over many realizations, is governed by a combination of the QKT Hamiltonian and a non-unitary channel which vanishes in the semiclassical limit, recovering the Classical Kicked Top. We also analyze individual quantum trajectories, where we explore the emergence of chaotic behaviour and revisit the role of the measurement process in the quantum-to-classical transition.

*Support from NSF is acknowledged

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X29 DQI: Hybrid Systems: Optomechanics and Microwave-Optical Transduction

BCEC 162A - John Teufel, NIST - Boulder - Tag(s): Focus
Quantum state transfer between microwave and optical frequencies is important in the development of modular quantum computation. Most schemes to realize such a hybrid interface are based on direct quantum transduction, which, nevertheless, has to fulfill stringent requirements such as high conversion efficiency and low added noise. Despite all the recent remarkable efforts, in practice, building a direct microwave-optical quantum transducer still remains a challenge. A possible way out is to generate entanglement between the two modes and use it as a resource for microwave-optical modes transfer through teleportation. In this work, we propose a heralded scheme to entangle microwave and optical modes via parametric down conversion in a generic cavity piezo-optomechanical system. By post-selecting a two-mode squeezed vacuum state, entangled microwave-optical photon pairs can be generated. The entanglement is verified by the Bell inequality violation for a wide range of feasible parameters, showing the potential of the entangled source for realizing quantum state transfer between microwave and optical frequencies.

In Part A: We will propose the experimental scheme for entanglement generation and detection.

*Supported by AFOSR MURI program, UChicago MRSEC (NSF DMR-1420709), NSF award NNCI-1542205, DOE and ARL.
An Optomechanical Transducer for Quantum State Transfer Between Infrared Light and Microwave. Part II: Measurement Results*  
GREGORY A PEAIRS (Presenter), Physics, University of California, Santa Barbara, MING-HAN CHOU, RHYS G POVEY, Institute for Molecular Engineering, University of Chicago, KEVIN SATZINGER, Physics, University of California, Santa Barbara, AUDREY BIENFAIT, HUNG-SHEN CHANG, CHRISTOPHER CONNER, ETIENNE DUMUR, JOEL GREBEL, YOUPENG ZHONG, ANDREW N CLELAND, Institute for Molecular Engineering, University of Chicago — Optomechanical systems provide a very interesting approach to frequency conversion between the microwave and optical domains, and in particular could provide a means to couple superconducting qubits to infrared telecommunications-wavelength signals. This capability would provide a compelling means to long-distance quantum communication. We have combined an aluminum nitride-based interdigital transducer (IDT) with a silicon-based one-dimensional optomechanical resonator, which together promise the necessary optomechanical and electromechanical coupling rates that would allow us to efficiently convert signals between infrared light and microwave electrical signals. We will present recent results using this device, including characterization of the electromechanical and optomechanical elements as well as classical operation using continuous-wave and time-domain signals.

*This work is supported by the Air Force Office of Scientific Research MURI program, the UChicago MRSEC (NSF DMR-1420709), and the Army Research Lab, and made use of the Pritzker Nanofabrication Facility, supported by the National Science Foundation’s award NNCI-1542205. E.D. was supported by LDRD funds from Argonne National Laboratory, and A.N.C. was supported in part by the DOE, Office of Basic Energy Sciences.

Two dimensional optomechanical crystal designs for microwave-optical transduction*  
RHYS G POVEY (Presenter), MING-HAN CHOU, GREGORY A PEAIRS, AUDREY BIENFAIT, HUNG-SHEN CHANG, CHRISTOPHER CONNER, ETIENNE DUMUR, JOEL GREBEL, YOUPENG ZHONG, ANDREW N CLELAND, University of Chicago — Conversion between microwave and optical frequencies via transduction with optomechanical devices is a topic of significant current interest, particularly for applications in quantum communication [1-3]. This process requires cooling the microwave-frequency mechanical resonator to the ground state, typically at mK temperatures. One dimensional optomechanical crystals have been operated in the quantum limit [4], but are limited by laser heating. Two dimensional structures may afford better thermal performance with only a minor reduction in optomechanical coupling strength. In this talk I will discuss ongoing efforts towards a two dimensional optomechanical crystal and cavity design, whilst using piezoelectric materials to convert microwave electrical signals to mechanical motion.


*Supported by the AFOSR MURI program, UChicago MRSEC (NSF DMR-1420709), the DOE, the ARL, and used the Pritzker Nanofabrication Facility supported by NSF NNCl-1542205.

Microwave-mechanical-optical transducer chip design innovations for noise mitigation*  
PETER BURNS (Presenter), BENJAMIN BRUBAKER, MAXWELL URMEY, SARANG MITTAL, ANDREW P HIGGINBOTHAM, CINDY A REGAL, KONRAD LEHNERT, JILA, University of Colorado Boulder — Viewed as resources for quantum information processing, microwave and optical fields offer complementary strengths. We simultaneously couple one mode of a micromechanical oscillator to a resonant microwave circuit and a high-finesse optical cavity, thereby realizing a mechanically mediated electro-optic converter. We have operated this converter at T < 100 mK, and demonstrated conversion efficiency of 47% and added noise of 38 photons [1]. In order to reduce the added noise from mechanical decoherence, we have integrated phononic shielding around the mechanical element. Changing the superconductor to NbTiN further reduces noise in the microwave circuit and conversion process.


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9:12AM X29.00007: Low temperature measurement of SiGe properties for superconducting quantum circuits*  
MARTIN SANDBERG (Presenter), MARKUS BRINK, VIVEKANANDA ADIGA, JOSÉ CHAVEZ-GARCIA, JERRY M. CHOW, HANHEE PAIK, JASON ORCUTT, IBM Thomas J. Watson Research Center — Superconducting circuits is a promising technology for building a scalable quantum computer. One of the shortcomings of this technology is that there is at the moment no technology available to transport quantum information in and out of the cryogenic environment that the circuit operates in. In order to transfer quantum information from the chip out to a room temperature environment the signal has to be converted from single microwave photons to something that will not be awash by the thermal noise at 300K. Lately there has been several proposals for how to enable such conversion using microwave to optical transducer. One approach is to exploit the electro-optical effect in strained SiGe. SiGe is a mature technology for on chip optics but is not well explored for superconducting circuits. We have fabricated quantum circuits in the form of transmon style quantum bits (qubits) on a substrate containing SiGe with a thin buffer layer of epitaxial Si. We find that that the introduction of SiGe in the substrate stack does not degrade the coherence properties of the transmon qubit. From the coherence measurements we are able to extract bounds for the loss tangent of SiGe at millikelvin temperatures.

*This work was funded by LPS/ARO under CQTS program, contract number W911NF-18-1-0022.

9:24AM X29.00008: Circuit cavity optomechanics approaching the ultrastrong coupling regime  
GABRIEL PETERSON (Presenter), University of Colorado, Boulder, SHLOMI KOTLER, FLORENT LECOCQ, X. Y. JIN, KATARINA CICAK, RAYMOND SIMMONDS, JOSE AUMENTADO, JOHN TEUFEL, National Institute of Standards and Technology — Many of the recent advances in quantum control and measurement of cavity optomechanical systems were enabled by the ability to reach the strong coupling regime, where the parametrically-enhanced optomechanical coupling rate is larger than any decoherence rate in the system. Ideally, the coupling could be further increased to the ultrastrong regime, where it approaches or exceeds the mechanical resonance frequency. In this talk, I will present experimental progress on a new architecture for cavity optomechanics where a mechanically compliant vacuum-gap capacitor resonates with a 3-dimensional microwave cavity. Compared to the planar superconducting microwave resonators used in previous experiments, the cavity resonator provides a similar vacuum coupling rate but superior power handling capability, allowing us to achieve driven optomechanical coupling rates improved by an order of magnitude over previous results. This architecture for microwave cavity optomechanics could therefore enable a new generation of experiments in the ultra-strong coupling regime.

9:36AM X29.00009: Generation of nonclassical states using quantum emitters in the metal-dielectric surface  
KARUN MEHTA, SHUBHRANGSHU DASGUPTA (Presenter), Indian Institute of Technology Ropar — We show that it is possible to generate optical photons in nonclassical states from a metal-dielectric interface using quantum emitters on the interface. The photons thus emitted into the surface plasmon (SP) mode from the initially excited emitters radiate out in free space in a cone-shaped geometry. When detected at two detectors, they exhibit anti-coalescence, a clear signature of nonclassicality. This also indicates that the photons are prepared in the path-entangled N00N-like states. These photons can be used for long-distance communication through free space or fiber. This technique is further scalable to a large number of photons. Such a system can therefore be employed as a building block for a distributed quantum network. We emphasize that our setup is different from the previously reported works in which the emitters get coupled to either propagating SP mode in a nanowire or the guided mode of a nanofiber, instead of the propagating SP mode on the interface. We find that the transmission probability of the photons into the free space is close to 0.7 from a silver-air interface, and therefore it is indeed feasible to implement our model using available technology.

9:48AM X29.00010: A three-dimensional optomechanical system for experiments in the quantum limit*  
BINDU MALINI GUNUPUDI (Presenter), SOUMYA RANJAN DAS, ROHIT NAVARATHNA, SUDHIR KUMAR SAHU, SOURAV MAJUMDER, VIBHOR SINGH, Indian Institute of Science — At low temperatures, microwave cavities are often preferred for the readout and control of a variety of systems. In this work, we present design and measurements of two independent mechanical resonator device coupled to a 3-dimensional rectangular waveguide cavity. We show that with a suitable modification to the electromagnetic field corresponding to the fundamental mode of the cavity, achieved by coupling a mechanical resonator, the circuit parasitic capacitance can be reduced significantly to as low as 13.7 ff. We perform measurements in the optomechanically-induced absorption (OMIA) regime on both the mechanical resonators, and demonstrate a single photon coupling strength of 12.5 Hz and a cooperativity of 40 for each mode. In addition, utilizing a low-impedance environment between the two-halves of the cavity, our design has the flexibility of incorporating a DC bias across the mechanical resonator which is often a desired feature in tunable optomechanical devices. With further improvements in device parameters, this system has the potential to reach the strong-coupling regime, enabling a wide range of quantum optomechanical experiments.

*We acknowledge support by the DAE under the Young Scientist Research Award, and by the UGC under the DSK Fellowship program.
10:00AM X29.00011: Study of coherent microwave-to-optical transduction using on-chip rare-earth ion devices*
JOHN BARTHOLOMEW (Presenter), JAKE ROCHMAN, JONATHAN KINDEM, ANDREI RUSKUC, ANDREI FARAON, Caltech — Quantum transducers will allow application-specific quantum hardware to accelerate the realization of large scale networks of entangled qubits. Rare-earth ions (REIs) in transparent crystals are one system suited to the development of quantum transducer technologies because of their ability to transfer entanglement between their highly coherent optical, electron-spin, and nuclear spin transitions. To harness this appeal, it is important to realize an integrated, on-chip architecture for REI quantum technologies to facilitate network connectivity with other quantum systems.

We will present the fabrication and characterization of on-chip REI devices based on $^{171}$Yb-doped yttrium orthovanadate ($^{171}$Yb:YVO$_4$). The devices combine nanophotonic waveguides or cavities with planar microwave waveguides. Waveguides allow spectroscopic measurements of the optical and spin transitions over broad frequency ranges facilitating studies in a variety of applied magnetic fields. We will report on the potential of this architecture for microwave to optical transduction, including its performance at zero-magnetic field, and suggest avenues for increasing the transduction efficiency.

*This work was supported by the Office of Naval Research and Northrop Grumman.

10:12AM X29.00012: Towards on-chip cavity-enhanced microwave to optical conversion using erbium doped crystals*
JAKE ROCHMAN (Presenter), JOHN BARTHOLOMEW, IOANA CRAICIU, CHUTING WANG, TIAN XIE, JONATHAN KINDEM, KEITH SCHWAB, ANDREI FARAON, Caltech — Generating remote entanglement between distant superconducting circuits via optical photons represents a crucial milestone towards the development of future quantum networks. Ensembles of rare-earth ions (REIs) coupled to optical and microwave cavities offer a promising architecture to achieve bidirectional coherent microwave to optical conversion by harnessing the strong coupling of REI ensembles to microwave and optical fields.

Here, we present an integrated platform composed of a superconducting microwave resonator and an amorphous silicon photonic resonator coupled to an erbium ensemble doped in the yttrium orthosilicate substrate. Our platform enables resonators with high quality factors in both the optical and microwave domain, while maintaining sufficient overlap between the optical and microwave fields required for the magneto-optical converter to achieve high efficiency. We present the fabrication of optical and microwave resonators and characterization of the platform's metrics such as microwave resonator losses due to static magnetic fields and circulating optical photons in the optical resonator.

*Jake Rochman acknowledges support from NSERC. The authors acknowledge support from the ONR Young Investigator Award and ARO/LPS CQTS.

10:24AM X29.00013: Photon super-bunching from a generic tunnel junction  
CHRISTOPHER LEON (Presenter), ANNA ROSLAWSKA, ABHISHEK GREWAL, OLLE GUNNARSSON, KLAUS KUHNKE, KLAUS KERN, Stuttgart, Max Planck Institute for Solid State Research — Generating correlated photon pairs at the nanoscale is a prerequisite to creating highly integrated optoelectronic circuits that perform quantum computing tasks based on heralded single-photons. Here we demonstrate fulfilling this requirement with a generic tip-surface metal junction. When the junction is luminescing under DC bias, inelastic tunneling events of single electrons produce a stream of visible photons of plasmonic origin whose super-bunching index is 17 when measured with a 53 picosecond instrumental resolution limit. The effect is electrically rather than optically driven – absent are pulsed lasers, down-conversions, and four-wave mixing schemes. This discovery has immediate and profound implications for quantum optics and cryptography, notwithstanding its fundamental importance to basic science and its ushering in of heralded photon experiments on the nanometer scale.

Prior poster presentation: http://conferences.au.dk/ecoss2018/scientific-programme/nam/

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Reliable characterization for improving and validating accurate elementary quantum operations*  

TAKANORI SUGIYAMA (Presenter), University of Tokyo, SHINPEI IMORI, Hiroshima University, FUYUHIKO TANAKA, Osaka University — A reliable method for characterizing elementary quantum operations that is suitable for improving and validating their accuracies is indispensable for realizing a practical quantum computer. Current standard methods, e.g., randomized benchmarking, quantum tomography, and gate-set tomography, are not sufficient because they lack reliability or are not suitable for the improvement and validation. A new characterization method, called regularized self-consistent quantum tomography (RSCQT), is an attractive alternative and has superior properties such as (i) the high reliability guaranteed by the asymptotic convergence of predicted probability distributions to the true probability distributions, (ii) applicability of the estimates to conventional validation protocols, and (iii) availability of detailed information of errors on the operations. Here we derive the asymptotic convergence rate, which would be optimal, and show numerical results on 1-qubit system, which confirm the theoretical results and prove that RSCQT is useful in practice.

*This work was supported by JSPS KAKENHI Grant Numbers JP16K13775 and JST ERATO Grant Number JPMJER1601.
8:36AM X34.00002: Computer-assisted quantum dot tuning for quantum computation and simulation [Invited]
LIEVEN VANDERSYPEN (Presenter), QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Much progress was made using electrostatically defined semiconductor quantum dots as the basis for quantum computation and simulation. In these experiments, a desired potential landscape is formed in a two-dimensional electron gas by individually adjusting the voltages applied to multiple gate electrodes. As a result, the filling of each dot, its electrochemical potential and its tunnel coupling to neighboring dots or to reservoirs are precisely controlled. Next, control signals for initialization, manipulation and read-out of individual charges and spins are calibrated. Despite this encouraging progress, the field could move faster if tuning and calibration tasks were more extensively assisted or taken over by computer automation. We started work several years ago on automating the initial tuning of coupled quantum dots to the few-electron regime [1] and the subsequent setting of the interdot tunnel coupling [2]. In parallel, we also invested in efficient (fast) measurement methods and the use of virtual gates [3] that allow real-time manual tuning and speed up computer-assisted tuning as well. Currently, our focus is on automating repetitive tasks such as calibration or compensation for background charge switches. I will present our past and present tuning efforts and summarize recent physics experiments on 2x2 and 8x1 quantum dot arrays that are enabled by these tuning methods.

9:12AM X34.00003: Automated Tuning of Tunnel Couplings and Gate Operations for Semiconductor Spin Qubits [Invited]
PASCAL CERFONTAINE (Presenter), JULIAN DAVID TESKE, RENE OTTEN, SIMON HUMPOHL, MICHAEL A WOLFE, PATRICK BETHKE, HENDRIK BLUHM, JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, 52074 Aachen, Germany — Quantum computers require large numbers of qubits with access to high-fidelity initialization, control and readout. While spin qubits in gate-defined quantum dots have demonstrated many of these properties, they need to be individually tuned by adjusting the voltages applied to electrostatic gates. This is a manual and time-consuming process [1] which will become unfeasible for large arrays of qubits. To address this challenge we present an iterative machine-learning algorithm [2] for automated fine-tuning of quantum dots. We estimate the system response by Bayesian updates and thus reduce the number of required measurements. Benchmarks show that the algorithm is able to adjust the tunnel and lead couplings in a singlet-triplet (ST) qubit in GaAs within 5 iterations.

In addition to the calibration of static dot parameters, high-fidelity quantum operations require precise tuning of time-dependent voltage pulses with respect to incoherent and coherent errors. While decoherence can be reduced by numerical pulse engineering, inaccuracies in the qubit model used for pulse engineering can cause coherent errors in the experimental implementation. In order to remove these errors, we present a self-consistent calibration routine for single- and two-qubit gates [2], which can be extended to a larger number of qubits and different sets of quantum gates. We apply this approach to a ST qubit in GaAs, and show experimentally that single qubit gate fidelities of 99.5% can be reached [3]. We use an accurate qubit model to simulate the performance of the calibration routine, and show that two-qubit gate fidelities of 99.9% (99.99%) should be achievable in GaAs (Si).

[2] All our software packages maintaining high software-engineering standards are available open source, see www.quantuminfo.physik.rwth-aachen.de/code

9:48AM X34.00004: Strategies for Automated Tune-up of Quantum Dot Arrays [Invited] SEÁN M MEENEHAN (Presenter), HRL Laboratories, LLC — As quantum dot qubit devices grow beyond two or three dots, computer-aided tools for calibration and control become essential. The first stage in tuning up any quantum dot spin qubit is determining an appropriate set of voltage biases such that all dots are loaded in the desired charge configuration, a task which is already complex at the three-dot level. In this talk we describe an automated process, based on single-dot measurements, simple image analysis, and linear compensation modeling of the device, which enables estimation of arbitrary charge states for a multi-dot system. Crucially, the desired bias state is estimated in a way that keeps all inter-dot tunneling rates within an acceptable range. This ensures relevant charge transitions remain visible, even for dots far away from the electron reservoir, and allows navigation of subsequent charge stability diagrams using image processing techniques. We demonstrate that this method can fully automate tuning of a six dot Si/SiGe device into a configuration appropriate for exchange-only qubit operation, including location of appropriate bias windows for spin preparation and measurement, and a validating demonstration of coherent spin rotations.
Fulfilling the promise of quantum technologies requires to be able to measure and tune several devices; fault-tolerant factorization using a surface code will require ~10^8 physical qubits. A long-term approach, based on the success of integrated circuits, is to use electron spins in semiconducting devices. A major obstacle to creating large circuits in this platform is device variability. It is very time consuming to fully characterize and tune each of these devices and this task will rapidly become intractable for humans without the aid of automation.

I will present efficient measurements on a single quantum dot performed by a machine learning algorithm. This algorithm employs a probabilistic deep-generative model, capable of generating multiple full-resolution reconstructions from scattered partial measurements. Information theory is then used to select the most informative measurements to perform next. The algorithm outperforms standard grid scan techniques in different measurement configurations, reducing the number of measurements required by up to 4 times.

I will also show the use of Bayesian optimisation to tune a single quantum dot device. By generating a score function, we can make the algorithm find the operating regime of a device. We tune the device to the single-electron tunnelling regime searching in a high-dimensionality parameter space in less than a thousandth part of the time that it requires manually.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X35 DQI: Characterization and Reduction of Noise in Quantum Computing Architectures I

8:00AM X35.00001: AI for qubits [Invited] LEV BISHOP (Presenter), IBM Thomas J. Watson Research Center — I present theoretical and experimental progress in applying classical AI techniques toward improving transmon-based qubit systems, including readout, hamiltonian estimation and gate calibration.

8:36AM X35.00002: Investigating Crosstalk and Correlated Errors with Randomized Benchmarking on Multiple Qubits* CHRISTIAN KRALFUND ANDERSEN (Presenter), STEFANIA BALASIU, JOHANNES HEINSOO, ANTS REMM, SEBASTIAN KRINNER, JEAN-CLAUDE BESSE, SIMONE GASPARINETTI, CHRISTOPHER EICHLER, ANDREAS WALLRAFF, ETH Zurich — Quantum computing with superconducting circuits has recently shown progress in implementing multi-qubit quantum processors with promising performance. To ensure scalability of these systems for quantum applications, it is critical that any errors remain small, local, and uncorrelated when increasing the number of qubits. In particular, the threshold theorem for quantum error correction is typically derived under the assumption of uncorrelated errors and constant error rates for each qubit. In this talk, we will present characterizations of cross-talk during gate operations using an extended simultaneous randomized benchmarking (RB) protocol. We apply sequences of randomly chosen elements from the single qubit Clifford group simultaneously on up to four qubits and use single-shot readout to measure individual qubits and all $σ_z$-correlators between the qubits. From these measurements, we estimate the multi-qubit error as the average $n$-qubit infidelity per application of $n$ single-qubit Clifford gates. We find the correlated errors to be composed mainly by two-qubit correlations. We also extend this method to analyse the crosstalk and correlated errors induced during two-qubit RB.

*We acknowledge support by ODNI, IARPA, via the US ARO grant W911NF-16-1-0071 and by the NCCR QSIT.

8:48AM X35.00003: Pairwise Perturbative Ansatz for Quantum Process Tomography Part 1: Theory* LUKE GOVIA (Presenter), GUILHEM RIBEILL, MATTHEW WARE, HARI K KROVI, Raytheon BBN Technologies — As candidate quantum processors increase both in size and fidelity, so too does the need for robust verification and validation of their operation. Full characterization of these devices would be highly desirable; however, standard quantum process tomography scales exponentially with the number of qubits. Even for small scale systems, the experimental resource requirements make full tomography very challenging in practice. To circumvent this, we present an ansatz to describe an arbitrary quantum process on a multi-qubit system that only requires characterization of two-qubit processes, such that the number of measurements scales only quadratically with the number of qubits. Our Pairwise Perturbative Ansatz (PAPA) builds a description of the multi-qubit process from tomographic reconstruction of the reduced two-qubit processes on all pairs of qubits in the system. In part 1 of this talk we outline the PAPA approach to multi-qubit process tomography, and show through theoretical simulation how it can be used for excellent characterization of multi-qubit quantum processes.

*This work was funded by the U.S. Army Research Office under Contract No: W911NF-14-C-0048.
In part two of this talk we present a Pairwise Perturbative Ansatz (PAPA) reconstruction of a three qubit process. For this demonstration, we perform GST characterization on neighboring pairs of qubits in a fully connected three qubit system. The local GST reconstructions constrain the global process. As outlined in part one, this data is used to bootstrap a description of a three qubit process from multiple two-qubit reconstructions. Such an ansatz could lead to characterization techniques that scale favorably in the number of qubits while making few assumptions about the structure of system noise.

*This material is based upon work supported by the U.S. Army Research Office under Contract No: W911NF-14-C-0048. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the U.S. Army Research Office.*

Characterization of realistic noise environments is crucial to the design of optimally tailored control methods for error suppression, and to the validation of microscopic models of noise. In particular, spatial correlations between noise afflicting distinct qubits are important in the determination of thresholds for fault-tolerant quantum computation. Recently, spin-locking relaxometry has been implemented to measure the single-qubit spectrum of quantum noise in superconducting circuits. In this talk, we present a generalization of this technique to two-qubit systems, enabling to simultaneously reconstruct the single-qubit and cross-correlation spectra of quantum dephasing noise. We also present simulations showing how this technique can be experimentally benchmarked using two superconducting qubits exposed to engineered photon shot noise from a common microwave cavity mode.

*This research was funded by the FRQNT, by ARO grant No. W911NF-14-1-0682; and by the Department of Defense via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.*

To investigate these assumptions experimentally, there is a need to extend established noise spectroscopy techniques from single- to multi-qubits systems. In this work, we present experiments on correlated dephasing of two superconducting qubits due to photon shot noise in a shared microwave cavity. Utilizing both free and driven evolution protocols, we demonstrate a frequency-selective method to probe the two-qubit correlations, and show how quantum noise spectroscopy techniques can reconstruct both single-qubit and two-qubit cross-spectra.

*This research was funded by the ARO grant No. W911NF-14-1-0682; and by the Department of Defense via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.*
We illustrate our work with data from both simulation and demonstration of the protocol run through the full stack at Rigetti Computing. By incorporating a model of the experiment that is aware of the controllable parameters, these tools can often help to identify and characterize Fourier-sparse drift in quantum gates, measurements, and state preparation operations. Cumbersome at best, in this talk, we discuss a suite of quantum circuit experiments and data analysis tools that is capable of identifying and characterizing Fourier-sparse drift in quantum gates, measurements, and state preparation operations. Identifying the source of this drift is a critical first step on the path to mitigating it, but techniques to do so have been cumbersome at best. In this talk, we discuss a suite of quantum circuit experiments and data analysis tools that is capable of identifying and characterizing Fourier-sparse drift in quantum gates, measurements, and state preparation operations. Furthermore, the effect of imperfect measurement bases and the resulting projections must be considered. In this work we adapt the framework of RB to MZM qubits with measurement-based gates and expand upon it by offering a protocol to directly characterize the fidelity of the underlying measurements themselves.

Randomized Benchmarking of Majorana Based Qubits

KENNETH RUDINGER, ERIK NIELSEN, ROBIN BLUME-KOHOUT, Sandia National Laboratories — The performance of a quantum computer depends critically on a large number of highly-tuned parameters. Time dependence (drift) in these parameters is generally unheralded, but can have a pernicious and possibly devastating impact on quantum gate fidelities. The effect of impermanent measurement bases and the resulting projections must be considered. In this work we adapt the framework of RB to MZM qubits with measurement-based gates and expand upon it by offering a protocol to directly characterize the fidelity of the underlying measurements themselves.
10:36 AM X35.00012: Calibration for single-qubit gates using robust phase estimation* WILLIAM KIRBY (Presenter), Tufts University, SHELBY KIMMEL, Middlebury College — Constructing single-qubit unitary gates with high accuracy is necessary for most implementations of gate-based quantum computation. A crucial component of this task is gate calibration, which requires methods for measuring the discrepancies between actual, physical gate implementations and ideal gates. In this talk we describe improved practical methods for quantifying such discrepancies using robust phase estimation, which requires only weak assumptions about the initial accuracies of the gate implementations.

*This work is supported by the NSF Graduate Research Fellowship Program under Grant No. DGE-1842474.

10:48 AM X35.00013: Calibrating two-qubit gates via robust phase estimation* KENNETH RUDINGER (Presenter), Center for Computing Research, Sandia National Laboratories, GUILHEM RIBEILL, LUKE GOVIA, MATTHEW WARE, Raytheon BBN Technologies, SHELBY KIMMEL, Department of Computer Science, Middlebury College — Robust phase estimation (RPE) is a Heisenberg-limited characterization protocol for learning the phases of quantum gate operations. Unlike many other similar techniques, RPE requires neither ancillae qubits nor highly accurate state preparation and measurement. Additionally, the computational requirements of RPE are minimal, needing nothing more complex than inverse trigonometric functions. To date, RPE has been used for single-qubit gate characterization and calibration. We extend RPE for two qubits, showing that it may be used to learn the phase for any standard two-qubit gate (e.g., CNOT, CPHASE, Molmer-Sorensen, SWAP, cross-resonance, etc.). We provide both numerical and experimental results.

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Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X36 DCMP: Novel f- and d-electron Materials: Skutterudites and Pnictides BCEC 205C
- Tag(s): Invited

8:00 AM X36.00001: Dynamical Mean Field Theory and the Iron Pnictides and Chalcogenides* [Invited] GABRIEL KOTLIAR (Presenter), Rutgers University and Brookhaven National Laboratories — Dynamical mean field theory (DMFT) in its combination with realistic electronic structure methods, now enables the computation of physical properties of materials starting from first principles. It also gives unexpected insights into the physics of strongly correlated systems.

We will illustrate these two aspects of the method, using the theory of Hund metals as an example. These are systems which derive their correlations from the Hund rule coupling rather than the Hubbard U. Primary examples are the iron pnictides and chalcogenides and the ruthenates. In this talk I will describe recent progress in understanding this class of materials using Dynamical Mean Field Theory and advanced quantum impurity solvers. We will stress in which way Hund correlations are different from those of materials near a Mott insulating state and on how the normal state characteristics of Hund metals impact their superconducting states at lower temperatures[2].

We will conclude with current directions to address outstanding challenges in this field[3].


*[1,2] Work on the theory of Hund metals is supported by NSF DMR
[3] Work on the development of Dynamical Mean Field Theory based electronic structure methods is supported by the DOE DMR Computational Material Science program.
Overview of Experimental Results on Filled Skutterudites with Pt-Ge framework

ROMAN GUMENIUK (Presenter), Institute for Experimental Physics, Freiberg University of Mining and Technology, WALTER SCHNELLE, ANDREAS LEITHE-JASPER, YURI GRIN, MPI CPfS — Filled skutterudites are compounds with the body-centred (space group \textit{Im}-3, \(a = 9\) Å) crystal structure and total chemical formula \(MT_4X_{12}\) (structure type LaFe\(_4\)P\(_{12}\)), where \(M\) = alkaline, alkaline-earth, rare-earth or actinide metal, \(T\) is a transition metal of Fe-subgroup and \(X\) is a pnictogen-atom. Their structural arrangement belongs to the group of the so-called cage-compounds, where positively charged filler-atoms (i.e. \(M\)-component) are situated inside large voids formed by a covalently bonded atomic framework (i.e. \(T_4X_{12}\)). Such a combination of different types of chemical bonding together with vibrational dynamics of the filler results in numerous exciting physical phenomena (e.g. superconductivity, heavy fermion and Kondo behaviours, charge-density wave, thermoelectric properties etc.). In the past decade we succeed in the preparation and study of the physical properties of filled skutterudites with the new Pt-Ge framework and total formula \(MPt_4Ge_{12}\) (\(M\) = Sr, Ba, Ce, Pr, Nd, Eu, Sm). {Sr, Ba, La, Pr}Pt\(_4\)Ge\(_{12}\) are superconductors with high transition temperatures (i.e. up to \(\sim 8\) K). The complete characterization of their properties, which included \(\mu\)SR and penetration depth measurements, revealed LaPt\(_4\)Ge\(_{12}\) to be a multi-gap superconductor, while the PrPt\(_4\)Ge\(_{12}\) is an unconventional superconductor with nodes in the energy gap. CePt\(_4\)Ge\(_{12}\) is found to be a system at the very border between typical intermediate valence and true Kondo lattice behaviour. SmPt\(_4\)Ge\(_{12}\) is a high-pressure phase with the moderate heavy fermion behaviour. Filled skutterudites {Nd, Eu}Pt\(_4\)Ge\(_{12}\) show Curie-Weiss paramagnetism in the temperature range 10-400 K and complicated magnetic structures with multiple orderings below 2 K.

Comprehensive Study of Electronic Structure of Rare-Earth (R) Filled Skutterudites, RPT\(_4\)Ge\(_{12}\)

KHANDKER F. QUADER (Presenter), Kent State University — Materials whose properties are influenced by presence of f-electrons are of current interest. Experiments on rare-earth filled skutterudites demonstrate an intriguing array of thermodynamic, transport and superconducting properties, and bring to fore theoretical challenges posed by f-electron systems. First principle calculations, such as density functional theory (DFT), sparse in the skutterudites, can provide valuable information about electronic structures that can be compared with experiments, and utilized in further theory development. The talk will discuss a comprehensive electronic structure study on a series of rare earth filled skutterudites, RPT\(_4\)Ge\(_{12}\) (\(R\) = La, Ce, Pr), aimed at shedding light on aspects that may be useful for understanding some of their properties: consequences of progressive increase of f-electrons in the series; role of correlation “\(U\)” between the f-electrons and its importance relative to spin-orbit coupling; the nature and variation of 3D Fermi surfaces with the number of f-electrons and “\(U\)”. The calculated Fermi surfaces may be relevant to the currently debated issue of multi-band versus single-band superconductivity; the density of states (DOS) and bands can be compared with resonant photoemission spectroscopy and specific heat measurements, and provide estimates of effective masses; the pseudogaps in DOS may be useful for understanding possible thermoelectric applications. These DFT calculations were cross-checked with VASP and Wien2K programs, and done for different exchange functionals; hence may serve as benchmark calculations for these materials.

*This work is funded in part by a QuantEmX grant from ICAM and the Gordon and Betty Moore Foundation, Grant GBMF5305.
Correlated materials are known to give rise to interesting physical properties such as superconductivity, colossal magnetoresistance, metal to insulator transitions, orbital and charge ordering, etc. In this talk I will present theoretical results for d- and f-systems, obtained with a method based on a combination of density functional theory (DFT) and dynamical mean field theory (DMFT). Due to recent development of forces for structural relaxations in DFT+DMFT method, we are now able to gain further insight into the couplings between electronic and structural degrees of freedom in the vicinity of a Mott transition, thus giving us predictive power for the electronic and structural properties of the correlated materials. Applying this method to AMnO3 (A=Bi,La) oxides, we find unusual electronic states with orbital selectivity, such as Site- and Orbital-Selective Mott state or Orbital-Selective Mott state. I will describe the electronic properties of such states and I will argue that: (1) these switchable novel states are a consequence of a highly sensitive interplay of the lattice with the electronic degrees of freedom of the correlated d-electrons and sp-electrons of the A ions; (2) based on the new understating of these electronic states we can explain the resonant x-ray scattering measurements, which till now could not be explained by other theoretical models. In addition, by comparing the DFT+DMFT structural relaxations at finite temperatures with the experimental crystal structures, we show that DFT+DMFT can capture the fine structural distortions induced by these unusual electronic states much better than DFT, thus confirming the predictive power of the DFT+DMFT method. I will end my talk discussing theoretical correlated electronic structure of filled skutterudites RPt4Ge12 (R=Ce,Pr) and comparison with experimental photoemission spectroscopy data.

*This work is supported by the U.S. Department of Energy as a part of the Computational Materials Science Program.

Soft-modes and electronic topological transitions in p- and d-electron materials

MICHAEL WIDOM (Presenter), Carnegie Mellon University — The Fermi surface of a metal can be altered through the application of isotropic pressure, symmetry-breaking anisotropic strains, or chemical substitution. Changes in Fermi surface topology, such as the opening of a gap, or the creation or disappearance of a pocket, are known as Lifshitz transitions, and can dramatically influence the electronic, magnetic and mechanical properties of a material. This talk will focus on two examples of such transitions: the Burgers distortion that transforms body centered cubic metals to hexagonal close packed is driven by a Jahn-Teller-Peierls transition associated with a pseudogap in d_{xy} orbitals created by symmetry breaking; the collapse transitions in tetragonal AFe2As2 pnictides (A = Ca, Sr, Ba) are driven by the disappearance of a p_z electron pocket upon the application of pressure. These collapse transitions are contrasted with the discontinuous tetragonal to orthorhombic transition in CaFe2As2, which is thermodynamic rather than mechanical in character. Both the Burgers distortion and the collapse transition are connected with soft mode behaviors.

*This work was supported by the Department of Energy under grant DE-SC0014506.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X39 GMAG DMP: Magnons, Spin Waves, and Magnetic Dynamics

Topological magnons on a kagome lattice

RANJANI SESHADRI (Presenter), DIPTIMAN SEN, Indian Institute of Science — A system of spins on a kagome lattice interacting via the nearest-neighbor XXZ interaction (anisotropy ratio Δ) and Dzyaloshinskii-Moriya interaction (strength D) is found to have a very rich phase diagram. In the classical limit, five distinct phases with different ground-state spin configurations are found by varying the two interaction parameters. In some of these phases, spin-wave theory using the Holstein-Primakoff transformations is used to find the bulk energy bands of the magnons. In the ferromagnetic phase, where all the spins point along the +z direction, the bulk bands are separated from each other by finite energy gaps. Finding the Chern numbers here, one finds that there are four topologically distinct phases sharing the same ground state spin-configuration. Hence an infinite strip of the system hosts robust edge states which are directly related to the Chern number of the bands. The other phases, however, are found to have gapless magnon bands.
8:12AM X39.00002: Spin waves in doped graphene with in-plane magnetic fields* MATTHEW ANDERSON (Presenter), CARSTEN ULLRICH, University of Missouri — Plasmonics in graphene and related 2D materials has attracted much interest, with many prospects for novel applications. However, the dynamics of collective spin excitations and spin waves in 2D materials has been much less explored. Here, we study the spin-wave excitations of itinerant electrons in doped graphene in the presence of in-plane magnetic fields. We calculate the spin-wave dispersions using time-dependent density-functional methods within a standard tight-binding approach. Dynamical exchange-correlation effects are treated using the Singwi-Tosi-Land-Sjolander (STLS) approach, generalized for systems with noncollinear spins.

*This work was supported by Research Corporation and by DOE Grant No. DE-SC0019109

8:24AM X39.00003: Relation between unidirectional magnetoresistance and magnon generation by spin current* IGOR BORISENKO (Presenter), VLADISLAV DEMIDOV, Physics, University of Muenster, SERGEI URAZHDIN, Emory University, SERGEJ DEMOKRITOV, Physics, University of Muenster — Ferromagnet/spin Hall effect (SHE) material bialayers are central to modern active nanomagnetic devices. The unidirectional magnetoresistance (UMR) observed in such structures – the asymmetry of resistance with respect to the current direction – has been explained in terms of spin-dependent electronic transport [1], or alternatively the effects of SHE-induced magnon generation [2].

We report on electrical measurements of UMR in a Permalloy/Pt bilayer, performed in conjunction with magneto-optical Brillouin light spectroscopy of spin current-driven magnon population. We show that the current dependence of UMR closely follows the dipolar magnon density, and that both dependences exhibit the same scaling over a large temperature range of 80-400 K. These findings demonstrate a close relationship between spin current-driven magnon generation and UMR, and indicate that the latter is likely dominated by the dipolar magnons. Our results may facilitate the development of new magnetoelectronic approaches for the characterization of SHE-induced magnetization dynamics.


*NSF DMR-1504449 and ECCS-1804198

8:36AM X39.00004: How to generate whispering gallery magnons* [Invited] KATRIN SCHULTHEISS (Presenter), Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, ROMAN VERBA, Institute of Magnetism, National Academy of Sciences of Ukraine, FRANZISKA WEHRMANN, KAI WAGNER, LUKAS KÖRBER, TOBIAS HULA, TONI HACHE, ATILIA KÁKAY, Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, AHMAD A AWAD, Department of Physics, University of Gothenburg, VASYL S TYBERKEYCH, ANDREI SLAVIN, Department of Physics, Oakland University, JÜRGEN FASSBENDER, HELMUT SCHULTHEISS, Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — One of the most fascinating topics in current quantum physics are hybridized systems, in which resonators of different quantum systems are strongly coupled. Prominent examples are circular resonators with high quality factors that allow the coupling of optical whispering gallery modes to microwave cavities or magnon resonances. However, the coupling to magnons with finite wave vectors has not yet been achieved due to the lack of efficient excitation schemes.

Here, we present the generation of whispering gallery magnons with unprecedented high azimuthal wave vectors via nonlinear 3-magnon scattering in a µm-sized magnetic disk exhibiting a vortex state. These modes show a strong localization at the perimeter of the disk and practically zero amplitude in an extended area around the vortex core. They originate from the splitting of the fundamental radial magnon modes, which can be resonantly excited in a vortex state by an out-of-plane microwave field. We will shed light on the basics of this non-linear scattering mechanism from experimental and theoretical point of view. Using Brillouin light scattering (BLS) microscopy, we investigated the frequency and power dependence of this nonlinear mechanism. The spatially resolved mode profiles give evidence for the localization at the boundaries of the disk and allow for a direct determination of the modes’ wavenumbers. Furthermore, time resolved BLS in combination with pulsed microwave excitation revealed the temporal evolution of the 3-magnon splitting and its dependence on the applied microwave power.

*Financial support from the Deutsche Forschungsgemeinschaft within programme SCHU 2922/1-1 is gratefully acknowledged. Samples were prepared at the Nanofabrication Facilities (NanoFaRo) at the Institute of Ion Beam Physics and Materials Research at the Helmholtz-Center Dresden-Rossendorf (HZDR). K.S. acknowledges funding within the Helmholtz PostDoc Programme.
Spin and Charge Pumping and Spin Wave Emission by Magnetic Domain Wall Annihilation:
Quantum-Classical Micromagnetics Approach*  
MARKO PETROVIC (Presenter), PETR PETR PLECHAC, Department of Mathematical Sciences, University of Delaware, BRANISLAV NIKOLIC, Department of Physics and Astronomy, University of Delaware — Recent experiments on magnetic domain wall collisions [1] showed their importance in generating short-lived spin wave bursts, low-power signals which can be used in future spintronics devices. Using a new, time-dependent method to propagate the non-equilibrium density matrix (the TD-NEGF method) combined with the classical Landau-Lifshitz-Gilbert (LLG) equation [2], we analyze spin and charge currents produced by an annihilation of two colliding domain walls in a magnetic material coupled to two electron reservoirs. The advantage of this approach is in its self-consistent coupling between quantum electron spin and classical magnetic moments which gives rise to a dynamical Gilbert damping and allows for calculation of the exact charge current pumped out of the system, in contrast to an approximate solution given by the perturbative spin motive force formula combined with the LLG equation [3]. The pumped currents provide enough information to indirectly determine details of the annihilation event.


*This project was supported by ARO MURI Award and NSF.

Magnon Damping in Yttrium Iron Garnet Films at Millikelvin Temperatures*  
SANDOKO KOSEN (Presenter), ARJAN F. VAN LOO, Department of Physics, University of Oxford, LAURA MIHALCEANU, DMITRY BOZHKO, ALEXANDER SERGA, Department of Physics, Technische Universitaet Kaiserslautern, ALEYX KARENOWSKA, Department of Physics, University of Oxford — Magnon-based quantum devices require low damping materials to maintain coherence. One of the most promising candidates is yttrium iron garnet (YIG). A ferrimagnetic insulator, YIG has the narrowest known linewidth of any practical material at room temperature. Bulk YIG has been shown to have low damping at millikelvin (mK) temperatures. However, there is some debate about whether this is the case in YIG films. Much of the uncertainty centres around the fact that the low-temperature magnetic behaviour of the substrate upon which high-quality samples are grown -- gadolinium gallium garnet (GGG) -- is not fully understood.

In this work, we study magnon damping in YIG films with and without GGG substrates by measuring the resonance linewidth at low temperatures. We observe that GGG contributes to significantly increased damping at low temperatures. Further measurements up to 9K reveal that temperature-peak processes are active above 1K and the presence of additional damping at mK temperatures which we attribute to the two-level fluctuators. Upon saturating the fluctuators, linewidths of 1.4 MHz are achievable in substrate-free YIG films at 20 mK, lower than the measured linewidth in the same films at room temperature.

*- EPSRC grant EP/K032690/1 (All authors)
- LPDP Indonesia (SK)

Non-linear parallel pump FMR studies in magnetic insulators*  
ANEESH VENUGOPAL (Presenter), TAO QU, RANDALL VICTORA, Electrical Engineering, University of Minnesota — Non-linear magnetic response of magnetic insulator materials is often used in the realization of radio-frequency (RF) devices. Although in use, there exists physical aspects that still need investigation for such devices. Here, we use high performance parallel computing based CUDA simulations and a theoretical model for magnon scattering to explore the direct and parametric generation of magnons, excited by microwaves in parallel pumped configurations. The sample is 10-100s of um and the response is largely dominated by the demagnetization fields in the sample. The DC applied magnetic field is in-plane and the RF field is linearly polarized and parallel to the DC field. We first determine the dispersion relation which plays a vital role in the understanding of nonlinear magnons. We then study the effect of ferrimagnet thickness, damping constant, RF frequency and power as well as DC applied magnetic field, on properties like frequency response, operational bandwidth, and power absorption of the material. It is found that the degree of non-linearity can be controlled using parameters like RF power. Analytically, Holstein and Primakoff based analysis is used to arrive at the threshold RF amplitude and dispersion relations.

*We would like to thank DARPA and XSEDE towards this project.
Magnon transport in quasi-two-dimensional van der Waals antiferromagnets* WENYU XING (Presenter), LUYI QIU, XIRUI WANG, YUNYAN YAO, YANG MA, RANRAN CAI, SHUANG JIA, XINCHENG XIE, WEI HAN, International Center for Quantum Materials, Peking University — The recent emergence of 2D van der Waals magnets down to atomic layer thickness provides an exciting platform for exploring quantum magnetism and spintronics applications. However, the potential of 2D van der Waals magnets for magnonics, has not been explored yet. In this talk, we will present the experimental observation of long distance magnon transport over several micrometers in quasi-2D van der Waals antiferromagnet MnPS$_3$. Experimentally, we exfoliated mechanically MnPS$_3$ flakes down to a few nanometers, and then fabricated the devices of non-local geometry where MnPS$_3$ is the transport channel of magnon. Then magnon is injected via thermal method and detected based on inverse spin Hall effect of platinum. As the quasi-2D MnPS$_3$ thickness decreases, a shorter magnon diffusion length is observed, which could be attributed to the surface-impurity-induced magnon scattering.

*National Basic Research Programs of China, National Natural Science Foundation of China, Key Research Program of the Chinese Academy of Sciences

Spin-wave Confinement and Coupling in Organic-Based Magnetic Nanostructures* MICHAEL CHILCOTE (Presenter), MEGAN HARBERTS, Physics, Ohio State University, BODO FUHRMANN, IZM, Martin-Luther-Universitat Halle-Wittenberg, KATRIN LEHMANN, Institute fur Physik, Martin-Luther-Universitat Halle-Wittenberg, YU LU, Chemistry, Ohio State University, ANDREW FRANSON, HOWARD YU, Physics, Ohio State University, NA ZHU, HONG X TANG, Electrical Engineering, Yale University, GEORG SCHMIDT, Institute fur Physik, Martin-Luther-Universitat Halle-Wittenberg, EZEKIEL JOHNSTON-HALPERIN, Physics, Ohio State University — We present the synthesis of a new class of organic-based magnetic nanostructures consisting of nanowires of V[TCNE]$_x$ that assemble along the ridges of a grooved substrate. These nanowires exhibit uniaxial magnetic anisotropy in direct contrast to the isotropic in-plane response of typical thin-films. When different magnon modes excited in these structures are brought into resonance by varying the orientation of an in-plane magnetic field, we observe anticrossing behavior, indicating strong coherent coupling between excitations. Furthermore, micromagnetic simulations using real nanowire profiles extracted from cross-sectional scanning electron microscopy faithfully reproduce the experimentally measured spectra without any free parameters, including spin-wave and other higher-order modes. These results introduce a new degree of freedom for organic-based magnetism and spintronics, and together with recent demonstration of encapsulation technologies and demonstrated functional microwave devices that exhibit high quality factors across a frequency range, suggest future promising applications in microwave electronics and quantum magnonics.

*This work was supported by NSF Grant No. DMR-1507775, NSF Grant No. EFMA-1741666, and DFG Grant No. SFB762.

Revisiting the Einstein-de Haas Effect* MICHAEL G DUNSMORE (Presenter), KAYTE MORI, MIRO BELOV, JOHN THIBAUT, VINCENT T.K. SAUER, JOSEPH E LOSBY, MARK FREEMAN, University of Alberta — The Einstein-de Haas (EdH) effect manifests the intrinsic connection between magnetic moment and mechanical angular momentum. In the original experiment [1], angular momentum changes induced in an iron cylinder by field-driven changes in the net magnetic moment were detected via resonant motion of a torsion pendulum. The miniaturization of torque sensors [2], combined with ultrasensitive optical detection, enables routine measurements of EdH effects. Millimeter to nanometer-scale sensors affixed to yttrium iron garnet structures were fabricated to explore the frequency-dependence of the EdH effect. Described are experimental methods for distinguishing EdH and conventional magnetic torques simultaneously.


*The authors wish to acknowledge support from the Natural Sciences and Engineering Research Council, Canada, the Canada Research Chairs program, and the Faculty of Science, University of Alberta.
10:24AM X39.00011: Observation of Ultrastrong Magnon-Magnon Coupling in YFeO$_3$ in High Magnetic Fields  

GARY NOE (Presenter), Department of Electrical and Computer Engineering, Rice University, MOTOAKI BAMBA, Department of Materials Engineering Science, Osaka University, XINWEI LI, Department of Electrical and Computer Engineering, Rice University, NING YUAN, JIASHU ZHANG, ZUANMING JIN, WEI REN, GUOHONG MA, SHIXUN CAO, Department of Physics, Shanghai University, DMITRY TURCHINOVICH, Fakultät für Physik, Universität Duisburg-Essen, JUNICHIRO KONO, Department of Electrical and Computer Engineering, Rice University — There is currently much interest in exploring resonant light-matter interaction in the ultrastrong-coupling (USC) regime where light and matter mix to an extreme degree and a variety of new phenomena emerge [1]. Recently, we have extended the concept of USC to a magnetic context in the form of matter-matter interaction [2]. Specifically, the exchange interaction of paramagnetic Er$^{3+}$ spins with an Fe$^{3+}$ magnon field in ErFeO$_3$ exhibited a large vacuum Rabi splitting. Here, we report another type of matter-matter USC between two magnon modes in YFeO$_3$. In rare-earth orthoferrite materials, there are ferromagnetic (FM) and antiferromagnetic (AFM) modes of magnons in the terahertz (THz) frequency range. By performing single-shot THz time-domain spectroscopy with a table-top pulsed magnet [3], we have investigated the magnetic field dependent magnon frequency and discovered anticrossing behavior for the FM and AFM magnon modes in high magnetic fields. The magnitude of the vacuum Rabi splitting suggests USC strength between the magnon modes when applying high magnetic fields at certain finite angles with respect to the crystallographic axes of bulk YFeO$_3$.


10:36AM X39.00012: Magnon-photon coupling in orthoferrites  

MARCEL BIALEK (Presenter), ARNAUD MAGREZ, JEAN-PHILIPPE ANSERMET, Institute of Physics, Ecole Polytechnique Fédéral de Lausanne — We study the magnon-photon coupling at THz frequencies [1]. The Purcell effect and magnon-polaritons were shown in ferromagnetic materials [2, 3]. It is interesting to observe these interactions in antiferromagnetic materials due to their high-frequency magnetic resonances. We report on an magnon-photon coupling in high-temperature antiferromagnets, bismuth ferrite BiFeO$_3$ (BFO) and dysprosium ferrite DyFeO$_3$ (DFO). We investigated polycrystalline samples of different thicknesses, thus having different sets of Fabry-Perrot-type cavity modes. We measured transmission spectra in 200-350 GHz frequency band at 300-600 K temperature range using frequency extenders to a vector network analyzer. Magnetic-resonance frequencies soften with rising temperature and cross with cavity modes. In BFO samples, we found that the width of the resonant line broadens at these crossings, consistent with the Purcell effect. In DFO samples, our data show avoided crossings of resonances with cavity modes, which is an indication of magnon-polaritons.


10:48AM X39.00013: Spin Waves Across 3-Dimensional, Close-Packed Nanoparticles*  

KATHRYN KRYCKA (Presenter), JAMES J RHyne, SAMUEl D OBERDICK, National Institute of Standards and Technology, AHMED M ABDELGAWAD, Department of Physics, Carnegie Mellon University, JULIE BORCHERS, National Institute of Standards and Technology, YUMI IJIRI, Department of Physics and Astronomy, Oberlin College, SARA MAJETICH, Department of Physics, Carnegie Mellon University, JEFFREY W LYNN, National Institute of Standards and Technology — While there is much practical and theoretical interest in characterizing magnons within 3-dimensional self-assembled nanoscale systems, few experimental techniques are appropriate. Here inelastic neutron scattering, although intensity limited, is utilized to measure inter-nanoparticle spin waves, or magnons, which arise from coupling between 8.4 nm manganese ferrite nanoparticles that are self-assembled into a close-packed lattice, yet physically separated by oleic acid surfactant. The observed magnons are dispersive, respond to an applied magnetic field, and display the expected temperature-dependent Bose population factor. Moreover, the dispersion yields a non-negative energy gap only when the effective Q is reduced by the inter-particle spacing, confirming that it is a collective excitation between the nanoparticles, rather than originating within individual nanoparticles. The experimental results are well explained by a limited parameter model which treats the 3-dimensional ordered, magnetic nanoparticles as dipolar-coupled superspins.

*We acknowledge support from grants DE-SC0019237 (Department of Energy), DMR- 1508249 (National Science Foundation), and the DMR- 1508249 (Center for High Resolution Neutron Scattering).

Friday, March 8, 2019 8:00 AM - 10:48 AM
8:00AM X40.00001: Probing spin correlations using angle resolved photoemission in the coupled metallic/Mott insulator system PdCrO$_2$ [*Invited] VERONIKA SUNKO (Presenter), Max Planck Institute for Chemical Physics of Solids, FEDERICO MAZZOLA, University of St Andrews, SOTA KITAMURA, Max Planck Institute for the Physics of Complex Systems, SEUNGYUN KHIM, PALLAVI KUSWAHA, Max Planck Institute for Chemical Physics of Solids, OLIVER J CLARK, MATTHEW WATSON, IGOR MARKOVIĆ, DEEPNARAYAN BISWAS, University of St Andrews, LEONID POUROVSKII, Collège de France, TIMUR KIM, TIEN-LIN LEE, PARDEEP K. THAKUR, Diamond Light Source, HELGE ROSNER, Max Planck Institute for Chemical Physics of Solids, ANTOINE GEORGES, Collège de France, RODERICH MOESSNER, TAKASHI OKA, Max Planck Institute for the Physics of Complex Systems, ANDREW P. MACKENZIE, Max Planck Institute for Chemical Physics of Solids, PHIL D C KING, University of St Andrews — A nearly free electron metal and a Mott insulating state can be thought of as opposite ends of the range of possibilities for the motion of electrons in a solid. In the magnetic oxide metal PdCrO$_2$, these two coexist as alternating layers. Using angle resolved photoemission, we surprisingly find sharp band-like features in the one-electron removal spectral function of the correlated subsystem. We show that these arise because a hole created in the Mott layer moves to and propagates in the metallic layer while retaining memory of the Mott layer's magnetism. This picture is quantitatively supported by a strong coupling analysis capturing the physics of PdCrO$_2$ in terms of a Kondo lattice Hamiltonian. Our findings open new routes to use the non-magnetic probe of photoemission to gain insights into the spin-susceptibility of correlated electron systems.

*We acknowledge support from the European Research Council (tGrant Nos. ERC-714193-QUESTDO and ERC-319286-QMAC), the Royal Society, the Leverhulme Trust (Grant Nos. RL-2016-006 and PLP-2015-144R), the Max-Planck Society and the International Max-Planck Partnership for Measurement and Observation at the Quantum Limit. We acknowledge PhD studentship support from EPSRC (grant numbers EP/L015110/1 and EP/K503162), and the IMPRS for the Chemistry and Physics of Quantum Materials. We thank Diamond Light Source for access to beamlines I09 (Proposal No. SI19479) and I05 (Proposal No. SI17699), which contributed to the results presented here.

8:36AM X40.00002: Magnetic proximity effect in Pt/α-Fe$_2$O$_3$ bilayers [*the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Grant No. DE-SC001304]*

SISHENG YU (Presenter), YANG CHENG, ADAM AHMED, FENGYUAN YANG, Ohio State University — Recently antiferromagnetic insulators play an important role in spintronic research including the spin superfluid [1] and long distance spin transport [2]. In this work, we find the magnetic proximity effect (MPE) in non-magnet Pt on antiferromagnetic insulator α-Fe$_2$O$_3$ bilayers. Off-axis sputtering was used to grow the high-quality bilayers as confirmed by atomic force microscopy and X-ray diffraction. Magneto-transport reveals anomalous hall signals at different temperature is observed. To elucidate these features, angle-dependent magnetoresistance (ADMR) measurements at different magnetic fields and temperatures have been conducted to isolate the contributions of anisotropic magnetoresistance (AMR) and spin Hall magnetoresistance (SMR). We also find non-trivial MR signals from field sweeps that reflect novel surface magnetism from the uncompensated moments in α-Fe$_2$O$_3$.


8:48AM X40.00003: Magnetic proximity effect (MPE) in Pt/YIG and Pt/Al:YIG heterojunctions* XIAO LIANG, YUPENG ZHU, ZHENH PENG, LONGJIANG DENG, LEI BI (Presenter), University of Electronic Science and Technology of China — Generation and manipulation of spin current in magnetic insulators, such as yttrium iron garnet (YIG) thin films have attracted great research interest recently. A variety of novel spintronic phenomena have been observed in the example system of Pt/YIG. To correctly interpret these observations, an important question and on-going debate is whether magnetic proximity effect (MPE) exists and its structural origin at this interface.

In this report, we present a joint study of the MPE in Pt/YIG and Pt/Al:YIG interfaces using first-principle calculations and transport characterizations. Theoretically, we demonstrate YIG crystal orientations and interface defects strongly influences MPE in Pt. Experimentally, we used diamagnetic Al$^{3+}$ ions to dope YIG at the tetrahedral site. The anomalous Hall resistance in Pt is found to be linearly proportional to the MPE induced magnetic moments predicted by first-principle calculations. Our findings demonstrate that the interface tetrahedral Fe-Pt exchange coupling is the origin of MPE at Pt/YIG heterojunctions, which can also be controlled by defect engineering at the interface.

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Ministry of Science and Technology of China MOST No. 2016YFA0300802

9:00AM X40.00004: First-Principles Studies of Influences of Capping Layers on Perpendicular Magnetic Anisotropy (K$_i$) in X/Co$_2$FeAl/MgO (X = 4d/5d transition metals) Structures SICONG JIANG (Presenter), SAFDAR NAZIR, KESONG YANG, University of California, San Diego — The Co$_2$FeAl/MgO based magnetic tunnel junctions (MTJs) with interfacial perpendicular magnetic anisotropy (K$_i$) have attracted extensive interests because of their potential utilization in spin-transfer-torque magnetic random-access memory (STT-MRAM). In this study, we systematically investigated the capping layer impact on the K$_i$ magnitude in Co$_2$FeAl/MgO system with 4d/5d transition metals (TMs) using density functional theory calculations. Our results show that TM capping layers, such as W, Pb, and Bi can effectively increase the K$_i$ values as compared to the uncapped structures. The results are explained in terms of atomic resolved K$_i$ contributions due to different orbital hybridizations. This work shed light on research and development of novel MTJs with high thermal stability during data storage in STT-MRAM in the future.

9:12AM X40.00005: Spin Seebeck Effect in Y3Fe5O12/NiO/Pt Thin Film Heterostructures EGECAN COGULU (Presenter), DEBANGSU ROY, Department of Physics, New York University, TAO LIU, MINGZHONG WU, Department of Physics, Colorado State University, HENDRIK OHLDAG, Advanced Light Source, Berkeley National Lab, ANDREW D KENT, Department of Physics, New York University — The spin Seebeck effect (SSE), where a thermal gradient in a ferromagnet generates spin current, has been in the focus of spintronics studies as it is one of the most efficient ways to generate spin currents. Also, antiferromagnets are gaining attention recently due to their properties like zero net magnetization, low magnetic susceptibility and very fast spin dynamics. In this work, we report SSE measured in Y3Fe5O12(YIG) (20 nm)/NiO(2 nm)/Pt (5 nm) structures as a function of temperature (5 K to 300 K) with the YIG magnetized in-plane, using a lock-in technique that probes the response at the first and second harmonic. By varying the current amplitude, magnetic field direction and temperature we characterize the amplitude of SSE in a comparative study with and without antiferromagnetic layer. Our results show that not only is spin transport possible through thin NiO layers but there is also an increase in the SSE effect magnitude at intermediate temperatures (~150 K). We correlate this increase in the SSE magnitude with an increase in the magnetic susceptibility of NiO shown by our XMLD/XMCD measurements. Our results suggest that the SSE can be used to characterize the response of thin antiferromagnetic materials and optimize their spin-transport characteristics.

9:24AM X40.00006: Spin transport and standing spin waves generation in heavy metal-magnetic insulator-ferromagnet hybrid structures YABIN FAN (Presenter), LUQIAO LIU, Microsystems Technology Laboratories, MIT — Magnons (or spin waves) are collective excitations of electrons' spin angular momenta in magnetic or antiferromagnetic materials. The excitation and tunability of magnons in low-damping magnetic insulators, e.g., the yttrium iron garnet (YIG), is particularly interesting because it could offer much longer magnon propagation length and potential broad spintronics applications.

Here, we study a platinum/YIG/permalloy hybrid structure, where YIG is the magnetic spacer and permalloy (Py) is a low-damping ferromagnetic metal. Through external microwave excitation, the YIG layer and the Py layer can be excited to reach the ferromagnetic resonance modes individually, and we have detected the spin current signal from the Py spin pumping process transmitted through the YIG layer and converted to voltage signals in the platinum (Pt) layer by the inverse spin Hall effect. More importantly, we have detected additional resonance peak and spin pumping voltage signals which are corresponding to the perpendicular standing spin waves (PSSW) in the YIG layer. At specific frequency, this PSSW in YIG could be coupled with the magnon mode in Py, which could possibly facilitate the magnon spin transport from the Py layer to the bottom Pt layer.
Spintronic Properties and Spin-Orbit-Torque Switching Characteristics of Pt/REIG Heterostructures  ETHAN ROSENBERG (Presenter), JACKSON BAUER, Massachusetts Institute of Technology, LUKÁŠ BERAN, Charles University in Prague, CAN AVCI, ETH Zurich, GEOFFREY S BEACH, CAROLINE ANNE ROSS, Massachusetts Institute of Technology — Ferrimagnetic insulator (FMI) thin films with perpendicular magnetic anisotropy (PMA) have recently attracted attention for spin-orbit torque (SOT) switching applications. We report the properties of epitaxial terbium iron garnet (TbIG) and europium iron garnet (EuIG) thin films with PMA. EuIG can be grown with PMA on (100) and (111) GGG substrates, making it ideal for orientation-dependent studies. For instance, Pt/EuIG had similar (001) and (111) Im[\Gamma] in contrast to similar studies on the Pt/CFO system. The TbIG films had a low Ms at room temperature due to their magnetic compensation point of 330K, and AHE measurements of Pt/TbIG showed a sign change at the compensation point. In addition, the (111) Im[\Gamma] of Pt/TbIG was similar to the Pt/EuIG system. Finally, we report the SOT switching characteristics of Pt/TbIG going through its compensation point, as well as the orientation dependence of the SOT switching characteristics of the Pt/EuIG system.


Probing boundary magnetization with spin Hall magnetoresistance in high T_N boron-doped magnetoelectric Cr_2O_3*  WILL ECHTENKAMP (Presenter), ATHER MAHMOOD, CHRISTIAN BINEK, University of Nebraska – Lincoln — Voltage controlled magnetization is a promising route for next-generation low-energy magnetic recording and logic devices. Utilizing magnetoelectric Cr_2O_3 based heterostructures, electric control of ferromagnetic exchange bias has been achieved up to the bulk Néel temperature. Recently spin Hall magnetoresistance has been shown to be present in Cr_2O_3 Pt bilayers, potentially providing a readout mechanism of the antiferromagnetic order parameter which avoids the need for a ferromagnet. In this study we combine this novel readout mechanism with the technique of boron-doping the Cr_2O_3 which increases the Néel temperature up to 400 K. Using a process of magnetoelectric annealing, spin Hall magnetoresistance in boron-doped Cr_2O_3 films is examined for the first time, with significant implications for future spintronic devices.

*This work was supported through MRSEC DMR-1420645, by E2CDA a joint initiative between NSF and SRC, by NRI & the Nebraska Center for Materials and Nanoscience.

Interfacial electronic states and correlated magnetic order across BiFeO_3/La_{0.7}Sr_{0.3}MnO_3 complex oxide heterointerfaces*  BO-CHAO HUANG (Presenter), Department of Physics, National Taiwan University, Taipei, Taiwan; and Institute of Physics, Academia Sinica, Taipei, Taiwan; and Institute of Atomic and Molecular Sciences, P. Yu, State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, and Collaborative Innovation Center of Quantum Matter, Beijing, China; an; YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan; and Institute of Physics, Academia Sinica, Taipei, Taiwan, CHIA-SENG CHANG, Institute of Physics, Academia Sinica, Taipei, Taiwan, RAMESH, Department of Physics, University of California Berkeley, California, USA, R. E. DUNIN-BORKOWSKI, PH. EBERT, Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, Germany, YA-PING CHIU, Department of Physics, National Taiwan University, Taipei, Taiwan; and Institute of Physics, Academia Sinica, Taipei, Taiwan, — Atomic-scale electronic states across termination engineered BiFeO_3/La_{0.7}Sr_{0.3}MnO_3 (BFO/LSMO) complex oxide heterointerfaces have been revealed using cross-sectional scanning tunneling microscopy and spectroscopy. The evolution of the Mn, O, and Fe states across MnO_2-BiO and La_{0.7}Sr_{0.3}O-FeO interfaces are demonstrated. Analysis of spectroscopy provides the electronic results of interfacial band gaps and interface bound charges at two kinds of terminations in the BFO/LSMO system. The result exhibits the MnO_2-BiO terminated interface with wide band gaps and dominant Mn^{4+} oxidation state, which can refer to an antiferromagnetic state at the interface. In contrast, the metallic behavior of the La_{0.7}Sr_{0.3}O-FeO terminated interface can be correlated to the ferromagnetism at the interface.

Reference:

*This work was supported by Ministry of Science and Technology of Taiwan, ROC under contrasts MOST 106-2628-M-002-011-MY3.
Emergent magnetic textures across SrRuO$_3$/SrMnO$_3$ interfaces

ARIJIT DAS (Presenter), PING ZHANG, ADAM J WATSON, TAMALIKA BANERJEE, Spintronics of functional materials, Zernike Institute for Advanced Materials, University of Groningen — Strongly correlated oxides by virtue of their correlation with lattice, spin and orbital degrees of freedom promote emergent phenomena at heterointerfaces. In SrRuO$_3$, a canonical correlated oxide, ferromagnetism arises due to coupling of oxygen octahedral distortion to hybridization of O 2p and Ru 4d orbitals. Furthermore, tunability of different physical properties at interfaces between thin films of SrRuO$_3$ and SrTiO$_3$ (100), either by tailoring strain or termination plane control can lead to the coexistence of different magnetic states. In this work, we investigate the emergence of an unconventional exchange bias at interfaces between thin SrRuO$_3$ films and SrMnO$_3$ thin films, a G-type antiferromagnet. We find that the competing interfacial exchange coupling between Ru $4^+$ and Mn $3+/4^+$, and the differences in local orbital bonding lead to differences in magnetic interactions at the bilayer interfaces. The magnetic ordering is manifested as an unconventional exchange bias in magnetization studies. We further observe a field dependent magnetic phase around 50 K from the M-T studies while the Tc of SrRuO$_3$ in the bilayer system is found to be $\sim$100 K. We analyze these observations along with unconventional features that is observed in the Hall magnetotransport data.

Unusual Magnetotransport Properties of Epitaxial NiCo$_2$O$_4$ Thin Films at Ultralow Temperatures*

ZHIGANG CHENG (Presenter), Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, XUEGANG CHEN, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln, XIANG ZHANG, LI LU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln — The inverse spinel NiCo$_2$O$_4$ (NCO) is a room temperature ferrimagnetic material that is promising for developing nanoscale energy and spintronic applications. In this work, we report the unusual thickness-dependent magnetotransport properties of high quality epitaxial NCO thin films. We have characterized the longitudinal magnetoresistance (MR) and Hall effect in NCO films with thickness varying from 5 unit cell (~4.1 nm) to 30 uc (24.6 nm) at ultralow temperatures down to 100 mK. The 10 and 30 uc films exhibit an intrinsic linear negative magnetoresistance, which persists up to 17 T without showing any saturation or upturn, while the 5 uc sample exhibits a positive MR that is possibly due to 2D weak antilocalization (WAL). We also observe robust anomalous Hall effect in the 10 and 30 uc samples, while the switching hystereses are in opposite directions. We discuss the effects of the Berry curvature, disorder scattering, and dimensionality crossover on the observed unusual thickness effect.

*This work was supported by National Key R&D Program of China Grant No. 2018YFA0305604, National Science Foundation of China (NSFC) Grant No. 11874403, NSF under Award No. DMR-1710461 and the Nebraska MRSEC (Grant No. DMR-1420645).

Simulation of Hall sign change in ferromagnet SrRuO$_3$*

SHIH-JYE SUN (Presenter), Applied Physics, National University of Kaohsiung, HSIUNG CHOU, Physics, National Sun Yat-Sen University — We employed a modified two-band model to theoretically investigate the mechanism of Hall sign change in SrRuO$_3$, in which an mpurity band couple with conduction and valence bands. Apparently, our theory can interpret the experimental results, which implies the proposed impurity band arising from Ru vacancies is an important factor in Hall sign change. We found that the electron density in the impurity band is getting increase as the impurity band energy approaches the chemical potential resulting in a decrease of Curie temperature of SrRuO$_3$. Besides, the Hall sign change occurs at the Curie temperature only when the band oupling is weak. Further more, the increase of the Ru vacancies makes the impurity band become solid but suppress the Curie temperature. Moreover, from the theoretical prediction a more relatively intrinsic p-type SrRuO$_3$ has higher Curie temperature and opposite for intrinsic n-type SrRuO$_3$.

*We would like to thank the Ministry of Science and Technology of Taiwan for Grant No. MOST 107-2112-M-390-002 (Shih-Jye Sun) and MOST 107-2112-M-110-012 (Hsiung Chou)
8:00AM X41.00001: Stabilizing spin spirals and isolated skyrmions at low magnetic field exploiting vanishing magnetic anisotropy [Invited] MARIE HERVE (Presenter), Physikalisches Institut, karlsruhe institute of technology, BERTRAND DUPÉ, Institut für Physik, Johannes Gutenberg Universität Mainz, RAFAEL LOPES, MAXIMILIANO MARTINS, Serviço de Nanotecnologia Laboratório de Nanoscopia, Centro de Desenvolvimento da Tecnologia Nuclear, TIMOFEY BALASHOV, Physikalisches Institut, karlsruhe institute of technology, LUKAS GERHARD, Institute of Nanotechnology, karlsruhe institute of technology, JAIRO DINIZ, Institut für Physik, Johannes Gutenberg Universität Mainz, WULF WULFHEKEL, Physikalisches Institut, karlsruhe institute of technology — The stabilization of non-collinear chiral magnetic structure is usually attributed to a large Dzyaloshinskii-Moriya interaction (DMI). DMI is enhanced at surfaces and interfaces via the hybridization of the magnetic atoms with 5d elements. Here, we show that a strong DMI is not a necessary condition to obtain a chiral magnetic order in ultra-thin films. Our spin-polarized scanning tunneling microscopy study show that Co/Ru(0001) possesses a spin spiral ground state, although the DMI is weak. Under moderated magnetic field (~150 mT) isolated skyrmion can be stabilized. We attribute the stability of this spin texture to the vanishing of the magnetic anisotropy energy.

8:36AM X41.00002: Correlating Induced Magnetization and the Dyzaloshinskii-Moriya Interaction in Skyrmion-host Metallic Multilayers* RYAN NEED (Presenter), National Institute of Standards and Technology, SABIT KARAYEV, DURGA KHADKA, University of Miami, PATRICK QUARTERMAN, BRIAN KIRBY, National Institute of Standards and Technology, SUNXIANG HUANG, University of Miami — In metallic multilayers, skyrmions can form at interfaces between a 3d elemental ferromagnet (e.g., Co, Fe) and a 5d nonmagnetic element (e.g., Ir, Pd), where broken inversion symmetry and large spin-orbit coupling enable Dzyaloshinskii-Moriya interactions (DMI) to generate chiral magnetic structures. Skyrmions in these systems can be moved through the material by small spin currents and thus present a promising opportunity to realize new, low-energy magnetic storage technologies. Here, we examine prototypical Pt/Co/Pt and Pt/Co/Ir heterostructures to address the question of how the strength of the net DMI of a multilayer structure corresponds to the strength of the proximity-induced magnetism (PIM) that exists in the Stoner-susceptible 5d metals. Specifically, we compare DMI strength, as measured by the spin-orbit torque induced effective field under an in-plane bias magnetic field, to the magnitude of the PIM in Pt and Ir, as determined by X-ray magnetic circular dichroism. We also use resonant reflectometry at the Pt and Ir L3 edges to extract magnetic depth profiles to understand how PIM changes as a function of Pt and Ir layer thickness.

*This research was performed while the author held an NRC Research Associateship award at the National Institute of Standards and Technology.

8:48AM X41.00003: Point-Group Dependence of Dzyaloshinski-Moriya Micromagnetics* AHSAN ULLAH (Presenter), BALAMURUGAN BALASUBRAMANIAN, ANDREI SOKOLOV, LANPING YUE, SHAH VALLOPPILLY, XINGZHONG LI, LI, WENYONG ZHNAG, DAVID SELLMYER, RALPH SKOMSKI, Nebraska Center for Materials and Nanoscience and Department of Physics and Astronomy,, University of Nebraska, Lincoln, Nebraska 68588-0299, USA — The micromagnetic realization of Dzyaloshinski-Moriya interactions (DMI) is investigated, with particular reference to spin spirals and skyrmions in crystals with cubic symmetry. The analysis starts with a group-theoretical analysis and explains the micromagnetism by a magnetic gyration tensor that is loosely related to the vector D of the DMI. In contrast to conventional wisdom, the DMI free-energy term $D \mathbf{M} (\nabla \times \mathbf{M})$ is not caused by broken inversion symmetry but reflects the presence of chiral building blocks (motifs) in the crystal structure. The scalar D includes not only DMI but also magnetocrystalline and magnetostatic contributions. In micromagnetic calculations, this D should never be used for noncubic structures, such as uniaxial tetragonal, rhombohedral, and hexagonal crystals. Furthermore, $D = 0$ for the cubic point groups $T_h$, $O_h$, and $T_d$, which include half- and inverse Heusler alloys ($T_d$), in spite of their broken inversion symmetry and nonzero atomic-scale DMI. The theoretical findings are used to discuss skyrmions in a range of related alloys: MnNiGa and MnNiSn, which crystallize in the centrosymmetric hexagonal Ni2In structure (point group $D_{6h}$), and Heusler-type cubic compounds MnNiIn and MnNiAl.

*This research is supported by DOE/BES (DE-FG02-04ER46152).
9:00AM X41.00004: Magnetic domain texture and Dzyaloshinskii-Moriya interaction in systems with perpendicular exchange bias

RISALAT KHAN (Presenter), School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK, THOMAS FORREST, Diamond Light Source, Didcot, Oxfordshire OX11 0DE, UK, HANS T. NEMBACH, Quantum Electromagnetics Division, National Institute of Standards and Technology, Boulder, Colorado 80305, USA, MANNAN ALI, School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK, JUSTIN SHAW, Quantum Electromagnetics Division, National Institute of Standards and Technology, Boulder, Colorado 80305, USA, CHRISTOPHER HUGH MARROWS, THOMAS MOORE, School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK — We sputter-deposited polycrystalline multilayers of Pt/Co/IrMn and Pt/Co/FeMn exhibiting perpendicular exchange bias (PEB). These multilayers are of interest because of the coincidence of the Dzyaloshinskii-Moriya interaction (DMI) with a vertical exchange field that could remove the need for an externally applied field to stabilise skyrmions [1]. We measured the exchange bias as a function of the layer thickness of Co, IrMn, and FeMn.

Utilising Kerr microscopy and XMCD-PEEM imaging, the domain morphology of the ferromagnetic (FM) layer (Co) was studied when crossing over the paramagnet to antiferromagnet (AFM) phase transition of the coupled AFM layers (IrMn and FeMn). The domain texture is influenced by the FM-AFM exchange coupling. A domain created by nucleation has rough edges, while a domain cooled through the transition maintains its smooth appearance.

The DMI brings about chiral magnetic order, such as Néel domain walls and skyrmions. The DMI was investigated in these systems, particularly how it is affected by the AFM spin order. The DMI was measured at different phases of the AFM layers. We quantified the DMI by Brillouin light spectroscopy [2].


9:12AM X41.00005: Universality of Defect-Skyrmion Interaction Profiles*

IMARA LIMA FERNANDES (Presenter), JUBA BOUAZIZ, STEFAN BLUEGEL, SAMIR LOUNIS, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425, Jülich, Germany — Magnetic skyrmions are prime candidates for future spintronic devices. However, incorporating them as information carriers hinges on their interaction with defects present in any device. We map from full ab initio [1], the energy profile of single magnetic skyrmions interacting with single-atom impurities, establishing a generic shape as function of the defect’s electron filling. Depending on their chemical nature, foreign 3d and 4d transition metal adatoms or surface-implanted defects can either repel or pin skyrmions in Pd/Fe/Ir(111), which we relate to the degree of filling of bonding and anti-bonding electronic states inherent to the proximity of the non-collinear magnetic structure. Similarities with key concepts of bond theories in catalysis and surface sciences imbue the universality of the shape of the interaction profile and the potential of predicting its interaction. The resulting fundamental understanding may give guidance for the design of devices to generate and control skyrmions.


*Funding provided by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 — DYNASORE).

9:24AM X41.00006: Determining the lifetime of metastable skyrmions*

JAMES ROWLAND (Presenter), MOHIT RANDERIA, Ohio State University — The question of the lifetime of metastable skyrmions in a ferromagnetic background is of both fundamental importance and of practical significance for memory applications. We address this question for a chiral magnetic thin film with ferromagnetic exchange \( J \), Dzyaloshinskii-Moriya interaction \( D \), and anisotropy \( K \) in an external field \( B \). We present results for skyrmion lifetimes based on novel numerical and variational approaches for analyzing the saddle-point in configuration-space paths that lead to skyrmion decay. Our results highlight the importance of the ratio of the film thickness \( L \) to the helical pitch length \( L_D = 2\pi J/D \) in understanding skyrmion decay. We show that Bloch point singularities play a crucial role in skyrmion decay even for small \( L/L_D \). The role of anisotropy and external field in determining skyrmion size and stability will also be discussed and comparison with previous results presented.

*JR and MR acknowledge support from DARPA Grant No. D18AP00008.
Quantum Collapse of a Skyrmion

AMEL DERRAS-CHOUK (Presenter), EUGENE M CHUDNOVSKY, DMITRY GARANIN, CUNY Graduate Center and Herbert H. Lehman College — We analytically and numerically investigate the quantum collapse of a small skyrmion in a thin magnetic film with Dzyaloshinskii-Moriya interaction (DMI). The stability threshold determined by the DMI, the external magnetic field, and the underlying atomic lattice has been computed. The Lagrangian describing the coupled dynamics of the skyrmion size and the chirality angle has been derived. An instanton solution of the equations of motion that corresponds to the skyrmion underbarrier contraction via quantum tunneling has been obtained. The tunneling rate has been computed and the conditions needed to observe quantum collapse of a skyrmion in a magnetic film have been elucidated [1].


Interfacial Dzyaloshinskii-Moriya interaction at an epitaxially grown ferromagnetic and heavy metal interface

KEMAL SOBOTKIEWICH (Presenter), University of Texas at Austin, AIDAN J LEE, Ohio State University, XIN MA, KEVIN OLSSON, DAVID LUJAN, University of Texas at Austin, ADAM S AHMED, FENG YUAN YANG, Ohio State University, XIAOQIN (ELAINE) LI, University of Texas at Austin — We study Dzyaloshinskii-Moriya interaction(DMI) in a series of epitaxially grown CoFe/Pt films using momentum-resolved Brillouin light scattering. The symmetry breaking present in the bilayer allows interfacial DMI, which is expected to depend on atomic alignment at the interface. Different CoFe alloys are studied. Co(25)Fe(75) is of particular interest because it exhibits exceptionally low magnetic damping [ref]. By controlling the chemical composition, thickness and growth conditions, one can tune the DMI parameter along with other magnetic properties of the film. We can measure these different properties using a single technique, Brillouin Light Scattering, allowing for a full characterization of the tunable parameters which could allow for engineering materials with the desired combination of properties.

Berry Phase and Exchange Contributions in Antiskyrmion Hosting Heusler Compound Mn1.5XY

JACOB GAYLES (Presenter), YAN SUN, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids — Recently, the Heusler compounds Mn1.4PtSn and Mn1.4Pt0.9Pd0.1Sn were shown to stabilize an antiskyrmion lattice above room temperature. This Heusler compound forms in a superstructure with the D2d symmetry, which allows for an anisotropic Dzyaloshinskii-Moriya interaction (DMI) perpendicular to the tetragonal axis. We use density functional theory calculations of Mn1.5XY to extract the relevant exchange interactions that determine the rich phase diagrams in these materials. The exchange interactions are between the large moments on the Mn atoms ~4 μB, which show magnetic states that are non-collinear ferrimagnetic up to the spin reorientation. The major role of the DMI and anisotropy are due to the X ion, either Rh, Pd, Ir, or Pt which also influence the exchange interactions. The Fermi level can be tuned by the Y ion, either In, Sn or Sb. We last calculate the anomalous Hall effect and topological Hall effects in these regimes, to capture the influence of the electronic structure on the Berry curvature.

Dzyaloshinski-Moriya Interactions and Berry Curvature in Magnetic Nanoparticles

RALPH SKOMSKI (Presenter), BALAMURUGAN BALASUBRAMANIAN, AHSAN ULLAH, RABINDRA PAHARI, DAVID SELLMYER, University of Nebraska - Lincoln — Noncentrosymmetric crystals, such as B20-ordered MnSi, have long been known to exhibit spin spirals in the bulk and skyrmions with quantized topological charge in thin films. We have theoretically and experimentally investigated the skyrmions of magnetic nanoparticles produced by cluster deposition. Our research includes CoSi, which is nonmagnetic in the bulk but magnetically ordered in nanoparticle form. The size confinement imposed by the nanostructuring suppresses the formation of spin spirals and skyrmions but leads top the formation of curling-type spin structures with nonzero Berry curvature and nonzero contribution to the topological Hall effect (THE). Concerning the nanoparticle material, there is an important distinction between centrosymmetric materials and various types of materials without inversion symmetry, especially polar and chiral crystal structures. With respect to the spin states, the former corresponds to broken chirality, whereas the latter imply a violation of chiral symmetry. It is interesting to note that moderately strong Berry curvatures and unquantized THE contributions may also be caused in nanoparticles with inversion symmetry and due to magnetostatic interactions.

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10:24AM X41.00011: Signatures of novel spin phases in thermal conductivity of the chiral skyrmion material Cu$_2$OSeO$_3$*  
ARTEM AKOPYAN (Presenter), NARAYAN PRASAI, University of Miami, BENJAMIN TRUMP, GUY G. MARCUS, Johns Hopkins University, SUNXIANG HUANG, University of Miami, TYREL MCQUEEN, Johns Hopkins University, JOSHUA COHN, University of Miami — We report measurements of thermal conductivity ($\kappa$) as a function of magnetic field in single crystals of the chiral skyrmion material Cu$_2$OSeO$_3$ in the temperature range $0.5 \leq T \leq 15$ K. Traversing phase boundaries associated with the low-temperature skyrmion and tilted conical spin phases, recently identified in small-angle neutron scattering studies,$^{a,b}$ gives rise to sharp signatures in $\kappa(H)$ for $H \parallel \langle 100 \rangle$ that are attributed to changes in the magnon thermal conductivity. Different crystallographic orientations for the applied field and heat flow will be discussed.


*This material is based on work supported by the U.S. DOE, Off. of BES, Div. of Mater. Sci. and Eng., under grant No. DE-SC0008607 (UM). Work at JHU was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. DOE, Off. of Sci., Off. of BES, under Award Number DE-SC0019331, and the NSF, Div. of Mater. Res., Sol. St. Chem., CAREER grant No. DMR-1253562.

10:36AM X41.00012: High pressure and magnetic field induced new phase in skyrmion Cu$_2$OSeO$_3$  
LIANGZI DENG (Presenter), HUNG-CHENG WU, RABIN DAHAL, MELISSA GOOCH, ZHENG WU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston TX 77204, HUNG-DUEN YANG, Department of Physics, National Sun Yat-sen University, Kaohsiung, 804 Taiwan, CHING-WU CHU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston TX 77204 — In recent years, there has been an enormous experimental research effort on skyrmion materials because of their peculiar topological properties. From a technological perspective, the magnetic skyrmions offer great potentials as information carriers in future robust, high-density, and energy-efficient spintronic devices. Ever since the discovery of skyrmion states in Cu$_2$OSeO$_3$ by Y. Tokura's group in 2012, Cu$_2$OSeO$_3$ has attracted considerable interest due to its complex magnetism, which is very sensitive to external perturbations, such as temperature, magnetic field, and pressure. Earlier high pressure studies on Cu$_2$OSeO$_3$ reveal that the ferrimagnetic transition temperature increases and the skyrmion state in magnetic H-T phase diagram could be enlarged under pressure up to 1.38 GPa. Recently, our group was able to establish the magnetic phase diagram in Cu$_2$OSeO$_3$ under pressure up to 45 GPa. Signatures of high pressure and magnetic field induced new phase in Cu$_2$OSeO$_3$ were detected. Structural analysis under high pressure in Cu$_2$OSeO$_3$ is ongoing to gain greater insight into the complex magnetism. Details of the experimental results will be shared and discussed in the presentation.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X43 DCMP: New Developments in Topological Materials BCEC 210B - Ashvin Vishwanath, Harvard Univ - Tag(s): Invited
8:00AM X43.00001: Two-dimensional topological superconductivity in Pb/Co/Si(111)* [Invited] TRISTAN CREN (Presenter), Institut des NanoSciences de Paris, CNRS-Sorbonne University, GERBOLD MÉNARD, SPEC, CEA Saclay, ANDREJ MESAROS, Laboratoire de Physique des Solides, CNRS-University Paris Saclay, CHRISTOPHE BRUN, FRANÇOIS DEBONTRIDDER, Institut des NanoSciences de Paris, CNRS-Sorbonne University, DIMITRI RODITCHEV, LPEM, ESPCI-Sorbonne University, PASCAL SIMON, Laboratoire de Physique des Solides, CNRS-University Paris Saclay — The examination of supposedly well-known condensed matter systems through the prism of topology has led to the discovery of new quantum phenomena that were previously overlooked. Just like insulators can present topological phases characterized by Dirac edge states, superconductors can exhibit topological phases characterized by Majorana edge states. In particular, one-dimensional topological superconductors are predicted to host zero energy Majorana fermions at their extremities. Zero bias anomalies localized at the edge of proximity induced superconducting wires were recently interpreted as fingerprints of the emergence of topological superconductivity [1,2].

By contrast, two-dimensional (2D) superconductors have a one-dimensional boundary which would naturally lead to propagating Majorana edge states characterized by a Dirac-like dispersion. We have recently observed some hint of dispersive Majorana edge states in a single atomic layer Pb superconductor. This material has strong triplet correlations but is not topological by itself [3]. We will show that by applying a Zeeman field with the help of a buried Co-Si nanomagnet one can provoke a transition to a topological state [4].

In addition to their dispersive edge states, 2D topological superconductors are also supposed to support localized Majorana bound states in their vortex cores. We will show that some recent measurements seem to support this theoretical prediction [5].

References

*This work was supported by the French Agence Nationale de la Recherche through the contract ANR Mistral, and by the Région Ile de France through the DIM Nano-K project ETERNAL.

8:36AM X43.00002: Fractional Excitonic Insulator* [Invited] CHARLES KANE (Presenter), Physics and Astronomy, University of Pennsylvania — We argue that a correlated fluid of electrons and holes can exhibit a fractional quantum Hall effect at zero magnetic field analogous to the Laughlin state at filling 1/m. We introduce a variant of the Laughlin wavefunction for electrons and holes and show that for m=1 it describes a Chern insulator that is the exact ground state of a free fermion model with $p_x + i p_y$ excitonic pairing. For m>1 we develop a composite fermion mean field theory, and we will give several pieces of evidence that our wavefunction correctly describes this phase. We will present physical arguments that the m=3 state can be realized in a system with $C_6$ rotational symmetry in which energy bands with angular momentum that differ by 3 cross at the Fermi energy. This leads to a gapless state with $(p_x + i p_y)^3$ excitonic pairing, which we argue is conducive to forming the fractional excitonic insulator in the presence of interactions. Prospects for numerics on model systems and band structure engineering to realize this phase in real materials will be discussed.


*This work was done in collaboration with Yichen Hu and Jörn Venderbos and was supported by a Simons Investigator grant from the Simons Foundation and by NSF Grant number DMR-1120901.
New invariants, complete classification and fast diagnosis for topological crystalline insulators*

CHEN FANG (Presenter), Chinese Academy of Sciences — Topological crystalline insulators have nontrivial band topology jointly protected by onsite symmetries of time reversal and charge conservation, as well as by spatial symmetries of lattice. Different types of lattice symmetries correspond to different topological invariants in the bulk and distinct characteristic surface states. We discuss newly discovered $Z_2$ invariants in 3D protected by rotation (screw) symmetry, inversion symmetry and roto-reflection symmetry, respectively. Each of the new invariants in the bulk is related to the $(d-2)$-dimensional edge states on the boundary. With the new invariants, we establish a complete classification of topological crystalline insulators for each of the 230 space groups in 3D, along with explicit, microscopic constructions for each class. To search for corresponding materials for the topological states in these new classes, we have established quantitative mappings from symmetry eigenvalues of valence bands to topological invariants all space groups. Applying these mappings, we have developed a fully automated diagnosis algorithm for all nonmagnetic crystals. The algorithm is applied to diagnosing 39519 materials, in which 8056 are found topological.

Observation of tunable Dirac interface states in topological crystalline insulator superlattice*

BADIH ASSAF (Presenter), Physics, Ecole Normale Superieure and University of Notre Dame, GAUTHIER KRIZMAN, THANANYAN PHUPHACHONG, Physics, Ecole Normale Superieure, GÜNTHER BAUER, GUNTHER SPRINGHOLZ, Institut für Halbleiter- und Festkörperphysik, Johannes Kepler University, GÉRALD BASTARD, ROBSON FERREIRA, LOUIS-ANNE DE VAULCHIER, YVES GULDNER, Physics, Ecole Normale Superieure — Topological crystalline insulators (TCIs) are unique topological systems. Their Dirac surface band structure - tightly linked to the crystal symmetries - can be tuned using a variety of external knobs. By stacking TCI Pb$_{1-x}$Sn$_x$Se in a superlattice of alternating trivial and non-trivial topology, we dramatically enhance the optical response of its topological Dirac states and succeed in demonstrating the tuning of their energy gap with temperature. We use magneto-optical infrared Landau level spectroscopy to probe the band structure of those topological states in MBE grown high mobility TCI/trivial superlattices for magnetic fields up to 15T and temperatures between 4.2K and 200K. By simply varying the sample temperature, we show that one can tune the penetration depth of surface states into the TCI layer and the inter-surface hybridization across this layer. As a result, we observe a tuning of the Dirac gap over a range extending from 5meV to 60meV. We pave the way for further realization of tunable quantum phases using TCI superlattices.

Wilson Loops, Wyckoff Positions, and Wannier Functions: New Developments in Stable and Fragile Topology

BARRY BRADLYN (Presenter), Department of Physics and Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign — The interplay of topology and geometry has been -- and continues to be -- a rich area of study for condensed matter physics. Recently, we have realized that spatial symmetries allow for the stabilization of topological phases much more exotic than those that can be found with time-reversal symmetry alone. Examples include topological crystalline insulators, "hourglass Fermion" phases, and Dirac and double-Weyl semimetals. In this talk, I will review recent developments in the theory of band representations which highlight the role of Wannier functions and holonomy in explaining the origins of topological crystalline behavior. I will show how this relates to several new ideas, such as symmetry indicators, topological phases with high co-dimension boundary states, and the "fragile" topology of isolated groups of bands. Finally, I will discuss how non-symmorphic symmetries can protect novel topological surface states, which can be diagnosed through the holonomy of Bloch functions.
Ultrafast electron imaging and diffraction of non-equilibrium structural dynamics in the charge-density wave system 1T-TaS\textsubscript{2}^* [Invited] CLAUS ROPERS (Presenter), University of Göttingen — Time-resolved electron imaging, diffraction and spectroscopy are exceptional laboratory-based tools to trace non-equilibrium phenomena in materials with a sensitivity to structural, electronic and electromagnetic degrees of freedom. The capabilities of these approaches are largely governed by the quality of the beam of electrons used.

This talk will discuss recent advances made by employing high-coherence ultrashort electron pulses from nanoscale field emitters, which substantially enhance the achievable image resolution in both real and reciprocal space. We have recently developed two complementary experimental techniques with ultimate surface sensitivity and spatial resolution, respectively, namely Ultrafast Low-Energy Electron Diffraction (ULEED) [1] and Ultrafast Transmission Electron Microscopy (UTEM) [2].

These methods are applied to study non-equilibrium dynamics in the prominent charge-density wave (CDW) material 1T-TaS\textsubscript{2} after femtosecond optical excitation. Specifically, we study structural phase transitions between different CDW phases and the optical excitation of fluctuation modes. In one set of experiments, ULEED is used to investigate the transient population of phonons and phase modes (phasons). For the transition between the domain-like nearly-commensurate (NC) CDW phase and the incommensurate (IC) phase, we identify the importance of dislocation-type topological defects in the periodic lattice distortion for establishing long-range phase-order. Finally, a new contrast mechanism for UTEM is developed that allows for ultrafast real-space domain imaging upon the structural phase transition.


*This work was funded by the European Research Council (ERC-StG “ULEED”, Project ID: 639119) and the German Research Foundation (SFB 1073, Project A05).
Ultrafast time-resolved x-ray scattering reveals diffusive charge order dynamics in La$_{2-x}$Ba$_x$CuO$_4$.

Charge order (CO) is ubiquitous in the high-Tc cuprates but its relation to superconductivity is still unclear. While static charge order seems to anticorrelate with superconductivity, charge order fluctuations may favor or enhance Cooper pairing. Here, we investigate the collective CO dynamics in the prototypical cuprate La$_{2-x}$Ba$_x$CuO$_4$ with time-resolved resonant soft x-ray scattering. By suddenly quenching the CO diffraction peak with ultrafast optical pump pulses and probing its recovery in the time domain with resonant soft x-rays, we find that CO excitations in the energy range 0.4-2.0 meV are overdamped and diffusive. At energy scales lower than 0.4 meV, the CO phase exhibits dynamical critical scaling, a universal behavior associated with the propagation of topological defects. Our observations imply that charge order is dynamic and may play a role in establishing superconducting pairing.

*This study was supported by the DOE Office of Science under award no. DE-FG02-06ER46285. Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515. P.A. acknowledges support from the Gordon and Betty Moore Foundation’s EPiQS initiative through grant GMBF-4542. M.M. acknowledges support from the Alexander von Humboldt foundation.

Exploring ideal charge-density-wave in superconducting YBCO via innovative uses of X-ray FEL and the pulsed magnet.

Increasingly compelling evidence of various forms of non-superconducting electronic orders, such as charge/spin density waves (CDW/SDW), in the cuprate high-Tc superconductors has fundamentally altered our understanding of the essential physics of these materials. However, it has been difficult to establish the nature of the quantum (zero-temperature) phases that compete and/or coexist with superconductivity. In order to overcome this difficulty, it is necessary to destabilize superconducting long-range order at low temperatures by a high magnetic field. In this context, we performed x-ray scattering at an x-ray free electron laser (FEL) in the presence of pulsed high magnetic fields. This approach provides us with the new insight to understand the intertwined phenomena between CDW and SC in YBa$_2$Cu$_3$O$_x$ (YBCO) cuprates at magnetic fields, as well as an ideal CDW phase. More details will be touched in this presentation.

*SLAC National Accelerator Laboratory, supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515.
8:00AM X46.00001: Probing Ultrathin Functional Layers and Buried Interfaces with Advanced X-ray Spectroscopic Techniques [Invited] ALEXANDER GRAY (Presenter), Temple University — Rational design of low-dimensional electronic phenomena at oxide interfaces is considered to be one of the most promising schemes for realizing new energy-efficient logic and memory devices. An atomically-abrupt interface between paramagnetic LaNiO3 and antiferromagnetic CaMnO3 exhibits interfacial ferromagnetism, which can be tuned via a thickness-dependent metal-insulator transition in LaNiO3. A rich cation picture, emerging from the polarity mismatch and electronic reconstruction at the interface, is considered to be the driving factor for this phenomenon. Once fully understood, such emergent functionality could turn this Mott-interface system into a key building block for the above-mentioned future devices. In this talk, I will discuss three recent studies, in which we utilized a combination of x-ray spectroscopic and electron imaging techniques to investigate the electronic-structural origins of this emergent phenomenon. Starting with the building blocks of this heterojunction (CaMnO3 and LaNiO3), we used a combination of hard x-ray photoemission (HAXPES) and x-ray absorption spectroscopy (XAS) to establish a direct link between the in-plane strain and the oxygen-vacancy content in CaMnO3 [1]. Then, by using a combination of XAS and scanning transmission electron microscopy (STEM), we examined the nature of the metal-insulator transition in LaNiO3 in the ultrathin limit (<2 u.c.) [2]. Finally, we utilized a combination of HAXPES and standing-wave photoemission spectroscopy (SW-XPS) to demonstrate a depth-dependent charge reconstruction at the LaNiO3/CaMnO3 interface [3]. Our findings suggest a new strategy for designing functional Mott oxide heterostructures by tuning the interfacial cation characteristics via controlled manipulation of thickness, strain, and ionic defect states.


8:36AM X46.00002: Resistive switching in tunnel junctions with a single-crystal La2NiO4 electrode* SHIDA SHEN (Presenter), MORGAN WILLIAMSON, Department of Physics and Texas Materials Institute, University of Texas at Austin, GANG CAO, Department of Physics, University of Colorado-Boulder, JIANSHI ZHOU, Texas Materials Institute, University of Texas at Austin, MAXIM TSOI, Department of Physics and Texas Materials Institute, University of Texas at Austin — We study the resistive switching in tunnel junctions with single-crystal La2NiO4 electrodes. Such electro-resistive devices are promising candidates for future nonvolatile memory and reconfigurable logic applications thanks to their simple structure, scalability and endurance. Our tunnel junctions were prepared by painting a spot of conductive silver epoxy on the surface of La2NiO4 single crystal. The interface between the silver and the semiconducting single crystal served as a natural barrier forming planar normal metal/insulator/semiconductor (N-I-S) tunnel junctions with resistances ranging from a few tens to tens of thousands of Ohms. The current-voltage measurements performed on such junctions at room temperature demonstrated a bias-driven resistive switching with ratios above 1000% and high endurance. In situ measurements with two junctions (N-I-S-I-N) demonstrate the polarity-dependent resistive switching of the two (N-I-S and S-I-N) junctions and show no contribution from the bulk of the La2NiO4 crystal. Such an interfacial nature of the switching phenomenon is promising for fabrication of thin-film planar devices to be used in nonvolatile memory and logic.

*This work was supported in part by NSF grants DMR-1712101 and DMR-1122603 and by KAUST Award No. OSR-2015-CRG4-2626

8:48AM X46.00003: Spontaneous epitaxy of VO and stabilization of interface phase of V2O3 during vanadium metal deposition on SrTiO3 in vacuum AGHAM POSADAS (Presenter), University of Texas at Austin, SUNAH KWON, MOON KIM, University of Texas at Dallas, ALEXANDER DEMKOV, University of Texas at Austin — The deposition of vanadium metal on SrTiO3 results in the spontaneous scavenging of oxygen ions from SrTiO3 to oxidize vanadium to VOx, where x = 0.5-1.2, depending on the temperature. At sufficiently high temperature, the VOx forms as an epitaxial film on both SrTiO3 (100) and SrTiO3 (111). Surprisingly, the oxygen scavenging and epitaxy persist for thicknesses over 300 Å with no sign of degradation. Additionally, when vanadium is deposited on SrTiO3 (111), an interfacial phase of hexagonal V2O3 with 2x2 surface reconstruction is formed, which is stable for three monolayers, before rocksalt VO(111) starts to be formed. We describe the growth process and layer by layer characterization of the films using in situ reflection high-energy electron diffraction (RHEED), x-ray and ultraviolet photoelectron spectroscopy (XPS and UPS), and reflective electron energy loss spectroscopy (REELS), as well as ex situ grazing incidence in-plane x-ray diffraction and cross-sectional scanning transmission electron microscopy.
Tunability of the Metal–Insulator Transition in VO₂/TiO₂ Heterostructures*  
GUOXIANG HU (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, QIYANG LU, ILKKA KYLANPAA, JARON KROGEL, Materials Science and Technology Division, Oak Ridge National Laboratory, PAUL KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory, HO NYUNG LEE, Materials Science and Technology Division, Oak Ridge National Laboratory, PANCHAPAKESAN GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory —  
The metal–insulator transition in strongly correlated vanadium dioxide (VO₂) has attracted considerable interest. It has been shown that formation of oxygen vacancies (VO) in VO₂ can suppress this MIT completely without any structural transition. Since VO can be introduced via tuning the thickness or type of capping oxide layers, in this work, we studied the control of MIT in VO₂ by interfacing with a TiO₂ capping layer. Using a combined approach with experimental measurements and theoretical calculations, we find that a TiO₂ capping layer on an epitaxial VO₂ thin film suppresses the MIT in VO₂. Density functional theory (DFT) calculations, benchmarked against more accurate many-body quantum Monte Carlo (QMC) calculations, provide information on the VO formation energy profile across the VO₂/TiO₂ interface. It is found that the VO₂/TiO₂ interface can facilitate the VO migration from TiO₂ to VO₂, and it is this migration that is responsible for the suppression of MIT in VO₂. Our study highlights the crucial role of VO introduced by a capping layer in tuning the MIT in epitaxial VO₂ thin films, which is useful for developing advanced electronic and ionic devices.  

*This work was supported by the Center for Predictive Simulation of Functional Materials, a DOE-BES center.

Origin of Suppression of Metal-Insulator Transition in Non-Stoichiometric VO₂*  
PANCHAPAKESAN GANESH (Presenter), Oak Ridge National Laboratory, FRANK LECHERMANN, University of Hamburg, ILKKA KYLANPAA, JARON KROGEL, PAUL KENT, Oak Ridge National Laboratory, OLLE HEINONEN, Argonne National Laboratory —  
Rutile (R) phase VO₂ is a quintessential example of a strongly correlated bad-metal, which undergoes a metal-insulator transition (MIT) concomitant with a structural transition to a V-V dimerized monoclinic (M) phase below T_{MIT} ~ 340K. In particular, doping vanadia thin-films with oxygen vacancies (VO) has been shown to completely suppress this MIT without any structural transition[1]. We explain this suppression by elucidating the influence of oxygen-vacancies on the electronic-structure of the R phase VO₂, explicitly treating strong electron-electron correlations using dynamical mean-field theory (DMFT) as well as diffusion Monte Carlo (DMC) techniques. We show that VO's tend to change the V-3d filling away from its nominal half-filled value, with the e^{\pi}_{g} orbitals competing with the otherwise dominant a_{1g} orbital. Loss of this near orbital polarization is associated with a weakening of electron correlations, which removes a charge-density wave (CDW) instability along the V-V dimerization direction above a critical doping concentration, thereby suppressing the metal-insulator transition. Our study also suggests that MIT is predominantly driven by a correlation-induced CDW instability. [1] Phys. Rev. Applied 7, 034008 (2017).  

*This work was supported by CPSFM, a DOE-BES center.

Depth-profiling metal-oxygen hybridization and orbital polarization in isovalent perovskite oxide heterostructures*  
PAUL ROGGE (Presenter), Department of Materials Science and Engineering, Drexel University, PADRAIC SHAFER, Advanced Light Source, Lawrence Berkeley National Laboratory, GILBERTO F L FABBRIS, Advanced Photon Source, Argonne National Laboratory, WEN HU, NSLS-II, Brookhaven National Laboratory, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, MARK DEAN, Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, STEVEN J MAY, Department of Materials Science and Engineering, Drexel University —  
Heterostructures of complex oxides have been successfully deployed to realize new electronic properties, with much of this work motivated by interfacial charge transfer effects that change the local charge density. Here, we synthesized superlattices of the isovalent perovskite oxides SrFeO₃ and CaFeO₃ using molecular beam epitaxy to investigate structural-induced changes in the orbital character of carriers across oxide interfaces while retaining the same nominal charge density. Using resonant x-ray reflectivity at the oxygen K-edge, we demonstrate that the Fe-O hybridization in CaFeO₃ and SrFeO₃ differs and is additionally modified at the interface. Further, using linearly polarized photons we find that the reflectivity at the Fe L-edge is polarization-dependent, which is attributed to strain-induced orbital polarization in the Fe 3d electron orbitals. By modeling the resonant reflectivity, we correlate changes in the Fe orbital polarization with changes in the Fe-O hybridization across the SrFeO₃-CaFeO₃ interface and reveal the presence of a hybridization superstructure.  

*P.C.R. and S.J.M. were supported by the Army Research Office, grant number W911NF-15-1-0133.
SUMMAYYA KOUSER (Presenter), Department of Physics and Astronomy, Vanderbilt University, SAURABH GHOSH, Department of Physics and Nanotechnology, SRM University, JOHN BREHM, Department of Physics and Astronomy, Vanderbilt University, ALBINA Y BORISEVICH, Center for Nanophase Materials Sciences, Oak Ridge National Lab, SOKRATES T PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — Structurally designing materials by combining two or more different materials for realizing interesting emergent properties to target a desired functionality reduces the need for serendipity. One of the nascent strategies for pursuing new acentric compounds focuses on layering centrosymmetric materials in a particular fashion that lifts inversion symmetry while retaining other electronic, magnetic or optical functionalities found in the constituent materials, thus enabling new multiferroics or narrow bandgap polar semiconductors. Here, we formulate an approach to functionalize a polar metal i.e., \((Ca_{1-x}Sr_xFeO_3)_m/(SrFeO_3)_n\) into an insulating ferroelectric constructed from metallic oxide components \(CaFeO_3\) and \(SrFeO_3\). We have investigated several odd and even superlattices with different periodicities (e.g. \(m \times n = 1x1, 2x2, 1x3, 3x1\) etc). We find that the trigger for such a metal-to-insulator (M-I) transition is the disproportionation of the oxidation states of the central Fe ions. We find that appropriate periodicity and cation ordering is critical for the desired transition. The present work opens a door for designing ferroelectrics with tunable energy gaps by inducing controlled M-I transitions.

*This work is supported by DOE grant numbers DE-FG02-09ER46554

CHENYI GU (Presenter), MIN GU, ZHOUSHEN YUAN, YUEFENG NIE, PENG WANG, College of Engineering and Applied Sciences, Nanjing University, XIAOQING PAN, Department of Physics and Astronomy, University of California, Irvine — Charge transfer at complex oxide interfaces can give rise to a rich variety of exotic two-dimensional phenomena. Recently, an antiferromagnetic to nonmagnetic transition was reported at the LaTiO_3/LaFeO_3 interface based on the observation of Ti and Fe valence change by X-ray photoelectron spectroscopy. Nonetheless, a direct spatially resolved measurement with atomic resolution to support the charge transfer truly happens at the interface is lacking. Here, we investigate the valence variations of Ti and Fe at the LaTiO_3/LaFeO_3 interface by a combination of molecular beam epitaxy and aberration corrected scanning transmission electron microscopy. We demonstrate that the charge transfer from Ti to Fe occurs near the interface accompanied by minor cation intermixing, and the charge transfer depth is two unit cells. Our work provides a spatially resolved observation of charge transfer at this interface, and lends significant credence to charge transfer designs in functional oxide interfaces.

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Fundamental Research Funds for the Central Universities (No.020514380136, No.021314380058)

MARTA GIBERT (Presenter), Physik Institut, University of Zurich — Epitaxial heterostructures offer multiple strategies to manipulate the interplay between the different degrees of freedom in transition metal oxides. Interfacial structural and electronic couplings are key to tune the functionalities of these materials and even allow access to novel electronic phases. Perovskite nickelates are interesting materials displaying a metal to insulator transition, with the insulating state characterized by two inequivalent Ni sites. A particular antiferromagnetic order is also stabilized in this low-temperature bond disproportionated state. Through the growth of NdNiO_3/SmNiO_3 superlattices, it will be shown that the existence of a single or double metal-insulator transition temperature can be controlled as function of the layer periodicity. The structural and electronic mechanisms driving this behaviour will be discussed.

Heterostructures also offer large versatility from a synthesis point of view. For example, a double-perovskite heterostructure such as La_2NiMnO_6 can be reproduced as a \((111)_{\text{Lp}}\)-Oriented LaNiO_3/LaMnO_3 superlattices when 1 monolayer-thick layers are considered. The magnetic properties of the high Curie-temperature ferromagnetic La_2NiMnO_6 heterostructure, synthesized both through a thin film and a superlattice approach, will also be presented.
10:36AM X46.00010: Electronic properties of \((001)_{\text{pc}}\) and \((111)_{\text{pc}}\) SmNiO\(_3\)/NdNiO\(_3\) superlattices  
CLARIBEL DOMINGUEZ ORDONEZ (Presenter), University of Geneva, MARTA GIBERT, Physik-Institut, University of Zurich, JENNIFER FOWLIE, SARA CATALANO, University of Geneva, MICHEL VIRET, Service de Physique de l'Etat Condensé, CEA, NICOLAS JAOUEN, Synchrotron SOLEIL, JEAN-MARC TRISCONE, University of Geneva — Rare earth nickelates (R\(\text{NiO}_3\) (RNO), R = rare earth) stand out for their unique metal to insulator transition (MIT) upon reducing temperature (T\(_{\text{MIT}}\)), accompanied by an unusual antiferromagnetic ordering at T\(_{\text{Néel}}\leq T_{\text{MIT}}\). In bulk, NdNiO\(_3\) (NNO) exhibits T\(_{\text{Néel}}\leq T_{\text{MIT}}\), whereas SmNiO\(_3\) (SNO) displays T\(_{\text{Néel}}\leq T_{\text{MIT}}\). It has been shown that the T\(_{\text{MIT}}\) and T\(_{\text{Néel}}\) of the corresponding films can be tuned over a wide temperature range by means of epitaxial strain. Moreover, by growing along the \((111)_{\text{pc}}\) crystallographic direction, one can induce splitting of T\(_{\text{MIT}}\) and T\(_{\text{Néel}}\) over a temperature range never achieved for films grown in the \((001)_{\text{pc}}\)-orientation \([1]\). Here, we adopt a new strategy to study the interfacial matching constraints in R\(\text{NiO}_3\)-based heterostructures and their impact on the electronic properties by growing \((001)_{\text{pc}}\) and \((111)_{\text{pc}}\)-oriented \(\text{m(SNO)/n(NNO)}\)\(_N\) superlattices (SLs). We have found that the T\(_{\text{MIT}}\) and T\(_{\text{Néel}}\) of the whole system depend on the superlattice wavelength (\(\Lambda=m+n\)) with a single T\(_{\text{MIT}}\) for the shortest superlattice period (\(\Lambda\)). In order to understand the evolution of the lattice distortions with the SL periodicities and how interfacial coupling affects T\(_{\text{MIT}}\) and T\(_{\text{Néel}}\), theoretical predictions will be shown. 
\[1\] Catalano et al., APL Materials 3, 062506. (2015)
8:12AM X47.00002: Structural and electronic properties of ferroelectric domain walls in GeTe from first principles* 

DJORDJE DANGIC (Presenter), Tyndall National Institute, Cork, Ireland, ÉAMONN MURRAY, Imperial College London, UK, STEPHEN B FAHY, University College Cork, Ireland, IVANA SAVIC, Tyndall National Institute, Cork, Ireland — Domain walls in ferroelectric oxides can have significantly different properties than their bulk counterparts [1]. This represents a new avenue for the manipulation of material properties for specific purposes. GeTe is a ferroelectric material that is also one of the best performing thermoelectrics, combining beneficial electronic properties with low lattice thermal conductivity [2] and mechanical stability [3]. In this work, we have performed first principles calculations to understand how domain walls affect structural and electronic properties of GeTe. We have identified five different types of domain walls. We find that strong strain-order parameter coupling is present at all of them, which is beneficial for the lattice thermal conductivity reduction. We also show that some of the domain walls are conducting along their planes and insulating out-of-plane. The n- and p-type conduction of these domain walls, discovered in our calculations, presents an opportunity for tuning the electronic transport properties of GeTe for thermoelectric applications.


*This work is supported by Science Foundation Ireland PI Award 15/IA/3160.

8:24AM X47.00003: Investigation of the structural, electronic and thermoelectric properties of GeX (X=S, Se, Te) monochalcogenides* 

AIDA SHEIBANI (Presenter), RAAD HALEOOT, BOTHINA HAMAD, University of Arkansas — Electronic band structure calculations were performed using density functional theory (DFT) for the orthorhombic structure of GeS and GeSe compounds, and the trigonal structure of GeTe. These compounds exhibit a semiconductor behavior with band gaps of 1.23, 0.899, and 0.68 eV for GeS, GeSe and GeTe, respectively. Based on these DFT calculations their thermoelectric properties were obtained using Boltzmann transport theory. Different procedures were adopted to increase the thermoelectric properties of these compounds including doping and lowering the dimensionality.

*This work was supported by Arkansas NASA EPSCOR Research Infrastructure Development (RID) grant number 002276-00001A. The calculations were performed using the High Performance Computer Center at the University of Arkansas.

8:36AM X47.00004: First-principles Study of Phonon Drag Effect in SiGe Alloys* 

QIAN XU (Presenter), JIAWEI ZHOU, TEOHUAN LIU, GANG CHEN, Department of Mechanical Engineering, Massachusetts Institute of Technology — Phonon drag is the effect that Seebeck coefficients of semiconductors are often greatly augmented at low temperatures. Recent works have shown that it is important in many materials' thermoelectric (TE) performance even at room temperature, and the major phonons contributing to phonon drag are with longer mean free path (MFP) and lower frequency than those carrying heat. Meanwhile, the point defects in alloys tend to scatter phonons with short MFP and high frequency. Combining phonon drag with alloying might lead to better low-temperature TE materials.

We perform the first-principles calculations on the $zT$ value of n-type SiGe alloys with different doping levels at different temperatures. We found that phonon drag contributes significantly to the Seebeck coefficient, especially at lower temperatures. The Seebeck coefficient peaks around the composition of Si$_{0.15}$Ge$_{0.85}$ due to band convergence, which agrees with reported experimental data. Our first-principles calculations are able to provide guidelines for the design of better low-temperature TE materials.

*This work is supported partially by DOE EFRC (Grant No. DE-SC0001299, for fundamental studies on thermoelectrics), and partially by DARPA MATRIX program (Grant No. HR0011-162-0041 for supporting its thermoelectrics programs).
Thermoelectric properties of ternary chalcogenides and oxides from first principles calculations

HITOSHI MORI (Presenter), MASAYUKI OCHI, HIDETOMO USUI, KAZUHIKO KUROKI, Osaka University — Several ternary chalcogenide compounds have been reported as high-performance or promising thermoelectric materials. Previous works have shown that AgBiSe₂ and TlSbTe₂ have high ZT values of 1.5 and 0.87, respectively [1,2]. Even though there are many other possible candidates of ternary chalcogenides, thermoelectric properties of most of them have not been reported.

In the present study, in order to narrow down promising candidates, we analyze the thermoelectric properties of 20 chalcogenide and oxide compounds represented as ABCh₂ (Ch = O, S, Se, Te) by using first-principles calculation and Boltzmann equation. We find that the power factor of the compounds composed of A = Li, Na, B = Ga, In, and Ch = O are far higher than those of other compounds, which originates from the favorable electronic structure possessing quasi-one-dimensionality and multi valley degeneracy. It is also revealed that we can control the electrical conductivity along the c-axis by the substitution of A atom.


*This study was supported by JST CREST (Grant No. JPMJCR16Q6) and JSPS KAKENHI (Grant No. JP17K14108).

Lone-pair Driven Thermoelectrics at Room Temperature

SAIKAT MUKHOPADHYAY (Presenter), THOMAS REINECKE, United States Naval Research Laboratory — Identifying materials which offer crystal-like charge transport and glass-like phonon transport for improved efficiency (ZT) of thermoelectric materials has been a challenging task. The complex interrelationship between these competing materials properties makes such materials rare. Here we report a series of new materials with promising thermoelectric properties; ZT ~ 0.8, at room temperature. This superior ZT stems from the high electrical conductivity and ultralow thermal conductivity; k ~ 0.3 W/m-K, as obtained from the two-channel model (phonons + oscillators). The calculated k is mainly dominated by the Einstein oscillators, which is similar to the cases with amorphous materials where mean free paths become comparable with the characteristics atomic bond lengths. Very low-group velocities due to weakly bonded atoms and strong anharmonicity associated with S² lone-pair electrons explain such low-k in these systems.

A search for good semi-metallic thermoelectric materials

MONA ZEBARJADI (Presenter), MAXIME MARKOV, SEYED EMAD REZAEI, SAFOURA NAYEB SADEGHI, KEIVAN ESFARJANI, University of Virginia — Heavily doped semiconductors are the most studied class of thermoelectric materials. The presence of the bandgap breaks the symmetry between electrons and holes, allowing large Seebeck coefficient values which are 2-3 orders of magnitude higher than metals. However, the optimal chemical potential in these materials requires a high level of doping usually larger than 10¹⁹ cm⁻³, resulting in low carrier mobility. Semimetals have properties in between semiconductors and metals with Seebeck coefficient values in between. Since there is no bandgap, the Seebeck coefficient values are small for structures where in electron-hole bands are similar. For example, for Dirac semimetals and at the Dirac point, the Seebeck coefficient is zero. However, if there is a large asymmetry between electron-hole bands (that is there is a large effective mass difference), then the Seebeck coefficient of intrinsic semimetals can be as large as those of heavily doped semiconductors. This combined with large intrinsic carrier mobility, makes semimetals potential thermoelectric candidates. In this talk, I will present our search results for semimetals with large Seebeck coefficient values using first principles calculations.

*National Science Foundation grant number #1653268
Temperature effects on the thermoelectric properties of PbTe: a first-principles study

JIANG CAO (Presenter), JOSE QUERALES-FLORES, AOIFE R. MURPHY, Tyndall National Institute, STEPHEN B FAHY, University College Cork, IVANA SAVIC, Tyndall National Institute — Thermoelectric materials are of intense interest for energy harvesting applications, because they convert waste heat into electricity. PbTe is one of the most efficient thermoelectric materials. It has a direct narrow gap that increases strongly with temperature [1]. Here we study how the temperature dependence of the electronic bands influences the thermoelectric transport properties of PbTe from first principles. The calculated temperature variation of the direct gap accounts for both thermal expansion and electron-phonon coupling [2]. The temperature dependence of the electronic bands is modeled using a two band Kane model. We also build accurate models of phonon bands and electron-phonon scattering from first principles [3]. By solving the Boltzmann equation, we calculate the thermoelectric transport properties of PbTe in very good agreement with experiments. We find that the temperature variation of the direct gap has substantial effects on these properties, leading to a high figure of merit $zT$ over a broader range of doping concentrations at high temperatures.

[2] J. D. Querales-Flores et al, 1809.02643

This work is supported by Science Foundation Ireland PI Award 15/IA/3160.

Electrical and thermal properties of 2D semimetallic transition metal dichalcogenides TiSe2 and ZrTe2

SEYED EMAD REZAEI, SAFOURA NAYEBSADEGHI, MONA ZEBARJADI, KEIVAN ESFARJANI (Presenter), University of Virginia — 2D materials have manifested a variety of interesting electrical and thermal properties. In this work, we have investigated the electrical and thermal properties of semi-metallic TiSe2 and ZrTe2 using density functional theory calculations. The effect of several exchange-correlation potentials on the band structure and thermoelectric properties has been investigated. We have also shown that tensile strain will open a gap and cause a corresponding non-linear change in electrical transport properties of these materials. Finally phonons and thermal conductivity of ZrTe2 were calculated, and its thermoelectric properties assessed.

Thermal Transport of Part-crystalline Part-liquid Materials

WENQING ZHANG (Presenter), Department of Physics, Southern University of Science and Technology — Multi-component materials usually manifest crystal structure with chemical bond hierarchy, exhibiting the part-crystalline part-liquid (PCPL) or part-crystalline part-amorphous state as the emerging candidates of thermoelectric materials. These materials contain at least two different types of sublattices, one crystalline and another one strongly disordered or liquid-like, leading to extremely low lattice thermal conductivity. This talk presents a survey on the general characteristics of the thermal transport in the part-crystalline materials. We also develop an approach to simulate the complex thermal transport process. We also compare the results in Green-Kubo method and Boltzmann transport theory to elucidate the thermal conductivity of PCPL materials by using empirical interatomic potentials fitting to the liquid-like thermoelectrics like Cu2Se. The contribution to thermal transport from each structural component, i.e. the rigid-crystalline, strongly disordered, and/or liquid-like parts, are respectively analyzed, and the underlying mechanism is elucidated. Based on the observation, a general trend about the thermal transport in a large group of materials is analyzed. Relationship to minimum thermal conductivity is also discussed.

*NSF of China, Guangdong Province Team Project, and Shenzhen-city Scholarship

Abstract Withdrawn
10:36AM X47.00012: First principles study on the thermoelectric properties of delafossite compounds

HIDETOMO USUI (Presenter), KAZUHIKO KUROKI, Osaka University — Thermoelectric materials should have the coexistence of large power factor $PF = \sigma S^2$ and low thermal conductivity for the enhancement of thermoelectric efficiency. It is however difficult to obtain good thermoelectric materials because the power factor is maximized at a certain doping level due to the relationship between the Seebeck coefficient and the electrical conductivity. We proposed that the "pudding mold type band", which has a flat portion at a band edge gives rise to large power factor [1,2].

Recently, PtCoO$_2$ has been found to possess extremely small resistivity and high mobility.[3] The electronic band structure of PtCoO$_2$ exhibits the pudding mold type shape, which suggests the possibility to possess large thermoelectric performance. We study the thermoelectric properties of PtCoO$_2$ from first principles calculations within the Boltzmann transport theory and the rigid band approximation. It is found that the power factor can be enhanced due to high mobility by controlling the carrier concentration.


10:48AM X47.00013: First-principles study of LaOBiPbS$_3$ and its analogous compounds as thermoelectric materials

KEIYA KUREMATSU (Presenter), MASAYUKI OCHI, HIDETOMO USUI, KAZUHIKO KUROKI, Department of Physics, Osaka University — LaOBiPbS$_3$ is a kind of pnictgen-dichalcogenide layered compounds, which have recently been investigated as thermoelectric materials owing to their low thermal conductivity and high controllability of constituent elements [1, 2]. However, thermoelectric performance of LaOBiPbS$_3$ is not very high and that of its analogous compounds is still unknown. In this study, we theoretically investigate the thermoelectric property of LaOBiPbS$_3$ and its analogous compounds: LaOPnTtCh$_3$ ($Pn = As, Sb, Bi$; $Tt = Sn, Pb$; $Ch = S, Se$). We find that there are two key factors for increasing thermoelectric performance: one is the spin-orbit coupling, mainly controlled by $Pn$, and the other is the hybridization between $Pn$ in the $PnS_2$ layer and $Ch$ in the rock-salt layer, which determines the gap size. In fact, we find that LaOSbPbSe$_3$, which optimizes these key factors but has not been synthesized yet, can have a power factor that is about 5 times as large as that of the known compound LaOBiPbS$_3$.

Reference:

*This work was supported by JST-CREST Grant Number JPMJCR16Q6 and JSPS KAKENHI Grant Numbers JP17H05481, JP17K14108.

Friday, March 8, 2019 8:00 AM - 10:36 AM

Session X48 GSNP: Statistical and Nonlinear Physics I

Focus
8:00AM X48.00001: Interlocking of Sheared Non-convex Hexapods* YUCHEN ZHAO (Presenter), Department of Physics, Duke University, Durham, NC, USA, JONATHAN BARÉS, Laboratoire de Mécanique et Génie Civil, Université de Montpellier, CNRS, Montpellier, France, ROBERT P BEHRINGER, Department of Physics, Duke University, Durham, NC, USA — Packings of non-convex or elongated particles can form free-standing structures like walls or arches, due to particle interlocking effects leading to geometric cohesion. Interlocking effects have been studied for various particle shapes and aspect ratios, but the microscopic origins of the stabilization of rigid structures remains unclear. We report on experiments on hexapods that consist of three orthogonal sphero-cylinders, whose centers are bonded at one origin. The diameter and lengths of the sphero-cylinders are 3, 10, 20 and 30 mm, respectively. We subjected aggregates of spheres or hexapods to quasistatic direct shear and developed novel techniques to measure structural information such as particle positions, orientations, and bending. For spheres and 10 mm hexapods, we observed plasticity phenomena consistent with the Mohr-Coulomb model. For 20 and 30 mm hexapods, however, we observed strain-stiffening during shear. By analyzing X-ray microcomputed tomography data collected during the shearing process, we found that the onset of strain-stiffening is associated with particle bending and that particles that bend significantly tend to be aligned with the compression direction of the shear.


8:12AM X48.00002: Study of Electrical Percolation in CrO$_2$/Cr$_2$O$_3$ nanoparticle composite system SHIVA POKHREL (Presenter), BRENDON WATERS, EHAB H ABDELHAMID, ZHI FENG HUANG, BORIS NADGORNY, Wayne State University — Percolation is a random probabilistic process that triggers a phase transition in disordered systems. In this work we investigate the classical percolation behavior in a CrO$_2$/Cr$_2$O$_3$ half-metal/insulator composite system. Cr$_2$O$_3$ was obtained by annealing of CrO$_2$ powder in air; composite samples with varying volume fraction were prepared by mixing Cr$_2$O$_3$ with CrO$_2$. The percolation threshold and the power law scaling exponent near the threshold were identified by studying the changes in the electrical resistance of the pellets with different volume fractions. Experimental results are compared with theoretical calculations, which were carried out via the combination of mechanical contraction method and Monte Carlo simulations for this binary composite system of non-overlapping hard spherocylinders.

8:24AM X48.00003: Robotic active matter on a deformable surface generates an analog gravity system SHENGKAI LI (Presenter), YASEMIN OZKAN AYDIN, CHARLES XIAO, Georgia Institute of Technology, GABRIELLA H SMALL, Physics and Astronomy Department, Swarthmore College, JENNIFER RIESER, PABLO LAGUNA, DANIEL GOLDMAN, Georgia Institute of Technology — Many analog gravity models of general relativity (GR) have been developed (e.g. in fluids and Bose-Einstein condensates) with goals to probe GR-like phenomena in the laboratory. One common analog is to study the dynamics of freely moving objects (like marbles) on two-dimensional curved or elastic sheets. Such systems have issues which prevent them from functioning as analog gravity models, including dominance of Earth's gravity over metric dynamics, the inability to model time-like curvature effects, and dissipation which limits persistent dynamics. Here, we circumvent these issues by developing an exact analog gravity system based on an active matter system: a robot car driving on a deformable membrane. We observe qualitative GR-like features including circular and precessing orbits around a central depression. We extract a dynamical system that describes our experiments. Remarkably it is the self-propelled aspects of the car that allow a formal mapping to Einstein's equations in 2+1 dimensions, thus creating an accurate GR model whose parameters can be tuned to mimic different astrophysical situations (e.g. Schwarzschild metric around a black hole).

8:36AM X48.00004: Membrane Diffusivity Driven Microtubule-Based Active Nematics* JOSEPH LOPES (Presenter), LINDA S. HIRST, AMANDA TAN, University of California, Merced — Biomimetic systems formed from active nematics provide important insights into how far-from-equilibrium materials can demonstrate assembly, motion, and replication. Active nematics produce collective motion through the interaction between moving particles. Here we couple motor proteins to a lipid membrane and perform gliding assays with dense microtubule populations. We observe the formation of an active nematic phase during gliding, driven by the microtubules propensity to not cross each other when bound to a diffusive surface. In the dilute case microtubules will coalesce into bundles for short term durations, and as density is increased the physical anisotropy of the microtubules forces the formation of the nematic phase. The lipid membrane is a tunable surface that can be deposited on a variety of geometries making this a promising system for the development of more complicated active matter investigations.

*NSF-CREST: Center for Cellular and Biomolecular Machines at UC Merced (NSF-HRD-1547848) NSF DMR 1808926
Dendritic crystal growth of ammonium nitrate from aqueous solution  ANDREW DOUGHERTY (Presenter), Lafayette College — Dendritic crystal growth is an important example of nonequilibrium pattern formation that involves both nonlinear and noise-driven effects. The resulting large-scale structures are sensitively dependent on relatively small effects, such as surface tension, and on small anisotropies in those quantities. In this work, we report new results for the dendritic growth of ammonium nitrate from supersaturated aqueous solution. This system has been studied previously by van Driel et al.[1] and shown to exhibit several different morphologies, including both steady state dendritic growth and a state with persistent tip-splitting behavior. Specifically, we present new measurements of the tip radius \( r \), growth speed \( v \), and sidebranch spacing \( \lambda \), along with initial estimates of the product \( Dd_0 \), where \( D \) is the chemical diffusion constant and \( d_0 \) is the capillary length. We then compare the resulting estimate of \( \sigma^* = 2 d_0 D / v r^2 \) with the values for other materials and with theoretical expectations.


Twisted states in low-dimensional hypercubic lattices* YOUNG SUL CHO (Presenter), SEUNGJAE LEE, HYUNSUK HONG, Chonbuk National University — Twisted states with non-zero winding numbers have been observed in a ring composed of sinusoidally coupled identical oscillators. In this presentation, we consider finite-sized \( d \)-dimensional hypercubic lattices, namely square \((d=2)\) and cubic \((d=3)\) lattices with periodic boundary conditions. For identical oscillators, we observe new states where the oscillators belonging to each line (plane) for \( d=2 \) (\( d=3 \)) are phase synchronized with non-zero winding numbers along the perpendicular direction. We note that these states can be reduced into twisted states in a ring with the same winding number if we regard each subset of phase-synchronized oscillators as one single oscillator. For nonidentical oscillators, we observe similar patterns with slightly heterogeneous phases in each line \((d=2)\) and plane \((d=3)\) for random configurations.

*This work was supported by the NRF Grants No. 2017R1C1B1004292 (Y. S. C) and No. 2018R1A2B6001790 (H. H).

Drainage through holes drives Arctic sea ice melt ponds to the critical percolation threshold* PREDRAG POPOVIC (Presenter), MARY C SILBER, DORIAN S ABBOT, University of Chicago — During the summer, vast regions of the Arctic sea ice are covered by meltwater ponds that significantly lower the ice reflectivity and accelerate melting. Ponds develop over the summer melt season through an initial stage of rapid growth followed by drainage through macroscopic holes. Recently, we showed that ponds after drainage resemble percolation clusters near a critical percolation threshold. Here, we explore the physical mechanism behind this previously-unrecognized constraint on pond evolution. We show that organization towards the percolation threshold is a consequence of pond drainage through macroscopic holes. The threshold sets the upper limit and scales the pond coverage throughout its evolution after the beginning of drainage. Furthermore, we show that, after rescaling, pond coverage fraction as a function of number of open holes follows a universal curve. This curve governs pond evolution during and after pond drainage, which allows us to formulate an equation for pond coverage evolution that captures the dependence on ice properties.

*This work was supported by the NSF under award number 1623064 and NASA Earth and Space Science Fellowship.

Disconnectivity graphs in planted spin-glass problems KATJA BISWAS (Presenter), HELMUT KATZGRABER, Physics, Texas A&M University — A disconnectivity graph is a simplified representation of a high-dimensional energy landscape consisting of low-energy pathways between different minima in the landscape. As such, one can use disconnectivity graphs to obtain insights into the accessibility of different minima in the energy landscape, and therefore make predictions for the computational effectiveness of different optimization methods. In this talk different disconnectivity graphs for different planted spin-glass problems are presented, and their similarities and differences discussed.

Floating elastic membrane in rotation : shape of interface and wrinkling instability LUCIE DOMINO (Presenter), Laboratoire PMMH, ESPCI Paris, DOIREANN O’KIELY, DOMINIC VELLA, University of Oxford, ANTONIN EDDI, Laboratoire PMMH, ESPCI Paris — When rotated at constant speed, the surface of a liquid takes the well known shape of a parabola. If the surface of the liquid is covered with a thin elastic membrane, the force balance is modified, which changes the obtained shape. We study the influence of the elastic properties of the membrane on this shape, and compare with experiments. We also report the apparition of a buckling instability at the edges of the floating membrane : radial creases appear and grow closer to the center as rotation speed is increased.
Geometric Stiffening and Softening of an Indented Floating Thin Film

MONICA RIPP (Presenter), Physics, Syracuse University, VINCENT DÉMERY, Physics, Université de Lyon, TENG ZHANG, Mechanical and Aerospace Engineering, Syracuse University, JOEY PAULSEN, Physics, Syracuse University — Thin sheets can behave nonlinearly while the local material response is purely linear. We separate two distinct mechanisms for geometric nonlinearities by studying the normal-force response of an indented polymer film on a liquid bath, using experiments, simulations, and theory. First, we show that the force reaches a plateau at large indentation, causing the effective spring constant of the system to soften, and we use a simple geometric model to capture this behavior at large slopes [1]. Then, we map out the full phase diagram at small slopes, supporting recent predictions [2] that the system stiffens out of the typical linear response for small deflections. Our results provide a prototypical example of how multiple distinct geometric nonlinearities may arise under monotonic driving.


Support from NSF-DMR-CAREER-1654102 and NSF-IGERT-1068780 is gratefully acknowledged.

Simulating the dynamics of actuated thin elastic sheets

SILAS ALBEN (Presenter), ROBERT D. DEEGAN, ALEX A. GORODETSKY, University of Michigan — We develop a method to simulate the dynamics of thin elastic sheets under time-dependent external or internal forces, e.g. contact forces, temperature change, or chemical reactions within the sheet. The dynamics are difficult to simulate efficiently due to numerical stiffness resulting from the in-plane stretching term in the elastic energy. We present a semi-implicit time discretization that allows the dynamics to be simulated stably with essentially no time-step constraint, allowing for fast simulations. We show examples for thin sheets, bilayers, and models of active gel materials, using different spatial geometries and different types of spatial discretizations.

We acknowledge support from the Michigan Institute for Computational Discovery and Engineering (MICDE).

Damage propagation in a model cohesive granular medium

MARIE-JULIE DALBE (Presenter), NICOLAS VANDENBERGHE, EMMANUEL VILLERMAUX, IRPHE, Aix-Marseille University, CÉDRIC BELLIS, LMA, CNRS — Understanding how a crack propagates in a heterogeneous medium is essential in numerous fields, since this process can lead to catastrophic events. The opening of a crack can lead to the emission of an elastic wave, which can interfere with the rest of the material, and provide energy to open new cracks. In particular, in a brittle material, the critical stress leading to rupture is different from one experiment to another. This is usually imputed to the presence of defects, which are weaker points in the material, making crack propagation easier. The interaction of the elastic waves emitted by a crack opening, and existing defects is still not fully understood.

We study a model material made of a monolayer of glass grains attached by individual elastic bridges. Using a high-speed camera, we can follow the propagation of elastic waves in this material as well as the crack opening dynamics. We can in particular observe the interaction of existing cracks and defects.

Mechanism of large-scale flow reversals in turbulent thermal convection

YIN WANG (Presenter), Department of Physics, Hong Kong University of Science and Technology, PIK-YIN LAI, Department of Physics, National Central University, Taiwan, HAO SONG, 3College of Physics and Energy, Shenzhen University, P. R. China, PENGER TONG, Department of Physics, Hong Kong University of Science and Technology — We report a new kind of convective instability for turbulent thermal convection in a closed thin disk cell. It is found that the convective flow stays over a long steady “quiet period” having a minute amount of heat accumulation, followed by a short and intermittent “active period” with a massive eruption of thermal plumes to release the accumulated heat. The rare massive eruption of thermal plumes disrupts the existing large-scale circulation across the cell and resets its rotational direction. The distribution function of the plume eruption amplitude is found to follow the generalized extreme value statistics with an upper bound, which changes with the physical properties of the convecting fluid. The experimental findings have important implications to many closed convection systems of geophysical scale, in which massive eruptions and sudden changes in large-scale flow pattern are often observed.

This research was supported by the Research Grants Council of Hong Kong SAR.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X49 DPOLY: Charged and Ion-Containing Polymers BCEC 252A - Di Jia, Khatcher Margossian, University of Massachusetts, Amherst
The increasing environmental concerns and global warming, attributed to conventional energy production, have motivated researchers to scout for clean energy harvesting (EH) strategy from pollutant-free and natural energy resources. Inspired by naturally occurring mechnano-electroactive materials, flexo-ionic devices consisting of a flexible solid polymer electrolyte membrane (PEM), consisting of an ionic compound and a polymer matrix host, laminated between two compliant carbonaceous electrodes were developed. The laminated flexo-ionic PEMs can generate electrical potential and current via ion diffusion/polarization by subjecting the PEM assembly under mechanical deformation. By varying cation sizes and valencies of ionic compounds in the development of these PEMs, the effects of ion size and valency on flexoelectric properties (i.e. output voltage and current/polarization), ionic conductivity, viscoelastic and mechanical properties were investigated as a function of ion concentration and mode of mechanical stimuli involving intermittent square (low frequency) and dynamic oscillatory (high frequency) displacement. The synergic effect of these factors and their roles in mechano-electrical energy conversion will be discussed.

*Supported by NSF-DMR-Polymers #1502543

The present article describes a novel phenomenon of polarity flipping during mechano-electrical energy conversion subjected to bending deformation of flexible polymer electrolyte membranes (PEM), which were originally developed for polymeric ion conductors in solid Li-ion batteries. This bending induced electrical polarization is analogous to flexoelectricity found in insulators and dielectric materials. However, the basic principle of flexoelectricity in PEMs operates based on electrical energy generation driven by ion polarization/depolarization across the PEM subjected to a pressure (or stress) gradient during bending. The observed flexoelectric coefficient (~323 μC/m), i.e., a measure of the converted mechano-electrical energy, is the highest among all flexoelectric materials hitherto reported. Of particular importance is that the present work is the first to demonstrate the occurrence of polarity switching, i.e., reversal of the polarization direction with increasing succinonitrile (SCN) concentration, attributable to changing ionic size of solvated Li-SCN complexes.

*Supported by NSF-DMR-Polymers #1502543

Coating lithium anode with flowable polymer layer may effectively suppress lithium dendrite growth at high current density.[1] Although the underlying mechanism is poorly explored, the sensitivity on dielectric permittivity and thickness of the polymer layer has been identified.[2] A coarse-grained simulation of lithium deposition in presence of polymer coating, which explicitly incorporates the dielectric heterogeneity, is presented. It was found that the more effective coatings are more adaptable, have modest elasticity, and maintain integrity during deposition. Higher polymer dielectric permittivity and coating thickness inhibit the growth of dendrite, but inevitably sacrifice battery performance.


*This research has been supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U.S. Department of Energy through the Advanced Battery Materials Research (BMR) Program (Battery500 Consortium).
Ion Transport in Well-Aligned Block Copolymer Electrolytes*

PETER BENNINGTON (Presenter), DANIEL SHARON, MOSHE DOLEJSI, PAUL F NEALEY, SHRAYESH PATEL

Institute for Molecular Engineering, University of Chicago — The independently tunable electrical and mechanical properties of block copolymer electrolytes (BCPEs) makes them attractive candidates for ion exchange membranes. However, these materials often show a lower conductivity even after accounting for the reduced volume fraction of the conducting phase. This reduction in conductivity has been ascribed to the tortuosity of the conducting pathways, poorly connected domains, grain boundaries, and low mobility near the BCP interface. It is often difficult to differentiate these nanoscale hinderances to transport in microns-thick membranes due to the inability to fully control the orientation of the BCP domains. Here, we present a new approach to this problem wherein we can fully align the conductive domains of a BCPE along the direction of the electric field produced by interdigitated electrodes (IDEs), thus enabling us to divorce morphological from molecular-level effects. We observe that a low mobility region near the block copolymer interface might explain the lower conductivity of BCPEs compared to an equivalent volume fraction of homopolymer electrolyte.

*We gratefully acknowledge support by U.S. Department of Energy, Basic Energy Sciences, Argonne National Laboratory, Materials Sciences and Engineering Division.

Phase Behavior of Salt Doped A/B/A-B Ternary Polymer Blends*

SHUYI XIE (Presenter), EN WANG, DANIEL J MEYER, TIMOTHY LODGE

University of Minnesota — The phase prism of a pseudoternary polymer blend system containing low molar mass poly(ethylene oxide) (PEO) and polystyrene (PS) homopolymers, a PS–PEO block copolymer (SEO), and lithium bis(trifluoromethanesulfonamide) (LiTFSI) is constructed. The addition of salt increases the segregation strength, and thus causes both macroscopic and microscopic phase separation. The phase behavior of the ternary system is studied in detail, including isothermal slices at different temperatures and isopleths with different phi_PEO/phi_h ratios. Also, a bicontinuous microemulsion (BμE) channel is located, and the structure as a function of salt concentration and temperature is investigated. Moreover, the congruency condition near the BμE channel will be discussed. This work may serve as a benchmark for experimental design of polyelectrolyte systems with tunable ionic conductivity and high mechanical modulus and help understand the physics underlying the structure and dynamics of ion-containing A/B/A-B ternary blends.

*This work was supported by the Office of Basic Energy Sciences (BES) of the U.S. Department of Energy (DoE), under Contract DE-FOA-0001664.

Detection of the Order-to-Disorder Transition in Block Copolymer Electrolytes Using Quadrupolar 7Li NMR Splitting*

LORENA GRUNDY (Presenter), GURMUKH SETHI, MICHAEL GALLUZZO, NITASH BALSARA

Chemical and Biomolecular Engineering, University of California, Berkeley — Mixtures of block copolymers and salts have been studied for use as safe electrolytes for batteries with energy-dense lithium metal anodes. Locating the order-to-disorder transition (ODT) in these systems is important, because microscopic morphology has a profound impact on bulk properties including ionic conductivity and mechanical rigidity. In this study, the ordered morphologies in a series of mixtures of polystyrene-\(\text{b}\)-poly(ethylene oxide) and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) salt are shown to be aligned due to exposure to the magnetic field in an NMR instrument, which is confirmed using small-angle X-ray scattering (SAXS). This alignment results in quadrupolar triplet peak splitting in \(^7\text{Li}\) NMR, which disappears above the \(T_{\text{ODT}}\). The \(T_{\text{ODT}}\) identified using this novel NMR method is consistent with that determined using SAXS.

*Funding for this work was provided by the National Science Foundation through Award DMR-1505444. Small Angle X-Ray scattering work at the Advanced Light Source was supported by contract no. DE-AC02-05CH11231. Work at the Stanford Synchrotron Radiation Light Source at SLAC National Accelerator Laboratory was supported by contract no. DE-AC02-76SF00515. NMR work was supported by the UC Berkeley College of Chemistry NMR Facility.
9:12AM X49.00007: Counterion condensation and ionic conductivity in microphase separated block copolymer electrolytes*  CHRISTOPHER ARGES (Presenter), QI LE, KE LE, REVATI KUMAR, Louisiana State University — Ion-conducting polymer electrolytes are central components to many types of electrochemical cells spanning batteries, fuel cells, and water purification units. Ionic conductivity is an important property of these materials as it controls the thermodynamic efficiency of electrochemical systems. Many studies correlate micro-structure attributes of polymer electrolytes to ionic conductivity. However, the impact of counterion condensation, a proxy for the extent and strength of ion-pairing, on ionic conductivity has received less attention and its impact on ionic conductivity is not clearly known. This talk highlights our effort to study counterion condensation in thin film ion-conducting block copolymer electrolytes with precisely defined microstructures. Ionic conductivity and 2D AFM force mapping, combined with all-atomistic molecular simulations, substantiate that microphase separated block copolymer electrolytes are less prone to counterion condensation resulting in lower resistances to ionic charge transport. These findings motivate future studies to probe counterion condensation in precisely defined block copolymer electrolyte microstructures as function of solvation and charge density.

*U.S. Department of Energy Office of Basic Energy Sciences Award #DE-SC0018989

9:24AM X49.00008: Compositionally Asymmetric Block Polyelectrolyte Morphologies*  SEBASTIAN RUSSELL (Presenter), ALAN C WEST, OLEG GANG, Chemical Engineering, Columbia University, MONICA OLVERA DE LA CRUZ, Material Science and Engineering, Northwestern University, LUIS M. CAMPOS, Chemistry, Columbia University, SANAT KUMAR, Chemical Engineering, Columbia University — The delicate balance of (short ranged) enthalpic interactions and entropic factors direct the self-assembly in nonionic diblock copolymers (BCPs) which is exploited in a broad range of applications, e.g., lithography, energy storage, membrane separations, and optics. We demonstrate that such behavior is profoundly altered when one block carries a charged trisaminocyclopropenium (TAC) ion at each monomer. These charged-neutral copolymers (CNBPs) display strongly asymmetric morphology maps with the unique aspect that the minority component, the charged block, has a strong propensity to form the continuous matrix. Such observations, coupled with the unexpectedly low TAC dielectric constant (~2.5) lead us to postulate that the CNBP morphology is strongly modified by long-range electrostatics. This conjecture is verified by detailed geometric calculations and quantitatively captured by a simplistic scaling model derived from surfactant self-assembly principles. This fundamental insight into the role of strong electrostatics on CNBP self-assembly has attractive implications for ion transport in polymeric media while simultaneously improving their mechanical properties.

*LMC thanks the NSF (NSF CAREER DMR-1351293) for funding.

9:36AM X49.00009: Mechanisms of Ion Diffusion as a Function of Microstructure in Ionomer Melts  JONATHAN BOLLINGER (Presenter), MARK STEVENS, AMALIE FRISCHKNECHT, Sandia National Laboratories — Understanding how the mechanisms and relative rates of ion transport depend on melt morphology and polymer architecture is a fundamental issue in ionomers. The low dielectric constant of the polymer backbone drives microscale aggregation of charged-groups and counterions, which can greatly impact ion conductivity. For some melts, aggregates can percolate and provide pathways for free ions to move independent of polymer dynamics; in other cases, isolated aggregates are favored and transport happens through infrequent collision-exchange events. We perform molecular dynamics simulations of coarse-grained ionomer melts that span these morphologies to understand charge mobility as a function of polymer architecture and background dielectric constant. For percolated networks, counterion diffusion depends weakly on these variables and results from discrete step motions along more static pathways of bound charged-groups. In contrast, charge mobility varies widely for systems that form clusters as the probability of ion exchanges is sensitive to the length scale and dielectric nature of the polymer-backbone regions between clusters. We explicitly measure the time scales of these distinct mechanisms and show that they directly underlie diffusion coefficients of the charged species.

9:48AM X49.00010: Structural and Dynamical Properties of Water and Salt ions in Confined Geometries of Block Copolymers  DIPAK ARYAL (Presenter), RITUPARNA SAMANTA, VENKATRAGHAVAN GANESAN, University of Texas at Austin — Understanding the transport properties of water and salt ions in confined geometries of block copolymers is crucial for water purification including others nanotechnology and biotechnology. Here, we investigate the local diffusivities along with supporting structural properties of water and salt (Na⁺ and Cl⁻) ions in the different regions from the pore with varieties of sizes made by morphologies of liner triblock copolymers such as lamella, cylinder, and gyroid using dissipative particle dynamics (DPD) mesoscale simulations. Besides, we extend our study to investigate the water and salt permeability through the membranes. Our results suggest that diffusivities of water and salt ions in the different region of pores are different than in the bulk phases. Under the confined conditions, the mobility of water and salt ions are perturbed by the additional interaction forces that arise from the blocks that have preferable water selectivity, which ultimately reduces the local molecular diffusion. Further, the geometries of block copolymers with different sizes of pore also influence the structural and dynamical properties of water and salt ions.
10:00AM X49.00011: Phase Separation of Polymer Mixtures with Highly Concentrated Ions  ISSEI NAKAMURA (Presenter), Physics, Michigan Technological University — The fluctuation of electrostatic potentials and the dielectric contrast between species often play a crucial role in the liquid-liquid phase separation of electrolytes, but the effect of correlation between the two on the phase behavior remains elusive. Accordingly, we develop a Ginzburg-Landau theory that simultaneously accounts for the two effects for liquid mixtures containing polymer and ionic liquid. Our theory suggests that both effects can be equally important to consider the trend of the phase boundary of the liquid-liquid phase separation involving highly concentrated ions. Moreover, our present results of ionic liquids compare favorably with those calculated by the Gaussian approximation (or the one-loop expansion) of self-consistent field theory. We also show that a comparison between theory and experiment suggests that the fluctuation effect may also be significantly suppressed in ionic liquids. <div class="grammarly-disable-indicator"> </div>

10:12AM X49.00012: Effects of Molecular Polarity and Polymerization on Ion Solvation in Polymer Melts  CAMERON SHOCK (Presenter), ISSEI NAKAMURA, Physics, Michigan Technological University, MARK STEVENS, AMALIE FRISCHKNECHT, Sandia National Labs — We study the solvation energy of ions in polymerized and non-polymerized dipolar solvents using molecular dynamics simulations. We use a coarse-grained Stockmayer fluid model to observe the effects on solvation energy for monovalent, divalent, and trivalent ions due to varying solvent dipole moments. We show that increasing polymer chain lengths leads to significantly more negative solvation energies of ions. This is because in polymerized solvents, chain connectivity leads to higher local packing fraction of solvent dipoles near the ion and hence a stronger dielectric response. Also, there is a substantial difference between simulation results and the predicted Born solvation energy using Onsager theory for dielectrics. We hypothesize that the compressibility of solvents and local dipolar structure are key to understanding the difference between simulated and predicted results.

10:24AM X49.00013: Peering into Phase-Separated Perfluorinated Sulfonic-Acid Ionomers with Energy-Tunable X-rays  GREGORY SU (Presenter), ISVAR CORDOVA, AHMET KUSOGLU, CHENG WANG, Lawrence Berkeley National Laboratory — Ion-containing polymers such as perfluorinated sulfonic-acid (PFSA) ionomers play a critical role as the ion-conducting electrolyte in various electrochemical energy devices such as polymer-electrolyte fuel cells, redox flow batteries, and solar fuel generators. The ion transport properties in PFSA are controlled by the nanoscale phase-separation of hydrophilic and hydrophobic domains. Next-generation membranes leverage new chemistries that enable good conductivity without requiring high relative humidity. As with well-studied PFSA like Nafion, understanding the structure-property relationships in these new materials is critical to optimizing performance. Here, synchrotron X-rays with energies tuned to the sulfonic-acid functional group provide enhanced contrast to reveal the phase separation in dry and wet PFSA membranes with various chemistries. These studies elucidate connections among molecular architecture, morphology and transport properties that can be used as design rules for ionomer membranes and highlight the capabilities of X-rays to understand structure and chemistry in ion-containing polymers in general.

10:36AM X49.00014: Macroion Complexation and Conformation of Neutral Polymer in Solution  MANUELA FERREIRA (Presenter), BENXIN JING, YINGXI ELAINE ZHU, Chemical Engineering, Wayne State University — Unusual electric charging and conformational behavior of neutral polymers, such as poly (ethylene oxide) (PEO), in polar solvents have been reported in the past. To further explore the charging mechanism, we compare the effect of simple small ions and multivalent macroions on the electrical potential and conformation of PEO in solutions of varied polarity. Measured electrical potential indicates that multivalent macroions can effectively bind with PEO to cause significant increase of the effective charges of a PEO chain, which is accompanied with the collapse of PEO chain in polar solvents as determined by single-molecule laser spectroscopy. In contrast, little change of PEO electrical potential and conformation is observed with lithium salt added solutions. More interestingly, as further increasing macroion concentration, unconventional liquid-liquid separating coacervate complexation is observed with macroion-added PEO solution, leading to a facile process of PEO-based ionomers.

10:48AM X49.00015: Diffusion of Charged Macromolecules under Strong Electric Repulsion*  KUO CHEN, JINGFA YANG, JIANG ZHAO (Presenter), Chinese Academy of Sciences — The complicity of diffusive motion of individual charged macromolecules under strong electrostatic interaction has been puzzling for decades. As an effort to explore the mystery, diffusion of polyelectrolyte molecules is investigated at single molecular level. By dual-color fluorescence correlation spectroscopy, the diffusion of different sodium polystyrene sulfonate (NaPSS) molecules is discriminated and their mutual correlation demonstrates the strong coupling of the diffusion of different molecules, leading to the abnormal diffusion of individual NaPSS molecules. After the proper correction of the correlation function, the self-diffusion of NaPSS demonstrates a two-stage feature – a fast and slow diffusion modes. The results have exposed a new species in the multiple diffusion modes in polyelectrolyte solution.

*Financial support by National Natural Science Foundation of China is appreciated.
**8:00AM X50.00001: Rapid and non-destructive optical patterning of conjugated polymers for device applications**

[Invited] ADAM MOULE (Presenter), IAN E. JACOBS, JUN LI, ZAIRA I. BEDOLLA VLDEZ, TUCKER L. MURREY, University of California, Davis — A significant obstacle for the industrial development of organic electronic devices is the lack of a patterning technology having the disruptive power that photolithography exerted in traditional microelectronics. Here we present a new scalable patterning technology for organic semiconductors that takes advantage of the existing photolithography infrastructure and is compatible with digital direct-write patterning and sequential roll-to-roll (R2R) solution coating. The Moule group works on a series of solubility control techniques including the use of marginal solvents and polymer doping, that reduce the solubility of polymers at room temperature, but allow patterning at elevated temperatures. Using these techniques, we are able to **vertically stack** and **laterally pattern** mutually soluble polymer layers, which are vital processing steps needed to expand the use of organic semiconductors in device applications. Optimization of these techniques has yielded diffraction limited film patterning with regular features of 200-300 nm with only solution processing steps and direct write laser patterning. We have also recently shown that vertically patterned layers are stable, even with solvent exposure times of hours. This presentation will cover the fundamentals of optical patterning of organic semiconductors and delve into details of how to create doped microdomains, dopant diffusion, and the relationship between polymer crystallinity, dopant diffusion rate, and pattern fidelity.

*Early work on this project was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Award No. DE-SC0010419. Since September of 2016, this project was supported by the U.S. National Science Foundation Scalable Nanomanufacturing Award No. 1636385.

**8:36AM X50.00002: Branched Side Chains Influence the Efficacy of Doping in Conjugated Polymers**

ELAYNE THOMAS (Presenter), Materials Department, University of California, Santa Barbara, EMILY C DAVIDSON, Department of Materials Science and Mechanical Engineering, Harvard University, REIKA KATSUMATA, Polymer Science and Engineering, University of Massachusetts, Amherst, RACHEL SEGALMAN, Materials Department and Department of Chemical Engineering, University of California, Santa Barbara, MICHAEL L. CHABINYC, Materials Department, University of California, Santa Barbara — The principles that govern effective charge transfer between dopants and semiconducting polymers are poorly understood. It is currently unclear how the position of the dopant in the thin film can affect carrier mobility. Here, we report the evolution in spectroscopic and electrical properties of a model conjugated polymer upon exposure to two types of dopants: a strong oxidant (F₄TCNQ) and a strong acid (HTFSI). The model polymer was poly(3-(2′-ethyl)hexylthiophene) (P3EHT), a branched side chain analogue of the well-characterized polymer P3HT. We find that F₄TCNQ forms a charge transfer complex (CTC) with P3EHT resulting in a maximum electrical conductivity of 3×10⁻⁵ S cm⁻¹. We postulate that the branched side chains of P3EHT constrain the position of F₄TCNQ within the P3EHT crystallites, resulting in partial charge transfer between the donor and acceptor. Conversely, protonation of the polymeric backbone from HTFSI increases the electrical conductivity of P3EHT to 4×10⁻³ S cm⁻¹, two orders of magnitude higher than when F₄TCNQ is used. This work shows that a favorable energetic offset between the donor and acceptor is not sufficient to predict the charge transfer mechanism, but also relies on structural constraints of incorporating a dopant molecule into the polymer film.
Understanding the molecular doping process of semiconducting polymers through in-situ conductivity measurements and structural characterization

MARK DITUSA (Presenter), Physics, University of Chicago, TENGZHOU MA, GARRETT GROCKE, Institute for Molecular Engineering, University of Chicago, JENS NIKLAS, OLEG POLUEKTOV, Chemical Sciences and Engineering, Argonne National Laboratory, SHRAYESH PATEL, Institute for Molecular Engineering, University of Chicago — Polymers with conjugated semiconducting backbones show promise for use in organic electronics, such as thin film transistors, organic photovoltaics and the emerging technology of organic thermoelectrics. Molecular doping is a vital step in the controlling the charge transport of semiconducting polymers. Here, we report on how molecular doping affects the conductivity of polythiophene-based polymers over the course of vapor doping, and how different dopants (fluorinated TCNQs) with variable HOMO-LUMO overlap with our polymers affect the observed conductivity trends. Through in situ conductivity experiments, we show that for all three dopants tested, the conductivity follows a distinct profile that shows rapid increase of conductivity up until an optimal time, after which it falls and then equilibrates between 90% to 50% of the optimal conductivity. In conjunction with our in situ conductivity experiments, we report on scattering and spectroscopy experiments such as GIWAXS, UV-Vis, and EPR spectroscopy on polymer-dopant films at various time-points throughout the doping process. This study shows the potential of these methodologies for use on various polymer-dopant pairings to further advance our understanding of molecular doping dynamics.

*NSF GRFP under Grant No. (DGE-1746045).

Electrical and magnetic characterization of doped conjugated polymers with pendent stable radicals

ALBERT PARK (Presenter), Applied and Engineering Physics, Cornell University, YIREN ZHANG, Materials Science and Engineering, Cornell University, STEPHEN MCMILLAN, NICHOLAS HARMON, MICHAEL FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, CHRISTOPHER K OBER, Materials Science and Engineering, Cornell University, GREGORY FUCHS, Applied and Engineering Physics, Cornell University — Conjugated polymers such as poly(3-hexylthiophene-2,5-diyl) (P3HT) are being considered as potential backbone materials for organic radical battery electrodes to increase conductivity over unconjugated backbones, without sacrificing the electrochemical activity of radical groups. This is important for efficient current collection. Although conjugated polymers are among the most conductive organic materials at ambient temperatures, covalent attachment of stable radical such as such as 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) to undoped, regioregular P3HT creates sterically hindrances that result in an exponential decrease of film conductivity as a function of radical content. To recover the conductivity, we dope the conjugated backbone using either iodine or 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ). We characterize electrical properties of the doped conjugated radical polymer by varying both the pendent radical concentration and the doping level. Additionally, we used electron paramagnetic resonance to investigate the interplay between polaron and stable radical electrons. Transport measurements confirm that the conductivity increases by a few to several orders of magnitude, depending on the dopant.

*We acknowledge support from the DOE (grant #DE-SC0014336)

Electronic and Optical Properties of N-doped BBL Polymer

SARBANI GHOSH (Presenter), IGOR ZOZOULENKO, Linkoping University — Since their discovery, conducting polymers have been widely studied over the last few years in many optoelectronic applications. Applying redox chemistry, the intrinsic conductivity of the polymers could be altered by adding/removing an electron to make the polymer as an n-type/p-type material, respectively. The charge transport in electronic devices depends on the performance of both the p-type and n-type materials. P-doped polymers have been extensively studied over n-doped polymers due to lack of stable n-doped polymers. The need of the hour is to study n-type polymer to improve the performance of organic electronic devices. Here we study n-doped poly(benzobisimidazobenzophenanthroline) (BBL) using ground-state and time-dependent (TD) density functional theory (DFT). High electron mobilities (~0.1 cm² V⁻¹ s⁻¹), high structural and thermo-oxidative stability make BBL as an ideal n-doped polymer. To understand the electronic structure and optical spectroscopy of n-doped BBL, a thorough theoretical study is carried out. Formation of polaron and bipolaron due to the reduction of BBL is analyzed by ωB97XD functionals DFT with the 6-31+G(d) basis set. UV visible absorption spectra from TDDFT calculations show the transition from polaron/bipolaron to the conduction band.
High-temperature side-chain dipolar glass polymer, sulfonylated poly(2,6-dimethyl-1,4-phenylene oxide) (SO2-PPO). No advanced dielectric materials for polymer film capacitor and gate dielectric in organic electronics. We design a new class of e.g., amide and sulfone groups. In this work, we explored the opportunity of side-chain dipolar glass polymers as high-k and low-loss dielectric applications because of the enhanced orientational polarization from highly dipolar groups, dipolar polarization and thus high dielectric constant of 6-8 was obtained for these SO2-PPOs. The discharged energy National Institute of Standards and Technology, LEE RICHTER, Materials Science and Engineering Division, National Institute of discuss how these processes relate to the observed Magneto-electroluminescence response.

We will present on key requirements to be able to observe TTA in Rubrene and DiFTES-ADT, in heterojunction-based OLED devices test structures. We will show that a sub-bandgap turn-on does not require higher order recombination processes such as TTA and is thus not a reliable measure. However, if competing interfacial recombination pathways are suppressed, TTA can be reliably observed in the luminescence-current density-voltage characteristics (L-J-V) in mid to high current densities. We will discuss how these processes relate to the observed Magneto-electro-luminescence response.
The Structural, Electronic and Optical Properties of γ-glycine Under Pressure: A First Principles Study

JAEHO SHIN ( Presenter), SEUNGHOOL YANG, CHUL-HO LEE, GUNUK WANG, KU-KIST Graduate School of Converging Science and Technology, Korea University — Since Aviram and Ratner initially proposed the possibility of a molecular-scale rectifier in 1974, diverse type of molecular diodes driven by a specific molecular itself or the asymmetric coupling has been extensively demonstrated [1-2]. In this study, we propose a new class of molecular diode based on a hybrid molecular junction system that is composed with the 2D semiconductor (MoS2 or WSe2) and the standard self-assembled monolayer (SAM) (alkyl- or conjugated molecules). The 2D semiconductor and the SAM are sandwiched between the Au probe tip and Au bottom electrode using conductive atomic force microscopy (CAFM) technique. In the case of the molecular junction with monolayer MoS2 and OPT2, the diode feature with rectification ratio > ~10^3 was observed. Furthermore, the rectification ratio can be programmed according to the number of MoS2 layers, the type of 2D semiconductor, molecular length, and molecular group. Our suggested rectifier architecture can provide potential benefits to simply implement the molecular diode function and propose the idea to improve the diode performance.


Electro-absorption in Metal Nanoparticles within Glass; Comparison with Quantum Dots in Nonconjugated Conductive Polymers

MRINAL THAKUR, JUSTIN VAN CLEAVE (Presenter), Photonic Materials Research Laboratory, Auburn University, AL 36849 — Quadratic electro-optic effect / Kerr coefficient of metal nanoparticles within glass and comparison with iodine doped nonconjugated conductive polymers have been recently reported. In this report, we will discuss results of the measurement of electro-absorption in gold nanoparticles in glass and compare the results with published data on electro-absorption in quantum dots within doped nonconjugated conductive polymers. The electro-absorption was found to increase quadratically with the applied electric field. The magnitude of electro-absorption appears to increase as d^{-3}, where d is diameter of metal nanoparticle. More detailed work on this is in progress. This dependence on d is similar to the recently reported results on Kerr coefficient. This is expected since electro-absorption is proportional to the imaginary part of \chi^{(3)} and Kerr coefficient is proportional to the real part of the same.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X51 DPOLY DBIO: Using Polymer Sequence to Control Material Properties

Lisa Hall, Ohio State University - Tag(s): Invited

Using PRISM theory and molecular simulations to understand the complex interplay of copolymer sequence and architecture on assembly in polymer solutions

ARTHII JAYARAMAN (Presenter), University of Delaware — In this talk I will present our recent work using molecular dynamics (MD) simulations and PRISM theory aimed at understanding effects of non-linear polymer architecture and sequence on structure and thermodynamics within polymer solutions. I will focus on amphiphilic copolymer solutions and show how copolymer architecture (linear, bottle brush, cyclic), sequence (diblock, triblock) and composition impact assembled micelle structure (i.e. shape, size, aggregation number) and thermodynamics (i.e. critical micelle concentration, disorder to order transition). I will also discuss how we use PRISM theory and MD simulations in a synergistic and sequential manner to screen through this large polymer design space to achieve our desired structure and thermodynamics in these polymer solutions.
8:36AM X51.00002: Impact of Structural Correlation and Monomer Heterogeneity in the Phase Behavior of Soft Materials and Chromosomal DNA* [Invited] ANDREW SPAKOWITZ (Presenter), Chemical Engineering and Materials Science and Engineering, Stanford University — Polymer self-assembly plays a critical role in a range of soft-material applications and in the organization of chromosomal DNA in living cells. In many cases, the polymer chains are composed of incompatible monomers that are not regularly arranged along the chains. The resulting phase segregation exhibits considerable heterogeneity in the microstructures, and the size scale of these morphologies can be comparable to the statistical correlation that arises from the molecular rigidity of the polymer chains. To establish a predictive understanding of these effects, molecular models must retain sufficient detail to capture molecular elasticity and sequence heterogeneity. This talk highlights efforts to capture these effects using analytical theory and computational modeling. First, we demonstrate the impact of structural rigidity on the phase segregation of copolymer chain in the melt phase, resulting in non-universal phase phenomena due to the interplay of concentration fluctuations and structural correlation. We then demonstrate how these effects impact the phase behavior in statistical random copolymers and in heterogeneous copolymers based on chromosomal DNA properties. With these results, we demonstrate that the spatial segregation of DNA in living cells can be predicted using a heterogeneous copolymer model of microphase segregation.

*This work was supported by the NSF Interfacial Processes and Thermodynamics Program, Award 1511373.

9:12AM X51.00003: Molecular Engineering Complex Coacervate Materials Using Sequence [Invited] SARAH PERRY (Presenter), Department of Chemical Engineering and Institute for Applied Life Sciences, University of Massachusetts Amherst — Polyelectrolyte complexation can be used in the self-assembly of a wide range of responsive, bioinspired soft materials. Material responses can include swelling and dissolution or liquid-to-solid transitions, which can be harnessed to facilitate encapsulation and the subsequent fabrication of functional materials. Drawing inspiration from proteins as sequence-controlled polymers, we utilize polypeptides as a model platform to study how the patterning or presentation of charges and other chemical functionalities affects the resulting self-assembly and material properties, including the ability to selectively uptake and stabilize globular proteins. Our experimental efforts are supported by the parallel development of computational approaches for modeling and predicting the phase behavior of patterned polymeric materials. The goal of this systematic investigation is the elucidation of molecular engineering design rules to facilitate the tailored creation of materials based on polyelectrolyte complexation that can both illuminate self-assembly phenomena found in nature, and find utility across a wide range of real-world applications.

9:48AM X51.00004: Sequence-controlled polymers: bridging the gap between biotic and abiotic macromolecules [Invited] JEAN-FRANCOIS LUTZ (Presenter), Institut Charles Sadron, CNRS — Over the last decades, synthetic polymers and biological macromolecules have been studied by different scientific communities. Man-made plastics are obtained by simple one-pot polymerization methods and exhibit therefore non-uniform molecular structures. Consequently, molecular polydispersity shall be taken into account in synthetic polymer chemistry and physics. In contrast, biopolymers are produced by precisely-controlled biosynthesis and have perfectly-defined molecular structures. Thus, they exhibit folding and organization properties that are difficult to attain with conventional synthetic materials. Hence, biochemistry and biophysics are disciplines on their own. Yet, in the last few years, the traditional boundaries between biological and non-biological polymers tend to disappear. Due to recent progress in synthetic polymer chemistry, it is today possible to synthesize a wide variety of uniform synthetic polymers. In particular, significant advances have been reported for the synthesis of sequence-controlled polymers, which are man-made macromolecules with perfectly-controlled primary structures. This new class of synthetic polymers open up unprecedented possibilities for tuning structure/property relationships. However, the physical chemistry of these novel materials has been barely investigated to date. In this talk, I will highlight recent approaches developed in my laboratory for the synthesis of uniform sequence-defined polymers. Particular emphasis will be put on the design of abiotic information-containing macromolecules, which are new functional polymers inspired by nucleic acids.
Segmented Ionones: Precision within disperse structures yields interesting microstructures and stimuli-responsive behavior*

MATTHEW GREEN (Presenter), Arizona State University — Ionones are polymers containing a permanent charged group in the polymer backbone and are of interest because of their synthetic versatility, unique morphologies, and ionic nature. The charge placement and the spacing between the charge segments enable the polymer properties to be tuned from glassy solids to rubbery films to viscous liquids. The use of long, soft segment spacers between charges produces a class of polymer called segmented ionones. When segmented ionones are prepared with halide counterions (i.e., strong basicity) they form thermoplastic elastomers and microphase separate into microstructures wherein the ionic domains can form a continuous, percolated network at sufficient volume fractions. This talk will discuss recent efforts to utilize the synthetic versatility of this class of polymer to prepare percolated ionic domains in microphase separated polymers that display a range of thermomechanical properties. Furthermore, the combination of synthetic versatility and electrostatic interactions can be used to influence the dispersion of nanoparticles in a segmented ionene matrix as well as influence the nanoparticle solubility in specific microdomains. Finally, the response to external stimulus (e.g., electrical, mechanical) will be discussed and connected to varying chemistries and microstructural features of the polymers.

*This work was supported in part by the Army Research Office (W911NF-18-1-0412).

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X52 DPOLY DBIO DFD GSNP: Polymer and Polyelectrolyte Rheology II: Large Deformations

8:00AM X52.00001: Entanglements in strongly strained high molecular weight polymer melts+ HSIAO-PING HSU (Presenter), KURT KREMER, Max Planck Institute for Polymer Research — We study highly entangled, fully equilibrated polymer melts [1] subject to strong isochoric uniaxial deformation in the non-linear viscoelastic regime by extensive molecular dynamics simulations. It is shown that the over-all conformations of the original paths as well as the primitive paths (PPs) affinely follow the deformation, while the distribution of entanglements along the PPs does not [2]. The signature of chain retraction predicted by the tube model right after deformation is verified qualitatively but not quantitatively in all directions [3]. Upon further relaxation an inhomogeneous distribution of topological constraints in the melts due to long-lived clustering of entanglements and the delayed relaxation in chain conformation is observed.


+European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013)/ERC Grant Agreement No. 340906-MOLPROCOMP

8:12AM X52.00002: Strain Hardening in Extensional Rheology of Polyolefin Multilayer Films ALEX JORDAN, Engineering and Technology Department, University of Wisconsin - Stout, KYUNGTAE KIM (Presenter), BONGJOON LEE, EAN LUDTKE, FRANK BATES, Department of Chemical Engineering & Materials Science, University of Minnesota, OLIVIER LHOST, Total Petrochemicals, CHRIS W MACOSKO, Department of Chemical Engineering & Materials Science, University of Minnesota — The interfacial strength between isotactic polypropylene (iPP) and polyethylene (PE) depends on commercial grades, i.e., detailed molecular structures of the polymers.¹ We utilized extensional rheology to understand molten iPP/PE interfaces. We produced iPP/PE multilayer films prepared from Ziegler-Natta catalyzed high-density PE (zHDPE) and isotactic PP (ziPP) as well as metalloocene catalyzed high-density PE (mHDPE), linear low-density PE (mLLDPE), and iPP (miPP). Films with 2, 160, and 640 alternating layers of ziPP/zHDPE, miPP/mHDPE, and miPP/mLLDPE were fabricated via multilayer coextrusion. Extensional rheology of the 160-layer miPP/mLLDPE system revealed a strain hardening behavior, which became more pronounced when the number of layers increased to 640, effectively quadrupling the interfacial area in multilayer films. The miPP/mHDPE system showed strain hardening only when the number of layers reached to 640. Strain hardening was not observed in individual mHDPE, mLLDPE, and miPP films, nor in their bilayers. We quantitatively model strain hardening in the multilayer films by adding the stress contribution from the equilibrium melt interfacial tension to the measured extensional contribution from the components.

¹ Jordan et al., Macromolecules 2018, 51, 2506.
8:24AM X52.00003: Molecular origin of extensional strain hardening in phenyl-containing polymer melts  
CARLOS LOPEZ-BARRON (Presenter), ExxonMobil Chemical Company, WESLEY ROTH BURGHARDT, MU SUNG KWEON, Northwestern University — We recently reported unexpectedly extensional strong strain hardening (SH) in poly(4-vinylbiphenyl) (PVBp) when subjected to uniaxial flow. We postulate that this behavior is due to a molecular rearrangement mechanism (supported by WAXS measurements) that involves flow-induced π-π stacking of the phenyl groups, which results in an enhancement of friction drag between polymer chains [PRL 119, 247801 (2017)]. To further elucidate the molecular mechanism of SH, we measure the time evolution of the molecular alignment using an extensional rheometer housed in a custom-built oven designed to facilitate in-situ synchrotron X-ray experiments. Based on the anisotropic 2D WAXS profiles, we defined two alignment factors, one for the backbone (Abb) and one for the π-π stacking (Aππ). Perfect correlation between Abb and Aππ are observed during extensional flow start-up and flow cessation. Moreover, linear relations between both Abb and Aππ and transient stress (σE+) are observed at stress values below 1 MPa. The resemblance between this behavior and the stress-optical rule observed in many polymeric liquids led us to propose a stress-WAXS rule (SWR): Abb=CbbσE+ and Aππ=CππσE+. Finally, we will discuss the validity of the SWR in PVBp and polystyrene.

8:36AM X52.00004: Macromolecular Dynamics, Extensional Rheology, Pinch-off Dynamics, and Printability of Aqueous Solutions of Flexible and Semi-Flexible Polymers  
JELENA DINIC (Presenter), VIVEK SHARMA, University of Illinois at Chicago — Liquid transfer and drop formation/deposition processes associated with printing, spraying and coating flows involve complex free-surface flows including the formation of columnar necks that undergo spontaneous capillary-driven instability, thinning and pinch-off. For simple Newtonian fluids, the interplay of capillary, inertial and viscous stresses determines the self-similar thinning and pinch-off dynamics. In rheologically complex fluids, extra elastic stresses alter the pinch-off dynamics. Here we show that dripping-onto-substrate (DoS) rheometry protocols that involve visualization and analysis of capillary-driven thinning of a columnar neck can be used for measuring extensional viscosity and extensional relaxation time of polymeric fluids. We investigate the role of chemical structure by contrasting behavior of aqueous solutions of flexible polyethylene oxide (PEO) with solutions of semi-flexible hydroxyethyl cellulose (HEC) and show that both flexibility and extensibility of chains dramatically influence the extensional rheology response and the macromolecular relaxation dynamics. We elucidate how macromolecular stretching and orientation modify excluded volume and hydrodynamic interactions, affecting extensional viscosity response as well as polymer relaxation dynamics.

8:48AM X52.00005: Brownian dynamics simulations of linear and non-linear semidilute polymer solutions in extensional flow*  
CHARLES YOUNG (Presenter), CHARLES E. SING, University of Illinois at Urbana-Champaign — Understanding the relationship between microstructure and bulk properties is an overarching goal in polymer rheology. This is particularly true for non-linear polymer architectures, where topological interactions resulting from chain crossing restrictions lead to flow rates which are locally much higher than the applied flow. Polymers can thus be deformed significantly from their expected conformations, modifying the molecular functionality and the bulk stress. Coarse-grained molecular simulations which satisfy crossing constraints are crucial for developing quantitative models of these phenomena. Using our iterative conformational averaging method for Brownian dynamics simulations, we present an explanation for unexpected dynamics in solutions of non-linear polymers first observed in single molecule imaging experiments. Starting from a solution of linear chains, we introduce trace ring or branched polymers and observe the effect on polymer relaxation and transient stretching in planar extensional flow. We determine the importance of hydrodynamic interactions for polymer solutions ranging from dilute to the entanglement concentration and show that non-linear polymers can exhibit accelerated or hindered relaxation below the overlap concentration.

*NSF Grant No. CBET-1803757

9:00AM X52.00006: Pinch-off Dynamics, Extensional Rheology and Printability of Polyelectrolyte Solutions  
LEIDY NALLELY JIMENEZ (Presenter), JELENA DINIC, VIVEK SHARMA, University of Illinois at Chicago — Biological macromolecules like proteins, DNA and polysaccharides, and many industrial polymers, are classified together as polyelectrolytes for in solution, the repeat units in their backbone are decorated with disassociated, charge-bearing ionic groups, surrounded by counter-ions. In diverse applications like inkjet printing, sprayable cosmetics and insecticides, paints and coatings that involve the formation of fluid columns or sheets that undergo progressive thinning and pinch-off into drops, the dominant flow within the necking filament is extensional in nature. The extensional rheology response of the charged macromolecular solutions are not as well understood as that of their uncharged counterparts. Here focus on the characterization of capillary thinning and pinch-off dynamics, extensional rheology and printability of two model systems: sodium (polystyrene sulfonate) and poly(acrylic acid) by using dripping-onto-substrate (DoS) rheometry technique. Due to an interplay of hydrodynamics-induced and charged-induced stretching, both the measured extensional relaxation times and the extensional viscosity values show salt- and polymer concentration-dependent behavior that is not expected or anticipated from the typical shear rheology response.
custom-built Taylor-Couette apparatus, operating in the fully turbulent flow regime, at Reynolds numbers between $10^4$ and $10^5$. As a specific example, we characterize the drag reducing properties of the aqueous mucilage extracted from flax seeds (*Linum usitatissimum*), and compare its performance to that of a commonly-used synthetic flexible homopolymer, namely, polyethylene oxide (PEO). The molecular and viscoelastic properties of the principal polysaccharide constituent in flax mucilage is also studied using size exclusion chromatography and extensional rheology techniques (CaBER). Finally, we compare the shear-induced degradation of both polymers under prolonged turbulent flow conditions, and explore the possibility of mitigating chain-scission processes by the use of appropriate ionic and non-ionic surfactant additives to modify the chain flexibility and develop polymer-surfactant complexes. The dilute mucilage solutions are seen to exhibit comparable drag reduction and degradation behavior as aqueous PEO, but on a much cheaper cost-basis, and can potentially serve as an effective, eco-friendly, and economical alternative to synthetic polymers in real-life drag reduction applications.

*Research performed with partial support from the Office of Naval Research (ONR)*

**9:48AM X52.00008: Rheology and Dynamic Adsorption of Polymer-Surfactant Complexes**  
CARINA MARTINEZ  
(Presenter), VIVEK SHARMA, Chemical Engineering, University of Illinois at Chicago — The rheological properties of polymer-surfactant mixtures play a significant role in applications ranging from enhanced oil recovery, pharmaceutical and biological fluids, cosmetics, food, and coating. Addition of an ionic surfactant to an aqueous solution of neutral polymer like polyethylene oxide is known to result in a shear rheological response with non-monotonic concentration dependent variation, attributed to association complexes formed by hydrophobic interactions between surfactant monomers and polymers chains, as well as charge effects. Furthermore, the formation of association complexes changes both dynamic and equilibrium surface tension. However, due to a lack of suitable techniques, extensional rheology response of polymer-surfactant mixtures has not been characterized in adequate detail, even though most processing flows, especially those involving drop formation or liquid transfer are influenced by extensional rheology and pinch-off dynamics. In this study, we examine how pinch-off dynamics and the extensional rheological response of polymer solutions are modified by the addition of ionic surfactants. We utilize dripping-onto-substrate rheometry protocols and show that shear and extensional rheology response display contrasting concentration-dependent variation.

**10:00AM X52.00009: A Model for Salt Effects on Semidilute Polyelectrolyte Solutions: Equilibrium and Dynamics**  
GUANG CHEN (Presenter), ANTONIO PERAZZO, HOWARD A STONE, Princeton University — Polyelectrolyte (PE) solutions are endowed with both viscous and elastic properties that differ significantly from uncharged polymer solutions. Owing to their universal existence and functionalities in biology and industry, PE solution physics have been widely studied yet are often restricted to specific assumptions, such as the presence of a theta solvent, rod/flexible chain configurations or weakly/strongly charge conditions. Here, we will present a theoretical model based on mean-field theory, which provides new insights and scaling laws for the chain conformation, relaxation time and viscosity of semidilute PE solutions in good solvents. By considering the elastic, excluded volume, and electrostatic energies due to the PE charges and double layer, our theoretical predictions agree well with experiments and offer interpretations for previously unexplained viscoelastic behavior of PE solutions in either high polymer density regimes or conditions with added salt. New criteria for the overlap concentration and other special regimes with varying salt concentrations and polymer density will also be discussed.

**10:12AM X52.00010: Entanglement density and crossovers of polyelectrolyte solutions**  
CARLOS LOPEZ (Presenter), WALTER RICHTERING, RWTH Aachen University — We present steady shear and oscillatory rheology data for flexible sodium polystyrene sulfonate (NaPSS) and semiflexible sodium carboxymethyl cellulose as a function of polymer concentration, degree of polymerisation and added salt. Semidilute non-entangled dynamics are well described by the Rouse model, in agreement with Dobrynin's model for flexible polyelectrolytes. Addition of salt leads to a decrease in chain dimensions and therefore in solution viscosity, the effect being much more pronounced for NaPSS than NaCMC, which can be understood as resulting from the intrinsic rigidity of NaCMC preventing chain collapse at high salt.

The entanglement concentration of NaCMC is found to be only weakly dependent on added salt concentration. This contrasts with the overlap crossover which increases by several orders of magnitude from salt-free conditions to 0.1 M NaCl. Further, we find that the entanglement density remains constant upon addition of salt despite significant changes in polymer conformation. Our results for entangled polyelectrolyte in salt-free and salt solutions strongly contradict several predictions of the current scaling models for polymer entanglement.
10:24AM X52.00011: Coarse grained simulations of migration of polyelectrolytes in a combination of flow fields and electric fields* ANGELO SETARO (Presenter), Rensselaer Polytechnic Institute — Separations can be accomplished by controlling the relative rate at which different molecules travel through a microfluidic device. In a flow, the rate of travel of a molecule is largely determined by its relative position in the flow profile. Thus, if one can control molecules relative positions within a flow profile, one can influence separation. It has been found that the electrophoretic mobility of certain molecules, such as double-stranded DNA, is dependent on their conformation, which is in turn dependent on the local shear rate. This opens the door to using flow rate as a means to modify polymer conformation and by extension polymer mobility. Though this potential method opens the door to a variety of separations, there remain a number of fundamental questions about the underlying mechanism. To address these, we use a combination of theoretical calculations and Brownian dynamics simulations to probe how the combination of velocity gradients and electric field gradients impact particle mobility and migration.

*We acknowledge support from NSF Grant CBET-1826788.

10:36AM X52.00012: Ultralow interfacial tension of polyelectrolyte coacervates using drop retraction method SAMIM ALI (Presenter), ANAND RAHALKAR, VIVEK PRABHU, National Institute of Standards and Technology — The interfacial tension of coacervates can be controlled by a number of physicochemical conditions, such as salt type and concentration, temperature, and polymer molecular mass. An improved understanding of these relationships will help advance applications such as polymer coatings, encapsulation media and wet adhesives. However, interfacial tension measurements are challenging due to the ultra-low magnitudes observed in polyelectrolyte coacervates. This presentation describes the use of shape retraction analysis of a deformed drop of dilute phase generated in situ in the coacervate. Our measurements confirm that the interfacial tension follows the mean field prediction of 3/2 scaling as a function of the difference between salt concentration and the critical salt concentration at which interfacial tension vanishes. The additional effects of temperatures and molecular mass will be described.

10:48AM X52.00013: Bubble dynamics in non-Newtonian fluids MARCOS REYES-MARTINEZ (Presenter), EDWIN CHAN, National Institute of Standards and Technology — Cavitation Rheology (CR) has been investigated as a novel technique for the characterization of the elastic and fracture properties of soft materials. In addition to measuring mechanical properties of solids, the formation and pressurization of a cavity, as dictated by some initial defect size, is an information-rich phenomenon that can illuminate the interfacial properties of fluids undergoing hydrostatic deformation. In this presentation, we explore the use of CR as a probe for the fluid properties of materials that display both Newtonian and non-Newtonian behavior. By tracking the evolution of the pressure inside the bubble and carefully analyzing the geometry of the bubble wall, we gain insight into properties of the fluid such as viscosity, bulk modulus and Poisson's ratio. For the case of a model shear thickening fluid, we observe pressurization rate dependence on the critical cavitation pressure and evidence of transient fracture at sufficiently high pressurization rates. Our observations have deep implications in advancing the study of high-rate deformation of non-Newtonian fluids and soft materials.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X53 GSOFT: Geometry and Topology of Active Matter BCEC 253C - Vincenzo Vitelli, Univ of Chicago - Tag(s): Invited

8:00AM X53.00001: Curvature-driven topological protection* [Invited] MARK BOWICK (Presenter), Kavli Institute for Theoretical Physics, University of California, Santa Barbara — Active systems on curved geometries are ubiquitous in the living world. Ordered polar flocks in the presence of spatial curvature are forced to be inhomogeneous and must also exhibit topological defects, even in the steady state, when the curved manifold is topologically non-trivial. I will discuss how dynamical symmetry breaking via spontaneous flow (flocking), together with spatial curvature, are the only ingredients necessary to produce long-wavelength symmetry-protected gapped sound modes. The steady state profile of an active polar flock on a two-sphere and a catenoid will be presented. The topologically-protected sound modes are localized to special geodesics on the surface (the equator or the neck respectively). These modes are the analogue of edge states in electronic quantum Hall systems and provide unidirectional channels for information transport in the flock, robust against disorder and backscattering.

*This work was supported by the National Science Foundation awards DMR-1609208, DGE-1068780, PHY-1125915 (KITP) and PHY-1748958 (KITP).
8:36AM X53.00002: Defect ordering and geometrical control in passive and active nematic liquid crystals [Invited]  LUCA GIOMI (Presenter), Leiden University — In this talk, I will discuss some recent theoretical and experimental work on active nematic liquid crystals confined on two-dimensional curved interfaces and highlight how the geometrical and topological structure of the environment can substantially affect collective motion in active materials, leading to spectacular life-like functionalities.

9:12AM X53.00003: Odd Elasticity in Active Metamaterials [Invited]  COLIN SCHEIBNER (Presenter), University of Chicago, ANTON SOUSLOV, Physics Department, University of Bath, DEBARGHYA BANERJEE, Max-Planck-Institute for Dynamics and Self-Organization, PIOTR SUROWKA, Max-Planck-Institute for the Physics of Complex Systems, WILLIAM T. M. IRVINE, VINCENT VITELLI, University of Chicago — The theory of elasticity provides a foundation for describing the mechanics of deformations of continuous media. However, elastic theories of active matter must confront a fundamental challenge: the starting point of elasticity, the elastic energy, is not well defined due to microscopic activity. We introduce Odd Elasticity as a generalized theory of continuum mechanics that breaks key symmetries of the elastic (stiffness) tensor otherwise required by conservation of energy. We show that odd elasticity describes solids in which activity depends on the deformation of microscopic bonds. As a minimal model that produces odd elasticity upon coarse graining, we consider active metamaterials in which internal torques are actuated in response to compression or extension of the beams. Our odd-elastic theory, corroborated by simulations, sheds light on a rich phenomenology, including activity-induced auxetic behavior, active elastic waves and instabilities. Our work revisits the foundations of continuum mechanics and provides a blueprint for the design of active elastic engines, which utilize a strain cycle to convert microscopic activity into useful mechanical work.

9:48AM X53.00004: The odd free surface flows of a colloidal chiral fluid [Invited]  WILLIAM T. M. IRVINE (Presenter), University of Chicago — TBD

10:24AM X53.00005: Topological defects in cell layers [Invited]  JULIA YEOMANS (Presenter), University of Oxford — TBD

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X54 DPOLY DBIO GSNP: Polymers and Biopolymers in Very Strongly Confined Environments II: Polymers in Nanochannels and Nanopores BCEC 254A - Ining Jou, University of Massachusetts Amherst - Tag(s): Focus

8:00AM X54.00001: Brownian Dynamics studies of a “Tug-of-War” of a DNA translocating through a two-nanopore system  SWARNADEEP SETH (Presenter), ANIKET BHATTACHARYA, Department of Physics, University of Central Florida, WALTER REISNER, Physics, McGill University, WILLIAM B DUNBAR, Two Pore Guys, Inc. — Two nanopore devices show potential for improved translocation control and error reduction through correlation of independent current channels accessed at each pore. We report Brownian dynamics (BD) simulation results for a dsDNA threading through a two-nanopore system using a coarse-grained model for the dsDNA and pore. Specifically, we study “tug-of-war” states, where the DNA is simultaneously present in both pores and the pores exert opposing electrophoretic forces. We extract the life-time of the tug-of-war as a function of biasing conditions, chain stiffness and inter-pore separation and investigate the correlation and cross-correlation functions of the chain translocation velocity through the pores. Our studies are expected to extend the single-pore translocation problem to dual nanopore pore systems and aide in the design of two-pore devices.
Methods for reducing and directly controlling the speed of DNA through a nanopore are needed to enhance sensing performance for direct strand sequencing and mapping of sequence-specific features. We have created a method for reducing and controlling the speed of DNA that uses two independently controllable nanopores operated with an active control logic. The pores are positioned sufficiently close to permit co-capture of a single DNA by both pores. Control logic then turns on constant competing voltages at the pores leading to a "tug-of-war" whereby the molecule is pulled from both ends by opposing forces. These forces exert both conformational and speed control over the co-captured molecule, removing folds and reducing the translocation rate. When the voltages are tuned so that the electrophoretic force applied to both ends of the molecule comes into balance, the life-time of the tug-of-war state is limited purely by diffusive sliding of the DNA between the pores (yielding a two order of magnitude enhancement in translocation time). We quantify the translocation slow-down as a function of voltage tuning and show that the slow-down is well described by a first passage analysis for a one-dimensional sub-diffusive process.

*This work was supported by Two Pore Guy's Inc (2PG).

8:24AM X54.00003: Simulations of extension distributions for DNA confined in nanochannels near the persistence length

ADITYA BIKRAM BHANDARI (Presenter), KEVIN DORFMAN, Department of Chemical Engineering and Materials Science, University of Minnesota, Twin Cities — DNA has been used extensively as a model system to study confined polymers. A particularly important application of strongly confined DNA is genome mapping, where DNA molecules labeled at sequence-specific sites along their backbone are stretched by confinement in nanochannels with widths close to the DNA persistence length. The distributions of the fractional extension obtained in genome mapping experiments are skewed-left from a Gaussian distribution. Mehlig and coworkers proposed an explanation for these skewed distributions by obtaining the asymptotic solution for a weakly correlated telegraph model of a channel-confined polymer in the limit of small channels and long chains. We have tested the predictions of this theory using pruned-enriched Rosenbluth method (PERM) simulations. The simulated distributions are in reasonable agreement with theory in the relevant asymptotic limits. However, deviations are observed as we move away from the strict inequalities in the limits of the theory, corresponding to situations that are more representative of experimental systems.

8:36AM X54.00004: Diffusion of DNA in confinement: From nanochannels to cells [Invited]

KEVIN DORFMAN (Presenter), Chemical Engineering and Materials Science, University of Minnesota — The key challenge in understanding the diffusivity of DNA in strongly confined systems is accounting for the hydrodynamic interactions between the polymer and its environment. I will present both experimental and theoretical results on the diffusion of DNA in two highly confined systems that illustrate the complexity of this problem.

In the first case, I will show how combining biased Monte Carlo simulations and confined hydrodynamics calculations leads to a complete picture for the friction of a semiflexible polymer confined to a square nanochannel. The regimes of hydrodynamic friction are closely related to those for the chain extension, including a Rouse-like regime at moderate confinement where the friction is independent of the fractional extension of the chain. Subsequent experimental measurements of DNA diffusion in the so-called “extended de Gennes” regime agree well with the model calculations.

In the second case, I will describe an experimental test of the viscoelastic Rouse model for the segmental motion of DNA within E. coli cells. When the cells are compressed under "Quake" valves, the mean-squared displacement of cytoplasmic particles slows down by over one order of magnitude but the exponent characterizing their subdiffusion is unchanged. In contrast, the corresponding exponent for the subdiffusion of segments of DNA on short time scales (~1 s) undergoes a statistically significantly change when the cells are compressed. These results suggest that factors other than the cytoplasmic viscoelasticity play a role in this non-equilibrium perturbation of the cells.
**Stochastic Resonance Behavior of DNA Translocation with an Oscillatory Electric Field**

JOU (Presenter), RHYS DUFF, MURUGAPPAN MUTHUKUMAR, University of Massachusetts Amherst — Stochastic resonance (SR) describes the synchronization between noise of a system and an applied oscillating field to achieve an optimized response signal. In this work, we use simulations to investigate the phenomenon of SR of a single stranded DNA driven through a nanopore when oscillating electric field (OEF) is added. The system is comprised of a MspA protein nanopore embedded in a membrane and different lengths of DNA are driven from one end of the pore to the other via a constant potential difference. We superimposed an OEF over the existing electric field. The source of noise is due to thermal fluctuations, since the system is immersed in solution at room temperature. Here, the signal optimization we seek is an increase in translocation time ($\tau$) of DNA through the protein pore. Normally, $\tau$ scales linearly with DNA length and inversely with driving force in a drift dominated regime. We found a nonmonotonic dependence of $\tau$ with the frequency of the oscillating field. This nonmonotonic behavior of $\tau$ is observed for all lengths of DNA, but SR occurs only for longer DNA. Furthermore, we also see evidence of DNA extension being influenced by the oscillating field while moving through the nanopore.

*National Institutes of Health (Grant No. R01HG002776-15)

**Spontaneous Transport of Single-Stranded DNA through Graphene-MoS2 Heterostructure Nanopores**

BINQUAN LUAN (Presenter), IBM Thomas J. Watson Research Center — The effective transport of a single-stranded DNA (ssDNA) molecule through a solid-state nanopore is essential to the future success of high-throughput and low-cost DNA sequencing. Compatible with current electric sensing technologies, here, I propose and demonstrate by molecular dynamics simulations the ssDNA transport through a quasi-two-dimensional nanopore in a heterostructure stacked together with different 2D materials, such as graphene and molybdenum disulfide (MoS2). Due to different chemical potentials, $U$, of DNA bases on different 2D materials, it is energetically favorable for a ssDNA molecule to move from the low-$U$ MoS2 surface to the high-$U$ graphene surface through a nanopore. With the proper attraction between the negatively charged phosphate group in each nucleotide and the positively charged Mo atoms exposed on the pore surface, the ssDNA molecule can be temporarily seized and released thereafter through a thermal activation, that is, a slow and possible nucleotide-by-nucleotide transport. A theoretical formulation is then developed for the free energy of the ssDNA transiting a heterostructure nanopore to properly characterize the non-equilibrium stick-slip-like motion of a ssDNA molecule.

**Determining the Free Energy and Kinetics of a Translocating Polymer Chain**

ZACHARY DELL (Presenter), MURUGAPPAN MUTHUKUMAR, University of Massachusetts Amherst — Polymer threading or translocation through nanopores is widely studied due to its ubiquity in biology and its recent use as a characterization method. In this work, we explored translocation of a chain from one spherical cavity to another, motivated by viruses and vesicles. The primary theoretical tool for studying a translocating chain is its free energy, which includes the free energy associated with the donor/acceptor compartments, and the polymer-pore interaction energy. In the first stage of the project, we focused on calculating chain free energy under spherical confinement, relevant for donor/acceptor compartments. Due to conflicting theoretical pictures, we implemented Monte Carlo simulations and investigated how the free energy relates to the confinement strength and how it varies when the chain is tethered. With the simulation results and previous translocation theories, we built a center of mass (CM) theory for polymer translocation. This theory establishes a physical interpretation for the translocation coordinate in terms of the CM. Also, our approach allows for the incorporation of hydrodynamics through the CM friction. Both the simulations and theory can be generalized to study other confined environments.

*National Institute of Health (Grant No. R01HG002776-15)

**Using capillaries with varying cross-section to study polymer dynamics and behavior under multiple confining length scales**

DAVID RING (Presenter), ROBERT RIGGLEMAN, DAEYEON LEE, University of Pennsylvania — Infiltrating polymers into cylindrical nanopores to induce confinement has led to the fabrication of a new class of nanostructured polymeric materials. The behavior of polymers during infiltration and under confinement has been elucidated with the help of computational studies, revealing a rich thermodynamic and kinetic landscape. These systems, however, focus on confinement with a single characteristic length scale. There are many situations in which polymers infiltrate into a porous medium with varying dimensions (e.g., a packing of nanoparticles). In this talk, we address the question of what happens when polymers are confined with more than one characteristic length scale. To that end, we have simulated capillaries with varying cross-sections and multiple well-defined points of confinement, including necks and voids. Using umbrella sampling, we can explore the free energy of an infiltrating polymer melt to characterize the impact of confinement on the driving force for infiltration. We also vary the diameter of the capillary mouths to characterize the effect of geometry on the start of infiltration as polymers move from the bulk to the confined pore. Lastly, we also investigate the effect of varying cross-section on the rheological components of the polymer.
10:00AM X54.00009: Polymer-Grafted Nanoparticle Translocation in Strongly Confining Nanochannels*  
MICHAEL HORE (Presenter), WILLIAM R LENART, GABRIELA T JUSTINO, Case Western Reserve University — The process of a particle moving from one region to another through a channel is central to many physical systems, including viral infection and water filtration. In this talk, we discuss the conformation of polymers that are grafted to a spherical nanoparticle surface, and the effect this has on the translocation of the particle through a single, confining nanochannel. Using self-consistent field theory (SCFT) coupled with Poisson-Nernst-Planck (PNP) theory, we investigate the distortion of the grafted polymer layer for nanoparticles undergoing translocation in strongly confining nanochannels, as well as the expected signatures that would be observed experimentally.

*This work was supported by an NSF CAREER Award from the Polymers program (DMR-1651002).

10:12AM X54.00010: Water mediated effects in alpha-helix formation inside nanotubes  
DYLAN SUVLU (Presenter), University of Maine, DAVE THIRUMALAI, Chemistry, University of Texas at Austin, JAYENDRAN C RASAIAH, University of Maine — We present replica exchange molecular dynamics studies of the phase diagram for alpha-helix formation of capped polyalanine in nanotubes (NT) open to a water reservoir as a function of the NT diameter and hydrophobicity. A helix forms only in a narrow range of diameters. Helix formation in polyalanine is driven by a small negative enthalpy and a positive entropy change at 300 K, in contrast to the large negative entropy change that destabilizes the helix and favors the coiled state in bulk water. To understand the sequence dependence of helix formation inside the NT, solvation thermodynamics are determined by forming a thermodynamic cycle with liquid and gas phase MD simulations. Polyalanine forms a more thermodynamically favorable helix in the presence of water inside carbon and boron nitride NT. This is attributed to a favorable solvent reorganization energy and solvation entropy. In contrast, polyserine forms a stable helix in the gas phase but not in the presence of water while inside the CNT. This is attributed to unfavorable water-mediated interactions. However, polyserine forms a helix in a BNNT inside the gas phase but only over a narrow temperature range in the liquid phase. These data have implications for understanding helix formation inside the ribosome tunnel.

10:24AM X54.00011: Free energy cost of localizing an end-monomer of a confined polymer  
JAMES POLSON (Presenter), ZAKARY R. N. MCLURE, University of Prince Edward Island — We develop and employ a simple Monte Carlo simulation method to calculate the free energy cost of localizing an end-monomer of a polymer to the inside surface of a confining cavity. The method is applied to a freely-jointed hard-sphere polymer chain confined to cavities of spherical, rectangular and cylindrical geometries. We consider cases where the other end of the polymer is free and where it is tethered to another point on the surface. We characterize the dependence of the free energy on the cavity size and geometry type, the localization position, the polymer length, and the effects of excluded volume interactions. The relevance of these results to the initial stages of polymer translocation through nanopores is discussed.

10:36AM X54.00012: Polymer Conformation & Diffusion in Symmetric Thin Film Confinement  
JAMES PRESSLY (Presenter), ROBERT RIGGLEMAN, KAREN WINEY, University of Pennsylvania — Polymer conformation and dynamics in thin film nanoconfined controls a variety of properties important for advanced coating technologies and nanoplatelet composites. In this study, we examine the effect of chain length and film thickness on polymer conformation, entanglement density, and center of mass polymer diffusion using coarse grained molecular dynamics simulations. Polymer chain lengths of N = 25-400 and were confined between parallel plates to create polymer film thicknesses of h = 5-40σ. The plates are composed of discrete beads with athermal polymer-plate interactions. The simulations indicate that the diffusion coefficient, D, increases as the film thickness decreases, with longer chains exhibiting a larger increase in D. This increase in the diffusion coefficient correlates with chain disentanglement as confinement increases, similar to previous simulations of polymers confined to cylindrical pores. While we observe slowed diffusion in the most confined cylindrical geometries associated with chain segregation, polymer diffusion confined in thin films increases monotonically with increasing confinement.
In unconfined systems ($H >> P$), we found the dependence of the isotropic-nematic transition volume fraction ($f_{IN}$) follows Onsager theory. For strongly confined polymer solutions, $f_{IN}$ decreases as $H$ decreases due to the increased segmental correlation length, and enhanced segmental alignment is found throughout the solution. For the isotropic to nematic transition, diffusion along the nematic director increased as the density increased while lateral diffusion decreased. Further increase in volume fraction leads to smectic transition. The transition volume fraction ($f_{NS}$) systematically shifts higher for more flexible polymers. Upon transition into the smectic phase, polymer diffusivity decreases sharply by two order of magnitude. For both I-N and N-S transitions, we found evidence of universal critical exponents near the transition density.

*MOST 107-2112-M-001-031-MY3

Friday, March 8, 2019 8:00 AM - 10:36 AM

Session X55 GSNP GSOFT: Shell Buckling I BCEC 254B - Shmuel Rubinstein, Harvard University - Tag(s): Focus

8:00AM X55.00001: Non-destructive prediction of the buckling load of soda cans and space rockets [Invited]
EMMANUEL VIROT (Presenter), EPFL - Harvard University — What is the critical load required to crush a soda can or a space rocket shell? Surprisingly, there is no good way to estimate it, because of the high defect-sensitivity of the buckling instability. Here we measure the response of (imperfect) soda cans to lateral poking and identify a generic stability landscape, which fully characterizes the stability of real imperfect shells in the case where one single defect dominates. We show that the landscape of stability is independent of the loading protocol and the poker geometry. Our results suggest that the complex stability of shells reduces to a low dimensional description and that tracking the ridge and the valley of the landscape of stability defines natural coordinates for describing the stability of shells. By using this new paradigm, we show that we can accurately and non-destructively predict the buckling load of real imperfect shell structures, thereby promising drastic reductions of the costs of structural engineering experimental tests.

8:36AM X55.00002: How localized imperfections modify the buckling threshold of cylindrical shells* EMILIO LOZANO (Presenter), ECPS, EPFL, SHMUEL RUBINSTEIN, SMRlab, Harvard University, TOBIAS SCHNEIDER, ECPS, EPFL — Shells buckle and collapse at load levels below the thresholds predicted by linear stability analysis. The reduction of the load-carrying capacity has been linked to extreme sensitivity to geometric imperfections. Historically, spatially extended periodic imperfections have been analyzed using linear and weakly nonlinear theory. Recent fully nonlinear approaches suggest however the importance of spatially localized imperfections. We thus characterize experimentally and numerically the effect of spatially localized imperfections in an axially loaded cylindrical shell. For different types of imperfections, the buckling thresholds as a function of its size shows similar behaviour. This suggests a universal failure mechanism due to local buckling.

*Supported by the Swiss National Science Foundation SNSF under grant 200021-165530
8:48AM X55.00003: Localized edge state equilibria control when a soda can buckles*  
EMILIO LOZANO, FLORIAN REETZ, Ecole polytechnique federale de Lausanne, EMMANUEL VIROT, Ecole polytechnique federale de Lausanne / Harvard SEAS, SHMUEL RUBINSTEIN, Harvard SEAS, TOBIAS SCHNEIDER (Presenter), Ecole polytechnique federale de Lausanne — Thin-walled cylindrical shells such as rocket walls (or soda cans) offer exceptional strength-to-weight ratios yet predicting at which load the structure becomes unstable and fails remains an unsolved problem. Shells buckle and collapse at loading conditions much below those predicted by linear stability theory. We thus propose a fully nonlinear approach and show that fully nonlinear equilibrium states located on the boundary of the unbuckled state's basin of attraction define critical perturbation amplitudes and guide the nonlinear initiation of catastrophic buckling. For a clamped thin cylindrical shell under axial compression a fully localized single dimple deformation is identified as the edge state—the attractor for the dynamics restricted to the stability boundary. Under variation of the axial load, the single dimple undergoes homoclinic snaking in the azimuthal direction, creating states with multiple dimples arranged around the central circumference. Once the circumference is completely filled with a ring of dimples, snaking in the axial direction leads to further growth of the dimple pattern. The bifurcation structure of the equilibria closely resembles that observed in the Swift-Hohenberg equation with quadratic-cubic nonlinearity.

*Supported by SNSF grant 200021-165530

9:00AM X55.00004: Interacting defects affect the buckling of imperfect spherical shells  
DONG YAN (Presenter), MATTEO PEZZULLA, PEDRO REIS, Institute of Mechanical Engineering, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland — The presence, distribution, and interaction of defects dictate the buckling strength of shell structures. Even if the sensitivity of shell buckling to imperfections has long been recognized, to date, the successful prediction of critical loads is restricted to cases with a single defect, of known geometry. However, in reality, shells typically contain a distribution of defects and their interaction has not been well studied. In this talk, we will focus on spherical shells with multiple defects and study the role of defect interactions in dictating the buckling pressure. In the experiments, we fabricate polymeric shells containing two precisely engineered geometric defects through a customizable coating technique. We vary the relative size and location of these two defects and quantify the relationship between buckling pressure and defect distribution. The experimental results are then contrasted against finite element modeling (FEM) simulations. Upon validation of the numerics, we use FEM to perform a broader and more systematic exploration of the parameter space. Our results provide a better understanding of defect interactions, which we hope will put us on a step to better predict the buckling pressure of practical shell structures.

9:12AM X55.00005: On Establishing Buckling Knockdowns for Imperfection-Sensitive Shell Structures*  
SYMEON GERASIMIDIS (Presenter), Civil and Environmental Engineering, University of Massachusetts, Amherst, EMMANUEL VIROT, EPFL/Harvard University, JOHN HUTCHINSON, SHMUEL RUBINSTEIN, School of Engineering and Applied Sciences, Harvard University — This presentation contributes to recent efforts aiming to revise long-standing knock-down factors for elastic shell buckling, which are widely regarded as overly conservative for well-constructed shells. The presented work focuses on cylindrical shells under axial compression with emphasis on the role of local geometric dimple imperfections and the use of lateral force probes as surrogate imperfections. Two buckling thresholds are identified (local and global buckling) and related for the two kinds of imperfections. Four sets of relevant boundary conditions are accounted revealing a strong dependence of the global buckling load on overall end-rotation constraint when local buckling precedes global buckling. A reasonably complete picture emerges, which should be useful for informing decisions on establishing knockdown factors.

*E.V. and S.M.R. acknowledge their involvement in a project directed at new methods for analyzing shell buckling headed by T. M. Schneider at EPFL. E.V. has been supported by this project. This work was also supported by the National Science Foundation through the Harvard Materials Research Science and Engineering Center (DMR-1420570).
Quasi-static experimental path-following*  ROBIN M NEVILLE (Presenter), RAINER GROH, ALBERTO PIRRERA, MARK SCHENK, ACCIS, University of Bristol — Our work aims to exploit structural nonlinearity in engineering, with a particular focus on aerospace applications, to develop well-behaved nonlinear structures [1].

In addition to improved numerical methods, experimental validation of nonlinear structures is critical in ensuring their use in engineering applications, especially in conservative industries such as commercial aviation.

Existing experimental techniques are unable to fully characterise the nonlinear response of even simple nonlinear structures, as they cannot measure structures with force-displacement responses that include limit points and snapping behaviour. An experimental method has been developed to extend our ability to measure the structural response of nonlinear structures [2]. In this presentation we will present our recent developments in experimental path-following on nonlinear structures.


*This work is funded by EPSRC through grant number EP/N509619/1

On the role of localised post-buckling equilibria in axially compressed cylinders*  RAINER GROH (Presenter), ALBERTO PIRRERA, University of Bristol — We revisit buckling of axially compressed cylinders by considering fully localised post-buckling states in the form of one or multiple dimples. Using a combination of nonlinear quasi-static finite element methods and numerical continuation algorithms, we trace the evolution of odd and even dimples into one ring of circumferential diamond waves. The growth of the post-buckling pattern with varying compression is driven by a homoclinic snaking sequence, with even and odd dimple solutions intertwined. The initially stable and axially localised ring of circumferential diamonds destabilises at a pitchfork bifurcation to produce a second circumferential snaking sequence that results in the Yoshimura pattern. Localised dimple solutions represent saddle points in the energy landscape providing an exponentially decreasing energy barrier between the stable pre-buckling and re-stabilised post-buckling wells. The significance of the Maxwell load as a measure for quantifying the onset of mountain-pass solutions and the reduced resilience of the pre-buckling state is assessed. Finally, conservative buckling loads for design are inferred by tracing critical boundaries of the snaking set.

*RG is funded by the Royal Academy of Engineering [RF20181718] and AP by the EPSRC [EP/M013170/1].

Powering the Renaissance: Methods to Reveal the Energy Landscapes in Thin Shell Buckling  JACK PANTER (Presenter), Department of Physics, University of Durham, JUNBO CHEN, TENG ZHANG, Mechanical & Aerospace Engineering, Syracuse University, HALIM KUSUMAATMAJA, Department of Physics, University of Durham — The extreme non-linearity of thin shell buckling introduces significant challenges to studying even the simplest geometries. Here, we develop a new approach by coupling efficient and powerful energy landscape methods to a conceptually simple discretized elastic mesh model. This highly versatile approach can probe the buckling energy landscape of any thin shell, or composite of thin shells, without the need for a priori assumptions about deformation morphologies or symmetries.

As an example, we investigate the landscape of an axially compressed cylinder, revealed to be remarkably rich and highly variable as a function of aspect ratio and compressive strain. Firstly, we observe that a relatively small, discrete set of sub-critical buckled states balloons in size as the aspect ratio is increased. We then use a string method to obtain the minimum energy pathways between any two minima. We show how experimental local probing techniques can access the true initial buckling transition for centrally-located dimples. By recursively connecting the local minima, we reveal the landscape to be dominated by a small number of multiply-dimpled states at small aspect ratios, becoming glassy and highly-connected at large aspect ratios, and featuring many multi-step pathways between minimum pairs.
10:00AM X55.00009: Buckling of thermalized cylindrical shells

ANDREJ KOSMRLJ (Presenter), Princeton University, DAVID R. NELSON, Harvard University — We explore how thermal fluctuations affect the buckling of thin cylindrical shells. It is known that for flat solid sheets thermal fluctuations effectively increase the bending rigidity and reduce the bulk and shear moduli. As a consequence, thermal fluctuations increase the critical buckling load. In cylindrical shells, thermal fluctuations also increase the bending rigidity and reduce the in-plane elastic constants. However, the additional coupling between the shell curvature, the in-plane stretching modes and the out-of-plane undulations leads to novel phenomena. In shells thermal fluctuations effectively generate compressive load. As a consequence, the critical axial buckling load for cylindrical shells is reduced due to thermal fluctuations, which is similar to the reduced buckling pressure for spherical shells, but different from the enhanced buckling load for flat sheets. Similar to spherical shells, we find that for cylindrical shells with a sufficiently large radius the thermally generated compression can be large enough that shells become unstable even in the absence of external load. Furthermore, we find that the critical radius also depends on the aspect ratio (length/perimeter) of cylindrical shells.

*This work was supported by NSF award DMR-1752100 (CAREER).

10:12AM X55.00010: Imperfection-insensitive thin wavy cylindrical shells under bending: Effect of local radius of curvature on buckling and imperfection-sensitivity.

KSHITIJ YADAV (Presenter), SYMEON GERASIMIDIS, Department of Civil and Environmental Engineering, University of Massachusetts, Amherst — The imperfection-sensitivity of thin cylindrical shells has long been an obstacle for their optimal applications. To nullify this behavior, a conservative knock-down factor method is utilized for the design of thin cylindrical shells. Alternatively, stiffeners are also used to increase their capacity and to reduce the imperfection-sensitivity. We explore wavy cross-sectional thin cylindrical shells under bending to investigate the impact of imperfections on their load carrying capacity. We found that thin wavy cylindrical shells are insensitive to imperfections under bending in contrast to thin circular cylinders. This insensitivity is achieved by reducing the local radius of curvature and consequently, the effective radius of the cylindrical shell is reduced. This way cylindrical shells become less sensitive to imperfections and increase their load carrying capacity.

10:24AM X55.00011: Out-of-plane buckling of architected sheets with non-periodic cut patterns

CONNOR MCMAHAN (Presenter), PAOLO CELLI, Caltech, BASILE AUDOLY, Caltech & LMS, CNRS, Ecole Polytechnique, CHIARA DARAIO, Caltech — We investigate the out-of-plane shape morphing capability of elastic sheets with architected cut patterns. These cuts result in arrays of tiles connected by flexible hinges. We demonstrate that a non-periodic cut pattern can cause a sheet to buckle into three-dimensional shapes, such as domes or patterns of wrinkles, when pulled at specific boundary points. This phenomenon stems from the geometric incompatibilities between regions that are designed to undergo different amounts of strain. Global buckling modes observed in experiments are rationalized by an in-plane kinematic analysis, and are reproduced in simulations of homogenized shell models implemented in the open-source finite-element platform FEniCS. Our work illustrates a scalable route towards the fabrication of three-dimensional objects with nonzero Gaussian curvature from initially-flat sheets.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X56 GSNP: Chaos and Nonlinear Dynamics

BCEC 255 - Adolfo Del Campo, University of Massachusetts Boston

8:00AM X56.00001: Renormalization Group for Barrier Escape: Crossover to Intermittency

DAVID HATHCOCK (Presenter), JAMES PATARASP SETHNA, Cornell University — We develop a critical theory of barrier crossing in overdamped systems with low barriers. Traditional calculations in reaction-rate theory typically assume the energy barrier separating two metastable states is much larger than the thermal energy of particles in the system. When the barrier vanishes, however, there is a qualitative change in behavior as the metastable states merge. Instead of escaping over a barrier, particles now slide down a sloping potential. We formulate a simple renormalization group description of this transition and derive the scaling form for the mean escape time with an arbitrary potential and spatially dependent noise. The renormalization group analysis unifies barrier crossing problems with the theory of intermittency, originally used to describe bursts of chaotic dynamics in discrete maps. This correspondence leads to an exact functional expression for the escape time that, in certain limits, recovers the results predicted by reaction-rate theory, intermittency theory, and deterministic dynamics.

*This work was supported by the Cornell Presidential Life Science Fellowship and NSF Graduate Research Fellowship Grant No. DGE-1650441.
**8:12AM X56.00002: Operator Scrambling and Fermi's Golden Rule**  BIN YAN (Presenter), LUKASZ CINCIO, WOJCIECH ZUREK, Los Alamos National Lab — The out-of-time-order correlator (OTOC) qualifies the scrambling of local operators over the entire system. It has been argued that at early times the OTOC exhibits an exponential growth with a rate bounded above by $2\pi/\beta$, where $\beta$ is the inverse temperature.

In this work, we show that for generic (0+1)D systems the OTOC is ultimately related to the thermal average of the Loschmidt echo, with the perturbation given by the coupling between subsystems. It is further argued that the exponential growth and the temperature dependence of the OTOC can be determined by the Fermi's golden rule.

*This research was supported by the DOE under the LDRD program at the Los Alamos National Laboratory. LC also acknowledges support by the DOE through the J. Robert Oppenheimer fellowship.

**8:24AM X56.00003: Universal entanglement spectra in random quantum circuits**  PO-YAO CHANG (Presenter), National Tsing Hua University, XIAO CHEN, Kavli Institute for Theoretical Physics, University of California at Santa Barbara, SARANG GOPALAKRISHNAN, CUNY College of Staten Island, and CUNY Graduate Center, JED PIXLEY, Rutgers University — We will discuss the time evolution of the entanglement spectra in a spin-1/2 chain under random unitary dynamics. We find that the reduced density matrix develops level repulsion on an O(1) time scale while the bandwidth of the entanglement spectrum is rapidly changing, well before the subsystem has fully thermalized. In this locally thermal regime, random matrix theory describes the correlations between nearby entanglement energy levels but fails to capture global level correlations in the entanglement spectral form factor or the entanglement density of states. We find this behavior is universal and holds for a multitude of other quantum circuits. We will provide a heuristic explanation of our results.

*P.-Y.C. was supported by the Rutgers Center for Materials Theory postdoctoral grant. S.G. acknowledges support from NSF Grant No. DMR-1653271. S.G. and J.H.P. performed part of this work at the Aspen Center for Physics, which is supported by NSF Grant No. PHY-1607611, and at the Kavli Institute for Theoretical Physics, which is supported by NSF Grant No. PHY-1748958.

**8:36AM X56.00004: Extreme Decoherence and Quantum Chaos**  ZHENYU XU (Presenter), LUIS PEDRO GARCIA-PINTOS, Department of Physics, Umass boston, AURELIA CHENU, Theoretical Division, Los Alamos National Laboratory, ADOLFO DEL CAMPO, Department of Physics, Umass boston — We study the ultimate limits to the decoherence rate associated with dephasing processes. Fluctuating chaotic quantum systems are shown to exhibit extreme decoherence, with a rate that scales exponentially with the particle number, thus exceeding the polynomial dependence of systems with fluctuating k-local interactions. Our findings suggest the use of quantum chaotic systems as a natural test-bed for spontaneous wave function collapse models. We further discuss the implications on the decoherence of AdS/CFT black holes resulting from the unitarity loss associated with energy dephasing.

*We acknowledge funding support by UMass Boston (project P20150000029279), the John Templeton Foundation, and the National Natural Science Foundation of China (Grant No. 11674238).
8:48AM X56.00005: Experimental Study of Quantum Graphs With Symplectic Symmetry*  LEI CHEN (Presenter), Department of Electrical and Computer Engineering, University of Maryland, College Park, EDWARD OTT, THOMAS M ANTONSEN, STEVEN ANLAGE, Department of Physics and Department of Electrical and Computer Engineering, University of Maryland, College Park — Quantum graphs had been introduced as a powerful tool to study quantum chaos. Graphs with time-reversal symmetry (TRS) and broken time-reversal symmetry (BTRS), which correspond to the Gaussian orthogonal ensemble (GOE) and Gaussian unitary ensemble (GUE) respectfully, had been previously explored experimentally. We are introducing a microwave network with special design to study the Gaussian symplectic ensemble (GSE) statistics, which may be useful for research in quantum dots with strong spin-orbit scattering and other quantum chaotic systems. Two geometrically identical subgraphs with GUE symmetry are constructed from coaxial cables connected by T junctions. BTRS properties are realized by making nodes with circulators. The two subgraphs are connected with two bonds, along which one has phase shift of π, and the other one has zero phase shift. The phase shift π and 0 are achieved by putting short and open circuit connector caps into the bonds respectfully. This trick ensures the graph has an antiunitary symmetry T which squares to -1. Statistical analysis of both experimental data and simulations based on the Random Coupling Model (RCM) for this GSE graph will be presented.

*We acknowledge support under contract AFOSR COE Grant FA9550-15-1-0171 and the ONR Grant N000141512134.

9:00AM X56.00006: Nonlinear wave chaos in superconducting billiards  MIN ZHOU (Presenter), THOMAS M ANTONSEN, EDWARD OTT, STEVEN ANLAGE, University of Maryland, College Park — The Random Coupling Model (RCM) has been shown to successfully predict the statistical properties of linear wave chaotic cavities in the highly over-moded regime. It is of interest to extend the RCM to strongly nonlinear systems. We have studied the statistics of harmonics generated in a billiard by a nonlinear circuit [1] and the case of a billiard with a single nonlinear port, both of which have a point-like nonlinearity. In this talk, we discuss measurements of the nonlinear S-parameters in superconducting billiards where the nonlinearity is continuously distributed. By taking advantage of the high power (up to +35 dBm) vector network analyzer (VNA), we observe that the S-parameters are power dependent. One billiard is a cut-circle quasi-2D microwave cavity which is made of Pb-plated copper. The granular Pb material has a dominant nonlinear resistance that manifests in the S-parameters. We find the noise from the measurement setup affects the statistics in such a low loss system. Another billiard which is made of Pb-plated copper. The granular Pb material has a dominant nonlinear resistance that manifests in the S-parameters. We find the noise from the measurement setup affects the statistics in such a low loss system.

9:12AM X56.00007: Enhanced Stability and Exceptional Points in Active Photonic Couplers  VASSILIOS KOVANIS (Presenter), YVERTAY ZHIYENBAYEV, CONSTANTINOS VALAGIANNOPOULOS, Physics Department, Nazarbayev University, YANNIS KOMINIS, Physics Department, NTUA — We consider active photonic couplers consisting of two coupled dissimilar waveguides with gain and loss. We show that under generic conditions, not restricted by parity-time or other types of symmetry, there exist finite-power, constant-intensity Nonlinear Supermodes, resulting from the balance between gain, loss, nonlinearity, coupling, and dissimilarity. These Nonlinear Supermodes are characterized by the amplitude ratio and the phase difference of the two electric wave fields, which can be tuned to have almost any desired value, by appropriate parameter selection. The asymmetry of the system is shown to result in non-reciprocal dynamics enabling directed power transport functionality. In turn, we systematically investigate the dynamical response of such asymmetric coupler in the context of a set of single-mode equations with gain/loss saturation included. Additionally, we point and map, in the parameter and in the solution space of this photonic structure, a rich set of Exceptional Points, corresponding to non-Hermitian degeneracies where two eigenvalues and eigenvectors coalesce. The importance of the Exceptional Points is crucial for the system response under noisy perturbations or other modulations as well as for sensing applications.

9:24AM X56.00008: Unwinding the model manifold: choosing similarity measures to remove local minima in sloppy dynamical systems  BENJAMIN FRANCIS (Presenter), MARK TRANSTRUM, Physics and Astronomy, Brigham Young University — We consider the problem of parameter sensitivity in models of complex dynamical systems through the lens of information geometry. In most cases, models are sloppy, that is, exhibit an exponential hierarchy of parameter sensitivities. We propose a parameter classification based on how sensitivities scale at long observation times. We show that for oscillatory models, sensitivities can become arbitrarily large, which implies a high effective-dimensionality on the model manifold. This translates to multimodal fitting problems and stands in contrast to the low effective-dimensionality previously observed in sloppy models with a single fixed point. We define a measure of curvature on the model manifold which we call the winding frequency that estimates the density of local minima in the model's parameter space. We then show how alternative choices of fitting metrics can “unwind” the model manifold and give low winding frequencies. This prescription translates the model manifold from one of high effective-dimensionality into the “hyper-ribbon” structures observed elsewhere. This translation opens the door for applications of sloppy model analysis and model reduction methods developed for models with low effective-dimensionality.
9:36AM X56.00009: Chaos and High Temperature Pure State Thermalization* YURI LENSKY (Presenter), XIAOLIANG QI, Physics, Stanford University — Classical arguments for thermalization of isolated systems do not apply in a straightforward way to the quantum case. Recently, there has been interest in diagnostics of quantum chaos in many-body systems. In the classical case, chaos is a popular explanation for the legitimacy of the methods of statistical physics. In this work, we relate a previously proposed criteria of quantum chaos in the unitary time evolution operator to the entanglement entropy growth for a far-from-equilibrium initial pure state. By mapping the unitary time evolution operator to a doubled state, chaos can be characterized by suppression of mutual information between subsystems of the past and that of the future. We show that when this mutual information is small, a typical unentangled initial state will evolve to a highly entangled final state. Our result provides a more concrete connection between quantum chaos and thermalization in many-body systems.

*This work is supported by the National Science Foundation through the grant No. PHY-1720504 (Yuri Lensky and Xiaoliang Qi), and by the Hertz Foundation (Yuri Lensky).

9:48AM X56.00010: Nucleation of Defect Turbulence in the Two-dimensional Complex Ginzburg-Landau Equation* WEIGANG LIU (Presenter), UWE CLAUS TAUBER, Virginia Tech — We numerically investigate nucleation processes in the transient dynamics of the two-dimensional complex Ginzburg-Landau equation towards its "frozen" state with stationary spiral structures. We are interested in the transition kinetics between a random initial configuration and the latter frozen state with a well-defined low density of quasi-stationary vortices. Nucleation is monitored using the characteristic length between the emerging shock structures. The average nucleation time for different system sizes is measured over many independent realizations to obtain good statistics. An extrapolation method as well as a phenomenological formula are employed to eliminate finite-size effects. The non-zero barrier for the nucleation of single vortex droplets in the extrapolated infinite-size limit suggests that the transition to the frozen state is discontinuous. We also investigate the nucleation of target waves which emerge if a specific spatial inhomogeneity is introduced. A long "fat" tails exists in the distribution of nucleation times in this case, which suggest that the associated transition may be continuous.

*This research is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-FG02-09ER46613.

10:00AM X56.00011: Thouless and Relaxation Time Scales in Many-Body Quantum Systems* MAURO SCHIULAZ (Presenter), Yeshiva University, E. JONATHAN TORRES-HERRERA, Instituto de Fisica, Benemerita Universidad Autonoma de Puebla, LEA SANTOS, Yeshiva University — We study the time scales involved in the relaxation process of isolated quantum many-body systems. Using experimental observables and a realistic many-body quantum model, we unveil three different time scales: a very short time that characterizes the early fast decay of the initial state, and two much longer times that increase exponentially with system size. These are the Thouless time, $t_{\text{Th}}$, and the relaxation time, $t_{\text{R}}$. The Thouless time refers to the point beyond which the dynamics acquire universal features, and relaxation happens when the evolution reaches a stationary state. We show that in chaotic systems, $t_{\text{Th}}<<t_{\text{R}}$, while for systems approaching a many-body localized phase, $t_{\text{Th}}$ tends to $t_{\text{R}}$. We also compare these results with those for random matrices, and study how self-averaging properties depend on time scales.

*M.S. and L.F.S. are supported by the NSF Grant No.–DMR-1603418. E.J.T.-H. acknowledges funding from VIEP-BUAP, Mexico.

10:12AM X56.00012: Capture and chaotic scattering of a charged particle by a magnetic monopole under a uniform electric field KOU MISAKI (Presenter), University of Tokyo, NAOTO NAGAOSA, University of Tokyo, Riken CEMS — Motivated by the realization of magnetic monopole of Berry curvature by the energy crossing point, we theoretically study the effect of magnetic monopole under a uniform electric field in the semiclassical dynamics, which is relevant to many physical situations such as relaxation through the diabatic point. We found that the competition between the backward scattering by the monopole magnetic field and the acceleration by the electric field leads to the bound state, i.e., capture of a particle near the monopole. Furthermore, the nonlinearity induced by the magnetic monopole leads to the chaotic behavior in the transient dynamics, i.e., the transient chaos. We computed characteristic quantities of the strange saddle which gives rise to the transient chaos, and verified that the abrupt bifurcation occurs as we tune the system parameter toward the parameter region in which the system is integrable.
10:24AM X56.00013: PULSEDYN: Open source code for dynamical simulations of strongly nonlinear systems  RAHUL KASHYAP (Presenter), SURAJIT SEN, University at Buffalo, The State University of New York — We present PULSEDYN which is an open source C++ code written with the goal of performing highly accurate and late time simulations on strongly and weakly nonlinear chains while requiring minimal effort on the user's part. PULSEDYN offers a suite of potentials and solvers and simulations and may be set up using a parameter file and running the code provided as an executable. PULSEDYN is also written with an emphasis on modularity, allowing for easy changes to be made to the code. PULSEDYN is available to download from Github and is accompanied by documentation and a detailed user manual [1]. We show standard results reproduced from literature using PULSEDYN for benchmarking purposes. We then use PULSEDYN to demonstrate how a strongly nonlinear Fermi-Pasta-Ulam-Tsingou system transitions from quasi-equilibrium to the equipartitioned state and verify our results by correctly predicting the exact equilibrium specific heat of the system from the simulated equipartitioned state.


10:36AM X56.00014: The dynamics of the musical saw PETUR BRYDE (Presenter), LAKSHMINARAYANAN MAHADEVAN, Harvard University — The musical saw is played by first being bent into an S–curve before it is bowed - this geometry allows for vibration modes that are localized near the point of inflection. To understand this, we consider how the spectrum of a curved plate or beam is controlled by a spatially varying curvature profile. Using a recent geometric interpretation of Anderson-like localization that links the underlying eigenvalue problem and a closely related elliptic problem allows us to determine the conditions for and extent of mode localization and suggests an explanation for the sweet sound of the saw.

10:48AM X56.00015: Thermodynamics of Turing Machines* ARTEMY KOLCHINSKY (Presenter), DAVID WOLPERT, Santa Fe Institute — Turing Machines [TMs] are the canonical model of computation. Using results from thermodynamics of computation, we investigate bounds on the amount of work required to perform calculations using TMs. First, we consider the minimal amount of work required to run a given input program on a TM. We also consider the minimal amount of work required to produce a given string as an output of a TM, in analogy to Kolmogorov complexity (which asks about the length of the shortest program needed to produce a given string on a TM). We analyze two ways of implementing a TM, one of which is shown to require less work than any computable implementation. We also show that unlike the Kolmogorov complexity of a string which can be arbitrarily large, the minimal amount of work required to produce a given string is bounded by a constant.

*Grant No. FQXi-RFP-1622 from the FQXi foundation, and Grant No. CHE-1648973 from the U.S. National Science Foundation.

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X57 GSNP: Mechanical Metamaterials II BCEC 256 - Johannes Overvelde, AMOLF

8:00AM X57.00001: Bidirectional Folding with Atomic Layer Deposition Bimorphs for Autonomous Micro-Origami* ITAI COHEN (Presenter), BARIS BIRCAN, MARC MISKIN, Physics, Cornell University, ROBERT J LANG, Robert Lang Origami, KYLIE J DORSEY, PAUL L MCEUEN, Physics, Cornell University — We present micron sized self-folding structures that consist of nanometer-thin, atomic layer deposited SiO$_2$-Si$_3$N$_4$ bilayers, built with conventional semiconductor fabrication methods. A bending response originating from strain differentials within these bilayer stacks is used as the fold actuation mechanism. This strain differential induced bending is controlled by ion exchange reactions in our nanoscale sheets, enabling us to produce radii of curvature at the order of microns within fractions of a second. By lithographically patterning these sheets and localizing the bending using flat photoresist panels, we create microscale origami devices that can sense chemical changes in their environment and respond by changing configurations according to prescribed mountain-valley fold patterns. Finally, we show that our fabrication approach offers a range of chemical, electrical and biological functions as well as a path to sequential folding through the programming of stacks.

*This research was performed in part at the Cornell Nanoscale Science and Technology Facility. This research was supported in part by NSF DMR 1435829.
8:12AM X57.00002: Computational design of multistable metamaterials  FERNANDO INIGUEZ-RABAGO (Presenter), YUN LI, JOHANNES OVERVELDE, AMOLF — Metamaterials’ properties arise not only from their chemical composition, but mainly from their periodic structure. While most of these materials are characterized by a fixed geometry, some materials are designed with internal hinging mechanisms. This allows them to be reconfigured with external stimuli, therefore exhibiting tuneable properties. However, these materials become dependent on the stimuli, and once removed the material will relax to the initial configuration. Previously we proposed a design strategy based on space-filling extruded polyhedra to create 3D reconfigurable materials comprising a periodic assembly of rigid plates and elastic hinges. Interestingly, for some of these structures we found additional stable configurations that are spatially admissible, but that cannot be reached without temporarily deforming the rigid faces. Here, we soften this constraint to open up new folding pathways. We introduce a computational approach to scan the energy landscape of these complex 3D structures, and show that our method closely mimics experimental implementations of locally actuated metamaterials. Using this approach, we find a wealth of multistable unit cells that can be assembled to create responsive materials capable of switching between different properties.

8:24AM X57.00003: Programmable Anisotropic Multi-stability in an Origami-inspired Metamaterial* SOROUSH KAMRAVA (Presenter), Northeastern University, RANAJAY GHOSH, University of Central Florida, ZHIHAO WANG, ASHKAN VAZIRI, Northeastern University — In this project, we design, develop, fabricate and study a new class of 3D origami-inspired metamaterials with highly anisotropic mechanical instability and controlled reconfigurability. This metamaterial is constructed by connecting star-shaped units that are formed by folding an array of interconnected Miura-ori patterns, also known as origami string. The origami string is a one degree of freedom slender mechanisms in which we substituted paper and creases with 3D printed faces and revolute hinges, respectively. The star-shaped unit exhibits mechanically rich and strongly nonlinear behavior that includes bi-stability and reconfigurability. In addition, we introduce a 3D combination of star-shaped units with zero effective Poisson's ratio in three orthogonal directions allowing its behavior in each loading direction to be programmed independently. The mechanical instability of this metamaterial in each orthogonal direction directly depends on the characteristics of star-shaped units aligned in that direction. Also, our study provides a framework to program the star units and create the desired properties in each orthogonal direction of the 3D metamaterial.

*United States National Science Foundation, Division of Civil, Mechanical, and Manufacturing Innovation, Grant No.1634560.

8:36AM X57.00004: Topological defects in complex mechanical metamaterials  ANNE MEEUSSEN (Presenter), Designer Matter Department, AMOLF, ERDAL C. OGUZ, YAIR SHOKEF, School of Mechanical Engineering, Tel Aviv University, MARTIN VAN HECKE, Huygens-Kamerlingh Onnes Laboratory, Leiden University — While topological defects play a crucial role in condensed matter, they are not widely explored in mechanical metamaterials. We introduce a systematic strategy to design frustrated metamaterials with local or topological defects. We uncover their distinct mechanical signatures, and show how defects can be harnessed to engineer a desired response. Our work presents a new avenue to systematically introduce frustration and defects with a topological signature in mechanical metamaterials.

8:48AM X57.00005: Propagation of Pop-ups in Kirigami Shells  AHMAD RAFSANJANI, School of Engineering and Applied Sciences, Harvard University, LISHUAI JIN (Presenter), School of Mechanical Engineering, Tianjin University, BOLEI DENG, KATIA BERTOLDI, School of Engineering and Applied Sciences, Harvard University — Kirigami-inspired metamaterials are attracting increasing interest because of their ability to achieve extremely large strains and shape changes via out-of-plane buckling. While in flat kirigami sheets all ligaments buckle simultaneously leading to a continuous phase transition, here we demonstrate that kirigami shells can also support discontinuous phase transitions. Specifically, we show via a combination of experiments, numerical simulations and theoretical analysis that in cylindrical kirigami shells the buckling induced pop-up process initially localizes near an imperfection and then, as the deformation is increased, progressively spreads through the structure. Notably, we find that the width of the transition zone, as well as the stress at which propagation of the instability is triggered, can be controlled by carefully selecting the geometry of the cuts and the curvature of the shell. Our study significantly expands the ability of existing kirigami metamaterials and opens avenues for the design of the next generation of responsive surfaces, as demonstrated by the design of a smart skin that significantly enhance the crawling efficiency of a simple linear actuator.
9:00AM X57.00006: Kirigami surfaces: programmable mechanical response via hierarchical design* NING AN (Presenter), State Key Laboratory for Strength and Vibration of Mechanical Structures and School of Aerospace, Xi’an Jiaotong University, Xi’an 710049, People’s Republic of China, AUGUST G DOMEL, John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA, AHMAD RAFSANJANI, Department of Materials, ETH Zürich, 8093 Zürich, Switzerland, JINXIONG ZHOU, State Key Laboratory for Strength and Vibration of Mechanical Structures and School of Aerospace, Xi’an Jiaotong University, Xi’an 710049, People’s Republic of China, KATIA BERTOLDI, John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA — Kirigami - the ancient Japanese art of cutting paper - has recently inspired the design of highly stretchable and morphable mechanical metamaterials that can be easily realized by embedding an array of cuts into a thin sheet. An attractive feature of these systems is that they are manufactured as a simple flat surface with cuts and then exploit elastic instabilities to transform into complex three-dimensional configurations. In this study, we focus on a thin elastic sheet perforated with a hierarchical pattern of cuts and demonstrate that the hierarchy significantly enhances the programmability of the system. In particular, we show that, by tuning the geometric parameters of this hierarchy, not only a variety of different buckling-induced 3D deformation patterns can be triggered, but also the stress-strain response of the surface can be effectively programmed. Finally, we show that when multiple hierarchical surfaces of various geometric patterns are brought together to create one combined heterogenous surface, the mechanical response can be further tuned and complex stress-strain curves can be achieved.

*Ning An was supported by the China Scholarship Council as a visiting scholar at Harvard University.

9:12AM X57.00007: Morphing origami shells: the case of the Miura ori HUSSEIN NASSAR (Presenter), MAE, University of Missouri, Columbia — Origami has become a source of inspiration in design across multiple scales. Its rules stipulate that a 3D shape must be folded from a single flat sheet: cutting and gluing are prohibited. Although seemingly restrictive, these rules have allowed artists, and more recently scientists, to construct surprisingly intricate shapes while guaranteeing an advantageous assembly-free fabrication based on a single process: folding. Origami-inspired structures have a second advantage: their folding/unfolding mechanism can be leveraged to adapt to a changing environment. Indeed, local folds aggregate and bring on large changes in shape, curvature and elongation on a global scale. The talk advocates for a way of describing origami tessellations as a class of morphing, yet kinematically constrained, shell structures rather than a mere discrete assembly of hinged plates. A purely kinematical continuum theory of these shells is suggested and exemplified in the case of the Miura origami tessellation. Various finite deformation modes (large strains, large curvatures) are successfully predicted and explained by the theory and are subsequently numerically constructed under suitable boundary conditions. The results demonstrate the rich morphing abilities of origami shells.

9:24AM X57.00008: Nonlinear elastic response of a topological mechanical metamaterial JOSHUA SOCOLAR (Presenter), Physics Department, Duke University, YUXUAN CHENG, Physics Department, Wuhan University — We consider the static response of a finite 1D lattice of pivoting rigid bars connected end-to-end by harmonic springs of zero equilibrium length. The linearized model is equivalent to the Kane-Lubensky model of rigid rotors and is topologically polarized when the pivot point of each bar is off center. We fix the angular displacement of the leftmost bar and solve the nonlinear torque balance equations for the equilibrium configuration. For the unpolarized case, we find an algebraic decay of the rotation angle θ_n due to nonlinear effects associated with the bulk zero mode. For one sign of the polarization, θ_n decays exponentially and the elastic energy is nearly zero, consistent with the excitation of the zero mode at the left edge. For the other sign, θ_n also decays exponentially with the same decay length as the zero mode, but with a finite energy, and there is a turning point beyond which θ_n grows exponentially toward the free boundary. Numerical solutions are explained in detail by an analysis that necessarily includes terms of up to fifth order in θ_n. The results provide insight into numerical results for the directional response of a 2D mechanical graphene model to an externally applied local strain.

9:36AM X57.00009: Geometric information and rigidity percolation in floppy origami SIHENG CHEN (Presenter), L MAHADEVAN, SEAS, Harvard University — Floppy origami structures have many folded configurations and are thus natural candidates for storing information geometrically. To address how we might harness this idea, we study the effect of folds and constraints in a planar tessellation inspired by the simplest globally coordinated origami pattern known as Miura-ori. Introducing folds randomly along the diagonals of the quads in Miura-ori makes the rigid structure floppy. We show how the number of degrees of freedom in the system varies with the increase in the density of constraints, first linearly, and then nonlinearly. In the nonlinear regime, mechanical cooperativity sets in via an inherent redundancy that depends on the assignment of constraints, and the degrees of freedom in the system depends on the density of constraints in a scale-invariant manner. The redundancy in the constraints shows a percolation transition at a critical constraint density \( \rho_c \). Our work shows how floppy origami can be used to store information in a scale-invariant way, and how we can control its rigidity exquisitely by taking advantage of a percolation transition.
Topological Directional Response in the Continuum Limit of Mechanical Metamaterials

ADRIEN SAREMI (Presenter), D. ZEB ROCKLIN, Georgia Institute of Technology — Flexible mechanical metamaterials display an exciting variety of novel deformation properties, including programmability, nonlinearity and robustness. However, these functionalities, which rely on nonuniform deformations of the microscopic unit cell of which the metamaterial is composed, are not captured by conventional elastic theory, creating a challenge in examining their actual large-scale properties. We address this via micromorphic continuum elasticity, which treats deformations that are nonuniform locally yet vary smoothly over larger lengthscales. We examine in particular topological edge and interface modes and directional response analogous to that observed by Kane and Lubensky in discrete models. We identify a new counting argument between modes of deformation and constraints that ensures mechanical criticality in the continuum, leading to a novel correspondence between a bulk topological invariant and boundary modes. Finally, we explore the lengthscales of deformations governed by this theory for given system geometries, elastic properties and disorder.

Topological edge floppy modes in quasicrystals

DI ZHOU (Presenter), LEYOU ZHANG, XIAOMING MAO, Department of Physics, University of Michigan, Ann Arbor — Quasicrystals (QCs) are fascinating materials that exhibit physics properties not available in crystals, such as rotational symmetries forbidden in lattices, physics of higher dimensions, and self-similarity. The interplay of these unique features with topological states of matter can offer a rich variety of interesting phenomena. In this talk, we discuss topological mechanics in 2-dimensional quasicrystalline parallelogram tilings. We use the Penrose tiling as our example to demonstrate how these boundary modes arise with a small geometric perturbation to the tiling. The same construction can also be applied to disordered parallelogram tilings to generate topological boundary floppy modes. We find that, due to the unusual rotational symmetry of quasicrystals, the resulting topological polarization can exhibit orientations not allowed in periodic lattices. Our result reveals new physics about the interplay between topological states and quasicrystalline order and leads to novel designs of quasicrystalline topological mechanical metamaterials.

The topological basis of function in flow and mechanical networks

JASON W ROCKS (Presenter), ANDREA LIU, ELENI KATIFORI, University of Pennsylvania — Recently, both flow networks and mechanical networks have been shown to be remarkably tunable. By tuning the local node connectivity, it is possible to robustly control the propagation of inputs in order to achieve a wide variety of specific tasks. However, the network architectures used to achieve such tasks demonstrate significant design flexibility, blurring the relationship between structure and function. Here we seek to identify the structural features responsible for function in tuned networks. Using persistent homology, we show that networks develop large-scale topological features when they are tuned, which are similar for different networks with the same function, regardless of the details of the local link topology. These features correlate strongly with the tuned response, providing a clear relationship between structure and function.

Using tunable origami for active energy absorption

ZHONGYUAN WO (Presenter), JULIA RANESES, EVGUENI FILIPOV, University of Michigan — Energy absorption devices are widely used to mitigate damage from collisions and impact loads. Due to the inherent uncertainty of possible impact characteristics, passive energy absorbers with fixed mechanical properties are not capable of serving in different application scenarios. Therefore, origami-inspired structures, which possess the ability to reconfigure and deploy, are a qualified candidate for a novel active design. In this work, we apply the constrained zipper-coupled Miura-ori tubes (deployable and stiff after locking) as the basis to a tubular energy absorber. Numerical and experimental (static and dynamic) studies are performed to quantify the response of these novel structures. This work shows that the reconfigurable origami could change their stiffness and the total amount of energy they absorb. These behaviors are suitable for creating systems with on-demand properties that adapt to different impact scenarios.

*NSF-EFRI-1741618

*The authors acknowledge funding from the ZF Automotive Research Award and the Office of Naval Research (Grant N00014-18-1-2015). J.R. acknowledges support from the SURE program at the University of Michigan.
10:36AM X57.00014: Atomic layer deposition for membranes, metamaterials, and machines*  KYLE J DORSEY (Presenter), TANNER G PEARSON, School of Applied and Engineering Physics, Cornell University, EDWARD P ESPOSITO, Laboratory of Atomic and Solid State Physics, Cornell University, BARIS BIRCAN, YIMO HAN, School of Applied and Engineering Physics, Cornell University, SIERRA RUSSELL, Nanoscale Engineering, SUNY Polytechnic, DAVID ANTHONY MULLER, School of Applied and Engineering Physics, Cornell University, ITAI COHEN, PAUL L MCEUEN, Laboratory of Atomic and Solid State Physics, Cornell University — Ultra-thin films of inorganic materials are well-suited for fabrication of micron-scale actuators because they can sustain small radii of curvature, are compatible with semiconductor processing, and are chemically robust. We leverage atomic layer deposition (ALD) to produce free-standing mechanical devices with sub-5 nm film thicknesses. We fabricate cantilevers from ALD films to characterize the mechanical properties. We find that ALD films are elastic and exhibit a bending stiffness on the order of $10^{-15}$ J. These measurements enable fabrication of cantilever springs with ultra-low spring constants suitable for micron-scale machinery. ALD mechanical metamaterials are fabricated by patterning of both the film and its substrate. Corrugations transferred into the ALD film enhance its bending stiffness and enable bending anisotropy, while cuts etched into the film soften the in-plane response. We integrate these results to produce magnetically actuated three-dimensional devices with applications in micromachinery.

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Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X58 GSOFT: Granules and Glasses BCEC 257A - Wen Zhang, University of Science and Technology of China

8:00AM X58.00001: Structural and topological nature of plasticity in sheared granular materials*  YUJIE WANG, YIXIN CAO, Physics, Shanghai Jiao Tong University, TIQIAO XIAO (Presenter), Shanghai Institute of Applied Physics, WALTER KOB, University of Montpellier and CNRS — Upon mechanical loading, granular materials yield and undergo plastic deformation. The nature of plastic deformation is essential for the development of the macroscopic constitutive models and the understanding of shear band formation. However, we still do not fully understand the microscopic nature of plastic deformation in disordered granular materials. Here we used synchrotron X-ray tomography technique to track the structural evolutions of three-dimensional granular materials under shear. We establish that highly distorted coplanar tetrahedra are the structural defects responsible for microscopic plasticity in disordered granular packings. The elementary plastic events occur through flip events which correspond to a neighbor switching process among these coplanar tetrahedra (or equivalently as the rotation motion of 4-ring disclinations). These events are discrete in space and possess specific orientations with the principal stress direction.

*The work is supported by the National Natural Science Foundation of China (No. 11175121 and 11675110).

8:12AM X58.00002: The Jamming Energy Landscape is Hierarchical and Ultrametric*  ROBERT DENNIS (Presenter), ERIC CORWIN, Physics, University of Oregon — Recent infinite dimensional mean field results have shown that the energy landscape of glasses forms a hierarchically structured ultrametric space. We directly explore this prediction in low dimensional finite size systems. Starting in an energy minima of an over-jammed system, we apply a small random perturbation to the positions of our particles and re-minimize in order to find new minima. By enumerating these minima and calculating the distance between their force networks, we produce a small correlated portion of the overlap matrix. This matrix exhibits a clear hierarchical structure and shows the signature of an ultrametric space. That such a hierarchy exists for the jamming energy landscape provides direct evidence for the existence of a marginal phase created by the Gardner transition.

*We gratefully acknowledge support from the NSF under Career Grant No. DMR-1255370 and a grant from the Simons Foundation No. 454939.
8:24AM X58.00003: Jammed packings behave similarly under random force and shear  PETER MORSE (Presenter), Syracuse University, ELISABETH AGORITSAS, École Normale Supérieure, M. LISA MANNING, Syracuse University, FRANCESCO ZAMONI, École Normale Supérieure, ERIC CORWIN, University of Oregon — Mean-field calculations suggest that in infinite dimensions, the response of a system to global shear and random forces may be equivalent. Whether or not this is true in 2d or 3d systems remains an open question. To address this, we develop a method for driving 2d jammed packings of disks by quasi-static persistent random forces and demonstrate that the response is similar to what is observed in athermal quasi-static shear simulations. We also investigate the gap and small force statistics in these randomly forced packings as well as the spatial organization of vibrational modes and particle rearrangements in order to compare to similar observations under shear. We expect that the results of this work may have interesting applications in understanding emergent behavior in active matter systems.

8:36AM X58.00004: Characteristic temperatures predicted from inherent structures*  JIANHUA ZHANG (Presenter), WEN ZHENG, NING XU, University of Science and Technology of China — We calculate the correlation and linear response to external forces for inherent structures (metastable solid states at zero temperature) of different systems. Borrowing the idea of fluctuation-dissipation relation for thermodynamically equilibrated systems, we obtain a temperature-like quantity purely from the correlation and response of inherent structures. For systems with Lennard-Johns, Weeks-Chandler-Andersen, and harmonic particle interactions, we surprisingly find that the temperature-like quantity agrees well with the crystallization or onset temperature for crystal or glass forming liquids. Our study indicates that some equilibrium information can be obtained just from nonequilibrium metastable solid states, which thus proposes a novel way to calculate characteristic temperatures. Our results also suggest that effective temperatures previously calculated in ageing glasses may be simply the onset temperature of glass forming liquids.

*This work is supported by the National Natural Science Foundation of China (Grants No. 11734014)

8:48AM X58.00005: ABSTRACT WITHDRAWN —

9:00AM X58.00006: Landau Theory of Complex Spherical Packing Phases*  DUNCAN MCCLENAGAN (Presenter), Department of Physics and Astronomy, McMaster University, KAI JIANG, School of Mathematics and Computational Science, Xiangtan University, ANCHANG SHI, Department of Physics and Astronomy, McMaster University — A large number of complex spherical phases, such as the Frank-Kasper phases (e.g., the \( \sigma \), A15, C14 and C15 phases), have been observed in various soft matter systems. Understanding the formation of these novel ordered structures presents an interesting challenge to the soft matter community. We are developing Landau theories that are capable of describing the occurrence and stability of these phases. Our research indicates that the A15 and \( \sigma \) phases may emerge as stable or metastable phases in systems described by a Landau theory derived from the statistical mechanics of block copolymers. We will discuss our results and their significance to the mechanisms for the formation of complex spherical phases in soft matter systems.

*This research is supported by the Natural Science and Research Council (NSERC) of Canada.

9:12AM X58.00007: Glass Transition in Supercooled Liquids with Medium-Range Crystalline Order.  INDRAJIT TAH (Presenter), Tata Institute of Fundamental Research Hyderabad, SHILADITYA SENGUPTA, University of Tokyo, SRIKANTH SASTRY, Physics, Jawaharlal Nehru Centre for Advanced Scientific Research, CHANDAN DASGUPTA, Physics, Indian Institute of Science, SMARAJIT KARMAKAR, Tata Institute of Fundamental Research Hyderabad — The origin of the rapid dynamical slowdown in glass forming liquids in the growth of static length scales, possibly associated with identifiable structural ordering, is a much debated issue. Growth of medium range crystalline order (MRCO) has been observed in various model systems to be associated with glassy behavior. Such observations raise the question of whether molecular mechanisms for the glass transition in liquids with and without MRCO are the same. In this study we perform extensive molecular dynamics simulations of a number of glass forming liquids and show that the static and dynamic properties of glasses with MRCO are different from those of other glass forming liquids with no predominant local order. We also resolve an important issue regarding the so-called point-to-set method for determining static length scales, and demonstrate it to be a robust method for determining static correlation lengths in glass formers.
9:24AM X58.00008: Softening of rapidly heated nanoscale glassy films of methylbenzene

RINIPAL KAUR (Presenter), VLADISLAV SADTCHENKO, Chemistry, The George Washington University — Using Fast Scanning Calorimetry (FSC), we investigated the impact of thin film confinement on softening and vaporization of glassy films of methylbenzene in the limit of high heating rates. The glassy films of distinct thicknesses ranging from 2 to 1800 nm were grown by vapor deposition and subjected to heating with rates in excess of $10^5$ K/s. For the films with thicknesses above 20 nm, the resulting softening kinetics strongly implied a surface facilitated mechanism: the softening originated at surfaces of a sample and progresses into its bulk via a transformation front. Yet, according to our analysis, the kinetic parameters for the softening front propagation differed significantly for the films with thicknesses below and above 300 nm. For example, the apparent activation energy barrier for the front propagation almost doubled for thicker films. We interpret these results in the framework modified Wilson-Frenkel model of softening front propagation and discuss their implications for past FSC studies of nanoscale vapor-deposited glassy films.

9:36AM X58.00009: Surface facilitated softening of rapidly heated glasses: recent experimental results and the fundamental mechanisms

VLADISLAV SADTCHENKO (Presenter), ULYANA CUBETA, RINIPAL KAUR, Chemistry, The George Washington University — Under certain conditions, e.g., during rapid heating, stable vapor-deposited, ordinary glassy, and even viscous liquid films can undergo softening by surface facilitated mechanism: the softening originates at the surface of a sample and progresses into its bulk via a transformation front. Despite years of research on this phenomenon, no simple theoretical model is currently available for quantitative description of glass softening by a propagating front. Based on our recent fast scanning calorimetry studies of surface facilitated glass softening and melting of superheated molecular crystals, we developed a comprehensive analytical description of the softening front propagation. This description is essentially a modification of well-established Wilson-Frenkel theory of non-equilibrium phase transitions. We present further experimental evidence in support of this analytical approach, and discuss the model's advantages, formalism, limitations, and applicability under a variety of experimental conditions.

9:48AM X58.00010: Stagnant zone formation in a 2D granular bed under penetration*

HONGYI XIAO (Presenter), MATT HARRINGTON, DOUGLAS DURIAN, University of Pennsylvania — Penetration into a granular material is a process that is both rich in physics and important in engineering applications. Here, we present experiments with a rectangular indenter penetrating horizontally into 2D granular beds. The penetration force experienced by the indenter shows a linear increase with the penetration depth, and this force is larger for penetration into elongated particles than that into circular-shaped particles. Particle positions are tracked, and local particle-based strains are calculated, showing a triangular-shaped stagnant zone in front of the indenter, and two shear bands along the edge of the stagnant zone. A structural function, $Q_k$, is used to characterize the local packing anisotropy, which reveals unique structural signatures as well as different structure-dynamic relations for the stagnant zone and the shear bands. The linear force law and the distinct regions observed here agree with a recent continuum model for granular penetration [1], while the structural information extracted here further demonstrates the microscopic difference between shear jammed and shear localized regions.


*Funded by NSF grants MRSEC/DMR-1120901 and MRSEC/DMR-1720530.

10:00AM X58.00011: Intruder spacing induces particle jamming during intrusion into granular media

SWAPNIL PRAVIN (Presenter), Temple University, ENDAO HAN, HEINRICH M JAEGER, The University of Chicago, S. TONIA HSIEH, Temple University — Robotic feet often encounter granular substrates that can display complex behavior ranging from solid to fluid in a single step. The effects of foot morphology on the interaction between feet and granular substrates remain poorly understood. Inspired by the presence of toes on animal feet, the goal of this study was to characterize the effect of spacing between two intruders ("toes") on granular material behavior. To this end, we measured and numerically simulated the force response to intrusion of two parallel square rods into dry poppy seeds while varying the rod gap spacing. Our results show that a peak in total force occurs at a gap of ~3 particle diameters, which was 20 % greater than the force at large separation (>11 particle diameters), beyond which the total produced force plateaued. We propose that this peak in force is the result of particle jamming between the intruders. To quantify the degree of particle jamming, interparticle forces were calculated from simulations. As expected, the total number of strong forces—identified as force chains—indicated greater particle jamming at gap spacings close to those corresponding to the peak force. These findings indicate that intruder separation and particle jamming can significantly affect force response to granular intrusion.
A New Calculation of Stretched Exponential Time Dependence in As2Se3 Structural Glass

CHRIS NELSON (Presenter), Physics and Astronomy, St. Cloud State University — It has been shown by a number of authors that the relaxation times of structural glasses satisfy a stretched exponential dependence with a particular value for the exponent $\beta$ at the glass temperature. Previously, this author used a free energy approach involving frustration in locally preferred structures to calculate the NQR distribution, the correct glass and Kauzzmann temperatures, as well as the spike in the heat capacity for the structural glass As$_2$Se$_3$. Here we calculate the correct relaxation time exponent ($\beta=3/5$) based on a statistical mechanical approach using the same approach. In addition, we show that this time dependence is entirely determined by the cooperative behavior of said structures, and at the glass transition temperature the system + bath is non-equilibrium steady state.

Presenting New Generation Amorphous Glassy Alloys “NGAGA”

DIPTI SHARMA (Presenter), Science, WIT, JOHN MACDONALD, Chemistry and BioChemistry, WPI, NEERAJ MEHTA, Physics, BHU — This work explores the details of “New Generation Amorphous Glassy Alloys (NGAGA)”. Several decades ago, single glassy material was explored, and one single glass transition of a single amorphous glassy material can be seen i.e. Amorphous Selenium. Later, binary glassy alloys appeared where an example of SeTe can be seen and glass transition of binary glassy alloys were explored as single but shifted glass transition. Then tertiary amorphous material came into research field i.e. SeTeAg and showed either shorter or wide and shifted kinetics of glass transition with doped material. But as time advanced, New Generation Amorphous Glassy alloys with four materials in one, appeared i.e. SeTeSnAg those brought very different results in glassy behavior. In this work, we are going to discuss changes occurred in NGAGA and in their kinetic behavior. From 1st generation to 4th generation, glassy alloys were made in our lab and studied and showed significant results in the research area of soft condensed matter and material Physics.

Keywords: Amorphous material, glassy alloys, material, transition, kinetics, Calorimetry, thermal behavior, new generation material.

Rigid clusters versus rigid regions in frictional granular packings and their role in packing mechanics

J. M. SCHWARZ (Presenter), KUANG LIU, Department of Physics, Syracuse University, JONATHAN E KOLLMER, Department of Physics, University of Duisburg-Essen, SILKE HENKES, Department of Mathematics, University of Bristol, KAREN DANIELS, Department of Physics, North Carolina State University — Force-chains are a well-established signature of granular packings yet their role in packing mechanics remains elusive. We explore two new complementary mechanical signatures, namely that of rigid clusters and that of rigid regions. To determine rigid clusters, we implement a frictional version of a (3,3) pebble game on experimental packings of photoelastic disks undergoing a jamming transition. To determine rigid regions, we compute the dynamical matrix in the presence of friction and use a threshold-based criterion to determine which regions are rigid. While the rigid cluster decomposition depends on the topology of the contact network, the latter approach depends both on the topology and forces of the contact network. We find that the rigid clusters correlate well with the rigid regions, particularly near the jamming transition. We also observe “partial rigidity” with both signatures containing holes of floppiness involving groups of disks in the contact network and we look for correlations between rigid clusters/regions and force chains. In some cases we find that spanning force chains can dictate the boundary of a rigid cluster/region, while in other cases there is little correlation, hinting at the complexity of the problem.

*NSF-CMMT-1507938/James S. McDonnell Foundation

Granular drag induced by oblique impact

KAI HUANG (Presenter), VALENTIN DICHTL, FELIX RECH, Experimentalphysik V, University of Bayreuth — Considering granular medium as a complex fluid with a finite yield stress, an object moving inside has to locally unjam and mobilize the surrounding particles in order to step forward. Consequently, granular drag depends strongly on the local rheological behavior. Using a recently developed bi-static radar system capable of tracking a metallic object with a diameter down to a few millimeters, we monitor the trajectory of a projectile penetrating obliquely into a granular medium and characterize the velocity dependent granular drag in both vertical (along gravity) and horizontal directions. Recent advances in this particle tracking technique and the possibility of using it as a local rheometer for granular media will be discussed.

*This work is partly supported by the German Research Foundation through Grant No. HU1939/4-1.

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X59 GSOFT: Soft Composites: Mechanics and Structure I

University of San Diego - Tag(s): Focus
8:00AM X59.00001: Glassy Dynamics in Composite Biopolymer Networks* [Invited] JOERG SCHNAUSS (Presenter), TOM GOLDE, MARTIN GLASER, TINA HÄNDLER, CARY TUTMARC, IMAN ELBALASY, JOSEF A. KAS, Leipzig University, HARALD HERRMANN, German Cancer Research Center, DAVID M SMITH, Fraunhofer Institute for Cell Therapy and Immunology — The cytoskeleton is a highly interconnected meshwork of strongly coupled subsystems providing mechanical stability as well as dynamic functions to cells. To uncover central biophysical principles, it is essential to investigate not only one distinct functional subsystem but rather their interplay as composite biopolymeric structures. Here, these effects caused by composite structures will be especially addressed with the two key elements of the cytoskeleton actin and vimentin IF. In contrast to previous studies, entangled conformations of these reconstituted composite networks can be described by a superposition of two non-interacting scaffolds. Key elements are the ability to compare different compositions with comparable architectural features as well as to identify polymer-specific interactions, which are typically ignored in most established models. We have experimentally identified inter-filament interactions as a key factor that can overwrite scaling predictions of the classical semiflexible polymer physics by comparing results of networks of actin, vimentin IF, keratin IF and synthetic double-crossover DNA nanotubes. Acquired results of the linear and non-linear bulk mechanics are captured in the frame of an inelastic glassy wormlike chain model allowing to address the diversity of the polymer types based on their specific interactions, which lead to differing relaxation behaviors for the different polymer types. Accounting for this molecular diversity, the composite effects can be expressed as a superposition of the non-interacting scaffolds.

*We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG) and by the European Research Council (ERC).

8:36AM X59.00002: Actin crosslinker density tunes mesoscale mechanics in actin-microtubule composites* SHEA RICKETTS (Presenter), MADISON FRANCIS, University of San Diego, LEILA FARHADI, University of Massachusetts Amherst, JACOB WALES, Rochester Institute of Technology, MICHAEL RUST, University of Chicago, MOUMITA DAS, Rochester Institute of Technology, JENNIFER ROSS, University of Massachusetts Amherst, RAE ROBERTSON-ANDERSON, University of San Diego — The physical interactions between semiflexible actin filaments, rigid microtubules and the suit of smaller proteins that crosslink both filaments, allows the cytoskeleton to precisely tune its structure and mechanics to enable a vast array of cellular processes such as cytokinesis. Here we use optical tweezers microrheology to determine how steric entanglements versus chemical crosslinking impacts the nonlinear mesoscale mechanics of actin-microtubule composites. We create co-polymerized and co-entangled composites of actin and microtubules with varying concentrations of actin crosslinkers. We optically drive microspheres through the crosslinked composites at speeds much faster than the relaxation rates and distances larger than network mesh size. We simultaneously measure the force the filaments exert on the microspheres during and following the strain. We map network stiffness, relaxation profiles, and spatial heterogeneities to the concentration of actin crosslinkers in composites.

*This work was funded by a NSF CAREER Award #1255446, a NIH NNIGMS Award #R15GM123420, and a W.M. Keck Foundation Research Grant.

8:48AM X59.00003: Modeling composite cytoskeletal networks using effective medium theory* JACOB WALES (Presenter), Rochester Institute of Technology, SHEA RICKETTS, University of San Diego, LEILA FARHADI, University of Massachusetts, Amherst, MICHAEL RUST, University of Chicago, JENNIFER ROSS, University of Massachusetts, Amherst, RAE ROBERTSON-ANDERSON, University of San Diego, MOUMITA DAS, Rochester Institute of Technology — The mechanical response of most eukaryotic cells is due to their cytoskeleton, a polymeric scaffold made up of two major types of biopolymers, actin filaments (F-actin) and microtubules, which have very different mechanical properties. The cytoskeleton is responsible for a number of cellular functions including maintaining cell shape, rigidity, and facilitating movement. Here we seek to investigate, understand, and predict the structure-function properties of engineered cytoskeletal scaffolds with tunable mechanics. We study composite networks of F-actin and microtubules using an effective medium theory, and characterize their mechanical response using rigidity percolation theory. We obtain the shear rigidity of these networks as a function of the concentrations of F-actin and microtubules, the type of crosslinking, and the concentration of the crosslinkers. Our results may help to elucidate the design principles of smart biopolymer composites with adaptive mechanical properties.

*This work was funded by a W.M. Keck Foundation Research Grant.
The addition of sticky nanoparticles in a physically associated hydrogel matrix is considered. It is shown that the nanoparticles assortatively self-assemble into a percolated nanoparticle network at volume fractions far below the percolation threshold of a pure sticky nanoparticle hydrogel. Concurrently, it is shown that hydrogel undergoes substantial mechanical reinforcement, as manifested by the emergence of a low-frequency plateau in the viscoelastic shear moduli as determined via rheology, and the increased elastic moduli as determined via cavitation. Nanoparticles added beyond the percolation threshold are shown to bolster the connectivity of the percolated nanoparticle network, as revealed by mechanical measurements as well as structure factor calculations. These results provide fundamental insights into the self-assembly, and mechanical consequences therein, of multicomponent reversible hydrogels.

*We acknowledge financial support from the NSF MRSEC DMR-1420382.

9:36AM X59.00007: Mechanical structure function properties and fracture toughness of Articular Cartilage modeled as a biopolymer double network* LEIJA SUTTER (Presenter), ANDREW B SINDERMANN, School of Physics and Astronomy, Rochester Institute of Technology, THOMAS S WYSE JACKSON, LENA BARTELL, Department of Physics, Rochester Institute of Technology — We present results on cracking and fracture toughness of biopolymer double networks, with Articular Cartilage (AC) as our model system. AC is a soft tissue that covers the ends of bones and distributes mechanical loads at the joints in our knees and elbows. Adult AC has very few cells, and its network-like extracellular matrix primarily determines its mechanical response. As a material, AC is remarkable. It is only a few millimeters thick and has minimal regenerative capacity, yet can withstand large forces over our lifetimes during which it undergoes 100-200 million loading cycles without fracturing. The molecular mechanism underlying this exceptional toughness is not well understood. Here we investigate the mechanical structure-function properties underlying the fracture toughness of AC by using a framework that combines a double network model of AC with rigidity percolation theory. We study how the stress relaxation and crack propagation in the double network depend on its composition and on loading conditions. Our results may help to formulate a quantitative criterion for fracture in AC and similar soft and biomaterials akin to the Griffith criterion for fracture of brittle materials.

*The research was funded by the National Science Foundation via the award NSF/DMR- 1808026
On the interplay between two rigidity transitions in disordered semiflexible polymer-tissue networks

AMANDA PARKER (Presenter), Physics, Syracuse University, M. CRISTINA MARCHETTI, Physics, UC Santa Barbara, M. LISA MANNING, J. M. SCHWARZ, Physics, Syracuse University — Low-connectivity semiflexible polymer networks undergo a rigidity transition from floppy to rigid as shear strain is increased beyond some finite value. Collections of cells with no gaps between them (confluent tissues) also undergo a rigidity transition from fluid to solid, as a parameter characterizing the shape of an individual cell is varied. Both transitions are driven by geometric constraints, though in confluent tissue, topology also plays an important role. We present numerical studies of a vertex model of a two-dimensional confluent tissue embedded in a two-dimensional semiflexible polymer network, with mechanosensitive coupling between the two systems. We study how a rigidity transition in one system may or may not induce rigidity in the other, depending on the nature of the coupling. In addition to going beyond studying the onset of rigidity in a single network construct, the semiflexible polymer-tissue network is relevant to cancer in which cancerous tissue (a tumor) is surrounded by and interacts with an extracellular matrix, consisting primarily of cross-linked collagen, a semiflexible polymer.

*This work is supported by NSF-POLS 1607416.

Ensemble dynamics of large DNA molecules within entangled and crosslinked cytoskeleton networks

DEVYNN WULSTEIN (Presenter), KATHRYN REGAN, SHEA RICKETTS, RAE ROBERTSON-ANDERSON, RYAN J. MCGORTY, University of San Diego — The cellular interior is highly crowded. How biological macromolecules, such as DNA, diffuse through these environments has yet to be fully elucidated. We mimic the crowded cellular environment by creating custom-designed co-polymerized networks of actin and microtubules that are crosslinked at various motifs. We study the effect of the co-entangled and co-crosslinked cytoskeleton networks on the ensemble dynamics of large circular and linear DNA molecules using selective-plane illumination differential dynamic microscopy (SPIDDM). As a digital Fourier microscopy technique, SPIDDM measures dynamics over a large range of length and time scales that supplement and expand on the dynamics measured using single-molecule tracking of DNA in the same environments. We find interesting differences between ensemble and single-molecule dynamics over the temporal and spatial scales probed.

*This work was funded by NIH NNI-GMS Grant No. R15GM123420

Polypelectrolyte composite: hyaluronic acid mixture with DNA

TOMISLAV VULETIC (Presenter), IDA DELAČ MARION, Institut za fiziku, Zagreb, SIGRID BERNSTORFF, Elettra-Sincrotrone Trieste, KREŠIMIR SALAMON, Rudjer Bošković Institute, DANIJEL GRRGICIN, Institut za fiziku, Zagreb — Biomacromolecules are mostly polyelectrolytes (PE), dissociating into polyions and small counterions. Their long-range electrostatic interaction leads to arrangements different than for neutral polymers and generates difficulties in physical understanding. For the last decade we have addressed these by studying the structure and dynamics of two semirigid (bio)PEs, DNA and HA (hyaluronic acid). Here we present a study of mixtures of DNA and HA, as a system of like-charged semi-rigid chains, differing, however, by the respective persistence lengths of 50 and 1 nm. We studied salt-free mixtures across a broad range of concentration ratios c_{HA}/c_{DNA}=0.05-50 (c=5-200 g/L). By polarizing microscopy we established that DNA and HA form clearly separated thread-like domains defined and oriented by solution shear. We applied small angle x-ray scattering (SAXS) and observed a PE correlation peak at q* wave vector, ascribed to DNA subphase and thus reporting on its effective concentration c_{DNA}*. From c_{DNA}* it was possible to infer the c_{HA}* of HA subphase. We found a ratio G= c_{HA}*c_{DNA}*=0.85 across the studied range. As there is the osmotic pressure, P equilibrium between DNA and HA subphases, the constant G indicates that P~c^{9/8} scaling commonly found for DNA and other highly charged PEs is valid also for HA which does not feature counterion condensation – so it's not due to the concentration dependence of the latter. Furthermore, as for HA all counterions contribute to P, the HA osmotic coefficient f_{HA}^* is a measure of f_{DNA}. We found the latter to be 0.28 and corroborated previous workers who found the concentration of counterions controlling the osmotic pressure to be double the Manning-condensation theory value for DNA.

*This work was supported by UKF, Croatia under Grant 17/13 and by ERDF grant KK.01.1.1.01.0001 for the Croatian Center of Excellence CEMS.
8:00AM X60.00001: Speaking Science to Power: Providing S&T Advice to Governments [Invited] JOHN HOLDREN (Presenter), Harvard University — This presentation discusses the opportunities and challenges for scientists and technologists in advising government policy-makers on science and technology for policy and policy for science and technology. It draws on the author’s five decades of experience as an academic engaging U.S. and non-U.S. governments on science and technology issues, most of it in parallel with an academic career but also, from January 2009 to January 2017, as President Obama’s Science Advisor and the Senate-confirmed Director of the White House Office of Science and Technology Policy. Considerable attention will be given to the contrasts between science and technology policy under Obama versus under Trump, including suggestions for dealing with the particular challenges posed by the latter.

9:12AM X60.00002: Federal Policy Making: Perspectives from Inside and Outside Government [Invited] CELIA MERZBACHER (Presenter), Independent consultant — Federal policy decision making is influenced by many factors and actors, including science and the scientific community. Drivers, incentives, and metrics vary among stakeholders inside and outside of government, which can make it difficult to find a mutually agreeable path. Yet action can be swift when what is made possible by science and technology (S&T) intersects a national need or threat. Policy makers in government must keep abreast of S&T advances relevant to their mission, whereas those outside government who seek to influence policy must be credible and understand how the various parts and agencies of government work. The process of federal policy making will be explored through examples, ranging from microelectronics to nanotechnology to quantum technology.

9:48AM X60.00003: Advice from a Scientist-Policy Maker on Giving Advice to a Policy Maker [Invited] ANDREW ZWICKER (Presenter), Princeton University and NJ State Legislature — As a member of the APS, I have met with and offered advice to federal policy-makers and their staff multiple times. Since 2016, I have also been a member of the NJ Legislature where I am the only scientist, and am the Chair of the Science, Innovation, and Technology Committee. In that role, I meet regularly with scientists and other stakeholders on a multitude of state legislative issues. Based upon my experiences, it is clear to me that effective scientific policy advice must, of course, start with an understanding of the background of the people you are speaking to and a presentation that is clear, jargon-free, and has a specific request. However, the assumption is most often to begin with the "big picture" and put the request at the end, but that is the opposite of what I have found to be effective. In addition, one must understand that while clear science policy advice is important, final policy decisions are most often made based upon a variety of complex factors, from fiscal restraints to competing interests. If these are known and acknowledged in the meeting there is an opportunity to maximize the impact. I will offer examples and practical advice based upon both my scientific and legislative background.

10:24AM X60.00004: Science Legislative Fellow Advisors for State Legislatures* [Invited] NATHAN PHILLIPS (Presenter), Earth and Environment, Boston University — As a science fellow in the California legislature during 2014; in my current work to initiate a science policy fellowship program in Massachusetts; and in working alongside colleagues to bring science fellowships to nine other states, key recurring lessons learned which I will share in this talk are:

1. Science fellows in state legislatures are as valuable for how they think as for what they know.

2. State-level science policy fellowships not only benefit policymakers and policymaking, but powerfully benefit the scientific community and enterprise.

3. Professional rewards and fulfillment are of a different nature for state legislative science fellows than for academic scientists, but are no less rewarding nor fulfilling.

I will draw off my own anecdotes and experiences as a scientist in state legislatures to illustrate these points. I’ll also discuss the vast diversity of potential science fellowship program structures and how they may be appropriately matched to the diversity of states, political geography and legislative structures.

*California Council on Science and Technology
Gordon and Betty Moore Foundation
Simons Foundation

Friday, March 8, 2019 8:00 AM - 11:00 AM
8:00AM X61.00001: Design of graphene-based catalysts for Belousov Zhabotinsky reaction*  
D JAYA PRASANNA KUMAR, SACHIN VERMA, KABEER JASUJA, PRATYUSH DAYAL (Presenter), Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Use of hybrid materials containing structures at different length scales has gained significant traction because of their ability to provide multifunctional characteristics to soft materials. Here, we focus on the Belousov-Zhabotinsky (BZ) reaction, which represents a nonlinear chemical oscillator, and show that its dynamics can be tuned by using hybrid 2D materials, i.e., graphene-based nanosheets decorated with different nanoparticles (NPs). Specifically, we demonstrate that through the careful choice of NP decorations in designing our catalytic mats, frequency of chemical oscillations in the BZ reaction system can be increased four times. Further, we reveal that this observed behavior is attributed to enhanced access to active catalytic sites on NPs, as well as the rapid shuttling of electrons facilitated by the highly conductive graphene platform. We also perform modelling and simulation studies and our results reveal a strong correlation between the rate of charge transfer and the frequency of chemical oscillations. In essence, we showcase the ability of a 2D material, like graphene, to influence the dynamics of an oscillatory chemical reactions and anticipate that our approach will open up new avenues to tune the dynamics of chemical oscillators.

*DST-SERB (EMR/2016/007778)

8:12AM X61.00002: Self-moving reaction droplets synergized by graphene-based nanocomposites*  
D JAYA PRASANNA KUMAR (Presenter), PRATYUSH DAYAL, Department of Chemical Engineering, Indian Institute of Technology Gandhinagar — Chemo-mechanical transduction to perform locomotion is one of the characteristics of biological systems that has inspired the design of self-moving biomimetic systems. Here, we harness self-oscillating Belousov-Zhabotinsky (BZ) reaction, synergized by graphene-based catalytic mats to demonstrate spontaneous motion of the BZ reaction droplet in surrounding oil. Specifically, we synthesize graphene-based catalytic mats by decorating Ce and Ru nanoparticles (NP) on graphene nanosheets, thereby creating a 0D-2D heterostructures, and subsequently, use these mats to catalyze the BZ reaction. Our results demonstrate spontaneous locomotion of BZ droplets in oil bath due to the Marangoni flow that is brought about by the interaction between BZ reaction intermediates and surrounding oil. We further demonstrate that the velocity of the droplet motion is dependent upon the conductivity of the catalytic mats. In particular, we show two-fold increase in the droplet velocity when RuNP decorated graphene sheets are used to catalyze the BZ reaction instead of the traditional solution based BZ catalysts. Our findings can be used to design self-moving synthetic objects and opens up new avenues to control their behaviour through the use of 0D-2D hybrid nanomaterials.

*DST-SERB: EMR/2016/007778

8:24AM X61.00003: Enzyme-coated liposomes as dual-direction self-propulsive motors  
AMBIKA SOMASUNDAR (Presenter), Chemical Engineering, Penn State University, University Park, SUBHADIP GHOSH, Chemistry, Penn State University, University Park, FARZAD MOHAJERANI, Chemical Engineering, Penn State University, University Park, PAUL CREMER, Chemistry, Penn State University, University Park, DARRELL VELEGOL, Chemical Engineering, Penn State University, University Park, AYUSMAN SEN, Chemistry, Penn State University, University Park — Directional migration in response to specific chemical signals is critical for the survival of biological organisms. This enables living cells to move towards food, escape away from toxins, transport cargo and coordinate collective behavior. Controlling the motion of a motor either towards or away from chemical species is the first step in designing adaptive life-like synthetic motors. Model protocells derived from phospholipids and other amphiphiles have been studied and their movement through catalysis has been observed. However, control of directionality based on chemical cues (chemotaxis) has been difficult to achieve. In this talk, I will discuss both positive and negative chemotaxis of autonomous liposomal protocells based on the interplay between positive enzymatic catalysis-induced chemotaxis and solute-phospholipid interaction-based negative chemotaxis. In doing so, I will systematically rule out currently available mechanisms of colloidal transport and propose a potentially new and previously unrecognized mechanism of transport due to the Hofmeister effect. This opens up the possibility of other mechanisms for the transport of biological colloids.

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8:36AM X61.00004: Enhanced Diffusion and Chemotaxis of Catalytically Active Enzymes* [Invited] RAMIN GOLESTANIAN (Presenter), Department of Living Matter Physics, Max Planck Institute for Dynamics and Self-Organization, JAIME AGUDO-CANALEJO, TUNRAYO ADELEKE-LARODO, PIERRE ILLIEN, University of Oxford — Enzymes have been recently proposed to have mechanical activity associated with their chemical activity. In a number of recent studies, it has been reported that enzymes undergo enhanced diffusion in the presence of their corresponding substrate, when this substrate is uniformly distributed in solution. Moreover, if the concentration of the substrate is non-uniform, enzymes and other small molecules have been reported to show chemotaxis—biased stochastic movement in the direction of the substrate gradient—typically towards higher concentrations of this substrate, with a few exceptions. The underlying physical mechanisms responsible for enhanced diffusion and chemotaxis at the nanoscale, however, are still not well understood. We will review the available experimental observations of both enhanced diffusion and chemotaxis, and discuss critically the different theories that have been proposed to explain the two. We put particular emphasis on an equilibrium model recently introduced by us, which describes how the diffusion of dumbbell-like modular enzymes can be enhanced in the presence of substrate, thanks to a binding-induced reduction of the internal fluctuations of the enzyme. We then turn to chemotaxis, beginning with an overview of the chemotaxis-like diffusiophoretic behavior of micron-sized colloids in solute gradients, followed by a discussion of why chemotaxis at the nanoscale requires special consideration. Next, we review the experimental evidence of nanoscale chemotaxis, and describe a number of shortcomings and pitfalls in the phenomenological models for chemotaxis introduced in some of those works. Finally, we discuss a microscopic model for chemotaxis including both non-specific interactions and binding between enzyme and substrate recently developed by us, which overcomes many of these shortcomings, and is consistent with the experimental observations of chemotaxis.

*NSF under MRSEC Grant number DMR-1420620 and EPSRC.

9:12AM X61.00005: Single Molecule Imaging of Nanoscale Self-Propelled Active Matter MENGQI XU (Presenter), JENNIFER ROSS, University of Massachusetts Amherst, LYANNE VALDEZ, AYUSMAN SEN, Chemistry, Penn State University — Active matter composed of ensembles of self-propelled particles display exciting emergent properties. When coupled to larger objects, enzymes can act as the propulsion of self-propelled particles displaying exciting emergent properties. When coupled to larger objects, enzymes can act as the propulsion of self-propelled particles, and recent studies have shown that these enzymes have exciting self-propelled properties, as well. Studies using fluorescence correlation spectroscopy (FCS) or macroscopic observation have revealed that enzymes can perform enhanced diffusion depending on the substrate concentration. The mechanism for enhanced diffusion remains unclear. We report new results using single particle tracking with total internal reflection (TIRF) microscopy to observe this emergent activity of active enzymes to test proposed mechanisms that could result in enhanced mobility of active enzymes. Using urease as a model enzyme, we observe that the diffusion of individual enzymes increases three fold as a function of substrate. This diffusion is unaffected by the background concentration of enzymes. Further, we find that the oligomerization state is unchanged by the presence of the substrate, implying that the enzyme does not significantly change size upon binding of substrate. This work effectively eliminates some previously-postulated theories of the mechanism of enzymatically enhanced diffusion.

9:24AM X61.00006: Engineering active matter at the nanoscale with DNA nanotechnology IBON SANTIAGO (Presenter), Physics of Synthetic Biological Systems, Technical University of Munich — Self-generated movement in response to internal or environmental events is a key characteristic of living organisms that distinguishes them from non-living things. Progress in bio and nanotechnology has enabled the creation of active particles that can convert energy into motion. Catalytic self-propelled motors are of fundamental interest in statistical biophysics and are also highly necessary in the context of artificial cellular systems. Although much research has been done on micron-sized motors, progress in catalytic nanomotors of sub-100 nm is still in its infancy.

This talk will present recent work in the synthesis, propulsion mechanism and measurement techniques of self-propelled particles. The chemical synthesis of nanomotors and new electrochemical characterisation tools to assess their motor behaviour will be presented. Finally, I will demonstrate the coupling of enzymatic nanomotors to propel larger structures mediated by DNA hybridization.

Catalytic enzymes are active matter — AH-YOUNG JEE (Presenter), TSVI TLUSTY, STEVE GRANICK, Institute for basic science — Recent studies suggest that the enhanced diffusion of catalytically-active enzymes is promoted by super-diffusive “kicks” generated by the catalytic events. Pursuing this idea, we have explored methods to vary systematically the turnover frequency, $k_{\text{cat}}$, which defines how many substrate molecules are consumed in a given time. Our measurements using fluorescence correlation spectroscopy in super-resolution mode (FCS-STED) enable us to illuminate this matter. The contrast between motions in the presence of inhibitor and of substrate is especially interesting.

Directing Self-Propelled Enzymes and Enzyme-Coated Vesicles Using Chemical Signals* [Invited] AYUSMAN SEN (Presenter), Pennsylvania State University — The ability to move both towards and away from specific chemical signals is a critical survival mechanism in living systems. The motion itself arises from the harnessing of free energy from enzymatic catalysis. A variety of enzymes has been shown to undergo positive chemotaxis, moving up their substrate concentration gradient. We propose a general expression for the active movement of an enzyme in a concentration gradient of its substrate. The proposed model takes into account both the substrate-binding and catalytic turnover step, as well as the enhanced diffusion effect of the enzyme. The model is general, has no adjustable parameters, and only requires three experimentally defined constants to quantify chemotaxis. Model enzyme-functionalized synthetic protocells have also been studied and they exhibit both positive and negative chemotaxis based on the interplay between positive enzymatic catalysis-induced chemotaxis and solute-lipid interaction-based negative chemotaxis. Controlling the extent and direction of chemotaxis holds considerable potential for designing cell mimics and delivery vehicles that can reconfigure their motion in response to environmental conditions.

*The work was supported by the National Science Foundation (DMR-1420620 and CHE-1740630).

Exploring, exploiting, and ignoring history dependence in active droplet simulations* JOSEPH ALBERT (Presenter), VINCENT HENRY CRESPI, Pennsylvania State University — Active droplets are an appealing model system for studying self-propelled particles because of their high symmetry and simple composition. Nonetheless, their mechanism of action is complex - they are driven by a self-maintained concentration gradient that results in history-dependent motion.

This talk presents several formulations of this system which can be used to analyze and simulate active droplet systems. From these we establish how spherical droplets can emulate persistent motion of polar swimmers by storing orientation information in their local emission cloud. We show that this simplified picture of a droplet’s dynamics is sufficient to describe its response to an external potential or time-dependent force.

Simulations of interacting droplets suggest that Vicsek-like variables are sufficient to describe the system’s state. However, the pairwise interactions between particles are can be highly anisotropic and asymmetric, reflecting the system's history dependence at higher Péclet numbers.

*This work was funded by the Penn State MRSEC, Center for Nanoscale Science, under the award NSF DMR-1420620.

Sideways self-propulsion of Janus rods* NAVEEN REDDY (Presenter), Hasselt University, DUGYALA VENKATESHWAR RAO, Chemical Engineering, Indian Institute of Science Education and Research (IISER) Bhopal, JAN FRANSAER, Materials Science, KU Leuven, CHRISTIAN CLASEN, Chemical Engineering, KU Leuven — The sideways self-propulsion behaviour of Janus rods will be presented [1-2]. Janus rods are prepared by consecutively sputter-coating platinum and gold on different sides of aligned polystyrene nano/micro-fibers produced via electrospinning. Self-propulsion is induced via the reaction of hydrogen peroxide at the Janus particle interface, and the effect of the particles shape on their self-propulsion trajectories is studied. We show that the self-propulsion trajectories change from straight to circular when the particle shape is changed from a straight to an ‘L’ shaped rod. In order to understand and quantitatively describe the particle shape effects, we have adopted a mathematical model developed by Hagen et al [3] to predict their trajectories. We show that the trajectory of irregularly shaped rods depends only on the particle shape. The predicted trajectories for various particle shapes are in good agreement with the experimental observations. We show that these sideways self-propulsion rods are effective in cargo transportation.

References

*FWO (Grant No. G077916N) and KUL (PDM/16/123)
ABHRAJIT LASKAR (Presenter), OLEG SHKLYAEV, ANNA CHRISTINA BALAZS, University of Pittsburgh — Catalyst-coated, hard particles can spontaneously generate fluid flows, which in turn propel the particles through the fluid. If the catalyst-coated object were a deformable sheet, the self-generated flows could affect not only the sheet's motion, but also its shape. By developing models that capture the interrelated chemical, hydrodynamic and mechanical interactions, we uncover novel behavior emerging from the previously-unstudied coupling between active, soft sheets and the surrounding fluid. The chemically-generated flows “sculpt” the sheet into various forms that yield different functionalities, which can be tailored by modifying the sheet's geometry, patterning the sheet's surface with different catalysts and employing cascades of chemical reactions. These studies reveal how to achieve both spatial and temporal control over the position and shape of active sheets and thus, utilize the layers to autonomously and controllably trap soft objects, perform logic operations and execute multi-stage processes in fluid-filled microchambers.

Friday, March 8, 2019 8:00 AM - 10:48 AM

Session X63 GSOFT DBIO: Out-of-Equilibrium Properties of Soft Materials and Biological Systems BCEC 259A - Stephen Whitelam, University of California, Berkeley - Tag(s): Focus

8:00AM X63.00001: Early Career Award for Soft Matter Research [Invited] APARNA BASKARAN (Presenter), Brandeis University — tbd

8:36AM X63.00002: Designing active colloidal architectures from diffusiophoretic interactions* ANTOINE AUBRET (Presenter), JEREMIE PALACCI, University of California, San Diego — In Nature, energy input is needed to develop advanced features, e.g. self-healing or self-regulation. I will show how we can extend this principle to the artificial world, using light to carve non-equilibrium interactions between synthetic microswimmers. Following sequential light-patterns, they autonomously assemble into robust self-spinning structures, or microgears. A rotor constitutes a dissipative building block that creates a repulsive, anisotropic potential of diffusiophoretic origin, which we characterize using Highly Inclined Laminated Optical sheets microscopy (HILO). The results agree with analytical and numerical predictions of a simple model of a rotor forming a hexapolar sink of fuel. We show that gears act as contactless ‘teeth’, synchronizing their motion, and constitute the fundamental components of synchronized micro-machineries that auto-regulate and whose dynamics is tuned by the spins of their internal components. The study demonstrate the potential of non-equilibrium interactions to program self-assembly and control dynamical colloidal architectures beyond static, equilibrium assemblies.

*This material is based on work supported by the National Science Foundation, Grant No. DMR-1554724. J.P. thanks the Sloan Foundation for support through grant FG-2017-9392.

8:48AM X63.00003: "Light driven motion of active microswimmers" POOJA ARYA (Presenter), DAVID FELDMANN, SVETLANA SANTER, Institute of Physics and Astronomy, University of Potsdam, Germany — We report on active colloids which can undergo light-driven self-propelled motion. The mechanism of self-propulsion is based on generation of local hydrodynamic flow at each micro-particle resulting from light-driven diffusioosmosis (LDDO) [1]. At the heart of this process is photosensitive azobenzene containing surfactant which undergoes a reversible trans-cis photo-isomerization with corresponding changes in hydrophobicity of the whole surfactant molecule. Active microparticles consist of porous silica and are negatively charged in water. When porous silica particles are dispersed in the solution of cationic photosensitive surfactant, they absorb partially the surfactant in trans-state, but the more hydrophilic cis-isomers are expelled out of the particles. Under illumination with blue light promoting trans-cis photo-isomerization, a continuous local hydrodynamic flow at a single particle is formed where cis-isomers leave the particle, while trans-isomers flow inside. The particles become active when one side of the porous surface is covered with a metal layer.

9:00AM X63.00004: Transport Processes in Active Fluids  KATHERINE KLYMKO (Presenter), CCSE, Lawrence Berkeley National Laboratory, JEFFREY EPSTEIN, Physics, Univ of California - Berkeley, KRANTHI K MANDADAPU, Chemical Engineering, Univ of California - Berkeley — We perform a coarse-graining analysis of the paradigmatic active matter model, Active Brownian Particles, yielding a continuum description in terms of balance laws for mass, linear and angular momentum, and energy. The derivation of the balance of linear momentum reveals that the active force manifests itself directly as a continuum-level body force proportional to an order parameter-like director field, which therefore requires its own evolution equation to complete the continuum description of the system. We derive this equation, demonstrating in the process that bulk currents may be sustained in homogeneous systems only in the presence of inter-particle aligning interactions. Further, we perform a second coarse-graining of the balance of linear momentum and derive the expression for active or swim pressure in the case of mechanical equilibrium.

9:12AM X63.00005: Competition between chiral self-replicators is mediated by surface growth dynamics  ASHISH B. GEORGE (Presenter), KIRILL KOROLEV, Boston University — Phase separation and self-assembly of chiral components underlie many biological and industrial processes. We study how chirality of the components impacts these processes. Motivated by recent experiments with microbes, we focus on two-dimensional growth of auto-catalytic or self-replicating agents. The dynamics, described by a chiral reaction-diffusion equation, recapitulate experimental findings in homochiral populations. We predict very unusual behavior when there are two distinct chiral components. Depending on the relative chirality of each, the population evolves to a stable mixed state with both components or a homochiral state where one component goes extinct. To explain our results, we derive an effective theory that couples component competition and growth front dynamics. The theory reduces to a chiral extension of the KPZ equation coupled to a Burgers’ equation with multiplicative noise. The solution of these equations exhibits bulges and dips on the surface at boundaries between domains with different chirality. These undulations in turn alter the motion of the domain boundaries and determine composition and spatial structure. Our findings suggest a new class of surface growth phenomena and can explain the rapid evolution of chirality in biological populations.

9:24AM X63.00006: Self-oscillating poroelastic instabilities  DAVID DYKSTRA (Presenter), NIGEL VISSER, CORENTIN COULAIIS, Institute of Physics, University of Amsterdam — Responsive materials changing shape in response to physical stimuli such as light, heat or chemical reactions are ubiquitous in nature and have recently sparked a myriad of applications, e.g. in smart coatings and soft robotics. So far, stimuli-responsive materials are not “active”: they cannot exhibit a perpetual motion unless the environmental conditions change. Here we show experimentally, numerically and theoretically how a simple system - a confined beam at the boundary of a solvent interface - can harness a combination of poroelastic swelling and elastic instabilities to generate perpetual oscillations. These oscillations are realised by rational design and optimisation of the time-dependent hysteretic loop coupling mechanical deformation to solvent transport within the structure. Our work provides general principles for active systems that operate autonomously, harnessing energy from their environment and as such offers new vistas for active metamaterials and soft robots.

9:36AM X63.00007: Dynamic clustering of passive colloids in an active bacterial bath*  SHREYAS GOKHALE (Presenter), JUNANG LI, ALEXANDRE SOLON, NIKTA FAKHRI, JEFFREY GORE, Massachusetts Institute of Technology — Active or self-propelled particles such as motile bacteria often exhibit exotic forms of self-organization on account of their intrinsically nonequilibrium dynamics. Further, it is known that these nonequilibrium dynamics can be harnessed to manipulate passive objects such as microscopic gears and motors. Here, using video microscopy experiments and numerical simulations, we show that the nonequilibrium fluctuations in a bath of motile *Pseudomonas aurantiaca* bacteria can spontaneously drive the self-assembly of suspended passive colloidal silica particles. In contrast to the phase separation between active and passive particles reported in previous computational studies, we observe a dynamic clustering phenomenon with frequent formation and fragmentation events. We demonstrate that the mean cluster size increases with increasing bacterial density. Moreover, we extract an effective attractive interaction energy scale from the distribution of bond lifetimes and show that it correlates well with the mean cluster size. We hypothesize that a local transient circulation of the bacterial velocity field around colloidal particles is responsible for the observed attractive interactions.

*S.G. thanks the Human Frontier Science Program (HFSP) for a cross-disciplinary postdoctoral fellowship.

9:48AM X63.00008: Large Deviation Functions for active Brownian particles  TREVOR GRANDPRE (Presenter), Physics, UC Berkeley, DAVID LIMMER, Chemistry, UC Berkeley, KRANTHI K MANDADAPU, Physics, UC Berkeley, KATIE KLYMKO, Lawrence Berkeley Lab — Large deviation Functions (LDFs) characterize fluctuations of extensive observables away from equilibrium and offer a route to relate those fluctuations to the systems response to external perturbations. LDFs are difficult to calculate analytically and sometimes numerically for complex interacting systems. For a system of interacting active Brownian particles, we show how a weighted many body expansion can be used to calculate LDFs for a wide variety of relevant observables such as the mass current, active work, and activity. These in turn can be used to understand diverse phenomena such as the Motility Induces Phase Separation (MIPS) and active transport.
Solids has brought new light to a multitude of problems - active foam provides a new platform to ask questions both in (phase). Stroboscopic analysis is used when studying cyclic forcing. Just like our understanding of active fluids and active evolution. Next, we study interactions between multiple active voxels with cyclic perturbations (in-phase and out-of-motion. We quantify this response of a single active voxel as a function of energy injected, symmetry and time course of injection triggers rearrangements in the structure involving neighbor swapping (T1), leading to cascades and global programmatically injected and removed from voxels in a 2D liquid soap foam in a Hele-Shaw cell. This cyclic energy such a material, where the activity of a single voxel is driven by volume oscillations. The platform allows air to be feedback. To the best of our knowledge, no abiotic "active" foam experimental systems currently exist. We have developed example include the central channel of the nuclear pore complex and liquid drops formed from multivalent interactions. Some biophysical interactions are typically non-specific and cannot be tuned. In contrast, macromolecular diffusion through networks can be controlled by binding and unbinding events between passing molecules and flexible chains. Some biophysical examples such as binding and unbinding rates, number of binding sites and chain elasticity, on diffusion is still poorly understood. Following a statistical mechanics approach, we have developed a diffusion model which shows that the maximum diffusion occurs for few occupied binding sites independent of other parameter choices. We show the validity of our findings by comparing model predictions with a macroscopic diffusion experiment designed to contain similar driving mechanisms and to allow tuning of key parameters including the number binding sites, activity and kinetic parameters. These findings will drive future research work and understanding of controlled active diffusion in dynamic networks.

*NSF CAREER award 1350090, NIHGMs R35 GM119755, Boettcher Foundation

Propagating Fronts in Columns of Fire Ants CALEB ANDERSON (Presenter), ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — For the past two decades, the study of active matter has revealed rich physics and universal behaviors, such as collective motion, across a wide variety of biological and synthetic systems with seemingly disparate particle interactions. Here we present our surprise observation and measurements of stable activity fronts propagating through 2 dimensional columns of thousands of fire ants. We then propose a model to explain the origin of these macroscopic non-linear fronts from simplified pairwise interactions between ants, and perform computer simulations that capture the experimental observations. Finally, we finish by comparing the fronts to other instances of collective motion observed in active systems.

Mechanics of Active Foam: Local Energy Injection in Addressable 2D Foam+ LAUREL KROO (Presenter), Department of Mechanical Engineering, Stanford University, MANU PRAKASH, Department of Bioengineering, Stanford University — The study of foam has inspired many insights into cellularized materials, including biological tissue. While cellular sheets superficially resemble passive foam structures, cells incorporate many layers of internal activity and feedback. To the best of our knowledge, no abiotic "active" foam experimental systems currently exist. We have developed such a material, where the activity of a single voxel is driven by volume oscillations. The platform allows air to be programatically injected and removed from voxels in a 2D liquid soap foam in a Hele-Shaw cell. This cyclic energy injection triggers rearrangements in the structure involving neighbor swapping (T1), leading to cascades and global motion. We quantify this response of a single active voxel as a function of energy injected, symmetry and time course of evolution. Next, we study interactions between multiple active voxels with cyclic perturbations (in-phase and out-of-phase). Stroboscopic analysis is used when studying cyclic forcing. Just like our understanding of active fluids and active solids has brought new light to a multitude of problems - active foam provides a new platform to ask questions both in foam physics and, by analogy, in tissue mechanics.

+This research was funded by NSF (GRFP, 1453190) and CZ Biohub.

Friday, March 8, 2019 8:00 AM - 11:00 AM
8:00AM X64.00001: Probing the dynamics of individual biomolecules with 1-μs resolution* [Invited] THOMAS PERKINS (Presenter), JILA, NIST & University of Colorado Boulder — Protein folding occurs as a set of transitions between structural states within an energy landscape. An oversimplified view of the folding process emerges when transiently populated states are undetected because of limited instrumental resolution. To achieve state-of-the-art performance, we integrated several recent technical advances that improve the precision, stability, and accuracy of AFM-based single molecule force spectroscopy. Using modified cantilevers optimized for 1-μs resolution, we reexamined the unfolding of individual bacteriorhodopsin (bR) molecules in native lipid bilayers. The experimental data revealed the unfolding pathway in unprecedented detail. Numerous newly detected intermediates—many separated by as few as 2–3 amino acids—exhibited complex dynamics, including frequent refolding and state occupancies of <10 μs. Equilibrium measurements between such states enabled the folding free-energy landscape to be deduced. These results sharpen the picture of the mechanical unfolding of bR. Finally, recent efforts to improve the quantity and quality of AFM studies of diverse biomolecules, including nucleic-acid structures and globular proteins, will be discussed.

*This work was supported by the National Science Foundation (MCB-1716033; Phy-1734006) and the National Institute of Standards and Technology.

8:36AM X64.00002: Destabilization of nucleosomes by HMGB proteins and FACT complexes [Invited] MICAH J MCCAULEY, RAN HUO, EMILY NAVARRETE, Northeastern University, NICOLE BECKER, QI HU, MOLLY NELSON HOLTE, Department of Biochemistry and Molecular Biology, Mayo Clinic College of Medicine and Science, UMA M MUTHURAJAN, Department of Chemistry and Biochemistry, University of Colorado, IOULIA ROUZINA, Department of Chemistry and Biochemistry, Ohio State University, KAROLIN LUGER, Department of Chemistry and Biochemistry, University of Colorado, GEORGES MER, L. JAMES MAHER, Department of Biochemistry and Molecular Biology, Mayo Clinic College of Medicine and Science, NATHAN ISRAELOFF, MARK WILLIAMS (Presenter), Northeastern University — Nucleosome disruption plays a key role in many nuclear processes including transcription, DNA repair and recombination. We combine atomic force microscopy (AFM) and optical tweezers (OT) experiments to probe the effects of various motifs of High Mobility Group B (HMGB) proteins on nucleosome stability. We find that the double box Hmo1 and the single box Nhp6A from \textit{S. cerevisiae} destabilize and unwind DNA from the H2A-H2B dimers that are part of the histone octamer. Unlike Nhp6A, Hmo1 also releases half of the DNA held by the (H3-H4)$_2$ tetramer. Despite this destabilization, the octamers appear intact, and the remaining (H3-H4)$_2$ tetramer interactions with the DNA are also destabilized. We also probe the human histone chaperone protein FACT (facilitates chromatin transcription), which also contains an HMGB box. We find that FACT (including the subunits Spt16 and SSRP1) binds directly to the nucleosome, specifically disrupting the H2A-H2B dimer interaction with DNA. Disruption leads to the release of that DNA from the nucleosome and the ejection of these dimers from the octamer, revealing a mechanism for regulation of chromatin assembly. Differences in nucleosome destabilization point to complementary roles that HMGB proteins play in chromatin remodeling.

9:12AM X64.00003: Single ligand and receptor binding spectroscopy using an atomic force microscopy* LINA ALHALHOOLY (Presenter), Physics, North Dakota State University, MATTHEW CONFELD, Pharmaceutical Sciences, North Dakota State University, YONGKI CHOI, Physics, North Dakota State University — Binding and unbinding between individual ligands and receptors were measured and quantified using an atomic force microscopy (AFM). Initially, the cell stiffness is characterized by force-distance measurements using ligand-free AFM tips and compared to several cancer and non-cancerous cells. Then, we measured the unbinding force with peptide-coated AFM tips, targeting specific cell receptors. The unbinding force between the ligand and receptor was measured to be an order of 100 pN. Such individual, specific interaction measurements were further supported by pre-blocking the cell receptors with the excess, free ligands.

*This research was supported by the NIGIM/NIH R15GM122063 and 1P20GM109024 (Pilot Project).
9:24AM X64.00004: Single Molecule Studies of a Novel Mechanism of Bacterial Transcription Initiation*  
DEBORA TENENBAUM (Presenter), JANE KONDEV, JEFF GELLES, Brandeis University — In bacteria, gene transcription begins with the binding of an RNA polymerase (RNAP) core enzyme to the initiation factor σ, which allows it to recognize promoter sequences on the DNA and initiate RNA synthesis. In the canonical transcription cycle, upon reaching the termination sequence and releasing the transcript, RNAP detaches from the DNA and is free to restart the process. However, previous work in our lab has shown that following termination, bacterial RNAP frequently remains bound to the DNA template, and sometimes exhibits one-dimensional sliding over thousands of basepairs. Moreover, in the presence of free σ factor molecules in solution, the sliding, DNA-bound polymerase is often observed to restart transcription. This mechanism of transcription initiation might have implications for the transcriptional coupling of nearby genes.

In this talk, I will describe single-molecule fluorescence-microscopy experiments we are doing to further characterize this novel mechanism of transcription initiation in vitro, and to evaluate its role in the coupling and coordination of gene expression.

*This work was supported through grants from the National Institutes of Health.

9:36AM X64.00005: Single-molecule orientation mapping in 3D using a novel optical design  
ABHISHEK KUMAR (Presenter), University of Maryland, College Park, JAMES M MARR, Materials Measurement Laboratory, National Institute of Standards and Technology, ANTHONY MAUTINO, University of Maryland, College Park, MARK MCLEAN, JEREMIAH WOODCOCK, JEFFREY GILMAN, STEPHAN STRANICK, Materials Measurement Laboratory, National Institute of Standards and Technology, VERONIKA SZALAI, JAMES LIDDLE, Physical Measurement Laboratory, National Institute of Standards and Technology — Single molecule (SM) localization-based super-resolution techniques have revolutionized the application of optical microscopy because of their ability to image structures below the diffraction limit in widefield. Fluorescent dyes and proteins used for SM imaging absorb and emit photons via an emission dipole, and any restriction on the motion of the dipole creates an asymmetry in the observation of the emission. Mapping this dipolar orientation can be a useful reporter of the local environment of molecules, and help improve localization accuracy for super-resolution imaging. We present a simple and flexible optical design, that can be incorporated into a standard optical microscope, to enable mapping the orientation of single molecules by simultaneously imaging 4 polarization orientations. A single camera is used to acquire all 4 channels, and fine adjustment controls for each channel minimize optical aberrations. We have used nanofabricated aperture arrays, fluorescent beads and single molecules embedded in a polymer matrix to characterize the system.

9:48AM X64.00006: Single molecule study of the stability of G-quadruplex DNA as an anti-cancer drug target  
PARASTOO MALEKI (Presenter), HAMZA BALCI, Kent State University — In targeted therapy, small molecule drugs are utilized to detect specific targets. G-quadruplex (GQ) structures are such a target for targeted cancer therapy. GQ is a physiologically significant secondary structure of DNA or RNA, which is formed by guanine-rich sequences. Studies on cancer cells show that stabilizing the GQ structures in telomeres with small molecules reduces telomerase activity and proliferation of cancer cells. However, the underlying dynamics of small molecule-GQ interactions are not known. In this study, we performed single molecule measurements to study how stability and dynamics of GQ are impacted by its interactions with several different small molecules. Moreover, we investigated the impact of these molecules on folding dynamics of the GQ structure. We observed significant enhancement in GQ stability in the presence of small molecules, as measured by the fraction of GQ molecules that remained folded against Bloom helicase mediated unfolding at the single molecule level. In addition, our measurements showed that folding of GQ takes place faster than our time resolution over all salt concentrations we studied (2-150 mM KCl) with or without small molecules, making it challenging to identify the impact of small molecules.
Single-Molecule Activity of φ29 DNA Polymerase Monitored by Nanoscale Transistors

CALVIN LAU (Presenter), KRISTIN NICHELLE GABRIEL, NAREN德拉 KUMAR, SUDIPTA MAJUMDAR, ARITH RAJAPEAKSE, WONBAE LEE, GREGORY WEISS, PHILIP G COLLINS, University of California, Irvine — Single-molecule techniques are enabling the rapid advancement of next-generation DNA sequencing. Recently, electronic nanocircuits functionalized with DNA polymerases have arisen as a new, potentially high-density and high-throughput platform for single-molecule DNA sequencing and enzyme kinetic studies [1]. Here, we describe single-molecule electronic measurements of φ29 DNA polymerase, an enzyme having extremely high fidelity and processivity. Using φ29 linked to carbon nanotube transistors, base-by-base activity of individual polymerase molecules was continuously monitored for up to 30 min as the enzymes replicated single-stranded templates. Base incorporation rates averaged 20 s⁻¹ but varied widely. Rates up to 200 and 400 s⁻¹ occurred when φ29 encountered homopolymeric sequences of poly(dT) and poly(dC), respectively. On the other hand, the processing of poly(dA) and poly(dG) sequences was dominated by pauses lasting 50 to 300 s. Such observations of sequence-dependent activity demonstrate how single-molecule methods can excel over traditional, ensemble-based techniques like PCR sequencing and gel chromatography assays.


Reliable extraction of energy landscape properties from critical force distributions

SUDEEP ADHIKARI (Presenter), KEVIN BEACH, University of Mississippi — The structural dynamics of biopolymers such as proteins are described in the context of their conformational energy landscapes. In pulling experiments using optical tweezers, features of the energy landscapes are extracted from the probability distribution of the critical force at which the polymer unfolds, and typically the analysis is based on rate equations having Bell-Evans form. We argue that this analysis is inadequate and leads to unreliable landscape parameters in many common situations. We propose a modified closed-form expression for the distribution of critical forces that works better for parameter extraction and is valid even up to fast pulling rates. We present results based on simulated data that confirm the utility of our new formula.

Quantifying Collective Dynamics in the Ribosome

MARIANA LEVI, PAUL WHITFORD (Presenter), Northeastern University — The functional dynamics of molecular assemblies often involve large-scale collective rearrangements. While these motions occur in a high-dimensional space, experiments are typically only able to simultaneously measure a small number of interatomic distances. Accordingly, a major challenge in single-molecule studies is to identify kinetically-relevant degrees of freedom. To address this issue for the ribosome, we use a range of theoretical models and molecular dynamics simulations in order to simulate hundreds of spontaneous large-scale (~30-50 Å) conformational transitions at various points of the elongation cycle. With these large data sets, we are assessing the ability of experimentally-accessible coordinates to capture the rate-limiting free-energy barriers. This analysis suggests design strategies for next-general experiments, as well as helps rationalize controversial/contradictory experimental observations. Finally, these calculations provide a quantitative foundation that is allowing us to study the precise relationship between structure and dynamics in the ribosome.

Relaxation spectrum of a concentration quench of Brownian particles.

AYKUT ERBAS (Presenter), UNAM, Bilkent University, JOHN FREDERICK MARKO, MONICA OLVERA DE LA CRUZ, Northwestern University — Single-molecule or SPR (Surface Plasmon Resonance) experiments rely on the relaxation of concentration quenches of initially surface-bound molecules into confined reservoirs to determine molecular kinetic rates. Similarly, biological processes such as exocytosis, in which small molecules are emitted into the intracellular cleft for cellular communication, can be considered to be a relaxation process of an effective concentration quench. We study a model system closely related to the above cases in which weakly interacting Brownian particles are released from their binding sites into a confined volume by using molecular dynamics simulations and scaling arguments. Our results suggest that the rebinding rate of released particles exhibits various power laws until the confined volume is entirely filled by the particles. Furthermore, the cumulative rebinding rate, which is the time integration of the rebinding rate, exhibits a novel plateau behavior. This plateau is a result of the decreasing number of collisions between sparsely-placed binding sites and dissociated ligands. Our results can have important consequences for molecular signaling as well as for the interpretation of kinetic measurements of ligand-receptor interactions.
10:48AM X64.00011: Incorporating photo-artifacts into the analysis of single molecule FRET measurements

IOANNIS SGOURALIS (Presenter), Arizona State University — Single molecule experiments, such as those measuring FRET, encode precise information on individual molecules free of bulk averaging. Nevertheless, because smFRET assessments employ conventional fluorescence microscopy setups, artifacts such as background photons, shot-noise, cross-talk, and fluorophore blinking are limiting factors that necessitate the use of advanced analysis methods. In our recent work we employ infinite hidden Markov models and propose a novel formulation to model and analyze smFRET measurements that contains nonparametric statistics with an explicit representation of the fluorophore photo-physics. As a result, our method combines the advantages of traditional hidden Markov models while it avoids the associated state-space size restrictions or other model selection assumptions. For this, we carefully formulate the measurement process itself accounting for the photo-physics on the individual donors and acceptors in addition to the other experimental characteristics. As a result, our framework obtains accurate estimates even when recorded intensities are excessively noisy, photo-blinked, and also of short duration. Finally, our estimates remain accurate even when fluorophore photo-states alternate at scales comparable to those of the FRET efficiency itself.

Friday, March 8, 2019 8:00 AM - 11:00 AM

Session X65 DBIO GSOFT: Physics of Development and Stem Cells

University - Tag(s): Focus

8:00AM X65.00001: The mechanics of epithelial folding* [Invited] ADAM MARTIN (Presenter), HANNAH YEVICK, Biology, MIT — Throughout the lifespan of an organism, tissues are remodeled to shape organs and organisms and to maintain tissue integrity and homeostasis. Apical constriction is a ubiquitous cell shape change of epithelial tissues that promotes epithelia folding and cell/tissue invagination in a variety of contexts. Apical constriction promotes tissue bending by changing the shape of constituent cells from a columnar-shape to a wedge-shape. Drosophila gastrulation is one of the classic examples of apical constriction, where cells constrict to fold the primitive epithelial sheet and internalize cells that will give rise to internal organs. We find that the apical constriction of these cells constrict via repeated contractile pulses of the cytoskeleton, specifically actin filaments and the molecular motor myosin II. Contractility of the cells results in anisotropic tension, which is essential for the proper orientation of the fold. We are investigating mechanisms that pattern contractility across the tissue to ensure robust folding.

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American Cancer Society
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8:36AM X65.00002: Lineage and state dynamics in stem cell differentiation* [Invited] ALLON KLEIN (Presenter), Systems Biology, Harvard Medical School — High-dimensional single cell measurements allow capturing snapshots of dynamic transitions in biological systems. Over the past few years, measurements such as single cell RNA-Seq (RNA-Seq) have come to be routinely used in stem cell biology. However, as single cell measurements necessarily destroy cells, they do not definitively reveal long-term dynamic behaviors. Various theoretical models have been invoked to link static snapshots to dynamics, all necessarily making assumptions. I will describe the assumptions underlying one such model of a Fokker-Planck type, and its limitations. I will then show how the combination of lineage data in single cell transcriptomes allows explicitly testing dynamic inference models on single cell RNA-Seq data. Our results show the successes but also failures of dynamic inference, and provide a test demonstrating the existence of "hidden variables" underlying cellular dynamics as measured by RNA-Seq. The results and methods are applied to the lineage hierarchy of hematopoiesis.

*The presentation will cover work supported by NIH grants 5R33CA212697-02 and 1R01HL14102-01, the Chan-Zuckerberg Initiative grant 2018-182714, and the Harvard HSCI Blood Pilot Program DP-0174-18-00. AMK additionally acknowledges funding support by the Burroughs-Wellcome Fund CASI award, and by the Edward J Mallinckrodt foundation.
Animals vary more in size than in proportions; a possible quantitative version of this observation would be that organisms exhibit scaling, so that the dimensions of different body segments all vary in proportion to the overall size of the organism. If this were true, pattern formation in biological systems would be qualitatively different from that in the non-biological pattern forming systems that we understand, such as Rayleigh-Benard convection and directional solidification. A relatively pure version of this question is accessible in the early development of insect embryos, where a "blueprint" for the final segmented body plan is visible in striped patterns of gene expression. We measure the positions of these stripes in an ensemble of 100+ embryos from a laboratory strain of *Drosophila melanogaster*, under controlled conditions. These embryos vary in length by only 4% (rms), yet we can resolve the scaling of stripe positions with length. The resulting 1% accuracy of relative positions is so high as to exclude alternatives, such as combinations of unscaled signals from the two ends of the embryo.

*Supported in part by the NSF Center for the Physics of Biological Function (PHY--1734030), Center for the Science of Information (CCF-0939370), and grant PHY-1607612; and by HHMI.

The formation of somites is a self-organizing mechanical process that has received little attention so far. In this work, we build a 2D computer model of mesenchymal to epithelial transition process to explore the cellular mechanisms that promote somite organization. We focus on the first stage of somite formation, the establishment of the dorsal layer as an anterior propagating wave of cell maturation. First we explore and discuss the separate and combined contributions of cell polarization, adhesion and elongation to the formation of the dorsal layer. Finally, we explore the process of apical constriction and show how the forming layer is segmented into discrete units.

*NIH Grants R01 GM076992, U01 GM111243 and R01 GM077138

In order to study experimental signatures of the limiting-pool mechanism, we consider a simple model of the self-assembly of two spherical structures from a common pool of building blocks. Using theory and simulations, we analyze the time series of the sizes of the spherical structures and make specific predictions about their autocorrelation functions. We then compare these theoretical results to fluorescence data from experiments that measure nucleoli size as a function of time in late stages of *C. elegans* embryo development. This approach can be used in other experimental systems to quantitatively test for the limiting-pool mechanism, and can be extended to other size-control mechanisms.

*NSF grants DMR-1610737, the Simons Foundation grant 400108
ANDREW MUGLER, Purdue University — Morphogen profiles allow cells to determine their position within a developing static disorders in the system due to coupling to other dynamical processes. We developed a deep-learning based live cell imaging and analysis procedure to trace single cell trajectories in high-dimensional morphology space. Using TGF-β induced Epithelial-to-Mesenchymal transition (EMT) in human HK2 cells as a model system, we experimentally depicted the quasi-potential landscape of EMT, identified three distinct morphology states that are correlated with different expression levels of EMT regulators and markers. We further reconstructed an extended state network that depicts coupling between cell cycle and EMT, and quantified the transition matrix from single cell data. In many aspects the single cell studies are analogous to the more established single molecule approaches in molecular biophysics, while the transition process under study is complicated by existence of dynamic and static disorders in the system due to coupling to other dynamical processes.

10:00AM X65.00007: Structural redundancy in supracellular actomyosin network connections enables robust tissue folding  HANNAH YEVICK (Presenter), PEARSON MILLER, JORN DUNKEL, ADAM MARTIN, Massachusetts Institute of Technology — It is essential for the fate of an organism that key morphogenetic processes occur reproducibly. While much is known about how genetic regulation achieves robustness, less is known about how a tissue mechanically ensures reproducibility. Gastrulation is an indispensable stage of development. Drosophila fruit fly gastrulation is driven by myosin-dependent constriction and this robust large-scale movement requires coordinated forces at the tissue level. Yet, how the cytoskeleton is connected across the constricting tissue to realize shape change is unknown. We demonstrate a high degree of robustness in Drosophila gastrulation whereby ablating many cells doesn’t halt shape change. To understand this robustness, we integrated concepts from graph theory to analyze the connectivity of a supracellular network of myosin connections that links cells in the tissue. We found that a dense meshwork of tissue scale connections ensures structural redundancy and that even when large numbers of connections are lost some paths across the tissue persists and folding proceeds. We propose that in the same way that redundancy ensures the large-scale function of telecommunication or transportation networks under localized failures, the organization of myosin activation enables robust morphogenesis.

10:12AM X65.00008: Diffusion vs. direct transport in the precision of morphogen readout  SEAN FANCHER (Presenter), ANDREW MUGLER, Purdue University — Morphogen profiles allow cells to determine their position within a developing organism, but there are multiple mechanisms by which these profiles form, and in some cases the mechanism is still not agreed upon. Here we derive fundamental limits to the precision of morphogen concentration sensing for two canonical mechanisms: the diffusion of morphogen through extracellular space and the direct transport of morphogen from source cell to target cell, e.g. via cytonemes. We find that direct transport establishes a morphogen profile without adding extrinsic noise. Despite this advantage, we find that for sufficiently large values of population size and profile length, the diffusion mechanism is many times more precise due to a higher refresh rate of morphogen molecules. We compare our predictions with data from a wide variety of morphogens in developing organisms.

10:24AM X65.00009: Intracellular crowding as mechanoregulator of intestinal organoid growth via modulating Wnt-receptor complex phase transition*  YIWEI LI (Presenter), JILIANG HU, MING GUO, Mechanical Engineering, Massachusetts Institute of Technology — Enormous amounts of essential intracellular events are crowdedly packed inside picoliter-sized cellular space. However, the significance of the physical properties of cells remains underappreciated due to a lack of evidence of how they impact cellular functionalities. Here, we show that the degree of intracellular crowding serves as a mechanoregulator of intestinal organoid growth via modulating Wnt/β-catenin signaling. Intracellular crowding varies upon stimulation by different types of extracellular physical and mechanical cues, and leads to a significant enhancement of Wnt/β-catenin signaling by promoting phase transition of LRP6 receptor complex. By enhancing intracellular crowding using either osmotic or mechanical compression, we show that expansion of intestinal organoids was facilitated through elevated Wnt/β-catenin signaling and greater intestinal stem cells (ISCs) self-renewal. Our results provide an entry point for understanding how intracellular crowdedness functions as a mechanotransducer linking extracellular physical cues with intracellular signaling, and potentially facilitate the design of engineering approaches for expansion of stem cells and organoids.

*This work is funded by NSF.
Population variation in human pre-implantation embryo development, or: how I learned to stop worrying and love IVF data.  

BRIAN LEAHY (Presenter), HELEN YANG, RONALD ALEXANDER, VINOTHAN MANOHARAN, DANIEL NEEDLEMAN, Harvard University — The early mammalian embryo is the physicist's dream for studying development. Between fertilization and implantation in the uterus, the mammalian embryo undergoes a global reorganization (compaction) followed by a symmetry-breaking differentiation (blastocyst formation), with no external direction from the mother. While studies on mouse embryos illuminate the mechanisms of development, the genetic homogeneity of lab mice obscures the natural variability in mammalian development. Here, we examine thousands of videos of human embryos recorded during IVF procedures to explore the natural variability in mammalian pre-implantation embryo development. We leverage this variability to infer possible regulatory mechanisms in early development. Finally, we will discuss our work on extending non-invasive 3D microscopy to imaging human embryos.

Biophysical studies of metabolic control in mouse oocytes and embryos  

XINGBO YANG (Presenter), TIM SANCHEZ, MARTA VENTURAS, DANIEL NEEDLEMAN, Molecular and Cellular Biology, Harvard University — While a great deal is known about pathways and enzymology of carbohydrate metabolism, it is still poorly understood how metabolic fluxes are modulated during development and in response to environmental factors, or degraded in disease. Mounting evidence suggests that defects in metabolism may cause chromosome segregation errors in eggs and embryos, leading to age related infertility in women, but the possible underlying mechanisms remain unclear. We are developing and testing a coarse-grained biophysical model of enzyme engagement of electron carriers, with the goal of extracting metabolic fluxes from fluorescence lifetime imaging microscopy measurements. We are attempting to construct a theory of the control of mitochondrial respiration and cytoplasmic fermentation in mouse oocytes and embryos by using this approach in conjunction with metabolic manipulations. Our preliminary results argue that the fluxes through these pathways can be redirected in response to perturbations, but this is accompanied by large changes in cell biological features, including disassembly of the spindle, which we speculate might underlie the connection between metabolic defects and chromosome segregation errors.

Systematic mutagenesis of oncocin reveals enhanced activity and insights into the mechanisms of antimicrobial activity*  

PIN-KUANG LAI (Presenter), KATHRYN GELDART, SETH RITTER, YIANNIS KAZNESSIS, BENJAMIN HACKEL, University of Minnesota — Oncocin is a proline-rich antimicrobial peptide that inhibits protein synthesis by binding to the bacterial ribosome. The aim of this work is to improve the antimicrobial activity of oncocin by systematic peptide mutagenesis and activity evaluation. We discovered that a pair of cationic substitutions (P4K and P7K/R) enhanced the activity by 2 to 4 fold (p<0.05) against multiple Gram-negative bacteria. An in vitro transcription / translation assay indicated that the increased activity was not because of stronger ribosome binding. Instead a cellular internalization assay revealed a higher internalization rate for the optimized analogs thereby suggesting a mechanism to increase potency. In addition, we found that the optimized peptides' benefit is dependent upon nutrient-depleted media conditions.

*This work was supported by grants from the National Institutes of Health (R01GM121777 and R01GM111358) and by a grant from the National Science Foundation (CBET-1412283). We acknowledge computational support from the Minnesota Supercomputing Institute and from the Extreme Science and Engineering Discovery Environment, which is supported by the National Science Foundation.
Quantifying the Formation and Dissolution of Multilayer Regions in the Expansion of Twitching Bacterial Colonies

ERIN SHELTON (Presenter), Department of Physics, University of Guelph, LORI BURROWS, Department of Biochemistry and Biomedical Sciences, McMaster University, JOHN DUTCHER, Department of Physics, University of Guelph — Type IV pili (T4P) are very thin (5-8 nm in diameter) protein filaments that can be extended and retracted by certain classes of Gram-negative bacteria including P. aeruginosa [1]. These bacteria use T4P to move across viscous interfaces, referred to as twitching motility. Twitching can occur for isolated cells or in a collective manner [2]. In collective motion, the advancing front of an expanding colony consists of finger-like protrusions consisting of many aligned bacteria, with 5 to 30 cells across the fingers, followed by cells that twitch within a lattice-like pattern. During the outward radial motion of the fingers along an agar-glass interface, cells can vertically displace the agar to form multilayer regions. Using our custom-built, temperature- and humidity-controlled environmental chamber, we have studied the formation and dissolution of multilayer regions within fingers for a range of agar concentrations. We find that there is a minimum finger width required for the stability of multilayer regions.


Magnetotactic bacterial scattering in porous media hinders transport

AMIN DEHKHARGANI (Presenter), NICOLAS WAISBORD, THOMAS COONS, JEFFREY S. GUASTO, Tufts University — Swimming cells exhibit complex surface scattering behaviors in both natural and engineered porous habitats, impairing their persistent random walks. Using microfluidics experiments complemented with Langevin simulations, we study how the scattering of magnetotactic bacteria (MTB) within a lattice of obstacles modifies cell transport, and how guidance by an external field augments their mobility. MTBs are used as a model biological system, because they share motility mechanisms with many other bacterial species, and their swimming direction is easily manipulated via an external magnetic field. We show that both the diffusive and directed mobility of the cells decreases markedly in the presence of porous microstructure compared to bulk fluid. Moreover, the spacing between the obstacles and the degree of the disorder in the lattice play a key role in the magnitude of the observed reduced mobility. These results are an important step toward understanding the physical ecology of swimming cells in quiescent porous media as well as for controlling micro-robots in complex environments.

Cargo carrying capacity of a single bacterium

PRANEET PRAKASH, AMITH ZAFAL ABDULLA, MANOJ M. VARMA (Presenter), Indian Institute of Science — In recent times, several groups have demonstrated bio-hybrid micro-robots where bacteria are attached to “cargo” such as polystyrene beads, which are transported using the power generated by bacterial motility. A system consisting of a single bacterium pulling a load is important for a clear understanding of such bacteria powered devices. Previous reports of cargo delivery by single bacteria have relied on attaching the cells to very small particles (~ 1 micron dia.) so that statistically only one cell can bind due to steric restriction. Such an approach is not effective, as dynamics of a single cell carrying a large load, say ~ 10 micron dia., cannot be studied. Systems describing single bacterium carrying such large size cargo have not been described so far to the best of our knowledge. In this talk, we ask a very general question, namely, what is the maximum load of a spherical cargo which can be transported by a flagellated swimmer at a specified speed. We present a technique to attach single loads as large as 12 micron diameter to micron sized single bacteria. Further, results from our experiments and theoretical analysis suggests the crucial role of tuning the flagellar geometry and the torque-speed characteristics of the flagellar motor to maximize cargo carrying capacity.
Three-dimensional imaging and force mode analysis of microflows induced by swimming *Chlamydomonas reinhardtii* KYLE WELCH, Department of Chemical Engineering and Materials Science, University of Minnesota, SANTOSH KUMAR SANKAR, Department of Mechanical Engineering, University of Minnesota, BO-KAI ZHANG, XINLIANG XU, Complex Systems Division, Beijing Computational Science Research Center, JIARONG HONG, Department of Mechanical Engineering, University of Minnesota, XIANG CHENG (Presenter), Department of Chemical Engineering and Materials Science, University of Minnesota — Understanding the fluid flow induced by microswimmers is paramount to revealing how they interact with each other and their environment. Here, we present a three-dimensional (3D) measurement and characterization of the flow field induced by motile planktonic algal cells, Chlamydomonas reinhardtii. A single alga is captured and held stationary by a micropipette, which beats its flagella in a characteristic breaststroke pattern. We track the 3D flow field around the alga by employing fast holographic imaging on 1 um tracer particles, which leads to a nominal spatial resolution of ~ 54 nm along the optical axis and ~ 44 nm in the imaging plane. The method allows us to image the flow around a single alga continuously over thousands of flagellar beat cycles and show time-averaged and phase-binned 3D flow fields. We analyze these 3D flow fields and determine the dominant force modes of the flagellar motion of C. reinhardtii. Our study demonstrates the power of holography in imaging detailed microscopic flows and provides crucial information for understanding the detailed locomotion of swimming microorganisms.

*The research is partially supported by NSF CBET-1702352. K.W. acknowledges the support of the Natural Sciences Foundation of China International Fund for Young Scientists.*

Length regulation of multiple flagella that self-assemble from a shared pool of components THOMAS FAI (Presenter), LISHIBANYA MOHAPATRA, JANE KONDEV, Brandeis University, ARIEL AMIR, Harvard University — The single cell biflagellate Chlamydomonas reinhardtii has proven to be a very useful model organism for studies of size control. We consider a model of flagellar length control whose key assumption is that proteins responsible for the intraflagellar transport (IFT) of tubulin are present in limiting amounts. We show that this limiting-pool assumption and simple reasoning based on the law of mass action leads to an inverse relationship between the rate at which a flagellum grows and its length, which has been observed experimentally, and has been shown theoretically to provide a mechanism for length control. We extend our length-control model to two flagella by considering different mechanisms of their coupling. Within our theoretical framework we conclude that, if tubulin and IFT proteins are freely exchanged between flagella, simultaneous length control is not possible if the disassembly rate is constant. However, if disassembly depends on the concentration of IFT proteins at the tip of the flagellum, simultaneous length control can be achieved.

Encounter rates between motile bacteria and sinking particles JONASZ SLOMKA (Presenter), VICENTE I. FERNANDEZ, ROMAN STOCKER, ETH Zurich — Many marine microbes rely on sinking particles of organic matter as their food source. Once attached to a particle, bacteria can solubilize its organic matter and convert it into biomass. This process hinders carbon from sinking to the deep ocean (a process known as the ‘biological pump’) and thus affects the magnitude of carbon flux in the ocean. Carbon consumption by bacteria is preceded by their encounter with sinking particles, whose quantification is needed to understand the biological pump. Here, we theoretically predict these encounter rates by combining the Stokes flow around the particle with Jeffrey's equation for a rod in flow. We show that elongated bacteria - unlike spherical particles often used in encounter rate estimates – break the fore-aft symmetry of the flow streamlines, with major consequences on encounter rates. Specifically, for small to intermediate sinking speeds, this symmetry-breaking implies that elongated swimmers are up to hundred times more likely to encounter the sinking particle than spherical bacteria with the same volume. We find that the mechanism for this encounter rate enhancement is the hydrodynamic focusing of elongated swimmers downstream of the sinking particle, which leads to their preferential attachment to the back of the particle.
9:24AM X66.00008: Collective bacterial vision  HARSHITHA SHANKAR KOTIAN (Presenter), Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India, SHALINI HARKAR, Robert Bosch Centre for Cyber Physical Systems, Indian Institute of Science, Bangalore, India, SHUBHAM JOGE, AYUSHI MISHRA, Molecular Reproduction, Development and Genetics, Indian Institute of Science, Bangalore, India, AMITH Z. ABDULLA, Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India, VARSHA SINGH, Molecular Reproduction, Development and Genetics, Indian Institute of Science, Bangalore, India, MANOJ M. VARMA, Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India — Bacteria are well studied primitive organisms and an ideal system for physical scientists to study how simple systems perform complex tasks. Swarming is one such complex collective phenomenon of producing surfactant to ease their motility on a semi solid surface (nutrient supplemented 0.6% agar). We perturbed the swarming pattern of *Pseudomonas aeruginosa* (PA) by incorporating inert obstacles (PDMS) in the agar plate thus creating local depletion of nutrient and water rich agar surface. To our surprise, we noticed that the bacteria as they colonize the surfaces with such obstacles effectively avoid them by changing the course of their path at a distance as far as 5 mm thus ‘seeing’ (sensing) them at \( \sim \) thousand body lengths. We refer to this phenomenon as “collective bacterial vision”. We demonstrate a fluid dynamic model that can guide them around these obstacles. Our model leads to further questions such as, is it possible for a single bacterium to possess “bacterial vision”? What is the grouping cost and ideal group size? Is there a need for information transfer in the group? Is this phenomenon a completely active or completely passive or a delicate balance between them? We will describe our attempts to address some of the above questions though most of them are still open.

9:36AM X66.00009: Bacterial growth curves are predictable from cellular Raman spectra*  KEN-ICHIRO F. KAMEI (Presenter), KOSEKI J. KOBAYASHI-KIRSCHVINK, YUICHI WAKAMOTO, Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo — Raman microscopy is an imaging technique that has been applied to cells to obtain Raman spectra that reflect the abundances of various biomolecules. It allows distinguishing cellular states in a label-free and non-destructive manner. Previously, employing spontaneous Raman scattering, we showed that cellular Raman spectra and transcriptomes could be linked in both *S. pombe* and *E. coli*, and that the transcriptomes could be reconstructed from Raman spectra (Kobayashi-Kirschvink et al., *Cell Systems*, 2018). Considering that omics information, which characterizes cellular states with *molecular* resolution, is linked to Raman spectra, we next asked whether Raman spectra could be linked to *macroscopic* quantities of cellular states. Our recent experimental and computational study indicates that different cellular states of single-gene knockout *E. coli* strains were distinguished by Raman spectra, and the entire population growth curves of different strains could be predicted by Raman spectra from cells in exponential phase. These results suggest that cellular Raman spectra have the potential to integrate macroscopic and microscopic characterizations of cellular states.

*Japan Society for the Promotion of Science KAKENHI (grant number 15KT0075 and 15H05746)

9:48AM X66.00010: Imaging the emergence of collective swarming in light-controlled bacteria*  YI PENG (Presenter), ZHENGYANG LIU, KECHUN ZHANG, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota — Collective motions of active matter as illustrated by bird flocks, fish schools and bacterial swarms demonstrate the intriguing emergent behaviors of living systems. While moving independently at low density, active entities move collectively with its neighbors at high density, exhibiting orientational order at a scale larger than their individual sizes. Although such a disorder-order nonequilibrium phase transition has been previously studied, detailed kinetics of this transition has not been explored in experiments. Here, using engineered *E. coli*, whose locomotion can be reversibly controlled by light, we experimentally study the kinetic pathway of the swarming transition in 3D bacterial suspensions. We trigger bacterial swarming by tuning light intensity and image the emergence of collective motion. We map the phase diagram of bacterial swarming as functions of bacterial concentration, swimmer velocity and the number fraction of active swimmers. Moreover, we find that the swarming transition occurs in a nucleation manner and characterize the incubation time of the transition. Our results reveal the microscopic dynamics of the emergence of bacterial swarming and provide insights into the nonequilibrium phase transition in active matter.

*NSF CBET-1702352, DARPA YFA-D16AP00120
Myxococcus xanthus is a rod shaped soil bacterium that lives in collectives of many millions of cells. These groups of cells exhibit different collective behaviors which benefit the bacteria depending on the external environment. When \( M. \) xanthus are in favorable conditions, colonies will swarm and spread out to explore new territory, resulting in thin layers only a few cells thick. Our goal is to understand how the motility of individual bacteria along with local interactions can lead to the collective behaviors that exist on length scales significantly larger that of the individuals. Using a confocal laser scanning microscope we image layers of cells with single cell resolution while simultaneously obtaining height maps of the layer thickness across the sample. From these images we are able to extract flow and director fields of the bacteria over time. Topological defects in director fields are connected to pressure fluctuations in active nematic systems which can lead to local changes in layer thickness. By combining height maps with director and flow fields, we are able to examine how the active nematic nature of the system can result in thickness changes in bacteria layers.

*This work was supported in part by the NSF, through the Center for the Physics of Biological Function (PHY-1734030)

**Self-organization of swimmers drives long-range fluid transport in bacterial colonies**

Microbes commonly live in structured communities that affect human health and influence ecological systems. Colony mode of bacterial growth on solid substrates (e.g. food products) is closely related to biofilm development, and it is a main approach to study structured microbial communities. Heterogeneous populations, such as non-motile and motile populations, often coexist in bacteria colonies. Here we discovered that motile cells in sessile colonies of peritrichously flagellated bacteria can self-organize into motile bands that can drive long-range fluid transport at a constant speed of \( \sim 30 \) μm/s, providing a stable high-speed avenue for material transport at the colony scale. These findings present a unique form of large-scale self-organization and active transport in bacterial colonies.

*This work was supported by the Research Grants Council of Hong Kong SAR (RGC numbers 2130439 and 2130493), and from the National Natural Science Foundation of China (NSFC 21473152).

**Bacterial Surface Motility is Modulated by An Abiotic Jamming Transition and is Independent of Chemotaxis and Individual Motility**

Bacillus subtilis is a model organism for the study of directed, collective motion over surfaces with groups exhibiting motility on length scales three orders of magnitude larger than themselves in a few doubling times. While genetic and chemical studies clearly show that surface tension gradients and water availability are required for this 'ultrafast' group motility, the relative importance of chemosensing, exogenous nutrient gradients, and individual motility are largely unknown from an experimental viewpoint. We demonstrate that contrary to simulations of bacterial growth on surfaces, \( B. \) subtilis does not rely on chemotaxis for direction, that the rate of dendritic expansion of the colony is faster when bacteria are motile but that the same type of group motility is possible even with non-motile cells, and that water availability is likely a control parameter modulating an abiotic jamming transition that determines whether the group remains fluidized and therefore motile.

*The University of Oregon
Despite decades of microbiology research, we lack a practical understanding of how bacteria migrate through host tissues in disease and through soils in bioremediation to consume environmental pollutants. Models of bacterial motility neglect how the impact of cells on their microenvironment dynamically influences subsequent motion of cells. We aim to unravel how the multi-scale dynamic feedback between bacterial motility and nutrient consumption gives rise to emergent behaviors. We find that E. coli suspension droplets in two-dimensional confinement spontaneously separate into two populations according to a self-generated oxygen gradient: immotile cells cluster in a droplet center and motile cells congregate near an outer air interface. We show how cluster formation and size depend on the interplay between oxygen consumption, diffusion, and bacterial motility. Understanding the impact of gradient-consumption feedback on population scale dynamics will better inform population level microbial behaviors like biofilm formation and migration.

*Project X fund

Friday, March 8, 2019 11:15 AM - 1:51 PM

Session Y01 DCMP: Interactions and Dynamics in Topological Semimetals BCEC 106

11:15AM Y01.00001: Quantum oscillations in Dirac/Weyl semimetals due to strain and external fields  DMITRY PIKULIN (Presenter), Microsoft, RONI ILAN, Tel-Aviv University — I will discuss how strain can cause quantum oscillations in Dirac/Weyl semimetals. In particular, I will concentrate on quasiclassical trajectories formed by strain alone and how they are modified in presence of external field. I will mention both bulk and bulk-boundary quantum oscillations.

11:27AM Y01.00002: Theory of spin torque in Weyl semimetals with magnetic texture*  DAICHI KUREBAYASHI (Presenter), Center for Emergent Matter Science, RIKEN, KENTARO NOMURA, Institute for Materials Research, Tohoku University — We theoretically study the spin-transfer torque, a fundamental physical quantity to understand the electrically-induced dynamics of magnetic texture. We calculate the electrically-induced non-equilibrium spin density of a Weyl semimetal (WSM) and obtain the analytical expression of the spin torque corresponding to a non-adiabatic spin-transfer torque. Importantly, the strength of the obtained spin torque outstrips that of conventional ferromagnetic metals when magnetization varies steeply. Furthermore, due to the suppression of longitudinal conductivity in this regime, the dissipation due to Joule heating for the spin-transfer torque is smaller than that in conventional ferromagnetic metals. We also analyze the dynamics of the domain walls driven using the spin-transfer torque and find that the velocity of the domain wall is one order of magnitude greater than that of a conventional ferromagnetic nanowire. Consequently, the fast-control of domain walls can be achieved with smaller dissipation in the WSM. Therefore, the WSM can be a new candidate for application to spintronics devices such as the racetrack memory.

*This work was supported by the KAKENHI Grant No. JP17K05485 and No. JP15H05854. D. K. is supported by the RIKEN Special Postdoctoral Researcher Program.

11:39AM Y01.00003: Counting formula for the pseudo Landau levels visible in an energy spectrum*  TOSHIKAZE KARIYADO (Presenter), International Center for Materials Nanoarchitectonics, National Institute for Materials Science — One interesting feature of Dirac/Weyl systems is that spatial modulation, for instance given by strain, can be regarded as a gauge filed. This “pseudo” gauge field can generate pseudo magnetic field, and enables us to observe magnetic like phenomena such as Landau level formation or quantum oscillations even without external magnetic field. Here, by considering a simplest situation to have finite pseudo magnetic field, we derive a concise formula to count the number of pseudo Landau levels clearly visible in the energy spectrum. The derived formula is numerically verified in a toy model. Equipped with the formula, we also discuss the possible realization of the pseudo Landau levels in existing Dirac materials, particularly in antiperovskite Sr$_3$SnO series.

*This work was supported by JSPS KAKENHI Grants No. JP17K14358.
11:51AM Y01.00004: Topological semimetal coupled to nano-mechanical resonator  KUN WOO KIM (Presenter), Physics of Complex Systems, Institute for Basic Science, JUNHO SUH, Korea Research Institute of Standards and Science — The detection of gapless Dirac point in semimetals is an important issue for the characterization of topological phase. While the direct measurements of spectral functions and magneto-conductance are widely employed, the strength of electronic signal is vanishingly small near Dirac point due to its low density of states. Here, we propose a way to detect the presence of Dirac node through the coupling to a nano mechanical resonator. Playing as a nonlinear circuit element, the quantum capacitance of topological semimetal induces an abnormal frequency shifting in the resonator near Dirac node. This quantum and mechanical setup will be ideal for the characterization of various topological matter and its boundary states.

12:03PM Y01.00005: Dirac cones protected by chiral symmetry in wallpaper groups*  CHING-KAI CHIU (Presenter), Kavli Institute for Theoretical Sciences, YANG ZHESEN, Chinese Academy of Sciences, CONGCONG LE, Kavli Institute for Theoretical Sciences — Dirac cones in 2D Brillouin zone (BZ) can be protected by chiral symmetry. The spinless and spin-1/2 systems preserving chiral symmetry can be realized in time-reversal symmetric superconductors and correspond to symmetry class BDI and DIII respectively. Since the total winding number in the entire BZ is zero, there are at least two Diracs cones in the BZ. Furthermore, crystalline symmetries lead to duplicate Dirac cones and additional constraints. The minimal numbers of the Dirac cones in the BZ under different symmetries might be different. In this talk, we classify the minimal numbers of the Dirac cones protected by chiral symmetry in all 17 wallpaper groups for class AIII, BDI, and DIII.

*CKC is supported by the Strategic Priority Research Program of the Chinese Academy of Sciences, Grant No. XDB28000000.

12:15PM Y01.00006: Stability of the Semimetallic Phase in strongly interacting Weyl semimetals*  JOHAN CARLSTROM (Presenter), EMIL J BERGHOLTZ, Stockholm University — Using a combination of analytical arguments and diagrammatic Monte Carlo simulations, we show that the corrections to the dispersion in interacting Weyl semimetals are determined by the ultraviolet cutoff and the inverse screening length. If both of these are finite, then the diagrammatic series is convergent even in the low-temperature limit, which implies that the semimetallic phase is protected by a symmetry of the self energy. We also find that the frequency dependent part of the self energy gives an extremely small correction to the Greens function of the interacting system, implying that the impact of interactions almost entirely takes the form of a renormalisation of the single particle dispersion.

*This work was supported by the Swedish research council (VR) and the Wallenberg Academy Fellows program of the Knut and Alice Wallenberg Foundation. Computations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at the High Performance Computing Center North in Umeå, Sweden.

12:27PM Y01.00007: Strain-induced nonlinear spin Hall effect in topological Dirac semimetal*  YASUFUMI ARAKI (Presenter), Institute for Materials Research, Tohoku University — Topological Dirac semimetals (TDSMs) form a new class of three-dimensional topological semimetals, characterized by pair(s) of doubly-degenerate nodal points (Dirac points) in their momentum(k)-space band structures. They show the intrinsic spin Hall effect (SHE), which comes from the k-space topology around the Dirac points. This spin Hall conductivity is topologically protected, while it cannot be easily tuned or enhanced at linear response. In order to overcome this problem, I theoretically propose that an electric field applied to a lattice-strained TDSM gives rise to an additional "nonlinear spin Hall current", namely the spin current perpendicular to and quadratic in the electric field [1]. The spin current response is obtained by the Boltzmann transport theory, regarding the strain as a pseudomagnetic field for the Dirac electrons. The nonlinear SHE arises as the hybrid of the regular Hall effect driven by the pseudomagnetic field (strain) and the anomalous Hall effect from the k-space topology. This behavior implies that one can obtain a rectified (dc) pure spin current out of an alternating (ac) electric field, which renders the TDSM an efficient spin-current injector.


*This work is supported by JSPS KAKENHI Grant Number JP17K14316.
12:39PM Y01.00008: Enhanced conductance of Weyl semimetals with strain-induced chiral magnetic fields in the ultra-quantum limit  JAN BEHRENDS (Presenter), TCM Group, Cavendish Laboratory, University of Cambridge, JENS BARDARSON, Department of Physics, KTH Royal Institute of Technology, RONI ILAN, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University — Magnetotransport is one of the key signatures of Weyl semimetals. It is believed to reveal the chiral anomaly, the nonconservation of chiral charge, by showing a large negative magnetoresistance for longitudinal transport. With the realization of chiral magnetic fields, fields that act with opposite sign on the two chiralities, transport experiments in presence of those fields come in sight. In this work, we show that the conductivity in the ultra-quantum regime of a disordered Weyl semimetal subjected to a chiral magnetic field in transport direction increases with the field strength and width of the sample. We relate this increment to the spatial separation of counterpropagating modes in those samples. Our results are based on tight-binding simulations and supported by analytical arguments. We argue how this effect can be used in devices that need spatial separation of charge carriers.

12:51PM Y01.00009: Ferromagnetic Weyl semimetal phase and anomalous Hall effect in stacked Kagome lattice* AKIHIRO OZAWA (Presenter), KENTARO NOMURA, Institute for Materials Research, Tohoku University — Recently, Weyl semimetals, which have three-dimensional linear dispersions near the Fermi energy have been intensively investigated. Especially, ferromagnetic Weyl semimetals are drawing attentions as a system which implements some novel transport phenomena such as the anomalous Hall effect. It is reported that ferromagnetic Weyl phase is realized in stacked Kagome material Co3Sn2S2 by experiment and first principle calculation. In this presentation, we study the electronic state and the phenomena such as the anomalous Hall effect. Our results are based on tight-binding simulations and supported by analytical arguments. We relate this increment to the spatial separation of counterpropagating modes in those samples. Our results are based on tight-binding simulations and supported by analytical arguments. We argue how this effect can be used in devices that need spatial separation of charge carriers.

*This Work was supported by KAKENHI Grants-in-Aid (No. JP15H05854) from the Japan Society for the Promotion of Science (JSPS) and GP-Spin at Tohoku University.

1:03PM Y01.00010: Semiclassical transport theory in Weyl semimetals beyond the relaxation time approximation* TOBIAS MENG (Presenter), TU Dresden — In this talk, I will detail new insights into transport in Weyl semimetals based on the semiclassical Boltzmann approach treated beyond the relaxation time approximation. This approach allows us to investigate the impact of various scattering mechanisms, and to make a step towards a more realistic description of transport experiments in Weyl semimetals. In particular, I will discuss Weyl-specific signatures in the low-field magnetotransport beyond the well-known negative quadratic magnetoresistance.

*We acknowledge funding by the Deutsche Forschungsgemeinschaft through the Emmy Noether Programme ME 4844/1-1 and through SFB 1143.

1:15PM Y01.00011: “Hinge” surface states in Weyl semimetals TOBIAS MENG (Presenter), TU Dresden — In this talk, I will detail new insights into transport in Weyl semimetals based on the semiclassical Boltzmann approach treated beyond the relaxation time approximation. This approach allows us to investigate the impact of various scattering mechanisms, and to make a step towards a more realistic description of transport experiments in Weyl semimetals. In particular, I will discuss Weyl-specific signatures in the low-field magnetotransport beyond the well-known negative quadratic magnetoresistance.

1:27PM Y01.00012: Non-local spin-spin coupling in topological semimetals SONU VERMA, DEBASMITA GIRI, KESHAV PAREEK, Physics, Indian Institute of Technology Kanpur, HERBERT FERTIG, Physics, Indiana University Bloomington, ARIJIT KUNDU (Presenter), Physics, Indian Institute of Technology Kanpur — We study the spin-spin coupling in finite-geometry topological semimetals employing the RKKY theory of interaction among impurity spins. The impurity spins can be on the surface of the geometry, where the mediated interaction between them can be through the topological surface states. Alternatively, the impurity spins can be on opposite surface of the system, where the mediated interaction can be through the semimetallic bulk states, giving rise to signatures of possible non-local effects.
Effects of long-range interactions on topological semimetals

SHOUVIK SUR (Presenter), PALLAB GOSWAMI, Physics & Astronomy, Northwestern University — In the presence of long-range interactions the low energy dynamics in a metal usually undergoes significant re-adjustments, leading to a state that qualitatively differs from that in the non-interacting limit. The band structures of many three dimensional systems host topologically protected nodal-points or nodal-lines. In such semimetals long-range interactions play an important role in both the native phase, and upon tuning to a topological or geometric quantum critical point. Here we study the interplay of long-range interactions and topology in a nodal-point semimetal.

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y03 DCMP: Transport in Topological Systems: Theory and Experiment BCEC 107B

11:15AM Y03.00001: Configuration-sensitive transport at the domain walls of a magnetic topological insulator*

YANFENG ZHOU (Presenter), ZHE HOU, QING-FENG SUN, School of Physics, Peking University — We report on the transport of a two-terminal device containing a domain wall (DW) in a magnetic topological insulator (TI). In the low-energy case, the transport behaviors of the magnetic TI are dominated by chiral edge states (CESs) at the device edges as well as at the DW. We calculate the band structures of magnetic TIs with both a Bloch wall and a Néel wall. For a Bloch wall, two copropagating CESs at the DW are doubly degenerate, while for a Néel wall a split is present. Consequently, the transport is strongly dependent on the DW configuration. In the Bloch wall case, the incoming electron with zero energy is totally reflected regardless of the system parameters. However, in the Néel case, the device functions as a chirality-based Mach-Zehnder interferometry, so that the transmission coefficient oscillates between zero and unity with changes in system parameters. By constructing the scattering matrix of the device from the effective Hamiltonian, these transport behaviors can be well understood.

*This work was financially supported by the National Key R and D Program of China (Grant No. 2017YFA0303301), NBRP of China (Grant No. 2015CB921102), NSF-China (Grant No. 11574007), and the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No.XDB28000000).

11:27AM Y03.00002: Conditions for fully gapped topological superconductivity in topological insulator nanowires*

RONI ILAN, Department of Condensed Matter Physics, Tel Aviv University, FERNANDO DE JUAN (Presenter), Donostia International Physics Center, Spain, JENS BARDARSON, Department of Physics, KTH Royal Institute of Technology — Among the different platforms to engineer Majorana fermions in one-dimensional topological superconductors, topological insulator nanowires remain a promising option. Threading an odd number of flux quanta through these wires induces an odd number of surface channels, which can then be gapped with proximity induced pairing. Because of the flux and depending on energetics, the phase of this surface pairing may or may not wind around the wire in the form of a vortex. We show that for wires with discrete rotational symmetry, a vortex is necessary to produce a fully gapped topological superconductor with localized Majorana end states. Without a vortex the proximitized wire remains gapless, and it is only if the symmetry is broken by disorder that a gap develops, which is much smaller than the one obtained with a vortex. These results are explained with the help of a continuum model and validated numerically with a tight binding model, and highlight the benefit of a vortex for reliable use of Majorana fermions in this platform.

*Marie Curie Programme under EC Grant agreement No. 705968 (F. J.). ERC Starting Grant No. 679722 and the Knut and Alice Wallenberg Foundation 2013-0093 (J. H. B.). Partial support by the National Science Foundation under Grant No. NSF PHY-1748958 (J. H. B.).
11:39AM Y03.00003: Topological Properties of Gapped Graphene Nanoribbons with Spatial Symmetries* KUAN-SEN LIN (Presenter), Department of Physics, University of Illinois, Urbana Champaign, MEI-YIN CHOU, Institute of Atomic and Molecular Sciences, Academia Sinica — To date, almost all of the discussions on topological insulators (TIs) have focused on two- and three-dimensional systems. One-dimensional (1D) TIs manifested in real materials, in which localized spin states may exist at the end or near the junctions, have largely been unexplored. Previous studies have considered the system of gapped graphene nanoribbons (GNRs) possessing spatial symmetries with terminations commensurate with inversion- or mirror-symmetric unit cells. In this work, we prove that a symmetry-protected $Z_2$ topological classification exists for any type of termination. Instead of the Berry phase, only the origin-independent part of it gives the correct bulk-boundary correspondence by the $\pi$-quantized values. The resulting $Z_2$ invariant depends on the 1D unit cell and is connected to the symmetry eigenvalues at the center and boundary of the Brillouin zone. Using cove-edged GNRs, we demonstrate the existence of localized states at the end of GNR segments and at the junction between two GNRs based on a topological analysis. The current results are expected to shed light on the design of electronic devices based on GNRs as well as the understanding of the topological features in 1D systems.

*This work is supported by a Thematic Project (AS-TP-106-M07) at Academia Sinica.

11:51AM Y03.00004: Quasi-one-dimensional first- and second-order topological insulators: Bi$_4$X$_4$ (X = Br, I)* CHIHO YOON (Presenter), Department of Physics and Astronomy, Seoul National University, CHENG-CHENG LIU, Beijing Key Laboratory of Nanophotonics and Ultrane Optoelectronic Systems, School of Physics, Beijing Institute of Technology, HONGKI MIN, Department of Physics and Astronomy, Seoul National University, FAN ZHANG, Department of Physics, The University of Texas at Dallas — Recently, quasi-one-dimensional materials Bi$_4$X$_4$ (X = Br, I) in both $\alpha$ and $\beta$ crystalline phases have been proposed as a promising platform for the realization of various topological insulator (TI) phases [e.g., PRL 116, 066801 (2016)]. This list includes the strong TI, the weak TI, and the second-order TI with helical hinge states. We perform first-principles calculations and construct an effective model for Bi$_4$X$_4$. These results allow us to derive all the aforementioned TI phases and guide future experimental studies.

*This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2018R1A2B6007837), Creative-Pioneering Researchers Program through Seoul National University (C.Y and H.M), the Global Ph.D Fellowship Program through NRF of Korea funded by Korean Government under Grant No. 2016H1A2A1907780 (C.Y.), and the Army Research Office and was accomplished under Grant Number W911NF-18-1-0416. (F.Z.)

12:03PM Y03.00005: PbSnSe: a model system to study topological phases* GAUTHIER KRIZMAN (Presenter), Department of Physics, Ecole Normale Superieure, BADIH ASSAF, Department of Physics, University of Notre-Dame, MILAN ORLITA, Laboratoire des Champs Magnétiques Intenses, THANYANAN PHUPHACHONG, Department of Physics, Ecole Normale Superieure, GUNTHER BAUER, GUNTHER SPRINGHOLZ, Department of Physics, Johannes Kepler Universität, LOUIS-ANNE DE VAULCHIER, YVES GULDNER, Department of Physics, Ecole Normale Superieure — Pb$_{1-x}$Sn$_x$Se hosts three-dimensional (3D) massive Dirac fermions across the entire composition range for which the crystal structure is cubic. In this talk, we will present a comprehensive experimental mapping of the 3D band structure of Pb$_{1-x}$Sn$_x$Se as a function of chemical composition (0<x<0.3), temperature (1.6<T<200 K), and magnetic field (0<B<34 T). We use magneto-infrared spectroscopy to determine all the Dirac parameters in the trivial and topologically non-trivial regimes.

In 3D Pb$_{1-x}$Sn$_x$Se topological insulators, an effective closure of the bulk energy gap with increasing temperature, magnetic field, or lead content is expected at the critical point of the phase transition. However, in this talk we experimentally demonstrate that such a gap closure consistently does not occur. Avoided-crossing of either bulk bands or N=0 Landau levels are evidenced. These results show that Pb$_{1-x}$Sn$_x$Se is a model system to study topological phases and the nature of the phase transition.

*This work is supported by Agence Nationale de la Recherche LabEx ENS-ICFP Grant No ANR-10-LABX-0010/ANR-10-IDEX-0001-02 PSL and by the Austrian Science Fund, Projects P 28185-N27 and P 29630-N27. It is also partly supported by a PSL scholarship.
12:15PM Y03.00006: Higher-order topology in two-dimensional crystals  FRANK SCHINDLER (Presenter), University of Zurich, WLADIMIR BENALCAZAR, The Pennsylvania State University, MARTA BRZEZINSKA, University of Science and Technology, MIKEL IRAOLA, Donostia International Physics Center, ADRIEN BOUHON, Uppsala University, STEPAN TSIRKIN, University of Zurich, MAIA VERGNIORY, Donostia International Physics Center, TITUS NEUPERT, University of Zurich — We study two-dimensional spinful topological phases of matter protected by time-reversal and crystalline symmetries. To define the topology we employ the concept of corner charge fractionalization: We show that corners in a higher-order topological phase can carry charges that are fractions of even multiples of the electric charge. These charges are quantized and topologically stable as long as all symmetries are preserved. We classify the topologies corresponding to different corner charge configurations for all 80 layer groups, and present their bulk topological indices. These can be calculated from the symmetry data and Brillouin zone Wilson loops. To corroborate our findings, we present tight-binding models and density functional theory calculations for various material realizations.

12:27PM Y03.00007: Exploring electronic properties of topological insulator Bi2Se3 using nuclear magnetic resonance  ROBIN GUEHNE (Presenter), GRANT V. M. WILLIAMS, SHEN V CHONG, MacDiarmid Institute for Advanced Materials and Nanotechnology, School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand, VOJTĚCH CHLAN, Department of Condensed Matter Physics, Charles University, Prague, Czech Republic, JUERGEN HAASE, Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany — The investigations of 3-dimensional topological insulators such as Bi2Se3 focus chiefly on the gapless surface states that emerge as a consequence of the special energy band inversion near the Fermi level induced by spin-orbit coupling. Not as much studied are the real-space effects in the bulk. The band inversion, for example, changes the wave function of the free carriers, compared to the topologically trivial counterpart. We will show that nuclear magnetic resonance (NMR) as a local, bulk probe can detect this band inversion through the electric quadrupole interaction that, in addition, measures the concentration of free carriers, e.g. originating from self-doping effects. NMR data in external fields up to 17 T, i.e., shifts, linewidths and quadrupole splittings, in doped single crystalline samples of Bi2Se3 are discussed.

12:39PM Y03.00008: Thermal Hall Effect Measurements on Topological Materials  LUKE PRITCHARD-CAIRNS (Presenter), University of Edinburgh, JEAN PHILIPPE REID, University of St.Andrews, ROBIN S. PERRY, University College London, DHARMALINGAM PRABHAKARAN, University of Oxford, ANDREW HUXLEY, University of Edinburgh — In the past few decades topology has become a central theme in condensed matter physics, allowing a more complete understanding of concepts such as the quantum Hall effect and of the class of materials termed topological insulators. Topological insulators were first predicted in 1987 and have subsequently been experimentally realised in a host of materials. A similar effect has been predicted to occur for SrCu2(BO3)2 (SCBO) but with one crucial difference; unlike those materials previously found, it is the spin waves that have a topological character rather than the conduction bands [3]. SCBO is therefore a bosonic topological material.

Theoretical predictions from [1] suggest that the topological nature of SCBO should be evident from thermal Hall effect measurements. In order to demonstrate the feasibility of these measurements, we have used our setup to reproduce those results from [2], which show a (magnon) Hall effect signal of a similar magnitude to that predicted for SCBO, and under similar conditions. We then present new thermal Hall data on the material SCBO, for which a positive result would be evidence for one of the first known bosonic topological insulators.

Selective Contact and Patterning of Topological Surface States by Interfacing with Trivial and Ferromagnetic Insulators*

ANKITA ANIRBAN (Presenter), Cavendish Laboratory, University of Cambridge, ABDUR REHMAN JALIL, Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, YUNBO OU, MIRKO ROCCI, Dept. Of Physics, Plasma Science and Fusion Center and Francis Bitter Magnet Lab, Massachusetts Institute of Technology, GREGOR MUSSLER, Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, JAGADEESH MOODERA, Dept. Of Physics, Plasma Science and Fusion Center and Francis Bitter Magnet Lab, Massachusetts Institute of Technology, CRISPIN BARNES, CHRISTOPHER J FORD, Cavendish Laboratory, University of Cambridge — Topological insulators (TIs) are a novel class of material which host helical surface states with exciting and unique electronic properties. They can provide insights into new physics and also pave the way for potential spintronic applications. Much work has been done to identify and characterise these surface states, but in order to utilise them towards multifunctional devices, we need a way to control the exchange gap opening in a tailored way and pattern them accordingly. We present results from devices which allow selective contact and patterning of topological surface states. We interface a TI with a ferromagnetic insulator to open up a gap in the Dirac cone, in an effort to have independent contact to the top and bottom surface states of a single TI film, enabling the characterisation and utilisation of the two surface states separately. We also study heterostructures with two TI layers separated by a trivially insulating tunnel barrier, allowing for a way of probing the dispersion relation of TIs using spin and momentum resolved tunnelling.

*ONR, NSF, CIQM, DPG-SPP 1666

The effect of lattice termination on the Zeeman gap of topological edge states in the quantum spin Hall insulator WTe2*

ALEXANDER LAU (Presenter), Kavli Institute of Nanoscience, Delft University of Technology, RAJYAVARDHAN RAY, Institute for Theoretical Solid State Physics, IWF Dresden, DANIEL VARJAS, ANTON AKHMEROV, Kavli Institute of Nanoscience, Delft University of Technology — We investigate the effect of the sample termination on the electronic properties of the recently discovered quantum spin Hall insulator WTe2. For this purpose, we have derived a minimal 4-orbital tight-binding model by means of a combination of symmetry considerations, density-functional theory calculations and experimental data. Here, we are going to present the results of our theoretical study including spectra of topological edge states and conductance calculations for various sample geometries with and without magnetic field. We observe that the edge-state dispersion considerably depends on the lattice termination: for some terminations the edge-state spectrum features a Kramers doublet, or Dirac point, of topological states inside the bulk energy gap. For others, this Dirac point is “buried” in the bulk continuum of bands. Here, we will show that this qualitative difference is strongly reflected in the electronic conductance under magnetic field. In particular, we find that the specific behavior is related to the type of Zeeman gap in the corresponding edge-state spectrum.

*We acknowledge support from the Netherlands Organisation for Scientific Research (NWO/OCW), as part of the Frontiers of Nanoscience program.

Bulk-boundary correspondence of non-Hermitian systems*

ZHONG WANG (Presenter), SHUNYU YAO, FEI SONG, Tsinghua University — An intriguing issue of non-Hermitian systems is the fate of bulk-boundary correspondence. We show that a previously overlooked “non-Hermitian skin effect” necessitates a non-Bloch bulk-boundary correspondence, which is based on a complex-valued Brillouin zone. This dramatic generalization of bulk-boundary correspondence is illustrated in the non-Hermitian Su-Schrieffer-Heeger models and Chern insulator models. We analytically obtain their topological phase diagrams, which are remarkably different from those of the Bloch Hamiltonians. As a natural formulation of the non-Bloch bulk-boundary correspondence, we introduce the non-Bloch topological invariants in the complex Brillouin zone (instead of the standard Brillouin zone with real-valued momentum), which faithfully predict the number of topological edge modes. Specifically, the chiral edge modes of two-dimensional non-Hermitian Chern bands are determined by the non-Bloch Chern numbers.

References:

*This work is supported by NSFC under Grant No. 11674189.
It has been shown that nanoribbon transistors consisting of InAs or GaSb channels can be processed by transferring epitaxial semiconductor layers onto a Si substrate, and further integrated into compound semiconductor CMOS circuits. In our research, we adapt this technique and study transferring epitaxial InAs/InGaSb topological insulator to Si/SiO2 or FM-insulator substrate. We will describe the processing for the QSH devices and present their low temperature transport data.

*The work is supported by NBRPC (No. 2014CB920901) and National Key R and D Program of China (No. 2017YFA0303301).

Magnetic topological insulators are an exciting new platform for the investigation of exciting time-reversal symmetry-breaking physics such as the quantum anomalous hall effect, inverse spin galvanic effect, axion electrodynamics, and spin orbit torque. These materials systems also have great potential for spintronic device applications, but practical development has so far been inhibited by the extremely low (around 30 K) Curie temperature of these materials. Interfacial proximity coupling to other magnetically ordered compounds has been suggested as a mechanism by which this challenge may be addressed. However, separating interfacial exchange coupling from less-desirable effects such as intermixing presents significant challenges. In this work, we use neutron and magnetic X-ray spectroscopy to assemble a depth and element-resolved picture of magnetism within topological insulator/antiferromagnet heterostructures. Our results support true proximity-induced magnetization in (Bi,Sb)2Te3 films interfaced with CrSb and MnTe, with enhanced ordering temperature and chiral magnetic structures. We show that the topology and magnetism of the (Bi,Sb)2Te3 may be readily controlled through exchange coupling with the adjacent antiferromagnet.

*The work is in part supported by ARO MURI.

Topological insulators (TI) have been widely studied due to their unique band structure. The Dirac cone band dispersion as well as spin-momentum locking at the surface enables the existence of Dirac plasmons with resonance frequencies in the THz range [1]. People have observed localized Dirac plasmons by etching TIs into stripe arrays [2]. There is limited experimental evidence for propagating surface plasmon polaritons in TIs. Due to the nature of TI surface states, the propagating surface plasmon will be both charge density wave and spin density wave. Here we present our work on exciting propagating Dirac plasmons in TIs by lifting off gold gratings on top of the TI surface. We demonstrate the tunability of the plasmon resonance frequency by varying the grating coupler period. Future work may also include other degrees of tunability, and the simulation of plasmon dispersion relation. The research on propagating Dirac plasmons give rise to new dimensions of plasmonic and spintronic applications with TI.


*Y.Wang and S.Law acknowledge funding from the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0016380.
First-Principles Prediction of Room Temperature Quantum Anomalous Hall Effect in 2D Oxalate-Bridged Metal Organic Complexes

LIZHI ZHANG (Presenter), University of Tennessee, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Quantum anomalous Hall (QAH) insulators are a highly promising class of materials for spintronic devices and quantum computations because of their precise quantization nature, robust properties against defects, and relatively low energy consumption for operation. To realize the QAH effect, quantum spin Hall (QSH) insulators must be utilized, which requires transition metal doping or surface functionality control. Here, we propose a new family of high temperature organic QAH insulators of 2D oxalate-bridged metal (M) organic complexes, \( M_2(C_2O_4)_3 \) (M=Re, Pt, Hg). First-principles calculations show the spin–orbit coupling gaps ~160 meV, with Curie temperature, calculated by non-linear spin wave theory based on the XYZ Heisenberg model, of greater than ~380 K, which indicates a room-temperature QAH effect. The first room-temperature organic QAH insulators with computationally proved high thermal stability can be realized experimentally.

*L.Z. was partly supported by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory. Computing resources were provided by the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the US Department of Energy under Contract No. DE-AC02-05CH11231.

Friday, March 8, 2019 11:15 AM - 1:27 PM

Session Y04 DMP DCOMP: Dielectric & Ferroic Oxides -- Understanding Vacancies and Dopants BCEC 107C - Donald Evans - Tag(s): Focus

11:15AM Y04.00001: First-Principles Study of Perpendicular Magnetic Anisotropy in Multiferroics

XUEZENG LU (Presenter), Northwestern University — Searching for materials with room-temperature electric-field control of magnetism has interested researchers for many years. Electric field assisted changes of perpendicular magnetic anisotropy (PMA) is a flourishing field owing to its application in magnetic random access memories (MRAMs). PMA has typically be explored in heterostructures comprised of ferromagnets and/or ferroelectrics, relying on interfacial effects whereby the strain generated by the substrate or changes in the electronic structures occur at the heterointerface due to the application of an electric field. Here we propose design rules, based on \((ABO_3)_1/(A'BO_3)_1\) superlattices and \(AA'B'B'O_6\) double perovskites exhibiting hybrid improper ferroelectricity (HIF), to realize potential in-plane electric-field control of PMA. Our studies show a change of PMA occurs in some ordered perovskite phases due to a polar-to-nonpolar phase transition driven by strain. Discovery of such phenomena allows us to formulate chemical and energetic design rules to facilitate the selection of other promising multiferroics for the applications in low-energy information storage and logic devices.

11:27AM Y04.00002: Ferromagnetic Resonance in BTO-BFO Films Grown on LSMO

GITI KHODAPARAST (Presenter), HAN-BYUL KANG, Virginia Tech, BENJAMIN MADON, Ecole Polytechnique, MIN GYU KANG, BRENDE N A MAGILL, DEE PAM MAURYA, SHASHANK PRIYA, Virginia Tech, HENRI-JEAN M DROUHIN, JEAN-ERIC WEGROWE, MARUCOS ALVES, Ecole Polytechnique — We synthesized epitaxial BTO-BFO films grown on LSMO with decreased leakage and improved multiferroic properties. This work provides new direction for ferromagnetic resonance studies in high quality BTO-BFO films. We observed small Gilbert damping (\( \alpha=0.004\)) and the absence of large inhomogeneous broadening, in a film with 80 nm thickness of BTO-BFO on LSMO (110). Magnetic insulators, such as BTO-BFO are potentially excellent candidates for pure spin current without the existence of charge current. This new materials system can provide opportunities for spin transfer in multifunctional materials where controlling magnetization or spin current, is crucial toward for developing nanoscale spin-based memory and devices.

*This material is based upon work supported by the Air Force Office of Scientific Research under award numbers: FA9550-14-1-0376 and FA9550-17-1-0341. D. Maurya acknowledges the support from office of basic energy science, department of energy DE-FG02-06ER46290.

M. Alves acknowledges the support from the Brazilian agency CNPq.
11:39 AM Y04.00003: Oxygen exchange kinetics in perovskite oxides: Effects of elastic strain, dislocations, and surfaces [Invited] BILGE YILDIZ (Presenter), Departments of Nuclear Sci. and Eng., and Materials Sci. and Eng., Massachusetts Institute of Technology — Interfaces between dissimilar oxides are attracting significant interest for their potential role in accelerating charge transport and surface reaction kinetics. If well understood and controlled, they can provide a new way to enable high-performance solid-oxide fuel cells, separation membranes as well as fast switching memristive devices. For example, recent studies have demonstrated that cobaltite hetero-interfaces exhibit orders of magnitude faster oxygen reduction kinetics compared with either single phase. The interfacial strain fields and electronic interactions between the two phases as well as the effect of these interactions on the surface chemistry are the likely mediators behind such an unprecedented enhancement. The underlying mechanisms must be understood quantitatively, so that we can go beyond isolated and empirically found interface or surface structures to rationally designing dissimilar oxide interfaces with superior properties. In this talk, I will present our findings on how elastic strains, dislocations, and surface chemistry affect the defect chemistry and the charge transport/transfer kinetics, by using atomistic computations and model experiments using thin films. These recent results are encouraging for an improved understanding of oxide hetero-interfaces and surfaces at elevated temperatures, and could enable the discovery of new interfaces with fast oxygen transport and oxygen reduction kinetics.

12:15 PM Y04.00004: Optical spectroscopic study on the oxygen vacancy formation in SrTiO3 single crystals YUNSANG LEE (Presenter), JUNHWI LIM, Soongsil University, SANG DON BU, Physics, Chonbuk National University — We investigated the changes in the emission characteristics of SrTiO3 (STO) single crystals under control of oxygen vacancies by using gamma-ray irradiation. The photoluminescence spectroscopy is useful in probing oxygen vacancies, since the intensity of the visible emission is nearly proportional to the amount of oxygen vacancies. The STO samples were prepared in the directions of (100), (110) and (111). The unirradiated samples were found to show visible emissions near 500 nm, indicating they should have initially had some oxygen vacancies. With the gamma-ray irradiation increasing up to 100 kGy, the visible emission was found to increase for all three directions of STO samples. Interestingly, the variation in emission was dependent on the surface orientation of the STO: the intensity variation was greatest in the (111) sample. We discussed our results in relation to the surface energy of the STO.

12:27 PM Y04.00005: Prediction and Direct Observation of Apical Oxygen Vacancies in YBCO STEVEN HARTMAN (Presenter), Institute of Materials Science and Engineering, Washington University in St. Louis, BERNAT MUNDET BOLOS, JAUME GAZQUEZ, Consejo Superior de Investigaciones Científicas, Institut de Ciencia de Materials de Barcelona, ROHAN MISHRA, Mechanical Engineering and Materials Science, Washington University in St. Louis — Prior study of the high-temperature superconductor YBa2Cu3O7-x (YBCO) has revealed the fundamental role of oxygen vacancies in controlling the material's superconductivity. At low oxygenation (x > 0.5), the vacancies are ordered in the CuO chains, and nearly all studies of the vacancies in YBCO, even for high oxygenation (x > 0) have focused on the chain vacancy for this reason. However, optimally doped YBCO (x = 0.06) has relatively few vacancies, and these do not form ordered patterns, which are easy to detect using diffraction techniques. In this work, we use first-principles calculations and scanning transmission electron microscopy (STEM) to investigate vacancy formation in optimally doped YBCO. Our calculations show that at optimal doping, vacancy formation at the apical site is equally favorable to chain vacancy formation. To confirm this prediction, we use the atomic resolution of STEM to provide direct observation of these apical vacancies under certain experimental conditions. We also characterize the effects of apical vacancies on YBCO's electronic properties, using the calculated density of electronic states and experimental electron energy loss spectroscopy.

12:39 PM Y04.00006: Coexistence of polar displacements and conduction in doped ferroelectrics: an ab initio comparative study* CHENGLIANG XIA (Presenter), YUE CHEN, The University of Hong Kong, HANGHUI CHEN, New York University Shanghai — Degenerately doped ferroelectrics may create an approximate polar metallic phase. We use first-principle calculations to investigate n-doped LiNbO3-type oxides (LiNbO3 as the prototype) and compare to perovskite oxides (BaTiO3 as the prototype). In rigid-band approximation, substantial polar displacements in n-doped LiNbO3 persist even at 0.3e/f.u., while that in n-doped BaTiO3 quickly get suppressed and completely vanish at 0.1e/f.u. Supercell calculations which use oxygen vacancies as electron donors support results from rigid-band approximation and provide more detailed charge distribution. We find that in n-doped LiNbO3, conduction electrons are not as uniformly distributed as in n-doped BaTiO3. Insulating and conducting Nb sites coexist but substantial cation displacements are observed throughout n-doped LiNbO3. Our work shows that polar distortions and conduction can coexist in a wide range of electron concentration in n-doped LiNbO3, which is a practical approach to create an approximate polar metallic phase. Our results also show that Li displacements are not solely induced by Nb-O displacements, which may shed light on the origin of ferroelectricity in LiNbO3.

*The authors are grateful for HKU Zhejiang Institute of Research and Innovation, New York University Shanghai.
12:51PM Y04.00007: Proton-transfer Ferroelectricity of Trans-Unitcell Ion-Displacement and Multiferroic Soliton in Sodium and Potassium Hydroxides  MENGHAO WU (Presenter), Huazhong University of Science and Technology — We show first-principles evidence of robust proton-transfer ferroelectricity with considerable polarization in sodium and potassium hydroxides, which are ready for commercial scale production. Moreover, even a small amount of proton vacancies can completely change the mode of proton-transfer from intra-unitcell to trans-unitcell, giving rise to a hitherto unreported type of multiferroic soliton with “mobile” magnetism and a tremendous polarization that can be two orders of magnitude higher compared with most perovskite ferroelectrics. Their vertical polarizations of thin-film are robust against depolarizing field, rendering various designs of 2D ferroelectric field-transistors with non-destructive readout and ultra-high on/off ratio via sensing the switchable metallic/insulating state.

1:03PM Y04.00008: Imaging current filaments created by the metal-insulator transition in vanadium dioxide* MARK FIELD (Presenter), Rigetti Computing, CHRISTOPHER HILLMAN, PHILIP STUPAR, Teledyne Scientific, EUAN RAMSAY, JAMES VICKERS, Thermo Fisher Scientific — Vanadium dioxide (VO2) undergoes a reversible metal-insulator transition at 67 °C, changing from a semiconductor at low temperatures to a metal at high temperatures. The crystal structure changes from monoclinic to rutile and this structural change is sufficient to modify the bandstructure. Current biasing a thin film of VO2 shows high resistivity Ohmic behavior at low currents, and at higher currents the resistance suddenly drops as the Joule heating is sufficient to trigger the metal - insulator transition. At this point the heating decreases allowing sections of the material to revert to a semiconductor, concentrating the current within a metallic filament. At intermediate currents the metallic filament forms but the low resistance path does not dissipate enough heat to maintain it, and thermal oscillations are observed where the filament repeatedly forms and collapses. In this work we image a metallic filament within a current biased thin film VO2 sample using a laser scanning microscope. We observe the evolution of the filament in time when the device is oscillating, following the formation and collapse of the filament, and measure the time scales for each process.

*Funding was provided by the Defense Advanced Research Projects Agency, contract number HR0011-12-C-0092.

1:15PM Y04.00009: Magnetism of BiFeO3 Nanoparticles across its ferroelectric phase transition* ALEXANDER CARDONA, EDWIN RAMOS, University of the Andes, ALEX HOJEM, Physics, UC San Diego, ANDREAS REIBER, University of the Andes, IVAN SCHULLER, Physics, UC San Diego, JUAN RAMIREZ (Presenter), University of the Andes — Multiferroics exhibit simultaneous magnetic and ferroelectric ordering. The archetypical multiferroic material, BiFeO3(BFO), has attracted much attention since it has both, high ferroelectric Curie temperature (1103 K) and, high antiferromagnetic Néel temperature (643 K) in bulk. Here we explore a new route of magnetic control via nano-structuration in the form of nanoparticles (NPs). We fabricated BFO NPs by the sol-gel method with different particle sizes. We have found that their magnetic properties at room temperature and down to 2K change drastically by varying the NP size. Here we present magnetometry studies at high temperature up to the ferroelectric phase transition crossing the antiferromagnetic ordering temperature. These measurements were contrasted with XRD at high temperature to map the structural phase transition associate to the ferroelectric distortion. Our results suggest that NP size also modifies the ferroelectric and antiferromagnetic transition, allowing for a full control of the multiferroic ordering.

*Partial Funding provided by Vicerrectoria de Investigaciones Universidad de los Andes and DOE grant DE-FG02-87ER-45332

Friday, March 8, 2019 11:15 AM - 12:51 PM

Session Y05 DCMP: Novel Techniques BCEC 108 - Daniel Arovas, University of California, San Diego

11:15AM Y05.00001: A Multi-Element Microcalorimeter X-ray Detector that processes Pulses in Real Time TERRENCE JACH (Presenter), National Institute of Standards and Technology, STEPHEN M. THURGATE, Murdoch University, ROBIN H CANTOR, Star Cryoelectronics, JOEL ULLOM, National Institute of Standards and Technology — Terrence Jach, NIST, Gaithersburg, MD, Stephen M. Thurgate, Murdoch University, Perth, Australia, Robin Cantor, Star Cryoelectronics, Santa Fe, NM, and Joel Ullom, NIST, Boulder, CO. We describe a microcalorimeter x-ray detector that operates up to 8 detector elements with full digital processing in real time. Each detector element employs a transition-edge sensor and two-stage SQUID electronics. The detector covers an energy range of 200 eV to 10 keV, with 5 eV resolution, at a count rate of 800/s. The processing includes pulse pileup rejection, digital filtering, peak fitting and an energy-calibrated histogram that displays a collective spectrum from all 8 detectors. The computer overhead is sufficiently low that we can envision a considerable expansion of the number of detectors.
11:27AM Y05.00002: Galeras Volcano internal structure characterization using geological and geophysics techniques as input to muon tomography studies* DENIS TORRES (Presenter), Physics, Universidad de Nariño, DAVID MARTINEZ, Physics, South Dakota School of Mines and Technology, ROBERTO TORRES, Servicio Geologico Colombiano, ALEX TAPIA, Physics, Universidad de Medellin, JAIME BETANCOURT, Physics, Universidad de Nariño, JAIRO RODRIGUEZ, Physics, South Dakota School of Mines and Technology, DAVID DUEÑAS, Physics, University of Cincinnati, DANILO ARTURO, Physics, Universidad de Puerto Rico — The Galeras Volcano (GV) activity has been monitored for several years due to it is surrounded by highly populated areas. Many populations have grown and settled in dangerous areas, this has increased the risk levels of these populations taking into account the GV recent history of eruptions and generation of pyroclastic flows. In this work, densities in the GV Complex and its variations were analyzed using geological studies and different geophysical methods, such as the seismic tomography of the P wave velocities and gravimetry. In the first method, layers are used at depths ranging from 4 to -10 km, taking 0 km as the sea level. It was obtained that the greatest density variation is between 2 and 0 Km with values between 2.16 and 2.43 g/cm³. Using the gravimetric method, a distribution map of densities ranging from 2.16 to 2.72 g/cm³ was obtained, the map shows a large number of low densities that can correspond to young bodies with little consolidation. The results obtained in this work will be a key input to enhance the developed GEANT4 simulations of GV within the project that aims to study the GV structure using the muon tomography technique.

*The speaker would like to thank the award received by FIP DS Program. The award will support speaker attendance to APS conference.

11:39AM Y05.00003: Studies in Baseplate-Pixel Sensor Gluing of the Pixel Strip Modules for the Compact Muon Solenoid Experiment Phase-2 Upgrade JEM GUHIT (Presenter), Mount Holyoke College, JAMES KEAVENEY, MARINO MISSIROLI, CMS, DESY — The upgrade program, Phase-2 of the High Luminosity LHC (HL – LHC), is planned to increase instantaneous peak luminosities to 5.0 x 10³⁴ cm⁻² s⁻¹. This study focuses on the Pixel-Sensor (PS) Module which will be installed in the end cap region of the Compact Muon Solenoid (CMS) detector. In order to prolong the lifetime of the modules during operation, an efficient cooling system has to be embedded within the components. The contact between the module and cooling is provided by a glue layer. Therefore, the study outlines the advances and improvements made on the gluing techniques between the baseplate and pixel sensor of the pixel strip (PS) modules to meet specifications. The automated assembly was commissioned by DESY (Deutsches Elektronen Synchrotron) to increase the building efficiency of the modules. Using two types of epoxy glues, a fast curing, and slow curing glue, the specifications were achieved by exploiting the precision of the motion stage to achieve a thin glue layer with excellent coverage. The techniques were tested and produced promising results. Further studies on improving the method and assembly of modules are being done at the Detector Assembly Facility (DAF) at DESY in Hamburg, Germany.

11:51AM Y05.00004: Photoelectric Effect And Mass-Energy Energy Equations Must IncludeRotational And Vibrational Kinetic Energy Factors As Well As Linear Kinetic Factors. Also Mass-Energy Equation Must Also Include Potential Energy Factors. STEWART BREKKE (Presenter), Northeastern Illinois University — Einstein originally proposed in his Special Theory of Relativity that at low speeds \( E_0 = m_0c^2 + \frac{1}{2}mv^2 \). However, the total energy at low speeds must include the rotational and vibrational kinetic energies as well as potential energies. Therefore the proper mass-energy equation at low speeds must be \( E_0 = m_0c^2 + \frac{1}{2}mv^2 + \frac{1}{2}I\omega^2 + kx_0^2 + Gm_1m_2/r + kQ_1Q_2/r \). Originally, Einstein proposed that the ejected electron in the Photoelectric Effect through collisions in the material has lost its original kinetic energy and only the energy from the impacting photon affects the linear kinetic energy of the ejected electron. However, also through collisions in the material the ejected electron all rotational and vibrational kinetic energy is lost and only the energy from the impacting photon is retained by the ejected electron. Therefore, the resulting equation for the Photoelectric must be \( hf = (\frac{1}{2}mv^2 + \frac{1}{2}I\omega^2 + \frac{1}{2}kx_0^2) \max + \phi \) to include the rotational and /or vibrational kinetic energies if present in the final Photoelectric Effect equation.
12:03PM Y05.00005: Ultralow-power nonlinear optics using optical nanofibers in metastable xenon atoms*

HARI LAMSAL (Presenter), JAMES FRANSON, TODD BUTLER PITTMAN, Department of Physics, University of Maryland, Baltimore County — Nonlinear optics (NLO) is a very broad field with applications ranging from frequency conversion and all-optical switching to quantum computing. For many of these applications, the use of low power lasers is desirable. Consequently, there is currently a push for the realization of new physical platforms enabling ultralow-power NLO. We study a promising ultralow-power NLO platform consisting of an optical nanofiber (ONF) suspended in a gas of metastable xenon atoms (Xe*). The origin of strong nonlinearity in this platform is due to the tight confinement of the ONF guided evanescent mode (~1 μm²) over a long distance (~1 cm), and a resonant interaction of the mode with the surrounding atoms. In this talk, I will describe how we develop our experimental “ONF in Xe*” platform, with ONF’s having long life, and no degradation of transmission through them. I then will explain the experimental result of ultralow-power (nWs level) saturation effects using the platform.

*This work is supported by National Science Foundation (NSF) (1402708).


JEFFREY LINDEMUTH (Presenter), Lake Shore Cryotronics (United States) — The Hall effect, discovered in 1879 by E. Hall, is the primary method to measure carrier density, mobility and carrier type in materials. The most common method for measuring the Hall effect in semiconductors uses a DC magnetic field. This method depends are reversing the direction of the magnetic field. For some applications, especially low mobility materials, the use of an AC field instead of a DC field provides better measurements. Using the field reciprocity theorem, it is possible to generate the same hall measurements without the use of an external AC field. The frequency of this “effective AC field” is determined by the rate of interchanging the current and voltage leads attached to the sample and is not limited by the induction of the magnet generating the DC field. The current excitation can also be modulated by switching the direction of the current leads. The frequency of the effective AC field and the AC current do not have to be the same. This provides the opportunity of dual frequency (AC field/AC current) hall measurements over a wide, and independent, frequency range. Measurements of low mobility (< 1 cm²/(V s) materials will be presented.

12:27PM Y05.00007: Morphology of copper using lateral electrodeposition suitable for low-temperature soldering of microelectronic devices*

SABRINA ROSA (Presenter), ARASH TAKSHI, University of South Florida — Lateral copper growth for the development of electroplating technique as a low-temperature soldering procedure allows modification of the morphology and properties of soldering joints. The approach is particularly useful for soldering electronic components to a plastic 3D printed substrate and printed circuit boards(PCBs). Miniaturization of PCBs has shown an improvement in the efficiency and properties of electronic devices leading to new applications. An electrode pattern was used with a separation gap of 1mm. A junction between the two working electrodes was reported to occur in less than 1 minute, this result ensures the participation of the electrolyte. Hydrogen bubbles released after the electrolysis caused the structure of the electroplated layer to be more porous suitable for sensors and other applications. The morphology of copper deposits based on the interaction with hydrogen was examined using Scanning Electron Microscopy (SEM) technique. Further experiments are required to optimize the soldering process for 3D approaches allowing interconnections of microelectronic devices.

*This work was supported by the National Science Foundation through NSF 1400017 and NSF Florida-Georgia Louis Stokes Alliance for Minority Participation Bridge to the Doctorate HRD #1612347.

12:39PM Y05.00008: Effect of Evaporation Boundary Condition on The Consolidation and Crack Propagation in Drying Colloidal Films*

HAN GAO, School of Mechanical Engineering and Automation, Beihang University, JIAJIA ZHOU, MASAO DOI, Center of Soft Matter Physics and its Applications, Beihang University, YE XU (Presenter), School of Mechanical Engineering and Automation, Beihang University — We investigate the dynamics of consolidation front growth and the subsequent crack propagation during the directional drying of colloidal film. By varying the geometry of the drying boundary, we observe that the shape of the consolidation front evolve from the shape of the boundary to one with smallest curvature. We also find the direction of the crack propagation keeps perpendicular to the consolidation front, resulting curved cracks. A theoretical model is developed to explain the evolution of consolidation front. Our finding allows us to explore other evaporation boundary conditions, such as temperature and humidity gradient, to control the direction of crack propagation in drying colloidal films.

*This work is supported by National Natural Science Foundation of China (Grant No. 11674019)

Friday, March 8, 2019 11:15 AM - 1:51 PM
11:15AM Y06.00001: The role of Joule heating in the voltage-triggered insulator-to-metal transition in VO$_2$.\textsuperscript{*}

ALYSON SPITZIG (Presenter), ALEX J FRENZEL, JEEHOON KIM, Physics, Harvard University, CHANGHYUN KO, SEAS, Harvard University, SHRIRAM RAMANATHAN, School of Materials Engineering, Purdue University, JENNIFER HOFFMAN, JASON D HOFFMAN, Physics, Harvard University — VO$_2$ undergoes a conductivity increase of up to five orders of magnitude as the temperature is increased through 341 K. Recently, the insulator-to-metal transition (IMT) has been triggered with an applied voltage, but debate remains as to whether the transition can be due to electric field effects alone, or whether Joule heating is necessary. Here, we use a conductive AFM tip to locally apply a voltage bias and measure the current through a VO$_2$ film. By fitting the $i/v$ curves immediately preceding the IMT to the temperature-dependent Poole-Frenkel conduction mechanism, we determine the local temperature of VO$_2$ in the insulating state. We find that the tip has locally warmed the film to 335 K ± 4 K immediately preceding the transition. Therefore, Joule heating plays a significant role in the voltage-triggered IMT in VO$_2$.

\textsuperscript{*}AS was funded by NSERC CGSM #6563, JDH was funded by Gordon and Betty Moore Foundation EPiQS Initiative Grant No. GBMF4536, NSF Grant No. DMR-1231319, sample fabrication funded by AFOSR Grant No. FA9550-08-1-0203.

11:27AM Y06.00002: Self-consistent GW study of VO$_2$\textsuperscript{*}

ANDREY KUTEPOV (Presenter), Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory — The question of the metal-insulator transition (MIT) in VO$_2$ remains open. Hybrid functionals [1] and non-self-consistent G$_0$W$_0$ [2] studies state that non-local exact exchange (EEX, included in hybrids and GW) is the most important. However, the arbitrariness of the percentage of EEX (hybrids) or of the starting point (G$_0$W$_0$) makes the agreement of the results with experiment not convincing. From the LDA+DMFT studies of VO$_2$ [3,4] it follows that strong on-site correlations are important for MIT. However, LDA+DMFT operates with local parameters (U and J) and the argument in favor of strong correlations might be just a consequence of missing the non-local EEX in LDA+DMFT. The talk will be about the role of self-consistency in GW approach, which eliminates dependence on the starting point. It will be shown that indeed the GW level of theory provide all necessary basis for description of MIT in VO$_2$ quantitatively.


\textsuperscript{*}This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences as a part of the Computational Materials Science Program.

11:39AM Y06.00003: Microstructural Engineering of the UV/Near-UV Photocurrent Production in VO$_2$ Thin Film Based Detectors\textsuperscript{*}

JASON CREEDEN (Presenter), SCOTT MADARAS, DOUG BERINGER, MELISSA R BEEBE, IRINA NOVIKOVA, ROSA ALEJANDRA Lukaszew, Physics, William & Mary — We sought to optimize the photosensitivity of VO$_2$ thin films in the near-UV (NUV) and UV regions after recent reports demonstrating it is possible to push the typical IR photoresponse of VO$_2$ into the visible spectrum via thin film growth on TiO$_2$:Nb substrates. By controlling the microstructure of the films via deposition parameters and substrate doping, we optimize VO$_2$ growth for TiO$_2$ and TiO$_2$:Nb substrates and compare their photocurrent response using 405 nm (NUV) and 254 nm (UV) light. We found that the VO$_2$ on TiO$_2$:Nb heterostructure demonstrates greater photocurrent response. By measuring the external quantum efficiency (EQE), we found a dramatic photosensitivity improvement for the VO$_2$ on TiO$_2$:Nb compared to undoped TiO$_2$ substrates. Notably, we demonstrated greater than 100% EQE for VO$_2$ on TiO$_2$:Nb for both wavelengths and an improvement in the EQE using UV in comparison to the NUV. Finally, we additionally propose a mechanism for this photoresponse which potentially allows for greater than 100% EQE.

\textsuperscript{*}We would like to thank the Defense Threat Reduction Agency (HDTRA 1-16-1-0056) for the continued support and funding for the project.
11:51AM Y06.00004: An infrared investigation of the insulator-to-metal transition in a thin, epitaxially strained VO₂ film* DAVID LAHNEMAN (Presenter), PATRICK MCARDLE, MUHAMMAD M QAZILBASH, Department of Physics, College of William & Mary, TETIANA SLUSAR, HYUN-TAK KIM, Metal-Insulator Transition Laboratory, Electronics and Telecommunications Research Institute — The insulator-to-metal transition temperature of vanadium dioxide (VO₂) can be tuned through epitaxial strain induced by lattice mismatch between a thin VO₂ film and the substrate. Here we report infrared and optical measurements on a very thin (~ 10 nm) VO₂ film on (001) TiO₂ substrate with an insulator-to-metal transition temperature of ~ 305 K, just above room temperature. We map the transition as it evolves in temperature using near-field imaging at a wavelength of ~10μm from a mid-infrared laser. Using our tabletop home-built argon plasma light source, we obtain the broadband near-field infrared spectra on the pristine substrate and the film-substrate system.

*M.M.Q. acknowledges support from NSF DMR-1255156

12:03PM Y06.00005: Correlation-driven metal-insulator transitions in hydrogenated VO₂* SE YOUNG PARK (Presenter), Center for Correlated Electron Systems (CCES), Institute for Basic Science (IBS), SO YEUN KIM, Department of Physics and Astronomy, Seoul National University, STEFFEN BACKES, Centre de Physique Théorique, Ecole Polytechnique, France, BYUNG CHEOL PARK, Center for Correlated Electron Systems (CCES), Institute for Basic Science (IBS), JUNWOO SON, HYOJIN YOON, Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), TAE WON NOH, Center for Correlated Electron Systems (CCES), Institute for Basic Science (IBS), SILKE BIERMANN, Centre de Physique Théorique, Ecole Polytechnique, France — We investigate the electronic and optical properties of hydrogenated HₓVO₂. We find doping-dependent metal-insulator transitions as increasing hydrogen content from the optical conductivity measured by spectroscopic ellipsometry, showing a gap opening with a structural transition forming V-V dimer as increasing the H doping. The insulating phase is investigated using density functional and dynamical mean-field theory. We identify the orbital-ordered paramagnetic insulating phase as the ground state of HVO₂ in which both the dimer-induced bonding-antibonding splitting and the orbital ordering stabilized by electron correlations play an important role in the metal-insulator transition. We compare the calculated optical conductivity of the metallic and insulating phases with experimental data and discuss the increase in the charge transfer energy with high hydrogen content.

*This work is supported by the Institute for Basic Science in Korea (Grant No. IBS-R009-D1).

12:15PM Y06.00006: Insights into the anomalous thermal properties of VO₂ from synchrotron spectromicroscopy SUHAS KUMAR, Hewlett Packard Labs, STEPHANIE BOHAICHUK (Presenter), Stanford University, LU CHEN, University of Michigan, ADITYA SOOD, Stanford University, DAVID A SHAPIRO, Lawrence Berkeley National Laboratory, HAIDONG ZHOU, University of Tennessee, AARON M LINDENBERG, Stanford University, LU LI, University of Michigan, STANLEY WILLIAMS, Hewlett Packard Labs, ERIC POP, Stanford University — Within the last year there have been reports on two distinct anomalous behaviors of the thermal conductivity of VO₂ across its insulator-metal transition, namely: (1) a violation of the Wiedemann Franz law and (2) a giant peak in thermal conductivity during the transition. These have not been captured by physical models, and an understanding of their origin requires in situ probing of both the electronic and structural transitions in VO₂ with very high spatial and thermal resolution. Here we performed temperature-controlled scanning X-ray absorption spectromicroscopy (SXASM), using synchrotron radiation with <30 nm spatial resolution, on single crystal VO₂ that exhibited these anomalies in thermal conductivity. SXASM revealed distinct signatures of the Mott electronic transition and the Peierls structural distortion, which occurred at slightly different temperatures, with the electronic transition occurring first. These results are combined with measurements of thermal conductivity, Seebeck coefficient, and electrical conductivity. We juxtapose these multi-dimensional data sets to shine light on possible correlations between the different transitions and the anomalous changes in VO₂ thermal properties.
**12:27PM Y06.00007: Modulating metal-insulator transitions in VOX by tuning oxygen stoichiometry**  
MINHAN LEE (Presenter), YOAV KALCHEIM, JAVIER DEL VALLE, IVAN SCHULLER, Department of Physics and Center for Advanced Nanoscience, University of California - San Diego — Thermally driven metal-insulator transitions (MITs) in vanadium oxides (VOX) have been of special interest in fundamental physics and oxide electronics. The existence of multi-valence states of vanadium leads to a complicated vanadium-oxygen phase diagram. Moreover, for thin films, finite size or strain effects can alter the physical and thermodynamic properties of the V-O system. Therefore, precise oxygen stoichiometry control in these oxide films remains an outstanding issue and a clear phase stability diagram has not yet been found. We demonstrate a gas evolution technique to precisely modify the oxygen stoichiometry in VOX thin films grown on sapphire substrates. By carefully tuning the temperature-oxygen partial pressure-time relationship, controlled phase evolution between VO2, V2O3 and Magnéli phases (VnO2n-1) was achieved, along with the detailed characterization of their electrical transport and structural properties. Moreover, we show that high quality films, with well-defined MITs can be synthesized this way.

*This work was supported by the AFOSR grant FA9550-14-1-0202, funded by the Vannevar Bush Faculty Fellowship program and funded by the Office of Naval Research through grant N00014-15-1-2848. J. del Valle acknowledges support from Fundación Ramón Areces.

**12:39PM Y06.00008: Non-Gaussian resistance noise behavior across the metal-insulator transition in VO2 thin films**  
AHMED ALI (Presenter), DASHARATH ADHIKARI, COLIN P KILCOYNE, SAMBANDAMURTHY GANAPATHY, Physics, University at Buffalo — Vanadium dioxide (VO2) thin films exhibit a sharp metal-insulator transition (MIT) at a critical temperature ~ 330 K. The significance of a Peierls-type instability or a Mott-Hubbard-type transition near Tc has been a topic of discussion for many years. We present results from a resistance noise spectroscopy study of VO2 thin films that show that the power spectral density (PSD) of the fluctuations near Tc show a marked deviation from the metallic and insulating phases. The PSD increases by orders of magnitude and deviates from a typical 1/f behavior near Tc. The probability density function (PDF) of the fluctuation is non-Gaussian in nature in thin films near Tc whereas the fluctuations are Gaussian at all temperatures in single crystal nanobeams. Our results suggest that the transition likely occurs as a single domain phenomenon in nanobeams whereas the nucleation and propagation of multiple domains of opposite phase are significant near Tc in thin films. The influence of the coexistence of phases on electrical transport will be discussed based on our analysis of the 1/f behavior, PSD, PDF and the second spectrum of noise.

**12:51PM Y06.00009: Resonant Hard X-ray Emission Spectroscopy of VO2 Thin Films in Metallic and Insulating Phases**  
SUNG SOO HA (Presenter), SEOKJUN CHOI, MOHD FAIYAZ, Gwangju Institute of Science and Technology, SUYONG LEE, Pohang Accelerator Laboratory, Pohang University of Science and Technology, DO YOUNG NOH, Gwangju Institute of Science and Technology — Resonant X-ray emission spectroscopy (XES) was carried out to study the metal-insulator transition (MIT) of vanadium dioxide. The Vanadium K-beta emission spectra including kβ2,5 and kβ1,3 both in the metallic and insulating phase were monitored with an x-ray energy resolution of about 1.6 eV at the 3rd generation Pohang Accelerator Laboratory using a highly oriented pyrolytic graphite (HOPG) spectrometer in von-Hamos geometry. The K-beta emission intensities were monitored as the excitation x-ray energy was scanned through the Vandium K-edge to obtain the X-ray absorption near edge structure (XANES) profile. In both the emission spectra and the XANES profile, the difference between the insulating and metallic phase was clearly observed. We also observed distinct resonant behavior in the elastic/inelastic scattering intensity. The physical interpretation of the resonant behavior will be discussed in relation with the energy band structure of the insulating and metallic phase of VO2.

*This work was supported by the National Research Foundation of Korea (NRF) through NRF-2015R1A5A1009962(SRC), and a grant provided by GIST in 2018.*
Resistance fluctuation of V$_2$O$_3$ films near the metal-insulator transition

LIYANG CHEN

Presenter, PANPAN ZHOU, Rice University, YOAV KALCHEIM, IVAN SCHULLER, University of California San Diego, DOUGLAS NATELSON, Rice University — The metal-insulator transition in the correlated material V$_2$O$_3$ is a highly studied phenomenon. Recent research has shown the nanotextured phase coexistence around the transition temperature ($T_c$) in V$_2$O$_3$ films, but the dynamic electronic properties are still not well resolved. Here, we study resistance fluctuations as a function of time in both low frequency (< 300 kHz) and higher frequency (225MHz-580MHz) ranges, comparing them to show the dynamic properties at both low and high frequency. We performed measurements at temperatures above $T_c$, close to $T_c$, and below $T_c$. We found 1/f type noise close to and below (yet near) $T_c$ as expected at low frequencies, and similar resistance fluctuation noise (mean square voltage fluctuations proportional to the square of the bias current) at higher frequency. However, the integrated noise intensity at high frequency exceeds our expectation based on an extrapolation of the observed low frequency data. More detailed measurements and experiments are ongoing to reveal the mechanism that causes the resistance fluctuations in V$_2$O$_3$ films near the metal-insulator transition.

The authors acknowledge support from the U.S. DOE office of Science/Basic Energy Science Award DE-FG02-06ER46337.

The role of defects on the metal-insulator transition in V$_2$O$_3$ and VO$_2$

DARSHANA WICKRAMARATNE

Presenter, NRC Research Associate residing at, US Naval Research Laboratory, Washington, DC 20375, USA, NOAM BERNSTEIN, IGOR MAZIN, Center for Computational Materials Science, US Naval Research Laboratory, Washington, DC 20375, USA — V$_2$O$_3$ and VO$_2$, are prototypical strongly-correlated materials that undergo a metal-insulator transition (MIT). The MIT in both materials leads to a concomitant structural phase transition and a magnetic phase transition in V$_2$O$_3$. Recent experiments [PRB 91, 205123, 2015] explored the sensitivity of the MIT to defects and demonstrated the MIT phenomenon in V$_2$O$_3$ is sensitive to the presence of defects while it is robust in VO$_2$. To explore the underlying mechanisms for this behavior we performed first-principles calculations to assess the role of defects on the structural, magnetic and electronic properties of V$_2$O$_3$ and VO$_2$. In V$_2$O$_3$ we find defects disrupt the antiferromagnetic (AFM) order in the insulating phase. We also find small polarons form through self-trapping or due to defects. We assess the impact of this phenomenon on the spin-flip energy between the metallic paramagnetic and the insulating AFM state with the goal of understanding how this impacts the MIT temperature. In VO$_2$, we explore the impact of defects on the vanadium dimerization in the insulating phase and the impact on the MIT.

NB and IM were supported by Office of the Undersecretary of Defense for Research and Engineering’s Basic Research Office through the LUCI. DW was supported by a NRC associateship at the US NRL.

NMR and bulk studies on S=1/2 spin chain Bi$_6$V$_3$O$_{16}$

TANMOY CHAKRABARTY

Presenter, IVO HEINMAA, Physics, NICPB, VALERIY YU. VERCHENKO, Chemistry, Lomonosov Moscow State University, P L PAULOSE, DCMPMS, TIIFR, RAIVO STERN, Physics, NICPB — We report the NMR and bulk properties of a vanadium based S=1/2 spin chain compound Bi$_6$V$_3$O$_{16}$ in its low temperature phase where the magnetic V$^{4+}$ ions are arranged in a one-dimensional chain mediated by V$^{5+}$ and oxygen ions. We have carried out magnetic and heat capacity measurements, both static and magic angle spinning (MAS) $^{51}$V NMR measurements and analysis for unaligned powder sample. The magnetic susceptibility $\chi$ shows a broad maximum around 50 K signifying a short-range magnetic order which matches well with the S=1/2 Heisenberg chain model. In the NMR measurements, we only detected the non-magnetic $^{51}$V. The spin susceptibility calculated from the shift of the static $^{51}$V NMR spectra reproduces well the behavior observed in $\chi$. The MAS NMR experiments reproduce the trend observed in $\chi$ and static NMR with unprecedented accuracy, and confirm that there is only one site the V$^{4+}$ ions are occupying. We have also performed and analyzed spin-lattice relaxation measurements of $^{51}$V.

Department of Science and Technology, Government of India, Mobilitas-Plus Estonian fellowships (MOBJD295, MOBJD449), European Regional Development Fund (TK134), Estonian research council (PRG4) and Government of Estonia (IUT23-7)
SCOTT MADARAS (Presenter), JASON CREEDEN, DOUG BERINGER, IRINA NOVIKOVA, ROSA ALEJANDRA LUKASZEW, Physics, William and Mary — We have studied vanadium dioxide (VO2) films grown on titanium dioxide (TiO2) substrates to investigate the properties of the heterojunction that forms at the interface between substrate and film with the purpose of applying it as an UV photodetector. The use of niobium as dopant on TiO2 substrates has been shown to favorably modify the energy levels at the heterojunction thus promoting photocurrent generation when illuminated with UV light. To further investigate this electronic structure modifications we study the ultrafast dynamics of the insulator-metal-transition (IMT) in such samples by using a pump probe configuration. The samples are pumped with ~150 fs pulses of 400nm wavelength light, and the changes in electronic structure of the heterojunction region are detected via change in relative optical reflectance (ΔR/R) of a 800nm probe light. The VO2 on TiO2:Nb doped samples generate distinctive ΔR/R effects compared with the VO2 films deposited on plain TiO2 substrates samples that are undoped.

*This work is supported by Defense Threat Reduction Agency grant (HDTRA 1-16-1-0056)

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y08 DCMP DMP: Superconducting Devices and Applications BCEC 150 - Lei Wang, Yale Univ

11:15AM Y08.00001: Ferroelectric control of superconductivity in an oxide interface* PRASANNA KUMAR ROUT, YORAM DAGAN (Presenter), Tel Aviv University — We study the transport properties of two-dimensional (2D) interfaces between a (3D) ferroelectric oxide and a polar one. The interface is superconducting with a transition temperature of 300mK. From the analysis of the anisotropy of the critical fields we find that superconductivity is 2D in nature. The resistance and the Hall conductance of the interface exhibit a hysteretic behavior as a function of gate voltage. The area of the hysteresis loop becomes zero at the ferroelectric transition temperature. A hysteretic dependence on gate voltage is also seen for the superconducting transition temperature and critical fields. We discuss possible interplay between superconductivity and ferroelectricity at this interface.

*Support from the Israeli Science Foundation is acknowledged

11:27AM Y08.00002: Tunable superconducting devices with a reconfigurable artificial-spin-ice* YANGYANG LYU (Presenter), Nanjing University, XIAOYU MA, University of Notre Dame, JING XU, Northern Illinois University, YONGLEI WANG, Nanjing University, ZHILI XIAO, Argonne National Laboratory, HUABING WANG, Nanjing University, RALU DIVAN, JOHN E. PEARSON, Argonne National Laboratory, BOLDIZSAR JANKO, University of Notre Dame, WAI-KWONG KWOK, Argonne National Laboratory — Recent work has shown that the magnetic charges in an artificial spin ice can strongly influence the properties of materials in contact with the spin ice structure [Science 352, 962 (2016) & Nature Nano. 13, 560 (2018)]. Here, we present a novel heterostructure combining a newly-introduced artificial spin ice pattern with a superconducting MoGe film. The reconfigurable magnetic template produced by artificial spin ice strongly couples with the vortices in the superconducting film, which enables us to control its transport properties. We will demonstrate some tunable functions of this artificial-spin-ice and superconductor heterostructure.

*The experiments were supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division and by DOE BES under Contract No. DE-AC02-06CH11357 that also funds Argonne's Center for Nanoscale Materials (CNM) where the nanopatterning was performed. YYL and YLW was supported by NSFC under Contract No. 61771235.

11:39AM Y08.00003: Estimating the effect of grain boundaries on the superconducting superheating field in 2D Ginzburg-Landau Theory* ALDEN PACK (Presenter), MARK TRANSTRUM, JARED CARLSON, Brigham Young University — The Meissner effect is the expulsion of an applied magnetic field by a superconducting material. For large applied fields, a surface effect creates barrier to vortex nucleation so that the Meissner state may persist in a meta-stable state up to a critical, superheating field. We study the role of grain boundaries, including surface morphology and material inhomogeneity, on vortex nucleation within two-dimensional Ginzburg-Landau theory. Our simulations mimic conditions observed in Nb3Sn SRF cavities using in particle accelerators. We show how defects lower the superheating field and discuss implications for SRF cavity performance and development.

*This work was supported by the U.S. National Science Foundation under Award PHY-1549132, the Center for Bright Beams.
**11:51AM Y08.00004: Tunneling spectroscopy of Nb/Al bilayers for superconducting computing**  
ZAC BARCIKOWSKI (Presenter), University of Maryland, College Park, JOSHUA POMEROY, MICHAEL DAVID STEWART, National Institute of Standards and Technology — Niobium and aluminum, and the compounds made from them, are important materials in the superconducting computing community. However, much remains to be explored to understand the interaction of states between Nb based superconductors and Al, and how these properties can be used to improve tunnel junctions and cavities. Tunneling spectra of normal metal (N)/insulator (I)/superconducting bilayer (S) tunnel junctions are found to vary significantly as a function of the thickness of the bilayer elements. We present N/I/S tunnel junctions fabricated with various Al thicknesses in the superconducting bilayer electrode. Tunneling spectra are measured at 4 K and fit using Maki analysis to extract orbital depairing and spin-orbit parameters.

**12:03PM Y08.00005: Proximity effect of Nb/Al superlattice as a superconducting resonator**  
LONG CHENG (Presenter), SANGIL KWON, Institute for Quantum Computing, University of Waterloo, HAMID R. MOHEBBI, High Q Technologies LP, YONGCHAO TANG, DAVID CORY, GUOXING MIAO, Institute for Quantum Computing, University of Waterloo — Superconducting resonator has evoked growing interest due to the wide spectrum of applications, especially in the booming realm of quantum information and quantum computing. How to achieve high-Q resonators as well as the ones maintaining high Q in a modest magnetic field are the long-standing goals and persistently explored issues. Here we systematically study how the proximity effect influence the performance of Nb/Al superlattice resonators. We fabricate a series of Nb/Al superlattice resonators with total thickness of 50 nm, while the number of repetition ranges from 1 (ie, 25nm Nb/25 nm Al) to 20 (ie, (1.25nm Nb/1.25nm Al)20). The DC transport measurement shows the proximity effect becomes stronger with the increasing number of repetition, while microwave measurement shows non-monotonic dependence of Q value, which may be ascribed to the competition between the enhanced proximity effect and the reduced mean free path of electrons. Based on this work, we are able to find the optimal design for proximity enhancement, which may be beneficial for further exploring high performance resonators.

*Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery grant RGPIN-04178, and Ontario Early Researcher Award

**12:15PM Y08.00006: Ternary and higher order classical cryogenic memory cells**  
NIKETH NAIR (Presenter), YEHUDA BRAIMAN, Oak Ridge National Laboratory — For many classical cryogenic computing applications, a key issue in designing powerful and practical systems is the scaling of memory. In particular, the amount of circuitry required to build and access memory units has limited the amount of information that it is possible to store. A possible solution to this problem is to consider designs that store more information in a single memory unit. Therefore, it may be beneficial considering ternary and higher order multivalued memory systems that use the same number of Josephson junctions as binary units.

In this talk we will present a ternary cryogenic memory cell paradigm based on an array of inductively coupled Josephson junctions[1]. We show how reading, writing and resetting are implemented using single flux quantum (SFQ) current pulse inputs and outputs from the circuit. We further show how both destructive readout (DRO) and nondestructive readout (NDRO) can be implemented.


*Support for this work was provided by the US Department of Energy, Office of Science, Advanced Scientific Computing Research. Oak Ridge National Laboratory is managed by UT-Battelle, LLC for the US Department of Energy under Contract No. DE-AC05-00OR22725.
12:27PM Y08.00007: Vortex rectenna powered by environmental fluctuations*  
JANA LUSTIKOVA (Presenter), Institute for Materials Research, Tohoku University, YUKI SHIOMI, Quantum-Phase Electronics Center, University of Tokyo, NAOTO YOKOI, Institute for Materials Research, Tohoku University, NORIYUKI KABEYA, NORIAKI KIMURA, Center for Low Temperature Science, Tohoku University, KOICHIRO IENAGA, SHIN-ICHI KANEGO, SATOSHI OKUMA, Department of Physics, Tokyo Institute of Technology, SABURO TAKAHASHI, Institute for Materials Research, Tohoku University, EJI SAITO, Department of Applied Physics, University of Tokyo — A rectenna, standing for a rectifying antenna, is an apparatus which generates d.c. electricity from electric fluctuations. It is expected to realize wireless power transmission as well as energy harvesting from environmental radio waves. To realize such rectification, devices that are made up of internal atomic asymmetry such as an asymmetric junction have been necessary so far. Here we report a material that spontaneously generates electricity by rectifying environmental fluctuations without using atomic asymmetry [Lustikova et al., Nat Commun (2018)]. The sample is a common superconductor without lowered crystalline symmetry, but, just by putting it in an asymmetric magnetic environment, it turns into a rectifier and starts generating electricity. Superconducting vortex strings only annihilate and nucleate at surfaces, and this allows the bulk electrons to feel surface fluctuations in an asymmetric environment: a vortex rectenna. The rectification and generation can be switched on and off with only a slight change in temperature or external magnetic fields.

*This work was supported by JST ERATO Spin Quantum Rectification Project (JPMJER1402), JSPS KAKENHI (Nos. 16J03699, 17H04806, 18H04215, and 18H04311), and MEXT (Innovative Area “Nano Spin Conversion Science” (No. 26103005)).

12:39PM Y08.00008: Superconducting Microwave Circuits with High Kinetic Inductance Materials in High Magnetic Fields  
AZARIN ZARASSI (Presenter), JEN-FENG HSU, TZU-CHIAO CHIEN, XI CAO, MICHAEL HATRIDGE, SERGEY M FROLOV, University of Pittsburgh — We report our experimental progress towards a semiconducting nanowire Josephson junction fluxonium. We fabricate co-planar waveguide and meander nanowire superconducting resonators from NbTiN and NbN thin films. These resonators exhibit a wide range of intrinsic quality factors based on fabrication methods, including lift off versus etching. They maintain their quality factors in finite magnetic fields. These thin-film resonators provide large kinetic-inductance boosts where they can be used as the large shunting inductor in a fluxonium qubit where the nonlinear element is either a conventional Al/AlOx/Al Josephson junction or a semiconducting nanowire weak link.

12:51PM Y08.00009: Geometric Superinductors for Mesoscopic Physics*  
MATILDA PERUZZO (Presenter), ANDREA TRIONI, MARTIN ZEMLICKA, Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria, LISA ARNDT, FABIAN HASSLER, JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany, JOHANNES FINK, Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria — High impedance has recently risen as a tool for circuit engineering in cQED. For regular microwave circuits the agreed upon impedance is 50Ω, vacuum itself has an impedance of 377Ω. In the quantum realm however there is a threshold above which a superconducting circuit is considered high impedance, the resistance quantum RQ=6kΩ. In fact impedance of the environment affects the quantum fluctuations of phase and charge and when the quantum resistance is surpassed charge fluctuations are suppressed to below 2e. Most interesting is the behavior of the Josephson junction (a key element for superconducting qubits) in this regime. The low charge fluctuations allow for the measurement of Coulomb blockade and Bloch oscillations of charge. This work demonstrates how the use of geometric superconducting inductors can become a new method to achieve high impedance. The inductor consists of a superconducting high density planar coil suspended on a 220nm silicon membrane which can achieve characteristic impedances of 14kΩ while having a self-resonance frequency above 8GHz. We present this new circuit element and it’s applications for the measurement of Josephson junctions in the high impedance regime.

*We aknowledge support from the NOMIS Foundation
Quantum thermodynamics in superconducting circuits

JORDEN SENIOR (Presenter), ALBERTO RONZANI, BAYAN KARIMI, YU-CHENG CHANG, AZAT GUBAYDULLIN, JOonas T PELTONEN, QTF Centre of Excellence, Aalto University, CHIIDONG CHEN, Institute of Physics, Academia Sinica (Taiwan), JUKKA P PEKOLA, QTF Centre of Excellence, Aalto University — Quantum thermodynamics has become a field of increasing importance in recent years, the understanding of heat transport at the quantum limit, having broad ranging applications, for example in circuit QED experiments, and nanoscale physics.

By integrating the tools of ultra-sensitive microwave bolometry with those of superconducting circuits (qubits), we present a platform for investigating fundamental quantum thermodynamics in mesoscopic systems, and our initial experimental realizations.

We will present recent observations of flux-tunable photonic heat transport between thermal baths embedded in both equal (quantum heat valve) and unequal (quantum heat engine) resonant environments interfaced by a transmon qubit. We demonstrate that the coupling to the qubit mediates the interface between the classical and quasi-Hamiltonian regime for this transport in the static-flux limit [1], and present our initial findings for a driven-flux system.


This work was supported by the Centre for Quantum Engineering (CQE) at Aalto University, OtaNano, and VTT Technical Research Center.

Spectroscopy of the two unequal superconducting resonators coupled via transmon qubit for the realization of the quantum heat engine

AZAT GUBAYDULLIN (Presenter), JORDEN SENIOR, BAYAN KARIMI, QTF Centre of Excellence, Department of Applied Physics, Aalto University, YU-CHENG CHANG, Department of Physics, National Taiwan University, JOonas T PELTONEN, QTF Centre of Excellence, Department of Applied Physics, Aalto University, CHIIDONG CHEN, Department of Physics, National Taiwan University, JUKKA P PEKOLA, QTF Centre of Excellence, Department of Applied Physics, Aalto University — Progress in both superconducting circuit QED experiments and ultrasensitive nanoscale bolometry provide a unique platform for studying heat transport in the quantum limit, towards the realization of quantum heat engines and refrigerators [1,2]. Transmon qubits coupled to superconducting resonators have been considered as promising candidates for realizing such quantum systems, such as the recently demonstrated quantum heat valve [3]. This work is devoted to study both theoretically and experimentally the transmission spectrum of the resonator-qubit-resonator assembly, in both the equal (valve) and unequal (engine) resonators regimes. For the realization of the quantum heat engine, we study the flux-tunable photonic heat transport in the resonator-qubit-resonator assembly with unequal resonators terminated by mesoscopic normal-metal reservoirs. Additionally, a means to characterize a superconducting resonator shunted with a highly dissipative normal metal bolometer is presented.

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Spectroscopy of the two unequal superconducting resonators coupled via transmon qubit for the realization of the quantum heat engine

AZAT GUBAYDULLIN (Presenter), JORDEN SENIOR, BAYAN KARIMI, QTF Centre of Excellence, Department of Applied Physics, Aalto University, YU-CHENG CHANG, Department of Physics, National Taiwan University, JOonas T PELTONEN, QTF Centre of Excellence, Department of Applied Physics, Aalto University, CHIIDONG CHEN, Department of Physics, National Taiwan University, JUKKA P PEKOLA, QTF Centre of Excellence, Department of Applied Physics, Aalto University — Progress in both superconducting circuit QED experiments and ultrasensitive nanoscale bolometry provide a unique platform for studying heat transport in the quantum limit, towards the realization of quantum heat engines and refrigerators [1,2]. Transmon qubits coupled to superconducting resonators have been considered as promising candidates for realizing such quantum systems, such as the recently demonstrated quantum heat valve [3]. This work is devoted to study both theoretically and experimentally the transmission spectrum of the resonator-qubit-resonator assembly, in both the equal (valve) and unequal (engine) resonators regimes. For the realization of the quantum heat engine, we study the flux-tunable photonic heat transport in the resonator-qubit-resonator assembly with unequal resonators terminated by mesoscopic normal-metal reservoirs. Additionally, a means to characterize a superconducting resonator shunted with a highly dissipative normal metal bolometer is presented.

References:

This work was supported by the Centre for Quantum Engineering (CQE) at Aalto University, OtaNano, and VTT Technical Research Center.
1:27PM Y08.00012: 1D Josephson chains isolated from the environment by superinductors* WEN-SEN LU (Presenter), KONSTANTIN KALASHNIKOV, PLAMEN KAMENOV, WENYUAN ZHANG, MICHAEL GERSHENSON, Rutgers University, New Brunswick — Superinductors offer new types of functionality, including non-dissipative high-impedance isolation of quantum circuits from the environment [i]. In our work we studied the chains of Josephson junctions (JJs) and individual JJs isolated from the environment by the superinductors made of strongly disordered Aluminum [ii]. The superinductors have been fabricated as nanowire meanders with small in-plane dimensions (to reduce parasitics) and the kinetic inductance up to 3 µH. We measured the current-voltage characteristics of JJ circuits with the normal-state resistance of individual JJs varied between 1 kΩ and 100 kΩ, and we observed the transition between thermally activated phase diffusion and macroscopic quantum tunneling regimes. We will also discuss application of superinductors for the observation of Bloch oscillations in Josephson circuits.


*This work was supported by awards NSF DMR 1708954, NSF DMR-1838979, and ARO award W911NF-17-C-0024.

1:39PM Y08.00013: Microwave Microscopy of Materials Limitations of Superconducting RF Cavities* BAKHROM ORIPOV (Presenter), STEVEN ANLAGE, University of Maryland, College Park — There are considerable efforts world-wide to improve particle accelerators by using Superconducting Radio Frequency (SRF) cavities which are limited by surface defects which lead to cavity breakdown at high accelerating gradients. A novel near-field magnetic microwave microscope that can study these defects was successfully built using a magnetic writer from a conventional magnetic recording hard-disk drive. We study the 3rd harmonic response-$V_{3f}(T, H_{rf})$ because it is far more sensitive to rf field amplitude $H_{rf}$ and temperature $(T)$ than linear response measurements. In our experiments on Nb surfaces we observed 2 different classes of nonlinearity depending on the location of the probe, which we call Low-field and Periodic. In the low-field case we observe that $V_{3f}$ increases uniformly as a function of applied rf field amplitude, reaches a peak value and decreases back to 0. In the periodic case $V_{3f}$ has periodic dips at $H_{rf} = H_1(T), H_2(T), H_3(T)$... The periodic case nonlinear response can be linked to Josephson effect at or near the surface and is in good agreement with the nonlinear response expected from rf-current-biased Resistively and Capacitively Shunted Junction (RCSJ) model.

*This work is funded by US DOE through grant # DESC0017931 and CNAM.

1:51PM Y08.00014: Wafer Bonding Approach for Epitaxial Al/GaAs(001)/Al Tri-layers* ANTHONY MCFADDEN (Presenter), University of California, Santa Barbara, COREY RAE MCRAE, RUSSELL LAKE, National Institute of Standards and Technology (NIST), Boulder, MICHAEL A SEAS, University of California, Santa Barbara, JIANGUO WEN, JIE WANG, ILKE ARSLAN, Center for Nanoscale Materials, Argonne National Laboratory, DAVID PAPPAS, National Institute of Standards and Technology (NIST), Boulder, CHRIS PALMSTROM, University of California, Santa Barbara — Superconductor-insulator-superconductor (Josephson) junctions utilizing amorphous oxide barriers have been studied extensively, however relatively little work has been done using single crystal semiconductors in place of amorphous oxide barriers. This is likely due to difficulty in fabrication of such structures including symmetry mismatch of the semiconductor to the superconductor and the reactions and roughening that may occur at the temperatures needed for semiconductor growth. This work focuses on a wafer bonding approach, subsequent substrate removal, and superconductor regrowth for fabrication of Al/GaAs(001)/Al Josephson junctions. AlGaAs/GaAs/Al structures are grown by molecular beam epitaxy and wafer-bonded to Si. The substrate and sacrificial AlGaAs layers were removed by selective wet etching followed by surface cleaning in ultrahigh vacuum and aluminum regrowth. The wafer bond and Al/GaAs interfaces are studied by transmission electron microscopy. X-ray photoelectron microscopy is used to determine GaAs surface cleaning conditions compatible with the wafer bonding process following substrate removal. X-ray and electron diffraction are used to assess crystalline quality and orientation of the epitaxial aluminum.

*Laboratory of Physical Sciences, University of MD
2:03PM Y08.00015: Quantum Transport in 2DEGs in Epitaxial GaN Quantum Wells on Superconducting NbN
PHILLIP DANG (Presenter), GURU BAHADUR SINGH KHALSA, Cornell University, D. SCOTT KATZER, NEERAJ NEPAL, BRIAN DOWNEY, United States Naval Research Laboratory, ALEXEY SUSLOV, National High Magnetic Field Laboratory, HUILI XING, Cornell University, DAVID J. MEYER, United States Naval Research Laboratory, DEBDEEP JENA, Cornell University — The epitaxial integration of superconducting NbN with III-N semiconductors was previously demonstrated in our report [Yan et al, Nature 555, 183-189 (2018)]. We have investigated the magnetotransport properties in this superconductor/semiconductor heterostructure, of the two-dimensional electron gas (2DEG) in the GaN quantum well in magnetic fields up to 35 Tesla. The 2DEGs exhibited strong Shubnikov-de Haas (SdH) oscillations that showed indications of spin-splitting as well as Hall-effect resistance plateaus that approach the quantum Hall regime. By varying a gate voltage to sweep the Fermi level, we directly observe the change in carrier concentration through SdH measurements. The associated change in occupation of Landau levels allows us clear access down to the 3rd Landau level. We report our observations of electron scattering processes due to dislocations near the gate-induced pinchoff point of the transistor and compare the scattering of N-polar and Ga-polar HEMTs. We comment on possibility of reaching the quantum Hall state in this material system, which would open a path towards realizing proximitized quantum Hall and superconducting states in a superconductor/semiconductor heterostructure.

Friday, March 8, 2019 11:15 AM - 1:51 PM

Session Y10 DMP DCMP: Surface Science of Organic Molecular Solids, Films, and Nanostructures - Materials Synthesis, Deposition, and Device preparation BCEC 151B - Dane McCamey. - Tag(s): Focus

11:15AM Y10.00001: Magnetism of ultra-short one dimensional atomic chains* [Invited] NICOLAS VARGAS (Presenter), Physics, University of California, San Diego, CARLOS MONTON, Physics and Astronomy, University of Texas at San Antonio, FELIPE TORRES, MIGUEL G KIWI, Physics, Universidad de Chile, DORA ALTBIR, Physics, Universidad de Santiago de Chile, VAGSON CARVALHO-SANTOS, Physics, Universidade Federal de Viçosa, ALEXANDER A. BAKER, TREVOR M WILLEY, Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, IVAN SCHULLER, Physics, University of California, San Diego — Driven by almost a century of theoretical work, the physical realization of one dimensional (1D) magnets has become essential to address pressing problems such as quantum criticality, many-body, spin transport, the emergence of new (topological) magnetic phases, and the extent and persistence of short- and long magnetic interactions as a function of length.

We report structural and magnetic properties of one-dimensional Fe chains as a function of length in the 10 to 200 atoms range. These Fe chains are grown using iron phthalocyanine (FePc) thin films and FePc/ metal-free-phthalocyanine (H2Pc) superlattices (SLs). The length of 1D Fe chains is precisely controlled by the deposited thickness of the FePc layers.

Although structurally identical, 1D Fe chains formed in films and superlattices have different magnetic behavior. In films, the coercive field remains almost constant whereas in SLs increases with the length of the chain. This difference can be explained using a semi-classical model, which combines short range direct Exchange and Dzyaloshinskii-Moriya interactions. The increase of the coercive field in SLs is attributed to a magnetization reversal process which is governed by chiral symmetry breaking produced by a weak magnetic anisotropy. This anisotropy originates at the extreme of the Fe chains by proximity with the H2Pc layers and is observable by element selective X-ray absorption spectroscopy (XAS).

*Work supported by the Department of Energy's Office of Basic Energy Science under grant DE FG02 87ER-45332, the National Science Foundation under grant No. 1804414 and 1805585, and AFOSR Grant FA9550-16-1-0122.
11:51AM Y10.00002: Coordination dependence of cooperative effects in spin crossover [Fe(H₂B(pz)₂)(bipy)] thin film GUANHUA HAO (Presenter), XUANYUAN JIANG, Department of Physics and Astronomy, University of Nebraska-Lincoln, AARON MOSEY, Physics Department, Indiana University Purdue University-Indianapolis, ANDREW J YOST, Department of Physics and Astronomy, University of Nebraska-Lincoln, XIN ZHANG, Department of Chemistry, University of Nebraska-Lincoln, ALPHA N’ DIAYE, Advanced Light Source, Lawrence Berkeley National Laboratory, JIAN ZHANG, Department of Chemistry, University of Nebraska-Lincoln, RUIHUA CHENG, Physics Department, Indiana University Purdue University-Indianapolis, XIAOSHAN XU, PETER A DOWBEN, Department of Physics and Astronomy, University of Nebraska-Lincoln — The electronic state of Fe(II) spin crossover complex [Fe(H₂B(pz)₂)(bipy)] (pz = pyrazol-1-yl, bipy = 2,2'-bipyridine) thin film on Al₂O₃ has been investigated by magnetometry (SQUID) and X-ray absorption spectroscopy (XAS) in both the total electronic yield mode and the photo-luminescence yield mode. The transition temperature of the spin crossover transition has a 20 K difference between the cooling and heating sequence in magnetometry and X-ray absorption spectroscopy taken in both the total electronic yield and photo-luminescence yield modes, indicating cooperative effects in the Fe(II) spin crossover complex. The differences in the hysteresis loop for the spin crossover transition for this Fe(II) spin crossover complex at the surface of the molecular film, extracted from X-ray absorption taken in the total electronic yield mode, differs from the bulk, as obtained from magnetometry and photo-luminescence yield mode X-ray absorption. This indicates the intermolecular interactions between the spin crossover molecules, at the surface of the Fe(II) spin crossover complex thin film, differs from bulk.

12:03PM Y10.00003: Local charge accumulation at a trinuclear metal-organic nanostructure on a surface AGUSTIN SCHIFFRIN (Presenter), CORNELIUS KRULL, MARINA CASTELLI, School of Physics and Astronomy, Monash University, PROKOP HAPALA, Institute of Physics, Czech Academy of Sciences, ANTON TADICH, Australian Synchrotron, MARTINA CAPSONI, Department of Physics and Astronomy, University of British Columbia, MARK T EDMONDS, JOHN HELLERSTEDT, School of Physics and Astronomy, Monash University, SARAH A. BURKE, Department of Physics and Astronomy, University of British Columbia, PAVEL JELINEK, Institute of Physics, Czech Academy of Sciences, DHANEESH KUMAR, School of Physics and Astronomy, Monash University — Coordination chemistry relies on harnessing active metal sites within organic matrices. Polynuclear complexes — consisting of organic ligands bound to several metal atoms — are relevant due to their electronic and magnetic properties, and to their potential for functional reactivity pathways. However, their synthesis remains challenging, with few geometries and configurations that have been achieved. Here, we synthesize — via supramolecular chemistry on a noble metal surface — one-dimensional metal-organic nanostructures composed of terpyridine-based molecules coordinated with well-defined polynuclear iron clusters. Combining low-temperature scanning probe microscopy techniques, density functional theory and x-ray absorption spectroscopy, we demonstrate that the coordination motif consists of coplanar terpyridine groups linked via a quasi-linear tri-iron node with mixed positive valence and a metal–metal bond configuration. This unusual linkage is stabilized by local accumulation of electrons between cations, ligands and metal surface. This morphology, enabled by the bottom-up on-surface synthesis, yields an electronic structure that hints at a chemically active polynuclear metal center, paving the way for nanomaterials with novel catalytic and magnetic functionalities.

12:15PM Y10.00004: Electron Induced Disordering and Decomposition of Alkanethiol Self-assembled Monolayers on Au(111) JODI GRZESKOWIAK (Presenter), University at Albany, CARL VENTRICE, SUNY Polytechnic Institute — Self-assembled monolayers (SAMs) are used for applications such as molecular electronics, selective deposition, and other forms of surface modification. Lithography within the semiconductor industry is adopting shorter wavelengths of light such that the interaction of secondary electrons with the organic resist is becoming the primary mechanism for photo-initiated electro-chemical reactions. To study the interaction of low energy electrons with thin organic films, measurements have been performed on electron induced disordering and decomposition of 1-decanethiol molecules grown via vapor phase deposition on Au(111). These monolayers arrange into two phases commonly referred to as lying down and standing up. The lying down phase is a physisorbed layer that is only weakly interacting with the substrate via Van der Waals forces. Conversely, the standing up phase is a chemisorbed species that is more strongly bound to the substrate. Surface analysis techniques were used to characterize the monolayers before and after electron exposure. LEED was used to determine the structure of the SAM and the rate of disordering and decomposition. TPD was used to evaluate the thermal stability of the attached SAMs and the resulting desorption products after electron exposure.
Assessing Monomer and Aggregate Populations in Squaraine-Based Organic Solar Cells
Catherine Ryczek (Presenter), Adriana Cruz, Physics Department, Hamilton College, Zhila Hooshangi, Chemistry Department, Rochester Institute of Technology, Kristen Burson, Physics Department, Hamilton College, Christopher Collison, Chemistry Department, Rochester Institute of Technology — Higher efficiencies of organic photovoltaic (OPV) devices have often been correlated with structural order within the solid state active layer of the device. Structural order is thought to improve charge mobility and energy transfer since both rely on effective orbital overlap between molecules. Nevertheless, questions remain about the role of electronic aggregates since they may act as energy traps for excited state species after photoexcitation, thereby leading to reduced overall efficiency. We aim to demonstrate how OPV efficiency is indeed related to aggregate (vs. monomer) populations through quantitative measurement. Population can be measured through absorption measurements and with a knowledge of the extinction coefficient of the species in question, along with the path length for the light through the sample. Experimentally, we will focus on the thickness measurements for a set of squaraine films. Squaraines are interesting because their efficiencies are significantly impacted by the exact geometry of aggregation, which can be controlled through chemical tuning. We will therefore use AFM thickness measurements coupled with spectroscopic techniques to confirm the importance of aggregation for molecular design strategy and fully optimized OPV devices.

Tuning the tunneling decay coefficient in self-assembled monolayer junctions
Xiaoping Chen, Harshini Annadata, National University of Singapore, Bernhard Kretz (Presenter), David Egger, University of Regensburg, Christian Nijhuis, National University of Singapore — Having insight into charge transport across organic-inorganic interfaces is important for the development and improvement of molecular electronic devices. Within the regime of quantum tunneling transport, the charge transfer rate strongly depends on the tunneling decay coefficient $\beta$, which determines the decline of the current across the junction as a function of the length and the barrier height. For self-assembled monolayer (SAM) junctions, it is well-known that the value of $\beta$ depends on the specific electronic structure of the molecular backbone. In our combined experimental and computational study, we demonstrate that $\beta$ of a non-conjugated SAM junction can be lowered significantly by using different halogens as termination on one side of the molecular backbone. With our experiments we can also show that this lowering of the tunneling coefficient is correlated with a change in the dielectric constant. Furthermore, our calculations allow for understanding how the frontier orbitals and transmission channels are effected by the change of the end-group.

Coherent X-ray measurement of local step-flow propagation during growth on polycrystalline C$_{60}$ thin film surfaces
Randall Headrick (Presenter), Jeffrey Ulbrandt, Department of Physics and Materials Science Program, University of Vermont, Peco Myint, Division of Materials Science and Engineering, Boston University, Jing Wan, Yang Li, Department of Physics and Materials Science Program, University of Vermont, Andrei Fleurasu, Yugang Zhang, Lutz Wiegart, National Synchrotron Light Source II, Brookhaven National Laboratory, Karl Ludwig, Department of Physics, Boston University — Vacuum deposition of C$_{60}$ on a graphene-coated surface is investigated with X-ray Photon Correlation Spectroscopy in surface-sensitive conditions. Local step-flow is observed through the observation of oscillatory correlations in the later stages of growth after crystalline mounds have formed. An important aspect of the work is that coherent X-rays do not average over complex structures, and this allows us to monitor the growth on polycrystalline surfaces without loss of information. The experimental results show that the step-flow velocity must be nonuniform, and we model the velocity of each step-edge as being a simple function of the lengths of the terraces above and below it. This model predicts that the steps become almost stationary near the edges of the mounds where the local terrace length is very small, and the average slope of the surface is large. It was not previously known that such nonuniform and disordered step arrays as we have observed would follow such a simple growth law. This work shows that the use of coherent X-ray scattering provides an approach to better understand surface dynamics and fluctuations during crystal growth.

*This work was supported by the U.S. Department of Energy (DOE) Office of Science under Grant No. DE-SC0017802.
Differences in Self-Assembly of Spherical C₆₀ and Planar PTCDA on Rippled Graphene Surfaces*

YANLONG LI (Presenter), Physics, Virginia Tech, XIAOYANG LIU, Chemistry, Virginia Tech, CHUANHUI CHEN, Physics, Virginia Tech, JAMES DUCHAMP, RONG HUANG, Chemistry, Virginia Tech, TING-FUNG CHUNG, Physics, Purdue University, MAXWELL YOUNG, TAREK CHALAL, Physics, Virginia Tech, YONG CHEN, Physics, Purdue University, JAMES R HEFLIN, Physics, Virginia Tech, HARRY DORN, Chemistry, Virginia Tech, CHENGGANG TAO, Physics, Virginia Tech — It was recently recognized that two-dimensional (2D) graphene exhibits nonplanar aberrations such as a rippled surface. Understanding the self-assembly of organic semiconductor molecules on monolayer 2D curved graphene surfaces is a paramount issue for ultimate application. Herein, we report on the preparation of fullerene, C₆₀ and perylenetetracarboxylic dihydride (PTCDA) molecules adsorbed on a rippled graphene surface. We find that the C₆₀ form a quasi-hexagonal close packed (hcp) structure, while the PTCDA form a disordered herringbone structure. These 2D layer systems have been characterized by STM imaging and DFT approaches. The DFT results exhibit interaction energies for adsorbed molecule/rippled graphene complexes located in the 2D graphene valley sites that are significantly larger in comparison with adsorbed planar/molecule graphene 2D complexes. In addition, we report that the adsorbed PTCDA prefer different orientations when the rippled graphene peak regions are compared to the valley regions. This difference in orientations causes the PTCDA molecules to form a disordered herringbone structure on the rippled graphene surface.

*Y.L. and C.T. acknowledge the financial support provided for this work by the U.S. Army Research Office under the grant W911NF-15-1-0414.

Effect of Admixture on Domain Morphology Transitions in Phase Separation of PCBM:tn-ZnPc from CCl₃ Solution

RAYMOND PHANEUF (Presenter), MIRIAM CEZZA, University of Maryland, College Park — We present results of investigations aimed at understanding how small mutually immiscible organic molecules self-assemble into domains during phase separation from liquid solutions. As a prototypical system we investigated molecular mixtures consisting of tetrano zinc-phthalocyanine (tn-ZnPc), an electron donor, and [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM), an electron acceptor, in chloroform and deposited on native oxide-covered Si(111) substrates. Previously we showed that for a 1:1 mixture PCBM:tn-ZnPc which has much higher solubility, precipitates onto the silicon substrate with domain morphologies which vary widely over the range of supersaturation rates investigated. For the highest rates the domains are isotropic, and apparently amorphous – with a mesoscale near-periodicity. Slowing the supersaturation rate causes an abrupt change in the domain size and shape, to micron-scale faceted domains; we speculated that either (1) a transition from spontaneous decomposition kinetics to nucleation and growth of crystalline domains or (2) a "cascade" series of transitions through increasingly stable structures was responsible for this. Here we present results in which the admixture of PCBM:tn-ZnPc is varied systematically to distinguish between these two mechanisms.

Abnormal ionic conductance switching under sub-3nm fluid confinement*

SYLVIA XIN LI (Presenter), Chemical Engineering, Massachusetts Institute of Technology, NAM S KIM, Chemistry, University of Maryland, College Park, GARY W RUBLOFF, Materials Science and Engineering, University of Maryland, College Park, SANG BOK LEE, Chemistry, University of Maryland, College Park, MARK A REED, Electrical Engineering, Yale University — Nanoscale protein ion channels are essential to bridge chemical and electrical signals in biological systems. When the confinement length of fluids is below a few nanometers, new transport behavior is expected and continuum-theory might no longer be valid. However, characterization and understanding of ion transport under such extreme confinement is limited. Here we construct solid-state nanofluidic devices with accurate confinement lengths ranging from sub-3nm to 10nm via precise nanofabrication techniques. We perform diverse electrical measurements under both quasi-equilibrium and perturbed states. We observe abnormal ionic conductance switching and propose that these intriguing phenomena result from a complex interplay between ion-surface interaction and confinement effect. These new transport behaviors have potential implications in a wide of applications, such as water treatment, bio-sensing and energy storage and conversion.

*Nanostructures for Electrical Energy Storage (NEES), an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, and Basic Energy Sciences under Award number DESC0001160.
Competing on-surface reaction pathways of bifunctional anthracene precursors to obtain organometallic networks

AMELIA DOMINGUEZ-CELORRIO (Presenter), Instituto de Nanociencia de Aragón, Universidad de Zaragoza, Spain, DIEGO PEÑA, Centro Singular de Investigación en Química Química Biológica e Materiais Moleculares (CIQUS) and Departamento de Química Orgánica, Universidad de Santiago de Compostela, Spain, VERONIQUE LANGLAIS, Centre d'Elaboration de Matériaux et d'Etudes Structurelles - Centre National de la Recherche Scientifique, Toulouse, France, DAVID SERRATE, Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, Spain — On surface synthesis is a versatile bottom up fabrication approach to create covalent nanostructures with atomic precision. Several organic covalent structures have been created by this approach, such as graphene based structures or organometallic networks. Aiming at the synthesis of a porous network, we study the hierarchy of chemical reactions of 10-bromoanthracene-9-yl-boronic-acid (BABA) precursors that are vapour sublimated onto crystalline surfaces under ultra-high-vacuum conditions. Our scanning tunnelling microscopy and spectroscopy characterization unveils that BABA dehydration to produce boroxine rings and metal substitution of the halogen group take place simultaneously leading to the formation of an organometallic honeycomb network, similarly to the case of using a simple phenyl core instead of anthracene [1]. In our case, however, the competition between these two reactions is extremely dependent on the catalytic role of the substrate, its surface termination and its temperature during the deposition of the precursor. As a consequence, the reaction pathway can be readily controlled by the choice of the catalytic surface (Ag(001), Ag(111) or Ag(111)).


We acknowledge FEDER funds from Interreg POCTEFA program (grant TNSI/EFA194/16)

Friday, March 8, 2019 11:15 AM - 1:51 PM
Session Y19 DMP: Computational Materials Design and Discovery -- Synthesizability and Stability

Networks of materials: a complexity approach to material synthesizability

MURATAHAN AYKOL (Presenter), Toyota Research Institute, VINAY I HEGDE, Northwestern University, SANTOSH SURAM, LINDA HUNG, PATRICK HERRING, Toyota Research Institute, CHRISTOPHER WOLVERTON, Northwestern University, JENS HUMMELSHØJ, Toyota Research Institute — Network science can provide a new arsenal of methods for materials informatics to address some of the daunting challenges in the field of materials. [1,2] One such challenge we address in this talk is the laboratory synthesis of computationally designed materials. The art of synthesis itself is too complex to be treated with an all-encompassing, quantitative approach as yet, because it involves not only the modeling of the energy landscape of competing phases or the kinetics of transformations, but also abstract factors, such as experience of scientists, state-of-the-art in experimental methods, resources and more. We present one of the first examples of “networks of materials” in the form of thermodynamic equilibria derived from high-throughput computational phase diagrams and analyze the local and global properties of this network. [1] We discuss how synthesis probabilities of yet-to-be-made, novel inorganic materials can be predicted from the dynamics of this network via machine-learning, connecting high-throughput computational design and experiments.


Roadmap for the Synthesis of Exotic 2D Metastable Carbon using Topologically Assembled Precursors

PURUSOTTAM JENA (Presenter), HONG FANG, Virginia Commonwealth University — Metastable structures of matter often possess properties superior to those of their ground state. A case in point is diamond vs. graphite. Yet, many predicted metastable structures are dismissed as hard-to-realize in practice as their basins of attraction are either too shallow or too narrow or both. There is no available theoretical approach that can deliberately enhance the realizability of these structures and directly guide their experimental synthesis. Here, we introduce a new approach to create potential energy surfaces in which the volumes of the basin of attraction of targeted metastable structures are increased by design, while simultaneously suppressing the accessibility of the ground state as well as other isomers. This approach is based on topologically assembled precursors, followed by density functional theory relaxations, and is applied to realize high-energy carbon allotropes such as penta-graphene comprised entirely of pentagon rings, O-graphene comprised of five- and eight-membered rings and R-graphene comprised of four-, six- and eight-membered rings.
11:39AM Y19.00003: Disorder drives synthesizability of multi-component systems*  CORMAC TOHER (Presenter), COREY OSES, STEFANO CURTAROLO, Mechanical Engineering and Materials Science, Duke University — The factorial increase in the number of potential compositions with increasing number of elemental components is not reflected in the number of synthesized ordered chemical compounds [1]. We show that this is due to formation-entropy-gain exceeding formation-enthalpy-gain as more species are added to the mixture. An analysis of the dependence of formation enthalpy on the number of species [2] using data extracted from the AFLOW data repository [3] shows interesting trends about the interplay between entropic and enthalpic effects on the synthesizability of multi-component materials.


*The authors acknowledge support by DOD-ONR (N00014-15-1-2863, N00014-17-1-2090, N00014-16-1-2583, N00014-17-1-2876). S.C. acknowledges support from the Alexander von Humboldt Foundation. C.O. acknowledges support from NSF (DGF1106401).

11:51AM Y19.00004: Retrosynthetic Planning with Generative Models  SHINTARO FUKUSHIMA (Presenter), TOYOTA InfoTechnology Center, Co.Ltd., YUICHI MOTOYAMA, KAZUYOSHI YOSHIMI, Univ of Tokyo-Kashiwanoha — Recently, retrosynthetic planning with machine learning and deep learning has been studied actively. One of the powerful approach was the retrosynthesis based on the molecular similarity proposed by Coley et al. In this approach, similarities between the target product and products in the reaction database were calculated to find similar products. Next, candidate reactions were generated by modifying reactions of the similar targets. This method by Coley et al. is more accurate than other methods. However, its search space is limited because it is based on the matching with the existing reactions. In this presentation, we propose a method with generative models, such as GAN(generative adversarial network) or VAE(variational autoencoder ) in order to expand the search space. The idea of the proposed method is to learn a generative model with GAN or VAE, generate reactants with the generative model, and then a reaction with reaction prediction. We got new reactants with the proposed method. We applied our proposed method to US patent dataset. As a result, reactants which did not exist in the reaction database were produced. Besides, the accuracy of retrosynthesis was higher than the previous methods.

12:03PM Y19.00005: Fantastic Metastable States and Where to Find Them: A Computational Search for Superlattices with Enhanced Functional Properties*  JOHN BONINI (Presenter), KARIN RABE, Rutgers University, New Brunswick — Superlattice systems continue to be of great interest in the development of new or enhanced material functionalities. One exciting prospect is that the conditions of the superlattice allow for the stabilization of novel states not accessible in bulk materials. To find such states, and the conditions under which they are stabilized, we construct a database of first principles calculations which describe not only the ground state of each constituent material, but a number of local minima and how these states change with mechanical, electrical, and other conditions. A data-driven approach is used in structure determination where the most probable local minima are systematically identified through analysis of existing materials databases. The resulting data set can be used as input to the "bulk-layer model" [1] to rapidly identify superlattice combinations with desirable functional properties, as well as the superlattice "stacking method" [2] to carefully compute the ground state of a particular superlattice. Examples applying the method to perovskite oxide compounds and superlattices will be presented.

[2] https://doi.org/10.1103/PhysRevB.89.214108

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Evaluating Species Stability with First Principles Calculations

LAUREN WALTERS (Presenter), LIANG-FENG HUANG, JAMES M RONDINELLI, Northwestern University — Novel multicomponent materials such as BiCuOS and BiCuOSe are used in a wide variety of applications like structural materials, semiconductors, and catalysis; however, the complex chemistry of having multiple anions makes reliable synthesis of these products challenging. Here we describe an ab-initio approach to evaluate the thermodynamic stabilities of multicomponent solids in aqueous environments with variable environmental conditions. The approach allows us to generate electrochemical Pourbaix diagrams that can be used to guide hydrothermal synthesis of these complex phases. Furthermore, we utilize a revised Helgeson-Kirkham-Flowers model to incorporate nonstandard state conditions for aqueous ions as functions of temperature and pressure. Our work identifies the main factors needed for the informed synthesis of new complex transition metal compounds and routes to deliver long-term stability of copper-based alloys.

The authors were supported by the ONR MURI under Grant No. N00014-16-1-2280. Calculations were performed using the QUEST HPC Facility at Northwestern University.

Formation enthalpies for automated computational materials design

RICO FRIEDRICH (Presenter), DEMET USANMAZ, COREY OSES, Department of Mechanical Engineering and Materials Science, Duke University, ANDREW R SUPKA, MARCO FORNARI, Department of Physics and Science of Advanced Materials Program, Central Michigan University, MARCO BUONGIORNO NARDELLI, Department of Physics and Department of Chemistry, University of North Texas, CORMAC TOHER, Department of Mechanical Engineering and Materials Science, Duke University, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics and Chemistry, Duke University — The accurate calculation of formation enthalpies is crucial for computational materials design. For compounds chemically similar to their reference phases such as metal alloys, standard semi-local approximations to density functional theory (DFT) lead to accurate results [1]. When the phases are chemically dissimilar as in the case of oxides, DFT suffers from a lack of error cancellation leading to deviations of several hundred meV/atom compared to experimental values [2]. We use the automated computational materials design framework AFLOW [3] to benchmark correction schemes for ab initio formation enthalpies [2, 4]. These empirical methods can improve DFT predictions by a factor of 4 to 7. Zero-point vibrational and thermal contributions to the formation enthalpy are found to largely cancel each other.


We acknowledge support by DOD-ONR (N00014-15-1-2266, N00014-17-1-2090, N00014-16-1-2326, N00014-17-1-2876). R.F. and S.C. acknowledge support from the Alexander von Humboldt foundation. C.O. acknowledges support from the NSF under Grant No. DGF-1106401.

The Phase Stability Network of All Inorganic Materials

VINAY ISHWAR HEGDE (Presenter), NORTHWESTERN UNIVERSITY, MURATAHAN AYKOL, TOYOTA RESEARCH INSTITUTE, CHRISTOPHER WOLVERTON, Northwestern University — In the pursuit of unlocking structure-property relationships, a dominant paradigm in materials science has been the bottom-up investigation of how the arrangement of atoms and interatomic bonding in a material determine its macroscopic behavior. Here we consider a complementary approach, a top-down study of the organizational structure of networks of materials, based on the interaction between materials themselves. We unravel the phase stability network of all inorganic materials as a dense complex network of 21,000 thermodynamically stable compounds (nodes) connected with 41 million tie-lines (edges) defining their two-phase equilibria as computed by high-throughput density functional theory. The connectivity of nodes in the materials network shows a lognormal distribution, while the network itself shows small-world behavior, with a number of compounds acting as “hubs” having connections to nearly all other compounds. Analyzing the structure and topology of the materials network has the potential to uncover new knowledge inaccessible from the traditional atoms-to-materials approaches. We use the connectedness of materials in the network to derive a general, data-driven metric for reactivity, the “nobility index”, and quantitatively identify the noblest materials in nature.
12:51PM Y19.00009: Instabilities during solid-solid structural phase transformations provide guidance for the high-throughput materials discovery* NIKOLAI A ZARKEVICH (Presenter), Ames Laboratory, HAO CHEN, VALERY LEVITAS, Iowa State University, VITALIJ K PECHARSKY, DUANE D JOHNSON, Ames Laboratory — Electronic and lattice instabilities are studied during the solid-solid phase transformations in materials subjected to a general stress. The elastic instability criterion is proposed. The instability criteria are useful for the high-throughput discovery of novel materials. Our findings reveal novel, more practical synthesis routes for new or known high-pressure phases under predictable nonhydrostatic loading, where competition of instabilities can serve for phase selection.

*New methods were developed at Ames Laboratory, supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. Ames Laboratory is operated for the U.S. DOE by Iowa State University of Science and Technology under contract DE-AC02-07CH11358. Solid-solid phase transformations in materials exhibiting caloric effects were considered under auspices of CaloriCool(TM), which is supported by the Advanced Manufacturing Office of the Office of Energy Efficiency and Renewable Energy of the U.S. DOE. Non-linear mechanics was supported by NSF (CMMI-1536925), ARO (W911NF-17-1-0225), and Extreme Science and Engineering Discovery Environment (XSEDE) (high-performance computational resources allocation MSS170015).

1:03PM Y19.00010: Exploring the landscape of nonlinear mechanical metamaterials EDER MEDINA (Presenter), SEAS, Harvard University, PATRICK FARRELL, Mathematical Institute, Oxford University, CHRISTOPHER RYCROFT, KATIA BERTOLDI, SEAS, Harvard University — Nonlinearities have recently emerged as a powerful tool for designing mechanical metamaterials, as they lead to systems with a complex and programmable response. Currently, nonlinear responses have primarily been explored through traditional experimental techniques and standard single-solution numerical solvers. Here, we use an in silico continuation method to discover multiple configurations with associated different properties for a single loading parameter. We test the method on simple porous structures under compressive loading; as the load increases, we discover bifurcating families of stable and metastable states. Using this method we find structures that can switch between energy-releasing and energy-harvesting configurations, and structures that are geometrically hysteretic. Physical experiments are conducted to validate the results.

1:15PM Y19.00011: Expanding the elemental space of atomic laminates by a theoretical/experimental approach MARTIN DAHLQVIST (Presenter), JOHANNA ROSEN, IFM, Linkoping University — More than 50 years ago a family of atomically laminated compounds were discovered, being comprised of a transition metal M, an A-group element, and carbon and/or nitrogen X, and therefore being referred to as MAX phases. The exploration of the taxonomy of these can be accelerated by theoretical design on the atomic level combined with combinatorial experimental synthesis. Here, we use predictive phase stability calculations to probe transition metal (M) alloying in MAX phases and identify several chemically ordered structures. Subsequent materials synthesis of these indicates a potentially large family of thermodynamically stable phases, with Kagomé-like and in-plane chemical ordering, and with incorporation of elements previously not used for MAX phases, including Y and W. In extension, we suggest a matching set of novel two-dimensional MXenes, from selective etching of the A-element and, when so required, the alloying metal. The here demonstrated structural design on both 3D and 2D atomic levels expands the property tuning potential of functional ceramics.

1:27PM Y19.00012: Symmetry induced stability in alkali doped calcium-silicate-hydrate* ONGUN OZCELIK (Presenter), NISHANT GARG, CLAIRE WHITE, Princeton University — CO₂ emissions originating from the construction industry have a significant impact on global warming where the production of ordinary Portland cement clinker is responsible for approximately 8% of all human-made CO₂. Alkali doped calcium-silicate-hydrate (C-S-H) is a critical silicate material since the use of blended cements and alkali-activated materials in construction industry can substantially reduce human-made CO₂ emissions. However, the effect of alkali doping (Na and K) on the long-term stability and associated durability of C-S-H remains an open question. Here, using first principles quantum chemistry calculations on the model crystalline phase clinotobermorite, we show that there is a strong interplay between the thermodynamic stability of alkali doped C-S-H and the symmetry of the alkali atoms in the structure. We investigate the associated structural mechanisms by calculating the migration barriers of alkali atoms within the material, the electronic charge distribution in the material and the variation of basal spacing by using both computational methods and X-ray diffraction analysis.


*We acknowledge funding from the Wilke 1989 Innovation Fund and the Princeton Center for Complex Materials, a MRSEC supported by NSF Grant DMR 1420541
IVOR LONCARIC (Presenter), PREDRAG LAZIC, Division of Theoretical Physics, Rudjer Boskovic Institute, Zagreb, Croatia — Sulfosalts form a vast mineral group which may be imagined as chemically analogous to oxides, with O replaced by S. However, the metal cations in sulfosalts generally have tetrahedral S coordination, and the chemical variety is much greater than in oxides, owing to the several possible oxidation states of sulfur. Structurally they range from the very simple to the very complex, and also span the whole range of anisotropies, from chainlike to fully 3D. They are less ionic than oxides, thus they display surprising crystallochemical flexibility and superior tunability of the valence of the transition metal ions. This results in a large variety of interesting electronic, magnetic and mechanical properties. Here we present an initial study of a particular class of sulfosalts, based on murunskite. The electronic structure is discussed with respect to possible signatures of thermoelectricity and superconductivity.

*We thank the HRZZ support - IP-2018-01-7828.

Friday, March 8, 2019 11:15 AM - 2:03 PM

Session Y20 DMP: Hybrid Perovskites -- Lattice Vibrations BCEC 157A - Yan Li, University of Utah - Tag(s): Focus

11:15AM Y20.00001: The Impact of Lattice and Charge Fluctuations on Carrier Dynamics in Halide Perovskites
MATTHEW Z. MAYERS, Department of Chemistry, Columbia University, LIANG TAN, Department of Chemistry, University of Pennsylvania, DAVID EGGER (Presenter), Institute of Theoretical Physics, University of Regensburg, ANDREW RAPPE, Department of Chemistry, University of Pennsylvania, DAVID REICHMAN, Department of Chemistry, Columbia University — While halide perovskites (HaPs) have shown great technological promise for use as materials in energy devices, several of their unique optoelectronic properties remain incompletely understood. We develop a microscopic theory that is aimed at describing pertinent physical effects related to the carrier transport and optical properties of HaPs. It captures the nuclear displacements to all orders and goes beyond assuming linear electron-phonon coupling in calculating the dynamics of carriers and band gap characteristics. We combine the theory with first-principles calculations and apply it to the paradigm HaP compound MAPbI3. Our results explain intriguing experimental findings related to the charge-carrier mobility and optical properties, including their temperature dependencies. The findings of our work demonstrate that orbital overlap fluctuations in the lead-halide structure play a leading role in determining the optoelectronic features of HaPs.

ALI KACHMAR (Presenter), Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), WISSAM SAIDI, Mechanical Engineering and Materials Science, University of Pittsburgh — Temperature can have a dramatic effect on the solar efficiency of methylammonium lead iodide (CH3NH3PbI3) absorbers due to changes in the electronic structure of the system even within the range of stability of a single phase. Herein using first principles density functional theory, we investigate the electron band structure of the tetragonal and orthorhombic phases of CH3NH3PbI3 as a function of temperature due to electron-phonon coupling and thermal expansion. Our results show that the band gap increases with temperature for the two CH3NH3PbI3 phases in excellent agreement with experimental results. We also found that temperature have a significant effect on the effective masses and Rashba coupling especially in the tetragonal phase. At room temperature, electron-phonon coupling is found to enhance the effective mass by a factor of two, and to diminish the Rashba coupling by the same factor compared to T=0 K values.

*WAS acknowledges a start-up fund from the Department of Mechanical Engineering and Materials Science at the University of Pittsburgh.

AYALA COHEN (Presenter), Weizmann Institute of Science, DAVID EGGER, University of Regensburg, ANDREW RAPPE, University of Pennsylvania, LEEOR KRONIK, Weizmann Institute of Science — We consider the Br vacancy in CsPbBr3 as a prototype for the impact of lattice dynamics on defect energetics in halide perovskites (HaPs). Using first-principles molecular dynamics based on density functional theory, we find that the static picture of defect energetics breaks down; the energy of the VBr level is found to be dynamic, oscillating by as much as 1 eV on the ps time scale at room temperature. These significant energy fluctuations are correlated with the distance between the neighboring Pb atoms across the vacancy and with the electrostatic potential at their atomic sites. The unusually strong coupling of lattice dynamics and defect energetics bears important implications for both experimental and theoretical analysis of defect characteristics in HaPs and may hold significant ramifications for carrier transport and defect tolerance in this class of photovoltaics.
Lattice dynamical properties of halide-perovskites from infra-red spectroscopy and first-principles calculations
CHRISTIAN GEHRMANN (Presenter), Institute of Theoretical Physics, University of Regensburg, MICHAEL SENDNER, SEBASTIAN BECK, Kirchhoff Institute for Physics, Heidelberg University, ROBERT LOVRINCIC, Institute for High Frequency Technology, TU Braunschweig, DAVID EGGER, Institute of Theoretical Physics, University of Regensburg — Halide perovskites (HaPs) are intriguing optoelectronic materials. It is of particular interest to understand how the outstanding optoelectronic properties of HaPs are related to their vibrational properties, especially in light of the possibility that phonons might be the dominant source of scattering for charge carriers at room temperature. Studying the lattice dynamics of the all-inorganic CsPbBr₃ as well as the hybrid MAPbBr₃, we here present our findings on how the A-site cation as well as its potential orientation effects influence the vibrational properties of HaPs. To this end, we show results from first-principles calculations, based on density functional theory, and compare these with experimental data obtained from far infra-red spectroscopy. Finally, we present results related to the LO phonons that are not infra-red active, but inherently contained in our calculations and experimentally accessible through reflectance measurements.

Vibrational Dynamics of Hybrid Organic-Inorganic Perovskites
DEPEI ZHANG (Presenter), Department of Physics, University of Virginia, TIANRAN CHEN, NIST Center for Neutron Research, National Institute of Standards and Technology, ALEXANDER CHEN, Department of Chemical Engineering, University of Virginia, MAIKO KOFU, Material and Life Science Experimental Facility, Japan Proton Accelerator Research Complex, WEI-LIANG CHEN, Center for Condensed Matter Sciences, National Taiwan University, DOUGLAS L ABERNATHY, Spallation Neutron Source, Oak Ridge National Laboratory, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CRAIG BROWN, LELAND HARRIGER, GUANGYONG XU, NIST Center for Neutron Research, National Institute of Standards and Technology, RYOICHI KAJIMOTO, Material and Life Science Experimental Facility, Japan Proton Accelerator Research Complex, YU-MING CHANG, Center for Condensed Matter Sciences, National Taiwan University, JOSHUA CHOI, Department of Chemical Engineering, University of Virginia, SEUNGHUN LEE, Department of Physics, University of Virginia — Vibrational modes, which are connected to the electronic properties of hybrid organic-inorganic perovskites (HOIPs) through the structural transition, electron-phonon coupling, and hot-phonon bottleneck effect, is an important topic for perovskite solar cells. This talk focuses on the phonon modes of two perovskite materials, MAPbI₃ (MA = CH₃NH₃) and FAPbI₃ (FA = HC(NH₂)₂). We have performed inelastic neutron scattering, Raman scattering, and density-functional theory (DFT) calculations on both systems. Our analysis well reproduces the low-temperature inelastic neutron scattering spectra for MAPbI₃ and FAPbI₃, and illuminates the connection between the vibrational dynamics and the organic molecules.

Rotational Dynamics of Organic Cations in the [CH₃(CH₂)₇NH₃]₂PbI₄ Perovskite
XIAO HU (Presenter), DEPEI ZHANG, TIANRAN CHEN, ALEXANDER CHEN, University of Virginia, DANIEL PAJEROWSKI, Oak Ridge National Laboratory, GUANGYONG XU, National Institute of Standards and Technology, WEI-LIANG CHEN, National Taiwan University, MINA YOON, Oak Ridge National Laboratory, YU-MING CHANG, National Taiwan University, JOSHUA CHOI, SEUNGHUN LEE, University of Virginia — The biggest challenge of the 3D high-efficiency perovskite solar cells, such as CH₃NH₃PbI₃ and CH(NH₂)₂PbI₃, is their device instability. 2D perovskite compounds such as butylammonium methylammonium lead iodide perovskite, [CH₃(CH₂)₃NH₃]₂(CH₃NH₃)₁Pb₃I₁₇, present a solution to this problem. Here we present our recent quasi-elastic neutron scattering on a powder sample of the 2D 1-layer system ([CH₃(CH₂)₇NH₃]₂PbI₄) as a function of temperature. Upon cooling, this system undergoes an orthorhombic phase(ACam) to another orthorhombic phase(Pbca) and further to a monoclinic phase(P2₁/a). Our group theory and density functional theory analysis show that the rotational dynamics is dominated by C₃ rotation of NH₃ and CH₃ groups. The relaxation rate of the C₃ modes decreases with decreasing temperature through the orthorhombic-to-orthorhombic transition. On the other hand, in the low-temperature monoclinic phase, the C₃ rotation becomes very slow to detect. The relevance of this finding to electronic properties will also be discussed.

The work is supported by the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, under Award DE-SC0016144.
Lead halide perovskites are polaronic materials

XIAOYANG ZHU (Presenter), Columbia University — Lead halide perovskites have been demonstrated as high performance materials in solar cells and light-emitting devices. These materials are characterized by coherent band transport expected from crystalline semiconductors, but dielectric responses and phonon dynamics typical of liquids. Here we explain the essential physics in this class of materials based their dielectric functions or dynamic symmetry breaking on microscopic level. We show that the dielectric function of a hybrid organic-inorganic lead halide perovskite (LHP) possesses combined characteristics of a polar liquid and a ferroelectric material. The latter response in the THz region may lead to dynamic and local ordering of polar nano domains by an extra electron or hole, resulting a quasiparticle which we call a ferroelectric large polaron, a concept similar to solvation in chemistry. Compared to a conventional large polaron, the collective nature of polarization in a ferroelectric large polaron may give rise to order(s)-of-magnitude larger reduction in the Coulomb potential and introduce potential barriers to charge carrier scattering. The ferroelectric large polaron may explain the defect tolerance and low recombination rates of charge carriers in lead halide perovskites, as well as providing a design principle for high performance semiconductors from nano, molecular, and hybrid materials. [Science, 2016, 353, 1409; Science Adv. 2017, 3, e1701217; Nature Mat. 2018, 17, 379].

Large Polaron Formation and its Effect on Electron Transport in Hybrid Perovskite

FAN ZHENG (Presenter), LIN-WANG WANG, Lawrence Berkeley National Laboratory — Many experiments have indicated that large polaron may be formed in hybrid perovskite, and its existence is proposed to screen the carrier-carrier and carrier-defect scattering. However, detailed theoretical study of the large polaron and its effect on carrier transport at the atomic level is still lacking. In this work, using CH$_3$NH$_3$PbI$_3$ as an example, we implement tight-binding model fitted from the density-functional theory to describe the electron large polaron ground state and to understand the large polaron formation and transport at its strong-coupling limit. We find that the formation energy of the large polaron is around -12 meV for the case without dynamic disorder, and -55 meV by including dynamic disorder. By performing the explicit time-dependent wavefunction evolution, together with the rotations of CH$_3$NH$_3^+$ and vibrations of PbI$_3^-$ sublattice, we studied the diffusion constant and mobility of the large polaron state. On one hand, the vibration of the sublattice provides additional driving force for carrier mobility, on the other hand, the large polaron polarization further localizes the electron, reducing its mobility.

Impact of the exchange-correlation functional on the analysis of static and dynamical structural properties of MAPbI$_3$

HUBERT BECK (Presenter), CHRISTIAN GEHRMANN, DAVID EGGER, Institute of Theoretical Physics, University of Regensburg — Hybrid organic-inorganic halide perovskites (HaPs) have shown many properties that are advantageous for efficient renewable energy applications. Several of the open questions for these systems can be addressed by first-principles calculations applying density functional theory (DFT). However, in order to achieve reliable insight from such calculations, it is important to understand which of the various microscopic effects in the different DFT-related approximations play an important role in the calculations. Here, we present an investigation on the importance of various theoretical aspects in the DFT calculations of the structural properties for MAPbI$_3$. We focus on a comparison of calculations varying the DFT functional, the account of van-der-Waals interactions as well as the inclusion of spin-orbit coupling. Our computed unit-cell volumes and bulk moduli are compared to results of experiments, addressing the relative importance of these effects on calculations of structural properties of MAPbI$_3$. Finally, we also present results on the impact of temperature-induced structural fluctuations on calculating the structural properties of MAPbI$_3$. 

*Joint Center for Artificial Photosynthesis, supported by the U.S. Department of Energy under Award number DE-SC0004993.
Magneto-Raman Spectroscopy on multiferroic metal-organic framework 

[(CH$_3$)$_2$NH$_2$]Co(HCOO)$_3$$^\ast$ RACHAEL RICHARDSON (Presenter), DAMIOLA OLOGUNAGBA, Florida A&M University, ZHENG-GUANG LUI, National High Magnetic Field Laboratory, NAN HUANG, University of Tennessee-Knoxville, DMITRY SMIRNOV, National High Magnetic Field Laboratory, DAVID GEORGE MANDRUS, University of Tennessee-Knoxville, KOMALAVALLI THIRUNAVUKKARASU, Florida A&M University — Metal-organic frameworks (MOFs) are a class of nanoporous compounds where organic groups are used in combination with transition metal ions to obtain multifunctional materials. The family of MOFs perovskites ABX$_3$ comprised of methylammonium (A= (CH$_3$)$_2$NH$_2$) and metal (B=Co, Cu, Fe, Mn, Ni) cations with a formate (X=HCOO$_3$) anion are studied because of their multiferroic properties [1]. Therefore, several efforts have been made to understand the nature and strength of exchange interactions in these materials including magnetization at high magnetic fields up to 60 T and infrared spectroscopy at magnetic fields up to 35 T [2,3]. Concurrently, we performed magneto-Raman spectroscopy on [(CH$_3$)$_2$NH$_2$]Co(HCOO)$_3$ at magnetic fields up to 31T to probe the magneto-elastic coupling, the results of our investigations and its implications will be discussed.

$^\ast$Work at NHMFL was supported by NSF DMR-1157490, DMR-1644779 and the state of Florida. The project is also funded by DoN HBCU/MI program.

Acoustic phonon instabilities and central peaks at the Brillouin zone boundary in the organic-inorganic perovskite CH$_3$NH$_3$PbCl$_3$$^\ast$ MANILA SONGVILAY (Presenter), University of Edinburgh, MARYAM BARI, YE ZUO-GUANG, Department of Chemistry and 4D labs, Simon Fraser University, GUANGYONG XU, PETER M GEHRING, WILLIAM RATCLIFF, NIST Center for Neutron Research, National Institute of Standards and Technology, KARIN SCHMALZL, Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at ILL, FRÉDÉRIC BOURDAROT, INAC, MEM/MDN, Université Grenoble Alpes, CEA, BERTAND ROESSLI, Laboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institut (PSI), CHRIS STOCK, University of Edinburgh — Lead halide hybrid perovskites consist of an inorganic framework hosting a molecular cation located in the interstitial space. These compounds have been extensively studied as they have been identified as promising materials for photovoltaic applications. In particular, the interaction between the molecular cation and the inorganic framework has been suggested to influence the electronic properties. CH$_3$NH$_3$PbCl$_3$ undergoes several structural transitions associated with both distortion of the octahedra and orientational ordering of the CH$_3$NH$_3$ cation. We have measured the low-frequency lattice dynamics using neutron spectroscopy. We report an anomaly in the acoustic phonon linewidth towards the high-symmetry point Q$_{X}$=(2, 1/2, 0) when approaching the transitions, and a hardening of the entire phonon branch with decreasing temperature. Measurements at the Brillouin zone edges Q$_{X}$=(2, 1/2, 0), Q$_{M}$=(3/2, 1/2, 0) and Q$_{R}$=(3/2, 3/2, 5/2) show central peaks appearing at the lower temperature transition. We discuss the presence of both central peaks and acoustic phonon instabilities as evidence of a strong coupling between the inorganic framework and the molecular cation.

$^\ast$We acknowledge funding from the EPSRC and the STFC

Diffuse Neutron and X-ray Scattering from Cesium Lead Bromide$^\ast$ MATTHEW KROGSTAD (Presenter), ALEX RETTIE, STEPHAN ROSENKRANZ, DUCK YOUNG CHUNG, Materials Science Division, Argonne National Laboratory, MERCOURI KANATZIDIS, Department of Chemistry, Northwestern University, FENG YE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, XING HE, OLIVIER DELAIRE, Department of Mechanical Engineering and Materials Science, Duke University, RAYMOND OSBORN, Materials Science Division, Argonne National Laboratory — Cesium lead bromide has attracted recent attention, along with other lead halide perovskites, due to its optoelectronic properties. It has been proposed that the long carrier life supporting these properties is due to local polar fluctuations. To investigate the short-range lattice distortions that such fluctuations would imply, diffuse neutron and x-ray scattering experiments were performed on single crystals of CsPbBr$_3$ across range of temperatures spanning two structural phase transitions. Significant diffuse scattering indicating short-range displacement correlations was found in all three structural phases. In particular, diffuse neutron scattering from CsPbBr$_3$ shows distinct elastic and inelastic features, distinguishing between static and dynamic forms of local displacement correlations.

$^\ast$This work was funded by DOE, BES, DMSE.

Friday, March 8, 2019 11:15 AM - 1:39 PM

Session Y23 GIMS: X-rays 8CEC 158 - Tag(s): Focus
Effectively Pin-hole Collimated USAXS as a Premier Tool to Quantitatively Analyze Anisotropic Hierarchical Porous Microstructures*  
TABBETHA DOBBINS (Presenter), AARON HOPKINS, Rowan University, JAN ILAVSKY, Advanced Photon Source, Argonne National Laboratory, MILAD MILAD AZAMI-GHADKOLAI, RAJENDRA BORDIA, Dept. of Materials Science & Engineering, Clemson University — The 2D collimated Bonse-Hart USAXS instrument was used to study the anisotropic and hierarchical pore microstructures in freeze-cast lithium titanate (Li₄Ti₅O₁₂). USAXS data with scattering vector q=0.0001Å⁻¹ to 0.02Å⁻¹ were collected at sample orientations from -10° to 190°. I vs. azimuthal angle polar data at q values of 0.0003Å⁻¹, 0.0006Å⁻¹, 0.001Å⁻¹, and 0.005Å⁻¹ were also collected. Six Li₄Ti₅O₁₂ samples differing by salt and gel additives and lithium titanate particle size were measured. Samples are strongly anisotropic at low q (aspect ratio of 0.3 to 0.4) for intercolumnar porosity and mildly anisotropic at high q (aspect ratio of 0.8) for interparticle pores. Models suggests the pore microstructures are comprised of two large anisotropic populations: 1μm (Φ=0.77; SA=2.88m²/cm³) and 0.5μm (Φ=0.05; SA=0.35m²/cm³) and two small, relatively isotropic populations: 38nm (Φ=0.02; SA=1.38m²/cm³) and 14nm (Φ=0.16; SA=35.3m²/cm³).

*The Clemson University portion of this work was supported in part by the National Science Foundation EPSCoR Program under NSF Award # OIA-1655740. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

High Magnetic Field X-ray Diffraction at the National High Magnetic Field Laboratory (NHMFL)*  
DREW REBAR (Presenter), ALEXEY E KOVALEV, National High Magnetic Field Laboratory, DALLAS MANN, MICHAEL SHATRUK, Chemistry and Biochemistry, Florida State University, YAROSLAV MUDRYK, VITALIJ K PECHARSKY, Ames Laboratory, Iowa State University, KAYA WEI, JULIA H. SMITH, ALEXEY SUSLOV, THEO SIEGRIST, National High Magnetic Field Laboratory — We develop a custom high magnetic field x-ray diffraction system for measurements in the 25 T Florida split coil magnet at the DC Field Facility of NHMFL, Tallahassee, FL, to probe spin-lattice coupling at extreme steady-state magnetic fields. This allows thermal cycling of materials with first order transitions and thermal relaxation of highly conductive or magnetocaloric materials. The system utilizes a Mo rotating anode X-ray source and PILATUS 300K-W X hybrid pixel array detector customized to tolerate the fringe fields of the split coil magnet. We plan to further modify the diffractometer with an elliptical mirror system which will enhance intensity and create a convergent x-ray beam configuration. We present a study of the magnetocaloric material, AlFe₂B₂, highlighting the evolution of the unit cell volume in field and a study of the magnetostrictive material, GdNi, highlighting the evolution of the crystal axes at high field.

*This research is supported by NSF-DMR grant MRI-1625780. NHMFL is supported by the National Science Foundation Cooperative Agreement No. DMR-1644779 and the State of Florida. The Ames Laboratory is operated for the U. S. Department of Energy by Iowa State University of Science and Technology under contract No. DE-AC02-07CH11358.

High Resolution Digital X-Ray Detection via Optical Interrogation of Electro-Optic Materials  
GEORGE HERRING (Presenter), LAMBERTUS HESSELINK, Stanford University — We report on the development of a high resolution (greater than 30 lp/mm), high quantum efficiency x-ray detector in the 40 to 60 keV range using non-linear optics. Typical indirect x-ray detectors use a scintillation material to convert high energy x-ray photons into a larger number of lower energy visible photons. Indirect x-ray detectors with the previously stated specifications have a low quantum efficiency due to the combination of a thin scintillation material, which has little x-ray stopping power, and a limited ability of the optical train and CMOS sensor to collect the visible photons. Instead of using a scintillator to convert incident x-rays into lower energy visible photons, we explore the use of non-linear optics to convert incident x-rays into a localized change in the index of refraction, which can be measured with optical interferometry. The non-linear optic consists of a biased Pockels Cell. When x-rays interact with the cell they release space charges which modify the electric field within the cell and thus changes its index. With this new design of x-ray detector, we explore the tradeoffs between x-ray stopping power, transverse spatial resolution, temporal resolution, and signal to noise ratio.
Bulk metallic ribbons have inherent rough surfaces. The non-trivial surface scatterings could mislead USANS data as the scattering of the Cu50Zr50 alloy disappeared under the surface neutron contrast-matched environment, indicating that the scattering originated not from its internal structure but from the surface. This confirms the homogeneity at the atomic level sustains to a micrometer. On the other hand, the crystallized alloy showed a strong scattering under the matching environment due to the structural heterogeneity inside the alloy. This technique can apply to the bulk samples when the transmission is high enough, not causing multiple scattering.

*We acknowledge partial financial support from KAERI and KIST (KIST funding number: 2G10480, 2V06030).
12:27PM Y23.00007: A high quality multilayer x-ray monochromator for third generation synchrotron sources
MATTHEW DECAMP (Presenter), KARL UNRUH, University of Delaware, ANTHONY DICHIARA, RAY CONLEY, Argonne National Labs — The ability to provide high spectral resolution with high dynamic photon flux is a hallmark of third generation synchrotron sources. However, under most circumstances, only two modes of operation are currently available for user studies, monochromatic and polychromatic modes. In polychromatic operation, the spectral bandwidth can exceed 1keV, which is often too large for accurate structural reconstruction in solid-state systems. In contrast, monochromatic operation comes at significant cost to photon flux, making the study of transient structural changes difficult to measure.

In this work we describe the design and performance of a new multilayer monochromator for use at hard x-ray synchrotrons. This monochromator can provide users with both a tuneable bandwidth and increased photon flux sufficient for rapid structural determination. Our results demonstrate that this multilayer monochromator can provide widely tunable hard x-ray, possessing energy bandwidth of 20-100eV, and photon fluxes that significantly exceed standard double crystal monochromators. This capability not only has implications for time-domain materials research, but could be utilized on a variety of x-ray scattering/spectroscopic techniques.

12:39PM Y23.00008: Critical-Dimension Grazing-Incidence Small Angle X-Ray Scattering: Enhancing the latent signal using Bragg scattering*
DINESH KUMAR (Presenter), Computational Research, Lawrence Berkeley National Laboratory, GUILLAUME FREYCHET, ISVAR CORDOVA, Advanced Light Source, Lawrence Berkeley National Laboratory, JOSEPH WALTER STRZALKA, X-ray Science Division, Argonne National Laboratory, PATRICK NAULLEAU, Center for X-ray Optics, Lawrence Berkeley National Laboratory, RONALD J PANDOLFI, Computational Research, Lawrence Berkeley National Laboratory, PETER ERCUUS, CHENGYU SONG, Molecular Foundry, Lawrence Berkeley National Laboratory, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Laboratory — The semiconductor industry is continuously pushing the limits of photolithography, with feature sizes now under 10 nm. X-ray scattering\(^1\) has emerged as a possible contender to determine the average shape of a line grating with a sub-nanometer precision. However, to fulfill its promise, faster algorithms must also be developed to interpret and extract metrics from reciprocal space scattering data. We are presenting a novel, fast, and accurate X-ray technique and analysis algorithm: Critical Dimension Grazing Incidence X-ray Scattering, CD-GISAXS

The CD-GISAXS technique operates in grazing incidence configuration with a continuous azimuthal rotation of the sample, thus does not require high-energy X-rays to penetrate the wafer and greatly reduces the data acquisition times, permitting analysis within the framework of the DWBA. The Bragg rods coming from the line gratings, intersect with the momentum transfer vector of the elastic X-ray scattering at a single point above the horizon. The Bragg rods can be scanned by rotating the momentum transfer vector, and therefore the sample.


*1. Center for Advanced Mathematics for Energy Research Applications
2. DOE Early Career Award to Alexander Hexemer

12:51PM Y23.00009: Applications of Thin Film Atomic Layer Deposition Superconducting Titanium Nitride to Astronomical Measurements*
CALDER SHEAGREN (Presenter), PETER BARRY, RITOBAN BASU THAKUR, RONG NIE, Kavli Institute for Cosmological Physics, University of Chicago, ERIK SHIROKOFF, QING YANG TANG, Department of Astronomy and Astrophysics, University of Chicago — Microwave Kinetic Inductance Detectors (MKIDs) are an appealing option for conducting millimeter-wave astronomy and measuring the Cosmic Microwave Background due to their ease of fabrication and multiplexing. MKIDs make detections when a microwave photon breaks Cooper pairs in the superconducting metal, modifying the kinetic inductance of the metal and the resonant frequency of the on-chip resonator. A material of interest for fabricating MKIDs is Atomic Layer Deposition titanium nitride (ALD TiN) due to its high kinetic inductance and low critical temperature. We can precisely control these characteristics of the TiN by tuning deposition parameters such as thickness, stage temperature, and nitrogen flow. This method also admits high quality factors, allowing for increased multiplexing, and wafer-level uniformity with film thicknesses in the range of 4-18 nm. We present measurements of the critical temperature and internal quality factor of ALD TiN resonators under the variation of various ALD parameters as it relates to fabricating MKIDs.

*This work was supported by NSF grant no. AST-1554565, the Kavli Institute for Cosmological Physics, and the Pritzker Nanofabrication Facility at the University of Chicago, which receives support from SHyNE under NSF grant no. NNCI-1542205.
1:03PM Y23.00010: The status of the ultra-high resolution spectroscopy at the HFIR* FANKANG LI (Presenter), Neutron Sciences Directorate, Oak Ridge National Laboratory, HAO FENG, JIAZHOU SHEN, Physics Department, Indiana University Bloomington, MORRIS LOWELL CROW, MASAAKI MATSUDA, Neutron Sciences Directorate, Oak Ridge National Laboratory, STEVEN PARNELL, Faculty of Applied Sciences, Delft University of Technology, ROGER PYNN, Physics Department, Indiana University Bloomington, JAIME FERNANDEZ-BACA, Neutron Sciences Directorate, Oak Ridge National Laboratory — To measure the crystal lattice distortion or the lifetime of weak interactions among quasiparticles, such as phonons, electrons and magnons, with high resolution, the key is to break the inverse relationship between the resolution and useable flux. By using the Larmor precession of the neutron spin inside a given magnetic field, its momentum or energy change during the interactions with sample can be measured with ultra-high resolution. Therefore, this unique property of neutron provides us with another approach to overcome some of the limitations of conventional neutron scattering instruments. Also, it can make the best use of all the available neutrons by allowing the use of large divergent beams. The progress on upgrading the HB-1 polarized triple axis spectrometer at the High Flux Isotope Reactor of ORNL with superconducting magnetic Wollaston prisms will be presented. For neutron diffraction, the achievable resolution of the absolute peak splitting and relative lattice distortion (Δd/d) can be 2×10⁻⁴ and 1×10⁻⁶ relatively. While for inelastic scattering, for example phonon linewidth measurements, the resolution can be <10µeV.

*This research is sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory.

1:15PM Y23.00011: Oxidation state sensitive 3D atomic mapping of oxide-supported catalysts through X-ray Standing Wave (XSW) excited X-ray photoelectron spectroscopy (XPS)* ANUSHEELA DAS (Presenter), NARAYANACHARI KVVL, BO-HONG LIU, DENIS T KEANE, MICHAEL J BEDZYK, Northwestern University — XSW excited XPS was used to study the hydroxylated surface of rutile TiO₂ (110) single crystal, where the excess unpaired electrons of the hydroxyls play a critical role in surface chemistry and photocatalytic processes. The experiments were performed at APS DND-CAT 5IDC using a 7 keV incident beam. The hydroxylated O 1s binding energy was 2.4 eV higher than that of the bulk-like O atoms and was found to have a different XSW coherent fraction and position. Summation of these Fourier components for 3 symmetry inequivalent hkl Bragg peaks generate a chemical state sensitive 3D atomic map of oxygen. We also studied monolayer coverages of vanadium oxide (catalytic material) supported on the same surface. Collecting V, O and Ti 1s XPS signals as we scanned across a Bragg peak at different stages of a redox reaction allowed tracking of surface sites for chemically distinct V atoms, important for understanding their catalytic behaviour. These results coupled with DFT calculations will give unique insights into this as well as other related oxide supported catalysts.

*Northwestern University (NU) Institute for Catalysis in Energy Processes under DOE Grant DE-FG02-03ER15457, NU MRSEC program (NSF DMR-1121262), NU Center for Hierarchical Materials Design program under NIST Grant 70NANB14H01

1:27PM Y23.00012: Testing for the Continuous Spectrum of X-Rays Predicted to Accompany the Photoejection of an Atomic Inner Shell Electron* PHILIP JACOBSON (Presenter), ANDRIJA RASOVIC, SONGQI JIA, YUE LI, ARTHUR CAMPELLO, CHASE GODDARD, STANISLAV STOUPIN, J. Y. PETER KO, YUCHAO CHEN, JUSTIN OH, GWEN GARDNER, CARL FRANCK, Cornell University — For decades, experimental evidence for an elegant prediction of quantum electrodynamics has been sought: the detection of a broad spectrum of X-rays at low energies expected upon sudden ejection of an inner shell electron following absorption of an incident high energy photon. We report here on a recent attempt that provides a significantly reduced upper limit on the process that is consistent with contemporary theory and contradicts earlier observations. The Cornell High Energy Synchrotron Radiation Source (CHESS) was employed to deliver a 46 keV incident beam on solid copper film targets. To suppress extraneous events detection of scattered photons was performed in coincidence with the fluorescent decay of the K shell hole produced by photoejection. Through variable thickness targets we assessed secondary processes.

*This work is based upon research conducted at the Cornell High Energy Synchrotron Source (CHESS) which is supported by the National Science Foundation under award DMR-1332208. This work made use of the Cornell Center for Materials Research Shared Facilities which are supported through the NSF MRSEC program (DMR-1719875).

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y24 DAMOP DCMP: Topological States in AMO Systems II BCEC 159 - Chuanwei Zhang, University of Texas at Dallas - Tag(s): Focus
In this talk we present a new class of phases of matter called higher-order topological phases. Such systems exhibit gapped boundaries that are themselves lower-dimensional topological phases. Furthermore, they manifest topologically protected states at intersections between multiple surfaces. These states can, e.g., carry fractional charge, or be chiral propagating modes. We show that some of the simplest examples of these phases are connected to materials with quantized electric quadrupole moments, and illustrate how they can be realized in a variety of meta-material systems. We will also review the first experimental evidence for these phases in meta-material contexts. To characterize these new insulating phases of matter, we introduce a new type of invariant that had been previously overlooked, and we show how these invariants can predict a collection of new phenomena.

*This project was supported by the US National Science Foundation (NSF) Emerging Frontiers in Research and Innovation (EFRI) grant EFMA-1627184 and U.S. National Science Foundation under grant DMR-1351895.

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**Topologically Protected Photonic Modes in Composite Quantum Hall/Quantum Spin Hall Waveguides**

SHUKAI MA (Presenter), Department of Physics, University of Maryland, College Park, BO XIAO, Department of Electrical and Computer Engineering, University of Maryland, YANG XU, KUEIFU LAI, GENNADY SHVETS, Cornell University, STEVEN ANLAGE, Department of Physics, University of Maryland, College Park — Photonic topological insulators (PTI) are a new class of structures that can support backscattering-free propagating waves at an interface between topologically non-trivial structures. In the bi-anisotropic meta-waveguide (BMW) PTI designs, by carefully tuning the geometrical and electromagnetic properties, we can emulate the electronic quantum spin Hall (QSH) effect using its electromagnetic analog. A magneto-optical material added to the structure will introduce a quantum Hall (QH) photonic bulk insulator on the BMW basis. The combined photonic systems with multiple topological phases supporting reflection-free edgemodes are proposed and experimentally demonstrated. The spin degree of freedom of such topologically protected edgemodes determines their unique pathways through these systems, free from backscattering and able to travel around sharp corners. As an example of their novel properties, we demonstrate a full 4-port circulator based on composite QH and QSH back-scattering free waveguides.

*This work was supported by ONR Grant No. N000141512134, AFOSR COE Grant FA9550-15-1-0171, DOE under grant DESC 0018788, the NSF under Grants No. DMR-1120923, No. PHY-1415547 and No. ECCS-1158644.

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**Interacting Hall Response in Quantum Gas Experiments**

SEBASTIAN GRESCHNER (Presenter), MICHELE FILIPPONE, THIERRY GIAMARCHI, Department of Quantum Matter Physics, University of Geneva — Recent experiments with ultracold quantum gases in artificial magnetic fields have shown the possibility to study the Hall effect in quasi one-dimensional highly tunable ladder systems. In this context we theoretically analyze the properties of the reactive Hall response on ladder models with strongly interacting bosons and fermions. We compare different methods for the computation of the static Hall coefficient and discuss its dependence on the various methods or limits considered. In the cases relevant for recent experiments in synthetic dimensions, we find a surprising universal behavior of the weak field Hall coefficient of single component phases in the case of an SU(M) symmetric interaction. For strong magnetic fields we study the interesting properties of the quantum-Hall effect in various quantum phases on ladder geometries including vortex-lattice, biased ladder or Laughlin like states.

*Swiss National Science Foundation

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**Higher Order Floquet Topological Insulators with Anomalous Corner States**

BIAO HUANG (Presenter), University of Pittsburgh, W.VINCENT LIU, University of Pittsburgh and Shanghai Jiaotong University — The theoretical and experimental discovery of topological insulators of higher multipole nature, dubbed “higher order topological insulators” (HOTI), has triggered heated discussions in recent studies. But so far, all researches have been limited to static systems due to the lack of higher order topological invariants constructed for a genuine dynamical system. Here, we report a Floquet-driven model showing the anomalous corner states and a construction of dynamical topological invariant built upon evolution operators $U(t)$. We show that the bulk static nested quadrupoles, constructed by eigenstates of the static Floquet operator $U_F = U(T)$, vanish identically, while corner states emerge in all energy gaps with quantized charges due to the dynamical topology. The signature of such an anomalous Floquet phase in cold atom experiments is also discussed via corner particle dynamics and a band tomography. Our work paves the way to the systematic study of HOTI in regimes far away from equilibrium.

*U.S. ARO (W911NF-11-1-0230), AFOSR (FA9550-16-1-0006), and MURI-ARO (W911NF-17-1- 0323)
Here we focus on recent results challenging the usual viewpoint, the occurrence of higher-order exceptional points where a macroscopic fraction of the states coalesce at a single point with a geometrical multiplicity of one [2] and where the system becomes devoid of extended states [2].

A scheme to generate such higher-order exceptional points in lattices will be presented together with an argument [3] regarding the separation of the spectrum into topological states and localized states originated by higher-order exceptional points.


*We thank FondeCyT 1170917.

12:39PM Y24.00006: Non-Hermitian adiabatic transport in the space of exceptional points*  
JUDITH HOELLER  
(Presenter), NICHOLAS READ, JACK HARRIS, Yale Univ — An $n \times n$ non-Hermitian Hamiltonian matrix $H$ can describe a dissipative system, such as $n$ coupled weakly dissipative classical harmonic oscillators. Under full parametric control over $H$, the parameter space contains a connected -- but not simply-connected -- subspace of $n$th order exceptional points, at each of which $H$ is equivalent to an $n \times n$ Jordan block. We show that smooth variations of parameters during time $T$, along a loop within that space, can single out one state that is least dissipative and evolves adiabatically. Its complex adiabatic phase is $T$ times a Puiseux series in powers of $T^{-1/n}$; the coefficient at order $T^0$ is the Berry phase, which is a multiple of $2\pi/n$ (modulo $2\pi$) and only depends on the homotopy class of the loop within the space of $n$th order exceptional points.

*We acknowledge support from Yale University (JH) and from AFOSR grant FA9550-15-1-0270 and ONR MURI N00014-15-1-2761 (JGEH).

12:51PM Y24.00007: Topological symmetry classes for non-Hermitian models and connections to the bosonic Bogoliubov–de Gennes equation*  
SIMON LIEU  
(Presenter), Imperial College London — The Bernard-LeClair (BL) symmetry classes generalize the Altland-Zirnbauer classes in the absence of Hermiticity. Within the BL scheme, time-reversal and particle-hole symmetry come in two flavors, and “pseudo-Hermiticity” generalizes Hermiticity. We propose that these symmetries are relevant for the topological classification of non-Hermitian single-particle Hamiltonians and Hermitian bosonic Bogoliubov–de Gennes (BdG) models. We show that the spectrum of any Hermitian bosonic BdG Hamiltonian is found by solving for the eigenvalues of a non-Hermitian matrix which belongs to one of the BL classes. We therefore suggest that bosonic BdG Hamiltonians inherit the topological properties of a non-Hermitian symmetry class and explore the consequences by studying symmetry-protected edge instabilities in a one-dimensional system.

*Imperial College President's Scholarship

1:03PM Y24.00008: Stability of Non-Hermitian Phases  
DAN BORGNIA  
(Presenter), Harvard University — Recent work on non-Hermitian physics in condensed matter systems has focused on the classification of new topological phases. The notion of a gap usually used to describe the stability of Hermitian phases is not sufficient in the presence of loss and gain terms. This work uses known results in the theory of pseudo-spectra and Jordan Normal Forms to detail the stability of novel non-Hermitian phases under different disorder profiles in 1D with some generalizations into higher dimensions. We find agreement with previous work in simple chiral models and single parameter disorder distributions of our generalized stability arguments.
Topological charge pumping in the interacting bosonic Rice-Mele model*  ANDREW HAYWARD
(Presenter), Institute for Theoretical Physics, Georg-August-Universität Göttingen, CHRISTIAN SCHWEIZER, MICHAEL LOHSE,
MONIKA AIDELSBURGER, Fakultät für Physik, Ludwig-Maximilians-Universität München, FABIAN HEIDRICH-MEISNER, Institute for Theoretical Physics, Georg-August-Universität Göttingen — In recent years, demonstrations of topological Thouless charge pumping have been performed with ultra-cold atoms. We discuss our recent work [1] investigating charge pumping in the Bosonic Rice-Mele model and verify that the charge pumping remains quantized as long as the pump cycle avoids the superfluid phase. In the limit of hardcore bosons, the quantized pumped charge can be understood from single-particle properties such as the integrated Berry curvature constructed from Bloch states, while this picture breaks down at finite interaction strengths. These two properties -- robust quantized charge transport in an interacting system of bosons and the breakdown of a single-particle invariant -- could both be measured with ultracold quantum gases extending a previous experiment [2]. We also relate the structure of the spectral flow of the entanglement spectrum to the properties of the charge pump.


*Supported by the DFG - project number 277974659 via Research Unit FOR 2414. Additional support from the DFG - project number 282603579 (DIP), the European Commission (UQUAM Grant No. 5319278), the Nanosystems Initiative Munich Grant No. EXC4, and the NSF, Grant No. NSF PHY-1748958.

Topologically robust defect states in two-fold PT-symmetric systems  SANG-JUN CHOI
(Presenter), JUNG-WAN RYU, HEE CHUL PARK, Center for Theoretical PCS, Institute for Basic Science — The emergence of topologically robust states has been understood in terms of the bulk-edge correspondence; they appear at the boundary between two insulating systems whose topology cannot be continuously deformed into another. However, is its converse true? Here, we find that at the boundary where two topologically trivial insulating system meets, a robust localized state can appear. We provide a new topological identification where two-fold PT-symmetry of the system protects the emergence of such a state against continuous deformations. Moreover, we show the localization length of the topological defect state is insensitive to a wide range of parameters, and the defect states in the known systems fall into our topological identification.

Topological insulators in synthetic dimensions  DAVID LONG (Presenter), PHILIP CROWLEY, Boston University, IVAR MARTIN, Materials Science Division, Argonne National Laboratory, ANUSHYA CHANDRAN, Boston University — Few level quantum systems driven by multiple incommensurate external tones exhibit temporal analogs of many real-space topological phenomena. I will discuss how a qubit driven by two tones realizes a topological insulator in frequency space and identify the symmetry protecting the insulator. The edge modes of the topological insulator can robustly transfer a large amount of energy between the drives for symmetry-broken initial states.

Interaction-induced multivaluedness and topological change between quantum current and its variance  CHIH-CHUN CHIEN (Presenter), University of California, Merced, MEKENA METCALF, Sandia National Lab, CHEN-YEN LAI, Los Alamos National Lab, MASSIMILIANO DI VENTRA, University of California, San Diego — The variance of a quantum observable has been an important quantity in quantum mechanics, and it can reveal additional information beyond the average. By analyzing the parametric curves of the quantum current versus its variance, we found a general change of topology due to the interactions. We consider a benzene-like lattice with fermions driven by a magnetic flux for the isolated system and a three-site lattice connected driven by two particle reservoirs for the open system. In both systems, there is a one-to-one correspondence between the current and its variance in absence of interactions. When the interactions are introduced, the parametric curves exhibit loop structures and show multivalued correspondence between the current and its variance. The phenomena could be realizable using available cold-atom technology.

Order-from-disorder effects and Zeeman field tuned quantum phase transitions in a bosonic quantum anomalous Hall system

FADI SUN (Presenter), JINWU YE, Mississippi State University — We study possible many body phenomena in the recent experimentally realized weakly interacting quantum anomalous Hall system of spinor bosons by Wu, et.al, Science 354, 83-88 (2016). At a zero Zeeman field $h = 0$, by incorporating order from disorder effects, we determine the quantum ground state to be a $N = 2$ XY-antiferromagnetic superfluid state and also evaluate its excitation spectra. At a finite small $h$, the competition between the Zeeman energy and the effective potential generated by the order-from-disorder leads to a canted antiferromagnetic superfluid state, then drives a second order transition to a spin-polarized superfluid state along the z direction. The transition is in the same universality class as the zero density superfluid to Mott transition. Scaling behaviours of various physical quantities are derived. The ongoing experimental efforts to detect these novel phenomena are discussed.

*The work is supported by AFOSR FA9550-16-1-0412.

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y27 DQI: Quantum Foundations III BCEC 160C - John DeBrota, University of Massachusetts Boston - Tag(s): Focus

11:15AM Y27.00001: Reconstructing quantum space-time from agents' subjective experiences* [Invited] LIDIA DEL RIO (Presenter), ETH Zurich — Within a global physical theory, a notion of locality allows us to find and justify information-processing primitives, like non-signalling between distant agents. Here, we propose exploring the opposite direction: to take agents as the basic building blocks through which we test a physical theory, and recover operational notions of locality from signalling conditions.

For example, in quantum theory, the tensor product rule allows us to describe independent systems jointly, and imposes a notion of locality of actions. However, if one is given a global system, there is no prior reason for considering some factorization of the system's state space as 'the only physical one.' Thus, if multiple agents observe the same system, their individual factorizations of the state space do not necessarily coincide, but can be related by an isomorphism. We may then explore how a group of agents could find out the relation between their individual factorizations of a global space, given only the operational experimental data for each agent, together with communication, under different constraints.

This factorization problem is a generalization of the marginal problem and of self-testing, both of which assume a fixed tensor factorization behind the different local descriptions. It can be applied to derive conditions for a common space coordinate set shared by a group of agents, and as such it is a first step towards operational quantum relativistic theories.

*FQXi Large Grant "Physics of the Observer"

11:51AM Y27.00002: Locally Causal Quantum Mechanics in Space-Time MORDECAI WAEGELL (Presenter), Chapman University — I introduce a reformulation of quantum mechanics as a theory of physical fields in space-time which obey the constraints of special relativity. Instead of being described by a single de-localized wavefunction in configuration space, the fundamental subsystems within a composite system are each described by a continuum of local relative wavefunctions in space. Each relative wavefunction is defined on a particular world-line through space-time, using only the past states and coupling unitaries of the systems within the past-interaction-cone, and thus obeying explicit local causality. As a result, the narrative and causal structures of this reformulation are Lorentz covariant - unlike single-wavefunction descriptions. This model explains violations of Bell inequalities while obeying local causality, but entanglement correlations are not physically obeyed until Alice's and Bob's measurement results are compared locally in space-time. Explaining their experiences in this experiment then necessitates the existence of multiple Alices and multiple Bobs who got different measurement outcomes, and thus we arrive at a locally-branching many-worlds interpretation of quantum mechanics in space-time which obeys local causality - unlike global-branching many-worlds models.
12:03PM Y27.00003: Quantum Clocks: Gravitation and Relativity* ALEXANDER R. H. SMITH (Presenter), Dartmouth College, MEHDI AHMADI, Santa Clara University — Time enters quantum theory through its appearance as an external classical parameter in the Schrödinger equation. In general relativity, time is defined operationally as what is indicated by a clock and the spacetime metric encodes the relationship between different clocks. Reconciling these two different notions of time in a quantum theory of gravity leads to the problem of time, one aspect of which is the disappearance of time in the Wheeler-DeWitt equation.

Motivated by this problem, the conditional probability interpretation (CPI) posits that time evolution emerges from entanglement shared between a clock and system of interest, the joint state of which does not evolve with respect to a background time and satisfies a Wheeler-DeWitt equation. After reviewing the CPI, I will present a generalization in which the clock and system interact — we should expect such a coupling when the gravitational interaction between the clock and system is taken into account. I will demonstrate how such clock-system interactions result in a time-nonlocal modification to the Schrödinger equation. Furthermore, I will demonstrate how time dilation becomes probabilistic within the CPI framework and recover on average the special relativistic result.

*Dartmouth College Society of Fellows and NSERC

12:15PM Y27.00004: Quantized Electromagnetic-Field Propagation in General Non-Local and Non-Stationary Dispersive and Absorbing Media* VERNE JACOBS (Presenter), United States Naval Research Laboratory — We develop dynamical descriptions for the propagation of quantized electromagnetic fields, in the presence of environmental interactions. These descriptions are systematically and self-consistently developed in the complimentary Schrödinger and Heisenberg pictures. An open-systems (non-equilibrium) quantum-electrodynamics and quantum-statistical description is thereby provided for electromagnetic-field propagation in general non-local and non-stationary dispersive and absorbing optical media, including a fundamental microscopic treatment of decoherence and relaxation processes due to environmental collisional and electromagnetic interactions. Particular interest is centered on entangled states and other non-classical states of electromagnetic fields, which may be created by non-linear electromagnetic interactions and detected by the measurement of various electromagnetic-field correlation functions. Accordingly, we develop dynamical descriptions based on general forms of electromagnetic-field correlation functions involving both the electric-field and the magnetic-field components of the electromagnetic field, which are treated on an equal footing.

*Work supported by the Office of Naval Research through the Basic Research Program at The Naval Research Laboratory.

12:27PM Y27.00005: Spacetime formulation for time crystals and continuous variables TIAN ZHANG (Presenter), University of Oxford, OSCAR DAHLSTEN, Department of Physics, Southern University of Science and Technology — In ordinary, non-relativistic quantum theory, especially in quantum information, space and time are treated differently. For example, time is a parameter rather than an operator; states are defined across the whole space but only at one time. These go against our intuition from relativity as well as classical probability theory. Thus, space-time density matrices have been introduced and here we discuss one of these formulations called pseudo-density matrix (PDM) which treats space and time indiscriminately. As a first application, we use this formulation to analyse time crystals via quantum error correction, which is the first time to discuss time crystals in the language of quantum information. We achieve the same result as the absence of continuous time crystals and formulate discrete time crystals in terms of quantum error correction. NMR experiments have been conducted to verify the results. We also extend this space-time formulation to the continuous variables via a generalisation for Wigner function, and discuss Gaussian case in particular. This is the first step we take to understand temporal vs spatial modes in quantum fields and black holes. We want to analyse temporal correlations in black hole information paradox.
12:39PM Y27.00006: Using Fisher Information to Analyse Inter-measurement Quantum Particles*  DAVID ARVIDSSON SHUKUR (Presenter), University of Cambridge and MIT, CRISPIN BARNES, University of Cambridge, NICOLE YUNGER HALPERN, Harvard-Smithsonian Center for Astrophysics and Harvard University — A debated question in quantum mechanics is how to describe and interpret a quantum particle between observations. Previous discussions have mainly been centred on controversial and interpretation-dependent weak values. In this talk we provide an operational methodology for the analysis of inter-measurement quantum particles. We assume that absolutely perfect quantum evolutions are impossible, and that all interactions include some disturbances. By calculating the quantum Fisher information with respect to these disturbances we obtain a quantitative tool to map out the past path of quantum particles and to investigate the “quantumness” of post-selected experiments. We relate the Fisher information to the Kirkwood-Dirac quasiprobability distribution by decomposing the density matrix of the quantum state in terms of the projectors of the final measurement and the generator eigenbasis of the relevant interaction. We then show that when the Fisher information of a post-selected experiment exceeds its standard maximum, there exist negative quasiprobabilities in the representation, revealing violations of noncontextuality. Our methodology provides a new approach to investigating the foundations of quantum mechanics.

*The EPSRC
The Sweden-America Foundation

12:51PM Y27.00007: Noninformative prior of the quantum statistical model in the qubit system*  FUYUHIKO TANAKA (Presenter), Osaka University — In quantum process tomography, we often encounter a parametric family of qubits with less symmetry and estimate the parameter from experimental data. If we use Bayes estimates, then we have to choose a default probability distribution over the parameter space, which is called a noninformative prior. While the effect of the prior becomes smaller with the large amount of data, the choice of the noninformative prior based on a certain criterion has been of theoretical interest. In this talk, we consider a suitable definition of a noninformative prior in a general parametric family of qubits.

In the classical Bayesian statistics, there is no universal criterion and still there are many works on the choice of a noninformative prior like the famous Jeffreys prior. The most famous one is Bernardo's criterion, which deals with the maximization of the mutual information. However, its formal extension is troublesome because the quantum relative entropy between two pure states diverges.

Recently the author proposed another way based on the quantum detection game, which is well-defined in pure-states model. In this talk, as further development, we extend the argument to general qubit models, which yields Bures geometry.

*This work was supported by JSPS KAKENHI Grant Numbers 16H04382.

1:03PM Y27.00008: Uncertainty relations for time averaged weak values*  ELI POLLAK (Presenter), Chemical and Biological Physics, Weizmann Institute of Science — Time averaging of weak values using the quantum transition path time probability distribution leads to the establishment of a general uncertainty principle for the weak values of two not necessarily Hermitian operators. This new principle is a weak value analog of the Heisenberg-Robertson strong value uncertainty principle. It shows that complementarity does not prevent the simultaneous determination of weak values of non-commuting operators. When the time fluctuations of the weak values of the two operators under consideration are proportional to each other there is no uncertainty limitation on their variances and, in principle, their means can be determined with arbitrary precision. This will be exemplified by considering weak value uncertainty relations for the time-energy, coordinate-momentum and coordinate-kinetic energy pairs, and an analysis of spin operators and the Stern-Gerlach experiment in weak and strong inhomogeneous magnetic fields. We find that anomalous spin values are associated with large variances implying that their measurement demands increased signal averaging. These examples establish the importance of considering the time dependence of weak values in scattering experiments.

*Israel Science Foundation
1:15PM Y27.00009: Three-Particles Aharonov-Bohm Effect* YUTAKA SHIKANO (Presenter), Quantum Computing Center, Keio University — Recently, we showed the successful experiment on the three-particles Aharonov-Bohm effect using the tapped ion [A. Noguchi, YS, K. Toyoda, S. Urabe, Nature Communications 5, 3868 (2014)]. In this experiment, there still remain several fundamental questions on the identical particles. Inspired by our experiment setup, we can discuss the properties of the identical particles from the Aharonov-Bohm effect perspectives. The phase shift by changing the particle status leads to give an answer to the following question when the Aharonov-Bohm phase can be acquired. As the minimum setup, three particle setting is considered. Maybe, it is possible to be generalized to the N-body particles. Furthermore, the dynamical non-locality aspects will be discussed if possible.

*This work is financially supported by a grant from The Precise Measurement Technology Promotion Foundation, JSPS KAKENHI (Grant Nos. 16K05492, 16K05410, 17H02797, 17K05082) and Collaborative Research Project of Laboratory of Materials and Structures.

1:27PM Y27.00010: Topological barriers for charged quantum systems* ISMAEL PAIVA (Presenter), YAKIR AHARONOV, MORDECAI WAEGELL, JEFF M TOLLAKSEN, Chapman University — The Aharonov-Bohm effect introduced a surprising influence of topology on the dynamics of quantum systems. The discovery of such a phenomenon unveiled that the evolution of a quantum system with charge traveling around a solenoid is affected by the magnetic flux on it, even though the solenoid only produces electromagnetic field on its interior. Here, making use of the concept of modular variables, which evidence the dynamical nonlocality presented in quantum mechanics, we argue that this effect allows solenoids to be used as barriers of energy for charged quantum systems. Moreover, we present and discuss a thought experiment, as well as its numerical simulation, where a configuration of solenoids inside a cavity can trap some quantum states in a certain subregion of it.

*Ismael L. Paiva acknowledges financial support from the Science without Borders Program (CNPq/Brazil).

1:39PM Y27.00011: Quantum simulation of a general PT-symmetric two-level system* CHAO ZHENG (Presenter), Department of Physics, North China University of Technology — The evolution of a two-level quantum system with a general PT-symmetric Hamiltonian is simulated as a subsystem in a four-dimensional Hilbert space, which makes it possible to simulate any two-level PT-symmetric quantum system using a conventional quantum mechanics system. We studied the ability to simulate and investigate novel quantum systems and phenomena using a conventional Hermitian quantum computer. The quantum circuits are given for a qubit and two qudit systems.

*This work was supported by the National Natural Science Foundation of China Grant No. 11705004, Open Research Fund Program of the State Key Laboratory of Low-Dimensional Quantum Physics No. KF201710.

1:51PM Y27.00012: Computing with a single qubit faster than the computation quantum speed limit* NIKOLAI SINITSYN (Presenter), Theoretical Division, Los Alamos National Laboratory — The possibility to save and process information in fundamentally indistinguishable states is the quantum mechanical resource that is not encountered in classical computing. I demonstrate that, if energy constraints are imposed, this resource can be used to accelerate information-processing without relying on entanglement or any other type of quantum correlations. In fact, there are computational problems that can be solved much faster, in comparison to currently used classical schemes, by saving intermediate information in nonorthogonal states of just a single qubit. There are also error correction strategies that protect such computations.

*the LDRD program at LANL
2:03PM Y27.00013: Problems with Decoherence in Quantum Geometrodynamics* MAANELI DERAKHSHANI (Presenter), Utrecht University — I illustrate some severe conceptual and technical problems that arise in attempts to apply quantum decoherence concepts to "quantum geometrodynamics" (i.e. Dirac constraint quantization of classical general relativity in the Hamiltonian formulation). In particular, I show that the Problem of Time, the Hilbert Space Problem, and the conceptual dependence of decoherence on time evolution and Hilbert space structure implies: 1) suppression of interference cannot take place between components of a superposition of quantum-gravitational (i.e. Wheeler-DeWitt) wave functionals; 2) approximate diagonalization of the reduced density matrix (associated with said superposition) in the 3-geometry basis cannot take place, and such a reduced density matrix is mathematically ill-defined; 3) time-dependent functional Schroedinger equations for the matter components of said superposition cannot be derived in a semiclassical approximation. I conclude, contrary to extant claims in the quantum gravity literature, that quantum decoherence concepts cannot be consistently applied to quantum geometrodynamics. I then suggest that quantum decoherence concepts can only be sensibly applied to quantum gravity theories that posit classical time parameters or matter-clock variables at a fundamental level.

*N.A.

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y29 DQI: Semiconducting Qubits: Automation of Tune-up BCEC 162A - Natalia Ares

11:15AM Y29.00001: Silicon MOSFET quantum dots with simplified metal-gate geometry* EDUARDO BARRERA (Presenter), FRANCOIS SFIGAKIS, FERHAT AYDINOGLU, JONATHAN D BAUGH, Institute for Quantum Computing, University of Waterloo, Waterloo, Canada — Silicon (Si) CMOS spin qubits have become a promising platform for a future quantum information processor due to recent demonstrations of high fidelity single and two qubit gates [Veldhorst et. al., Nature 526.7573 (2015)], compatibility with industrial CMOS process and promising prospects for scalability. Typical Si spin qubits devices consist of gate-defined quantum dots, each defined by several metal gates, which pose a challenge to scaling the technology up. Hence, future designs of Si spin qubits will need to reduce the fabrication complexity and adopt a scalable design.

Here, we introduce a two metal-layer MOSFET quantum dot device that reduces the number of metal gates and simplifies the dot tune-up procedure. By performing electron counting measurements with a charge sensor, we determine that the accumulation gate defining the electron reservoir can tune the dot-reservoir tunnel rate by about 10 decades/V. Magnetospectroscopy measurements up to 6 T reveal electron spin filling in the few electron regime from which we estimate a valley splitting of about 290 μeV.

*The authors would like to thank NSERC, the Waterloo Institute for Nanotechnology, the Canada First Research Excellent Fund, and the University of Waterloo's Quantum NanoFab facility.

11:27AM Y29.00002: Single electron charge shuttling in a linear quantum dot array* ADAM MILLS (Presenter), DAVID ZAJAC, MICHAEL GULLANS, FELIX SCHUPP, THOMAS HAZARD, JASON R PETTA, Princeton University — Recent advances in silicon spin qubits have pushed single qubit fidelities beyond 99.9% [1,2] and have lead to the realization of two-qubit gates based on exchange coupling [3-6]. In order to advance spin qubits to the next level of technological complexity, it is important to start investigating how to scale up to larger multi-component architectures. These architectures must allow for arbitrary coupling of spatially separated qubits, demanding the development of inter-qubit quantum state transfer procedures. Here we demonstrate shuttling of a single electron across a linear array of 9 series-coupled Si quantum dots in ~50 ns with an approach that is extendable to larger quantum dot arrays.


*Research sponsored by ARO grant No. W911NF-15-1-0149 and the Gordon and Betty Moore Foundation's EPIQS Initiative through grant GBMF4535. Devices were fabricated in the Princeton University Quantum Device Nanofabrication Laboratory.
11:39AM Y29.00003: Electron shuttling based error-correction architectures using quantum dot qubits* VEIT LANGROCK (Presenter), DAVID PETER DIVINCENZO, Institute for Theoretical Nanoelectronics (PGI-2), JARA-FIT Institute for Quantum Information, FZ Jülich, Germany — Spin-qubits based on electrons in gate-defined quantum dots [1] are currently one of the major candidates for quantum computers realized in semiconductor hosts. The inherent dot mobility provided by the conceptual ease of electron shuttling in such gate-defined systems is a powerful resource which has been incorporated as a vital component in proposals for fault-tolerant spin-qubit architectures [2,3], with the assumption that such operations can be realized with very high fidelity and on relatively short time scales. We address the issue of decoherence for such shuttling devices and present a possible realization of a scalable fault-tolerant quantum memory based on more realistic device models.


*VL acknowledges support from Helmholtz IVF grant 'Scalable solid state quantum computing'.

11:51AM Y29.00004: Simulating coherent electron shuttling in quantum dots BRANDON BUONACORSI (Presenter), BENJAMIN D SHAW, JONATHAN D BAUGH, Institute for Quantum Computing, University of Waterloo, Canada — Coherent transport of electron spins is required for several proposed large-scale architectures based on quantum dot spin qubits [1,2]. In [1], spin singlets are distributed across neighboring computational nodes by sequential single-electron tunneling through a linear array of quantum dots. We adopt a simplified metal-gate geometry for silicon MOS dots and use the Nextnano software to determine the potential landscape as a function of varying gate voltages, subsequently solving the time-dependent Schrodinger equation in 1D to simulate coherent shuttling. An algorithm is presented that calculates time-dependent voltages that maintain a desired fidelity with the ground state orbital wavefunction. These tools are used to vary the geometrical device parameters to maximize the electron shuttling velocity. We further show that the essential physics can be captured in an effective Hamiltonian model, which allows us to explore how spin-orbit and valley states affect the shuttling fidelity and maximum velocity.


12:03PM Y29.00005: Algorithm for automated tuning of a quantum dot to the single electron regime.* MAXIME LAPOINTE-MAJOR (Presenter), JULIEN CAMIRAND LEMYRE, DANY LACHANCE-QUIRION, SOPHIE ROCHELLE, MICHEL PIORO-LADRIERE, Institut quantique and Département de Physique, Université de Sherbrooke, Sherbrooke, Québec, J1K 2R1, Canada — Tuning quantum dot devices to an operational target is a time-consuming process. In this work, we have developed an algorithm adapted to quantum dots measured by charge detection with a single electron transistor (SET). The program uses a computer-controlled visual approach, where the tuning of the quantum dot is performed with an intuitive heuristic approach. Small size stability diagrams of the dot and reservoir gates are measured in an adaptive sequence until the last electronic transition of the quantum dot is found. For each stability diagram, the charge detector background is removed and the electron occupancy transitions are identified. From these transition points, lines are reconstructed using a modified Hough transform and other image detection tools. Preliminary tests on previously measured stability diagrams show reliable performances of the algorithm for different samples. This work is a step towards fast automatized initialization of quantum dots arrays.

*This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Canada Foundation for Innovation (CFI). This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund.
12:15PM Y29.00006: Control of a GaAs “QuByte” in the single electron regime – adding dots one-by-one  
CHRISTIAN VOLK (Presenter), ANNE-MARIJE ZWERVER, QuTech, TU Delft, PIETER EENDEBAK, Netherlands Organization for Applied Scientific Research (TNO), SJAAK VAN DIEPEN, QuTech, TU Delft, FLOOR VAN RIGGELEN, Netherlands Organization for Applied Scientific Research (TNO), UDITENDU MUKHOPADHYAY, JUAN PABLO DEHOLLAIN, TOIVO HENSGENS, QuTech, TU Delft, CHRISTIAN REICHL, WERNER WEGSCHEIDER, Solid State Physics, ETH Zürich, LIEVEN VANDERSYPEN, QuTech, TU Delft — Spin qubits based on semiconductor quantum dots (QDs) are promising building blocks for quantum computation. So far, research mainly focused on devices with up to four QDs. However, quantum algorithms, quantum simulations and mediators to exchange quantum information require larger and scalable systems. Though, controlled filling becomes challenging with an increasing number of QDs due to cross-capacitances and electron latching effects.

We develop a scalable technique, the ‘n+1 strategy’ where, starting from a double QD, subsequent QDs will be added one-by-one. We measure the capacitive coupling between all relevant gates and the QDs in order to create a parameter set of virtual gates. That allows individual control of chemical potentials and thus the number of electrons on each QD and furthermore the adjustment of tunnel rates.

We successfully use this technique to tune up a linear array of eight QDs ‘QuByte’ in GaAs so they are occupied by one electron each.

12:27PM Y29.00007: Towards Autonomous Tuning of Double Quantum Dots  
JANA DARULOVA (Presenter), Institute for Theoretical Physics, ETH Zurich, SEBASTIAN PAUKA, ALICE MAHONEY, School of Physics, The University of Sydney, JOHN HORNIBROOK, Microsoft Corporation Sydney, NATHAN WIEBE, CHRISTOPHER GRANADE, Microsoft Corporation Redmond, WA, MAJA C CASSIDY, DAVID REILLY, Microsoft Corporation Sydney, MATTHIAS TROYER, Microsoft Corporation Redmond, WA — Defining quantum dots in semiconductor or semiconductor/superconductor heterostructures is an essential step in initializing solid-state qubits. To date, the majority of the repetitive procedure of finding suitable gate voltages defining a quantum dot is done manually. However, as the complexity of devices as well as the number of devices per chip grows, this approach becomes unfeasible.

Current approaches either require significant, manually measured input, or address specific parts of the tune-up only. In both cases, only one well known device has been addressed.

In this talk we present an alternative autonomous automated solution for the tuning of gate-defined quantum dots which requires as input only the device layout. Our approach is able to characterize unknown devices and determine suitable gate voltages defining either a single or double quantum dot. We also discuss the extraction of the full capacitance matrix and performance of different classifiers when applied to both theoretical and experimental data.

JULIAN DAVID TESKE (Presenter), SIMON HUMPOHL, RENE OTTEN, PATRICK BETHKE, PASCAL CERFONTAINE, HENDRIK BLUHM, JARA-FIT Institute Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, 52074 Aachen, Germany — In the search for a technology best suited for quantum computation, spin qubits based on gate-defined quantum dots have demonstrated very favorable properties, one remaining challenge is their tuning into a suitable operating regime. Since this requires accurate tuning of the voltages applied to all electrostatic gates, this is a time-consuming procedure [1]. Thus, the automation of these tuning procedures is a necessary requirement for the operation of a quantum processor based on gate-defined quantum dots, which is yet to be fully addressed.

We present an algorithm for the automated fine-tuning of quantum dots, and benchmark its performance by tuning tunnel and lead coupling on a GaAs singlet triplet qubit. We employ a Bayesian approach called Kalman filter to estimate the gradients of the parameters of interest as function of gate voltages. Our benchmarks demonstrate the ability of reaching the operation regime within 3 to 5 iterations, corresponding to 10 to 15 minutes of lab-time.

ANDREW MOUNCE (Presenter), PHILLIP J LEWIS, CARA MONICAL, N. TOBIAS JACOBSON, ALBERT GRINE, MARTIN RUDOLPH, JOHN ANDERSON, JOEL R. WENDT, TAMMY PLUYM, DAN R WARD, KURT W. LARSON, MICHAEL P LILLY, MALCOLM S. CARROLL, Sandia National Laboratories — Tune-up and analysis of quantum dots (QD) is an arduous manual task consisting of a sequence of steps that builds upon one another. The tuning and analysis complexity is increasing as designs extend from QDs to multi-objects (e.g., donor-QD coupling and multi-QDs). The process can be simplified by utilizing image recognition techniques and automation. In this talk, I will present image analysis techniques which extract information from transport and charge sensing stability plots. These analysis modules can determine parameters such as tunnel rates and charge configurations in the QD systems. We identify the necessary combination of tune-up steps and feedback from analysis modules (i.e., output parameters for the next scan) that can automate tuning to few-electron charge sensing. This talk presents some of the proof-of-concepts, details and key future challenges.

*N Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

1:03PM Y29.00010: A Flexible Control System for Quantum Dot Qubits*  
NIZAR MESSAOUDI (Presenter), Keysight Technologies, AZFAR BADAROUDINE, LARISSA NJEJIMANA, Département de Génie Électrique et Informatique, Université de Sherbrooke, GIDGET HEINTZ, Keysight Technologies, MARC-ANTOINE GENEST, MICHEL PIORO-LADRIERE, Institut quantique et Département de physique, Université de Sherbrooke — The advancement of Quantum Dot qubit technology is paving the way to fault-tolerant quantum computing systems. Although spin qubits are still at a relatively early stage, their strong robustness against noise makes them extremely attractive. However, quantum architectures still rely on classical electronics for control and readout. While traditional instrumentation has been used to manipulate and detect qubit spins, they lack the scalability necessary to move from single qubit to multi-qubit experiments. Even if the instruments can be synchronized for signal phase coherence, they lack the flexibility that is required for researchers to explore new control techniques and qubit architectures. This flexibility can be achieved through Digital Signal Processing (DSP) realized on Field Programmable Gate Arrays (FPGA). FPGAs allow the implementation of a range of DSP algorithms while also providing absolute time determinism. This paper discusses the use of commercial FPGA based instruments to implement a spin-qubit control system. A lock-in amplifier is implemented in the FPGA of the digitizer and quantum dot Coulomb blockade measurements are compared to when using a dedicated lock-in amplifier.

*This project was supported by the Natural Sciences and Engineering Research Council of Canada

1:15PM Y29.00011: Scalable tuning of InAs quantum dots embedded in photonic structures  
JOEL GRIM (Presenter), ALLAN S BRACKER, MAXIM ZALALUTDINOV, SAMUEL CARTER, U.S. Naval Research Laboratory, ALEXANDER C. KOZEN, ASEE postdoctoral research fellow at the U.S. Naval Research Lab, MIJIN KIM, KeyW corporation, CHUL SOO KIM, U.S. Naval Research Laboratory, JEROME THOMAS MLACK, NRC Research Associate residing at the Naval Research Laboratory, MICHAEL K YAKES, U.S. Naval Research Laboratory, BUMSU LEE, NRC Research Associate residing at the Naval Research Laboratory, DANIEL G GAMMON, U.S. Naval Research Laboratory — The prospect of integrated quantum optics platforms based on semiconductor quantum dots (QDs) has driven quantum semiconductor research for decades. This has resulted in advanced demonstrations of single photon emission and switching, quantum transistors, and qubit-photon interfaces. However, the variation in QD emission energies – which prevents interfacing QDs with each other and photonic elements such as cavities and waveguides – has thus far limited these demonstrations to one or two QDs. We have developed an approach that addresses this challenge by laser-patterning strain via local phase transitions of a conformal thin film deposited on the surface of photonic architectures. Using this approach, InAs QDs can be tuned across the entire inhomogeneous distribution, with a spectral resolution down to the homogeneous linewidth, and sub-micron spatial resolution. We show that a scalable number of QDs embedded in the same bridge waveguide can be tuned into resonance. We also demonstrate that the emission energies of QDs embedded in photonic crystal cavities and waveguides can be tuned with this approach.

Deep Reinforcement Learning Based Control of Coherent Transport by Adiabatic Passage of Spin Qubits

RICCARDO POROTTI (Presenter), DARIO TAMASCELLI, Dipartimento di Fisica, Università degli Studi di Milano, MARCELLO RESTELLI, Dipartimento di Elettronica, Informazione e Bioingegneria, Politecnico di Milano, ENRICO PRATI, Istituto di Fotonica e Nanotecnologie, Consiglio Nazionale delle Ricerche — Several tasks, involving the temporal evolution of a system of qubits, require stochastic methods to identify the best sequence of gates and the interaction time among qubits. The great success of deep reinforcement learning (DRL) methods to identify the best strategy in problems involving a competition between short and long-term rewards, has suggested its application to quantum information (QI) as well.

To extend the application of DRL to the transfer of QI, we focus on Coherent Transport by Adiabatic Passage (CTAP) on a chain of three semiconductor quantum dots (QDs). This task is usually performed by the so-called counter-intuitive sequence of gate pulses, which can coherently transfer an electronic population from the first to the last site of an odd chain of QDs, leaving the central depopulated.

We apply a technique to find a near-optimal gate pulse sequence without explicitly providing any preliminary knowledge of the underlying physical system to the DRL agent. Using the advantage actor-critic algorithm, with a small neural network as a function approximator, we trained a DRL agent to select the best action during the evolution to achieve the same results previously found only by ansatz solutions. The method naturally extends to systems affected by dephasing and loss.

Controllable Approximations for Spin Qubit Design - Jacob's Ladder of Device Modelling*

ANDRE SARAIVA (Presenter), CHRISTOPHER ESCOTT, Silicon Quantum Computing, UNSW, ANDERSON WEST, ROSS LEON, RUICHEN ZHAO, Univ of New South Wales, HENRY YANG, Silicon Quantum Computing, UNSW, ANDREW STEVEN DZURAK, Univ of New South Wales — Some key quantities for spin qubits - tunnel rates, exchange coupling and electronic correlations in general - are hard to describe within the most commonly adopted approximations. Tunnel rates and the exchange coupling are small corrections to the total electronic energy, so that variational methods often fail to predict these quantities. Electronic correlations can be accurately calculated for few electrons through full CI, for example, but are difficult for many electrons. We discuss some of the limitations of these approaches and how to overcome these with state-of-the-art methods that are controllable. We review two methods to improve the accuracy of these quantities: the Path Integral Monte Carlo method for tunnel rates and exchange coupling; and the Density Functional Theory applied to the effective mass Hamiltonian for the many electron problem. Both methods have controllable approximations that may be systematically improved by enhancing the computational effort.

GPU-Accelerated Simulations of Single and Two Electron-Spin Qubit Operations in Semiconductor Devices.*

HUGO LEPAGE (Presenter), ALEKSANDER LASEK, DAVID ARVIDSSON SHUKUR, CRISPIN BARNES, University of Cambridge — Although experimental physicists can control the output of electron-spin setups in the lab, it is hard to know exactly what happened to the particles during the manipulation. We present GPU-accelerated simulations that provide valuable insights into how a particle behaves while in the metaphorical “black box” that is the experimental device. In particular, we show how the most general measurements can be implemented for dynamic qubits via a POVM protocol. We provide high fidelity simulations of entanglement distillation for electrons carried by surface acoustic waves. Furthermore, we compare two methods for generating entanglement between electron-spin qubits using the power-of-SWAP operation. By using realistic experimental parameters, we show that entanglement generation via electron-electron collisions in a harmonic channel cannot be implemented for multidimensional systems. We provide an alternative by demonstrating that a method based on the exchange energy across a tunnel barrier is more viable than previously thought. These findings pave the way to designing efficient entangling quantum logic gates.

*This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 642688.
Controlling spatial entanglement in interacting two electrons trapped in superlattices

DUNG PHAM (Presenter), SATHWIK BHARADWAJ, YUCHEN WANG, Department of Physics, Worcester Polytechnic Institute, Worcester, MA 01609, L RAMDAS RAM-MOHAN, Department of Physics, Electrical and Computer Engineering and, mechanical engineering, Worcester Polytechnic Institute, Worcester, MA 01609 — Entanglement properties of two-electron systems have been the subject of considerable interest in recent years. Solutions to the Hamiltonian in few-electron systems require special techniques to evaluate computationally demanding Coulomb integrals. Here we develop a fully variational action integral formalism to obtain the coordinate space wavefunctions for two electrons trapped in semiconductor superlattices. The entanglement in such systems have contributions from not only the spin part but also from the spatial correlations of the confining potential. The latter contribution has been neglected in most considerations. We show that the probability distributions of electrons largely deviate from those of the widely-used slater-determinant representation. We demonstrate that the entanglement in such systems can be controlled by varying physical parameters, and by applying external fields. The entanglement resonances associated with anti-crossings of eigenstates are displayed for the first time, and these can be manipulated through geometric changes and by the applied electric field.

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Session Y34 DCMP: The Physics of Computing and Computing with Physics

11:15AM Y34.00001: Digital-Analog Quantum Computing [Invited] MIKEL SANZ (Presenter), University of the Basque Country, Bilbao, Spain — Purely digital classical computers are rather recent devices which are a consequence of the impressive technological development in miniaturization of electronics and microchips. However, until only few decades ago, digital computers had not sufficient computational power for most applications, so they usually employed analog parts for specific hard calculations. The situation nowadays in quantum computing is similar due to the small number of coherent controllable qubits allowed by current platforms. Even doubling the number of qubits yearly, a purely digital approach with error correction will not allow us to solve relevant problems in the following decades. Here, we will explore in detail a universal digital-analog approach employing the ubiquitous Ising Hamiltonian as the resource. We use this global Hamiltonian, together with local rotations, to generate an arbitrary unitary and we find efficient protocols, polynomial in the number of single-qubit rotations, to produce relevant families of Hamiltonian, such as arbitrary two-body Hamiltonians or, in general, k-body Hamiltonians. We introduce the concept of banged digital-analog quantum computing, in opposition to the stepwise, when single-qubit rotations are much faster than the natural time-scale of the Hamiltonian, which allows us to compute without switching on/off the global interaction. Employing natural models of errors, we compare the performance of digital against both stepwise and banged digital-analog protocols showing that, in general, digital-analog approaches perform better both in time and fidelity. Finally, we will also show that this emerging digital-analog approach can be applied not only to quantum simulations, but also to quantum algorithms. Indeed, we provide an efficient digital-analog description of the Quantum Fourier transform, comparing its performance against the pure digital approach in the presence of errors.

11:51AM Y34.00002: The physics and challenges of neuromorphic computing with spintronic nanooscillators [Invited] JULIE GROLLIER (Presenter), CNRS/Thales lab — TBD
12:27PM Y34.00003: MemComputing: leveraging memory and physics to compute efficiently* [Invited] MASSIMILIANO DI VENTRA (Presenter), University of California, San Diego — In this talk I will discuss how to employ memory (time non-locality), in a novel physics-based approach to computation: Memcomputing [1, 2, 3]. As examples, I will show the polynomial-time solution of prime factorization, the search version of the subset-sum problem [4], and approximations to the Max-SAT beyond the inapproximability gap [5], using polynomial resources and self-organizing logic gates, namely gates that self-organize to satisfy their logical proposition [4]. I will also show that these machines are described by a Witten-type topological field theory, and they compute via an instantonic phase, implying that they are robust against noise and disorder [6]. The digital memcomputing machines we propose can be efficiently simulated, are scalable and can be easily realized with available nanotechnology components.


*Work supported in part by MemComputing, Inc. (http://memcpu.com/) and CMRR.

1:03PM Y34.00004: Benchmarking NISQ-era quantum processors [Invited] JAY GAMBETTA (Presenter), IBM Thomas J. Watson Research Center — As the field marches towards quantum advantage with near-term quantum processors, it becomes imperative to characterize, verify, and validate performance. An outstanding scientific challenge in the community is a scalable set of metrics or experiments which can shed light on the usability of a device for near-term algorithms. Moreover, it becomes critical to explore techniques to extend the computational reach of noisy systems, be it through understanding underlying non-idealities, or more efficient circuit compilation. In this talk I will review the work we are doing at IBM to develop a NISQ device and our recent results.

1:39PM Y34.00005: Accelerating Deep Neural Networks with Analog Memory Devices [Invited] CHARLES MACKIN (Presenter), PRITISH NARAYANAN, HSINYU TSAI, STEFANO AMBROGIO, AN CHEN, GEOFFREY W. BURR, IBM Research--Almaden — Over the next few years, special-purpose hardware accelerators based on conventional digital-design techniques will optimize the GPU framework for Deep Neural Network (DNN) computations, increasing speed and reducing power for both “training” and “forward-inference.” During training, DNN weights are adjusted to improve network performance through repeated exposure to the labelled data-examples of a large dataset. During forward-inference, already trained networks are used to analyze new data-examples.

Even after the improved computational performance and efficiency that is expected from these special-purpose digital accelerators, there would still be an opportunity for even higher performance and even better energy-efficiency from neuromorphic computation based on analog memories (including both memristors and Phase-Change Memory).

In this presentation, we discuss the origin of this opportunity as well as the challenges inherent in delivering on it, with some focus on materials and devices for analog volatile and non-volatile memory. We review our group’s work towards neuromorphic chips for the hardware acceleration of training and inference of Fully-Connected DNNs [1-4]. The presentation will discuss the impact of real device characteristics – such as non-linearity, variability, asymmetry, and stochasticity – on performance, and describe how these effects determine the desired specifications for the analog resistive memories needed for this application. We present some novel solutions to finesse some of these issues in the near-term, and describe some challenges in designing and implementing the CMOS circuitry around the NVM array. The talk will end with an outlook on the prospects for analog memory-based DNN hardware accelerators.

11:15AM Y36.00001: Engineering Quantum States of Matter for Atomic Clocks [Invited] JUN YE (Presenter), National Institute of Standards and Technology Boulder — Precise engineering of quantum states of matter and advanced laser technology are elevating the performance of optical atomic clocks to new levels. These increasingly powerful measurement capabilities are promising greater opportunities for probing fundamental and emerging phenomena.

11:51AM Y36.00002: Geodesy and metrology with a transportable optical clock* [Invited] CHRISTIAN LISDAT (Presenter), Physikalisch-Technische Bundesanstalt — The development of optical clocks that can be transported and operated outside metrology laboratories promises exciting new and competitive measurement methods for geodesy, where chronometric levelling is considered as a complementary method to measure height differences [1-4].

To perform such tasks in a competitive way, it is not sufficient to demonstrate the clock performance in the laboratory, but transportable clocks need to show reproducibility of their frequency at the level of few parts in $10^{17}$ and better in the various locations to which they are transported and where they are used.

At Physikalisch-Technische Bundesanstalt (PTB), we have developed such a transportable optical clock [5] that has been tested for the applications described above by measurement campaigns outside the laboratory. I will present results of the measurement campaigns we have performed so far and discuss the perspective of our apparatus for chronometric levelling.

*We acknowledge support by the German Research Foundation (DFG) within CRC 1128 geo-Q, the Marie-Curie Action ITN FACT, and the EMRP project ITOC. The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union.

12:27PM Y36.00003: Geopotential measurements with synchronously linked optical lattice clocks [Invited] MASAO TAKAMOTO (Presenter), RIKEN — The recent progress of optical lattice clocks has improved the accuracies to $10^{-18}$, which outperforms the realization of the SI second. We will present the development of the optical lattice clocks and their applications in geodetic measurements.

1:03PM Y36.00004: Atomic clock performance beyond the geodetic limit* [Invited] ANDREW LUDLOW (Presenter), National Institute of Standards and Technology Boulder — We present recent updates in the development of optical lattice clocks, with particular emphasis on systems using ultracold ytterbium. Over the last several years, the intersection of quantum control, optical coherence, and precision measurement has afforded substantial progress in the development of these clock systems. Measurements can now reach $10^{-18}$ precision or better, at a level capable of beyond state-of-the-art geodesy through determination of the gravitational redshift. We will highlight a variety of Yb clock measurement campaigns that have recently been carried out, including optical frequency ratio measurements with other optical clocks. These measurements are analyzed in the context of beyond-Standard-Model physics, such as fundamental constant variation and dark matter searches. Finally, we will discuss prospects for continued improvements and future measurement applications.

*NIST, DoD, NASA, DARPA
Two clock transitions in neutral Yb for the highest sensitivity to variations of the fine-structure constant

Invited: MARIANNA SAFRONOVA (Presenter), SERGEY G PORSEV, University of Delaware, CHRISTIAN SANNER, JUN YE, JILA, NIST and University of Colorado, Boulder — We propose a new frequency standard based on a $4f^{14} \, 6s6p \, ^3P_0 \rightarrow 4f^{13} \, 6s2 \, 5d \, (j=2)$ transition in neutral Yb [1]. This transition has a potential for high stability and accuracy and the advantage of the highest sensitivity among atomic clocks to variation of the fine-structure constant $\alpha$. We find its dimensionless $\alpha$-variation enhancement factor to be $K=-15$, in comparison to the most sensitive current clock (Yb$^+$ E3, $K=-6$), and it is 18 times larger than in any neutral-atomic clocks (Hg, $K=0.8$). Combined with the unprecedented stability of an optical lattice clock for neutral atoms, this high sensitivity opens new perspectives for searches for ultralight dark matter and for tests of theories beyond the standard model of elementary particles. Moreover, together with the well-established $^1S_0 \rightarrow ^3P_0$ transition one will have two clock transitions operating in neutral Yb, whose interleaved interrogations may further reduce systematic uncertainties of such clock-comparison experiments.


Friday, March 8, 2019 11:15 AM - 1:51 PM

Session Y39 GMAG DMP: Magnetic Sensors, Devices, and Applications  

11:15AM Y39.00001: PicoTesla Magnetic Sensors based on Magnetic Tunneling Junctions with Double-staged Flux Concentrators*  
GUANYANG HE (Presenter), YIOU ZHANG, LIJUAN QIAN, GANG XIAO, Brown University, QIANG ZHANG, J. CARLOS SANTAMARINA, TADEUSZ W. PATZEK, XIXIANG ZHANG, King Abdullah University of Science and Technology — Highly sensitive magnetic tunneling junction (MTJ) sensors have shown great potential as the best miniaturized, low-cost, solid-state magnetic sensors, strongly needed in different applications. We have fabricated high performance MTJ sensors and pushed the magnetic sensing limit to a high level, mainly by incorporating double-staged magnetic flux concentrators (MFC), one on the MTJ chip level and the other on a macroscopic level, to amplify the external field. After multiple optimizations on MFC fabrication conditions, it has increased the sensitivity of the MTJ sensor by a large factor of 517 to 775.4%/Oe in terms of magnetoresistance response. The sensor coercivity is only 0.12 Oe which is desired for sensing application, as we will show that the low-field detectability of magnetic sensor have direct relations with its coercivity. By integrating such MTJ sensors from wafers to integrated circuits, our sensor prototype has achieved detectable field limit of 30pT per root hertz at 10 kHz. We will also present the noise spectrum and the sensitivity spectrum of it and discuss its detectabilities based on these information.

*The work was supported by National Science Foundation through Grants No. DMR-1307056, and by King Abdullah University of Science and Technology (KAUST).

11:27AM Y39.00002: Circumventing Magnetostatic Reciprocity: a Diode for Magnetic Fields*  
JORDI PRAT-CAMPS (Presenter), University of Sussex, PATRICK MAURER, GERHARD KIRCHMAIR, ORIOL ROMERO-ISART, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences — Lorentz reciprocity establishes a stringent relation between electromagnetic fields and their sources. For static magnetic fields, a relation between magnetic sources and fields can be drawn in analogy to Green's reciprocity for electrostatics. So far, the magnetostatic reciprocity principle remains unchallenged and the magnetostatic interaction is assumed to be symmetric (reciprocal). Here we show that a linear and isotropic electrically conductive material moving with constant velocity is able to circumvent the magnetostatic reciprocity principle and realize a diode for magnetic fields. This result is demonstrated by measuring an extremely asymmetric magnetic coupling between two coils that are located near a moving conductor. The possibility to generate controlled unidirectional magnetic couplings implies that the mutual inductances between magnetic elements or circuits can be made extremely asymmetric. Other strategies to break magnetic reciprocity based on novel kinds of magnetic metamaterials will be also discussed.

*This work is supported by the European Research Council (ERC-2013-StG 335489 QSuperMag), the Austrian Federal Ministry of Science, Research, and Economy (BMWF) and the European Union’s Horizon 2020 research and innovation programme (grant agreement No 737087).
11:39AM Y39.00003: picoTesla Magnetoelectric Sensors with Low-Curvature Nano-Plate Resonators  ALEXEI
MATYUSHOV (Presenter), Physics/Electrical and Computer Engineering, Northeastern University, ZHENYUN QIAN, MOHSEN
ZAEIMBASHI, CHENG TU, HUAIHAO CHEN, MENGHUI LI, MATTEO RINALDI, NIAN XIANG SUN, Electrical and Computer
Engineering, Northeastern University — Prior studies have shown the effectiveness of piezoelectric/magnetostrictive MEMS
magnetometers featuring a nano plate resonator and using the ΔE effect for highly sensitive detection of DC magnetic
fields. By monitoring changes in resonance frequency from applied magnetic fields, a sensitivity of a few Hz/nT has been
achieved in unshielded lab environments. With dimensions of ≤ 200 μm across, and < 1 μm thick, these devices offer the
advantages of small scale, including portability and low power consumption, as well as high spatial resolution in sensor
arrays. However, a thorough understanding of magnetic properties and other performance aspects in these
magnetometers has not been developed. In this study we report on the strong effects of resonator plate curvature on
sensor performance. It was found that the total resonance frequency shift dropped off exponentially with increasing
curvature by as much as two orders of magnitude. By fabricating a ΔE effect magnetometer with low curvature in the nano
plate resonator, we achieved maximum magnetic field sensitivity of 4.98 Hz/nT. High frequency stability was also
observed: an Allan deviation measurement yielded a minimum of 0.0245 Hz at 100 ms averaging time. This results in a
theoretical limit of detection of 1.56 pT/Hz1/2.

11:51AM Y39.00004: Brain MRI at ultra-low field: new multifunction instrument  KOOS C J ZEVENHOVEN (Presenter),
Aalto University — While conventional MRI uses increasingly high magnetic fields, another approach has emerged, where
the signal is detected in an ultra-low field (ULF) on the order of Earth’s field. Despite similarities, ULF-MRI differs from high-
field MRI in interesting ways. At ULF, the magnetic pulses can be applied silently and with an open-geometry coil system,
and the signal can be modeled from theory with high accuracy. The unique possibilities of ULF-MRI also include the
combination of MRI and magnetoencephalography (MEG), the measurement of the weak magnetic fields generated by
brain activity. ULF-MRI and associated methods such as current-density imaging (CDI) improve the localization of brain
activity.

Superconducting quantum-interference devices (SQUIDs) configured as pulse-tolerant sensors for ULF-MRI can also be
used for MEG. Compared to our first hybrid prototype, our current-generation system uses more robust techniques and
new software. Our dedicated amplifiers allow switching off even \( B_0 \) even during an imaging sequence, enabling the
encoding of 3D information for current-density imaging (CDI). We demonstrate the state of the art of ULF-MRI and
describe Dynamical Coupling for Additional dimensioNs (DynaCAN) – designing pulse waveforms to couple to a dynamical
system with memory.

12:03PM Y39.00005: Finite element study on magnetomechanical properties of magnetorheological elastomer
used in advanced mechanical systems.  WINNIE KIARIE (Presenter), NEELAM PRABHU GAUNKAR, DAVID C JILES, Iowa State
University, EDWARD BARRON, Dept., of Materials Science and Engineering, Iowa State University, MICHAEL D. BARTLETT, Dept. of
Electrical and Computer Engineering, Iowa State University — Magnetorheological Elastomers (MREs) constitutes a group of
materials referred to as ‘smart’ materials. These materials exhibit field-dependent material property which include change
in damping and stiffness properties of the material when subjected to an external magnetic field. This paper presents a
simulation study of magnetomechanical and thermal properties for a MRE used as a semi-active automotive suspension
bushing. Such suspension bushings isolate passengers from the undesirable effects of the surface over which the vehicle
is being driven on. It also enhances handling and driving comfort of the driver. The performance of semi-active suspension
bushing is highly dependent on the magnetic properties of the MRE. Therefore, electromagnetic simulation using finite
element analysis software is used to design and optimize on the MRE suspension bushing's response to magnetic field.
From the finite element analysis, the magnetic flux density developed within the MRE is observed to depend on the
permeability, thickness and magnetic shielding of the MRE.
Highly Sensitive Magnetic Sensor based on Magnetoelcetric Effect and Cross-Modulation Technique  
CUNZHENG DONG (Presenter), YIFAN HE, XIANFENG LIANG, HUAIHAO CHEN, YUYI WEI, NIAN XIANG SUN, Northeastern University — State of the art bulk magnetoelastic (ME) sensors composed of Metglas/PMN-PT fiber structures have been demonstrated to exhibit a low limit of detection (LOD) of 10 pT at 1 Hz. Because of the low cost and compact size, the ME magnetic field sensor has become competitive to other sensing technologies for applications demanding high sensitivity. The magnetic noise of ME sensors is the key parameter that results from the internal and external noise sources. To reduce the noise level, an active operation mode has been proposed. However, active ME sensors usually show a high magnetic noise over 200 pT/Hz at 1 Hz in the reports. Here, we demonstrate an ultra-sensitive ME sensors based on Metglas/PZT fiber heterostructures operating at the complete demagnetized state of Metglas. A strong correlation was observed between the limit of detection and the degree of demagnetization of Metglas in the ME sensors, which points to a new way of improving the magnetic field sensitivity of ultra-sensitive ME sensors. Our demonstrated ME sensors based on PZT/Metglas has shown LOD below 2pT and magnetic noise level of 9.1pT/Hz^{1/2} in the detection of magnetic field at 1Hz, which is one order of magnitude better than other best reported values for PZT/Metglas heterostructures.

Fabrication and characterization of ultra-soft PDMS based magnetorheological elastomers*  
ANDY CLARK (Presenter), JIAJIA LI, LILA HERNANDEZ, VIDYA RAMASWAMY, Bryn Mawr College, ELISE CORBIN, Cardiovascular Institute, Perelman School of Medicine, University of Pennsylvania, ALEXANDER BENNET, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, XUEMEI CHENG, Bryn Mawr College — Magnetorheological elastomers (MREs) are composite materials consisting of an elastomer matrix with embedded micro- or nano- sized ferromagnetic entities. Ultra-soft PDMS based MREs are promising candidates for dynamic cell culture substrata. In this work, we report the fabrication and magnetic characterization of PDMS based MREs. Sylgard 527 and carbonyl iron powder were mixed together at various ratios and cured at 60°C for 24 hours without applied magnetic field and with applied magnetic field of various field strength. Angular dependent magnetic hysteresis loops of MREs were measured using a vibrating sample magnetometer. MREs cured without magnetic field show no angular dependence in the major hysteresis loop, consistent with the isotropic distribution of iron particles in the MREs. Instead, hysteresis loops for MREs cured in magnetic field clearly display anisotropy as expected. The different first order reversal curve (FORC) distribution characteristics of the isotropic and anisotropic MREs agree with the structural difference of these two types of MREs.

A one-dimensional magnetoelectric sensor array for magnetic sketching*  
ZHAOQIANG CHU (Presenter), WEILIANG SHI, Peking University, XIANFENG LIANG, NIAN XIANG SUN, College of Engineering, Northeastern University, SHUXIANG DONG, Peking University — Although various magnetic sensors have been developed, it is still a challenge to get the imaging of magnetic objects safely and instantaneously, for example, magnetic imaging for capsule positioning, endoscope navigation, and detection of magnetic weapon that is hidden in/on human body. In this paper, a magnetic detecting and sketching system utilizing a one-dimensional magnetic sensor array with 56 magnetoelectric (ME) sensing units is proposed. The ME sensors used in this system are based on a (1-1) connectivity Metglas/piezo-fiber composite operating in longitudinally magnetized and transversely poled (L-T) mode. Simulation and experiment results show that the proposed magnetic detecting system not only can find the 2-D position of a running magnetic metal object, but also can identify its posture and length-diameter ratio. The proposed magnetic detecting method promises an outlook for medical magnetic positioning and security checking.

*This work was supported by the National Natural Science Foundation of China (Grant Nos. 51132001, 51072003) and The Beijing Municipal Science and Technology Projects (Grant Nos. Z131100003213020, Z151100003715003).
12:51PM Y39.00009: Superparamagnetic Fe₃O₄ magnetic nanoparticles and their potential for hyperthermia treatment for cancer* BIANCA PAOLA MENESES BRASSEA (Presenter), CAMILLE CYR, ISRAEL MARTINEZ, CRISTIAN BOTEZ, AHMED EL-GENDY, Physics Department, University of Texas at El Paso — The heating efficiency of Fe₃O₄ nanoparticles of different sizes synthesized using supercritical conditions of liquids, under different applied magnetic field intensities and frequencies, was investigated through experimental measurements of specific absorption rate (SAR). The synthesis conditions have been varied in order to obtain different sizes and shapes of Fe₃O₄ nanoparticles and to examine their effect on the SAR values. The morphology and crystal structure characterization of three samples revealed cubic-like shapes with average sizes of 63, 128, and 91 nm and formation of FCC Fe₃O₄ phase structure. The magnetic properties were characterized using magnetization dependent of magnetic field and temperature up to 3 T and 400 K respectively. The samples exhibit superparamagnetic-like behavior at room temperature with saturation magnetization Ms of 108, 74, and 77 emu/g and blocking temperatures Tₜ of 320, 235, and 192 K, respectively. SAR values at 400 Oe and 304 kHz were measured using D5 hyperthermia system to be 126, 33 and 73 W/g for sizes of 63, 91, and 128 nm, respectively. The results yield efficient heating and the nanoparticles perfect feasibility for magnetic hyperthermia treatment of cancer.

*Authors acknowledge the support from UTEP startup and Rising stars funding.

1:03PM Y39.00010: Preparation and Investigation of Carbon Coated (Fe-Fe₃C) Nanocomposites for Medical Applications* ARAM MANUKYAN, HARUT GYULASARYAN, EDUARD SHAROYAN, Laboratory of Solid State Physics, Institute for Physical Research, NAS of Armenia, Ashtarak-2, JENNIFER GRAY LYNN, Materials Characterization Lab, The Pennsylvania State University, Materials Research Institute, OSCAR BERNAL, ARMEN KOCHARIAN (Presenter), Physics Department, California State University, Los Angeles 90032 — Carbon-coated ferromagnetic (Fe-Fe₃C) nanocomposites have been synthesized via solid-phase pyrolysis of metal-organic compounds. Structure, morphology and magnetic characteristics of the nanocomposites were investigated by electron microscopy, X-ray diffraction, Raman spectroscopy, STEM-TEM images, EDX line-scan profiles and magnetometry. The magnetic characteristics such as saturation magnetization, coercivity and heating saturation as well as the specific absorption rate (SAR) make these materials attractive for magnetic hyperthermia applications. Hysteresis loop of the (Fe-Fe₃C)@C nanocomposites is of special interest as it shows almost square-like behaviour, where Mₛ/M(200 Oe) = 0.75. The limitation of the magnetic field amplitude and - frequency (H x f) ≤ 10.625x10⁶ Oe/s makes this factor important that provides a high energy absorption even in case of low magnetic fields.

*This work was supported by a grant from the Russian-Armenian (Slavonic) University at the expense of the Ministry of Education and Science of the Russian Federation. The work at CSULA was supported by the National Science Foundation-Partnerships for Research and Education in Materials under Grant DMR-1523588.

1:15PM Y39.00011: Ultrathin cobalt nanowires with high energy product MEIYING XING (Presenter), JEOTIKANTA MOHAPATRA, JACOB ELKINS, JULIAN BEATTY, J PING LIU, physics, university of texas at arlington — Uniform and single crystalline hexagonal close-packed (hcp) Co nanowires (NWs) have been synthesized by optimizing the precursor concentration and cleaning process in a hydrothermal process. The TEM image indicates that the prepared Co NWs have uniform size distribution with a mean diameter and length of 8 nm and 150 nm, respectively. As the radius of the Co NWs is smaller than coherent radius $R_{coh} = 3.65 l_{ex}$, where $l_{ex}$ is the exchange length, the ultrathin Co NWs exhibit the coherent magnetization reversal based on the Stoner-Wohlfarth mode. As a result, a pronounced coercivity of 11.4 kOe is achieved in the aligned Co NW assemblies. The high aspect-ratio, good crystallinity, uniform morphology and desired orientation of Co NW assemblies result in a record high energy product of 56.1 MGOe which is close to the theoretical value. The compaction of the prealigned NWs assemblies at various pressure results in packing density in the range from 5.3 to 7.3 g/cm³ and energy product as high as 20 MGOe. The obtained nanowire based permanent magnets with well controlled aspect ratios exhibited energy products in the intermediate range between Alnico and rare-earth containing magnets.

1:27PM Y39.00012: Search for the new rare-earth free iron-based permanent magnets*  OLGA VEKILOVA (Presenter), OLLE ERIKSSON, HEIKE C. HERPER, Uppsala University — Permanent magnets are irreplaceable for many technological applications. Therefore new magnetic materials, that are cheap and abundant, are vital for the modern society. A good permanent magnet must have a high Curie temperature, high saturation magnetization and uniaxial magnetocrystalline anisotropy. Rare-earth free Fe-rich systems like the hexagonal close-packed Fe3Sn compound are promising candidates. However, its magnetocrystalline anisotropy is planar. Alloying is a possibility for changing the easy axis of magnetization. We have calculated from first principles the electronic structure and magnetic properties of ferromagnetic Fe3Sn doped with Si, P, Ga, Ge, As, Se, In, Sb, Te, Pb, and Bi on the Sn sublattice as well as with the Mn phase-stabilizer on the iron sublattice. We discuss the influence of the different dopants on the magnetocrystalline anisotropies and Curie temperatures of Fe3Sn and suggest new stable/metastable ferromagnetic phases with uniaxial anisotropy suitable for the development of advanced permanent magnets.

*Authors acknowledge support from NOVAMAG project, under Grant Agreement No. 686056, EU Horizon 2020 Framework Programme.

1:39PM Y39.00013: High-Performance Thick On-chip Hard Magnets for MEMS Applications  YIFAN HE (Presenter), CHENGJU YU, Electrical and Computer Engineering, Northeastern University, SAMER HAIDER, Analog Devices, Inc., MOHSEN ZAEIMBASHI, Electrical and Computer Engineering, Northeastern University, GREGORY STEPHEN, Department of Physics, Northeastern University, JIAWEI WANG, YUIYI WEI, HUAIHAO CHEN, XIANFENG LIANG, CHENG TU, CUNZHENG DONG, Electrical and Computer Engineering, Northeastern University, DON HEIMAN, Department of Physics, Northeastern University, BAOXING CHEN, Analog Devices, Inc., NIAN XIANG SUN, Electrical and Computer Engineering, Northeastern University — We adopted two methods for thick on-chip hard magnets fabrication for MEMS application. (1) Dry packing of Nd2Fe14B powders. Nd2Fe14B powders were mixed with binder wax powders, then dry-packed into pre-etched trenches on silicon wafers under 10 MPa pressure and 100°C heating. An out-of-plane, in-situ magnetic field of 1000 Oe was applied during the process. (2) High pressure compression of Nd2Fe14B powders. Nd2Fe14B powders were packed into a metal mould and heated to 300°C with 850 MPa pressure applied. The sample was bonded onto the silicon chip with polyimide. The dry-packed Nd2Fe14B magnets showed a remanent out-of-plane magnetization of 330 emu/cc (Br = 0.42 T), a coercive field of 8.6 kOe (690 kA/m) and an energy product of 2.4~2.6 MGOe (19-21 kJ/m^3). It is also found that the out-of-plane magnetic field can boost the remanent magnetization in that direction. For high pressure compressed Nd2Fe14B magnets, a remanent out-of-plane magnetization of 446 emu/cc (Br = 0.56 T), a coercive field of 9.6 kOe (770 kA/m) and an energy product of 6.4 MGOe (50.5 kJ/m^3) were observed. Our demonstrated Nd2Fe14B on-chip hard magnets are compatible to MEMS fabrication process with a larger thickness of over 1mm and higher achieved energy product over published results for on-chip magnets.

Friday, March 8, 2019 11:15 AM - 1:51 PM

Session Y41 GMAG DMP: Magnetic Materials, Not Oxides  BCEC 209 - Patrick Quarterman, National Institute of Standards and Technology - Tag(s): Focus

11:15AM Y41.00001: Exploring the Magnetic Properties of the Iron-Nitrogen System+  TODD MONSON (Presenter), TYLER STEVENS, STAN ATCITTY, Sandia National Laboratories, BAOLONG ZHENG, YIZHANG ZHOU, ENRIQUE Lavernia, University of California, Irvine — The magnetic properties of the iron-nitrogen system have only been explored on a very limited basis. Theoretical predictions of the magnetic behavior of the different phases of iron nitride are limited and experimental data is quite sparse. By employing several different techniques which include solution based nanoparticle nitridation, electrochemical methods, and metathesis based reactions we have synthesized several different phases of iron nitride: FeN, Fe3N, Fe2N, Fe8N, and Fe24N10. Additionally, we have demonstrated a path for consolidating raw powders of iron nitride into bulk material, enabling additional characterization and application in macroscopic devices. Our difficulties and successes in synthesizing and processing these different phases of iron nitride will be described. Additionally, the magnetic properties of these seldom explored iron-nitrogen compounds will be summarized.

+Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
11:27AM Y41.00002: Mn-based Heusler Compounds with Low Magnetization* WENYONG ZHNAG, BALAMURUGAN BALASUBRAMANIAN, RABINDRA PAHARI, AHSAN ULLAH, SHAH VALLOPPILLY, RALPH SKOMSKI, DAVID SELLMYER (Presenter), Nebraska Center for Materials and Nanoscience and Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588-0299, USA — Heusler compounds with small or zero magnetization are of interest for spintronics applications, because they cause little or no fringing fields and may exhibit ultrafast dynamics and high spin polarization [1-3]. We find virtually zero room-temperature magnetizations in stoichiometric Ru$_2$MnSn and Pt$_2$MnGa Heusler alloys fabricated by rapid quenching from the melt. X-ray diffraction patterns show the formation of a $L_2_1$ structures with $a = 6.22$ Å and a tetragonal structure with $a = 4.02$ Å and $c = 7.24$ Å in Ru$_2$MnSn and Pt$_2$MnGa, respectively. Both systems show nearly linear $M(H)$ curves for intermediate field strengths of several T, and the slopes $dM/dH$ are used to characterize the spin structure. In Pt$_2$MnGa, which shows a helical spins structure with an ordering temperature of about 350 K [4], $dM/dH$ increases with decreasing spiral wave vector $q$. The complex spin structures of Ru$_2$MnSn and Pt$_2$MnGa are used to explain the electron-transport properties of the alloys.

References

*This research is supported by the NSF-DMREF: SusChEM (1729288) and NSF-NNCI (1542182) and NCMN-NRI.

11:39AM Y41.00003: First principles study on alkali-metal-based half-Heusler XCrZ ([X = Li, Na, K, Rb]; [Z = As, Sb]) THU THUY HOANG (Presenter), SUNG-HYON RHIM, SOON CHEOL HONG, Physics, The university of Ulsan — In this works, we present systematic study of strain effects on half-metallicity (HM) of alkali-metal-based half-Heusler XCrZ ([X=Na, K, Rb]; [Z=As,Sb]) using first-principles calculations. Among three structural phases α, β and γ, we focus on the β-phase, which is energetically most stable and compatible with zinc-blende (zb) structured CrAs and CrSb. Except LiCrZ, all compounds are HM, where the total magnetic moments per unit cell are 4 µB, obeying the modified Slater-Pauling rules ($M = N_v - 8$) [1]. In LiCrZ, on the other hand, HM emerges under tensile strain. Furthermore, HM and direct vs indirect band gap of XCrZ are investigated for different cation [X]$^+$, for strains. While uniform strain, hydrostatic limit, impacts little on the band gap, tetragonal distortion associated with sin-plane tensile strain influences valence band maximum of LiCrZ. In particular, indirect to direct gap transition occurs for tensile strain larger than 2% in LiCrSb, where the role of p-d hybridization is discussed.


11:51AM Y41.00004: Disorder and electron correlation effects in the ground state of Ni-Co-Mn-Sn alloys with Heusler structures* AKI PULKKINEN (Presenter), Physics, LUT (Finland), BERNARDO BARBIELLINI, Physics, LUT and Northeastern Univ., JOHANNES NOKELAINEN, Physics, LUT (Finland), VLADIMIR SOKOLOVSKIY, VASILIY D. BUCELNIKOV, MIKHAIL ZAGREBIN, Chelyabinsk State University, Chelyabinsk, Russian Federation, KATARIINA PUSSI, ERKKI LAHDERANTA, Physics, LUT (Finland), ALEXANDER GRANOVKY, Physics, Moscow State University, Moscow, Russian Federation — We consider ab-initio calculations of Co-doped Ni-Mn-Sn shape memory alloy. The Co doping leads to a decrease in both the martensitic transformation temperature and the Curie temperature of martensite and to an increase in the Curie temperature of austenite. Besides, large magnetisation changes occur in the vicinity of structural transformation. As a result, the tuning of Co and Mn contents can lead to favorable magnetocaloric properties . In this work, we focus on the effect of atomic disorder and electron correlation on the structural, magnetic and electronic properties of Ni-Co-Mn-Sn systems by using the Density Functional Theory (DFT) implemented in the VASP and SPR-KKR packages within a 32-atom supercell and the coherent potential approximation, respectively. The optimized atomic positions for compositions studied are obtained by the USPEX package. To study the effect of exchange-correlation, a series of ground state calculations were performed using both the GGA-PBE functional and Meta-GGA with SCAN functional of DFT.

* B.B. acknowledges support from the COST Action CA16218
12:03PM Y41.00005: Tuning magnetic anisotropy in the layered mixed halide series CrCl$_{3-x}$Br$_{x}$*  
FAZEL FALLAH TAFTI (Presenter), MYKOLA ABRAMCHUK, SAMANTHA JASZEWSKI, KENNETH METZ, GAVIN B OSTERHOUDT, YIPING WANG, KENNETH BURCH, Boston College — Magnetic anisotropy is the tendency of spins to align in a certain crystallographic direction - the easy axis. Without anisotropy, thermal fluctuations prevent magnetic ordering in two dimensions according to the Mermin-Wagner theorem. In layered materials, the two limits of the easy axis are in-plane (XY) and out-of-plane (Ising). Recent advances in exfoliation and device fabrication have led to the discovery of ferromagnetic ordering with Ising anisotropy in CrI$_3$ monolayers. It is theoretically conjectured that spin-orbit coupling (SOC) provided by halide atoms on the super-exchange path yields the magnetic anisotropy. Here, we design a unique experiment to probe this idea by growing a series of CrCl$_{3-x}$Br$_{x}$ crystals where SOC is tuned between CrCl$_3$ with XY and CrBr$_3$ with Ising anisotropy. We discover a continuous rotation of the easy-axis from XY to Ising with increasing x. Remarkably, the magnetic ordering temperature, optical gap, and inter-layer spacing are also tuned linearly with x. This is the first observation of a continuous rotation of the easy axis and the effect of SOC on the super-exchange path. Methods presented here can be extended to produce other metal mixed halides to fabricate tunable heterostructures and spintronic devices.

*This work was supported by DMR-1708929.

12:15PM Y41.00006: Tuning the magnetic properties of NiBr$_2$ with cobalt doping*  
HASITHA SURIYA ARACHCHIGE (Presenter), Department of Physics & Astronomy, University of Tennessee, Knoxville, TN 37996, USA, BINOD RAI, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, GANESH POKHAREL, Department of Physics & Astronomy, University of Tennessee, Knoxville, TN 37996, USA, ANDREW MAY, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, ADAM ACZEL, TRAVIS J WILLIAMS, MATTHIAS D FRONTZEK, Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, CRISTIAN BATISTA, Department of Physics & Astronomy, University of Tennessee, Knoxville, TN 37996, USA, DAVID GEORGE MANDRUS, Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA, ANDREW D CHRISTIANSON, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — The compound NiBr$_2$ crystallizes in the trigonal space group R-3m. Below $T_N$= 44 K, NiBr$_2$ exhibits antiferromagnetic order characterized by antiferromagnetically stacked sheets of ferromagnetically aligned Ni spins. A transition to a helical magnetic structure occurs below $T_C$=22.8 K with a propagation vector of at 4.2 K. Here we use neutron diffraction to study the tuning of the magnetic properties with cobalt substitution in single crystals for several compositions of Ni$_{1-x}$Co$_x$Br$_2$, where x = 0, 0.2, 0.25, 0.3, and 0.45. Our measurements show that the $T_N$ decreases with doping while changes in $T_C$ are more subtle. The neutron scattering studies further reveal that the 6 incommensurate spots in the parent compound give way to a ring of magnetic scattering reminiscent of that observed previously for Ni$_{0.92}$Zn$_{0.08}$Br$_2$.

*This work was supported by U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division and the Gordon and Betty Moore Foundation’s EPIQS Initiative.

12:27PM Y41.00007: Eu-Si nanowires formation on Si(100) studied by scanning tunneling microscopy and spectroscopy*  
AARON WANG (Presenter), TE-YU CHIEN, University of Wyoming — By depositing Eu onto a cleaned Si(100) surface at 400 °C, patterned nanowires are formed and visualized by scanning tunneling microscopy(STM). The nanowires are measured to be ~1.5 nm in diameter, ~1 Å in height and hundreds of nm or more in length. The spacing between the nanowires are found to be mostly 2.2 nm, 2.8 nm and 3.4 nm, i.e. with 0.6 nm increment. Interestingly, the topography images taken at positive and negative bias show single-wire and double-wire morphologies, respectively. Same observations are made in the $dI/dV$ mapping with positive and negative bias. Furthermore, $dI/dV$ spectra taken at the double-wire features (found while scanning at negative bias) exhibit peak-valley features in the valence band - a peak at -3.2 V and valley at -3.4 V. Similar peak-valley $dI/dV$ spectra were reported for the Pt/Si nanowires, which showed signs of strong Rashba spin splitting [1]. Further studies are underway in determining the possibility of strong Rashba effect in this Eu/Si nanowire systems.


*This work is financially supported by the U.S. National Science Foundation, Division of Materials Research (DMR) (Grants No. DMR-1710512).
Effect of Bi addition on the magnetic and structural properties of chemically synthesized Fe-Pt-Ni alloy

VIMAL DEEPCHAND (Presenter), FRANK M ABEL, University of Delaware, VASILEIOS TZITZIOS, Department of Chemical Engineering, Khalifa University of Science and Technology, GEORGE C HADJIPANAYIS, University of Delaware — L10 FePt has been chosen as the ideal candidate for heat assisted magnetic recording media due to its high magnetocrystalline anisotropy of ~70 Merg/cc, and thermal stability down to 3 nm [1]. Producing L10 alloys with high thermal stability, while reducing the Curie temperature is critical for the development of heat assisted magnetic recording media, and has led to the exploration of third element doping into the L10 FePt [2]. In this work, we studied the effect of bismuth addition on chemically synthesized FePt1-xNiₓ alloys, with x=0.2 – 0.4. The as-made particles showed an fcc structure, but after annealing at 700°C for 30 minutes a transformation to the L10 phase occurred. The addition of Bi appears to enhance the ordering of the L10 alloy relative to the ternary Fe-Pt-Ni but leads to the formation of a secondary phase. Thermomagnetic measurements show a reduction in Curie temperature compared to the Fe-Pt-Ni ternary alloy in the x=0.3 case, which suggests that Bi enters the structure of the L10 alloy. Current efforts are focused on varying the Bi content to optimize the magnetic and structural properties of Fe-Pt-Ni.


Concentration tuned tetragonal strain in alloys: application to magnetic anisotropy of FeNi1-xCox

ALEX WYSOCKI (Presenter), MANH CUONG NGUYEN, Ames Laboratory, Ames, USA, ANDREY POSTNIKOV, Universite de Lorraine, Metz, France, VLADIMIR ANTOPROV, Ames Laboratory, Ames, USA — We explore an opportunity to induce and control tetragonal distortion in materials using the ideas of Bain transformation path for multatomic systems with body- and face-centered symmetries. The concept is illustrated in the case of FeNi1-xCox magnetic alloy formed by substitutional doping of the L10 FeNi magnet with Co. Using electronic structure calculations we demonstrate that the tetragonal strain in this system can be controlled by concentration and it reaches maximum around x = 0.5. This finding is then applied to create a large magnetocrystalline anisotropy in FeNi1-xCox system. We demonstrate that this anisotropy can be significantly improved by delicate tuning the tetragonal distortion, electronic concentration and chemical anisotropy. We discuss possible experimental ways to create such magnet.

This work was supported by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy

Magnetic and Structural Properties of Melt-Spun Co-Ge Ribbons

ONUR TOSUN (Presenter), FRANK M ABEL, Physics and Astronomy, University of Delaware, BALAMURUGAN BALASUBRAMANIAN, RALPH SKOMSKI, DAVID SELLMYER, Physics & Astronomy, University of Nebraska, Lincoln, GEORGE C HADJIPANAYIS, Physics and Astronomy, University of Delaware — The Co-Ge materials is a key subsystem of Heusler alloys and have attracted much interest because they play an important role in the field of integrated circuits [1, 2]. In this work, we have investigated the magnetic and structural properties of Co-Ge melt-spun ribbons in an attempt to understand better the behavior of our Co2Ge nanoparticles prepared by the cluster-beam deposition technique. Melt-spun ribbons with different compositions and different wheel speeds were prepared. Our data showed that small variations in the Co content and wheel speed lead to different structures and magnetic properties. The ribbons with 65% Co composition are ferromagnetic at room temperature with Curie temperatures larger than 800 K in contrast to previous reports that claimed to be ferromagnetic at cryogenic temperatures [3]. The contradiction with the literature could be attributed to the difference in grain size in the ribbons and can explain the effect of size on the magnetic properties of our nanoparticles.


This work was supported by DOE Grants DE-FG02-90ER45413 and DE-FG02-04ER4612
magnetization is observed, but is consistent with a NixPy or spin-canted shell ~1 nm thick.

CHRIS LEIGHTON, Chemical Engineering and Materials Science, University of Minnesota — Recent advances in colloidal synthesis pathways have shown very similar kinetics, unless the intermediate substrate was consumed by an additional biocatalytic intermediate substrates or presence of an external magnetic field. The biocatalytic reactions proceeded through bulk solution performing biocatalytic cascades in two different states, solute suspension or aggregated, produced in the absence or functionalized with various enzymes (amyloglucosidase, glucose oxidase and horseradish peroxidase) were used to reconcile differences between the true mean blocking temperature, \( T_B \), and the zero field cooled magnetization peak. The resulting \( T_B \) vs. \( D \) yields an effective anisotropy surprisingly close to that of bulk Ni. Reduced saturation magnetization is observed, but is consistent with a Ni_{33}\% type or spin-canted shell ~1 nm thick.

*We acknowledge support from NSF-DMR#1809800 and NIH-NIBIB Trailblazer#1R21EB027405-01.  

1:27PM Y41.00012: Quantitative size-structure-magnetic property relationships in thoroughly-characterized metallic Ni nanoparticle assemblies* 

JOSEPH BATLEY (Presenter), MY NGUYEN, ISHITA KAMBOJ, Chemical Engineering and Materials Science, University of Minnesota, ERAY S. AYDIL, Chemical and Biomolecular Engineering, NYU Tandon School of Engineering, CHRIS LEIGHTON, Chemical Engineering and Materials Science, University of Minnesota — Recent advances in colloidal synthesis and other approaches have realized nanoparticles(NPs) with controlled structure, size, functionalization, and self-assembly. In magnetism, the focus on hard ferromagnetic(FM) NPs and oxides has left relatively little research on metallic soft FM NPs. Here, Ni NPs have been synthesized via injection of a Ni-oleylamine(OAm) complex into 200°C trioctylphosphine(TOP). Size control was obtained by varying TOP/OAm ratio, reaction time, and by differential centrifugation. Characterization was performed with X-ray diffraction, transmission electron microscopy, Raman and Fourier-transform infrared spectroscopy, and SQUID magnetometry. Polycrystalline FCC NPs are obtained, with mean diameter, \( D \), tunable from 4—22 nm, and dispersion, \( \sigma/D \approx 10-30\% \). Superparamagnetic blocking can thus be tuned between 15 and >300 K. Size distributions and inter-particle interactions are explicitly accounted for, quantitatively reconciling differences between the true mean blocking temperature, \( T_B \), and the zero field cooled magnetization peak. The resulting \( T_B \) vs. \( D \) yields an effective anisotropy surprisingly close to that of bulk Ni. Reduced saturation magnetization is observed, but is consistent with a Ni_{33}\% type or spin-canted shell ~1 nm thick.

*Work supported by 3M.  

1:39PM Y41.00013: Magneto-Controlled Biocatalytic Cascades with Logically Processed Input Signals – Substrate Channeling versus Free Diffusion* 

YAROSLAV FILIPOV (Presenter), Clarkson University, ANDREY ZAKHARCHENKO, SERGIY MINKO, Nanostructured Materials Lab, University of Georgia, EVGENY KATZ, Clarkson University — Magnetic nanoparticles (MNPs) functionalized with various enzymes (amyloglucosidase, glucose oxidase and horseradish peroxidase) were used to perform biocatalytic cascades in two different states, solute suspension or aggregated, produced in the absence or presence of an external magnetic field. The biocatalytic reactions proceeded through bulk solution diffusion of intermediate substrates or substrate channeling, when the systems were dispersed or aggregated, respectively. The both pathways have shown very similar kinetics, unless the intermediate substrate was consumed by an additional biocatalytic process called “filter” for brevity. In the presence of the “filter” process, the diffusional process in the bulk solution was significantly inhibited, while the process based on the substrate channeling was still active. The systems were switched reversibly between the inhibited dispersed state and the active aggregated state by removing and applying the external magnetic field, respectively. The signal-controlled biocatalytic cascades were considered as Boolean logic circuits with the inputs consisting of biomolecules and the magnetic filed on-off.

*Work was supported by the National Science Foundation (award CBET-1403208 and award No. 1604526).

Friday, March 8, 2019 11:15 AM - 2:15 PM
Session Y43 DCMP: Advances in the Quantum Control of Single Spins in Semiconductors

BCEC 210B - David Awschalom, University of Chicago - Tag(s): Invited

11:15AM Y43.00001: Multi-node quantum networks based on spins and photons [Invited] RONALD HANSON (Presenter), Delft University of Technology — TBD

11:51AM Y43.00002: Spin and Orbital Resonance Driven by a Mechanical Resonator* [Invited] GREGORY FUCHS (Presenter), Cornell University — I describe our experiments to drive spin and orbital resonance of single diamond nitrogen-vacancy (NV) centers using the gigahertz-frequency strain oscillations produced within a diamond acoustic resonator. Strain-based coupling between a resonator and a defect center takes advantage of intrinsic and reproducible coupling mechanisms while maintaining compatibility with conventional magnetic and optical techniques, thus providing new functionality for quantum-enhanced sensing and quantum information processing. Using a spin-strain interaction at room temperature, we demonstrate coherent spin control [1] and spin coherence protection [2]. At cryogenic temperatures, we use orbital-strain interactions driven by a diamond acoustic resonator to examine multi-phonon orbital resonance of a single NV center [3]. We drive a strong mechanical modulation of the orbital state energies in the side-band resolved limit and produce nine orders of coherent sidebands. When we match the resonator frequency to half of the orbital splitting, we demonstrate resonance between the orbital states using a transverse orbital-strain interaction. The resulting dressed orbital states display Autler-Townes splitting as a function of resonator amplitude that is well-described by a 2-phonon resonance process. Finally, we discuss orbital decoherence protection as means of engineering NV centers to be a better spin-photon interface as a potential application of these techniques.


*We gratefully acknowledge support from the Office of Naval Research (N000141712290).

12:27PM Y43.00003: Probing spin-phonon interactions in semiconductors with x-rays and Gaussian acoustics* [Invited] SAMUEL WHITELEY (Presenter), University of Chicago — Coupling defect spins to phonons provides routes to new quantum control methods, coherence protection, and integrating spin qubits with quantum transducers. Silicon carbide (SiC) substrates host optically addressable point defects with long-lived electronic spin registers. Additionally, SiC is a low loss acoustic material and supports wafer-scale fabrication techniques, making SiC an ideal material for hybrid spin-mechanical systems. We fabricate surface acoustic wave (SAW) resonators taking advantage of isotropic acoustic propagation properties to construct simple Gaussian geometries, which focus strain and minimize diffraction losses. We directly image the mechanical mode with nanometer-scale spatial resolution by using hard x-ray diffraction microscopy and frequency matching a SAW to the timing structure of a synchrotron [1]. The SAW resonators are then utilized for coherent manipulation of divacancy electron spin ensembles in the SiC. We demonstrate all-optical detection of acoustic paramagnetic resonance, which enables quantum sensing of phonons without magnetic microwaves. In addition, we measure coherent magnetically forbidden spin transitions with Autler-Townes splittings and Rabi oscillations on the divacancy spins, as well as show spatial mapping of spin driving which reveals spin coupling to shear [2]. Our model, comprising of ab initio calculations for the spin-strain coupling parameters, captures the salient features of the physics. These results offer a basis for three-level spin system control with phonons and paths to combining spin registers with nanomechanical devices.


*This work was supported by AFOSR, DOE, NSF GRFP, and UChicago MRSEC.
1:03PM Y43.00004: Quantum nano-photonics with rare-earth-doped materials* [Invited] ANDREI FARAON (Presenter), Applied Physics, Kavli Nanoscience Institute, Institute for Quantum Information and Matter, California Institute of Technology — I present quantum nano-photonics devices based on nanophotonic resonators coupled to rare-earth-ions in crystals. The rare-earth ions exhibit long coherence times on optical and microwave transitions, which makes them suitable for various quantum light-matter interfaces like quantum memories, single quantum bits and optical to microwave quantum transducers. We demonstrate on-chip optical quantum memories based on atomic frequency combs and optically addressable quantum bits based on single rare-earth ions where the quantum state can be mapped on Zeeman or hyperfine levels with long coherence time. Our solid-state nano-photonics quantum light-matter interfaces can be integrated with other chip-scale photon source and detector devices for multiplexed quantum and classical information processing at the nodes of quantum networks.

*National Science Foundation
Air Force Office of Scientific Research
Office of Naval Research

1:39PM Y43.00005: Theory of electrical readout of deep defect qubits in solids* [Invited] ADAM GALI (Presenter), Hungarian Academy of Sciences — Paramagnetic color centers with deep levels in the gap are candidates to realize qubits in solids, in particular, those color centers that show spin-dependent fluorescence that can be employed to initialize and readout the electron spin of single color centers, first demonstrated for the nitrogen-vacancy (NV) center in diamond [1]. It has been shown [2] that optical excitation can also lead to ionization of NV center that is also spin dependent. The resultant carriers, i.e., the photocurrent can be collected that is the ground of photocurrent detected magnetic resonance (PDMR).
In my talk, I will show the power and significance of ab initio atomistic simulation techniques that can provide deep insight into the microscopic mechanisms behind the observed phenomena, and how it can be applied to optimize the conditions of qubit measurements. In particular, I will show how ab initio theory can explain the two-photon ionization of NV centre [3] that is the base of PDMR measurements. Intricate details of back ionization reveal the optical spinpolarization process in NV centre [4] under continuous green laser excitation. Theory predicted that two-color excitation will increase the signal-to-noise ratio of PDMR signal of NV center in diamond that was confirmed in experiment [5]. We will discuss very prospective deep color centers, divacancies in silicon carbide [6,7], what could be the experimental conditions to realize PDMR signal from these qubits in this technologically mature semiconductor.


*EU H2020 Asteriqs, Hungarian NKFIH Grant Nos. 2017-1.2.1-NKP-2017-00001, 127902 and 127889

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y44 DCMP: Exotic Majorana Physics and Beyond BCEC 210C - Maissam Barkeshli, University of Maryland, College Park - Tag(s): Invited
11:15AM Y44.00001: Solid state realizations of Sachdev-Ye-Kitaev models* [invited] MARCEL FRANZ (Presenter), University of British Columbia — An intriguing connection, pointed out by Kitaev in 2015, exists between a simple model of Majorana fermions with random all-to-all interactions – the Sachdev-Ye-Kitaev (SYK) model – and the horizons of extremal black holes in two-dimensional anti-de Sitter space. This connection furnishes a rare example of holographic duality between a solvable quantum-mechanical model and Einstein gravity. It also opens up a possibility to study quantum black holes, realized holographically in a quantum mechanical model, in a tabletop experiment. In this talk I will review some of these developments and describe the recent efforts to bring the family of SYK models closer to experimental reality. The proposed experimental realizations employ both complex and Majorana fermions in various atomic and solid state systems. These include some of the standard platforms for Majorana zero modes (proximitized quantum wires and topological insulator - superconductor interfaces) as well as electrons in the lowest Landau level in a graphene flake with an irregular boundary.

*The work was supported by NSERC and CIfAR.

11:51AM Y44.00002: Approximating the Sachdev-Ye-Kitaev model with Majorana wires* [invited] AARON CHEW, Caltech, ANDREW ESSIN, UC Davis, JASON ALICEA (Presenter), Caltech — The Sachdev-Ye-Kitaev (SYK) model describes a collection of randomly interacting Majorana fermions that exhibits profound connections to quantum chaos and black holes. I will discuss a potential solid-state implementation based on a quantum dot coupled to an array of topological superconducting wires hosting Majorana zero modes. Interactions and disorder intrinsic to the dot mediate the desired random Majorana couplings, while an approximate symmetry suppresses additional unwanted terms. Random matrix theory and numerics show that this setup indeed emulates the SYK model (with certain corrections). Tunneling measurements provide an appealing first experimental test of this scenario.

*Research supported by the National Science Foundation through grant DMR-1341822; the Caltech Institute for Quantum Information and Matter, an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation through Grant GBMF1250; and the Walter Burke Institute for Theoretical Physics at Caltech.

12:27PM Y44.00003: Majorana Multiplexing [invited] YANG PENG (Presenter), California Institute of Technology — TBD

1:03PM Y44.00004: Quantum Engineering of Majorana Fermions* [invited] DIRK MORR (Presenter), University of Illinois at Chicago — The experimental observation of Majorana states in topological superconductors represents a major breakthrough in realizing their applications in topological quantum computing. This has stimulated the search for new possibilities to engineer Majorana states at the nanoscale, in particular using magnetic-superconducting hybrid (MSH) structures in which islands of magnetic adatoms are placed on the surface of s-wave superconductors.

In this talk, I provide several examples for the quantum engineering of Majorana fermions in MSH systems [1,2]. First, I will report the results of a theory-experiment collaboration demonstrating the ability to tune between a topological phase exhibiting chiral Majorana edge modes and a trivial phase in Fe-Re MSH structures using interface engineering [1]. Second, I will show that one can create a topological switch in MSH systems by imprinting magnetic skyrmions, allowing one to write and delete topological phases. Similarly, it is possible to engineer chiral Majorana states of arbitrary shape through the creation of magnetic domain walls. Third, I show that it is possible to continuously tune MSH systems between 2D and 1D topological phases using atomic manipulation, and thus to change the character of the associated Majorana modes. Finally, I will demonstrate that Josephson scanning tunneling spectroscopy is a crucial tool in identifying topological phases [3].


*This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-FG02-05ER46225
1:39PM Y44.00005: The Majorana-Hubbard Model* [Invited] IAN AFFLECK (Presenter), University of British Columbia — When a vortex lattice forms in a superconducting layer on a topological insulator a Majorana fermion is predicted to appear in each vortex core. Hopping and interaction terms between the Majorana fermions lead to a novel generalization of the Hubbard model. Furthermore, the hopping amplitude is predicted to vanish at a special value of the chemical potential in the topological insulator, allowing the phase diagram to be studied as a function of the ratio of interaction strength to hopping amplitude. I will present results on the interesting phase diagrams, which includes supersymmetric critical points, in both one and two dimensions.

*NSERC, CIFAR, UBC SBQMI

Friday, March 8, 2019 11:15 AM - 1:51 PM

Session Y48 GSNP: Statistical and Nonlinear Physics II BCEC 251 - Daniel Lathrop, University of Maryland, College Park

11:15AM Y48.00001: The Ising Model in Curved Geometries* NIKOLAS BREUCKMANN (Presenter), University College London, ANANDA ROY, Institut de Physique Theorique, CEA Saclay, BENEDIKT ANDREAS PLACKE, IQI, RWTH Aachen — The study of statistical mechanics in curved geometries has recently gained an increasing amount of attention. Particularly the Ising model in negatively curved spaces has been studied as a mean to understand exotic crystals, soft-matter and field theories in Anti-de Sitter spaces.

We analyze the Ising model on in the hyperbolic plane as well as 2+1-Anti-de Sitter (AdS) space using high temperature series-expansion and Monte-Carlo simulations. While series expansions have been performed on the hyperbolic plane before, we study a wider class of hyperbolic lattices and go to much higher order, allowing us to analyze the dependency of critical phenomena on the magnitude of curvature.

In the past Monte Carlo methods have been difficult to use as the curvature lead to severe boundary effects which persist even for large system sizes. We overcome this problem by constructing families of closed 2D surfaces of increasing area and compactified AdS spaces of increasing volume, akin to periodic boundaries in euclidean space.

It has been discussed into which universality class the Ising model in hyperbolic space falls. Our results strongly support that it falls into the mean-field universality class.

*NPB is a UCLQ fellow at UCL. AR is supported by the Alexander von Humboldt foundation.

11:27AM Y48.00002: Strong randomness criticality in the scratched-XY model ZHIYUAN YAO (Presenter), Institute for Advanced Study, Tsinghua University, TOBIAS PFEFFER, LODE POLLET, Department of Physics, University of Munich — We study the finite-temperature superfluid−normal-liquid classical phase transitions in a disordered two-dimensional XY model with power law distributed "scratch"-like bond disorder. While for weak disorder the transition is of Berezinskii-Kosterlitz-Thouless type, the transition in the strong disorder regime is in a different universality class with a non-universal jump of the superfluid stiffness. We show this new criticality can be described by the asymptotically exact theory of superfluid-insulator quantum phase transition in one-dimensional disordered boson systems and discuss possible experimental realizations.

11:39AM Y48.00003: Violation of a universal changeover in two-dimensional Potts models NIR SCHREIBER (Presenter), REUVEN COHEN, SIMI HABER, GIDEON AMIR, Mathematics, Bar Ilan University — We present a novel combinatorial approach which allows the determination of the critical temperature and the phase transition order of Potts models with multi-site interaction. Applying this approach to the hexagonal lattice, it is demonstrated that Potts models with local, range independent interaction may changeover from a continuous to a discontinuous phase transition, at a marginal value \( q_c \leq 3 \). Our theory is substantiated by Monte-Carlo simulations. In particular, it is numerically indicated that the system undergoes a first order transition for \( q=3 \). The latter is in agreement with a further prediction of \( q_c \leq 2 \), established under a mild assumption related to the asymptotic growth of hexagonal lattice animals. Our findings are in contrast to known cases where \( q_c=4 \) which were believed to represent a universal phenomenon. Thus, the universality of \( q_c=4 \) is violated.
11:51AM Y48.00004: Non-universal Dynamics of Three-Dimensional Magnetic Systems With Heisenberg Interaction
RIYA NANDI (Presenter), UWE CLAUS TAUBER, Virginia Tech — We numerically investigate the non-equilibrium critical dynamics in three-dimensional isotropic Heisenberg antiferromagnets. To account for the reversible terms arising from the microscopic dynamics of the system, we employ a hybrid simulation algorithm that combines reversible spin precession with relaxational Kawasaki spin exchange processes. We verify the dynamic exponent, and obtain a suitable aging scaling window. We observe and thus validate an older renormalization group prediction that, while the critical aging collapse exponent assumes universal value, the temporal decay exponent is found to be non-universal and dependent on the initial distribution of the spins.

*Research was sponsored by the U.S. Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.
The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Army Research Office or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein.

12:03PM Y48.00005: Exact many-body quantum scar states with topological properties in dimensions 1, 2, and 3
SEULGI OK (Presenter), KENNY CHOO, University of Zurich, CHRISTOPHER M MUDRY, Paul Scherrer Institute, CLAUDIO CASTELNOVO, Cavendish Laboratory, University of Cambridge, CLAUDIO CHAMON, Physics Department, Boston University, TITUS NEUPERT, University of Zurich — We provide a general construction of exact excited states in a class of certain non-integrable conserved quantum many-body Hamiltonians. These states have area law entanglement entropy, while they are spectrally embedded in states with volume law scaling. Our construction applies to models in arbitrary dimensions, and we exemplify it for scar states with properties usually associated to gapped ground states of symmetry protected topological phases or topologically ordered phases of matter, including the respective degeneracies.

*S. Ok and T. Neupert were supported by the the Swiss National Science Foundation (grant number: 200021 169061). K. Choo and T. Neupert were supported by the European Unions Horizon 2020 research and innovation program (ERC-StG-Neupert-757867-PARATOP).

12:15PM Y48.00006: Stability of quantum statistical ensembles with respect to random local measurements
BORIS FINE (Presenter), Skolkovo Institute of Science and Technology, WALTER HAHN, QuTech, Delft University of Technology — We define a quantum statistical ensemble as 'stable', if a small number of local measurements cannot significantly modify the total-energy distribution representing the ensemble. This stability criterion is applied to lattices of spins-1/2, for which different measures of the quantum ensemble stability are investigated. In the context of the foundations of quantum statistical physics, our results justify the use of statistical ensembles with narrow energy distributions such as canonical or microcanonical ensembles.

References:

*This work was supported by a grant of the Russian Science Foundation (Project No. 17-12-01587).

12:27PM Y48.00007: Quantum Heat Machines with Trapped Ions
SUMAN CHAND (Presenter), Physics, Indian Institute of Technology Ropar, ASOKA BISWAS — Quantum heat machines (QHM) are those quantum systems that convert heat into the useful form of work. Specific kinds of QHMs, namely the heat engines and the refrigerators, among others have been studied in quantum regimes, using discrete strokes or continuous strokes. Heat engines take the heat from a hot bath, deliver a certain amount of work, and release heat to the cold bath. In most of the proposals of QHMs it is assumed that the hot bath and the cold bath are physically separated and can be switched on or off in a controlled way, just as in the case of their classical counterpart. In quantum regime, however, the interaction between the system and the bath is never switched off. Therefore, newer strategies are required for a QHM that can be implemented in a realistic scenario, and also within the quantum framework. Here, we show how one can implement different strokes of an Otto engine, using a single trapped ion. Using two ions, one can even build a refrigerator. Further, we study how a QHM performs across the critical value of an external parameter, pertaining to the quantum phase transition

Reference
CHRIS KOSCHENZ (Presenter), CARSTEN TIMM, Technische Universität Dresden, Institute of Theoretical Physics / Condensed Matter Theory Group — We present a generalized Bogoliubov-Hartree-Fock theory, which allows to study magnetic ordering, charge ordering, and superconductivity on the same footing and gives additional information about the so-called mixed phases [1]. These phases emerge in parameter ranges where the system is potentially strongly affected by fluctuations and cannot be described by any set of usual Hartree-Fock states (Slater determinants) [1,2]. Furthermore, we show how to obtain the self-consistent set of order parameters in the normal and BCS states by straightforward unrestricted global minimization of the appropriate Landau functional [3]. This method allows us to study the coexistence and competition of various magnetic and superconducting order and can be used to study the possibility of additional phase transitions in the coexistence regime.


*We acknowledge Research Training Group GRK 1621 of Deutsche Physikalische Gesellschaft (DPG) for funding.

NATHANIEL RUPPRECHT (Presenter), DERVIS CAN VURAL, University of Notre Dame — Scientific inference involves obtaining the unknown properties or behavior of a system in the light of what is known, typically, without changing the system. Here we propose an alternative to this approach: a system can be modified in a targeted way, preferably by a small amount, so that its properties and behavior can be inferred more successfully. For the sake of concreteness we focus on inferring the future and past of Markov processes and illustrate our method on two classes of processes: diffusion on random spatial networks, and thermalizing quantum systems.

MATT WALKER (Presenter), MARIJA VUCELJA, University of Virginia — The Mpemba effect is an anomalous relaxation process in which a system starting at a hot temperature cools down faster than an identical system starting at an initially lower temperature when both are coupled to an even colder bath. The effect has been observed in water, clathrate hydrates, magnetic alloys, and driven granular gases. We search for an analogous to Mpemba phenomenon for the case of a Langevin particle diffusing and advecting on a potential energy landscape. The particle is diffusing with a diffusion constant, that corresponds to a temperature that is lower than specified by the initial condition. We study the Mpemba effect, or non-monotonic thermal relaxation, as a function of parameters specifying the potential landscape.

VIDUSHI ADLAKHA (Presenter), Department of Physics, University of Houston, PHILIPP G. MEYER, HOLGER KANTZ, Max Planck Institute for the Physics of Complex Systems, KEVIN E BASSLER, Department of Physics, University of Houston — We show that the anomalous diffusive behavior found in an aging system can be decomposed into three fundamental constitutive causes. A model process that is a sum of increments that are iterates of a chaotic dynamical system, the Pomeau-Manneville map, is examined. The increments can have long-time correlations, fat-tailed distributions and be non-stationary. Each of these properties can cause anomalous diffusion through what is known as the Joseph, Noah and Moses effects, respectively. The model can have either sub- or super-diffusive behavior, which we find is generally due to the combination of the three effects. Scaling exponents quantifying each of the three constitutive effects are calculated using analytic methods and confirmed with numerical simulations. They are then related to the scaling of the distribution of the process through a scaling relation. The work also discusses the importance of Moses effect in the anomalous diffusion of experimental systems.

*Work supported by the NSF through grant DMR-1507371 and AAUW (International Fellowship).
Universal First-Passage-Time Distribution of Non-Gaussian Currents

SHILPI SINGH (Presenter), PAUL MENCZEL, DMITRY S GOLUBEV, Aalto University, IVAN KHAYMOVICH, Max Planck Institute for the Physics of Complex Systems, JOONAS T PELTONEN, CHRISTIAN FLINDT, Aalto University, KEIJI SAITO, Keio University, ÉDGAR ROLDÁN, The Abdus Salam International Centre for Theoretical Physics, JUKKA P PEKOLA, Aalto University — I present our recent work on the fluctuations of the time elapsed until the electric charge transferred through a conductor reaches a given threshold value. For this purpose, we measure the distribution of the first-passage times for the net number of electrons transferred between two metallic islands in the Coulomb blockade regime. Our experimental results are in excellent agreement with numerical calculations based on a recent theory describing the exact first-passage-time distributions for any non-equilibrium stationary Markov process.

We present a simple analytical approximation for the first-passage-time distribution, which takes into account the non-Gaussian statistics of the electron transport, and show that it describes the experimental distributions with high accuracy. This universal approximation describes a wide class of stochastic processes and can be used beyond the context of mesoscopic charge transport. In addition, we verify experimentally a fluctuation relation between the first-passage-time distributions for positive and negative thresholds.

Electromagnetic properties of random materials

POUYAN KARIMI (Presenter), MARTIN OSTOJA-Starzewski, Mechanical Science and Engineering, University of Illinois at Urbana-Champaign — Scale dependence bounds on the electromagnetic properties are studied in the setting of spatially random linear materials with statistically homogeneous and spatially ergodic random microstructures. First, from the Hill-Mandel homogenization conditions adapted to electric and magnetic fields, uniform boundary conditions are formulated for a statistical volume element (SVE). From these conditions, rigorous bounds are obtained on the macroscale (effective) electrical permittivity and magnetic permeability. Using computational electromagnetism methods, these bounds are obtained through numerical simulations for composites of two types: (i) 2D random checkerboard (two-phase) microstructures and (ii) 2D Gaussian correlated microstructure. The simulation results demonstrate a convergence of these bounds to the effective properties with increasing length scales.

The authors gratefully acknowledge the partial support from the NSF IIP-1362146 (M.O.-S) as well as the Computational Science and Engineering (CSE) Fellowship (P.K.) at NCSA and the use of the campus cluster resources provided under the CSE program at the University of Illinois at Urbana-Champaign.

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y51 DBIO: Physical Mechanisms of Cell Fate Decision Making and Stem Cell Differentiation/Reprogramming

BCEC 253A - Wei Wang, Nanjing University - Tag(s): Invited

Trigger waves in cell signaling [Invited] JAMES FERRELL (Presenter), Stanford University — Untethered cytosolic proteins can move 10 µm or so in a few seconds by simple random walk diffusion. In a typical eukaryotic cell (with a radius of ~10 µm), this is fast enough to allow a cell to respond in a spatially coordinated fashion to many stimuli. Over larger distance scales, regulators are often spread via flow. For example, hormones like insulin and epinephrine make their way around the body via the circulatory system on a time scale of a minute or so, whereas random walk diffusion would take about 500 years. An alternative to flow for long-range biological communication is the trigger wave. Action potentials are trigger waves; so are calcium waves in neurons and fertilized eggs; and so are cAMP waves in aggregating slime molds.

Here we will show that mitosis spreads through Xenopus egg cytoplasm via a trigger wave of Cdk1 activation, and apoptosis spreads via a trigger wave of caspase activation. These findings explain how a large cell like a frog egg (~1.2 mm diameter) and function in a spatially coordinated fashion, and they show that trigger waves are a recurring theme in cell signaling.
transdifferentiation*  

12:27PM Y51.00003: Waddington landscape and pathways for stem cell differentiation, reprogramming and transdifferentiation* [Invited]  
JIN WANG (Presenter), Stony Brook University — Waddington landscape in biology gives a qualitative picture for understanding differentiation and development. However, the original Waddington landscape picture lacks physical foundations and quantifications. We developed a nonequilibrium landscape and flux theory for quantifying the Waddington landscape for differentiation, reprogramming and transdifferentiation. We found that the landscape for differentiation and development emerges from the underlying gene regulatory interactions with distinct stem cell and differentiated cell state attractors. Furthermore, the pathways for differentiation, reprogramming, and transdifferentiation among the stem cell and differentiation cell state attractors can be quantified. In addition, the kinetic speed of differentiation, reprogramming, and transdifferentiation can be quantified and associated with the landscape topography. We also show that the dynamics of the differentiation, reprogramming, and transdifferentiation processes are determined by both the landscape gradient and the rotational flux. We show that the flux can influence significantly the pathways and the kinetics of these processes. Importantly, flux may also provide a nonequilibrium driving force for the formation of different cell state attractors as the new active matter phases. We apply the landscape and flux theory to several biological differentiation processes including human stem cell development. We also identified the key genes and regulations for the differentiation and reprogramming based on the landscape topography and pathways. The relationship between development and cancer is also explored with the emergence of cancer stem cell state attractor. This study may provide useful clues for the practice of tissue engineering and cancer treatment.  

*NSF-PHY-76066, NSF-CHE-1808474

1:03PM Y51.00004: Setting the epigenetic stage for differentiation: a collective phenomenon [Invited]  
FABRIZIO OLMEDA, Max Planck Institute for the Physics of Complex Systems, STEPHEN CLARK, TIM LOHOFF, The Babraham Institute, HEATHER LEE, The University of Newcastle, WOLF REIK, The Babraham Institute, STEFFEN RULANDS (Presenter), Max Planck Institute for the Physics of Complex Systems — The self-organisation of cells during embryonic development is one of the most intriguing non-equilibrium processes in nature. How do cells coordinate their behaviour in order to build a living organism? Recent technological advances, for example in genomics, for the first time allow us to probe microscopic states of these processes with unprecedented detail. But how can detailed quantitative information on the microscopic scale be translated into a mechanistic understanding of the collective degrees of freedom that determine biological function at the cellular scale? In this talk, I will give the example of epigenetic patterning in early embryonic development to demonstrate how core concepts from non-equilibrium physics can help gain understanding of the collective processes underlying cell fate regulation.  

During early development, when the first cell fate decisions are made, the genome undergoes large-scale changes in epigenetic DNA modifications (DNA methylation) and chromatin structure. As a result of these processes cells carry distinct epigenetic marks that assign their fate during later stages of development and adulthood. But how are these epigenetic marks so robustly established? Combining novel methods from single-cell multi-genomics with non-equilibrium physics we find universal scaling behaviour in the processes leading to the establishment of epigenetic marks. We show that these phenomena result from long-range interactions mediated by the interplay between chemical and topological modifications of the DNA. Our work sheds new light on epigenetic mechanisms involved in cellular decision making. It also highlights how mechanistic insights into the molecular processes governing cell-fate decisions can be gained by the combination of methods from genomics and non-equilibrium physics.
Intracellular noise level determines ratio control strategy confined by speed-accuracy tradeoff

Robust and precise ratio control of heterogeneous phenotypes within an isogenic population is essential in the development and differentiation. However, the mechanisms of such ratio control are poorly understood. Here, we employ experimental and mathematical techniques to understand the combined effects of signal induction and gene expression stochasticity on phenotypic multimodality. We identify two strategies to control phenotypic ratios from an initially homogenous population, suitable roughly to high-noise and low-noise intracellular environments, and we show that both can be used to generate precise fractional differentiation. In noisy gene expression contexts, such as those found in bacteria, induction within the circuit's bistable region is enough to cause noise-induced bimodality within a feasible timeframe. However, in less noisy contexts, such as tightly controlled eukaryotic systems, spontaneous state transitions are rare and hence bimodality needs to be induced with a controlled pulse of induction that falls outside the bistable region. Finally, we show that noise levels, system response time, and ratio tuning accuracy impose tradeoff and limitations on both ratio control strategies, which guides the selection of strategy alternatives.

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y53 GSOFT: Towards Soft Active Metamaterials

Soft Active Metamaterials by Programing Ferromagnetic Domains*

Robust and precise ratio control of heterogeneous phenotypes within an isogenic population is essential in the development and differentiation. However, the mechanisms of such ratio control are poorly understood. Here, we employ experimental and mathematical techniques to understand the combined effects of signal induction and gene expression stochasticity on phenotypic multimodality. We identify two strategies to control phenotypic ratios from an initially homogenous population, suitable roughly to high-noise and low-noise intracellular environments, and we show that both can be used to generate precise fractional differentiation. In noisy gene expression contexts, such as those found in bacteria, induction within the circuit's bistable region is enough to cause noise-induced bimodality within a feasible timeframe. However, in less noisy contexts, such as tightly controlled eukaryotic systems, spontaneous state transitions are rare and hence bimodality needs to be induced with a controlled pulse of induction that falls outside the bistable region. Finally, we show that noise levels, system response time, and ratio tuning accuracy impose tradeoff and limitations on both ratio control strategies, which guides the selection of strategy alternatives.

This is an invited talk for Session Towards Soft Active Metamaterials.

*This work is supported by the National Science Foundation (CMMI-1661627) and the Office of Naval Research (N00014-17-1-2920) and the MIT Institute for Soldier Nanotechnologies.

Bifurcations in mechanical structures: from smart folding to folding smarts*

Self-folding structures (also known as 4D printing) have emerged as a potential technique for the fabrication of complex structures in three dimensions, much as origami artists fold an intricate shape from flat sheets of paper. Recently, it has become clear self-folding origami exhibits a complex, bifurcated configuration space with exponentially many branches - making self-folding difficult. I will describe recent work extending this analysis to more complex origami having 2 or more degrees of freedom and explore, in detail, how to program a structure to fold robustly despite the proliferation of misfolding pathways. Finally, I will describe how to use the bifurcations and nonlinearities in origami and other mechanical structures to design “smart materials” - metamaterials that can perform logical operations.

Putting stubborn flocks to work

Building on spontaneously flowing liquids assembled from colloidal rollers, I will show that (French) active colloids collectively protest and resist when one tries to waive their privilege to freely choose their direction of motion. I will show that the flows emerging from flocking transitions are intrinsically bistable and can proceed against external pressure gradients. I will theoretically explain this collective stubbornness showing that orientational elasticity and confinement conspire to protect the direction of spontaneous flows. Finally, I will show how to exploit the intrinsic bistability of confined polar liquids introducing a generic design principle for self-sustained microfluidic oscillators.
1:03PM Y53.00004: Manipulating the dynamics of active emulsions* [Invited] CHENYU JIN (Presenter), BABAK VAJDI HOKMABAD, KYLE A BALDWIN, CORINNA MAASS, Max Planck Institute for Dynamics and Self-Organization — Precise control and manipulation are crucial to various applications of active matter. For example, in guidance applications as in active microsensors, microreactors with targeted release or microfluidic droplet logic, we need to know and control the rules by which such entities can be guided, follow external stimuli and control their stability.

Nematic and isotropic oil droplets in aqueous surfactant solutions are well-controlled artificial active system with easily accessible tuning parameters such as temperature, liquid crystalline order or bulk viscosity. These active emulsions exhibit many properties such as wall guidance, chemotaxis, autochemotaxis, as well as tunable swimming dynamics. We demonstrate how the motion of the droplets can be controlled by topographical guidance, droplet topology and chemical gradients, and show avenues for technical application by adding internal compartments.

*supported by the DFG SPP 1726 “Microswimmers” and the Max Planck Society

1:39PM Y53.00005: Designing active topological networks [Invited] HENRIK RONELLENFITSCH (Presenter), Massachusetts Institute of Technology — Mechanical and phononic metamaterials with exotic characteristics, including negative elastic moduli or negative effective mass density, allow for precise control of mechanical functionality. Materials possessing spectral bandgaps are particularly interesting due to their ability to host topological edge modes that enable robust signal transmission even in the presence of defects. Active matter can induce and carry such topological modes through its inherent breaking of time-reversal symmetry. Here, I will present recent work by our group that aims at harnessing interactions between activity and topology to realize autonomously acting metamaterials. Specifically, we show how one can program desired spectral properties such as bandgaps directly into mechanical networks, and thus control topological excitations when time-reversal symmetry is broken. Furthermore, we demonstrate how these ideas can be generalized to design active electronic circuits that can self-select and sustain topological modes and how topology can be used to construct other precisely controllable current patterns.

Friday, March 8, 2019 11:15 AM - 1:15 PM

Session Y55 GSNP GSOFT: Shell Buckling II BCEC 254B - Pedro Reis, Ecole polytechnique federale de Lausanne - Tag(s): Focus

11:15AM Y55.00001: Mechanics of turning a page JIHYE MYEONG (Presenter), Seoul National University, ANNA LEE, POSTECH, HO-YOUNG KIM, Seoul National University — A mundane activity of turning a page arises not only in reading, but also in production of paper and textile. Here we analyze the shape and stability of a thin sheet of paper, bound to a book in one side and compressed from the other side, to gain mechanical understanding of the page turning. We start with describing the shape of a sheet that is buckled between the bound end and gripping fingers, using the Euler elastica. Then we predict the fate of the bent page when the external load is removed, to determine the condition for the page to turn to the other side. Upon corroborating our theory with experiments of various geometry and materials of thin sheets, we suggest the shortest path of fingers to turn pages for both lazy readers and efficient manufacturing robots.
**11:27AM Y55.00002: Swimming through shell buckling**  
ADEL DJELLOULI (Presenter), Harvard University, PHILIPPE MARMOTTANT, GWENNOU COUPIER, CNRS/Grenoble University, CATHERINE QUILLIET, HENDA DJERIDI, Grenoble University — Under pressure, a hollow elastic sphere becomes unstable and collapses. It reinflates back when the pressure is decreased. The hysteresis in shape sequence and in deformation velocity associated to this cycle makes this simple object a good candidate for becoming a swimmer able to move at low or high Reynolds number.

We explore this possibility through a macroscopic experiment in fluids of varying viscosities so as to explore different flow regimes. We show that not only the shape hysteresis leads to swimming but the fast buckling phase is an efficient mechanism for propulsion that implies inertial effects and subtle coupling between shape post-buckling oscillations and fluid flow patterns. Our modeling shows that such an inertial regime could even be reached at microscopic scale.

We anticipate that a conveyor made of a few of microbubbles with different shell thicknesses, would constitute a microrobot whose 3D displacement can be remotely controlled by ultrasonic waves.


*This research was made possible by ERC Grant No. 614655 Bubbleboost.

**11:39AM Y55.00003: Buckled Bundles and Beyond**  
ISAAC BRUSS (Presenter), Harvard University, GREGORY GRASON, Polymer Science and Engineering, University of Massachusetts - Amherst — Defects can elastically buckle 2D crystalline membranes (like graphene) into 3D shapes. Using a combination of numerical simulations and continuum elasticity theory, we show how the same is true for columnar structures (like nanotubes or protein fibers). This discovery builds upon the recently uncovered mapping between the inter-filament spacing in bundles and the metric properties of a curved surface. We show that shape instabilities are controlled by a single material-dependent parameter that characterizes the ratio of bending to cohesion energies. Along with a host of previously unknown shape equilibria—the filamentous analogs to the conical and saddlelike shapes of defective membranes—we find a profoundly asymmetric response to positive and negative disclinations in the infinite length limit that is without parallel to the membrane analog.

*This work was supported by the National Science Foundation through Grant No. DMR 1608862.

**11:51AM Y55.00004: Dynamic buckling of rings and annuli**  
OUSMANE KODIO (Presenter), FINN BOX, DOIREANN O’KIELY, VINCENT CANTELLI, ALAIN GORIELY, DOMINIC VELLA, University of Oxford — When an elastic ring is subject to an external pressure, it is known to buckle as a ‘figure of 8’; similarly an annulus subject to a strong internal tension is known to form two folds. Here we explore how these examples of mode-2 buckling change under dynamic loading. In particular, we show that the presence of inertia means that higher modes are observed at the onset of instability, and present results for the observed mode number as a function of the driving pressure. Our results are in accord with experiments in which an elastic ring is rapidly pulled inwards by surface tension. Surprisingly, we find that while inertia is required to observe higher modes, the actual selected mode does not depend on inertia. We explain this, and reconcile our observation of higher modes with earlier experiments that exhibited mode 2, by understanding the growth rate of instability.

*ERC Grant Agreement No. 637334*
12:03PM Y55.00005: Membrane morphology beyond polyhedra*  
HANG YUAN (Presenter), MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University — Conventional homogeneous or heterogeneous elastic crystalline membrane exhibits buckling transition from sphere to polyhedra. However, their morphologies do not go beyond polyhedra and cannot be externally controlled. We study the morphology of a closed crystalline membrane co-assembled with super-paramagnetic particles which is called magnetoelastic membrane. With additional competition from magnetic dipole-dipole interaction on top of elasticity, magnetoelastic membrane shows novel morphology beyond polyhedra. By systematically changing two dimensionless control parameters, we find a rich class of membrane morphologies. The morphology of magnetoelastic membrane can be manipulated by external magnetic field, providing promising applications for membrane shape control, design of micro-containers and targeted drug delivery systems.

*This work was supported as part of the Center for Bio-Inspired Energy Science, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award # DE-SC0000989.

12:15PM Y55.00006: Swelling and warpage of orthotropic plates  
HARRISON WOOD (Presenter), JAMES HANNA, Virginia Tech — While isotropic in-plane swelling problems for elastic sheets have been studied extensively in recent years, many shape-programmable materials, including nematic solids and 3d-printed structures, are anisotropic. Inspired by the warpage of engineered wood panels, we examine plates in which both the in-plane swelling and the material stiffness are highly orthotropic, leading to multiple separations in energy scales. For these orthotropic plates, in-plane swelling can produce configurations that approximate cylindrical shapes and twisted ruled surfaces.

12:27PM Y55.00007: Transverse edge extension underlies compression, buckling and wrinkling in thin solids  
MENG XIN (Presenter), BENJAMIN DAVIDOVITCH, University of Massachusetts Amherst — When a rectangular sheet whose short edges are clamped is stretched, elongated wrinkles appear, indicating the presence of transverse compression. So far, the mechanism by which longitudinal tension and edge clamping act jointly to generate transverse compression has not been clarified. Here we employ analytic tools and numerical simulations to compare this problem with a new variant, where instead of stretching and edge clamping one only imposes edge-localized transverse strain, pulling the corners outward. We find that, despite the absence of longitudinal tension in the new variant, both models exhibit similar transverse stress profile in planar state, thus revealing that the generic origin of compression is the transverse extension of edges relative to the bulk. This similarity in planar stress profiles underlies similarity in the near-threshold buckling patterns exhibited by the two models. In contrast, the two models are sharply distinct in their respective far-from-threshold regime: the deflection of the stretched sheet consists of small wavelength wrinkles whereas the edge-extended sheet does not develop wrinkles. This indicates the role of longitudinal tension in providing an effective substrate resistance, which is crucial for the emergence of wrinkle patterns.

12:39PM Y55.00008: A geometric theory of wrinkling for confined shells: Part 1*  
YOUSRA TIMOUNAY (Presenter), IAN TOBASCO, Department of Mathematics, University of Michigan, DESISLAVA V TODOROVA, ELENI KATIFORI, Department of Physics and Astronomy, University of Pennsylvania, JOSEPH D PAULSEN, Department of Physics, Syracuse University — The problem of joining a planar sheet to a surface with a different metric is a familiar frustration. Flat bandages don't stick as well to curved knuckles or elbows, and maps of the earth exaggerate areas near the poles. We study the deformations of ultrathin (~100 nm) elastic shells, which we manufacture on spherically-curved substrates and then transfer to a flat water bath. The sheets respond by forming distinct domains filled by smooth parallel wrinkles or by disordered buckled patterns. We show that the selection of these domains and the orientation of wrinkles within them depends sensitively on the shape of the boundary of the film. Remarkably, these complex patterns may be predicted by a theoretical model wherein the exposed surface area of the water bath is minimized. The derivation and solution of this model will be presented in the next talk. (This is part 1 in a 3-talk series).

*Support from NSF-DMR-CAREER-1654102 is gratefully acknowledged.
12:51PM Y55.00009: A geometric theory of wrinkling for confined shells: Part 2*  
IAN TOBASCO (Presenter), Department of Mathematics, University of Michigan, YOUSRA TIMOUNAY, Department of Physics, Syracuse University, DESISLAVA V Todorova, Department of Physics and Astronomy, University of Pennsylvania, JOSEPH D PAULSEN, Department of Physics, Syracuse University, ELENI KATIFORI, Department of Physics and Astronomy, University of Pennsylvania — Thin elastic shells readily take on shapes wildly different from their own. Motivated by the puzzle of determining the wrinkle patterns exhibited by shallow shells floating on a water bath, we obtain a fully rigorous asymptotic expansion of the energy (elastic and otherwise) valid in the high-frequency limit. After renormalizing by the typical energy of wrinkling, we derive a coarse-grained model in which an elastically compatible pattern is assigned energy proportional to the difference between its intrinsic undeformed area and its projected area in the plane. Energetically optimal patterns therefore maximize their projected area. Surprisingly, this limiting model turns out to be explicitly solvable in a large variety of cases, including for shells whose (possibly non-constant) curvature is of a known sign. We demonstrate our methods in many cases of interest, offering an ansatz-free explanation for the geometry of wrinkle patterns seen in confined elastic shells. (This is part 2 in a 3-talk series.)

*This work was partially supported by NSF Awards DMS-1515161 and DMS-1812831, and a Van Loo Postdoctoral Fellowship.

1:03PM Y55.00010: A geometric theory of wrinkling for confined shells: Part 3*  
DESISLAVA V Todorova (Presenter), Department of Physics and Astronomy, University of Pennsylvania, IAN TOBASCO, Department of Mathematics, University of Michigan, YOUSRA TIMOUNAY, JOSEPH D PAULSEN, Department of Physics, Syracuse University, ELENI KATIFORI, Department of Physics and Astronomy, University of Pennsylvania — Materials engineered through surface patterning are used for a broad array of applications, including flexible electronic and microfluidic devices, electronic skin, and many others. Microfabrication techniques based on elastic instabilities have attracted much attention because of their relative simplicity and potential for technological innovation. We employ Gaussian curvature as a mechanism for pattern formation: when a shallow curved shell is placed upon a liquid surface, well-defined domains of unidirectional wrinkles are formed. In the third part of this series of talks, we use finite element simulations and a theoretical approach based on the minimization of the elastic energy, to probe how the global arrangement of the patterns and wrinkling amplitude depends on the shape and curvature of the shell. We finally consider cases of shells with highly non-trivial boundary geometries and we demonstrate how this setup can be employed to harness surface structures with complex, yet predictable and controllable, topography. (This is part 3 in a 3-talk series).

*This work was partially supported by the NSF Award PHY-1554887, and by the MRSEC Grants DMR-1120901 and DMR-1720530.

Friday, March 8, 2019 11:15 AM - 1:15 PM

Session Y56 GSNP GSOFT: Machine Learning Approaches to Understanding Bulk Metallic Glasses and Other Amorphous Materials BCEC 255 - Corey O’Hern, Yale Univ - Tag(s): Focus

11:15AM Y56.00001: Machine Learning Stress Overshoot of Amorphous Solids*  
SHIYUN ZHANG (Presenter), WEN ZHENG, NING XU, Department of Physics, University of Science and Technology of China — When undergoing quasistatic shear, slow-quenched glasses exhibit an overshoot in shear stress, which decreases with the increase of quench rate and eventually evolves into a smooth crossover. However, the structure of glasses does not exhibit significant quench rate dependence. It thus remains unclear what determines the emergence of stress overshoot. Here, inspired by image recognition, we propose that stress overshoot of amorphous solids can be predicted from structures of solids using machine learning methods. Our results show that pure geometrical quantities such as local coordination number, bond orientational order and voronoi cell volume, which seem to weakly correlate with soft spots, have displayed very high predictive power of stabilities of amorphous solids, when combined with coarse-grain and machine learning methods. Besides, the stress overshoot in pinned systems suggests that our recently defined order parameter from the normal modes of vibration is a more general structure descriptor to identify stress overshoot. The high accuracy in identifying stress overshoot may imply that machine learning methods successfully capture the spatial correlation of the descriptor in some complicated way.

*National Natural Science Foundation of China (Grants No. 11734014)
11:27AM Y56.00002: Interplay of softness and rearrangements during avalanche propagation* GE ZHANG (Presenter), SEAN RIDOUT, ANDREA LIU, University of Pennsylvania — Disordered solids yield at a common shear strain of about 3%, but the behavior beyond yield is different for different systems and for systems with different histories. Foams can deform indefinitely without fracturing, many systems exhibit crackling noise or avalanche behavior, and still others exhibit shear banding and brittle fracture. Here we study an athermal, jammed packing of Hertzian particles that are sheared quasistatically. We identify the stress drops associated with rearrangements and then use steepest descent dynamics to study the evolution of the avalanches. We find that the avalanches consist of localized events that appear sequentially in well-separated locations of the sample. To understand this behavior, we exploit a machine-learning approach that has been developed to correlate local structure with dynamics in glassy systems. Following earlier work, we define a quantity softness that correlates with dynamical events during the avalanche process. We study the interplay of softness and dynamics: particles with higher softness are more likely to shift, while dynamical events affect local structure and hence softness. This interplay gives insight into the avalanche process.

*DOE DE-FG02-05ER46199/Simons327939

11:39AM Y56.00003: A Structural Measure of Effective- (Fictive-) Temperature and its Basis in Statistical Mechanics* MICHAEL FALK (Presenter), DARIUS D ALIX-WILLIAMS, Johns Hopkins University — The concept of fictive-temperature has long been utilized to characterize the processing dependence of glass structure, and has recently been shown to be predictive of metallic glass ductility. Some theories have hypothesized that it is actually a real temperature related to the configurational degrees of freedom of the glass, i.e. an ”effective-temperature,” notably the shear-transformation-zone (STZ) and soft-glassy-rheology (SGR) theories. Here we derive a thermodynamic integration scheme for calculating effective-temperature based on a 2-temperature hypothesis. To test this scheme we simulate a binary Cu-Zr metallic glass modeled with an EAM potential. Measures of the energy fluctuations associated with both the fast and slow degrees of freedom are measured during the glass quench. The resulting effective-temperature is consistent with estimates of fictive-temperature obtained from simulation in more heuristic ways. The results indicate that effective-temperature can be understood as a purely structural quantity. The method provides a means to measure the effective-temperature in the absence of fluctuations induced by shear and without resorting computationally expensive and impractical methods for explicitly measuring the configurational entropy.

*NSF DMR 1408685/1409560

11:51AM Y56.00004: Interaction potentials for bulk metallic glasses that can generate both brittle and ductile mechanical response* AYA NAWANO (Presenter), JAN SCHROERS, Department of Mechanical Engineering and Materials Science, Yale University, MARK SHATTUCK, Department of Physics and Benjamin Levich Institute, The City College of the City, University of New York, COREY SHANE O’HERN, Department of Mechanical Engineering and Materials Science, Yale University — Bulk metallic glasses (BMGs) have desirable mechanical properties such as high yield strength and elasticity compared to conventional alloys. However, BMGs are typically brittle, which limits their viability for structural applications. We perform molecular dynamics simulations to understand the ductility of model glass formers that interact via the Lennard-Jones, Stillinger-Weber, and embedded atom method potentials. We prepare binary BMGs over a range of cooling rates and perform athermal quasi-static uniaxial tension tests. We correlate the ductility with the fictive temperature, depth in the potential energy landscape, and measures of local structural order. We show that we can prepare samples that span a wide range of mechanical responses for all of the interaction potentials that we study. We also present a phenomenological spring network model that describes brittle and ductile response in terms of the number of springs that have broken and reformed in response to applied strain. We identify the parameters in the model that control the behavior of the stress versus strain curve, which allows us to achieve quantitative agreement with the results from the simulation of uniaxial tension.

*A. N. and C.S.O acknowledge support from NSF Grant No. CMMI-1462439.
12:03PM Y56.00005: Correlations in the shear flow of athermal amorphous solids: A principal component analysis
CELINE RUSCHER (Presenter), JOERG G ROTTLER, Stewart Blusson Quantum Matter Institute — Machine learning methods are increasingly being applied to problems in statistical physics, because they unveil aspects that would generally be neglected by traditional approaches. Here we apply principal component analysis, a method frequently used in image processing and unsupervised machine learning, to study the passage from the elastic to plastic flow regime in amorphous materials. Sets of particle displacements are obtained from simulations of a 2D amorphous model system in steady shear flow at different shear rates in the athermal limit. PCA produces a low-dimensional representation of the data, in which the principal directions clearly identify distinct differences between elastic (i.e. reversible) and plastic deformation. When deformation is accumulated over larger strains, shear localizes along bands, and PCA provides a quantitative measure of the increased degree of anisotropy in the flow patterns. We suggest that PCA can be a useful analysis technique that complements a traditional statistical description via correlation functions.

12:15PM Y56.00006: Analyzing the Internal Structure of Metallic Glasses through X-ray Absorption Fine Structure (XAFS) Spectroscopy*
HANYU ZHANG (Presenter), Case Western Reserve University, JENNIFER CARTER, Materials Science and Engineering, Case Western Reserve University, HAROLD CONNAMACHER, Electrical Engineering & Computer Science, Case Western Reserve University — This project aims to independently find the structure of metallic glasses through theoretical and experimental measures to see if current theoretical simulations yield the same structures as measured through experimental techniques. This is achieved by analyzing the accuracy of current molecular dynamics (MD) simulations to predict the amorphous structure of metallic glasses as characterized by x-ray absorption fine structure (XAFS) spectroscopy experiments. The influence of composition and processing techniques on the final structure is being explored on metallic glasses made from Ni, Co, Ta, and Nb. This project utilizes Large-scale Atomic/Molecular Massively Parallel Simulator (http://lammps.sandia.gov/), a MD software, to build the structures and Larch (Matthew Newville 2013) for data analysis. Used as a Python package, Larch gives us full control of the usage and implementation of our code. We are analyzing how closely the computer-generated structures matches with experimentally measured XAFS spectra. The validity of the computational approach has been tested using the pure crystalline solids.


*SOURCE at CWRU
CWRU Grad student funds

12:27PM Y56.00007: Local Yield Stress Analysis in Simulated 3D Glasses
DIHUI RUAN (Presenter), Johns Hopkins University, SYLVAIN PATINET, ESPCI, MICHAEL FALK, Johns Hopkins University — The ‘Local Yield Stress’ (LYS) method was developed to characterize the local structure of a atomistic model of a glass in a way that provides insight into its plastic response. The local yield stress is characterized as the incremental stress needed to induce a structural instability when an outer shell surrounding of a patch of atoms is deformed affinely along various shear orientations, while allowing the structure at the core to rearrange via athermal quasi-static (AQS) simulation. Here we generalize the LYS method to three-dimensional systems. We describe a method to democratically sample local shear orientations and triaxialities. By applying the LYS analysis to as-quenched glasses, we are able to identify the statistics of the local yield stress distribution. In order to assess to predictability and persistence of this measure, a correlation is computed between these local yield stresses and the observed plastic events when the glasses are undergoing shear deformation within in AQS simulations.
Bulk metallic glass design: What properties determine the glass-forming ability of multi-component alloys?

Yuanchao Hu (Presenter), Jan Schroers, Department of Mechanical Engineering & Materials Science, Yale University, Mark Shattuck, Benjamin Levich Institute and Physics Department, The City College of the City University of New York, Corey Shane O’Hern, Department of Mechanical Engineering & Materials Science, Yale University — Bulk metallic glasses (BMGs) possess a number of important properties, such as high strength and thermoplastic formability, which stem from the fact that they are structurally disordered in contrast to crystalline metals. Materials scientists have identified several features that are correlated with the glass-forming ability (GFA) of alloys. For example, good glass-formers are typically multi-component alloys composed of elements with atomic radii that differ by more than 10%. Most BMGs also possess a negative heat of mixing, which disfavors clustering of like atoms and hinders phase separation. However, researchers have not been able to a priori predict a new BMG-forming alloy. In this work, we perform computational studies of binary alloys to understand the relative contributions of geometric frustration and energetic frustration in determining the GFA. From a database of the heats of mixing and cohesive energies of binary atomic systems with atoms A and B, we show that most binary alloys follow a Berthelot combining rule, \( \varepsilon_{AB} = \left( \varepsilon_{AA} \varepsilon_{BB} \right)^{1/2} \), where \( \varepsilon_{AB} \), \( \varepsilon_{AA} \), and \( \varepsilon_{BB} \) are the depths of the attractive energy for pair interactions between AB, AA, and BB. We employ this mixing rule in molecular dynamics simulations of binary Lennard-Jones mixtures of atoms with equal sizes, but different cohesive energies. We measure the critical cooling rates of binary systems over the full range of cohesive energies and number fraction \( f_A \) of A and \( 1-f_A \) of B atoms. We show that good glass formers satisfy \( \varepsilon_{AA} > \varepsilon_{AB} > \varepsilon_{BB} \) when \( f_A < f_B \). We find that good glass-forming ability is determined by the conditions \( \varepsilon_{BB} << \varepsilon_{AA} \) and \( f_A < f_B \), and not correlated with the magnitude of the heat of mixing. In future studies, we will identify the variables that control the glass-forming ability in ternary alloys with atoms of different sizes and cohesive energies.

We acknowledge funding from Yale’s Center for Interface Structures and Phenomena (Y.H.) and the National Science Foundation Grant No. CBET-1605178 (C.O.).

Friday, March 8, 2019 11:15 AM - 1:51 PM

Session Y57 GSNP: Mechanical Metamaterials III BCEC 256 - Martin van Hecke, AMOLF

Non-reciprocal Dynamic Response of a Bilinear Lattice — Behrooz Yousefzadeh (Presenter), Brian J Ramirez, Chiara Daraio, Caltech — We report on the non-reciprocal dynamics of a one-dimensional bilinear lattice subject to continuous harmonic excitation. The bilinear nature of the lattice is due to elements within the unit cell that have different elastic moduli in compression and extension. We investigate the asymmetric wave propagation characteristics of bilinear lattices, and explain the results based on the nonlinear dynamics of the unit cell. We show that we can obtain different responses for the forward and backward configurations relying on either (i) the harmonic (frequency-preserving) operating range, or (ii) different onsets of instability. We discuss experimental realization of the unit cell based on 3D-printed macroscale structures.

This material is based upon work supported by the National Science Foundation under EFRI Grant No. 1741565.

Anomalous Collisions of Elastic Vector Solitons in Mechanical Metamaterials — Bolei Deng (Presenter), Harvard University, Vincent Tournat, Le Mans University, Pai Wang, Katia Bertoldi, Harvard University — We investigate via a combination of experiments and numerical analyses the collision of elastic vector solitons in a chain of rigid units connected by flexible hinges. Due to the vectorial nature of these solitons, very unusual behaviors are observed: while, as expected, the solitons emerge unaltered from the collision if they excite rotations of the same direction, they do not penetrate each other and instead repel one another if they induce rotations of opposite direction. Our analysis reveals that such anomalous collisions are a consequence of the large-amplitude characteristics of the solitons, which locally modify the properties of the underlying media. Specifically, their large rotations create a significant barrier for pulses that excite rotations of opposite direction and this may block their propagation. Our findings provide new insights into the collision dynamics of elastic solitary waves. Furthermore, the observed anomalous collisions pave new ways towards the advanced control of large amplitude mechanical pulses, as they provide opportunities to remotely detect, change or destruct high-amplitude signals and impacts.

*This work was supported by the National Science Foundation under Grant No. DMR-1420570 and EFMA-1741685 and from the Army Research Office under Grant No. W911NF-17-1-0147.
DOMINIC ROBE (Presenter), JUSTIN BURTON, Emory University — Amorphous materials show surprising and potentially useful acoustic properties at low frequencies. A notable example are the low-temperature acoustic properties of dielectric glasses, where quasi-localized, resonant states absorb energy and form memories of past excitations. To probe these phenomena at low-frequencies and over long times, we study the vibrational modes of quasi-2D networks of coupled oscillators using parallelized, GPU computing. We vary the degree of pre-stretching (tension) in the network, disorder in site masses, and disorder in the network connectivity. Even with a crystalline network structure, disorder in the site masses gives rise to low-frequency, quasi-localized modes, similar to those studied in glasses and jammed systems. The anharmonic properties of these modes become exceedingly important over thousands of cycles of oscillations. In addition, in order to realize some of these properties in the laboratory, we have developed a mechanical metamaterial fabricated from a silicon nitride layer on a silicon wafer using standard photolithography. The degree and type of disorder can be tuned prior to fabrication, leading to a high-Q, constituent-level visualization of vibrational modes in disordered materials.

*National Science Foundation DMR Grant No. 1455086

KOJI SATO (Presenter), RYOKICHI TANAKA, Tohoku University — It has been shown by Kane and Lubensky that certain classical chains admit topologically protected zero-energy modes that are localized on the boundaries. Although the static features of the localized modes are well captured by linearized equations of motion, the description of their dynamics requires fully nonlinear treatment. We study quasi-periodic solutions of the nonlinear equations of motion of one-dimensional classical chains. Such quasi-periodic solutions correspond to periodic trajectories in the configuration space of the discrete systems, which allows us to define solitons without relying on a continuum theory. Furthermore, we study the dynamics of solitons in inhomogeneous systems by connecting two chains with distinct parameter sets, where solitons show intriguing transmission/reflection properties at the boundary of the two chains.

SERGIO LEIVA (Presenter), CLAUDIO FALCON, ALVARO S NUNEZ, University of Chile — The interaction between phonons and an external elastic deformation within an elastic material can produce various controllable effects. It is known that these external elastic deformations endow the phononic dynamics (their wave equations) with a gauge structure similar to the one of electromagnetism, even though phonons are electrically neutral. An appropriately chosen deformation can generate an acoustic Hall effect among other experimental signals. We set out to study the elastic wave-dislocation interaction and then extend it to an interaction with a distribution of dislocations. Our formalism is based on finding an equation of motion for a wave in a medium with a static deformation in the regime in which the wave does not alter the deformation but its propagation is affected by the presence of this dislocation. With the above, we find an analogy between the Aharonov-Bohm effect and a dislocation. Our study provides a powerful tool to export topological properties to the context of elasticity and, with this, to produce more and better materials for nanoscience. The periodic case of the problem is also studied, and the new topological mechanical material arising from such periodic structure is discussed.

*Millenium Nucleus for Soft Smart Mechanical Metamaterials

MARTIN BRANDENBOURGER (Presenter), XANDER LOCSIN, CORENTIN COULAIS, University of Amsterdam — Over the last few years, there has been an explosion of activity on non-reciprocal metamaterials, namely, which transmit motion in one direction, but block it in the other. However, to date, non-reciprocal transmission has only been achieved for a limited range of frequencies and input magnitudes. Here, we introduce a novel robotic mechanical metamaterial that overcomes these limits. Each building block is a minimal robot that is able to sense the behavior of its neighbor and act consequently, which opens the way to new types of interactions. We leverage this platform to program asymmetric non-equilibrium interactions and show that the system as a whole supports first-of-their-kind unidirectionally amplified waves. As a result, the system achieves unprecedented broadband and attenuation-free unidirectional transport of mechanical energy.
Thermally-triggered tunable vibration attenuation in 3D-printed mono-material lattice metamaterials  

YANGBO LI (Presenter), SIYU CAO, YAN SHEN, China Three Gorges University — Phononic crystals, capable to tailor mechanical wave propagation and displaying omnidirectional band gaps, are vital for numerous potential applications such as wave filtering, waveguiding, acoustic cloaking, and energy harvesting. In raw materials, vibration mitigation depending on intrinsic damping feature usually cannot be adjusted easily and broad attenuation frequency ranges is still scarce in these materials. Here, we propose a novel approach and metamaterial design with the ability of thermally-triggered tunable vibration mitigation in multiple frequency ranges, which arise from the local resonance mechanism. The proposed method utilizes reversible Young's Modulus-temperature relationship of glassy polymer and non-uniformity of steady temperature field in solid structures. Through numerical simulations and low amplitude transmission testing, we demonstrate that the proposed method and metamaterials can exhibit broad and multiple omnidirectional band gaps. The finding reported here provides a new routine to design phononic metamaterial systems with tunable band gaps, offering a wide range of potential applications in harsh environmental conditions and being extended to baseline lattices with other topologies.

Electric-field-triggered instabilities in dielectric elastomer composites: application to tunable phononic crystals*  

MICHAEL JANDRON (Presenter), Naval Undersea Warfare Center, Newport, RI 02841, USA, DAVID HENANN, School of Engineering, Brown University, Providence, RI 02906, USA — Tunable phononic crystals offer promising directions for elastic wave control. When phononic crystals are composed of soft dielectric elastomers, their band-gaps may be manipulated through an applied electric field. In addition, the rich electromechanical instability landscape in these materials offers opportunities for enhanced tunability. In this work, we report on our numerical simulation capability and show how electrically triggered instabilities provide a new route to tunability in phononic crystals composed of dielectric elastomers. The result is a comprehensive view of the instability landscape in dielectric elastomer composites, the suggestion of favorable actuation arrangements, as well a general strategy for exploring enhanced band-gap tunability.

*This work is supported through the Naval Undersea Warfare Center In-house Laboratory Independent Research (ILIR) Program and Brown University School of Engineering.

Non-Abelian sound in mechanical metamaterials  

MICHEL FRUCHART (Presenter), VINCENZO VITELLI, University of Chicago — The propagation of mechanical waves in a medium is shaped by the microscopic arrangement of the oscillating elements. Here, we consider a material where the propagation of sound can be ruled by a band structure with a non-Abelian Berry connection stemming from the presence of an emerging non-crystallographic symmetry. This has dramatic consequences on the wave propagation inside an inhomogeneous medium and at interfaces.

Acoustic Bianisotropic Impedance and Hyperbolic Propagation in Metasurfaces  

LI QUAN (Presenter), Department of Electrical and Computer Engineering, The University of Texas at Austin, ANDREA ALU, Advanced Science Research Center, City University of New York — The strong analogies between electromagnetic and acoustic wave propagation have led to the discoveries of various forms of electromagnetic metamaterials and of their acoustic counterparts. However, the longitudinal properties of acoustics waves in fluid make the effective bulk modulus and effective impedance in acoustics inherently isotropic, which marks a strong difference, and a limitation of acoustic metamaterials and metasurfaces, compared to electromagnetics. Several important concepts in electromagnetics inherently require anisotropic impedance profiles, such as hyperbolic wave propagation, and therefore cannot find a direct counterpart in acoustics. Motivated by this limitation, in this talk we discuss a way to realize acoustic bianisotropy metasurfaces, relying on strong nonlocalities over the surface. Based on this approach, we introduce a design for hyperbolic acoustic metasurfaces with enhanced local density of states for sound, and inherent imaging and canalization properties. These design approaches based on strong nonlocality may also be extended to electromagnetics, offering a new path towards hyperbolic wave propagation.
1:15PM Y57.00011: Vortex Phase Singularities in Multiple Slit Interference Patterns in Chaotic Metamaterial Billiards  JORGE JOSE (Presenter), Indiana University Bloomington, NATALIA M LITCHINITSER, Electrical and Computer Engineering, Duke University — A wide range of diffractive wave interference patterns have been produced by using different planar slit configurations. In particular, situations have been recently studied having more than two slits to test the validity of the superposition principle in wave and quantum mechanics. Here we study the presence of vortex or phase singular fluctuations produced by interference patterns in chaotic billiards with a variable number of diffraction slits. We report numerical wave simulation results of integrable and non-integrable D-shape billiards, having a variable number of slit type configurations. Embedded in this D-shaped chaotic billiards we consider different combinations of positive (PIM) and negative index of refraction (NIM) materials. We compare the topological charge in the phase singularities and their correlations in the different interference pattern configurations produced. We studied closed and open billiards. We found different types of topological charge properties directly related on the geometry, the number of slits as well as the different embedded PIM and NIM configurations. The properties of the vortex pattern configurations and their correlations change dramatically as a function of the geometry of the cavity and the number of slit configurations.

1:27PM Y57.00012: Liquid crystal elastomer based mechanical metamaterials for lightweight extreme impact energy absorption*  SEUNG-YEOL JEON (Presenter), ZEYU ZHU, Mechanical Engineering, Johns Hopkins University, NICHOLAS TRAUGUTT, Mechanical Engineering, University of Colorado Denver, CRISTINA MARTIN LINARES, Mechanical Engineering, Johns Hopkins University, CHRISTOPHER YAKACKI, Mechanical Engineering, University of Colorado Denver, THAO NGUYEN, SUNG KANG, Mechanical Engineering, Johns Hopkins University — Liquid crystal elastomers (LCEs) are one of the most promising materials in the field of impact energy absorption, due to their exceptional energy dissipation behavior arising from the coupling of the relaxation dynamics of liquid crystal (LC) molecules and polymer chains. In this study, we report snapping-based metamaterials composed of LCEs for lightweight extreme impact energy absorption. We synthesized LCEs based on a two-stage thiol–acrylate reaction to program the order of LC molecules and chain alignment within beam elements. We characterized the energy absorption behaviors of the programmed LCE beams with bistability at various strain rates. We found that our LCE-based metamaterials show orders of magnitudes better specific energy absorption compared with previous works and their absorption capability is further enhanced as the strain rate increases. We could also tune the metastable energy states by controlling the strain rates. The combination of the inherent enhanced dissipation of LCEs with snapping-based architectures allows a new class of mechanical metamaterials with excellent energy absorbing capabilities.

*This work was supported by the start-up fund from Whiting School of Engineering at Johns Hopkins University and the Army Research Office (W911NF-17-1-0165).

1:39PM Y57.00013: Anisotropic Toughness and Crack Growth on Cubic SiC  FAZLE ELAHI (Presenter), MD Z HOSSAIN, University of Delaware — Molecular dynamics calculation is executed applying the Stillinger-Weber atomic interaction to explore the anisotropic properties of cubic SiC. A solid 3C-SiC with predefined edge crack is subjected to uniaxial tensile load along its crystallographic axis. Three major directions (100), (110) and (111) are studied in this work. The crack propagation path is noticeably different in three directions which in return bring variation in critical energy absorption rate. In (100) plane toughness is 70% higher than in (111) plane. The reason behind this variation is the crack propagation path through the atomic system. In (100) direction, Crack starts growing at 7% strain when the stress is 21.9 GPa. The crack face atoms rather than bonds which hinder the growth and require more energy to break. The sole criterion for growth is bond breaking which drive the crack to branch out and propagate through (110) crystallographic plane. At the point of bifurcation, the solid absorb some energy which increase the fracture toughness. However, in other two planes, (111) and (110), crack sees no obstacle and bonds are parallel to the loading direction. They require lower critical energy release rate for crack growth. So, the crack evolve through the straight path and contain lower toughness.
BRANKO BIJELJIC (Presenter), MARTIN BLUNT, QINGYANG LIN, ALI RAEINI, AHMED ALRATROUT, YOUSEF AL-KHULAIFI, AMER ALHAMMADI, YING GAO, Earth Science and Engineering, Imperial College London — Understanding of multiphase flow, transport and reaction phenomena in disordered porous media has recently been transformed by the advances in X-ray and NMR imaging, which inspired new concepts in pore-scale modeling. More accurate static and dynamic experimental description of solid and fluid(s) distributions in the pore space enabled simplifications in descriptions of spatio-temporal complexities through introduction of the intrinsic functions characterizing flow, transport and reaction in the form of distributions, rather than average values.

This concept is illustrated by the predictive modeling of flow and transport on micro-CT images of subsurface porous media validated against NMR experiments. Furthermore, a novel set of ideas used for characterising physical and chemical heterogeneity and their coupled impact on the effective reaction rates and dissolution patterns in multi-mineral porous media will be discussed.

One of the key breakthroughs was achieved by devising differential imaging tomography which provides full information of connectivity at sub-micron scale. Examples will be provided for multi-modal function description of single phase flow and transport, characterisation of initial and recovered oil from micro-porosity in steady-state two-phase flow, and determination of capillary-number dependent flow intermittency.

Furthermore, advances in in-situ characterisation of pore morphology and wettability will be presented, where a distinct pore-morphology signature is identified for unconsolidated and consolidated media. Both pore morphology and wettability have a large impact on the potential for layer flow. A distinct mixed-wet state can be identified where two fluid phases remain connected over a wide range of saturation. This state can be designed to improve oil recovery, the performance of batteries, fuel cells, catalysts, and other disordered porous materials.

11:51AM Y58.00002: Disorder-mediated wetting transitions in unstable imbibition  
AMIR PAHLAVAN (Presenter), Princeton University, LUIS CUETO-FELGUEROSO, Universidad Politécnica de Madrid, GARETH MCKINLEY, RUBEN JUANES, Massachusetts Institute of Technology — An archetypical example of pattern formation is the front instability that emerges when a less viscous fluid displaces a more viscous fluid in a Hele-Shaw cell. This instability, however, has been studied only in drainage—when the invading fluid is nonwetting. Here we show that the interplay between wettability and disorder leads to novel instability regimes. We inject a more wetting liquid into a rough Hele-Shaw cell filled with a less wetting, more viscous liquid. At low injection rates, the displacement is full across the cell gap. Above a critical injection rate, however, a wetting transition occurs and thin films of the invading liquid become entrained on the rough surfaces. This wetting transition is accompanied by a drastic change of the front instability, leading to a dendritic pattern. Our observations point to the crucial role of disorder in pattern formation during fluid-fluid displacement, and its important implications for multiphase flows in porous media.

12:03PM Y58.00003: Suppressing fingering instabilities using gradients in porous media  
NANCY B LU (Presenter), Chemical and Biological Engineering, Princeton University, JANINE NUNES, Mechanical and Aerospace Engineering, Princeton University, SUJIT DATTA, Chemical and Biological Engineering, Princeton University — Drainage, the displacement of a wetting fluid from a porous medium by an immiscible non-wetting fluid, arises in key technological problems including oil recovery, groundwater contamination, and waste CO2 sequestration. When the displacing non-wetting fluid is less viscous than the displaced fluid, Viscous Fingering occurs. By contrast, when the displacing fluid is more viscous than the displaced fluid, Capillary Fingering occurs. These two processes lead to disordered finger-like displacement pathways. For both cases, we find that a pore size gradient stabilizes the flow—the fluid flows uniformly without fingering. For Viscous Fingering, this stabilization only occurs below a threshold flow rate [1], while for Capillary Fingering, it only occurs when the gradient exceeds a static geometric criterion. Knowing these two suppression criteria provides a new way to control fingering instabilities in porous media.

Cooperative mobilization of emulsion droplets in porous media

SHIMA PARSA MOGHADDAM (Presenter), Harvard University, MOHAMAD ALI BJIARCHI, Sharif University of Technology, Iran, MARIA JIMENEZ, University of Granada, Spain, DAVID A WEITZ, Harvard University — We study the cooperative dynamics of monodisperse droplets in 2D porous media using confocal microscopy and particle tracking. The size of the droplets are of the same order of the pore sizes of the medium and are generated on demand and injected into the porous media. We measure the dynamics of the carrier fluid at pore level and track the mobilization of droplets simultaneously. We find that upon arrival or mobilization of one droplet, large pressure fluctuations emerge across neighboring pores. The pressure fluctuations result in cooperative mobilization of droplets. The behavior of emulsions within porous media is an important issue in industry and environmental studies such as water remediation.

Transport of Microgels in a Microfluidic Constrictive Channel*

SHUAIJUN LI (Presenter), JING FAN, City College of New York — The transport of soft bodies in narrow channels are remarkably common in biological systems and industrial processes. During the transport process, the soft body deforms and blocks the channel, and thus induces a pressure drop across the channel. In this work, we study the motion and deformation of microgels in a constrictive channel with a circular cross-section. Employing elasticity theory with small deformation assumption, we find the correlation among the built-up pressure, the mechanical properties of microgels, and the geometry of the channel. An approximate method is applied to estimate stress distribution at the contact surface between the deformable microgel and the channel. We then conduct experiments in constrictive micro-channels using microgels with well controlled sizes and mechanical properties to validate the effectiveness of our analysis. Compared to previous studies on microgel transport through constrictive channels, our result features an optimal balance between simplicity and accuracy. The methodology can be easily extended to various natural and engineered processes involving transport of soft bodies in narrow channels.

*Acknowledgment is made to the donors of the American Chemical Society Petroleum Research Fund for partial support of this research.

Fluid-solute-colloid interactions in porous media and its implications for enhanced oil recovery

SANGWOO SHIN (Presenter), University of Hawaii at Manoa — Flows of colloidal suspensions containing a variety of solutes in porous media are widely found in nature as well as artificial settings such as hydrocarbon recovery, blood flow, water purification, and coastal habitats. Such environments often exhibit spatiotemporal inhomogeneity in the solute and colloid distribution. While it is naively expected that the colloidal particles advect with the flow, non-equilibrium interactions between the fluid, solute, and the colloids may lead to unique colloidal dynamics. We present a number of scenarios in which the colloidal particles can be captured and accumulate continuously in localized regions in porous media despite the presence of strong pore flow due to the fluid-solute-colloid interactions. We link our findings to the chemical flooding process to provide useful insights into the enhanced oil recovery.

Phase change in disordered media: intermolecular forces control simultaneous evaporation and condensation

KE XU (Presenter), Massachusetts Institute of Technology, AMIR PAHLAVAN, Princeton University, RUBEN JUANES, Massachusetts Institute of Technology — We investigate phase change and fluid-fluid redistribution in porous media using micromodel experiments, in which air is injected to displace water. At late times, long after injection stops, we expect the system to arrive at a steady-state equilibrium configuration. Instead, we observe the condensation and growth of liquid droplets at the expense of the evaporation of liquid bridges. This is surprising, given that the liquid bridges are at lower pressure than the liquid droplets. We show that this counterintuitive behavior emerges from the influence of intermolecular forces on the instability of condensing thin liquid films. Our observations therefore point to a new physical mechanism for phase change in disordered media, which drives fluid organization at the pore scale, and has important implications for multiphase-flow properties at the macroscale.
this structure will be integral in robustly applying polymer solutions to groundwater remediation and EOR. We understand this switching as a dynamic coupling between single-polymer conformations and pore-scale flow. We directly observe the flow of polymer solutions in model porous media using confocal microscopy. However, we find that the flow is not purely chaotic, as is commonly assumed: it can adopt two distinct structures, which switch stochastically.

Enhanced oil recovery (EOR); in some cases, the modified flow allows the flooding fluid to sweep a greater portion of the aquifer or reservoir. This enhanced sweep is believed to be linked to unstable flow observed above a threshold flowrate.

Utilizing microfluidics, we flow a purely elastic fluid through a hexagonal array of cylindrical pillars at a range of flow speeds, where the transition to chaotic flow occurs at a critical ratio of the polymer relaxation time to flow time scale (Deborah number). We introduce finite disorder to the system – corresponding to a random perturbation of the pillars by 10% of the lattice spacing – delays the transition to Deborah number, De ~ 1, and reduces the magnitude of the chaotic velocity fluctuations. Larger disorders appear to completely suppress the transition within the tested flow range up to De ~ 5. Examination of the Lagrangian strain rate correlations reveal that disorder broadens the distribution of excitation frequencies in the system, suggesting a potential mechanism for stabilizing the elastic flow.

Disorder Suppresses Chaotic Viscoelastic Flow

Challenges associated with highly confined systems arise beyond critical flow conditions, but little is known about the implications of geometric order/disorder for this transition. Utilizing microfluidics, we flow a purely elastic fluid through a hexagonal array of cylindrical pillars at a range of flow speeds, where the transition to chaotic flow occurs at a critical ratio of the polymer relaxation time to flow time scale (Deborah number). We introduce finite disorder to the system – corresponding to a random perturbation of the pillars by 10% of the lattice spacing – delays the transition to Deborah number, De ~ 1, and reduces the magnitude of the chaotic velocity fluctuations. Larger disorders appear to completely suppress the transition within the tested flow range up to De ~ 5. Examination of the Lagrangian strain rate correlations reveal that disorder broadens the distribution of excitation frequencies in the system, suggesting a potential mechanism for stabilizing the elastic flow.

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1:51PM Y58.00012: Hydrogels dehydrate liposomes: the structural fate of lipid nanoparticles in the extracellular matrix*  
SARITH BANDARA (Presenter), THOMAS MOLLEY, HOJUN KIM, PRIYALINI BHARATH, University of Illinois at Urbana-Champaign, KRISTOPHER KILIAN, University of New South Wales, CECILIA LEAL, University of Illinois at Urbana-Champaign — Drug-loaded liposomes are the most successful nanomedicine to date, with multiple FDA-approved systems for a myriad of diseases. While liposome circulation time in blood and retention in tissues have been studied in detail, the structural fate of liposomes—and nanoparticles in general—in the body has not been extensively investigated. This presentation explores the structural fate of liposomes in a synthetic hydrogel system with the aim of understanding the possible restructuring effects that liposomes experience in the natural extracellular matrix. Small angle X-ray scattering, confocal microscopy, and cryogenic transmission electron microscopy data demonstrate that poly(ethylene glycol) (PEG), gelatin, and alginate hydrogels cause 200-nm liposomes of 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) to transform into micrometer-sized aggregates. These aggregates are composed of multilamellar vesicles around 100 nm in diameter with a mean interlamellar separation of 5.5 nm. Protecting the liposomes with a corona of PEG damps this restructuring effect, making the multilamellar vesicles formed less stable. We attribute this unilamellar to multilamellar transition to an osmotic driving force from the hydrogel environment.

*This work is supported by the NIH (1DP2EB024377-01).

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y59 GSOFT: Soft Composites: Mechanics and Structure II  
BCEC 257B - Moumita Das, Rochester Institute of Technology - Tag(s): Focus

11:15AM Y59.00001: Dynamics of interacting nanoparticles in complex polymeric solutions* [Invited]  
JACINTA CONRAD (Presenter), University of Houston — The nanoscale mechanisms underlying the unusual mechanical properties of polymer nanocomposites and other soft composites remain elusive. Because nanoparticles are of comparable size to heterogeneities present in many complex fluids, their dynamics cannot be described through the framework of micro rheology but rather decouple from the bulk fluid properties. Indeed, nanoparticles diffuse many orders of magnitude faster than expected when coupled to complex fluid relaxations on similar length scales, or much more slowly than expected when physically obstructed. Interactions between the nanoparticles, arising from high particle densities and/or chemical surface modifications, can further modify their dynamics. To understand the underlying physics of transport in this size regime, we measure the dynamics of nanoparticles and polymers in solution, which are simple models of polymer nanocomposites with well-controlled and tunable heterogeneities, using x-ray photon correlation spectroscopy and neutron spin-echo spectroscopy. Electrostatic charges lead to long-range interactions between the particles in organic solvents without disrupting the structure or dynamics of the surrounding polymer solution. The long-range interparticle interactions slow nanoparticle dynamics across the interparticle distance, even though the nanoparticle dynamics are subdiffusive and coupled to the polymer relaxations. Grafted polymers help to stabilize the nanoparticles in complex fluids and lead to soft physical interactions between the grafted particles and the surrounding polymer chains that alter their transport. Our work illustrates that the particle surface chemistry sensitively modifies the transport of nanoparticles through complex media.

*Welch Foundation (E-1869); NSF (CBET-1705968)

11:51AM Y59.00002: Deformation in polymer nanoparticle composites (PNC) at ultra high loading: interplay of jammed solids and glassy mechanics  
EMILY LIN (Presenter), ROBERT RIGGLEMAN, University of Pennsylvania — Polymer nanoparticle composites (PNC) with ultra high loading of nanoparticles (NP) (>50%) have been shown to exhibit simultaneously improved strength and stiffness without compromising, and sometimes even improving, the toughness compared to the neat systems. As a result, these composites have become an interesting class of material for a variety of applications. Furthermore, when the particle volume fraction approaches random-close-pack, these composite systems become a combination of a jammed solid (the random-close-packed NPs) filled with a glass-forming polymer in its interstices. In our study, we aim to understand the origin of these performance enhancements by examining the dynamics of both polymer and NPs during active deformation. We performed molecular dynamics simulation of coarse-grained, glass forming polymers equilibrated in the voids of a random-close-packed NP packing and subsequently applied uniaxial tensile strain to the bulk system. We examined the mechanical characteristics of the PNC systems with different polymer fill fractions at temperatures below the glass transition temperature. We also compared the NP rearrangement behavior in the presence of polymer to the neat NP systems to provide a molecular view of the toughening mechanism in these materials.
Visualization and Mechanical Study of a Transparent Filled Rubber

ZACH GAULT (Presenter), ZSOLT TERDIK, JOERG WERNER, FRANS A SPAEPEN, DAVID A WEITZ, Harvard University — Filled rubbers are composite materials containing two interpenetrating phases: crosslinked elastomers, and a ‘filler’ consisting of colloidal particle aggregates. Above a critical volume fraction, the colloidal aggregates form a system-spanning subnetwork that reinforces the elastomer network and introduces a new energy loss mechanism at low strains of only 1-5%. This loss mechanism, known as the Payne Effect, is one of the mechanical hallmarks of filled rubbers and is a major contributor to rolling friction in tires. We create a transparent model filled rubber which exhibits the mechanical hallmarks of traditional filled rubbers, but can be optically imaged. Fluorescent silica nanoparticles provide optical contrast needed to distinguish the two phases. With this system we can directly observe microstructural changes of filler particle aggregates during in situ shear deformation. We complement these observations with bulk rheological tests to gain new insight into the microscopic deformations underlying the Payne effect. By controlling filler loading and crosslink density, we can tune the microstructure of our composite to better understand the relation between its structure and mechanical properties.

Mechanical response of composite biopolymer networks in the vitreous gel in our eyes*

PANCY LWIN (Presenter), SCOTT FRANKLIN, DAVID ROSS, GEORGE THURSTON, MOUMITA DAS, Rochester Institute of Technology — The vitreous gel in the human eye is a viscoelastic composite network of stiff collagen fibers and softer hyaluronic acid (HA) polymers. Its material properties are critical to vitreous function, and ultimately to that of the eye, and depend on applied stresses, concentrations, and constituent filament stiffnesses. Although it has long been known to undergo dramatic changes with aging and disease, the key vitreous gel phase transitions and their mechanical consequences are not well understood. We mathematically model and investigate the mechanical response of the vitreous gel by modeling it as a composite network made of (i) a stiff network of collagen fibers, and (ii) a flexible polyelectrolyte network of HA. Our results relate the linear and nonlinear mechanical response of this composite network to the structure, micromechanics, and concentrations of the constituents, and may provide insights into mechanical changes associated with vitreous disorders.

*The research was funded by the National Science Foundation via the award NSF/CBET-1604712.

In situ mechanical reinforcement of polymer hydrogels via metal-coordinated mineralization

NIELS HOLTEN-ANDERSEN (Presenter), Massachusetts Institute of Technology — Over millions of years, various types of organisms have evolved the ability to synthesize exceptionally strong and tough organic-inorganic composites through cell regulated in situ mineralization of macromolecular material scaffolds. Borrowing inspiration from such complex biomimetic material processing, we have found that metal-coordinate polymer networks can be utilized as model macromolecular scaffolds for controlled in situ hydrogel mineralization. Starting with a monodisperse metal-coordinate polymer hydrogel network, we show that metal-ion coordination crosslinks can serve as nucleation sites for mineral growth, thereby allowing significant mechanical reinforcement upon limited mineralization of the polymer hydrogel scaffold. By targeting nanoscale mineral particle growth directly at the metal-coordinate network crosslink sites, we observe simultaneous significant increases in stiffness and magnetization of the resulting hydrogels with less than 0.1% volume of minerals. We demonstrate that the method of controlling mineralization of polymer hydrogel networks through metal-coordination is general, and therefore potentially offers a broad platform for the development of new bio-inspired organic-inorganic composite materials processing systems.

Confocal Microrheology of biopolymer Hyaluronan*

JARED WELCH (Presenter), SCOTT FRANKLIN, GEORGE THURSTON, MOUMITA DAS, DAVID ROSS, Rochester Institute of Technology — Hyaluronan is a biopolymer that is found throughout the human body in connective tissue. To investigate the viscoelastic properties of this material the diffusion of carboxylate spheres in buffered solutions containing varying concentrations of 60 kDa Hyaluronan was monitored using a confocal microscope. The solutions contained a mix of D2O/H2O to match the density of the spheres. The trajectories of the spheres were analyzed using one- and two-point microrheology analysis methods. At low concentrations of hyaluronan the dynamic viscosity was extracted using the Stokes-Einstein relation. We compare these viscosities with theoretical models and use them to estimate the overlap concentration. At high concentrations, the spheres move in a way that does not correspond to normal diffusion, and the mean-squared displacement vs. lag time displays an interesting concentration-dependent inflection point. We compare results from one- and two-point particle tracking analysis.

*This research is funded by the National Science Foundation via the award NSF/CBET-1604712.
A continuum model of the viscoelastic response of the vitreous gel
LOGAN MELICAN (Presenter), School of Mathematical Sciences, Rochester Institute of Technology, SCOTT FRANKLIN, GEORGE THURSTON, School of Physics and Astronomy, Rochester Institute of Technology, DAVID ROSS, School of Mathematical Sciences, Rochester Institute of Technology, MOUMITA DAS, School of Physics and Astronomy, Rochester Institute of Technology — The vitreous gel is a transparent, hydrated extracellular matrix filling the posterior cavity of the eye behind the lens and is surrounded by and attached to the retina. More specifically it is a composite material primarily made of a dilute network of stiff collagen fibrils and flexible polysaccharide (Hyaluronic Acid) chains within an aqueous solution. It has complex viscoelastic properties but becomes progressively fluid-like with age, leading to a number of pathologies. Here we develop a continuum mathematical model of the vitreous gel by drawing from two-fluid models of semi dilute polymer solutions. We solve a system of coupled partial differential equations for the soft and flexible networks, and the fluid via a combination of spectral and Runge-Kutta methods, and obtain the frequency dependent viscoelastic properties of the system as a function of polymer stiffness and density, and fluid viscosity. Our results will help to better understand rheological experiments on the vitreous, and provide new insights into the origin of vitreous liquefaction.

*This research is funded by the National Science Foundation via the award NSF/CBET-1604712.

Optical tweezers microrheology reveals the viscoelastic properties of entangled ring-linear DNA blends
KARTHIK REDDY PEDDIREDDY (Presenter), MEGAN LEE, RAE ROBERTSON-ANDERSON, University of San Diego — Solutions of entangled polymers display complex and intriguing viscoelastic properties that are still poorly understood. While the reptation model can describe the viscoelastic properties of entangled melts of linear polymers, the model is ill-equipped to deal with circular or ring polymers, blends of polymers of varying topologies, or solutions of polymers at concentrations near the critical entanglement concentration. DNA is an excellent model system for resolving this issue as it occurs naturally in linear and circular forms. Here, we use optical tweezers microrheology to measure the linear and nonlinear viscoelastic response of semidilute and entangled blends of circular and linear DNA. We characterize the dependence of viscoelastic properties on the ratio of circular and linear chains in the blend as well as the overall solution concentration. Our results show intriguing properties of blends compared to single-component systems including increased stiffness coupled with faster relaxation rates.

*This work was funded by AFOSR Grant No. FA9550-17-1-0249 and NSF-CBET-1603925

Phase behavior and morphology of multicomponent mixtures
SHENG MAO (Presenter), Princeton University, DEREK KULDINOW, Yale University, MIKKO HAATAJA, ANDREJ KOSMRLJ, Princeton University — Multicomponent systems are ubiquitous in nature and industry. While the physics of binary and ternary liquid mixtures is well-understood, the thermodynamic and kinetic properties of N-component mixtures (N>3) have remained relatively unexplored. Inspired by recent examples of intracellular phase separation, we investigate equilibrium phase behavior and morphology of N-component mixtures within the Flory-Huggins theory of regular solutions. In order to determine the number of coexisting phases and their compositions, we developed a new algorithm to construct complete phase diagrams, based on numerical convexification of the discretized free energy. Together with a Cahn-Hilliard approach for kinetics, we employ this method to study mixtures with N=4 and 5. We report on both the coarsening behavior of such systems and the resulting morphologies in 3D. The number of coexisting phases and their compositions can also be extracted with Principal Component Analysis (PCA) and K-Means algorithms. Finally, we discuss how to reverse engineer the interaction parameters and volume fractions of components in order to achieve a range of desired packing structures, such as nested "Russian dolls" and encapsulated Janus droplets.

*This work was supported by NSF awards no. DMR-1420541 and EEC-1559973.

Anisotropic self-assembly of polarizable colloidal mixtures
ZIWEI WANG (Presenter), ERIK LUIJTEN, Northwestern University — Particles with directional interactions represent promising building blocks for new functional materials and are often realized by particles with anisotropic shape or with patchy directional bonds. Here we demonstrate that binary suspensions of oppositely charged size-asymmetric colloids robustly self-assemble into a variety of anisotropic superstructures, resulting from the many-body dielectric effects which impart effective directionality to the inter-particle interactions. Via simulations, we illustrate how both local coordination number (connectivity) and fractal dimension can be well controlled through variation of the size ratio and the mismatch in relative permittivity. The mechanism we have identified offers a potential avenue to designing materials with controllable structural properties.
Beyond Bi-disperse: A study of propensity in a Kob-Andersen Quartet*
CORDELL DONOFRIO (Presenter), ERIC WEEKS, Emory University — We simulate the Kob-Andersen bidisperse glassformer system to study dynamics near the glass transition. As the name implies, the standard KA system is composed of two different sized particles. In our system we split the population of large particles into its own binary where half are increased in size and the other half decreased by the same (small) percentage. A similar binary is created for the small particles. Isoconfigurational ensemble runs are then made to understand the influence of slight “errors” in particle size. An isoconfigurational ensemble is a series of simulations, each with the same starting positions but with randomized velocities consistent with the temperature (following Widmer-Cooper et al, 2004). The “propensity” of each particle is defined as the average motion of that particle, averaged over this ensemble. While normally this is done with the exact same particles in the starting positions, having multiple variants of each particle size allows for slight changes to be made to the structure at the start of each run in the isoconfigurational ensemble. We seek to find how large of a change in structure is needed to remove propensity from the system.

*NSF (DMR-1609763)

Plant Inspired Soft Material Composite with Liquid Encapsulations
AMRITA KATARUKA (Presenter), Civil and Environmental Engineering, University of Illinois at Urbana Champaign, SHELBY HUTCHENS, Mechanical Science and Engineering, University of Illinois at Urbana Champaign — Plants are unique mechanical structures that combine high water content with structural elements. Unlike common soft material and liquid composites (ex: hydrogel), plants compartmentalize their water using semi-permeable membranes. We synthesize plant tissue analogs, idealized as closely packed water droplets surrounded by thin walls of PDMS, to understand their mechanical response. The analogs are created by high internal phase emulsion templating. We choose PDMS because it is highly stretchable and semipermeable yet does not swell in water. It also has a tunable modulus that allows us to capture the varied range of stiffness in flora. However, due to the high viscosity of PDMS prepolymer, adding large quantities of water to the emulsion demands very high shear force. Using microfluidics is also difficult because high pressure – required to make PDMS flow through the channels – easily ruptures device assembly. To overcome these challenges, we combine shear-mixing with centrifugation. The influence of viscosity ratio, amount of stabilizer, and fabrication specifics on droplet generation and structure are investigated. We find that with careful manipulation of the above governing parameters, the micromorphology of the composite can be designed to within plant-cell relevant ranges.

Programming shape changes in tri-stable bilayer structure*
SHICHENG HUANG (Presenter), LIN WANG, DONG WANG, XING GUO, GUANGCHAO WAN, Dartmouth College, JING FAN, Mechanical Engineering, City College of New York, ZI CHEN, Dartmouth College — The programmable shape transition in response to external stimuli has attracted increasing attention. Multi-stable structures represent a stimuli-responsive structure that features more than one stable shape and transition from one to another, appropriate for applications such as in micro-robotics. Although bi-stable structures have been extensively investigated, very few studies have been focusing on tri-stability of such structures. Here we design a partially bonded bilayer structure composed of a SMP layer and a rubber strip. When subjected to changes in temperature, this structure exhibits tri-stability and transits between hemihelical, left-handed and right handed-helical shapes. Theoretical analysis, experiments, and finite element simulations are conducted to identify the mechanism of the tri-stability and used to predict the deformed configuration given geometric and material parameters. Our work provides a facile strategy for fabricating smart reconfigurable structures for a broad range of applications in intelligent materials.

*Zi Chen acknowledges the startup fund from Thayer School at Dartmouth and the support from the Branco Weiss-Society in Science Fellowship. Jing Fan acknowledges the support from ACS Petroleum Research Fund and CUNY Advanced Science Research Center.

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y60 FPS: Iran, North Korea, and Nuclear Proliferation
BCEC 258A - Joel Primack, University of California, Santa Cruz - Tag(s): Invited, Undergraduate
11:15AM Y60.00001: 2019 Szilard Lectureship Award recipient - Scientists and Today's Struggles Against Nuclear Weapons: What Would Szilard Do? [Invited] ZIA MIAN (Presenter), Princeton University — Long standing arms control and nonproliferation arrangements intended to forestall, halt, reverse and eventually eliminate nuclear weapons programs are unraveling and prospects for near-term progress on this critical issue appear bleak. Alongside ambitious plans for modernization and further development of nuclear arsenals and production complexes, for some states the conditions for nuclear weapons use seem to be broadening rather than shrinking. One potentially hopeful development, the 2017 United Nations Treaty on the Prohibition of Nuclear Weapons, has elicited opposition rather than support from most nuclear-armed states. The turn away from restraint towards retrenchment of nuclear weapons and warfighting postures exposes some of the inherent contradictions in the project of arms control as a way to end the threat of nuclear war. This talk will look at what role scientists can play in the current conjuncture with a focus on lessons that might usefully be learned from the organizing initiatives involving Leo Szilard, a pioneer in efforts by physicists as citizen-scientists to transcend nationalism and to bring science and democracy to bear on the challenge of reducing and eliminating the risks from nuclear weapons.

11:51AM Y60.00002: Iran, North Korea, and the Renewed Challenge of Proliferation [Invited] R KEMP (Presenter), Massachusetts Institute of Technology — Nuclear weapons are now a 70-year-old technology. Since that time, progress in science and technology has made access to nuclear weapons easier for all who might seek them—yet, interestingly, there has been less nuclear proliferation in the last four decades than in the first three; and the nuclear proliferation of recent years has occurred has a different character than the proliferation seen in the first half of the nuclear age. This puzzle can be largely explained by the politics of the international system; but technology has also played an important role. Technologies have shaping the actual and perceived capabilities of states; and has provided justifications and means for circumventing different systems of control. This talk examines the cases of Iran and North Korea as archetypes for understanding how technological change might impact proliferation in the future. Particular focus will be given to the impact of the gas centrifuge, which has enabled proliferation; detection of clandestine programs; and to emerging technologies and policies that might help limit, control, or reverse proliferation.

12:27PM Y60.00003: Verification of Denuclearization [Invited] ALEXANDER GLASER (Presenter), Princeton University — A possible denuclearization of North Korea presents a historic opportunity to eliminate a nuclear weapons program. A viable process is likely to proceed in several phases and depend on verification approaches that are considered adequate and effective by all parties. Even in the best case, however, North Korea will retain an arsenal of nuclear weapons for an extended period of time, possibly for many years or even a decade, which will pose additional unique verification challenges. In particular, North Korea may initially not want to reveal the storage locations of its nuclear warheads, warhead components, and long-range missiles because this could provide a target list for an attack. This talk discusses possible concepts and required technologies that would allow monitoring a residual nuclear arsenal while addressing North Korea's security concerns and meeting the requirements of effective verification.

1:03PM Y60.00004: Can Neutrino Detectors Strengthen the Nonproliferation Regime? [Invited] RACHEL CARR (Presenter), Massachusetts Institute of Technology — For 40 years, physicists have explored the idea using neutrino detectors to monitor nuclear activities, especially reactor operations. The challenge is detecting these weakly interacting particles in detectors of reasonable size and cost in cases where their signals would add value to existing monitoring techniques. This talk surveys hypothetical neutrino use cases, including roles in verifying a nuclear test ban treaty, discovering undeclared reactors, monitoring fissile material production in known reactors, and providing information about nuclear waste products. Even with recent advances in neutrino detection, most of the applications remain strongly limited by basic physical or practical constraints. In a few cases, existing or foreseeable neutrino technology has potential to complement more conventional approaches.
1:39PM Y60.00005: Strengthening the Nonproliferation Regime*  [Invited]  FRANK VON HIPPEL (Presenter), Princeton University — In the US State Department’s 1946 Acheson-Lilienthal Report, the first official proposal for a nuclear-weapon-free world, three activities were identified as “dangerous”: uranium mining, plutonium separation and uranium enrichment. They are dual-use; they could be used to produce fuel for either nuclear reactors or nuclear weapons. The report therefore recommended that these activities be placed under ownership of an international Atomic Development Authority (ADA). The US and Soviet Union could not agree, however, on which would come first: US nuclear disarmament or verification that the Soviet Union did not have a nuclear-weapon program. Seven decades later, many countries mine uranium but only one non-nuclear-weapon state separates plutonium (Japan) and three (Brazil, Iran and Japan) have national enrichment plants while, as an alternative model, Germany, the Netherlands and the UK co-own a multinational enrichment company, URENCO, which owns the only enrichment plant in the United States. It may be too late for the ADA but perhaps it is not too late to phase out plutonium separation and national enrichment plants.

*John D and Catherine T MacArthur Foundation
Carnegie Corporation

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y61 GSOFT FIAP: Multiphase Physics: Soft Matter Research at the Interface of Industrial and Academic Interests 8CEC 258B - Joshua Dijksman, Wageningen University & Research - Tag(s): Careers, Focus, Industrial, Undergraduate

11:15AM Y61.00001: Moisture and density measurements in powders: from geophysics to pharmacy  [Invited]  MICHEL LOUGE (Presenter), Merck Sharp & Dohme — The quality of pharmaceutical powders depends on fine control of their density and moisture content. Meanwhile, their processing requires availability of non-invasive instrumentation. We exploit recent advances in quantitative measurements of complex dielectric permittivity in hyper-arid desert sands to design capacitance instruments that can detect subtle changes in density and moisture in pharmaceutical processes and storage. We illustrate the technique with measurements of non-linear moisture diffusion through an excipient powder.

11:51AM Y61.00002: Antigravity static frictional force on the walls of confined granular columns*  PAYMAN JALALI (Presenter), School of Energy Systems, Lappeenranta University of Technology, Lappeenranta, Finland, YUCHEN ZHAO, JOSHUA SOCOLAR, ROBERT P BEHRINGER, Department of Physics, Duke University, Durham, NC, USA — We measure the static frictional force exerted by a granular material on the side wall of a vertical tube as a function of the filling height. We consider a cylindrical tube of diameter \( D \) = 5.2 cm filled to heights up to 6\( D \), which is smaller than the Janssen screening length. We use either glass beads (4 mm monodisperse spherical beads) or sand (0.5 mm polydisperse quasi-spherical particles). The grains are added in discrete steps in such a way that the top of the column remains flat, with a fixed mass per step and a fixed waiting time between steps. For sand, the vertical force on the tube remains zero up to a height of approximately 2\( D \), then increases linearly in the downward direction. Surprisingly, for glass beads the force on the container rises in the upward direction up to a turning height \( h \sim 2D \), above which it declines linearly. The variation in frictional force during a waiting period between steps becomes large for heights near \( h \). Discrete element method simulations of frictional spheres show qualitative agreement with experiments.

*This work was supported by the Academy of Finland under Grant 311138 and NSF grant DMR-1809762.

12:03PM Y61.00003: Particle formation in spray drying of Amorphous Solid Dispersions: a challenge for soft matter physics  PEDRO VALENTE (Presenter), Hovione FarmaCiencia S.A. — In this presentation we discuss the mathematical modeling of the various concurrent physical phenomena that a polymer solution with an Active Pharmaceutical Ingredient (API) undergo prior to forming an amorphous solid dispersion particle, such as atomization, co-solvent evaporative dynamics, propensity for phase separation and shell formation. We show a set of case studies comparing computational predictions against data from spray drying experiments. The motivation of the work is to support the development of Amorphous Solid Dispersion powders of poorly water soluble APIs in hydrophilic polymeric matrices which is a commonly used strategy to increase the solubility and dissolution rate of oral-dosage forms. However, successful development of amorphous solid dispersions for optimal performance and stability depends on both the formulation (e.g. drug load, polymer system and surfactants) and on the manufacturing technology/process conditions. Optimizing the formulation and the process requires extensive laboratory work, which is often compromised by time and cost constraints. Therefore the ability to perform virtual experiments is highly advantageous and cost-effective.
Novel stratification phenomena have recently been discovered in drying suspensions of polydisperse mixtures of particles. In this process, molecular dynamics (MD) modeling has played an important role. One challenge faced by the MD approach is how to treat the solvent in a computational model. We use large scale MD simulations to study drying suspensions of a binary mixture of large and small particles. The solvent is first modeled explicitly and then mapped to a uniform viscous medium by matching the diffusion coefficients of the particles while keeping all the interactions unchanged. “Small-on-top” stratification of the particles, with an enrichment of the smaller ones at the liquid/vapor interface during drying, is observed in both models under the same drying conditions. Using the implicit solvent model, we study the effect of the initial film thickness and show that the degree of stratification is controlled by the Péclet number defined with the initial film thickness as the characteristic length scale. When the Péclet numbers of large and small particles are much larger than 1, the degree of “small-on-top” stratification is first enhanced and then diminished as the Péclet numbers are increased.

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Control Stratification in Drying Particle Suspensions via Temperature Gradients

*Supported by American Chemical Society Petroleum Research Fund (#56103-DNI6).

The drying of polydisperse particle suspensions has recently attracted great attention as the particles may stratify according to sizes after drying, which may lead to new fabrication methods of multilayered films. We use molecular dynamics simulations to study a drying suspension of bidisperse nanoparticles and demonstrate a strategy of controlling stratification. When the suspension is kept isothermal during fast drying, it can exhibit “small-on-top” stratification with the smaller particles accumulated in the top region of the drying film. However, when only the region near the substrate is thermalized, a negative thermal gradient develops in the suspension because of evaporative cooling. Since the associated thermophoresis is stronger for larger nanoparticles, relatively more larger nanoparticles migrate into the top region of the drying film. The net result is either diminished “small-on-top” or converted “large-on-top”. By imposing a positive thermal gradient in the drying suspension via thermalizing the vapor at a higher temperature than the solvent, we observe very strong “small-on-top” stratification. Possible experimental approaches to realize various thermal gradients are suggested.

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Cement cohesion from the structuring of ions and water

*Supported by American Chemical Society Petroleum Research Fund (#56103-DNI6).

The solvent itself can also exhibit a great deal of structure due to confinement and strong electrostatic forces. To investigate these effects, we combine a primitive model for ions and surfaces with an explicit representation of water. We find that the presence of water proves to have a strong impact on the ordering of ions and greatly enhances the strength of attraction between two surfaces. By identifying quantitatively the link between chemistry and cohesive forces in cement, these results may open new paths for designing stronger cements, more durable and more sustainable.

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Characterization of Multiphase Fluid Transport and Relative Permeability in Microporous Media with Low-Field NMR

Recent advances in low-field nuclear magnetic resonance (NMR) enable the studies of interfacial interactions at micro/nano scales. In this work, relative permeability for decane/water in a carbonate rock is measured with an unsteady-state method. NMR T2 relaxation time distributions of fluids help to distinguish the in-situ water/decane flow in rock while capturing transport behaviors of water displacing decane into pores at different sizes. Furthermore, the permeabilities of water and decane are predicted by the correlation between respective NMR T2 signal strength and mass, and they matches previous results achieved with the unsteady-state method. Additionally, thermal effects on fluid interactions are investigated experimentally for both water and decane. Our findings reveal the physics of multilayer flows in complicated porous media for subsurface energy applications.
Lattice Boltzmann simulations of complex flows in fibrous porous media*  
FANG WANG, ULF SCHILLER (Presenter), Clemson University — Flow phenomena in porous media are relevant in many industrial applications including filters, membranes, and biomedical implants. For instance, nonwoven membranes can be used as filtration media with tailored permeability range and controllable pore size distribution. Predicting the structure-property relations that arise from specific porous microstructures remains a challenging task, and theoretical approaches have been limited to simple geometries. Computer simulations are a cost-effective way of validating semi-empirical relations and predicting the precise relations between macroscopic transport properties and microscopic pore structure. In this contribution, we discuss lattice-based modeling approaches for multiphase flow in porous media and demonstrate their application to nonwoven fibrous membranes and coalescence filtration.

*This work was supported in part by the National Science Foundation EPSCoR Program under NSF Award OIA-1655740.

New Class of Model Porous Materials Prepared by Colloidal Self-assembly Methods  
HONGYU GUO (Presenter), China Spallation Neutron Source, Institute of High Energy Physics, CAS, YUN LIU, National Institute of Standards and Technology — Understanding the properties of complex fluids (both liquid and gas) in porous media is crucial for both fundamental science and application, especially for many industrial problems, such as water filtration, protein chromatography, reservoir capacity estimation and productivity of shale gas. Confinement, at the scale observed in many porous media, can lead to dramatic shifts in physical properties such as gas density, phase transitions, and diffusivity. With the development of many nanoscale processing techniques it has become increasingly urgent that detailed structural and phase behavior of materials be probed with the confinement length scales from 1 nm- 10 µm. For this purpose, a model porous material with well controlled pore properties (size, shape and surface chemistry) need be developed. We herein introduce a new class of model porous materials prepared by self-assembly of colloidal particles. The essential of NPs assembly is the controlling of interactions. We have used silica NPs as building blocks suspended in a lutidine/water mixture. This method can be scaled up to synthesize monolithic solid porous materials with almost any designed shape on the scale of a few millimeters to centimeters. They are glass-like solids and have enough mechanical strength.

Atmospheric Pressure Plasma - Soft Matter interactions for controlled Materials Synthesis*  
SHOMEEK MUKHOPADHYAY (Presenter), ZACHARY FISHMAN, MICHAEL LOEWENBERG, Chemical Engineering, Yale University — Atmospheric pressure plasmas are a unique system which has been recently harnessed by engineers in a large number of industrial applications like water treatment to medical applications. Obsidian Advanced Manufacturing (Yale university spinoff) has been pioneering an approach to directly print complex materials for applications like flexible electronics using the interaction of atmospheric pressure plasmas with liquid drops carrying suitable reactants. In this talk we will present some key results of the ongoing collaboration to understand and control the reaction diffusion dynamics in these complex non-equilibrium systems. The interactions of atmospheric pressure plasmas which are essentially non-equilibrium allows us to synthesize materials ( semiconductors and metals) with properties and shapes which are usually difficult using conventional techniques.

*National Science Foundation - 1745845

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y62 DCMP: Interfaces and Mixing - Non-equilibrium Transport Across the Scales  
BCEC 2S8C - Snezhana Abarzhi, Univ of Western Australia - Tag(s): Invited
11:15AM Y62.00001: First Principles Based Multiscale Atomistic Methods for Non-Equilibrium Transport Across Interfaces* [Invited] WILLIAM GODDARD (Presenter), chemistry, materials science, applied physics, california institute of technology
— This symposium is focused on Non-equilibrium transport and mixing across interfaces, with papers describing non-equilibrium coupling of transport at interfaces, including mesoscopic and macroscopic dynamics in fluids, plasmas, and other materials over scales from microns to celestial. Most such descriptions deal with the materials in terms of density and equations of state rather than specific atomistic structures and chemical processes. At interfacial boundaries, such atomistic information can be quite relevant, but it is not yet practical to couple phenomena at celestial scales with the atomistic descriptions of chemistry. The starting point for including such information is quantum mechanics (QM). But practical QM calculations are limited to 100's of atoms for 10's of picoseconds, far from the scales required to properly inform the continuum level about the atomistics. To bridge this enormous gap, we are developing practical methods to extend the scale of the atomistic simulation by several orders of magnitude while retaining QM accuracy for describing chemical processes. These developments are aimed toward including the relevant chemistry for systems with millions of atoms. We will describe the progress in accomplishing these extensions of first-principles-based atomistic simulations to larger scales while dramatically decreasing computational efforts.

*DOE JCAP (DE-SC0004993), DOE CMP (DE-SC0014607), NSF (CBET 1805022)

11:51AM Y62.00002: Interface dynamics: New mechanisms of stabilization and destabilization and structure of flow fields* [Invited] SNEZHANA ABARZHI (Presenter), Univ of Western Australia — Interfacial mixing and transport are nonequilibrium processes coupling kinetic to macroscopic scales. They occur in fluids, plasmas, and materials over celestial events to atoms. Grasping their fundamentals can advance a broad range of disciplines in science, mathematics, and engineering. This work focuses on the long-standing classic problem of stability of a phase boundary—a fluid interface that has a mass flow across it. We briefly review the recent advances and challenges in theoretical and experimental studies, develop the general theoretical framework directly linking the microscopic interfacial transport to the macroscopic flow fields, discover the new mechanisms of interface stabilization and destabilization that have not been discussed before for both inertial and accelerated dynamics, and chart perspectives for future research.

*2018 PNAS 201714500; https://doi.org/10.1073/pnas.1714500115. The work is supported by the University of Western Australia (AUS) via project grant 10101047, and the National Science Foundation (USA) via award 1404449.

12:27PM Y62.00003: Nanoscale view of assisted ion transport through the liquid-liquid interface* [Invited] MARK SCHLOSSMAN (Presenter), University of Illinois at Chicago — During solvent extraction, amphiphilic extractants assist the transport of metal ions across the liquid–liquid interface between an aqueous ionic solution and an organic solvent. Investigations of the role of the interface in ion transport challenge our ability to probe fast molecular processes at liquid–liquid interfaces on nanometer-length scales. Recent development of a thermal switch for solvent extraction has addressed this challenge, which has led to the characterization by X-ray surface scattering of interfacial intermediate states in the extraction process. We find that trivalent rare earth ions, Y(III) and Er(III), combine with bis(hexadecyl)phosphoric acid (DHDP) extractants to form inverted bilayer structures at the interface; these appear to be condensed phases of small ion–extractant complexes. The stability of this unconventional interfacial structure is verified by molecular dynamics simulations. The ion–extractant complexes at the interface are an intermediate state in the extraction process, characterizing the moment at which ions have been transported across the aqueous–organic interface, but have not yet been dispersed in the organic phase. In contrast, divalent Sr(II) forms an ion–extractant complex with DHDP that leaves it exposed to the water phase; this result implies that a second process that transports Sr(II) across the interface has yet to be observed. Calculations demonstrate that the budding of reverse micelles formed from interfacial Sr(II) ion–extractant complexes could transport Sr(II) across the interface. Our results suggest a connection between the observed interfacial structures and the extraction mechanism, which ultimately affects the extraction selectivity and kinetics.

*We acknowledge support from US Department of Energy (DOE), Office of Basic Energy Sciences (OBES) (DE-SC0018200). ChemMatCARS is supported by National Science Foundation Grant CHE-1346572.
1:03PM Y62.00004: Spiky Electric and Magnetic Field Structures in Flux Rope Experiments* [Invited] WALTER GEKELMAN (Presenter), SHAWN TANG, STEPHEN T VINCENA, Dept. of Physics, University of California, Los Angeles — Magnetic flux ropes are bundles of twisted magnetic fields and their associated currents. They are common on the surface of the sun (and presumably all other stars) and are observed to have a large range of sizes and lifetimes. One or more flux ropes are routinely generated in the Large Plasma Device at UCLA. The ropes are kink unstable and when they collide fully 3D magnetic reconnection occurs. The time dependent magnetic field, plasma flow, electron temperature, plasma density, and the space charge and inductive electric fields were measured at over 42,000 spatial positions throughout the plasma volume over several million rope collisions. Magnetic field lines are followed and used to derive quasi-seperatrix layers, locations where reconnection occurs. The complete data set was used to evaluate all the terms in Ohm's law, which resulted in unphysical plasma resistivity. It was then determined that in this situation Ohm's law is non-local. The resistivity was properly evaluated using the fluctuation dissipation theorem (Kubo resistivity). Time domain structures (TDS), sharp pulses in potential and magnetic field are generated during reconnection events and subsequent move from the reconnection region into the rope currents. The probability distribution function of the spike amplitudes is log-normal, the same as the fold of crumpled paper. A amplitude counting method is used to create a vector map of the magnetic field of the spikes. TDS observed by satellites are ubiquitous in the plasma surrounding the earth.

*This work is funded by DOE Office of Fusion Energy Science and the Physics division of the NSF. The work was done at the Basic Plasma Science Facility which is also funded by these agencies

1:39PM Y62.00005: Subdiffusive and superdiffusive transport in plane steady viscous flows* [Invited] MICHAEL ZAKS, Institute of Physics, Humboldt University of Berlin, ALEXANDER NEPOMNYASHCHY (Presenter), Technion - Israel Institute of Technology — Dispersion of particles in chaotic, turbulent or random flows has been studied for a long time. It is known that the action of advection on large spatial and temporal sales typically can be described as an (anisotropic) normal diffusion process. However, as found by Kraichnan in 1970, that is not the case for steady two-dimensional flows of incompressible viscous fluids. We show that the deterministic transport of particles through lattices of solid bodies or arrays of steady vortices can be anomalous. Motion along regular patterns of streamlines is typically aperiodic. Repeated slow passages near stagnation points and/or solid surfaces serve for eventual decorrelation. Singularities of passage times near the obstacles, determined by the boundary conditions, affect the character of transport anomalies. Flows past regular arrays of vorticies are subdiffusive; the temporal evolution of MSD displays some nontrivial similarity properties. Tracers advected through lattices of solid obstacles can feature superdiffusion. The particle transport in spatially irregular flows is also considered. The analytical predictions match the results of numerical simulations.

*The research was supported by Grant I-1271-303.7/2014 from the German-Israeli Foundation for Scientific Research and Development.

Friday, March 8, 2019 11:15 AM - 2:03 PM

Session Y63 GSOFT DBIO: Phase Separation in Biological Processes BCEC 259A - Daphne Klotsa, University of North Carolina at Chapel Hill - Tag(s): Focus

11:15AM Y63.00001: Protein phase separation and emergent material properties* [Invited] SHANA ELBAUM-GARFINKLE (Presenter), Advanced Science Research Center at GC/CUNY — Phase separation has emerged as a new paradigm currently revolutionizing our understanding of cell biology and intracellular organization. The assembly of biomolecules into condensed liquid phases (i.e condensates) appears to underlie the formation of membraneless organelles and other liquid compartments with roles in cell signaling, transcriptional regulation and cytoskeletal organization. Understanding the role of liquid material properties in condensate function and dysfunction requires new tools and approaches. We employ model in vitro systems and a combination of quantitative imaging and rheological tools to interrogate the nature of liquid material properties and their contribution to molecular processes and functions. We find that protein-protein and protein-RNA interactions can tune the material properties of condensates; Conversely, the viscous network of condensates can in turn modulate the molecular diffusion within droplets in a length scale dependent manner. This work provides important insight into the physicochemical rules that govern the regulation of protein/RNA liquid phases, from the cellular functions of membraneless organelles, to the potential misregulation of liquid phase separation in disease.

*NIH-NINDS
Controlling biological droplets with chemical reactions

David Zwick (Presenter), Max Planck Institute for Dynamics and Self-Organization — Phase separation has recently emerged as an important concept to understand the spatial organization of biological matter. In this talk, I will demonstrate that such biological droplets can be controlled by non-equilibrium chemical reactions that affect the droplet material. Such chemical reactions generate compositional fluxes, which control droplet sizes, counteract the effects of surface tension, and can position solid-like particles inside the droplet. I thus show that combining phase separation of proteins with post-translational modifications provides cells with a toolset to build and control compartments without membranes.

Stiffness gradients control phase separation in gels and cells

Kathryn Rosowski (Presenter), Robert Style, Tianqi Sai, Thomas Boddeker, Eric Dufresne, ETH Zurich — Living cells compartmentalize various processes using phase separation. The physical mechanisms which control this phase separation are not fully understood. However, the interior of the cell can be simply viewed as a closely packed elastic network, with well-regulated regions of lower or higher stiffness. Using droplet formation in a polymer gel as a model system, we found that phase separation can be controlled by the elasticity of the network, and that droplet size and location evolve over time under a stiffness gradient. Our findings further suggest that elasticity differences in cells may similarly regulate phase separation and could be used by cells to control droplet location.

How yeast harness 2D liquid-liquid phase separation to organize proteins and lipids in vacuole membranes

Sarah Keller (Presenter), Scott P Rayermann, Glennis E Rayermann, Alex J Merz, University of Washington — For decades, scientists have argued about how living cell membranes acquire and maintain liquid regions enriched in specific lipid and protein types. Physicists have long observed liquid-liquid demixing in artificial membranes. Clear identification of the same phase transition in a living biological membrane has heretofore been elusive. By directly imaging micron-scale membrane domains of yeast organelles both in vivo and cell-free, we show that the domains reversibly appear and disappear at a distinct miscibility transition temperature and that the domains merge quickly, consistent with fluid phases. Interesting physical phenomena underlie membrane domains. For example, domains are strongly coupled across both membrane faces (with a coupling parameter of ~0.02 kT/nm²). Similarly, liquid-liquid phase separation can occur near a critical point. Membranes behave as 2-dimensional Ising systems with conserved order parameter; and we have measured the membrane's effective critical dynamic exponent. A third example is that liquid domains coarsen. As expected, domain radius grows as time¹/³. These results have appeared in PRL (2012) and BJ (2013, 2015, and 2017) and Physics Today (2018).

Physics of non-equilibrium phase separation: Implications for stress granule formation in the cell cytoplasm

Chiu Fan Lee (Presenter), Imperial College London — Phase separation is exploited by biological cells to organize their cytoplasm. Although equilibrium phase separation is a well understood phenomenon, the cell cytoplasm is fundamentally different from a thermal system, with driven chemical reactions and directed movement being two hallmarks of its non-equilibrium nature. In this presentation, I will describe some of the universal features in non-equilibrium phase separation relevant to the cell cytoplasm. I will then discuss their implications for stress granules, which form in the cell cytoplasm when the cell is under stress.

References:


DNA Local Flexibility Dependent Formation of Liquid-like Droplets

Anisha Shakya (Presenter), John King, Center for Soft and Living Matter, Institute for Basic Science — Associative phase separation of biomacromolecules like proteins and nucleic acids into liquid-like droplets, termed liquid-liquid phase separation (LLPS), has been linked to lipid-membrane intracellular organization as well as aggregation mediated diseases. In this work, we have studied the role of sequence-dependent DNA flexibility in LLPS of multiple interacting components. We find that DNA local flexibility, encoded by the DNA sequence, not simply the overall charge density, determines the phase behavior in such systems.

The authors thank taxpayers who supported this work through the Korean Institute for Basic Science, project code IBS-R020-D1.
1:15PM Y63.00007: Azobenzene-doped, lipid-bilayer vesicles with light-responsive permeability: measuring mechanical response to photochemical excitation by micropipette aspiration* ARASH MANAFIRAD (Presenter), Physics, University of Massachusetts Amherst, LUCAS ANTONY, JUAN DE PABLO, Chemical Eng., University of Chicago, SANKARAN THAYUMANAVAN, University of Massachusetts Amherst, ANTHONY DINSMORE, Physics, University of Massachusetts Amherst — Inspired by the ability of cell membranes to control the permeability of selected solutes across the lipid bilayer membrane, we report on a synthetic system that switches permeability in response to light. We use experiments and simulations to study giant unilamellar lipid vesicles that contain a photoisomerizing unit (azobenzene) that channels photochemical excitation into mechanical energy within the membrane. In experiments with micropipette aspiration, we hold the vesicles at a constant tension and expose them to UV light with controlled dosage. The membrane surface area, interior volume, and stretching modulus are all measured in situ. We find a threshold molar fraction of azobenzene, below which there is no UV-stimulated response. Above that threshold, we find an extension of the aspirated projection length within seconds of exposure. Together with a prior study of glassy membranes, our experiments and simulations show the basic principles by which the injection of photochemical energy drives the membrane away from equilibrium switching membrane properties in a reversible manner. These results will allow us to mimic cell function and to design smart, responsive artificial systems.

*This work was supported by a MURI grant from the U.S. Army Research Office (W911NF-15-1-0568).

1:27PM Y63.00008: Microfluidic Fabrication of Asymmetric Lipid Vesicles* YUTING HUANG (Presenter), Physics and Applied Physics, Harvard University, LAURA ARRIAGA, Complutense University of Madrid, DAVID A WEITZ, Physics and Applied Physics, Harvard University — Lipid vesicles are aqueous volumes surrounded by a bilayer of lipid molecules, which are amphiphilic molecules with their head groups facing water and tail groups facing oil. These vesicles are simple models that mimic cell membranes and can be used for drug delivery. One interesting type of lipid vesicle is the asymmetric vesicle, in which its bilayer is composed of two dissimilar lipid monolayers. Importantly, all eukaryotic cell membranes exhibit this type of asymmetry and asymmetry is also proposed to enhance mechanical properties of the membrane. Here, we use microfluidics to fabricate mono disperse and highly controllable asymmetric lipid vesicles, which unlike the conventional methods that often end up with highly poly disperse samples. To achieve this, asymmetric vesicles are produced using water/oil1/oil2/water emulsions in a glass capillary device, with different lipids immersed in two different volatile oil phases. Using the asymmetric vesicles, we are trying to measure how mechanical properties are affected by this asymmetry and also how to improve the degree of asymmetry in our vesicles even more. In future, we envision asymmetric lipid vesicles could open a new door in the field lipid based drug delivery systems.

*NSF Collaborative Research grant DMR-1705775

1:39PM Y63.00009: Molecular dynamics of hydrophobic transport using monolayer-protected nanoparticles* MUKARRAM TAHIR, ALFREDO ALEXANDER-KATZ (Presenter), Massachusetts Institute of Technology — Proteins such as serum albumin contain apolar pockets in their three-dimensional structure that facilitate the transport of hydrophobic small molecules in biological settings. Nanoscale carriers that can similarly solubilize therapeutic compounds without requiring chemical modification have immense value as drug delivery systems. Here, we use molecular dynamics simulations to demonstrate that gold nanoparticles functionalized with alkanethiol ligands can passively encapsulate hydrophobic molecules. We focus on the encapsulation of long-chain fatty acids and study the thermodynamics and kinetics of incorporation into the nanoparticle’s surface monolayer as a function of chain length and unsaturation. We also characterize the structure of the nanoparticle and organization of the encapsulated molecules as a function of loading density and demonstrate that loaded nanoparticles release their cargo into lipid membranes upon contact with fluctuations such as lipid tail protrusions. These observations suggest the possibility of designing nanomaterials that can function as synthetic mimics of transport proteins and have applications in solubilizing apolar pharmaceutical compounds in the aqueous environment of biological systems.

*US DOE CSGF contract DE-FG02-97ER25308
Multivalent gene regulatory elements localize condensation of transcription machinery

KRISHNA SHRINIVAS (Presenter), Massachusetts Institute of Technology, BENJAMIN SABARI, Whitehead Institute, PHILLIP SHARP, Massachusetts Institute of Technology, RICHARD YOUNG, Whitehead Institute, ARUP K CHAKRABORTY, Massachusetts Institute of Technology — Enhancers are regulatory elements that cooperatively assemble the transcriptional machinery upon binding by sequence-specific transcription factors. Recently, we and others have hypothesized and demonstrated that the transcriptional apparatus forms liquid-like condensates, particularly at cell-type specific enhancer elements called super-enhancers. Many transcription factors (TFs) and coactivators phase separate \textit{in vitro}, but only at supra-physiological concentrations. A unified mechanism to describe how and why these condensates form around specific genomic loci at physiological conditions is unknown. Here, using a combination of simulation, and complementary \textit{in vitro} experiments, we propose that specific and multivalent enhancers nucleate localized condensation of TFs and coactivators at physiologic-like conditions. Using thermodynamic guiding principles, we predict key interactions that regulate condensate formation, as well as motif features encoded in DNA that drive phase separation and higher-order organization of the 3-D genome. Experiments validate our predictions, and many of these features are encoded and leveraged by mammalian genomes to assemble high amounts of transcription machinery, implicating phase separation in shaping the gene regulatory landscape.

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y64 DBIO DPOLY: Physics of Proteins and Nucleic Acids II: Structures, Dynamics, Interactions, and Energetics BCEC 259B - Aihua Xie, Oklahoma State Univ - Tag(s): Focus

11:15AM Y64.00001: The physical basis of computer-aided drug design: assessing and advancing the accuracy of binding affinity calculations* [Invited] MICHAEL GILSON (Presenter), University of California San Diego — Predicting the binding thermodynamics of proteins and small organic molecules is a key aim in computer-aided drug design. I will provide an introduction to this problem in physical chemistry, the statistical mechanical framework for models of binding, and computational approaches based on this framework. I will then describe some interesting and unexpected outcomes of blinded prediction challenges in this field and what they indicate about steps required to improve accuracy, notably the need for improve potential functions, also known as force fields. Finally, I'll present the approaches we are taking, in coordination with the Open Force Field Initiative, to improve the accuracy of force fields and thus speed the discovery of new medications.

*I thank the National Institutes of Health for support of this work (grants R01GM061300 and U01GM111528). These findings are solely of the authors and do not necessarily represent the views of the NIH. MKG has an equity interest in and is a co-founder of and scientific advisor of VeraChem LLC.

11:51AM Y64.00002: New strategies to predict protein-peptide interactions* [Invited] XIAOQIN ZOU (Presenter), Department of Physics and Astronomy, Dalton Cardiovascular Research Center, Department of Biochemistry, and Informatics Institute, University of Missouri - Columbia — Peptides are short polymer chains consisting of amino acids. They are flexible and often change conformations when they bind to proteins. Protein-peptide interactions play an important role in many cellular processes. In silico prediction of protein-peptide complex structure is highly desirable for mechanistic investigation of these processes and for therapeutic design. However, it is challenging to predict all-atom structures of protein-peptide complexes without any knowledge about the binding site and the bound peptide conformation, because of the large degrees of freedom involved in the system. In this talk, I will present our recent development of new strategies for predicting protein-peptide complex structures, based on the integration of information-driven modeling and physics/chemistry-based computational modeling of the interaction modes. The peptide is treated as a flexible structure during modeling, and the search space includes the whole surface of the protein. The methods have been systematically and extensively tested, and the results will be presented. The methods are computationally efficient. They can be used either as a standing-alone tool for large-scale protein-peptide docking or as an initial-stage sampling tool for protein-peptide structure refinement programs.

*NIH grants R01GM109980, R01HL126774, and R01HL142301, and NSF CAREER Award Grant DBI0953839
12:27PM Y64.00003: Effects of Small Compounds on Structure of Amyloid-β1-42 Monomer
FARBOD MAHMOUDINOBAR (Presenter), Physics, New Jersey Institute of Technology, ZHAOQIAN SU, Systems and Computational Biology, Albert Einstein College of Medicine, CRISTIANO DIAS, Physics, New Jersey Institute of Technology — Alzheimer’s disease is associated with deposits of Amyloid-β, an intrinsically disordered peptide. Molecular structure and aggregation rate of Aβ are observed to be significantly dependent on the properties of its aqueous environment. For example, NaCl is shown to accelerate Aβ fibril formation whereas 4-Aminophenol (4AP) and Inositol have been shown to reduce its aggregation rate. Despite many studies to investigate the effects of small molecules on aggregation of Aβ, its atomic interactions with small molecules that mediate various structures and behavior of this peptide are not well understood. To investigate Aβ molecular structures and to understand how Aβ properties are affected by compounds, we performed extensive Replica Exchange Molecular Dynamics (REMD) simulations on Aβ1-42 monomer with explicit solvent and small molecules. Our research reveals that each molecule affects different regions of Aβ1-42 and the peptide adopts distinguished structures compared to control system. Specifically, we observe that NaCl increases contact among residues K16-E22 and V38-I41 while 4AP increases K16-E22 and N27-G37 contacts and Inositol mainly disrupts the intrapeptide contacts. Effects of compounds on structural and physical properties of Aβ1-42 monomer will also be discussed.

12:39PM Y64.00004: Cluster-expansion theory for sequence-specific “fuzzy” interaction between a pair of intrinsically disordered proteins
ALAN AMIN, YI-HSUAN LIN (Presenter), SUMAN DAS, HUE SUN CHAN, University of Toronto — Intrinsically disordered proteins (IDPs) do not fold into a unique tertiary structure in isolation, likely because they are depleted in hydrophobic but enriched in polar, charged, and aromatic amino acids. While many IDPs become ordered upon binding to folded proteins, several IDPs have been recently discovered to retain their structural disorder when binding with each other via a so-called “fuzzy” mechanism. Just like interactions between folded proteins, such a fuzzy mechanism must be determined by the amino acid sequences of the IDPs. Here, we implement the cluster expansion method in statistical mechanics to develop an analytical theory for calculating the sequence-specific IDP-IDP binding affinity. We apply the theory to various IDP pairs selected from a set of 30 polyampholytic IDP sequences with the same amino acid composition but different charge patterns. The sequence-specific correlation between the double-chain binding affinities and single-chain conformations are systematically investigated. Our analytical theory provides a concise and powerful tool for high-throughput proteomic analysis of IDP-IDP interaction.

*This material is based on the work supported by Canadian Institutes of Health Research and Natural Sciences and Engineering Research Council of Canada

12:51PM Y64.00005: Conformation-Induced Conductivity Switching in Bacterial Protein Nanowires
SIBEL EBRU YALCIN (Presenter), J. PATRICK O’BRIEN, ATANU ACHARYA, YANGQI GU, PETER DAHL, SOPHIA YI, WINSTON HUYNH, SUBHAJYOTI CHAUDHURI, VICTOR BATISTA, NIHIL MALVANKAR, Yale Univ — Large-scale conformational changes in molecules are attractive because they can serve as information carriers for switches in memory and logic devices. Here we report the ability to control molecular conductivity via conformational switching at an unprecedented scale. Atomic force microscopy showed that individual Geobacter sulfurreducens protein nanowires undergo > 20 Å conformational change that propagates over their micrometer-lengths upon changing the environment. This increases the mechanical stiffness of nanowires by 4-fold and dc conductivity by 15,000-fold. Infrared nanospectroscopy revealed that this conformational change is driven by an internal structural transition. A suite of complementary experimental and computational methods such as X-ray diffraction, Raman, UV-Vis, fluorescence emission spectroscopy and circular dichroism further demonstrated this structural transition. Our studies thus establish nanoscopic approaches to visualize and quantify large-scale conformational changes in biomolecules and present novel strategies for tuning their structure and conductivity. Our work will guide the creation of a new class of programmable biomaterials with precisely controlled electronic and mechanical properties.

*Funded by NIH New Innovator and NSF CAREER Awards.
1:03PM Y64.00006: Computational Protein Redesign and Decoy Discrimination*  
ZHE MEI (Presenter), JOHN TREADO, ZACHARY LEVINE, COREY SHANE O'HERN, Yale Univ, LYNNE REGAN, The University of Edinburgh — A key aim of computational protein design is to understand how amino acid mutations affect the structure and stability of proteins. Recent studies have used molecular dynamics (MD) simulations to predict the response of wildtype proteins to mutations. However, MD structures can be trapped in local free energy basins, resulting in configurations that diverge significantly from experimental crystal structures. In this work, we construct a mutation dataset, which contains 32 pairs of single-core-residue mutated crystal structures and their corresponding wildtype structures. We perform replica-exchange MD (REMD) simulations on wildtype and mutant structures to obtain a series of possible protein conformations before and after the core mutations. We then perform residue repacking to determine whether the side chain conformations match those in the crystal structures. We also evaluate the local packing fraction and void geometry of the protein structures from REMD simulations to distinguish decoys from the crystal structures. The ability to distinguish experimental structures from decoys will enable unprecedented validation of MD simulations, and provide insight into novel structures that have not yet been experimentally characterized.

*NIH Training Grant, Grant No.1T32EB019941

1:15PM Y64.00007: Weighted ensemble simulations of biomolecules: Applications to peptides and proteins*  
HIROSHI FUJISAKI (Presenter), Physics, Nippon Medical School, KEI MORITSUGU, Yokohama City University, AYORI MITSUTAKE, Physics, Meiji University, HIROMICHI SUETANI, Oita University — Weighted ensemble (WE) method is an efficient way to numerically sample rare event trajectories generated by random dynamical systems, first introduced by Huber and Kim [1] and further extended by Zuckerman and coworkers [2].

We apply this method to a small peptide called chignolin, which only has 10 amino acids but is known to have at least two stable states, a folded and misfolded states. The main focus is to study the transitions between these two states of chignolin, and to extract the kinetic properties of chignolin at high temperature [3]. While applying the WE method, we use the diffusion map (a manifold learning technique) coordinates as order parameters and compare the result with those using more chemically intuitive coordinates (hydrogen bond distances). Furthermore, we also apply the WE method to proline isomerization of PIN1 enzyme and the global conformational change of adenylate kinase.


*Japan Society for the Promotion of Science (KAKEN 16K00059, 17KT0101, 25120011)

1:27PM Y64.00008: Identifying Trimerization Mechanisms of Human Islet Amyloid Polypeptide through Molecular Simulation  
ASHLEY GUO (Presenter), JUAN DE PABLO, University of Chicago — Human islet amyloid polypeptide (hIAPP, or human amylin) is implicated in the development of type II diabetes and is known to aggregate into amyloid fibrils. Early-stage aggregates have been shown to be cytotoxic, prompting study of prefibrillar oligomeric species and their aggregation mechanisms. Here, we build upon recent work that studied formation of the hIAPP dimer, which identified a dimerization pathway and its corresponding free energy profile, by studying and comparing hIAPP trimerization mechanisms. We use atomistic molecular dynamics simulations combined with the finite-temperature string method to identify favorable pathways for trimer formation, relevant intermediate structures, and free energy changes during trimerization. Specifically, we compare and contrast two trimerization scenarios: (1) formation of a trimer from three disordered hIAPP molecules, and (2) formation of a trimer from a single disordered hIAPP molecule added to an hIAPP dimer.
1:39PM Y64.00009: Direct experimental characterization of contributions from self-motion of hydrogen and from interatomic motion of heavy atoms to protein anharmonicity  ZHUO LIU, CHENXING YANG, School of Physics and Astronomy, Shanghai Jiao Tong University, JUAN HUANG, School of Life Sciences and Biotechnology, Shanghai Jiao Tong University, JUN LI (Presenter), School of Physics and Astronomy, Shanghai Jiao Tong University — One of challenges in biophysics is to understand the connection between protein dynamics and its function. The challenge partially arises from the fact that protein present a variety of local atomic motions and collective dynamics on the same time scales, and this has rendered difficult the experimental identification and quantification of different dynamic modes. Here, taking lyophilized protein as examples, we combined the deuteration technique and the neutron scattering experiment to separate the self-motion and the collective interatomic motion of heavy atoms in proteins. We found that the self-motions of protein hydrogen atoms present a resolution-time-dependent anharmonic onset, with the onset temperature increasing when decreasing the resolution time. This can be ascribed to the thermal activation of local side-group motions, mostly the methyl rotations. In contrast, the collective dynamics of protein heavy atoms exhibit a resolution-time-independent anharmonicity around 200 K. Further dielectric spectroscopy and Brillouin light scattering results suggest that the anharmonicity of the heavy atoms results from unfreezing of the relaxation of the protein structures on the laboratory equilibrium time (100-1000 s), which softens the entire bio-macromolecules.

1:51PM Y64.00010: ABSTRACT WITHDRAWN —

2:03PM Y64.00011: Topological analysis of morphological changes of proteins due to the differences of experimental conditions of X-ray structural analysis  HARU NEGAMI (Presenter), Graduate school of engineering, The University of Tokyo — In structural biology, it is an important problem how tiny local mutation of the protein affect its global structure. To understand the mechanism, we focus on a topological method called “Fatgraph models of proteins” [1]. The model is a topological two-manifold with boundary components (surface) which have one to one correspondence with three-dimensional protein structures listed on Protein Data Bank (PDB) [2] with several exceptions. The traits of each surface for each protein are described by invariants.

Although the model enables us to grasp the global structure of each protein, it is still unclear if the method is useful for comparison between several structures because there was no research on the effect of the differences of experimental conditions on protein structure.

Here, we investigated the effect of experimental conditions of X-ray analysis and the fatgraph invariants of proteins which share identical sequences. We found that the invariants are sensitive to the differences of the conditions and proposed a method to analyse the morphological changes due to the mutation.


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Session Y65 DBIO: Biological Navigation and Orientation BCEC 260 - Adam Fine, Yale Univ - Tag(s):

Undergraduate

11:15AM Y65.00001: Interaction of spermatozoa with micro structured surfaces*  ANTON BUKATIN (Presenter), St. Petersburg Academic University, PETR DENISSENKO, VASILY KANTSLER, University of Warwick — Spermatozoa navigation plays crucial role in the process of mammalian fertilization. Mechanical interactions in the heterogenous environment of the fertility such as surface scattering and rheotaxis are the key mechanisms in determining the sperm journey towards the ovum. Here we report an experimental study of interaction mechanisms for single human sperm cells scattering off solid surface boundaries of different curvature. The investigation is based on measuring the trajectories of the cells near curved surfaces of cylindrical pillars with diameters 50 – 500 um in a microfluidic device. By analysing several thousands of cells trajectories we built the scattering functions of interaction process. The results reveal the dependence of the scattering functions on the pillar size. We deduce that for the smaller pillars, 50 – 200 um in diameter, the scattering is primarily determined by the steric interactions, while the hydrodynamics starts playing a role for the larger pillar sizes. The results of the spermatozoa scattering dynamics can be used in designing new types of microfluidic devices for rapid selection of motile cells in-vitro.

*AB thanks Russian Science Foundation (18-74-00127); VK thanks Royal Society International Exchange Scheme (IE150384).
11:27AM Y65.00002: Measured effect of boundary distance on flagellar motor torque*  BRUCE RODENBORN (Presenter), MACKENZIE CONKLING, CESAR ROMERO, PHILIP LOCKETT, Centre College — Darnton et al. (2007) used resistive force theory to derive experimental measurements of the torque generated by bacterial motors in free swimming *Escherichia coli*. Recent reports have found similar torque values using both boundary element methods and slender body theory to model flagella swimming near a boundary (Das et al. 2018). Such numerical methods have also been used to model constrained bacteria swimming near a boundary, where their flagella act as micropumps (Dauparas et al., 2018). We use scaled macroscopic experiments to directly measure the torque on constrained, pumping flagella as a function of boundary distance. The helical flagella have a diameter ≈12 mm and are immersed in a fluid with viscosity 10^5 times that of water to ensure the Reynolds number in the experiments is much less than unity, just as in the bacterial experiments. We compare our nondimensionalized values to the numerical data and find good agreement, particularly in the dependence of motor torque on boundary distance. We also report a similar functional dependence of propulsive force measurements as a function of boundary distance.

*Centre College Faculty Development Fund
Kentucky NSF EPSCoR

11:39AM Y65.00003: Bacteria push the limits of sensory precision to navigate dynamic chemical gradients*  DOUGLAS BRUMLEY (Presenter), University of Melbourne, FRANCESCO CARRARA, ETH Zurich, ANDREW HEIN, University of California, Santa Cruz, YUTAKA YAWATA, University of Tsukuba, SIMON LEVIN, Princeton University, ROMAN STOCKER, ETH Zurich — The limited precision of sensory organs places fundamental constraints on organismal performance. An open question, however, is whether organisms are routinely pushed to these limits, and how limits might influence interactions between populations of organisms and their environment. By combining a method to generate dynamic, replicable resource landscapes, high-speed tracking of freely moving bacteria, a new mathematical theory, and agent-based simulations, we show that sensory noise ultimately limits when and where bacteria can detect and climb chemical gradients. Our results suggest the typical chemical landscapes bacteria inhabit are dominated by noise that masks shallow gradients, and that the spatiotemporal dynamics of bacterial aggregations can be predicted by mapping the region where gradient signal rises above noise.

*This work was supported by an HFSP Cross-Disciplinary Fellowship and a Discovery Early Career Researcher Award (D.R.B.), a Swiss National Science Foundation Early Mobility Postdoctoral Fellowship (F.C.), a James S. McDonnell Foundation Fellowship (A.M.H.), Army Research Office Grants W911NG-11-1-0385 and W911NF-14-1-0431 (S.A.L.), Simons Foundation Grant 395890 (S.A.L.), and a Gordon and Betty Moore Marine Microbial Initiative Investigator Award (R.S.).

11:51AM Y65.00004: A theory of searching for a target with partial information  GAUTAM REDDY (Presenter), MASSIMO VERGASSOLA, University of California, San Diego — Animals often need to find and navigate to distant targets, such as food, mates or prey, using partial information about their location. Search algorithms that deal with such scenarios have been proposed, but there is no theoretical framework that offers a standard baseline to compare the search efficiency of different algorithms. In this work, we propose a general theoretical framework to describe the task of a decision-making agent searching for a distant target emitting noisy cues. Within this framework, we define a notion of an `asymptotically optimal' search algorithm and show how its performance produces a lower bound to the expected cost of any other algorithm. We demonstrate how the optimal decision boundaries and the corresponding PDFs of search times can be computed in a simplified one-dimensional search task, and compare them to those of a previously proposed `Infotaxis' algorithm. Generic features of searching in higher dimensions are discussed.

12:03PM Y65.00005: Cell decision making at a microfluidic fork  VAMSI SPANDAN (Presenter), CHON U. CHAN, L MAHADEVAN, Harvard University — Many cell types, such as white blood cells, undergo directed migration during wound healing, development and immune response. A simple paradigm for this is related to the aphorism attributed to Yogi Berra "When you come to a fork, take it" - so that one can ask what happens when an active cell comes to a junction in a vasculature? Since the paths may have different mechanical resistance and/or chemokine concentrations, how does the cell respond by integrating multiple signals across different spatial-temporal scales and reject transient noise? We use a combination of numerical simulations and microfluidic experiments to understand the mechanochemistry of cellular decision-making at a confined bifurcation junction. The cell is modelled as a deformable, active acto-myosin cortex surrounding a fluid volume, with active stresses which are a function of the local hydrodynamic and chemical cues. We show how the system shows a range of phenomena reminiscent of critical slowing down, and noise-induced tipping, and compare the results with experiments on single cells moving through a confined microfluidic fork.
12:15PM Y65.00006: Variance Adaptation in Navigational Decision Making*  
JASON WOLK (Presenter), RUBEN GEPNER, DIGVIJAY S WADEKAR, SOPHIE DVALI, MARC H GERSHOW, New York University — Sensory systems relay information about the world to the brain, which enacts behaviors through motor outputs. To maximize information transmission, sensory systems discard redundant information through adaptation to the statistics of the environment. The behavioral consequences of sensory adaptation to environmental variance have been largely unexplored. We study how larval Drosophila adapt sensory-motor computations underlying navigation to changes in the variance of visual and olfactory inputs. We show that variance adaptation can be characterized by rescaling of the sensory input and that for both visual and olfactory inputs, the temporal dynamics of adaptation are consistent with optimal variance estimation. In multisensory contexts, larvae adapt independently to variance in each sense, and portions of the navigational pathway encoding mixed odor and light signals are also capable of variance adaptation. Our results suggest multiplication as a mechanism for odor-light integration.

*NIH 1DP2EB022359  
NSF 1455015

12:27PM Y65.00007: Individual and Automatic Training and Assay of Learned Navigational Behaviors in Drosophila larva*  
AMANDA LESAR (Presenter), JAVAN MF TAHIR, MARC H GERSHOW, New York University — Previous studies of olfactory learning in Drosophila larva show larva can learn through classical conditioning. While behavioral responses of trained larva have been studied, neural responses of freely moving, trained larva are unexplored. Previous training experiments present larva population with an odor and reinforcer in a small number of training trials, then allow larvae to make a decision in the presence of odor without reinforcer once. We develop a chamber which involves rigorous training and testing. The Y maze training chamber allows larva to make a decision, turn around, and go back to Y intersection to quickly make another decision, allowing us to study large number of decisions in short times in individual larva. We will study neural responses of trained versus untrained larva, while larva is making decisions, which can help us to connect stimulus, behavioral responses, and neural activity. We will present initial results for olfactory training of individual larva.

*NSF Award 1455015, NIH Award 1DP2EB022359

12:39PM Y65.00008: Internal bias vs. external sensory cues: the role of "handedness" in navigation decisions of invertebrate model systems  
MASON KLEIN (Presenter), ANGGIE FERRER, ROWANNE ALI, JOSHUA FORER, JOSEPH SHOMAR, Physics, University of Miami, KYOBI SKUTT-KAKARIA, ZACHARY WERKOVEN, BENJAMIN DE BIVORT, Organismic and Evolutionary Biology, Harvard University — How do the internal properties of individual animals combine with external environmental stimuli to produce a physical output? Answering this is important for understanding how the brain functions, and we examine the question using simple invertebrate animals, the Drosophila larva and C. elegans. Both animals have well-mapped brain circuits and limited behavioral repertoires, and exhibit exploratory behavior as they search for food, while at the same time responding to external stimuli. We focus on one specific internal property, the tendency of an animal to turn leftward or rightward (“handedness”). We find statistically significant bias in individual turning and drifting directions, but that turn and drift handedness are uncorrelated. This lack of correlation explains why even strongly left- or right-turning crawlers on average have similar diffusion rates as unbiased turners. Both handedness types are also weakly persistent, with frequent shifts to new biases.

We show that the internal bias (handedness) strongly affects, and in fact dominates, individual turning decisions in the presence of a temperature gradient, suggesting that inherent traits of individuals must be considered to achieve a more complete understanding of navigation and brain processing.
1:27PM Y65.00012: Motility Characteristics of Maze Navigating Fibroblasts

N. G. HALLFORS, Z. HUSAIN, KUST, J. TEO, NYU, G. ALHUSEIN, D. RUTA, A. F. ISAKOVIC (Presenter), KUST — Micropatterned substrates, in the form of mazes, are utilized to study cell migration. Highly motile cells such as fibroblasts rely on complex combination of forces exerted by the surrounding environment and neighboring cells to achieve motion. Substrate stiffness and topology of the patterned maze, together with the cell-cell neighbor interaction are shown to enhance or inhibit cells' self-propulsive behavior. Fluorescence imaging was used to quantify kinematics of the contractile motion of fibroblasts. It is shown that the density of cell population is a critical variable, and that, for sufficiently high densities, cells appear to self-organize into groups that move around (that is “solve the maze”) in qualitatively different manner we termed “rule following” and “cheating”. The motility analysis shows that Hurst exponent of cell dynamics shows a spread of values, indicating that only a fraction of cells follows near-diffusive dynamics, with other, non-diffusive modes of motion being clearly present as well. Similarly, the motility index and chemotactic index analysis show qualitatively more than one mode of cells.

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*Work supported in part by the UAE ICTFund. NGH acknowledges support from KUST Graduate School.
Development of flow-less linear gradient microfluidic devices

DRAGOS AMARIE (Presenter), ARTURO RUBEN DIAZ, ILEENE ASHLEY DIAZ, Physics and Astronomy, Georgia Southern University, DWAYNE G. STUPACK, Moores Cancer Center, University of California San Diego — Our previous work showed that by splitting and recombining the input flows through a combination of bifurcated and trifurcated channels one can generate a linear chemical gradient across a microfluidics chamber. However, when such devices are meant to study cell migration one must consider that physical factors of the microenvironment have influences in regulating cell fate. Such biomechanical cues have gained significant attention in recent years for their roles in defining fundamental cell properties, including motility, chemotaxis and migration. One such factor is the mechanical stress introduced by the flow in the gradient chamber that induces shear stress thus impacting the migration patterns. In this work we present a microfluidics device that generates highly linear chemical gradients into a cell culture chamber that is separated, flow-wise, from the gradient chamber and any investigated live cells will not experience any confounding fluid flows. The slope and the offset of the gradient can be manipulated with respect to experimental needs to enhance migration.

*This work was supported in part by the Office of the Provost and Vice President for Academic Affairs of Georgia Southern University.

Friday, March 8, 2019 11:15 AM - 2:15 PM

Session Y66 DBIO: Physics of Microbes II BCEC 261 - Katherine Copenhagen, Princeton University

11:15AM Y66.00001: Geometric localization of cell wall growth and shape determining proteins in *Helicobacter pylori*

BENJAMIN P BRATTON (Presenter), Princeton University, JENNIFER A TAYLOR, NINA R SALAMA, Fred Hutchinson Cancer Research Center, JOSHUA SHAEVITZ, Princeton University — The bacterial kingdom exhibits a wide variety of cell shapes. Our computational imaging framework allows us to extract 3D shapes of individual bacterial cells from fluorescence microscopy images. From these shapes we calculate geometric parameters such as local curvature, surface area, and the enrichment of fluorescent signals. The helical-rod shape of *Helicobacter pylori*, a human stomach pathogen, is important for its pathogenesis and is an ideal model system for studying complex bacterial cell shapes. In *H. pylori*, we have been investigating the geometric localization of the proteins and metabolic probes of cell wall growth. To propagate its helical shape, a cell must grow its longer, outer helical axis more than its inner one. Fluorescent, metabolic probes incorporated into the cell wall show enrichment of growth at both the outer and inner axes. Consistent with these labels, two of the proteins associated with cell wall homeostasis show geometric localization. MreB is enriched at regions of small and negative Gaussian curvature and CcmA is enriched at Gaussians curvatures of about 5 μm\(^{-2}\), similar to the curvature of the outer axis. These data are consistent with a model of helical-rod like growth that takes the simple rod and elaborates it by defining a outer helical axis.

11:27AM Y66.00002: Mechanical Forces to Trigger Morphological Changes in Motile Bacteria

RAVI CHAWLA (Presenter), RACHIT GUPTA, KATIE FORD, PUSHKAR LELE, Texas A&M University — Bacterial swarming is an important mechanism for flagellated bacteria to effectively cover large distances on soft surfaces, such as tissues. Swarming is likely initiated when the flagella sense higher viscous loads such as those experienced near solid boundaries. However, the underlying assumption that soft and porous surfaces cause significantly high loads on the flagella remains untested. Here, we developed an approach to estimate the hydrodynamic drag as a function of separation from soft interfaces. In one type of testing, optical trapping experiments were employed to estimate the diffusivities of tiny objects close to soft interfaces, using a novel flow-geometry. The method was validated by comparing results for transverse diffusion coefficients for single spherical particles near a no-slip solid boundary with predictions from Faxen's law. The data were in good agreement with published models. In a second type of testing, the surface-induced load on the flagellar motor was interpreted from the rates of swarming in two different strains that developed differential hydrodynamic thrust. These results are anticipated to help estimate the magnitude of mechanical forces necessary to initiate the transition of a bacterial cell to the swarmer state.

*NIH R01 Award (NIGMS), TEES
11:39AM Y66.00003: Bacterial Motors and Surface Sensing*  
PUSHKAR LELE (Presenter), Texas A&M University — Surface-sensing precedes the establishment of many types of bacterial colonies on surfaces. Evidence suggests that surface-sensing triggers transcriptional regulation as well as post-translational signaling that promote a variety of interesting cell phenotypes. The molecular mechanisms continue to remain unclear. I will discuss how motile cells discriminate between random forces arising due to Brownian motion and those arising due to surface contact. Our recent measurements that highlight the role of the flagella (otherwise known to be involved in motility) in surface-sensing and signaling will be discussed. Single molecule experiments that explain how flagella tune the sensitivities of modules involved in well-known signaling pathways will be presented. Data indicate an indirect link between the intracellular events and the external hydrodynamic drag acting on individual flagellum, and also hint at the regulation of certain surface-dependent phenotypes by these sensitive modules. I will conclude with a brief note on how mechanically-stimulated regulatory events influence a host of important processes such as bacterial competence, which regulates the uptake of extracellular DNA.

*R01GM123085

11:51AM Y66.00004: Determining the Metabolic Activity and Flow Boundary Conditions of Bacteria from Diffusion Measurements*  
LEVENT ASLANBAS (Presenter), AHMET C KIRLIOGLU, VURAL KARA, KAMIL EKINCI, Mechanical Engineering, Boston University — When live bacteria are adhered onto a microcantilever, the nanomechanical displacements of the microcantilever increase noticeably, suggesting that bacteria fluctuations drive the microcantilever to a higher amplitude than thermal fluctuations. Here, we have performed similar measurements by adhering various bacteria onto the surface of 8-μm-diameter microbeads. After bacteria adhesion, we image the Brownian motion of these single microbeads suspended in liquid by high-resolution optical microscopy. We then calculate the mean square displacements and diffusion constants from the trajectories of the microbeads. Interestingly, microbeads with non-motile bacteria show an unexpected diffusion profile: in a given interval, microbeads with dead bacteria on them tend to diffuse farther compared to those with live bacteria. We will discuss possible sources of this unexpected behavior, including modifications to the no-slip boundary condition on the surface of bacteria.

*We acknowledge support from NIH (R03AI126168).

RENATA GARCES (Presenter), University of Gottingen, SAMANTHA MILLER, The Institute of Medical Sciences, The University of Aberdeen, CHRISTOPH F. SCHMIDT, Department of Physics, Duke University — The ability to maintain a positive turgor pressure, by means of higher osmolarity of the cell interior than the exterior, is a requirement for proper metabolism in walled microbial cells. Turgor pressure is sensitive to changes in external osmotic conditions, and is drastically increased upon osmotic downshock, together with cell volume. Bacteria prevent lysis caused by excessive osmotic pressure through mechanosensitive (MS) channels: membrane proteins that release solutes (ions) in response to mechanical stress. The exact mechanism of channel gating in the natural setting, however, has been elusive due to the lack of experimental methods appropriate for the small dimensions of prokaryotes. We here present experimental data on the gating of MS channels of E. coli subjected to compressive force under iso-osmotic conditions. We indent living cells with micron-sized beads attached to the cantilever of an atomic force microscope (AFM) and characterize the mechanical response. We show that turgor pressure can be monitored through the measured response and quantify its value and fluctuations for individual single cells before and after MS channel gating.

12:15PM Y66.00006: Theoretical investigation of stochastic clearance of bacteria*  
HAMID TEIMOURI (Presenter), ANATOLY BORIS KOLOMEISKY, Chemistry, Rice University — Understanding mechanisms of bacterial eradication is critically important for overcoming the failures of antibiotic treatments. Current studies suggest that the clearance of large bacterial populations proceeds deterministically, while for smaller populations the stochastic effects become more relevant. We developed a theoretical approach to investigate the bacterial population dynamics under the effect of antibiotic drugs using a method of first-passage processes. It allows us to explicitly evaluate the most relevant characteristics of the bacterial clearance dynamics such as extinction probabilities and extinction times. In addition, we investigate the effect of fluctuations in the population growth rates on dynamics of bacterial eradication. It is found that fluctuations for some range of parameters increase the extinction probability and the extinction times, indicating slowing the bacterial clearance. We speculate that this might be a first step in developing of antibiotic resistance.

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Mechanotransduction in bacteria: how *Pseudomonas aeruginosa* actively probes and responds to substrate mechanics  MATTHIAS D KOCH (Presenter), ZEMER GITAI, JOSHUA SHAEVITZ, Princeton University — A growing body of evidence suggests that bacteria respond to mechanical cues such as shear flow or surface material properties, yet clear evidence that such mechanical features of the environment are integrated in a cell’s active decision making is lacking. Here, we demonstrate that the pathogen *Pseudomonas aeruginosa* employs arm-like, retractable appendages called pili to actively deform a substrate and probe its mechanical properties. We use a transcriptional fluorescence reporter to show that *Pseudomonas* tunes the expression of virulence factors based on substrate stiffness in the range of 0.1 – 1000 kPa. Using optical tweezers, traction force microscopy, and molecular modeling of the active motor components, we probe the mechanism of pilus-based mechanosensation. These results provide unique insights into the molecular functioning and control of pilus extension and retraction and how this is linked to twitching motility. We find evidence of an active bacterial mechanotransduction pathway that connects substrate mechanical properties to a genetic response via active surface deformation, similar to the mechanogenetic regulation found in stem cell differentiation.

Strength and longevity of non-genetic memory in sister bacterial cells.  HARSH VASHISTHA (Presenter), MARYAM KOHRAM, HANNA SALMAN, University of Pittsburgh — Phenotypic heterogeneity is a vital aspect of isogenic bacterial population related to the survival of the species. The focus of this study is to understand the origin of non-genetic phenotypic heterogeneity by observing the inheritance pattern of different cellular traits in the lineage of single bacterial cells using microfluidics and time-lapse microscopy. We aim to reveal the cellular factors responsible for this variability and estimate the timescale over which new phenotypes emerge. We have developed a unique microfluidic device that allows us to trap and follow E. coli sister cells for hundreds of generations in the same environment, and thus separating cellular effects from environmental ones. Our results reveal strong correlation of several measurable properties like cell size, cell-cycle duration and growth rate between E. coli sister cells for many generations while non-related cells growing in the same environment show almost zero correlation over the same period. These results allow us to quantitatively determine the strength and longevity of non-genetic memory in sister bacterial cells.

Mechanics and dynamics of filaments on curved membranes  FELIX WONG (Presenter), ETHAN GARNER, ARIEL AMIR, Harvard University — Protein filaments that bind to curved membranes exhibit rich behavior, as shown in previous studies of bacterial morphogenesis. Here we model the direct binding of protein filaments to membranes and show that it is typically energetically favorable for filaments to orient along the direction of largest curvature. We then model the dynamics of an ensemble of filaments, each translocating along the direction of largest curvature and subject to noise. We show that their macroscopic properties, such as localization, can vary significantly depending on membrane geometry. Finally, we discuss the implications of our study to bacterial morphogenesis and regulation of bacterial rod shape. Our work shows, from a physical perspective, how cellular-scale dynamics which dictates growth may arise from nanometer-scale properties.

Modes of Bacterial Aging and Death  MARYAM KOHRAM (Presenter), HARSH VASHISTHA, ZOLTAN NAGY OLTVAI, HANNA SALMAN, University of Pittsburgh — Currently, “biological aging” is well defined in human beings and multicellular organisms, and is one of the largest risk factors for most diseases. However, in single cell organisms there has been a sequence of various definitions. My research focuses on understanding the cellular processes responsible for senescence and death in *E. coli* bacteria as well as identifying cellular characteristics of aging. We employed an experimental setup consisting of a microfluidic device designed to trap single-cells while continuously supplying them with nutrients, allowing us to acquire images of the trapped cells. Analysis of these images provides long-term single-cell measurements of cell-size and protein content, which are then used to uncover aging effects and determine modes of cell death. Our data acquired thus far reveal two different phenotypes of cell death: 1. Part of the cells maintain their bacterial chromosome and enter a non-dividing phase. 2. A subset of the population loses its chromosome and so all cellular functions are obstructed. Our results indicate aging in all strains, which is marked by the increase in death rate with time. In addition, by comparing wild type and an ATP synthase *E. coli* mutant, we found different average lifetimes prior to undergoing these transitions.
**1:15PM Y66.00011: Rolling motion of uni-flagellated bacteria near a solid surface**  
GEORGE BARBOSA ARAUJO (Presenter), ZHAOYI ZHENG, JAY TANG, Brown University — Bacterial interaction with surfaces is ubiquitous in nature and is essential to many biological processes such as infection and biofilm formation. Here we study the tethering of uni-flagellated *Caulobacter crescentus* to a solid surface. In particular, we focus on weak reversible adhesion, which allows subsequent detachment. By applying an electrical field parallel to the surface, we observe that some initially tethered bacteria detach from the surface, but remain close to it. The detached cells perform rolling motion, a mixture of translation and rotation, different from the almost exclusive translation observed for nonmotile bacteria or swimming cells that are not previously attached. Our analysis of the rolling motion accounts for electrophoretic force, flagellar rotation, and the cell’s close proximity to the solid surface.

*NSF CBet1438033

**1:27PM Y66.00012: E. coli in Mazes**  
TRUNG PHAN (Presenter), ROBERT AUSTIN, Princeton University, RYAN MORRIS, University of Edinburgh, MATTHEW BLACK, Princeton University, JULIA BOS, Pasteur Institute — Bacteria often live in topologically complex environments. The path from a colony of bacteria which has exhausted its local supply of food to a source can have many branch points with false, dead-end leads. While chemotaxis can easily navigate bacteria to a food source in the presence of a food gradient, in a sufficiently complex and large maze chemotaxis will fail, leading to bacterial collapse at dead ends. Here, using nano and microfabrication, we made physical puzzles to study the collective behaviors of *E. coli* bacteria. We constructed mazes for bacteria to solve in order to get food and probed for their searching algorithms, with and without the presence of hydro flows.

*This work was supported by NSF PHY-1659940.

**1:39PM Y66.00013: High Throughput 3D Tracking of Bacterial Chemotaxis in Complex Environments**  
MARIANNE GROGNOT (Presenter), KATJA M. TAUTE, Rowland Institute at Harvard — Bacterial chemotaxis is an important survival mechanism by which motile bacteria bias their random walk trajectory to navigate chemical gradients. While chemotaxis has been studied extensively in *E. coli*, much less attention has been devoted to the diversity of bacteria with different flagellar architectures, or to motility in viscous or porous environments that more closely mimic the complexity of natural habitats. Current approaches for characterizing and comparing chemotaxis strategies are hampered by being either limited to the population scale, qualitative, low throughput, 2D, and/or dependent on theoretical models.

Here we present a simple yet powerful chemotaxis assay combining a recent high-throughput 3D tracking method with microfluidically created chemical gradients. With a typical throughput of above 3,000 individual trajectories in 5 minutes, we demonstrate that we can directly determine chemotactic drift velocities in diverse environments while simultaneously resolving 3D motility behavior, enabling unprecedented access to a mechanistic understanding and quantitative comparison of chemotactic strategies. We highlight the power of our assay by revealing the role of lateral flagella in the opportunistic pathogen *V. alginolyticus* for motility and chemotaxis in hydrogels.

**1:51PM Y66.00014: Bacterial Scattering from Convex Surfaces and its Effects on Motility and Chemotaxis**  
KENTARO HOEGER (Presenter), TRISTAN URSELL, University of Oregon — For many organisms across length scales, self-propulsion is a key mechanism for survival and nutrient acquisition in changing environments. The model microorganism *Escherichia coli* explores low Reynolds number environments executing ‘run-and-tumble’ chemotaxis in its search for resources. While many studies of chemotaxis and motility take place in open environments, typical real-world environments – like soils, sediments, or the mammalian gut – have physical structure across multiple length-scales which can alter or impede cellular trajectories. To understand how physical structure in the environment alters trajectories and attendant persistence lengths, we built microfluidic devices containing arrays of microscopic circular pillars and studied bacterial interactions with these structures through the lens of probabilistic scattering functions. We find that attractive interactions with the pillars and stochastic noise produce a complex set of probability distributions that characterize bacterial motion in structured environments. Thus, understanding how cells navigate chemical gradients and acquire resources in such complex environments is crucial to our understanding of microbial ecology and may enable design of devices for controlling bacterial motility.

*University of Oregon
Run-and-tumble motility enables equatorial magnetoaerotaxis

NICOLAS WAISBORD, MICHAEL STEHNACH (Presenter), Tufts University, CHRISTOPHER T LEFEVRE, CEA Cadarache/ CNRS/ Aix-Marseille Université, JEFFREY GUASTO, Tufts University — Guided by Earth’s magnetic field, magnetotactic bacteria (MTB) seek out microoxic environments in the sediments of swamps, lakes, and oceans for survival. To accomplish this, MTB synthesize magnetic nanoparticles that mechanically orient the cells along Earth’s magnetic field, which is mostly parallel to the water column over a broad range of latitudes. In the current paradigm, magnetotaxis provides a global orientation for the cells and facilitates a one-dimensional aerotactic search along naturally occurring, parallel oxygen gradients through ‘run-and-reverse’ motility. However, a variety of MTB species thrive at the equator, in spite of the orthogonal magnetic field and oxygen gradients. Using a microfluidic device and Helmholtz coil, we independently control an oxygen gradient and an orthogonal magnetic field, enabling precise measurements of MTB motility under equatorial conditions. In contrast to the current paradigm, we show that *Magnetococcus marinus* (MC-1) achieves ‘run-and-tumble’ motility, which facilitates exploration and aerotaxis perpendicular to the magnetic field. These results establish a new survival mechanism for equatorial magnetoaerotaxis in bacteria.